From atoms to landscapes through time: The chemical controls on carbonate precipitation and phosphate concentration in alkaline lakes



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"(...) this program does monitor itself and does have ideas about its ideas – but it cannot monitor its own processes in complete detail, and therefore has a sort of intuitive sense of its workings, without full understanding. From this balance between self-knowledge and self-ignorance comes the feeling of free will."

Douglas Hofstadter, *Gödel, Escher, Bach, an Eternal Golden Braid*

"Imagine a set of parts which, when placed in the proper supporting environment, spontaneously group themselves in such a way as to form a complex machine. (...) The information for the total conformation of the organism (or machine) is spread about in its parts; it is not concentrated in some single place."

Douglas Hofstadter, *Gödel, Escher, Bach, an Eternal Golden Braid*

"From our present perspective, the first step toward a possible reunification of knowledge was the discovery in the nineteenth century of the theory of heat, of the laws of thermodynamics. Thermodynamics appears as the first form of a 'science of complexity'."

Ilya Prigogine and Isabelle Stengers, *Order Out of Chaos*

"This statement is false."

Alternative version of the Epimenides paradox

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Over my years in Oxford I have had many different experiences, although nearly half of that time those were certainly unusual and challenging years for most people around the planet as well. With a pandemic hitting global proportions and its unfolding consequences, I am aware many struggled to adapt, and some are surely still recovering from its more general effects. Regardless of personal challenges in this and other respects, I believe I could experience the journey of having time to immerse in an exciting and rewarding research enterprise for four years. I have been incredibly fortunate to have the opportunity to work with my supervisor Nicholas J. Tosca, who trusted my capabilities to work on my own and gave me an enormous amount of freedom to pursue my own research interests. And even after moving to Cambridge to assume his new role he maintained his critical contributions, ingeniously indicating the directions to follow by posing challenging questions, pointing to the appropriate literature and extensively commenting on all my many rough drafts and ideas. I learned enormously from him. Many thanks for these invaluable feedbacks and also for sharing the alluring interest and fascinating discussions about the broad topic of origins of life research. I also thank my second supervisor here in Oxford, Gideon M. Henderson, for his willingness to assist me in scientific matters as well as other necessary aspects of academic life, and for introducing me to his "Climotope" research group discussions when any contact and all meetings could only be performed remotely. There I was presented to many interesting current work being developed with different applications for climate and environmental research. The positive encouragement from them both is greatly appreciated.

Additionally, I am also grateful to a large number of people, because there is generally no path in life where we can proceed entirely alone even in our individual journeys, such as conducting a PhD research, or in a broader sense regarding other aspects of life. Just like chemical reactions, events in life are differentiated by given initial conditions and are also path-dependent (and I imply more than a mere analogy here, which I hope to have the chance to explain more thoroughly some day). Thus, it is fundamentally important to be surrounded by good people, because one can support each other. And this turns out to be one of the most valuable

things in life, having good people around. These have not been easy times for many, and some probably felt and still feel the repercussions more than others. But I think it is generally fair to assume everyone has been more or less affected by the events that are still unfolding, with over two years of pandemic, several lockdowns of different degrees in different countries, isolation, and more recently a war crisis of sizeable proportions. These experiences only come to reinforce my belief, backed up in part by critical empirical observations and partly by philosophical thinking, that we are not absolute masters of our lives; we are all connected in an extensive network, and we all depend on one another, even though that may not be clearly noticeable or acknowledged from a first impression and shallow evaluation. All lives are affected even by events that are seemingly only distantly related. We are part of an enormous ecosystem, involving human societies and the natural ecosystem in which the latter are embedded. "Free will" to run our lives independently has only certain degrees of freedom, constrained by serendipity and by the broader context enveloping our immediate surroundings as well as the larger environment where human life happens to take its place. Therefore, after these final remarks I find that it is absolutely necessary to acknowledge the contribution of numerous people, even if not directly related to the research that has been undertaken, simply because I am aware other structures support my existence, thereby supporting my work.

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Abstract

From atoms to landscapes through time: The chemical controls on carbonate precipitation and phosphate concentration in alkaline lakes

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As some of the most biologically productive environments on the modern Earth, alkaline lakes may have figured prominently in the evolution of the global carbon cycle and in the chemical origins of life. Significant $CaCO_3$ supersaturation is a ubiquitous trait of alkaline lakes, controlling the geochemical evolution of lake waters as well as the mineralogy and sedimentary expression of their deposits. By definition, $CaCO_3$ supersaturation requires compounds that interfere or inhibit precipitation, yet the processes controlling $CaCO_3$ saturation in many alkaline lakes are poorly understood. In the pursuit to understand the essential physicochemical processes influencing non-skeletal $CaCO_3$ precipitation, this study focusses on the roles of aqueous phosphate and magnesium in influencing the dissolved carbonate system. It also dissects the roles of alkalinity and pH, addressing a comprehensive compilation of published water chemistry data of alkaline lakes from 16 countries in six continents, implementing a Pitzer ion interaction activity coefficient model to explore carbonate geochemistry and the potential role of these ions in maintaining $CaCO_3$ supersaturation. This survey reveals that ∼80% of the investigated lakes are supersaturated with respect to calcite ($0 < SI_{cal} < 2.9$). In fact, as pointed out by another study (Fukushi and Matsumiya 2018 [1]), alkaline lake waters are predominantly poised between monohydrocalcite and amorphous Ca-Mg carbonate saturations, being a strong indication that these phases control the water chemistry of alkaline lakes that have not yet become depleted in Ca^{2+} (*i.e.*, barring those alkaline lakes comprising soda lakes). This provides additional evidence indicating that the crystallisation of more stable $CaCO_3$ phases in these settings occurs preferentially

via the formation of more soluble precursors that will undergo recrystallisation likely via dissolution-reprecipitation, as also observed experimentally in a different study (Rodriguez-Navarro et al. 2016 [2]). Furthermore, the present comprehensive dataset is complemented with experimental observations demonstrating that small concentrations of total phosphate (ΣPO_4 $\geq$25 μmol/kg) inhibit specific $CaCO_3$ phases such as aragonite and allow supersaturations (Ω_{calcite}) above 70–100 (or SI_{cal} $\sim$1.85–2) to be maintained, whilst overall rates of $CaCO_3$ precipitation decrease with proportionally higher ΣPO_4. Together, these observations support previous suggestions that $CaCO_3$ supersaturation in alkaline settings must be sustained at least in part by kinetic inhibition of $CaCO_3$ nucleation and/or growth. Importantly, the natural alkaline lake water data paired with geochemical and thermodynamic calculations stemming from kinetic theory suggest that monohydrocalcite should be the predominant primary $CaCO_3$ phase forming in these lakes. The implications for the geological record of the precipitation via metastable intermediate phases, concerning the incorporation of trace metals and isotopic fractionation in the final, non-stoichiometric products forming in disequilibrium with their surroundings are also briefly discussed. The complete alkaline lake water chemistry database compiled in the present investigation, the modified implementation of the code "thermo_phrqpitz.tdat" (Plummer et al. 1988 [3]; Bethke et al. 2020 [4]), comprising the thermodynamic and geochemical database for equilibrium calculations used to assess the water chemistry dataset, as well as a MATLAB code developed in this study for determination of other geochemical relations investigated in this research are being stored in the online repository under the name "raphapietzsch/alkaline_lakes" on github.com. In a related direction but concerning environments for a plausible prebiotic chemistry, the study also shows that high phosphate concentrations, *i.e.*, $\Sigma PO_4 \approx$ 2–3 mol/kg at $[Ca^{2+}] \approx$ 4–5 mmol/kg and pH $\approx$ 9 are theoretically possible, carrying implications for scenarios of the emergence of life requiring high soluble phosphate levels. In contrast, even though some present-day alkaline lakes can reach $\Sigma PO_4 = \sim$100 mmol/kg and above, their maximum ΣPO_4 tends to be even lower, at $\sim$40 mmol/kg. This is likely the result of the high primary productivity taking place in these modern environments, in part due to the large availability of carbon as dissolved inorganic carbon (DIC) but also of other limiting nutrients such as nitrogen and phosphate itself. Conversely, ammonia volatilisation, a phenomenon that may occur as a result of high alkalinity in some lakes, may limit productivity, thereby allowing phosphate levels to increase without this constrain. Moving a step further, the knowledge from theory, geochemical modelling and experimental observations is combined with a detailed investigation of the ancient carbonate sediments from the Lower Cretaceous Barra Velha Formation, Santos Basin, offshore Brazil, in the South Atlantic ocean. These carbonate rocks are generally composed of two intriguing non-skeletal $CaCO_3$ textures, broadly referred to as calcite "shrubs" and "spherulites".

This latter investigation rests on multiple microanalytical techniques addressing the mineralogical, isotopic and geochemical composition of these carbonate rocks. It proceeds employing computational statistics to evaluate minor and trace element (including phosphorus) distribution between different carbonate mineral textures and phases. This permits an assessment of mineral formation in the context of fluid evolution and degree of diagenesis. These tasks ultimately underpin the goal to reconstruct a plausible scenario for the original environment of deposition of the Barra Velha Fm, including calcite saturation state, alkalinity and phosphorus concentrations and cycling. Building on this assessment and on the experimental and theoretical work above, the two main $CaCO_3$ morphologies bearing the hallmark of this Formation, the "shrubs" and the "spherulites" may be used at least as rough indicators of growth rate and saturation state, both increasing from shrubs to spherulites. The average P/(Ca + Mg) molar ratio values based on electron micro-probe analysis (EPMA) data for carbonate crusts, "shrubs" and "spherulites" in the upper part of the analysed interval are 1.45 ± 0.98, 1.13 ± 0.97 and 1.09 ± 0.90 mmol/mol, respectively. These values may suggest the waters from which these calcite minerals precipitated had $[Ca^{2+}]/ALK_T<0.75$. From these and additional data, it is inferred that lake waters had $\Omega_{calcite} > 14–45$ and possibly within the range of 100–180. Nonetheless, it is pointed out in the present study that possible antagonistic effects of dissolved SiO_2 and phosphate on carbonate precipitation and growth are presently not well constrained and should be investigated in future studies. Another relevant contribution of potentially wider implications for global budgets at the time of their formation is the maximum estimated volume of water implied in the deposition of these rocks, calculated to be in the order of 6×10^{19} L, ∼three orders of magnitude greater than the present volume of water in the Caspian Sea, the largest modern endorheic lake in the world. Finally, the picture emerging from the combination of theory, experimentation and geological investigation provided in this study establishes a robust framework for our understanding of the chemical controls on non-skeletal carbonate minerals deposited in sedimentary basins elsewhere. In turn, this extended knowledge may allow us to place better constraints on the chemical evolution of Earth's surface conditions dating as far as the existing sedimentary carbonate rock record goes back in time.

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Acronyms

ACC amorphous calcium carbonate. 6, 93, 104, 107–109, 163–165

ACMC amorphous Ca-Mg-carbonates. 6, 54, 58, 59, 76, 93

ACP amorphous calcium phosphate. 57, 65, 66, 68

AFM atomic force microscopy. 163

ALK alkalinity. 4, 11, 39–43, 65–68, 82, 93, 95, 154, 164, 170

AMC amorphous Mg-carbonates. 58, 59

ANC acid-neutralising capacity. 39, 49

BSE backscattered electrons. 135, 137, 138

BVF Barra Velha Formation. 12, 117, 119, 157, 159, 174–177, 184, 187, 200–203

CAP carbonate-associated phosphate. 117

CBE charge balance error. 33, 34, 56–58, 62, 67, 68, 72

CI confidence interval. 142

CLR centred-log ratio transformation. 128

CPA crystallisation by particle attachment. 6

DH Debye–Hückel. 17, 20, 22, 23, 29, 31

DIC dissolved inorganic carbon. 11, 40, 41, 43, 54, 63, 68, 72, 80–82, 90, 106, 156, 168, 169

DOM dissolved organic matter. 4

EDS energy dispersive X-ray spectrometry. 83, 86, 87, 124, 125, 135, 137, 138, 145, 153

EPMA electron probe microanalysis. 124, 125, 127, 135, 137, 145, 146, 148, 150, 151, 153–155, 184, 203–212

GWB The Geochemist's Workbench. 15, 24, 25, 27, 28, 57

HAP hydroxyapatite. 57, 65, 68, 69

IAP ion activity product. 16, 17, 58, 82

ICP-MS inductively coupled plasma mass spectrometry. 44, 45, 122, 193, 195

ICP-OES inductively coupled plasma optical emission spectrometry. 122, 130, 131, 133, 141

IRMS isotope ratio mass spectrometer. 126

ISE ion-selective electrode. 81, 86

Ksp (equilibrium) solubility product constant. 16, 24, 25, 58, 82, 163

LD limit of detection. 45, 46, 68, 133, 193, 194

MC-ICP-MS multicollector inductively coupled plasma mass spectrometer. 127

MHC monohydrocalcite. 6, 59, 69, 76, 87, 89, 90, 93, 107–110, 182

ML machine learning. 153

NMR nuclear magnetic resonance. 153, 187

OCP octacalcium phosphate. 27, 57, 66, 68, 72–74

OM organic matter. 168, 169

PCA Principal Component Analysis. 127, 148, 153

PCs principal components. 147

QEMSCAN Quantitative Evaluation of Minerals by SCANning electron microscopy. 125, 135, 137, 139, 145, 146, 153

SEM scanning electron microscopy. 83, 93, 125, 135, 137, 138, 145, 153

SI saturation index. 16, 58, 59, 61, 63, 65–70, 72

TLK terrace-ledge-kink. 3

VPDB Vienna Pee Dee Belemnite. 126

WDS wavelength dispersive X-ray spectrometry. 124

WS working solution. 80, 81, 88, 92

XANES X-ray absorption near-edge structure. 153, 187

XRD X-ray diffraction. 80, 93, 125, 130, 131, 133, 140, 141, 159, 169, 461

1 Introduction

1.1 Plain Language Summary

Linking observations of modern environments with experimental work and the investigation of the rock record is an old activity. However, in ancient times the scientific method was not yet established, and humanity had to wait for the intellectual and technical revolutions of the 16^{th} through 18^{th} centuries, setting the stage for our current modern approach. This is typified with the works of some selected 17^{th} and 18^{th} century naturalists, such as Nicolaus Steno (Niels Stensen), James Hutton and Abraham Gottlob Werner. However, knowledge is cumulative. New techniques are developed to address new and old problems, new questions are posed, and new challenges emerge. This work follows this old naturalist's tradition, well-established in Earth sciences, and tries to undertake a comprehensive approach with *relatively* 'simple goals': (1) to understand the chemical controls on carbonate sediment production in alkaline lakes, (2) to understand the interactions of $CaCO_3$ mineral formation with dissolved phosphate in these environments and in controlled experiments, and (3) to use this knowledge to interpret the sedimentary rock record, bearing the important caveat in mind that rocks and their constituent minerals

may always reflect multiple superimposing events, thus overprinting their primary (depositional) mineralogical, chemical, and morphological/physical attributes.

These tasks are of utmost importance because they provide fundamental knowledge about the chemical reactions involved in the process of mineral formation in chemically precipitated sediments. In turn, this potentially allows us to retrieve general information about the chemical conditions of their environment of deposition and also to predict new reactions once the already deposited rocks in sedimentary basins come in contact with later fluids, such as in the case of geological Carbon Capture and Storage (CCS). These goals also provide foundational principles that establish a robust framework to guide the systematic acquisition of new data and quantitatively inquiry about the evolution of the planet Earth from its remote past to its unfolding future. The latter in turn provides the basis to investigate the scenarios where life may have emerged on the ancient planetary surface, as well as the settings where life co-evolved with the planet, and finally how they may change as a result of continuing biological activity, including human activity.

1.2 Background

Carbonate minerals of sedimentary origin encompass a class of materials of major interest in Earth sciences. Among other sedimentary minerals, they represent a potentially rich archive of past surface environmental processes, whereby inquiring about the composition of past oceans, lakes and the atmosphere is possible (*e.g.*, Berner 1971 [5]; Holland 1984 [6]; Grotzinger and James 2000 [7]; Sumner and Grotzinger 2000 [8]). Importantly, they pave the way in our attempts to reconstruct elemental fluxes between the different compartments of the Earth system and therefore to understand major changes on the planetary surface. An improved knowledge in this respect offers in turn further opportunities for advancing our understanding of (bio)geochemical cycles through time and Earth's co-evolution with life (*e.g.*, Grotzinger 1990 [9]; Grotzinger and James 2000 [7]; Arndt and Nisbet 2012 [10]; Hao et al. 2020 [11]). In this respect, different crystal textures and morphologies

preserved as sedimentary carbonate minerals are regarded as important pieces in this larger puzzle, because they may hold additional information about the mechanisms of their crystallisation. Together with high resolution sedimentological and facies analyses, carbonate mineral textural and morphological attributes have been widely used by geologists as proxies to infer about the physicochemical conditions of past fluid conditions from which they precipitated (*e.g.*, Sumner and Grotzinger 1996 [12]; Sami and James 1996 [13]; Chafetz and Guidry 1999 [14]; Grotzinger and James 2000 [7]; Sumner and Grotzinger 2000 [8]; Pope and Grotzinger 2000 [15]; Richter et al. 2011 [16]; García-Veigas et al. 2013 [17]; Wright and Barnett 2015 [18]).

However, it remains a challenge to retrieve the information encoded in mineral textures and morphologies that may tell unambiguous details about the environmental conditions that drove their crystallisation, as well as re-crystallisation (Garcia-Ruiz 2000 [19]; Sumner and Grotzinger 2000 [8]). This stems from the fact that we still lack a complete understanding of the physicochemical controls on crystal morphology and fabric development, regarding for example, the relations between solution composition, role of inhibitors, and different pre-existing crystal faces and substrates. This clearly bears implications for our interpretations of the rock record and thereby to our abilities to comprehend and accurately reconstruct the history of ancient Earth's surface environments.

Following extensive observations made in experimental studies, it is broadly understood that, among other factors, the role of inhibitors (additives) and different saturation states will influence the mechanisms of crystal growth (Van Cappellen 1991 [20]; Pope and Grotzinger 2000 [15]; De Yoreo and Vekilov 2003 [21]; De Yoreo et al. 2015 [22]; Wang et al. 2012 [23]). For example, at low saturations crystal nucleation and growth behaves generally well within application of the models of classical growth and terrace-ledge-kink (TLK) theories (Figure 1.1). The latter predict that crystals will grow by molecules- or ion-by-ion attachment of solutes diffusing at the surface of substrate minerals and incorporation at kink

sites, producing spiral growth under conditions of low supersaturation (Burton et al. 1951 [24]; De Yoreo et al. 2015 [22]; Rodriguez-Navarro et al. 2016 [2]). However, the assumption that carbonate minerals grow in nature predominantly following this classical nucleation pathway, requiring low supersaturations, is contrasted with observations made in natural environments and in experiments. For example, calcites with >10 mol % $MgCO_3$ cannot be grown by this mechanism at low temperatures, whereas *in situ* observations show that layer-by-layer formation by step propagation is fully inhibited at Mg^{2+} concentrations significantly lower than those in modern seawater (Davis et al. 2000 [25]; Wang et al. 2012 [23]). Even so, abiotic calcite precipitated from seawater normally contains 11–14 mol % $MgCO_3$ (Morse et al. 2007 [26]).

Alkaline lakes tend also to be substantially supersaturated with respect to calcite, even though its precipitation and growth are often restricted to specific depositional settings, whereby both abiotic and biotic processes can be involved (*e.g.*, Della Porta 2015 [27]; Tutolo and Tosca 2018 [28]; Fussmann et al. 2020 [29]). This sustained supersaturation is often attributed to the presence of other solutes at moderate to high concentrations, such as dissolved organic matter (DOM), Mg^{2+} and ΣPO_4 (total inorganic phosphate) (Jellison et al. 1993 [30]; Fukushi and Matsumiya 2018 [1]; Ingalls et al. 2020 [31]) that are known to inhibit its growth and spontaneous nucleation (Reddy 1977 [32]; Mucci and Morse 1983 [33]; Gratz and Hillner 1993 [34]; Lin and Singer 2006 [35]; Mercedes-Martin et al. 2016 [36]).

In alkaline lakes Na-carbonates are frequently another relevant mineral product, that on their own provide information about the chemical evolution of the waters from which they precipitated (*e.g.*, Eugster and Jones 1979 [37]; García-Veigas et al. 2013 [17]). At the extreme end of alkaline and evaporitic lakes, Ca^{2+} concentrations may be somewhat low to yield significant precipitation of calcium carbonate minerals in short spans of time, but steady state or intermittent Ca^{2+} supply may rapidly or locally lead to supersaturation with respect to $CaCO_3$. In this extreme, Na-carbonates will predominate over $CaCO_3$, because high alkalinity (ALK) is provided

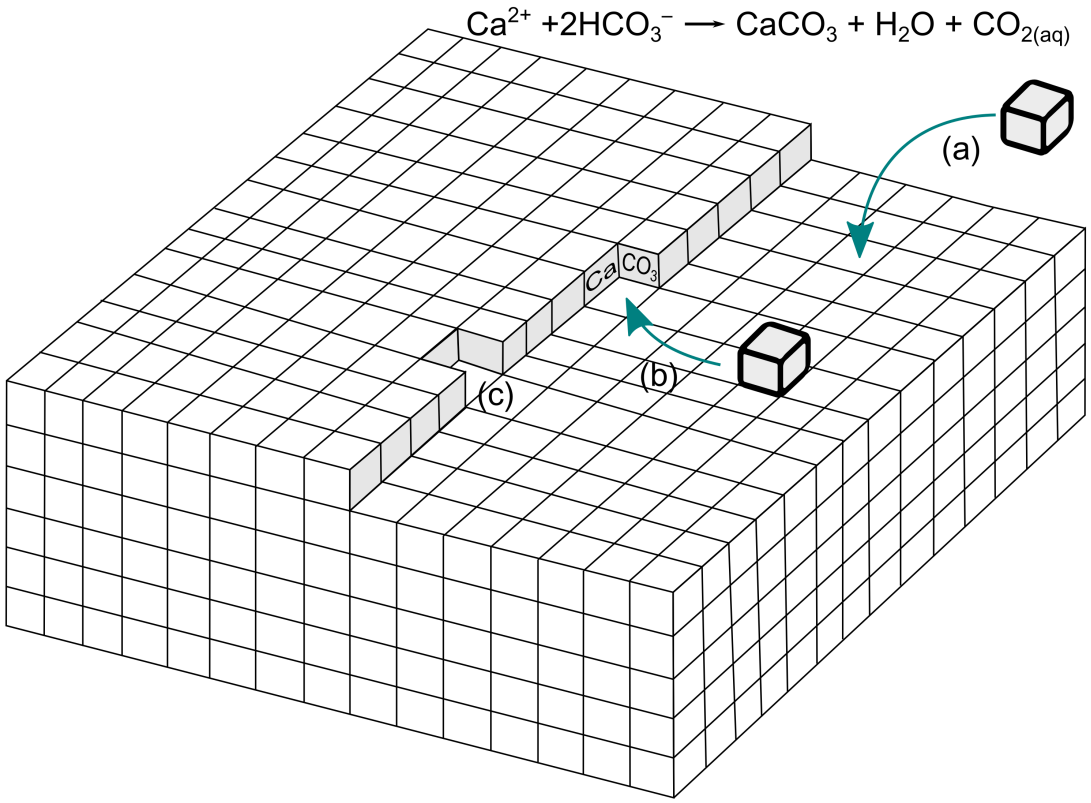


Figure 1.1: Simplified schematic or conceptual model in the frame of classical theory of crystal growth, conveying the idea of growth by ion-by-ion attachment, under low supersaturations (*i.e.,* approaching equilibrium). In this case, the growth of a calcium carbonate mineral is represented by the individual attachment of Ca^{2+} and CO_3^{2-} (following dehydration) ions. (a) an ion is transported through the fluid to the surface of the growing crystal; (b) the ion (also analogue to a *terrace adatom*) diffuses across the crystal surface to a *kink site* along the ledge; (c) a *step vacancy* or *double kink site*. Impurities arising from the presence of other heteroatoms may cause lattice strain and deformations to the crystal structure (not depicted).

by the concentration of alkaline cations and excess *carbonate alkalinity* (Eugster and Jones 1979 [37]; Al-Droubi et al. 1980 [38]). Even so, Na-carbonates may lend themselves as suitable analogues to investigate mechanisms and products of rapid growth from supersaturated solutions that may similarly affect more common $CaCO_3$ minerals. For example, the formation of millimetric-sized fibrous and dendritic $CaCO_3$ aggregates is less well-documented in laboratory experiments, perhaps due to the short timescales usually involved in such studies. Despite that they are commonly observed, among other settings, in modern springs, tufa and travertines, as well as some ancient deposits (*e.g.*, Pentecost 1990 [39]; Chafetz and

Guidry 1999 [14]; Pope and Grotzinger 2000 [15]; Jones 2017 [40]). However, owing to multiple interfering parameters and the large differences in gradients around a growing crystal and its relative size, it remains a virtually impossible task to actively monitor the microenvironment surrounding it in these systems (Jones 2017 [40]). Hence, a distinction between predominant and independent mechanisms controlling crystal growth is difficult to be clearly established in natural environments.

Importantly, a number of experimental studies have now extensively observed that calcium carbonate minerals nucleate and grow more commonly via alternative pathways to the classical mechanisms mediated by ion-by-ion attachment. These are related to higher supersaturations and involve the formation of clusters of intermediate metastable precursor phases (Gebauer et al. 2008 [41]; Rodriguez-Blanco et al. 2014 [42]; Purgstaller et al. 2016 [43]; Rodriguez-Navarro et al. 2016 [2]; Blue et al. 2017 [44]; Prus et al. 2019 [45]; Figure 1.2). Several of these studies have shown that the crystallisation of $CaCO_3$ polymorphs, including calcite, aragonite, vaterite and monohydrocalcite (MHC), normally proceed via formation of amorphous calcium carbonate (ACC) and/or amorphous Ca-Mg-carbonate (ACMC) phases, which are more soluble and thermodynamically less stable. The amorphous phases are comprised of nanoparticles that diffuse along the solid-liquid interface and attach to kink sites, in a way that is analogous to the classical growth model by ion attachment (Rodriguez-Navarro et al. 2016 [2]; Fig. 1.1). The amorphous phase then undergoes transformation to calcite via a dissolution-reprecipitation mechanism coupled to the interface, which may proceed producing intermediate phases such as MHC and vaterite (Rodriguez-Blanco et al. 2014 [42]; Purgstaller et al. 2016 [43]; Rodriguez-Navarro et al. 2016 [2]). At higher supersaturations, the free-energy barrier (ΔG^*) to nucleation will vary in shape and magnitude, driving the crystallisation pathway from monomer-based to crystallisation by particle attachment (CPA) (De Yoreo et al. 2015 [22]; Rodriguez-Navarro et al. 2016 [2]; Schoeppler et al. 2021 [46]). Whilst the latter mechanism refers specifically to processes occurring at the nanometer scale, a third type of particle aggregation known as *agglomeration process* occurs at the micrometer scale. It entails both

physical and chemical forces, such as Brownian motion, turbulent and van der Waal forces, thereby resulting in aggregates following transport and collision with another particle(s), attachment of particles and/or cementation (Lewis et al. 2015 [47]). These accretionary mechanisms from amorphous particle precursors and larger aggregates produce macroscopic polycrystalline morphologies and textures with complex non-coherent crystallographic properties (Schoeppler et al. 2021 [46]), which are indeed a characteristic of calcite textures observed in a range of sedimentary carbonate deposits, such as radiaxial, fascicular optic, and spherulitic aggregates (*e.g.*, Folk and Assereto 1976 [48]; Tucker 1983 [49]; Chafetz and Guidry 1999 [14]; Richter et al. 2011 [16]; Jones 2017 [40]).

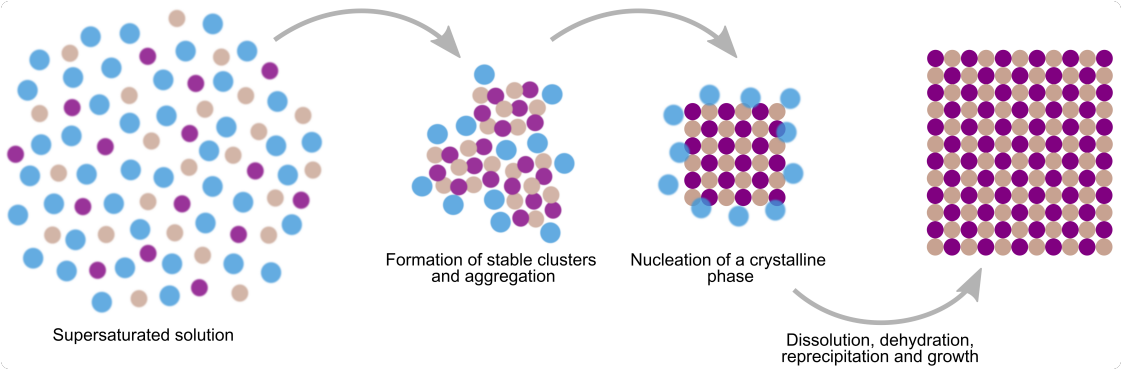


Figure 1.2: Conceptual model illustrating the general mechanism of nucleation and growth of an ionic crystal according to the *non-classical* view. In this case, pre-nucleation clusters, equivalent in composition to the crystalline phase, may form (*e.g.*, Gebauer et al. 2008 [41]) or, alternatively, populations of clusters comprising ions and ion-pairs lead to the nucleation of a crystalline nucleus (Henzler et al. 2018 [50]), all of which may eventually continue to grow, if the critical size is reached. Blue, beige and purple spheres represent water molecules, cations and anions, respectively.

The preceding observations represent therefore the main motivation of the present study. Here, I strive to investigate the mechanisms of homogeneous and heterogeneous nucleation of carbonate minerals ($CaCO_3$ and Na-carbonates) of relevance to sedimentary Earth's surface environments, exploring the links between the roles of relevant inhibitors (ΣPO_4 and Mg^{2+}) and $CaCO_3$ supersaturation. To investigate these links on carbonate nucleation, growth and fabric development in alkaline solutions of possible relevance to ancient marine and lacustrine environments, this study (1) examined the first-principles of equilibrium thermodynamics and kinetics

necessary to tackle complex multi-electrolyte solutions with high-ionic strength, (2) explored the aqueous chemistry of modern alkaline lakes from the published literature, (3) undertook free-drift and constant composition experiments simulating high $CaCO_3$ supersaturation under variable inhibitor concentrations and (4) probed ancient alkaline lake deposits preserved in the geological record.

With regards to the implications involving (1) fluid chemistry, (2) different mechanisms of precipitation of $CaCO_3$ and (3) the final products observed in the geological record, it becomes clear that understanding the links among these three steps is of paramount importance. This is because, as mentioned in the beginning, one common assumption is that the morphology and chemical (as well as isotopic) composition of the solid crystals reflect the physical and chemical conditions of their parent fluids. This forms, for example, the basis for the application of the concept of distribution or partition coefficients, where equilibrium conditions are often assumed and elemental or isotopic ratios in the solid are understood to follow a proportionality rule with respect to the same ratio in the parent fluid. In this case (under equilibrium), the distribution or partitioning of the elements or isotopes between the fluid and the solid are a function of the temperature and/or composition of that fluid, for example. If, on the other hand, the crystallisation is driven predominantly by kinetic (disequilibrium) processes, then it is possible that the composition of the solids (in terms of trace elements or their stable isotopes) may not directly reflect the composition of the parent fluids. The relevance of this difference then becomes obvious for studies inquiring about the geochemical composition of ancient sedimentary materials. This is because the geologist, the geochemist and the palaeoclimatologist often build their premises about the evolution of the planet's oceans, lakes, and atmosphere on the grounds that the chemical and textural compositions in those sediments preserve, map and can inform about the composition of their aqueous environment of deposition.

1.3 Thesis Objectives

The main objective of this thesis is to provide a framework to improve our understanding on the chemical controls on the nucleation and precipitation of calcium carbonate minerals in alkaline lakes, specifically focusing on the inhibitory roles of dissolved orthophosphate (and addressed as ΣPO_4, to refer both to PO_4^{3-} ion as well as to the other potentially present dissociated species of phosphoric acid). Are calcite and other $CaCO_3$ minerals supersaturated in all alkaline lakes? If they are supersaturated, what sustains the supersaturation? Do different levels of supersaturation and/or of inhibitory compounds affect the type and morphology of the precipitate?

For this wider goal and to answer these questions, this thesis pursued the following aims:

- **Aim 1: to quantitatively estimate the calco-phosphoric-carbonic acid system properties in alkaline and high ionic strength solutions** This goal aimed to improve the thermodynamic calculations applying the Pitzer ion activity interaction parameters for the determination of dissociation constants of H_3PO_4 in high ionic strengths solutions, coupling it to the carbonate system (chapter 2). This goal places meaningful constraints on the analyses and interpretation of the aqueous chemistry data of natural alkaline and experimental fluid samples, accounting for these ionic species and their interactions with other ions.

- **Aim 2: to quantitatively describe the general chemical characteristics and $CaCO_3$ saturation state in modern alkaline lakes driving carbonate mineral precipitation** In order to appreciate the possible physicochemical conditions present at the time of precipitation of ancient chemical sediments it is necessary to understand and clarify the general conditions governing the deposition of equivalent sediments in modern, *presumably* analogue environments. With this goal in mind, this study employed the knowledge developed in the preceding item and built an extensive

database of alkaline lake water geochemistry in search for regularities and broader patterns representative of most or all alkaline lakes of the world. (chapter 4). It also investigated the precipitation in carbonate minerals in controlled experiments (chapter 5).

- **Aim 3: to transfer the preceding fundamental principles and knowledge to retrieve information from ancient deposits, aware of inherent limitations involving other overprinting geologic processes** This aim attempts to reduce the gap between experimental observations, constraints from modern environments, and the interpretation of the ancient sedimentary rock record. For this purpose it quantitatively investigate the sedimentology, facies distribution, mineralogy, compositional and isotopic geochemistry of a Cretaceous alkaline lake deposit as a case study (chapter 6). Figure 1.3 summarises the workflow of this thesis.

1.4 Thesis Structure and Chapter Linkages

- **Chapter 2** introduces the thermodynamic principles necessary to understand the geochemistry of natural waters, the principles governing precipitation (and dissolution) of minerals as a result of a solution being saturated or not with respect to a mineral phase, with focus on carbonate and phosphate minerals. It also addresses the complications arising in complex multi-electrolyte solutions, that is, high ionic strength fluids, such as saline and alkaline waters that are the topic of the present research, and the theoretical framework employed to estimate the excess free energy in a solution (the driving force of precipitation) and the activity coefficients and activities of the ions of interest. In this respect, the chapter provides a new implementation of phosphorus chemistry at higher ionic strength and coupled with the carbonate system, building on previous experimental and theoretical thermodynamic work by Hershey et al. (1989) [51]. To the best of the author's knowledge, very few if any aqueous geochemical models have explicitly done such implementation and coupled

those two systems under such conditions. Therefore, this new development allows us to understand the thermodynamics of phosphate-bearing solutions under high carbonate alkalinity and pH conditions.

- **Chapter 3** Discusses in detail the central concept of alkalinity (ALK) that permeates this entire work, and describes a protocol for the preparation of internal standard solutions for calibration and measurements by potentiometric titration of natural and experimental samples with high alkalinity. It also provides details about the latter measurements, which together with pH determinations (or another independent known variable, such as pCO_2 or dissolved inorganic carbon (DIC)), allow the carbonate system to be fully constrained. This is extremely relevant for the ensuing discussion in chapters 4 and 5.

- **Chapter 4** creates a comprehensive database based on published fluid chemistry analyses of alkaline lake waters covering most parts of the world (from 16 countries and six continents). This large dataset permits the recognition of general patterns regarding the water chemistry of alkaline lakes and the saturation states with respect to main mineral phases. Therefore, this contribution enables these observations to be generalised and extended to place further constraints on the interpretation of the geologic record (Chapter 6), based on present-day alkaline lake water compositions.

- **Chapter 5** investigates the theoretical models describing homogeneous and heterogeneous precipitation and explores the thermodynamic driving force of nucleation, the saturation state, with experimental observations made in constant composition experiments and theoretical considerations. It ends summarising the implications our current understanding of theory and of experimental results bear on the interpretation of ancient sedimentary mineral deposits.

- **Chapter 6** employs some of the previous knowledge to the interpretation of a case study deriving from the ancient geologic record, the Lower Cretaceous

continental carbonates rocks of the BVF in Santos Basin, Brazil, considered the products of precipitation from ancient alkaline lakes. This chapter advances further with a new set of sedimentological and geochemical observations, employing computational tools for the interpretation of geochemical data that are useful in distinguishing compositional differences among distinct textures of the same carbonate mineral phase (*e.g.*, calcite) and between different phases (calcite and dolomite).

- **Chapter 7** summarises the major contributions of this thesis and discusses several limitations of the current work, which further drive the directions of future research.

1.5 Contributions and Publications

Chapter 2 and chapter 4 Pietzsch, R., Tosca, N.J., Henderson, G.M., 2022. Chemical controls on carbonate sediment production and phosphate concentration in alkaline lakes. Book of Abstracts, Goldschmidt Conference 2022, Honolulu.

Chapter 2 and chapter 4 Pietzsch, R., Tosca, N.J., Henderson, G.M., 2022. Chemical controls on carbonate sediment production and phosphate concentration in alkaline lakes. Book of Abstracts, Geochemistry Group Research in Progress Meeting 2022, Cardiff.

Chapter 6 Pietzsch, R., Tosca, N.J., Gomes, J.P., Roest-Ellis, S., Sartorato, A.C.,L., Tonietto, S.N., 2022. The role of phosphate on non-skeletal carbonate production in a Cretaceous alkaline lake. Geochimica et Cosmochimica Acta 317, 365-394. doi: 10.1016/j.gca.2021.09.032

Chapter 6 Pietzsch, R., Roest-Ellis, S., Tosca, N.J., 2020. A Cretaceous alkaline lake as an analogue for the prebiotic P-cycle? Book of Abstracts, Carbonate Forum 2020.

Chapter 3 and chapter 5 Pietzsch, R., Roest-Ellis, S., Tosca, N.J., 2019. An experimental investigation of chemical controls on fabric development in $CaCO_3$ systems. Book of Abstracts, 16^{th} Bathurst Meeting of Carbonate Sedimentologists, Palma de Mallorca.

Chapter 3 and chapter 5 Pietzsch, R., Roest-Ellis, S., Tosca, N.J., 2019. Chemical controls on fabric development in non-skeletal carbonates. Book of Abstracts, Goldschmidt Conference 2019, Barcelona.

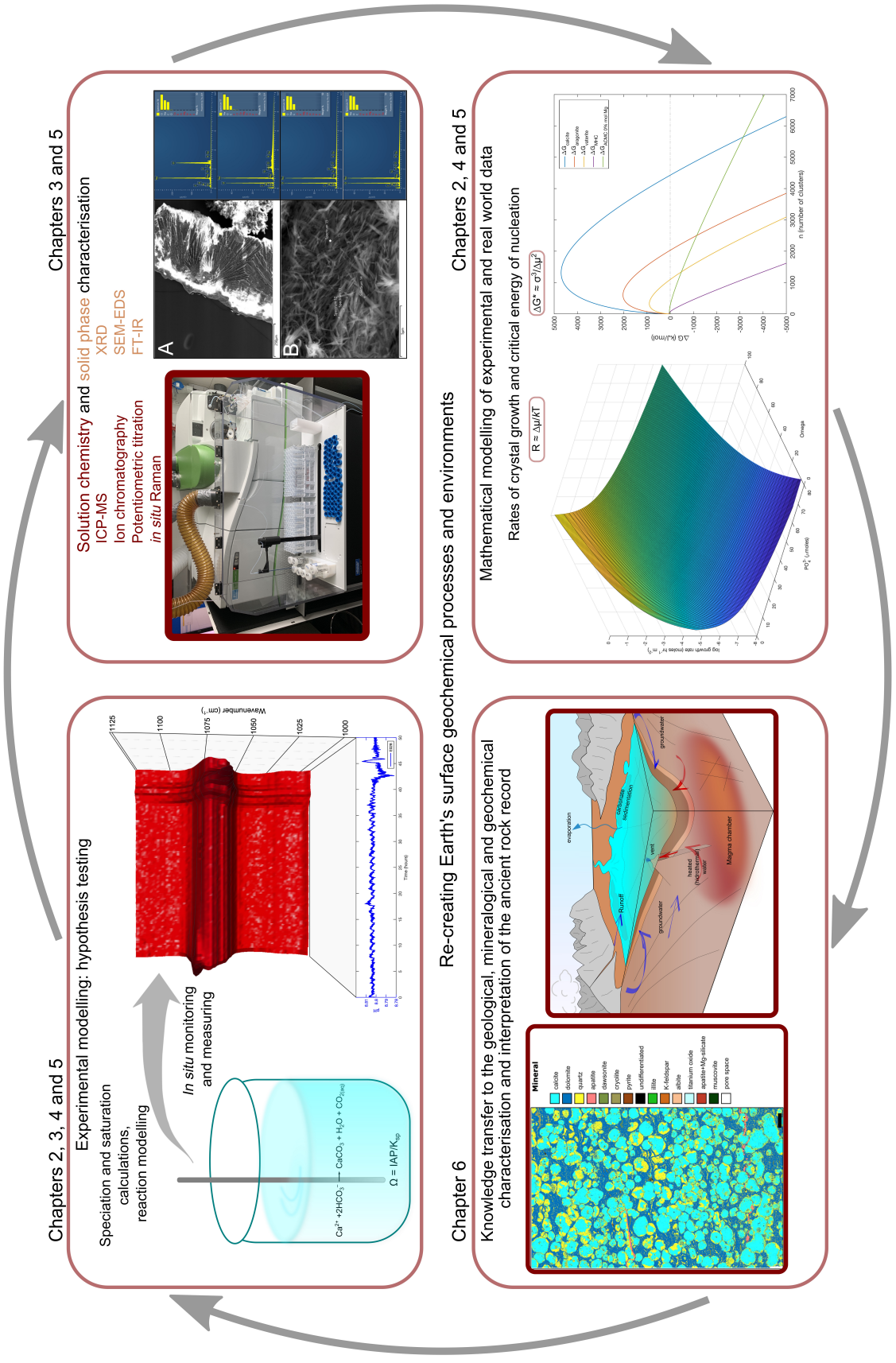


Figure 1.3: Summary of the general Workflow and main approaches used in this thesis, and how they relate to each other.

2

Review of Thermodynamic Theory and Description of Calculations

2.1 An Overview of General Concepts

This chapter is intended to provide only a brief overview of the thermodynamic principles and calculations entailed in the estimation of the general conditions of electrolyte solutions (*i.e.*, ion activities) and of mineral solubilities of relevance to the present study. This is because the theory is extensive and thorough overviews can be found in some classical works as well as in more recent literature (for example, Garrels and Christ 1965 [52]; Berner 1971 [5]; Truesdell and Jones 1974 [53]; Pitzer 1987 [54]; Stumm and Morgan 1996 [55]; Drever 1997 [56]; Brezonik and Arnold 2011 [57]; Anderson 2017 [58]). This overview also aims to clarify the calculations of equilibrium solubility constants for modification and inclusion of new entries in The Geochemist's Workbench (GWB) thermodynamic database "thermo_phrqpitz.tdat" (Plummer et al. 1988 [3]; Bethke et al. 2020 [4]). The modified database is a customisation with the aim of permitting thermodynamic equilibrium calculations of the water-carbonic acid-phosphoric acid system for highly alkaline and evaporitic waters. The "thermo_phrqpitz.tdat" code containing the

modifications explained below is made available on github.com under the repository "raphapietzsch/alkaline_lakes".

To estimate whether or not solutions and their solutes are in equilibrium conditions, in simple terms meaning that no visible change is occurring, such as precipitation or dissolution of a solid phase, the thermodynamic properties of solutions must be calculated. More rigorously, reactions are continuously taking place in solution, but under thermodynamic equilibrium the rates of forward and backward reactions, exemplified again as precipitation and dissolution, are equivalent and therefore no change is observed. If the rates are different the solution is no longer considered to be in equilibrium, because the reactions will progress preferentially in one direction or another. This is the kinetic definition of equilibrium, from which thermodynamic equilibrium constants (K) can also be derived, being in actuality their first and original conceptualisation (Brezonik and Arnold 2011 [57]). It may be also a more intuitive way of understanding equilibrium. In any case, the relevant thermodynamic properties here are the saturation states and saturation indexes with respect to the mineral phases of interest in this study, that is, the main Ca-Mg-Na-carbonates and Ca-phosphates phases considered in this work.

Thus, we begin defining the saturation state (Ω) of a solution with respect to a given solid phase

$$\Omega = IAP/Ksp \tag{2.1}$$

Where IAP is the ion activity product (IAP) and *Ksp* is the (equilibrium) solubility product constant (Ksp) (*e.g.*, for calcite, $10^{\breve{}8.48}$ at 25^{o}C, Plummer and Busenberg 1982 [59]). The SI, in turn, is simply defined as

$$\text{SI} = \log_{10}(\Omega) \tag{2.2}$$

Therefore, the values of $\Omega = 1$ or SI $= 0$ indicate the solution is at equilibrium with respect to a given solid phase. Numbers below these reference values therefore

imply the solutions are unsaturated, and thus dissolution of the mineral phase is expected, whereas values above suggest the solutions are supersaturated, and hence precipitation or crystal growth are expected instead. As mentioned, the IAP reflects the ion activity product of the relevant ions in solution that can react to form a given solid. The ion activity is often informally addressed as the effective or "true" thermodynamic concentration of ionic species available for reactions. This is because as a result of multiple competing electrostatic interactions among charged ions, arising from different hydration shells related to different charges and ion sizes, the structure and the free energy of the real, water-containing solution is affected and becomes different from that of an ideal solution (free of ions or "infinitely diluted solution"). This arises because dissociated (hence charged) ions in solution exert long-range electrostatic forces (Coulombic forces) upon one another, in turn lowering the values of their activity coefficients (defined below) (Garrels and Christ 1965 [52]; Drever 1997 [56]). It follows that activities (and activity coefficients) are a function of the change in chemical potentials and the free energy of a solution ($\Delta\mu$ and ΔG, respectively) with respect to a reference state, resulting from the variation in the concentration of the respective dissolved ions they relate to. The Debye–Hückel (DH) theory, developed in the early 1920s by Peter Debye and Erich Hückel, considers precisely these interactions and has been successful in describing the behaviour of electrolyte solutions and their ions in dilute conditions. It also forms the basis of more complex models incorporating diverse ion interactions in considerably concentrated brines, such as Pitzer's ion interaction activity coefficient model (*e.g.*, Pitzer 1987 [54]).

It cannot be emphasised enough that only changes in free energy and chemical potentials with respect to some reference state can be measured, but not their absolute values. The derivations to show that chemical potentials, free energy and the activity of some constituent i are directly related are carefully and thoroughly described by Anderson and Crerar 1993 [60]. It can be demonstrated that

$$\mu_i - \mu_i^\circ = RT\ln a_i \tag{2.3}$$

Where μ_i is the chemical potential of some constituent i, μ_i° is the chemical potential of the constituent in its pure form, R and T are the gas constant and the absolute temperature of the system of interest, respectively, and a_i is the activity of constituent i. In order to be more complete, it must be emphasised that the chemical potential is an important intensive state variable, reflecting the effective free energy of one mole of component i in a solution at specified T, P and concentration of interest. This means it expresses the change in total free energy of a solution when one mole of the constituent i is added at constant T and P to a sufficiently large quantity of that solution that no change can be observed in the other components present there (Anderson and Crerar 1993 [60]). This is expressed as

$$\mu_i = \bar{G}_i = \left(\frac{\partial \mathrm{G}}{\partial n_i}\right)_{T,P,\hat{n}_i} \tag{2.4}$$

Where $\bar{G}_i$ is the partial molar free energy of constituent i, G is the total free energy of the system (an extensive property or state variable, meaning that it depends on the mass of the system considered) and $\hat{n}_i$ refers to all constituents in solution other than the constituent i. These parameters, in turn, set the principles from which the concepts of activity and activity coefficients can be defined, which are the parameters we want to measure or derive from chemical analyses, measurement of fluid properties such as pH and additional calculations.

A rigorous definition of activity and activity coefficients has its roots even further, in the ideal solution and ideal mixing concepts deriving from Henry's law and Raoult's law, respectively, which are in turn derived from the ideal gas concept. Anderson and Crerar 1993 [60] discuss in great detail these concepts and how, in ideal systems[1], the activity equals the mole fraction (X_i) of a solute i in a liquid phase and both – the activity and the mole fraction – equate to the ratio between the fugacity of a substance i in a mixture (f_i) and the fugacity of pure i with respect to its own liquid phase (f_i°). The latter is designated the reference state for i at

[1]Despite being "merely" theoretical constructs, ideal systems are nevertheless very powerful models to compare our observations with, and hence provide profound insight into real systems, those that we are interested in investigating in the real world.

some given temperature T, because it is our choice (a convention) to define the pure i at that temperature as the reference state. The superscript $^\circ$ – introduced earlier with the parameter μ_i° – is often used to refer to some given reference or *standard state*, which represents a definition chosen because of its usefulness. Mathematically

$$a_i = X_i = \frac{f_i}{f_i^\circ} \tag{2.5}$$

When systems deviate from the ideal behaviour (true of real systems), Raoultian or Henryan activity coefficients (γ_R and γ_H, respectively) are introduced in equations 2.3 and 2.5 to account for such deviations. In these cases, equation 2.5 then becomes

$$a_i = X_i \gamma_R \tag{2.6}$$

Or

$$a_i = X_i \gamma_H \tag{2.7}$$

However, molalities are more useful instead of mole fractions or fugacities in studies of aqueous solutions, because they are directly measurable parameters. This requires the definition of some new specific standard state establishing the relationship between μ and m, the solute molality in the dilute solution region (where Henry's law is obeyed). Because μ_i is a state variable with a fixed absolute value for any system at equilibrium and the same applies to μ_i°, except that the choice of state is arbitrary at our convenience, therefore fixing μ_i° at a specifically chosen standard state, it follows that $(\mu_i - \mu_i^\circ)$ becomes a fixed quantity as well.

Relating μ to m requires some less than straightforward derivations, but it can nonetheless be shown that the relation $\mu_i - \mu_i^\circ = RT\ln a_i$ (eqn. 2.3) is equivalent to

$$\mu_i - \mu_i^\circ = RT\ln\frac{f_i}{f_i^\circ} \tag{2.8}$$

As well as to

$$\mu_i - \mu_i^\circ = RT\ln\frac{(\gamma_H m_i)}{(\gamma_H m_i)^\circ} \tag{2.9}$$

This latter expression relates the chemical potentials of a given state of interest and of a given standard state with the molalities and Henryan activity coefficients of that state with respect to the standard state (the term $(\gamma_H m_i)^\circ$). It may seem a long and unnecessary detour, but equation 2.9 simply redefines the activity term introduced in equations 2.3, 2.5—2.7 and 2.8 in terms of units that are more convenient to address in aqueous solutions. However, equation 2.9 still requires some redefining of the standard state, because in its present form it is implied that the ideal gas is the chosen standard state. Thus, it is a convention to set $(\gamma_H m_i)^\circ$ equal to 1.0, "obviously the best thing to do", quoting Anderson and Crerar 1993 [60], which is the "hypothetical ideal one molal" scale standard state. This reduces equation 2.9 to

$$\mu_i - \mu_i^\circ = RT\ln(\gamma_H m_i) \tag{2.10}$$

The definitions above provide some of the foundations on which the DH theory is built. The latter, in turn, results in the starting point to determine the activity coefficients and, thus, the activities of specific ions that are the desired parameters in most thermodynamic calculations aiming to assess the conditions expressed by equations 2.1 and 2.2.

As alluded to above, the DH model is a limiting law, signifying it assumes infinitely diluted solutions where the electrical interactions only occur over considerable distances, and the total concentration of dissolved species approaches zero (Berner 1971 [5]; Anderson 2017 [58]). This condition is analogue to the "Henryan" ideality mentioned above. In this special case the activity of a particular solute approaches its concentration because the activity coefficient approaches the value of 1. Therefore, from the preceding discussion the relations among activity, activity coefficient and (molal) concentration can be summarised by the more conventional expression

$$a_i = m_i\gamma_i \tag{2.11}$$

Where a_i corresponds to the ion activity of species i, m_i is the concentration of species i and γ_i is its activity coefficient. In turn, concentrations can be determined directly by chemical analyses, although speciation models are further required to estimate the distribution of, say, one same element in their possible different chemical species. Speciation introduces additional complexity to chemical modelling of aqueous solutions, particularly when dealing with multicomponent and concentrated solutions, because it will inevitably involve multiple acid-base equilibrium calculations of dissolved salts. Thus, it will only be discussed briefly below, with regards to the cases that are most directly relevant to this study. It is however implicitly assumed as a necessary step in the calculations of all individual activities and activity coefficients described herein. A further problem arises because of the physical fact that both cations and anions always exist together in solution and there is no way of measuring their activity coefficients separately. Therefore, some alternative approaches involving different conceptual models have been historically developed in attempts to tackle this physical imposition, among them the single-ion (MacInnes assumption) and the mean ionic activity coefficient model, the latter being the most widely used (Garrels and Christ 1965 [52]; Berner 1971 [5]; Truesdell and Jones 1974 [53]; Anderson and Crerar 1993 [60]; Drever 1997 [56]). For additional details regarding this issue specifically, the interested reader is referred to the cited literature and the references therein.

Assuming initially the effect on the free energy of an individual ion Debye and Hückel could derive the expression describing single ion activity coefficients behaviour of ions in very dilute solutions. They assumed this effect results from the electrical interactions with other ions of opposite charge, producing a spherical shell or "ionic atmosphere" around that ion (Truesdell and Jones 1974 [53]; Atkins and de Paula 2014 [61]; Anderson 2017 [58]). The classical expression of their extended model takes the form

$$log\gamma_i = \frac{-Az^2\sqrt{I}}{1 + \mathring{a}_i B\sqrt{I}} \tag{2.12}$$

The constants A and B depend on temperature, density and the dielectric constant of pure water at the investigated T and P, with the numerical values at 1 atm and 25^{o}C equal to 0.5085 and 0.3281, respectively. The å$_i$ is a constant estimated from experimental data, corresponding to the theoretical hydrated radius of a given ion (the DH distance of closest approach, in ångström units) (Truesdell and Jones 1974 [53]; Drever 1997 [56]; Anderson 2017 [58]). Truesdell and Jones (1974) [53] estimated several values of å$_i$ for corresponding major ions by fitting of experimental data, using a variation of eqn. 2.12 that extends its range of validity (further below). Finally, I corresponds to the ionic strength of the solution, and is given by

$$I = \frac{1}{2} \sum m_i {z_i}^2 \tag{2.13}$$

Where m_i corresponds to the total molal concentration of a given ionic species and z_i to its charge.

For solutions with $I \leq 0.1$ the extended DH equation tends to hold, describing well the expected behaviour of the solutes in solution. For higher values of ionic strength, modifications of the DH equation, such as the Davies (Stumm and Morgan 1996 [55]; Drever 1997 [56]) and the Truesdell and Jones (Truesdell and Jones 1974 [53]) equations, for up to $I \leq 0.7$ and $I \leq 2$ respectively, are more appropriate. The Davies equation (Davies 1962 [62]) is expressed as

$$\log\gamma_i = \frac{-Az^2\sqrt{I}}{1+\sqrt{I}} - 0.3I \tag{2.14}$$

Where Davies 1962 [62] introduced the empirical term $0.3I$ to a variation of the DH model, which makes this formulation still rather simple to apply in geochemical modelling and useful to solutions approaching the ionic strengths of seawater and at 25° C. Truesdell and Jones 1974 [53] employed a further variation of the DH equation, after Robinson and Stokes 1955 [63]:

$$\log\gamma_i = \frac{-Az^2\sqrt{I}}{1+\text{å}_i B\sqrt{I}} + bI \tag{2.15}$$

Which is a form of DH equation considering the adjustable parameter b that accounts for the effect of the decrease in concentration of solvent in concentrated solutions. To apply this equation, Truesdell and Jones 1974 [53] calculated the values of both constants å and b for major ions from experimental data of mean salt single-ion activity coefficients.

An advancement of these models was proposed by Helgeson 1969 [64] and Helgeson and Kirkham 1974 [65]. Their model aimed to tackle a difficult problem of great interest to geochemists, that is, to determine activities of minor and trace components that occur in concentrated aqueous solutions and over a wide range of temperatures (Anderson and Crerar 1993 [60]; Bethke 2008 [66]). Helgeson 1969 [64] defined a deviation function $\dot{B}$ (hence, the "B-dot" equation, as it is known), that corresponds to the difference between observed and predicted activity coefficients for an electrolyte, where he initially considered essentially NaCl solutions (Anderson and Crerar 1993 [60]; Bethke 2008 [66]). The $\dot{B}$ parameter was thus derived by fitting experimentally observed activity coefficients for NaCl at variable concentrations and temperatures, up to 3 molal and 300°C. This equation is considered accurate in predicting the activities of ionic species other than Na^+ and Cl^- to ionic strengths up to about 0.3 to 1 molal (Bethke 2008 [66]). The "B-dot" equation is thus

$$\log\gamma_i = \frac{-Az^2\sqrt{I}}{1 + \mathring{a}_i B\sqrt{I}} + \dot{B}I \tag{2.16}$$

Finally, for even higher ionic strengths, it becomes necessary to resort to more complex models to describe the state of the solution, such as the Pitzer ion activity interaction model. However, the latter also has limitations, perhaps the most significant one being that equilibrium constants for several reactions that may be relevant in concentrated brines have not been estimated in temperatures outside 25^oC. Despite this, the Pitzer model produces the most reliable results for concentrated and evaporitic solutions at surface temperatures and has therefore been used herein. Before describing it in some detail in the next section, we will address in the following the relevant reactions that constrain our system of interest and that have

been used in the customisation of the GWB "thermo_phrqpitz.tdat" database, as mentioned earlier.

We will first consider the carbonic acid system in association with calcium carbonate reactions, and later the case of the phosphoric acid system in association with calcium phosphates. The following discussion refers specifically to modifications implemented in the database called by The Geochemist's Workbench software and used for thermodynamic calculations addressed in the present study.

2.2 Reactions constraining the calco-carbonic-phosphoric acid system

Consider the familiar example of calcite: under the description "minerals" in the GWB "thermo.tdat" database we will find the value of $logK$ for calcite (at 25^{o}C) is 1.7130, whereas it is 1.9333 in the "thermo_hmw.tdat" (after Harvie, Møller and Weare 1984 [67]) database and, finally, is 1.8487 in the "thermo.com.V8.R6+.tdat" database.

Whichever value is used, the reaction considered in the GWB program usually takes the following form (see also The Geochemist's Workbench® GWB Essentials Guide; Bethke et al. 2020 [4]):

$$CaCO_3 + H^+ \longrightarrow Ca^{2+} + HCO_3^-$$

This reaction is one amongst a few different ways to represent the dissolution of calcium carbonate. It may be seen more often represent as:

$$CaCO_3 \longrightarrow Ca^{2+} + CO_3^{2-} \tag{2.17}$$

The Ksp of this reaction at 25^{o}C is (Plummer and Busenberg 1982 [59]):

$$Ksp = a_{Ca^{2+}} \cdot a_{CO_3^{2-}} = 3.31 \times 10^{-9} \qquad \therefore \qquad logKsp = -8.48 \tag{2.18}$$

The other important equilibrium reactions to have at hand, considering the carbonate system, that allow us to recast the equilibrium relations in different forms and to derive the respective value of Ksp related to these reactions are:

$$CO_{2(g)} \longrightarrow CO_{2(aq)} \qquad K_H = \frac{a_{CO_{2aq}}}{pCO_2} \tag{2.19}$$

$$CO_{2(aq)} + H_2O \longrightarrow H_2CO_3 \tag{2.20}$$

$$H_2CO_3 \longrightarrow H^+ + HCO_3^- \qquad K_1 = \frac{a_{H^+} \cdot a_{HCO_3^-}}{a_{CO_{2aq}} \cdot a_{H_2O}} \tag{2.21}$$

$$HCO_3^- \longrightarrow H^+ + CO_3^{2-} \qquad K_2 = \frac{a_{H^+} \cdot a_{CO_3^{2-}}}{a_{HCO_3^-}} \tag{2.22}$$

Where K_H, K_1 and K_2 are respectively the Henry constant and the first and second carbonic acid dissociation constants. GWB considers reaction (2.17) coupled with reaction (2.22) (which needs to be reversed for mass-balance reasons):

$$CaCO_3 \longrightarrow Ca^{2+} + CO_3^{2-} \qquad logKsp$$

$$H^+ + CO_3^{2-} \longrightarrow HCO_3^- \qquad -logK_1$$

We finally get

$$CaCO_3 + H^+ \longrightarrow Ca^{2+} + HCO_3^- \qquad new\, logKsp \tag{2.23}$$

The solubility product of this reaction is not the same as the Ksp value of $3.31 \times 10^{\breve{}9}$ (or logKsp = –8.48) because this new Ksp is a function of H^+ and $HCO_3^{\breve{}}$, as well as Ca^{2+} (and assuming the activity of $CaCO_3$ is 1):

$$Ksp = \frac{a_{Ca^{2+}} \cdot a_{HCO_3^-}}{a_{H^+}} \tag{2.24}$$

Quite simply, the new value of the Ksp could be found as indicated above, but to avoid confusions (such as directly subtracting $Ksp - K_1$, instead of their logarithms,

which will yield an incorrect result), it is handy to follow the step-by-step procedure that was used to calculate the new entry values in the modified database. Following Drever (1997) [56] we express reaction 2.22 in terms of $a_{CO_3^{2-}}$:

$$K_2 = \frac{a_{H^+} \cdot a_{CO_3^{2-}}}{a_{HCO_3^-}} \qquad a_{CO_3^{2-}} = \frac{a_{HCO_3^-}}{a_{H^+}} \cdot K_2 \tag{2.25}$$

And substitute in equation 2.18:

$$Ksp = a_{Ca^{2+}} \cdot a_{CO_3^{2-}} \quad \therefore \quad Ksp = a_{Ca^{2+}} \cdot \frac{a_{HCO_3^-}}{a_{H^+}} \cdot K_2 \quad \therefore \quad \frac{a_{Ca^{2+}} \cdot a_{HCO_3^-}}{a_{H^+}} = \frac{Ksp}{K_2}$$
$$\therefore \quad \frac{Ksp}{K_2} = new\,Ksp = 7.06 \times 10 \tag{2.26}$$

$$\therefore \quad log(new\,Ksp) = 1.8488 \tag{2.27}$$

Therefore, the value of $logKsp$ for calcite considering the reaction (2.23) at 25^{o}C is 1.8488.

Vaterite was also added to the same database (*i.e.*, the modified "thermo_phrqpitz.tdat"), whose data were available in the "thermo_minteq.tdat" database, but which in turn considers the reaction 2.17. Thus, the provided $logKsp$ = –7.9134 (at 25^{o}C) assumes reaction 2.17. Therefore, it is also necessary to convert this value to the appropriate reaction 2.23, in order to maintain consistency with the new database. Calculating the $logKsp_{(vaterite)}$ for the reaction $CaCO_3 + H^+ \longrightarrow Ca^{2+} + HCO_3^-$, at 25^{o}C:

$$\begin{aligned} Ksp_{new}vaterite &= \frac{Ksp_{(vaterite)}}{K_2}, \quad \text{or} \\ logKsp_{new}vaterite &= logKsp_{(vaterite)} - logK_2 \end{aligned} \tag{2.28}$$

Substituting numerically eqn. 2.28

$Ksp_{new}vaterite = -7.9134 - (-10.3290) = 2.4156$, where the value –10.3290 is the $logK_2$ determined by Plummer and Busenberg (1982) [59].

Similarly, we can recalculate the $logKsp_{(vaterite)}$ for the same reaction (2.23) at 0 and 100^{o}C:

$logKsp_{new}vaterite(0^oC) = -7.7427 - (-10.6392) = 2.8965$

$logKsp_{new}vaterite(100^oC) = -8.8588 - (-10.1658) = 1.3070$

Finally, the same procedures were applied to obtain the solubility product of octacalcium phosphate (OCP). Assuming its unit formula as $Ca_4(PO_4)_3H \cdot 2.25H_2O$ (Tung et al. 1988 [68]), The dissolution is cast as (in GWB):

$$Ca_4(PO_4)_3H \cdot 2.25H_2O + 2H^+ \longrightarrow 4Ca^{2+} + 3HPO_4^{2-} + 2.25H_2O \tag{2.29}$$

And therefore, the K_{OCP} is

$$K_{OCP(GWB)} = \frac{(a_{Ca^{2+}})^4 \cdot (a_{HPO_4^{2-}})^3}{(a_{H^+})^2} \tag{2.30}$$

Tung et al. (1988) [68] cast OCP dissolution as

$$Ca_4(PO_4)_3H \cdot 2.25H_2O \longrightarrow 4Ca^{2+} + H^+ + 3PO_4^{3-} \tag{2.31}$$

From which we get

$$K_{OCP} = (a_{Ca^{2+}})^4 \cdot (a_{H^+}) \cdot (a_{PO_4^{3-}})^3 \tag{2.32}$$

With a $K_{OCP} = 10^{\breve{}48.4}$ at 23.5^{o}C (Tung et al. 1988).

Considering now the phosphoric acid dissociation reactions, with the K_1, K_2 and K_3 values at 25^{o}C provided by Tung et al. (1988) [68],

$$H_3PO_4 \longrightarrow H^+ + H_2PO_4^- \quad , \quad logK_1 = 7.11 \times 10^{-3} \tag{2.33}$$

$$H_2PO_4^- \longrightarrow H^+ + HPO_4^{2-} \quad , \quad logK_2 = 6.31 \times 10^{-8} \tag{2.34}$$

$$HPO_4^{2-} \longrightarrow H^+ + PO_4^{3-} \quad , \quad logK_3 = 4.52 \times 10^{-13} \tag{2.35}$$

And then,

$$K_3 = \frac{a_{H^+} \times a_{PO_4^{3-}}}{a_{HPO_4^{2-}}} \tag{2.36}$$

Recasting it for $a_{PO_4^{3-}}$,

$$a_{PO_4^{3-}} = \frac{a_{HPO_4^{2-}}}{a_{H^+}} \times K_3 \tag{2.37}$$

Replacing 2.37 in 2.32

$$K_{OCP} = (a_{Ca^{2+}})^4 \cdot (a_{H^+}) \cdot (\frac{a_{HPO_4^{2-}}}{a_{H^+}} \cdot K_3)^3$$

We finally get

$$\begin{aligned} K_{OCP} &= \frac{(a_{Ca^{2+}})^4 \cdot (a_{HPO_4^{2-}})^3}{(a_{H^+})^2} \cdot (K_3)^3 \quad \therefore \frac{(a_{Ca^{2+}})^4 \cdot (a_{HPO_4^{2-}})^3}{(a_{H^+})^2} = \frac{K_{OCP}}{(K_3)^3} \\ \therefore K_{OCP(GWB)} &= \frac{K_{OCP}}{(K_3)^3} \end{aligned} \tag{2.38}$$

Therefore, $log_{K_{OCP(GWB)}} = -11.37$.

2.3 Additional geochemical calculations and the Pitzer model for the determination of the activity coefficients and thermodynamic dissociation constants of the phosphoric acid system

As mentioned before, the GWB "thermo_phrqpitz.tdat" database used in the present study is an implementation of the Pitzer model (Plummer et al. 1988 [3]). Additionally, to independently investigate the behaviour of the Ca-HPO_4 system in a high ionic strength solution departing from ideality, the dissociation constants of the phosphoric acid were calculated using the experimental data of Hershey et al. (1989) [51] and their evaluation of the Pitzer ion activity coefficient

model parameters. In this regard, it is worth highlighting that very few aqueous geochemical models if any have explicitly incorporated phosphorus chemistry at higher ionic strengths. Thus, the present work is a new development that allows us to understand the thermodynamics of phosphate-bearing solutions under such conditions.

The complete formulation of the Pitzer model is complex and long, being beyond the scope of the present text. Only a general account describing the essential background theory and steps taken to derive the final equations used in the present modelling are given below. Thus, the initial formulation of the Pitzer model is expressed by the following equation (Pitzer 1987 [54]; Drever 1997 [56]):

$$\frac{\mathbf{G}^{ex}}{n_w RT} = f^{\gamma} + \sum_i \sum_j m_i m_j \lambda_{ij} + \sum_i \sum_j \sum_k m_i m_j m_k \mu_{ijk} \tag{2.39}$$

This is the general Pitzer formulation, stating that departures from ideality in electrolyte solutions result from the interaction between the multiple ions in the solution (Pitzer 1987 [54]; Drever 1997 [56]; Anderson 2017 [58]). The $\mathbf{G}^{ex}$ stands for the excess Gibbs free energy per kilogram of water (*i.e.*, the difference between the actual free energy and the free energy the solution would have if the activities were equal to concentrations), n_w is the number of kg of water and m_i, m_j,... are the molalities of all solute species. R and T are again the gas constant and the absolute temperature, respectively. The first term on the right hand of eqn. 2.39 includes the extended DH limiting law shown in eqn. 2.12, adapted for empirical effectiveness (Pitzer 1987 [54]). The quantity λ_{ij} represents the short-range interaction between solute particles i and j in the presence of the solvent. Similarly, the quantity μ_{ijk} corresponds to the interaction among three species i, j and k. Higher order interactions are certainly possible, but are often omitted, which results in limitations if treating extremely concentrated solutions. Regardless, it is still possible to introduce virial coefficients for fourth and higher order interactions or to follow alternative methods in such extreme cases (Pitzer 1987 [54]). From standard definitions and thermodynamic transformations, it is possible to derive

the general equation for the activity coefficient from eqn. 2.39 (Pitzer 1987 [54]; Anderson 2017 [58]):

$$ln\gamma_i = \frac{\partial(\mathbf{G}^{ex}/n_w RT)}{\partial m_i} \tag{2.40}$$

where $m_i = n_i/n_w$, n_i being the number of moles of species i.

An important effect in complex electrolyte solutions is that an ion will form different chemical species in the form of ion pairs and ion complexes of, say, the same chemical element, reducing its overall availability for given reactions, simply because some species are already the most stable under a given condition. Because some species will contribute more to minimise the overall energy of the solution under those given conditions, they will therefore have greater likelihood than others of being the predominating species in that context (Anderson 2017 [58]). This might be said an alternative way of interpreting activity coefficients. In other words, the activity coefficients of ions in solution are directly related to the free energy of the system (the solution), their values therefore reflecting the (local) equilibrium distribution of the dissolved species under the given conditions.

The Pitzer model is a semi-empirical approach, whereby the preceding formulations derive directly from thermodynamic theory, but which on the other hand many of the parameters introduced in the next equations are only obtained through carefully designed experimentation. However, the requirement of electrical neutrality in ionic solutions makes impossible the determination of individual ionic activities. Furthermore, different combinations of the quantities λ and μ will arise in mixed electrolyte solutions, rendering the direct measurement of these properties impossible as well. Therefore, Pitzer and his co-workers introduced the terms B_{MX}, C_{MX}, Φ_{cc} and $\psi_{cc'a}$ that can be determined by fitting experimental data to measurable parameters such as molalities and ionic strength (Harvie et al. 1984 [67]; Pitzer 1987 [54]). These terms are defined further below for the phosphoric acid system as also used in the present study, following Hershey et al. (1989) [51]. The general equation that follows from these derivations assumes the form (Pitzer 1987 [54])

$$ln\gamma_M = z_M^2 f^\gamma \; + \; \sum_c m_c(2B_{cM} + ZC_{cM}) \; + \; \sum_a m_a(2\Phi_{Ma} \; + \; \sum_c m_c\psi_{cMa}) + \sum_c \sum_{c'} m_c m_{c'} \psi_{cc'M} \; + \; |z_M| \sum_c \sum_a m_c m_a C_{ca} \; + \; 2\sum_n m_n \lambda_{nM} \; + ... \tag{2.41}$$

where $ln\gamma_M$ is the activity coefficient of the cation M and the sums are over the various cations (c, c') and over the anions (a, a') interacting with M. An equivalent equation applies to the calculation of the activity coefficient of the anion X (Harvie et al. 1984 [67]; Pitzer 1987 [54]).

This general form was applied by Hershey et al. (1989) [51] in their experimental determination of the phosphoric acid dissociation constants, which were used in the present study for subsequent implementation in the modelling of the Ca-HPO_4 system behaviour in a concentrated solution. Equations 2.42 to 2.46 below provide the full algorithmic description of the terms used to solve eqn. 2.41:

$$f^\gamma = -0.392 * (sqrt(I)/(1 + 1.2 * sqrt(I)) + (2/1.2) * ln(1 + 1.2 * sqrt(I))) \tag{2.42}$$

Where f^γ is the Debye-Hückel (DH) term at 25^{o}C. Additionally:

$$B_{MX} = \beta_{MX}^{(0)} + (2 * \beta_{MX}^{(1)}/((\alpha_1^2) * I)) * (1 - (1 + \alpha_1 * sqrt(I))) * exp(-\alpha_1 * sqrt(I)) \tag{2.43}$$

$$B_{MX'} = (2 * \beta_{MX}^{(1)}/((\alpha_1^2) * I^2)) * (1 - (1 + \alpha_1 * sqrt(I) + (\alpha_1^2) * I)) * exp(-\alpha_1 * sqrt(I)) \tag{2.44}$$

$$C_{MX} = C_{MX}^{\phi}/(2 * sqrt(|Z_M * Z_X|)) \tag{2.45}$$

$$E = \sum_i |m_i * Z_i|/2 \tag{2.46}$$

Where M and X represent cations and anions, respectively, $\beta_{MX}^{(0)}$, $\beta_{MX}^{(1)}$, C_{MX}^{ϕ} are ion interaction parameters, B_{MX} and $B_{MX'}$ describe the interaction of pairs of oppositely charged ions represented by measurable combinations of the second virial coefficients, and C_{MX} is the single electrolyte third virial coefficient, which accounts

Table 2.1: Pitzer coefficients for phosphoric acid dissociation in Na-Cl and Na-Mg-Cl solutions, fitted from experimental data, Hershey et al. (1989) [51].

salt		$\beta^{(0)}$	$\beta^{(1)}$		C^{ϕ}
HCl		0.1775	0.2945		0.0008
NaCl		0.0765	0.2664		0.00127
Na_3PO_4		0.1781	3.8513		-0.05154
Na_2HPO_4		-0.05828	1.4655		0.02938
NaH_2PO_4		-0.0533	0.0396		0.00795
MgCl		0.35235	1.6815		0.00519
$Mg(H_2PO_4)_2$		-3.55	16.9		
$MgHPO_4$		-17.5	27.4		
i	j	k		Φ_{ij}	ψ_{ijk}
H	Na	Cl		0.036	-0.004
H_2PO_4	Cl	Na		0.1	-0.028
HPO_4	Cl	Na		-0.105	-0.003
PO_4	Cl	Na		-0.59	0.110
H	Mg	Cl		0	0
i	j		λ_{ij}		
H_3PO_4	Na		0.075*		
H_3PO_4	Cl		0		
$MgHPO_4$	Na		-0.124		

for short-range interaction of ion triplets. Finally, Z_i is the charge of the ion i, m_i is the molal concentration of ion i, and I is the ionic strength of the solution.

With these parameters constrained it is possible to calculate the activity coefficients of the species considered, with the additional terms Φ and ψ, which represent higher order parameters for the like-charged ions (*i.e.*, cation-cation or anion-anion) and for the triple ion interactions (*i.e.*, between cations and anions). These terms have been experimentally determined by Hershey et al. (1989) [51] for the phosphoric acid dissociation in Na-Cl and Na-Mg-Cl solutions (Table 2.1). Thus, the corresponding activity coefficients related to the phosphoric acid dissociation are given by the following expressions

$$\begin{aligned} \gamma_{H^+} = exp(f^{\gamma} + 2 * m_{Cl} * (B_{HCl} + E * C_{HCl}) + \\ m_{Na} * m_{Cl} * (B'_{NaCl} + C_{NaCl}) + m_{Na} * (2 * \Phi_{HNa} + m_{Cl} * \psi_{HNaCl})) \end{aligned} \tag{2.47}$$

$$\gamma_{H_3PO_4} = exp(2 * m_{Na} * \lambda_{H_3PO_4Na}) \tag{2.48}$$

$$\gamma_{H_2PO_4^-} = exp(f^\gamma + 2 * m_{Na} * (B_{NaH_2PO_4} + E * C_{NaH_2PO4}) + m_{Na} * m_{Cl} * (B'_{NaCl} + C_{NaCl}) + m_{Cl} * (2 * \Phi_{H_2PO_4Cl} + m_{Na} * \psi_{H_2PO_4ClNa})) \tag{2.49}$$

$$\gamma_{HPO_4^{2-}} = exp(4 * f^\gamma + 2 * m_{Na} * (B_{NaHPO_4} + E * C_{NaHPO4}) + m_{Na} * m_{Cl} * (4 * B'_{NaCl} + 2 * C_{NaCl}) + m_{Cl} * (2 * \Phi_{HPO_4Cl} + m_{Na} * \psi_{HPO_4ClNa})) \tag{2.50}$$

$$\gamma_{PO_4^{3-}} = exp(9 * f^\gamma + 2 * m_{Na} * (B_{NaPO_4} + E * C_{NaPO4}) + m_{Na} * m_{Cl} * (9 * B'_{NaCl} + 3 * C_{NaCl}) + m_{Cl} * (2 * \Phi_{PO_4Cl} + m_{Na} * \psi_{PO_4ClNa})) \tag{2.51}$$

$$K^*_{1P} = 2.146 - 0.5136 * sqrt(I) + 0.1606 * sqrt(I) \tag{2.52}$$

$$K^*_{2P} = 7.198 - 1.4040 * sqrt(I) + 0.6168 * I - 0.08114 * I^{(3/2)} \tag{2.53}$$

$$K^*_{3P} = 12.35 - 2.0992 * sqrt(I) + 0.9318 * I - 0.1291 * I^{(3/2)} \tag{2.54}$$

$$K_{1P} = K^*_{1P} * \gamma_{H^+} * \gamma_{H_2PO_4^-} / \gamma_{H_3PO_4} \tag{2.55}$$

$$K_{2P} = K^*_{2P} * \gamma_{H^+} * \gamma_{HPO_4^{2-}} / \gamma_{H_2PO_4^-} \tag{2.56}$$

$$K_{3P} = K^*_{3P} * \gamma_{H^+} * \gamma_{PO_4^{3-}} / \gamma_{HPO_4^{2-}} \tag{2.57}$$

Input data to determine K_1, K_2, and K_3 came from Table 1 (reproducing Table III of Hershey et al. 1989 [51]) and from [Na^+] and [$Cl^˘$] molal concentrations and ionic strength values assumed for a hypothetical alkaline and high ionic strength solution. Considering a hypothetical average alkaline solution with $I = 1.134$ molal (N = 232), [Na^+] = 0.706 molal (N = 232) and [$Cl^˘$] = 0.535 molal (N = 232), (applying the constraints CBE $\leq$ 10% and only samples with detected Ca^{2+} concentrations [see below], hence N =232) the final values of activity coefficients and the dissociation constants of phosphoric acid are shown in Table 2.2:

Table 2.2: Activity coefficients and dissociation constants for the phosphoric acid system in an average alkaline lake solution (ionic strength = 1.134, $[Na^+]$ = 0.706 molal and $[Cl^-]$ = 0.535 molal).

Activity coefficients	Stoichiometric pKs	Dissociation constants
$\gamma_{H} = 0.615$	$pK^*_{1P} = 1.78$	$K_{1P} = 4.67 \times 10^{-3}$
$\gamma_{H3PO4} = 1.112$	$pK^*_{2P} = 6.30$	$K_{2P} = 2.50 \times 10^{-8}$
$\gamma_{H2PO4} = 0.510$	$pK^*_{3P} = 11.02$	$K_{3P} = 1.10 \times 10^{-13}$
$\gamma_{HPO4} = 0.042$		
$\gamma_{PO4} = 0.0008$		

Finally, to model the role of Ca^{2+} in modulating ΣPO_4 concentrations in average alkaline lake waters (Chapter 4), the mean value of $a_{Ca^{2+}}$ was extracted from the alkaline lake water database. For this purpose, samples whose charge balance error (CBE) exceeded 10% and samples with undetected $[Ca^{2+}]$ values were excluded. Hence, from this subset with N = 232 the mean value of $a_{Ca^{2+}} = 0.0056$.

2.4 Directions for Future Work

The Pitzer equations and the semi-empirical parameters that are utilised have been a successful paradigm since the 1970s, allowing the estimation of equilibrium relations of an increasingly large number of ions in considerably concentrated brines at ambient temperature and pressure. However, considering the fundamental importance of dissociation/association constants, solubility products and activity coefficients to adequately treat such equilibrium relations in natural brines, there is still significant room for experimental improvement. Further refinement in the estimation of dissociation and equilibrium constants of relevance to our understanding of processes entailing mineral dissolution and precipitation reactions are still needed, and it is becoming clear that many relevant processes in sedimentary environments throughout Earth's history may have taken place at considerably concentrated aqueous solutions. For example, relevant prebiotic chemical reactions inorganically generating amphiphilic polymeric compounds may have been favoured in alkaline and restricted settings concentrating cyanide salts in the Hadean world (Toner and Catling 2019 [69]; Sutherland 2016 [70]).

Admittedly, one of the greatest limitations in studies in chemistry and geochemistry of natural surface environments and in aqueous geochemistry lies in dealing with dissociation and solubility constants. The name "constant" here is misleading, because they are not universal constants in the same sense of universal physical constants, such as the speed of light or Boltzmann's constant. They depended on temperature, pressure to a lesser degree, and strongly on the composition of the media - the solution's ionic strength. Ideally then, for solutions such as lakes and other compartments with much shorter water residence times than the oceans - for example, a restricted evaporating pond or a beaker - dissociation and solubility constants should be iteratively calibrated and recalculated. This makes the task of step-wise determination of the equilibrium relations (activity coefficients, activities, and saturation states of mineral phases) of evolving solutions computationally challenging, depending on the number of steps, salts, and acid-base reactions considered, and if accuracy is not to be sacrificed. Instead, if the recognition of more general trends and patterns is the main goal, sacrificing accuracy might be justified. This work has used in most cases equilibrium solubility and dissociation constants determined for pure phases, but in some cases has taken stoichiometric dissociation constants of the carbonic acid estimated for present-day seawater composition with a salinity of 35 as a reasonable assumption for other fluids of similar and higher salinities. Bearing this caveat in mind, and that this may result in discrepancies in terms of the accuracy achieved in the final results, it is believed that the general trends observed may still remain broadly preserved. However, future research should attempt to address these challenges.

3

Method for standard solution preparation for calibration of total alkalinity measurements by potentiometric titration of alkaline water samples

3.1 Introduction

Alkalinity is a fundamental parameter in natural waters and an essential property for constraining the carbonic acid system, its relationships involving speciation, mineral equilibria and saturation states in aqueous media. Therefore, by means of combining measurements of alkalinity with pH and elemental concentrations, fundamental thermodynamic relations can be determined, contributing to the prediction of which solid phases may be prone to dissolve or to precipitate in natural waters (*e.g.*, Morel and Hering 1993 [71]; Stumm and Morgan 1996 [55]; Drever 1997 [56]; Zeebe and Wolf-Gladrow 2001 [72]). Saline lakes with variable but usually high alkalinities in turn comprise nearly half of the total volume of lakes waters in the world, about 104,000 cubic kilometres out of 229,000 km^3, and are present on every continent (Vallentyne 1972, in Hammer 1984 [73]), and are dynamically influenced by local as well as global climates (Pecoraino et al. 2015 [74]; Edmonds et al. 2020 [75]).

Furthermore, as a result of the usually high alkalinity levels in these lakes, there is a proportionally high potential for absorption of atmospheric CO_2 in these water bodies (Lerman and Stumm 1989 [76]; Finlay et al. 2015 [77]; Edmonds et al. 2020 [75]).

Therefore, the precise determination of alkalinity in such waters is of paramount importance, since with the additional measurement of at least one other variable, such as pH, the carbonate system in any solution can be fully constrained (Stumm and Morgan 1996 [55]; Drever 1997 [56]; Zeebe and Wolf-Gladrow 2001 [72]). This in turn permits additional investigations addressing the state of mineral saturation in natural water bodies and about the response of these waters to climatic variations and increasing atmospheric CO_2 levels. Additionally, these parameters are also of utmost relevance to experimental studies trying to mimic natural conditions in the laboratory and to investigate how they respond to external forcings, such as increased CO_2 levels.

Alkaline lakes can have alkalinities varying roughly within three orders of magnitude, from less than 1 mmol/L to ∼2,500 mmol/L (see Chase et al. 2020 [78] for a recent review). Still, these are the extreme end-members, and alkalinity standards (conventionally as $CaCO_3$ solutions reported in mg $CaCO_3$/L) are available in the market for the lower range of alkalinity values more commonly dealt with by most researchers, such as marine (geo)chemists. However, these standards still do not take into account complex mixtures and the effect of multiple bases in the acid neutralising capacity (briefly addressed below), and clearly standards in the middle and more common range of alkaline lakes are lacking. The average alkalinity of world alkaline lake waters is 138 meq/L (or mmol/L), based on a metadata analysis of 229 reported values of water chemistry results compiled by Chase et al. (2020) [78], with examples such as Lake Van in Turkey and Lake Yoa in Chad possessing values around 155 and 300 mmol/L, respectively (Reimer et al. 2009 [79]; Darragui and Tardy 1987 [80]). $CaCO_3$ standard solutions from as low as 20 to 25000 mg $CaCO_3$/L (0.4 to 500 meq/L) are available from different suppliers; however, the

standards with concentration at the higher end are manufactured for measurements using spectrophotometric instruments, whereas ideally alkalinity is more accurately determined by potentiometric titration, which follows from its definition (detailed in the next section).

Here a protocol is proposed for the preparation of high alkalinity (188 mmol/kg) internal standard reference materials for calibrations of alkalinity determinations using potentiometric titration. The procedures allowing these determinations to be conducted using small sample volumes (∼1mL/1g) in a semi-automated way are also briefly described. Creating an alkaline lake titration standard is viewed as necessary, because of the increased relevance and prominence of these environments within the geochemical community and because such standards are visibly lacking. Determination of alkalinity of samples with expected high values require, like any other measurement, bracketing with measurements of a reference material, thereby increasing the confidence on the measured alkalinity value of natural and experimental fluid samples.

3.2 Methods

3.2.1 Definitions

The concept of alkalinity is complex and often misunderstood, and the source of misunderstanding may partly stem from considering it as a synonym with basicity. Although related by the general property of solutions containing proportionally low proton activities, the two should not be confused as inter-exchangeable terms. Basicity refers to the concentration (or, more specifically, the activity) of the conjugate base of an acid in an acid-base pair such as HB^+—B in a reaction of the kind $B + H_2O = OH^{\breve{}} + BH^+$ (Stumm and Morgan, 1996), whereby the higher concentration of the base, the greater the removal of H^+, and thereby the higher the pH will be. Another source of confusion is the fact that different definitions of total alkalinity exist, tending to reflect the legitimate interests of different communities,

who will apply concepts according to the convenience for their purposes (Wolf-Gladrow et al. 2007 [81]). Very briefly, total alkalinity is operationally referred to as the "acid-neutralising capacity (ANC)" or the "buffering capacity" of a solution, which are inter-exchangeable terms in this case. What this all means is that total ALK_T can be considered as a measure of the amount of proton acceptors in a given solution, in most surface natural waters being often and primarily represented by bicarbonate and carbonate ions alone (*e.g.*, Stumm and Morgan 1996 [55]; Drever 1997 [56]; Zeebe and Wolf-Gladrow 2001 [72]) such that

$$ALK_T \approx [HCO_3^-] + 2[CO_3^{2-}] \tag{3.1}$$

Which is equivalent to carbonate alkalinity, defined as:

$$CA = [HCO_3^-] + 2[CO_3^{2-}] \tag{3.2}$$

where the brackets denote concentrations.

Alkalinity is appropriately determined by potentiometric acid titration, whereby the progressive addition of a strong acid say, HCl results first in the conversion of all existing $CO_3^{2\breve{}}$ to $HCO_3^{\breve{}}$ and finally in the conversion of $HCO_3^{\breve{}}$ to CO_2. Because CO_2 is conventionally chosen as the zero level of protons, $CO_3^{2\breve{}}$ and $HCO_3^{\breve{}}$ are called proton acceptors with respect to carbon dioxide, and can each accept two and one protons, respectively (Wolf-Gladrow et al. 2007 [81]). Hence the factor 2 multiplying $CO_3^{2\breve{}}$ in eqn. 3.1 and eqn. 3.2. More generally, alkalinity represents the equivalent sum of all bases that are titratable with a strong acid (Stumm and Morgan 1996 [55]). In other words, this signifies that the higher the alkalinity is, the higher the concentration of bases in a given solution, and the greater the capacity the solution has to absorb a strong acid before reaching the "equivalence point", where $ALK_T = 0$ (defined below; see also Zeebe and Wolf-Gladrow 2001 [72] and Wolf-Gladrow et al. 2007 [81]). Total alkalinity is therefore broadly defined as the excess of proton acceptors over proton donors with respect to the chosen zero level of protons (Dickson 1981 [82]; Wolf-Gladrow et al. 2007 [81]):

$$ALK_T = [HCO_3^-] + 2[CO_3^{2-}] + [OH^-] - [H^+] \tag{3.3}$$

An additional important and useful relationship both in natural and experimental systems simulating natural waters is the total dissolved inorganic carbon (DIC), simply defined as:

$$DIC = [CO_2] + [HCO_3^-] + [CO_3^{2-}] \tag{3.4}$$

For experimental conditions targeting alkaline lakes possessing high pH and DIC values, standard reference and working solutions can be prepared by establishing a desired pH value and DIC concentration, whereby other parameters of the carbonic acid system can be fully constrained (*e.g.*, Stumm and Morgan 1996 [55]; Zeebe and Wolf-Gladrow 2001 [72]). Following calibration with certified buffers, the pH (*i.e.*, $[H^+]$, for simplicity hydrogen concentration considered equivalent to hydrogen activity) can be measured directly from solution with a pH meter electrode. The DIC is easily calculated from mass balance relations and gravimetric measurements of the reagents used in the preparation of the solutions. Once this is done, the carbonate species can be estimated from the following relations (Morse and Mackenzie 1990 [83]; Zeebe and Wolf-Gladrow 2001 [72]; Wolf-Gladrow et al. 2007 [81]):

$$a_{CO_{2(aq)}} = DIC / \left(1 + \frac{K_1}{a_{H^+}} + \frac{K_1 K_2}{(a_{H^+})^2}\right) \tag{3.5}$$

$$a_{HCO_3^-} = DIC / \left(1 + \frac{(a_{H^+})}{K_1} + \frac{K_2}{(a_{H^+})}\right) \tag{3.6}$$

$$a_{CO_3^{2-}} = DIC / \left(1 + \frac{(a_{H^+})}{K_2} + \frac{(a_{H^+})^2}{K_1 K_2}\right) \tag{3.7}$$

Where K_1 and K_2 represent the thermodynamic dissociation constants of the carbonic acid, not the stoichiometric dissociation constants (Zeebe and Wolf-Gladrow 2001 [72]; Wolf-Gladrow et al. 2007 [81]). Fig. 3.1 shows the theoretical

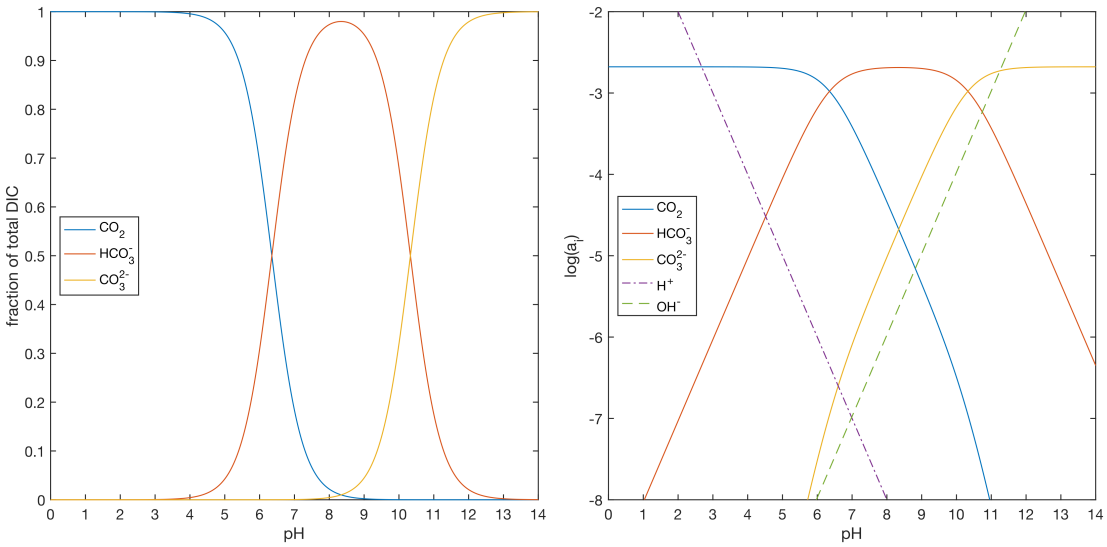


Figure 3.1: Relative proportion of carbonic acid species to total dissolved inorganic carbon, as a function of pH (left) and theoretical prediction of species activities in a simple carbonic acid–water system, as a function of pH (right).

thermodynamic relations among the different carbonic acid system species as a function of the total DIC and variable pH of the solution.

From the relations above, an expression for the determination of the total alkalinity (ALK_T), of more general use for natural waters and synthetic solutions, can be derived:

$$ALK_T = a_{CO_{2(aq)}} \times \left(1 + \frac{K_1}{a_{H^+}} + 2\frac{K_1 K_2}{(a_{H^+})^2}\right) + \frac{K_W}{a_{H^+}} - a_{H^+} \tag{3.8}$$

Therefore, any value of ALK_T can be calculated by specification of given DIC and pH values. This in turn allows target DIC, pH and ALK_T values to be established for synthetic solutions. Furthermore, alkalinity can also be defined from the requirement of electroneutrality in any given solution. This is relevant because the consistency of the value established above for alkalinity can be verified by means of chemical analysis and full characterisation of the composition of the solution. Thus, considering proton donors versus proton acceptors:

$$\begin{aligned} &2[Mg^{2+}] + 2[Ca^{2+}] + [Na^+] + [H_3PO_4] + [H^+] = \\ &[HCO_3^-] + 2[CO_3^{2-}] + [OH^-] + [HPO_4^{2-}] + 2[PO_4^{3-}] + [Cl^-] \end{aligned} \tag{3.9}$$

Equation 3.9 refers to a general alkaline standard solution, prepared for the purposes of the present study, and therefore considering only the ions relevant to this work. A more complete definition of the concept of proton donors *vs* acceptors, including both *conservative quantities* and *nonconservative species*, can be expressed including other major ions commonly found in abundance in most of Earth's surface waters (Drever 1997 [56]):

$$\begin{aligned} &2[Mg^{2+}] + 2[Ca^{2+}] + [Na^{+}] + [K^{+}] + [H_3PO_4] + [H^{+}] + [HSO_4^{-}] = \\ &[HCO_3^{-}] + 2[CO_3^{2-}] + [OH^{-}] + [HPO_4^{2-}] + 2[PO_4^{3-}] + [Cl^{-}] + [H_3SiO_4^{-}] \end{aligned} \tag{3.10}$$

According to Drever (1997), the ions "Na^+, K^+, Ca^{2+}, Mg^{2+}, and Cl^- can be regarded as *conservative* in the sense that their concentrations are unaffected by changes in pH, pressure, or temperature (within the ranges normally encountered near the Earth's surface and assuming no precipitation or dissolution of solid phases, or biological transformations)." The reason why HSO_4^- is included in the definition above (eqn. 3.10) as a proton donor despite its negative charge resides in the fact that this definition considers titrations where large pH variations might be expected, whereby this species can be expected to dissociate and contribute with a proton.

Thus, rearranging conservative species to the *left* and nonconservative species to the *right* (and considering our particular case represented by eqn. 3.9), we get:

$$\begin{aligned} &2[Mg^{2+}] + 2[Ca^{2+}] + [Na^{+}] - [Cl^{-}] = \\ &[HCO_3^{-}] + 2[CO_3^{2-}] + [OH^{-}] + [HPO_4^{2-}] + 2[PO_4^{3-}] - [H_3PO_4] - [H^{+}] \end{aligned} \tag{3.11}$$

And finally, this permits us to define ALK_T in another way, which is also equivalent to *titration alkalinity* (TA), which is derived from titration with a strong acid:

$$ALK_T = [HCO_3^{-}] + 2[CO_3^{2-}] + [OH^{-}] + [HPO_4^{2-}] + 2[PO_4^{3-}] - [H_3PO_4] - [H^{+}] \tag{3.12}$$

The advantage of the above definitions of ALK_T is that this parameter is invariant with changes in temperature and pressure (once defined in terms of moles per kilogram of solution), and thereby a sample can in general preserve its alkalinity

for long periods of time (Wolf-Gladrow et al. 2007 [81]; Sharp and Byrne 2021 [84]). Importantly, it follows from this definition that alkalinity is a conservative property because the individual terms are also conservative. Thus, alkalinity of a mix will be a weighted average of the components being mixed.

3.2.2 Preparation of solutions

Alkaline standard solutions were prepared using milliQ water (resistivity 18.2 MΩ · cm) and the following reagents: Na_2CO_3 (Sigma-Aldrich, 99.5%), NaCl (Sigma-Aldrich, 99.5%), 1 molal NaOH stock solution from NaOH pellets (Sigma-Aldrich, 98%), 0.1 molal NaH_2PO_4 stock solution from NaH_2PO_4 powder (Acros Organics, 99%), $MgCl_2$ (Sigma-Aldrich, 1 M), $CaCl_2$ (Sigma-Aldrich, 1 M). The target concentrations are indicated in Table 3.1. These concentrations are aimed to produce a solution with ALK_T ∼189 mmol/kg, DIC ∼100 mmol/kg and pH 10.5 ± 0.5. The recipe is shown in Table 3.2, and Fig. 3.2 illustrates the specified range.

Table 3.1: Concentration of internal standards for calibration of measurements of high alkalinity solutions.

Concentration (mmol/kg)	**ALK Standard Solution #1**	**ALK Standard Solution #2**	**ALK Standard Solution #3**	**ALK Standard Solution #4**
Na	200	200	300	300
Cl	0	4	100	100
DIC	100	100	100	100
PO4	0.1	0.1	0.1	0.1
Mg	0	1	0	1
Ca	0	1	0	1

Table 3.2: Recipe for preparation of ½ kg standard solution with the concentrations given in Table 3.1.

Concentration (g/0.5kg)	**ALK Standard Solution #1**	**ALK Standard Solution #2**	**ALK Standard Solution #3**	**ALK Standard Solution #4**
NaCl (solid)			2.93	2.93
Na_2CO_3 (solid)	5.3	5.3	5.3	5.3
NaOH (1 m stock)	0.17	0.17	0.17	0.17
NaH_2PO_4 (0.1 m stock)	0.5	0.5	0.5	0.5
$MgCl_2$ (1 m stock)		0.5		0.5
$CaCl_2$ (1 m stock)		0.5		0.5

Adding Ca and Mg to the standard solutions, while avoiding precipitation with spiking of adjusted concentration of ΣPO_4 may approximate them to real fluid

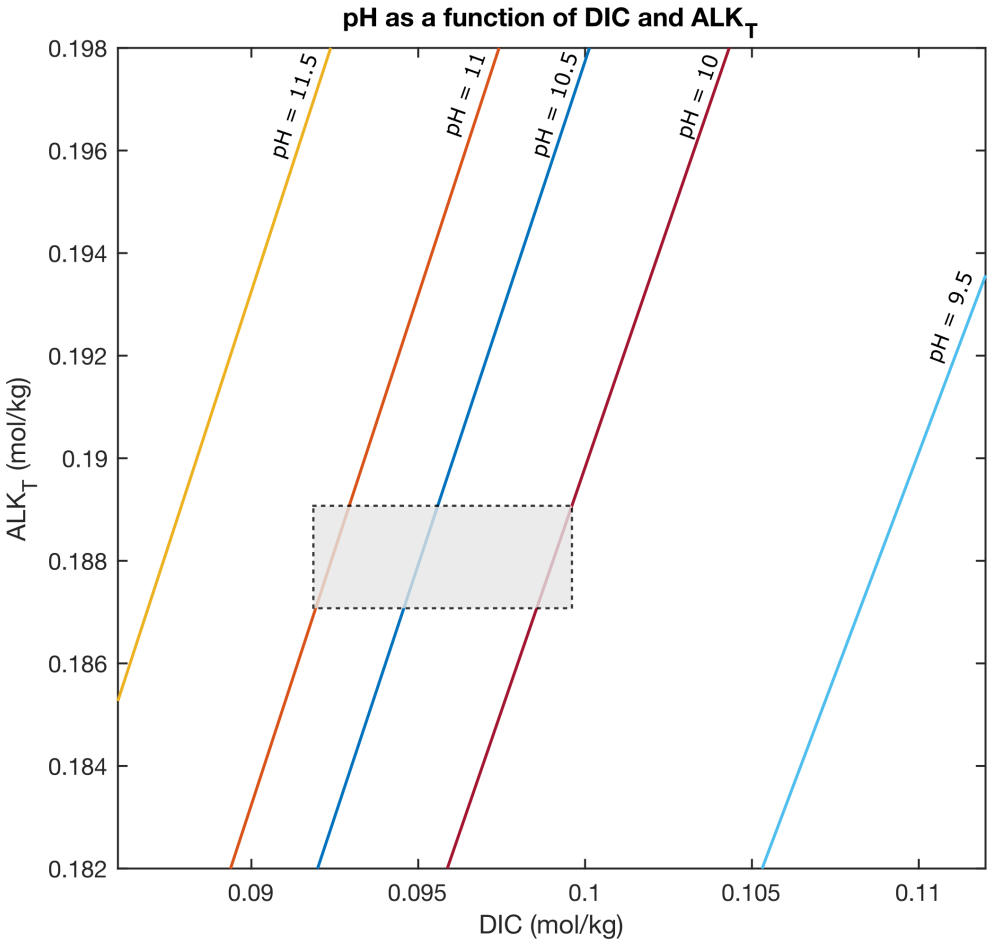


Figure 3.2: Estimated range of the standard solutions, applying the calculations above and following the recipe indicate in Table 2.

samples. This may also provide a comparative benchmark for the estimation of alkalinity from chemical analyses (based on conservative ions). Conversely, standard solutions without these cations may be useful to keep track of any undesired reactions during preparation of the whole set of standards, such as precipitation of solid phases (consequently changing their alkalinity).

In order to assure the target concentrations established by gravimetrically measuring and mixing the reagents in the desired proportions were satisfactorily achieved, the solutions were analysed by ion chromatography (Dionex ICS-5000 equipped with an AS-AP autosampler) and by ICP-MS (Perkin Elmer NexION 350D) for determination of anion and cation concentrations, respectively. Samples were diluted

in deionised, MilliQ-purified water for ion chromatography and in 2% HNO_3 acid for ICP-MS analysis, following a dilution factor of 1000× for chloride, 50× for phosphate, and 100× for cation analyses. Na analyses underwent further 50× automated inline dilution using a prep*FAST*® unit coupled to the ICP-MS. All concentrations reported herein in ppm units were converted to their equivalent molal units (moles, or millimoles, per kg of solution).

The Dionex instrument used at the School of Geography and the Environment, University of Oxford, is equipped with an Anion Electronically Regenerated Suppressor and an IonPac™ AS23-4μm column and analyses were carried out using a 4.5mM Na_2CO_3/0.8 mM $NaHCO_3$ solution as the eluent. Calibration range was from 0 to 20ppm (converted from the equivalent molal concentrations of ΣPO_4 and chloride). Six water-based standards were prepared and used for the calibrations, providing six points' calibration curves for each species of interest (chloride and phosphate): 0.5, 1, 2, 5, 10 and 20 ppm. Accuracy will depend on the calibration work and preparation, represented by each determination coefficient, which were better than 0.999 for chloride and than 0.995 for phosphate. The limit of detection (LD) was based on 3× the standard deviation of blanks and precision of the method in the range of 0–20 or up to 40ppm for chloride and phosphate was 0.01 (LD) ± 0.1 and 0.02 (LD) ± 0.03, respectively.

ICP-MS analyses were carried out in the Department of Earth Sciences, University of Oxford. For calibrations, the Certified Reference Materials (CRM) LGC6019 (river water from Henley-on-Thames) as well as the NRC Canada SLRS-6 and NASS-7 were used. Accuracy was based on analyses of the CRMs and measurement of each sample was based on five replicates, with dwell time of 10 msec, scanned 100 times. Analyses of Ca and Mg in the the LGC6019 followed 25× dilution factor of the CRM. Precision of the instrument detection (reproducibility) is defined as before as 3× the LD and was based on 3× the standard deviation of blanks. All blanks, standards and samples were also spiked with 1ng/g In and Rh, so that any general instrument drift could be normalised. The respective LD of Na, Ca, and

Mg were 0.024 mmol/kg (572 ppb value converted to mmol/kg), 0.0002 mmol/kg (8 ppb) and 0.0006 mmol/kg (15 ppb). Ca and Mg concentrations were <LD in blank sample analyses (MilliQ water and 2% HNO_3 acid used for dilution). Accuracy and precision were respectively ∼5% and ∼4% for Na, ∼8–15% and 1–3% for Ca, and 2–6% and 2–6% in both cases for Mg.

The alkalinity determined on the basis of the conservative species (eqns. 3.11 and 3.12), ignoring uncertainties related to the weighed masses of the reagents added together to make the final solution, yields similar results to the calculated alkalinity or that determined by the potentiometric method (below). For example, for the standard solution 2:

$$2[Mg^{2+}] + 2[Ca^{2+}] + [Na^{+}] - [Cl^{-}] = 2 \times 1 + 2 \times 1 + 200 - 4 = 200 mmol/kg \tag{3.13}$$

Which is in actuality only about 6% higher than the target value calculated initially (based on the equilibrated carbonate system) and determined by titration (below). Conversely, the alkalinity based on conservative species' concentrations deriving directly from chemical analyses would yield an associated uncertainty of ∼9% or 191.5–208.5 mmol/kg, based on the combined uncertainties coming from the individual precision of the analytical methods reported above. These lower and upper boundaries, in turn, represent an estimation as good as 2% or as bad as 10% of the alkalinity of ∼189 mmol/kg, which was set as the goal and was calculated with eqn. (3.8). This is a reminder of the importance of one having to resort to multiple different and independent methods to constrain with increasing confidence the value of a given parameter.

3.2.3 Titration configuration

Potentiometric titration was conducted in the 916 Ti-Touch autotitrator (Metrohm), and was initially performed using two different acid concentrations, 0.01 N and 0.1 HCl (Alfa Aesar), for comparison of efficiency (titration time), precision and accuracy. The set up was optimised for determination of alkalinity in small sample

volumes (∼1g or 1mL), carried out in a glass titration vessel with a thermostat jacket (Metrohm). This is a benefit in the case of experimental samples because it reduces the potentially detrimental effects of extraction of large aliquots of fluid for analysis, which might result in significant change of the overall experimental fluid conditions under investigation in a reactor vessel or in a beaker (following a major volume change, for example). For this purpose, a flat-membrane pH glass electrode (Metrohm) was used. pH buffers (Orion Application Solution, Thermo Scientific) traceable to NIST were used for calibration of the pH electrode at least once a day, and the temperature of buffer solutions as well as of the samples was recorded using a separate temperature sensor. Room temperature during alkalinity measurements was maintained at 20 ± 1°C. The autotitrator is programmable and titration parameters such as titration rate and temperature can be edited, to account for variations in the pH values arising from temperature fluctuations and to avoid overshooting of equivalence points (further below). Filtered (syringe filtered through 0.1 μm membranes) and unfiltered aliquots were initially compared. Following these procedures each time an additional measurement was made the pH and temperature sensors and the vessel were automatically rinsed and cleaned with deionised water and drained, and any remaining water was removed by drying gently with a soft tissue. After this new weighed aliquots of the solutions were pipetted in the vessel to start new measurements.

3.3 Results

Expected and successful titration measurements of high alkalinity fluid samples should produce titration curves such as those shown in Fig. 3.3 (bottom). Because of the initial high alkalinity and pH of the solutions, CO_3^{2-} ion is the species contributing the most to the total alkalinity. The progressive addition of HCl 0.1 N will therefore initially convert all CO_3^{2-} ion into HCO_3^- ions, corresponding to the first equivalence point – the first inflection point in Fig. 3.3 – and finally HCO_3^- ions will be converted to CO_2, *i.e.*, the second equivalence point, near pH 4.5. This is also known as the *proton condition*, which, in a simplified system where carbonate

alkalinity is considered equivalent to total alkalinity, can be represented as (Zeebe and Wolf-Gladrow 2001 [72]; Clark 2015 [85])

$$[H^+] = [HCO_3^-] + 2[CO_3^{2-}] + [OH^-] \tag{3.14}$$

The curves represented in this Fig. 3.3 (top) correspond to a subset of 18 measurements of three internal reference standards, measured in different days. Failed titration measurements can be promptly seen from observation of the titration curves, when for example either one of the inflection points is missing or the curve shows anomalous trends, whereby random and/or systematic measurement errors can be spotted immediately (Fig. 3.3, bottom). A sample of the *equivalence point recognition criterion* (ERC), related to the derivative of the potentiometric curve, and used to define the second equivalence point using the 916 Ti-Touch autotitrator (Metrohm), is shown in Fig. 3.4 (bottom). Following the manufacturer's definition, the ERC simply represents a measure for the size of the jump in the titration curve. Its value is compared with the equivalence point criterion defined in the method for the evaluation of the titration curve (Metrohm, 2017). Additionally, this graph (Fig. 3.4 (bottom)) also indicates more clearly titration measurements that were less accurate. Finally, Fig. 3.5 shows the control chart resulting from a first pilot test, reflecting a total of 83 measurements of all four variations of the standard solutions, performed between 8$^{\text{th}}$ June and 20$^{\text{th}}$ July 2021.

A last remark regarding Figures 3.3 and 3.4 should be pointed out, that is, it concerns the potential issues of adding about 2 mL of acid to about 1 mL of sample. Indeed, no dilution was applied to the samples taken to potentiometric titration. If it were the case, alkalinity could still have been measured by titration following the same principle but requiring a correction for the dilution factor. It would also have reduced the step involving the acid titration. Even so, as they are shown here the results seem satisfactorily reproducible, which suggests the protocol can be improved in further applications.

3.4 Summary

Alkalinity is a fundamental and essential parameter in natural waters. Its precise determination in lake waters is of paramount importance, since with the additional measurement of at least one another variable, such as pH, the carbonate system in any solution can be fully constrained. This in turn permits additional investigations addressing the state of mineral saturation in natural water bodies and about the response of these waters to climatic variations and increasing atmospheric CO_2 levels. Furthermore, these parameters are also of utmost relevance to experimental studies trying to mimic natural conditions in the laboratory and to investigate how they respond to external forcings, such as increased CO_2 levels. A metadata analysis of 229 reported values of water chemistry results compiled by Chase et al. (2020) [78] shows the average alkalinity of world alkaline lake waters is 138 meq/L (or mmol/L). $CaCO_3$ standard solutions from 20 to 25000 mg $CaCO_3$/L (0.4 to 500 meq/L) for calibration of alkalinity measurements are available from different suppliers; however, the standards with concentration at the higher end are suitable for spectrophotometric measurements, whereas ideally alkalinity is more accurately determined by potentiometric titration, which follows from its definition as ANC. More generally, alkalinity represents the equivalent sum of all bases that are titratable with a strong acid. Here a successfully tested protocol is thus proposed for the preparation of high alkalinity (188 mmol/kg) internal standard reference materials for calibrations of alkalinity determinations using potentiometric titration. The procedures allowing these determinations to be conducted using small sample volumes ($\sim$1mL/1g) in a semi-automated way are also briefly described.

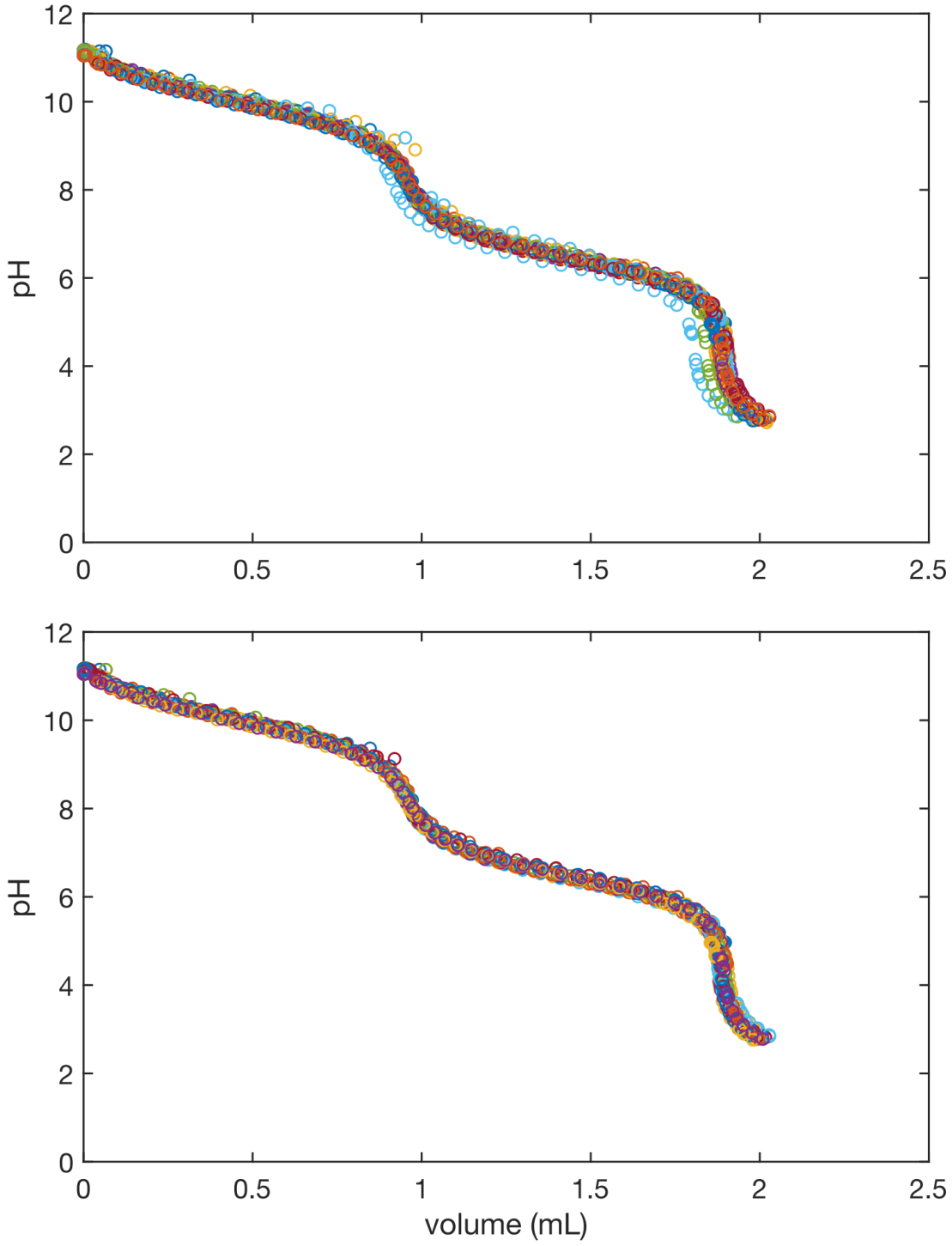


Figure 3.3: Above: Selected sample of titration curves for 18 measurements of standard solutions indicated in Table 1. Below: Selected sample of titration curves for 23 measurements of standard solutions indicated in Table 1, with some examples of random and systematic errors, for comparison with picture above.

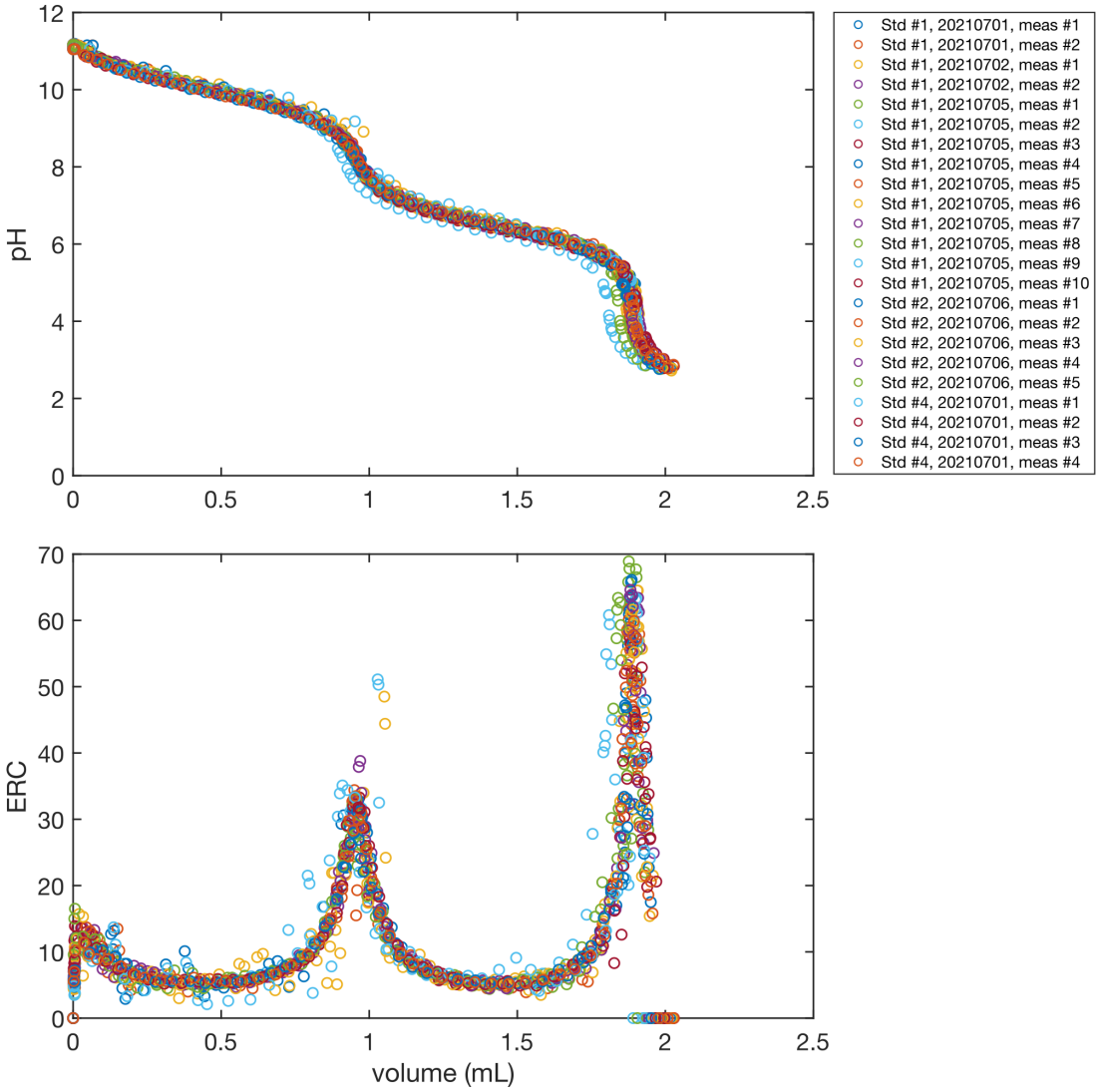


Figure 3.4: Above: As in previous picture, selected sample of titration curves for 23 measurements of standard solutions indicated in Table 1, with some examples of random and systematic errors. Below: Equivalence point Recognition Criterion (ERC), as defined in Metrohm (2017, p. 228 [86]), from the set of measurements shown above.

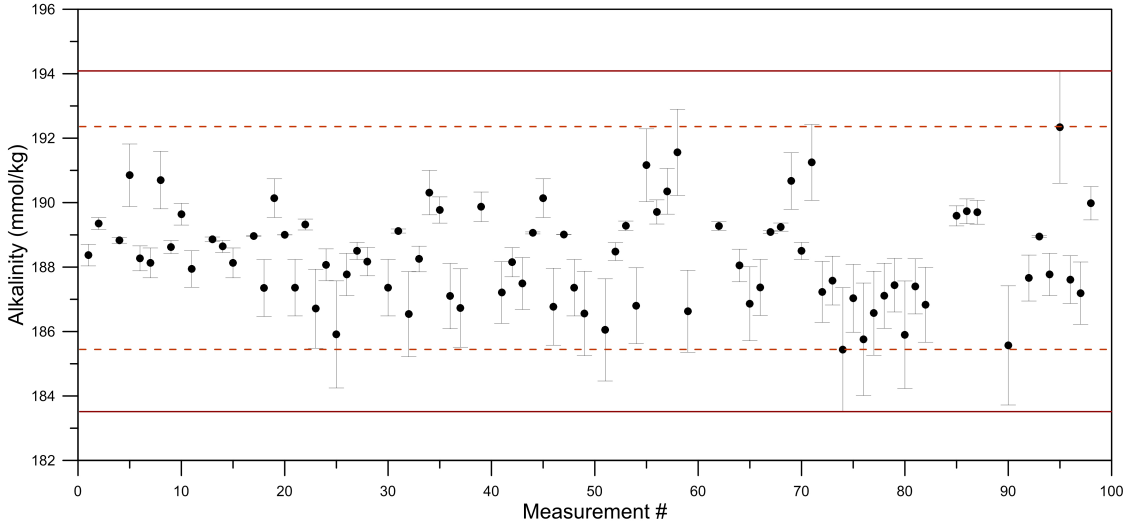


Figure 3.5: Calibration control chart for 83 measurements of the four solutions indicated in Table 1, performed between the 8th June and 20th July 2021. Dashed lines represent the limits of the actual measured values and continuous lines represent the limits of their associated uncertainties.

4

Chemical Controls on Carbonate Sediment Production and Phosphate Concentration in Alkaline Lakes

4.1 Introduction

Modern saline and alkaline lakes represent approximately half of all lake water volume on Earth, which in turn spans roughly 200.000 km^3 according to a recent assessment (Vallentyne 1972, in Hammer 1986 [73]; Cael et al. 2017 [87]). Diverse and unique characteristics place such lakes in a position of high relevance and well-deserving detailed studies. They draw the attention of a varied community of researchers, reflecting the numerous different perspectives and interests to study them, from ecology (Talling et al. 1973 [88]; Hammer 1986 [73]) to sedimentology (Renaut and Long 1989 [89]), geochemistry (Hardie and Eugster 1970 [90]), hydrology (Hillaire-Marcel and Casanova 1987 [91]) and palaeoclimate (Benson et al. 1996 [92]). Alkaline lakes specifically are (1) regarded as some of the most productive ecosystems on the modern Earth (Talling et al. 1973 [88]; Melack and Kilham 1974 [93]; Hammer 1986 [73]; Chase et al. 2020 [78]); (2) the resulting excess alkalinity may lend these environments as important sinks for atmospheric CO_2 (Talling et al.

1973 [88]; Lerman and Stumm 1989 [76]; Edmonds et al. 2020 [75]); (3) and finally, they may also have figured prominently in the chemical origins of life (Toner and Catling 2019 [69]; 2020 [94]).

Research on prebiotic chemistry has established some canonical principles that may emerge from plausible chemical pathways, given certain environmental constraints. Oligomerisation and polymerisation of larger organic molecules of relevance to an early biochemistry can thus be synthesised from simple inorganic feedstock compounds (Holland 1984 [6]; Sutherland 2016 [70]). Importantly, shallow alkaline lakes may have been able to provide the physicochemical conditions to achieve the necessarily high concentrations of specific inorganic molecules that have been pointed out as likely initial feedstock, thereby also sustaining the synthesis and polymerisation of essential organic compounds. These initial building blocks would have inevitably to contain the basic elements necessary to promote and sustain life, and specifically hydrogen cyanide (HCN), cyanide salts and inorganic phosphate, all of which can be concentrated in alkaline lakes under certain conditions, are favourable candidates (Toner and Catling 2019 [69]; 2020 [94], Sasselov et al. 2020 [95]). Perhaps not so surprisingly, timeless attributes defining alkaline lakes, such as enhanced DIC content in the forms of bicarbonate and carbonate, correlated with high concentrations of important limiting nutrients such as phosphate, are factors that may also contribute to the high productivity documented in modern alkaline lakes (Talling et al. 1973 [88]; Toner and Catling 2020 [94]).

Remarkably, alkaline lake waters tend also to be systematically supersaturated with respect to $CaCO_3$, predominantly poised at amorphous Ca-Mg-carbonate (ACMC) supersaturation (Fukushi and Matsumiya 2018 [1]), providing an interesting natural laboratory to investigate $CaCO_3$ precipitation mechanisms. However, the extent and degree of supersaturation in such lakes is likely to be variable and is predicted to decrease in terminally evaporitic basins evolving towards Na-carbonate brines, as thoroughly addressed by Hardie and Eugster (1970) [90]. Furthermore, even though it has been pointed out that the degree of supersaturation in some such lakes, *i.e.*,

the Mono Lake, is probably sustained by the presence of inhibitors such as dissolved phosphate (Jellison et al. 1993 [30]), a direct link has not yet been established.

In line with these observations and with more recent studies pointing to strong links between high alkalinity and phosphate concentration in modern and ancient alkaline lakes (Ingalls et al. 2020 [31]; Toner and Catling 2020 [94]) this study attempts to address these simple questions: Are all alkaline lakes supersaturated with respect to calcium carbonate minerals? Whether or not they are, what is the degree of supersaturation? Finally, what kinetic factors likely sustain $CaCO_3$ supersaturation in alkaline lakes?

4.2 Methods

4.2.1 Geochemical database

In the present study we built on previously available lake water chemistry datasets from alkaline lakes from several regions (Eugster 1970 [96]; Melack and Kilham 1974 [93]; Jones et al. 1977 [97]; Imhoff et al. 1979 [98]; Ashton and Schoeman 1983 [99]; Hirst 1995 [100]; Shvartsev et al. 2014 [101]; Fukushi and Matsumiya 2018 [1]; Guerreiro et al. 2019 [102]; Chase et al. 2020 [78]), to expand and use this new comprehensive database as a starting point for our investigations. The compilation includes data from more than 200 alkaline lakes from around the globe, located in six continents and 16 countries, including Australia, Austria, Bolivia, Brazil, Canada, Chad, China, Egypt, Italy, Kenya, Mongolia, Russia, South Africa, Tanzania, Turkey and the United States (Fig. 4.1). The complete database, including the raw water chemistry data, as well as the geochemical calculations, is provided in the appendix G and is also made available online on github.com under the repository "raphapietzsch/alkaline_lakes". The MATLAB code used to make the plots in this chapter is provided in the appendix I.

The original dataset consisting of the compilation above would result in 624 water samples (Supplementary Material in Appendix G). However, not all samples have information that allow for the full determination of the carbonate system (*i.e.*, at

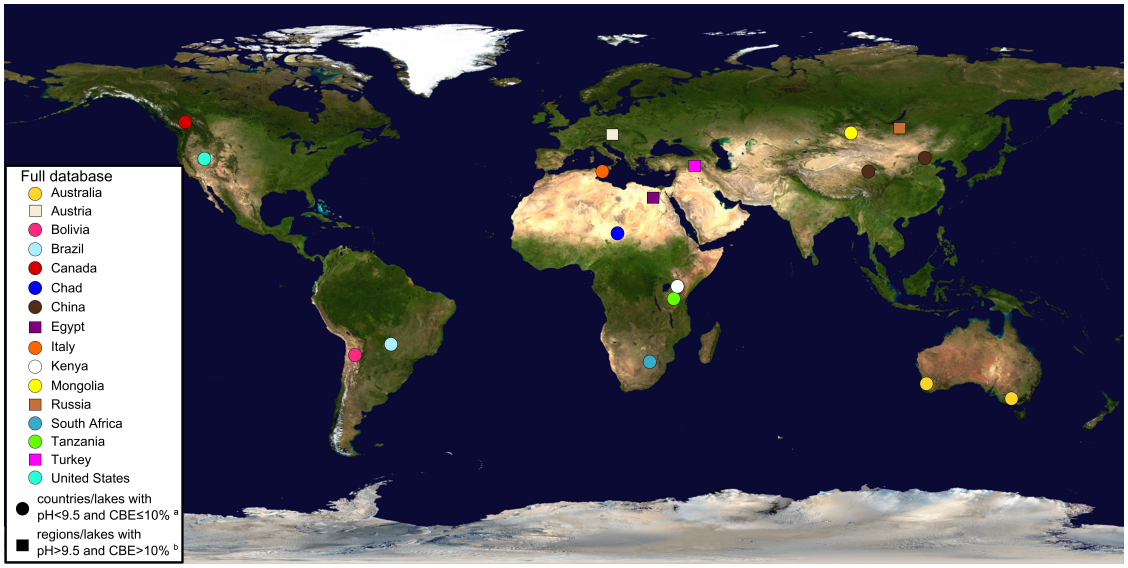


Figure 4.1: Map illustrating the countries and other main regions where the alkaline lakes are located, containing available published results of fluid chemistry analyses which were integrated in the present work. In total, 16 countries and six continents are represented in this new database. Some regions/countries encompass several different lakes, such as Bolivia, Canada and the United States. [a]countries/regions containing at least some lakes/water samples with pH<9.5 and charge balance error (CBE)≤10%. [b]countries/regions where all lakes/water samples lie above both pH>9.5 and CBE>10%. True-colour map credit of NASA ("Visible Earth, A catalog of NASA images and animations of our home planet").

least two variables, for example pH and pCO_2, or pH and alkalinity) and therefore the practical number of samples is reduced to 539. It is this subset that is the focus of the present contribution. Additionally, some relevant ions/compounds in alkaline lake waters, such as dissolved total phosphate (ΣPO_4) and aqueous silica ($SiO_{2(aq)}$), are not reported in the original studies or were in other instances below the detection limit. In all these cases, the empty entries were replaced by 1E–6 for "major elements/ions" (Na^+, K^+, Cl^-), 1E–9 for other ions/compounds of secondary relevance, assuming soda-type lake waters (*i.e.*, Ca^{2+}, Mg^{2+}, $SiO_{2(aq)}$), and 1E–12 for minor/trace compounds (*i.e.*, ΣPO_4). This is a necessary step because zero/null entries cannot be calculated, compromising the equilibrium calculation of the entire set of variables. Although the entries are somewhat arbitrary, it can be shown that the choice of altering these values does not affect the main results. However, it is important to bear in mind that certain mineral phases become artificially undersaturated in the final results, *e.g.*, phosphate mineral phases when no ΣPO_4

values were reported in the original source. Such cases are considered as "insufficient data" and are therefore removed from the plots and from any interpretations.

4.2.2 Geochemical modelling

Geochemical calculations for the determination of aqueous speciation, individual ion activities and mineral phases were made in GWB software Spec8 module, using a modification of the thermodynamic database thermo_phrqpitz.tdat (Plummer et al. 1988 [3]; Tosca et al. 2005 [103]; Tosca and McLennan 2009 [104]; Tosca et al. 2011 [105]). This database includes the Pitzer ion activity coefficient model parameters for several electrolytes and was here expanded to incorporate inorganic phosphate species and the mineral phases hydroxyapatite (HAP) and OCP as well as amorphous calcium phosphate (ACP). All calculations were performed at 25^{o}C, the temperature value for which most of the Pitzer parameters and equilibrium coefficients have been reliably determined. This assessment provides clues as to whether given mineral phases are saturated in natural and experimental conditions but do not precipitate, suggesting the formation of metastable precursor phases instead (Tosca and McLennan, 2009 [104]). Details of calculations and modifications to the database are provided in chapter 2.

Finally, following Chase et al. (2020) [78] and also acknowledging the challenge to obtain accurate analytical and thermodynamic data from complex fluid brines (Harvie et al. 1984 [67]) we constrained the investigation of this natural alkaline lake waters database to only those samples whose CBE was $\leq$10%. This restriction limits the number of valid samples from 539 to 281. There are at least a few reasons for roughly 48% of the samples being so far out of charge balance. One is obviously that no chemical analysis is complete, and different studies from the compilation above focussed on reporting elemental compositions and ions that were relevant to their investigations. Another possible effect arises from the difficulty in getting very precise pH measurements in saline solutions (*e.g.*, Golan et al. 2014 [106]). The combination of these two limitations will clearly have further effects on the

estimations of chemical species of cations and anions, which are the parameters the calculation of charge balance is based on, following the expression

$$CBE(\%) = \frac{|\Sigma(cat \times valence)| - |\Sigma(an \times valence)|}{|\Sigma(cat \times valence)| + |\Sigma(an \times valence)|} \times 100 \quad (4.1)$$

Where Σcat and Σan represent the summation over all major cations and anions, respectively, conventionally given in units of milliequivalents per L or per kg of solution (meq/L or meq/kg).

4.3 Results

Considering all fluid samples with full carbonate geochemistry constrained investigated in this study (N = 539), 80% of them are (super)saturated with respect to calcite ($SI_{cal} \geq 0$, where $SI = \log(IAP/Ksp)$, IAP is the ion activity product and *Ksp* is the solubility product constant). If the CBE constraint is imposed (CBE $\leq$ 10%), then ∼82% of the samples are supersaturated (Fig. 4.2). This later assessment takes into account 281 samples, including those with reported pH values that do not strictly reflect alkaline waters (here considered to be pH ≥8). Such measured pH values (pH <8) are normally associated with samples representing springs, streams, and wetland areas that feed into the lakes (Supplementary material in Appendix G).

When only samples with pH ≥8 and CBE $\leq$ 10% are considered, 79% of the water samples (191 out of 242) have $SI_{cal} > 0$, still covering a representative portion of the globe, with samples from 15 out of 16 countries and all six continents represented (some lakes such as Lake Neusiedl in Austria and Wadi El Raiyan in Egypt are cut off as a result of all water samples having CBE >10%). Fig. 4.3 shows a plot of $a_{Ca^{2+}}$ vs $a_{CO_3^{2-}}$ vs pH values and the mineral/amorphous phase saturation lines for various relevant $CaCO_3$ phases. ACMC are "amorphous-Ca-Mg-carbonates" with a $Ksp = 10^{((0.0175*mol\%Mg)\breve{}6.277)}$ determined by Purgstaller et al. (2019) [107], and AMC1 and AMC2 are "AMC" with $Ksp = 10^{\breve{}5.2}$ and $Ksp = 10^{\breve{}5.59}$ determined by Fukushi and Matsumiya (2018) [1].

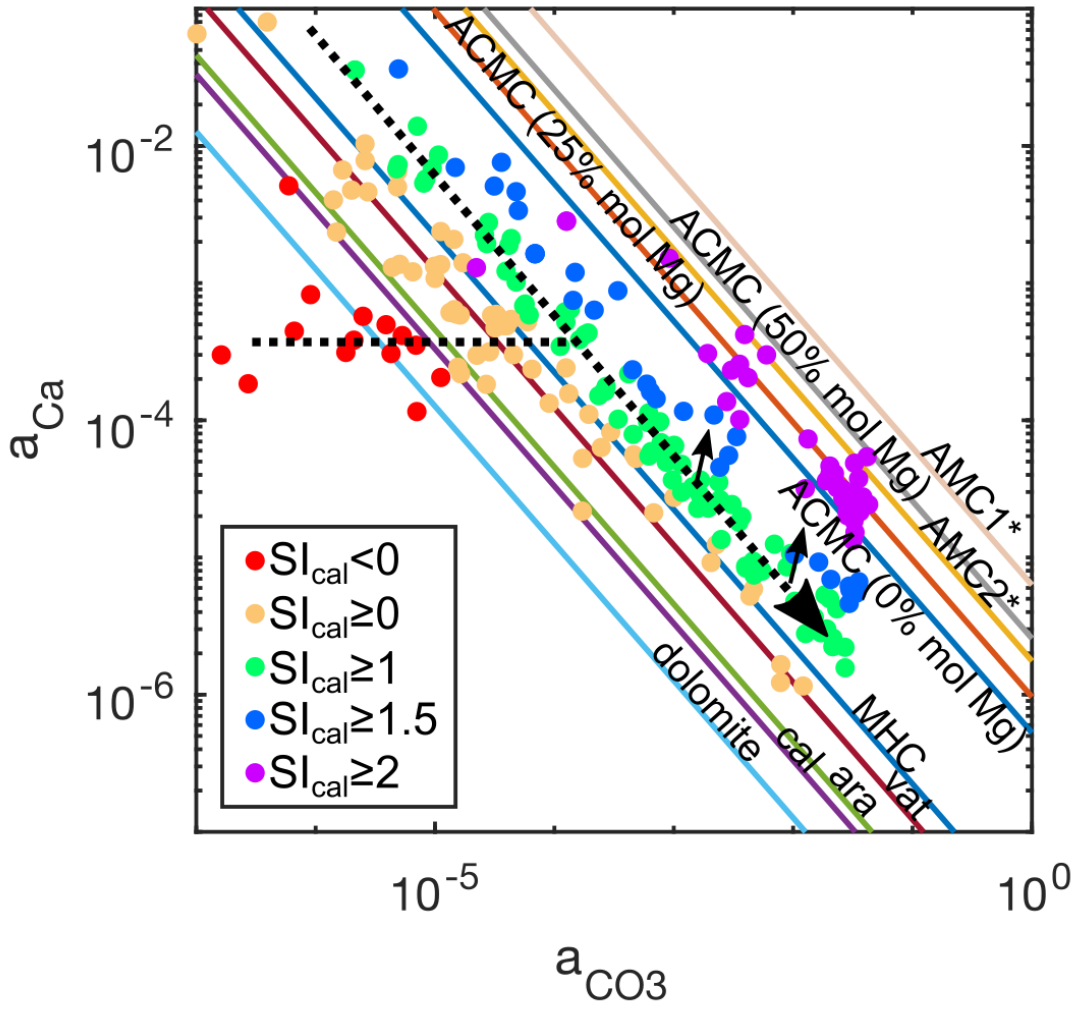


Figure 4.2: Plot showing the relationship between the activity of Ca^{2+} *vs* activity of CO_3^{2-}, calculated from natural lake water data, with saturation lines of various Ca-(Mg)-carbonate phases, in accordance to the solubilities estimated from different sources (Plummer and Busenberg 1982 [59]; Fukushi and Matsumiya 2018 [1]; Purgstaller et al. 2019 [107]). The dashed lines represent evaporation paths and presumably fluids evolving from different initial conditions. Samples are colour-coded according to the range in SI of calcite, indicated in the figure legend. cal: calcite; ara: aragonite; vat: vaterite; MHC: monohydrocalcite; ACMC: amorphous-Ca-Mg-carbonate; AMC: amorphous-Mg-carbonate.

It is also surprisingly remarkable to note how the saturation of these amorphous and metastable phases control the evolving chemistry of alkaline lakes under increasing evaporation and alkalinity conditions. The saturation state of $CaCO_3$ phases is clearly sustained through the paths of evaporation, increasing pH and alkalinity, even under declining $a_{Ca^{2+}}$ (Figs. 4.2–4.4A). The saturation state of Mg-carbonate

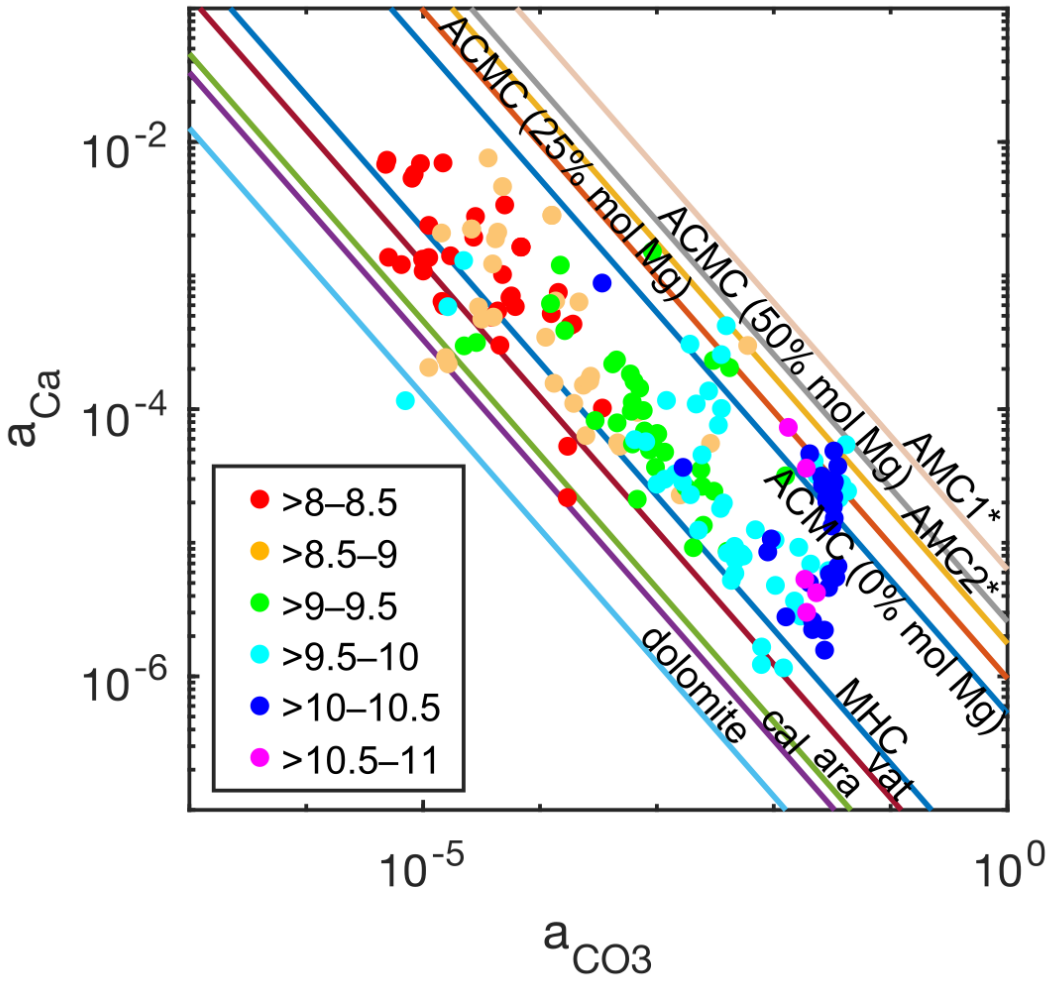


Figure 4.3: Same as in Figure 4.2, but colour-coding referring to pH range. Only samples with pH > 8 are considered in the plot.

phases is affected somewhat similarly, *i.e.*, controlled by more soluble and amorphous phases, but without a strong correlation with declining $a_{Mg^{2+}}$, until more advanced stages of evaporation and higher alkalinity and pH (Fig. 4.4B). Na-carbonate phases are shown for comparison, as well as because of their relevance in the late stages of evolution of alkaline lakes, when alkalinity builds up excessively as Ca^{2+} and Mg^{2+} ions become significantly depleted, and waters approach the saturation of minerals such as natron and trona (Fig. 4.4C). Fig. 4.4D illustrates the pathways of different initial conditions, reflected in waters with different initial Ca^{2+} concentrations (represented as $\log(a_{Ca^{2+}})$, converging towards natron saturation.

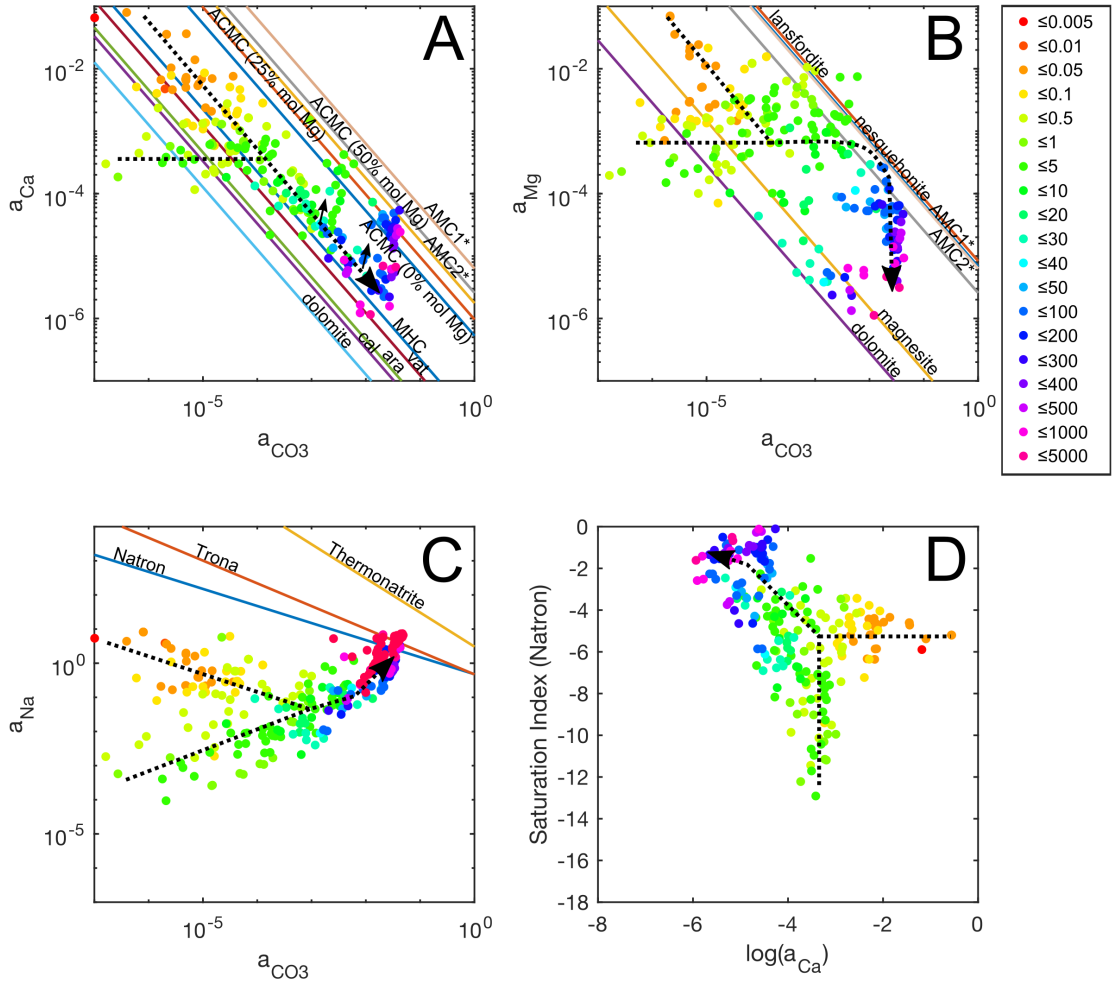


Figure 4.4: Activity and saturation index diagrams for 281 water samples whose CBE≤10%. (A) Activity of calcium ($a_{Ca^{2+}}$) *vs* activity of CO_3^{2-} ($a_{CO_3^{2-}}$) and solubility lines for various Ca-Mg-CO_3 crystal and amorphous phases. (B) $a_{Mg^{2+}}$ vs $a_{CO_3^{2-}}$ and solubility lines for various Mg-(Ca)-CO_3 phases. (C) a_{Na^+} vs $a_{CO_3^{2-}}$ and solubility lines for various Na-CO_3 minerals. (D) SI of natron versus $\log_{10}(a_{Ca^{2+}})$. The dashed lines represent evaporation paths and presumably fluids evolving from different initial conditions. Samples are colour-coded according to ALK/(Ca+Mg) ratio intervals, shown to the right. Thermodynamic mineral saturation data of Mg-(Ca)-CO_3 and Na-CO_3 phases from Marion 2001 [108] and Marion et al. 2011 [109].

4.4 Discussion

4.4.1 Constraints on carbonate production in alkaline lakes

In face of the preceding results, we return to our motivating questions, that is (1) are calcium carbonate minerals supersaturated in all alkaline lakes? (2) What is the degree of supersaturation? And (3) what kinetic factors likely sustain

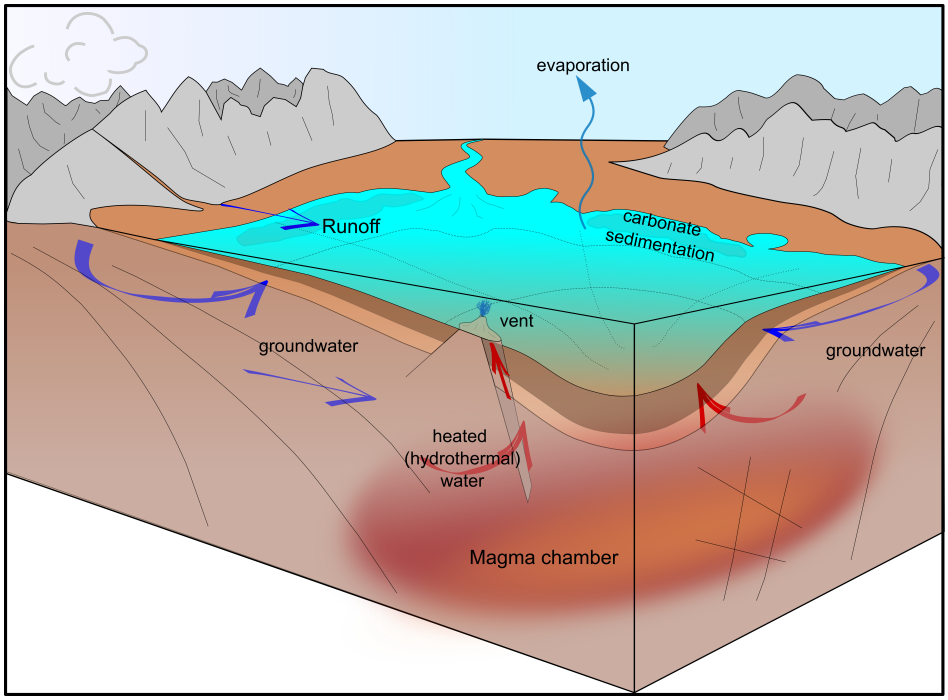
$CaCO_3$ supersaturation in alkaline lakes? The answer to question (1) is clearly not all of them, but this dataset suggests that roughly 80% of all alkaline lakes are supersaturated with respect to calcite specifically. Although all remaining lakes are unquestionably alkaline when the restrictions pH $\geq$8 and CBE $\leq$ 10% are applied, the fact that still not 100% of the samples are saturated/supersaturated with respect to calcite reflects yet another reality: some have [Ca^{2+}] that is too low and below detection limit, such as those from Lake Magadi in Kenya (Eugster 1970 [96]; Jones et al. 1977 [97]), lakes in Wadi Natrun in Egypt (Imhoff et al. 1979 [98]), Pretoria Salt Pan in South Africa (Ashton and Schoeman 1983 [99]), or a few samples from Lake Yoa in Chad (Darragi and Tardy 1987 [80]) and in Lake Abert, in the United Sates (Whitehead and Feth 1961 [110]; Phillips and van Denburgh 1971 [111]). In these cases, the lakes have become substantially depleted in Ca^{2+} and turned into Na-carbonate brines, approaching the saturation of these latter minerals, as indicated in the clear trends shown in Fig. 4.4C–D. However, it is important to highlight that the fact that [Ca^{2+}] may be low and below the detection limit of a given method does not imply there is no dissolved form of calcium in solution. By the same token, following from the definition of the saturation state (Ω, eqn. 2.1), a solution can still be saturated with respect to $CaCO_3$ under low Ca^{2+} but correspondingly high CO_3^{2-}.

This geochemical evolution of alkaline lake waters is in agreement with the early observations and ideas brought forward by Hardie and Eugster (1970) [90]. Investigating the evolution of closed basin lakes, they observed that the initial fluid composition and the ensuing mineral precipitation will establish chemical divides, or turning points, whereby both mineral assembly and fluid composition can be predicted from progressive concentration of evaporative brines. These authors have long documented that calcite precipitation (or coprecipitation of calcite and sepiolite) is a critical step in determining the evolution of evaporating solutions in closed basins, decisively dictating whether they will evolve into carbonate-rich or carbonate-poor brines. Our newly expanded compilation of alkaline lakes data clearly shows this trend, whereby low Ca^{2+} activities, resulting either from low

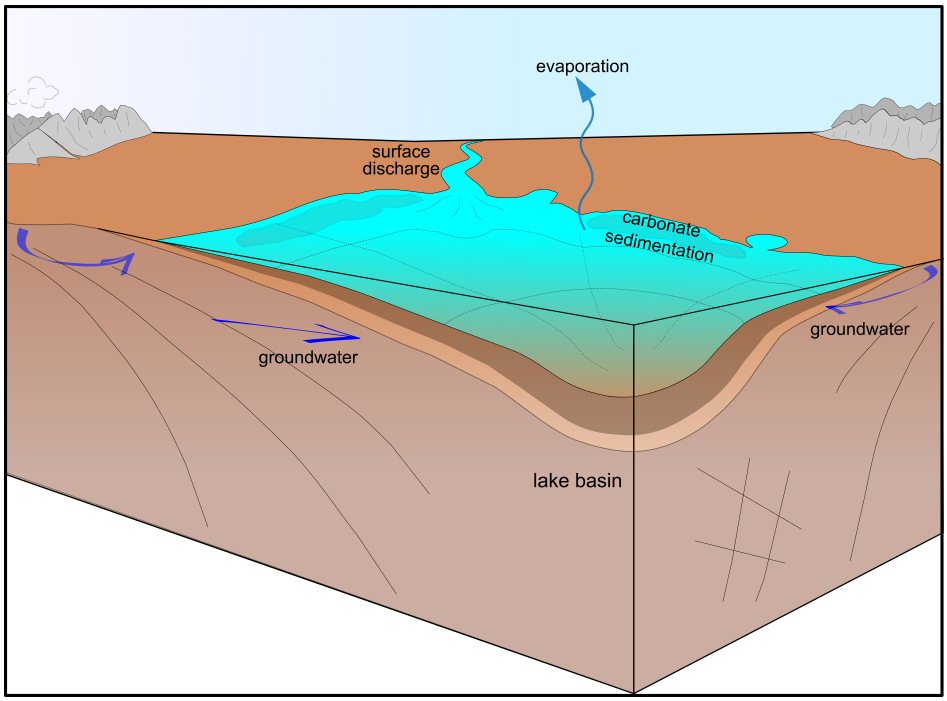
[Ca^{2+}] supply or early sequestration in precipitated Ca-carbonate minerals or both, allow the waters to evolve into high pH, high alkalinity, and high DIC solutions. The upper DIC concentration threshold is in turn controlled by the solubility of Na-carbonate minerals, which finally draws down the DIC as CO_3^{2-} once their saturation is reached (Fig. 4.4C).

Moving on to question (2), its answer is also striking: the degree of supersaturation with respect to calcite (SI_{cal}) tends to be significantly high, with ∼17% of the samples having $0 < SI_{cal} < 1$, whereas 45% of samples have $1 \leq SI_{cal} < 2$ and ∼17% of samples have $SI_{cal} \geq 2$ (Fig. 4.2; Supplement Material in Appendix G). That is, in summary, roughly 80% of all alkaline lakes surveyed have $SI_{cal} > 0$. This last point highlights another fact already pointed out above and in several other studies (*e.g.*, Warren 2010 [112]): Terminal (endorheic) salt pans in rain shadow zones that are not efficiently maintained for example by a fresher groundwater flux supply (insufficient hydraulic head/distant from recharge zones) and/or by runoff from drainage basins are more likely to become depleted in alkaline earth cations and become soda-type brines. Fig. 4.5 conveys conceptually the main hydrological influences in closed basins and the main factors affecting the fluxes of water in and out of such basins.

Thus, except for the very extreme cases of some hydrographically closed terminal lakes, the two preceding and important observations lead naturally to the formulation of question (3). Clearly, to maintain such high supersaturations in all other alkaline lakes (80% of them), some kinetic inhibition of $CaCO_3$ precipitation must be taking place, sustaining SI_{cal} in such a consistent trend. Many ions are known to inhibit calcite (and aragonite) precipitation, but Mg^{2+} and PO_4^{3-} are often considered to be the main ones (Reddy 1977 [32]; De Kanel and Morse 1978 [113]; Reddy and Wang 1980 [114]; Meyer 1984 [115]; Mucci 1986 [116]; Burton and Walter 1990 [117]; Dove and Hochella 1993 [118]; Lin and Singer 2006 [35]), and are thus the best candidates for further investigation, as also suggested by the general chemistry dominating alkaline lake waters.



(a) Rifting basin with influence of volcanism/magmatism generating hydrothermal water circulation, and additional groundwater and surface water discharge.



(b) Closed-lake basin, not necessarily connected with a rifting zone, but placed in a rain shadow area and located at distance from aquifer recharge zones.

Figure 4.5: Schematic representation of the main influences with respect to the hydrology dynamics in closed basins. Not depicted is the fact that differences in bedrock and catchment area geology will contribute distinctly with variable compositions in terms of fluxes of dissolved ions to the lake waters.

The effect of Mg^{2+} ions has been extensively investigated and generally accepted to inhibit calcite precipitation at Mg/Ca ratios above ∼5, favouring aragonite precipitation instead (Hardie 1996 [119]). This effect is often attributed to the increasing energy required to promote the dehydration of proportionally more aqueous Mg^{2+} into the calcite crystal lattice (Lippman 1973 [120]). On the other hand, $PO_4^{3\breve{}}$ is a strong inhibitor of both calcite and aragonite precipitation, as demonstrated in numerous studies (Reddy 1977 [32]; De Kanel and Morse 1978 [113]; Mucci 1986 [116]; Burton and Walter 1990 [117]; Dove and Hochella 1993 [118]; Lin and Singer 2006 [35]). It has also been shown to exert a stronger inhibitory effect than Mg^{2+} (Gratz and Hillner 1993 [34]), even at comparatively lower concentrations (Mucci and Morse 1983 [33]; Mucci 1986 [116]). The next two sections attempt to examine in greater detail the potential roles of these two ions in inhibiting and maintaining $CaCO_3$ supersaturation, in the broader context of average evaporitic and alkaline lakes.

4.4.2 Phosphate interactions with $CaCO_3$ in alkaline lake waters

The effects among $a_{PO_4^{3-}}$, $a_{Mg^{2+}}$ and SI_{cal} can be further visualised in Fig. 4.6, where it is shown a comparison of the saturation index of calcite with respect to $a_{PO_4^{3-}}$ (first row) and with respect to $a_{Mg^{2+}}$ (second row). The third row shows plots of $a_{PO_4^{3-}}$ vs $a_{Ca^{2+}}$ with the saturation lines for various Ca-phosphate phases. These plots reveal that all alkaline lake water samples with reported ΣPO_4 concentrations are supersaturated with respect to hydroxyapatite (HAP) and close to saturation with respect to less stable and amorphous Ca-phosphate (ACP). The columns reproduce the same plots but with samples colour-coded in bins reflecting different variables (ALK/(Ca+Mg), $a_{Ca^{2+}}$ and pH, in the first, second, and third column, respectively). Other possible Ca-phosphate mineral phases, such as fluorapatite and francolite, which are considered important diagenetic marine phosphate mineral phases (*e.g.*, Atlas and Pytkowicz 1977 [121]; Gunnars et al. 2004 [122]; Brady et al. 2022 [123]), are ignored in this assessment. Only a few selected phosphate phases

were considered because the main goal here was to set lower limits and ceilings to the controls on the solubility of phosphate in alkaline fluids. Likewise, based on the foregoing and subsequent discussions, upper thresholds based on some more likely amorphous phases such as OCP and ACP, are deemed more important phases to account for, rather than the more insoluble fluorite or the complex francolite series.

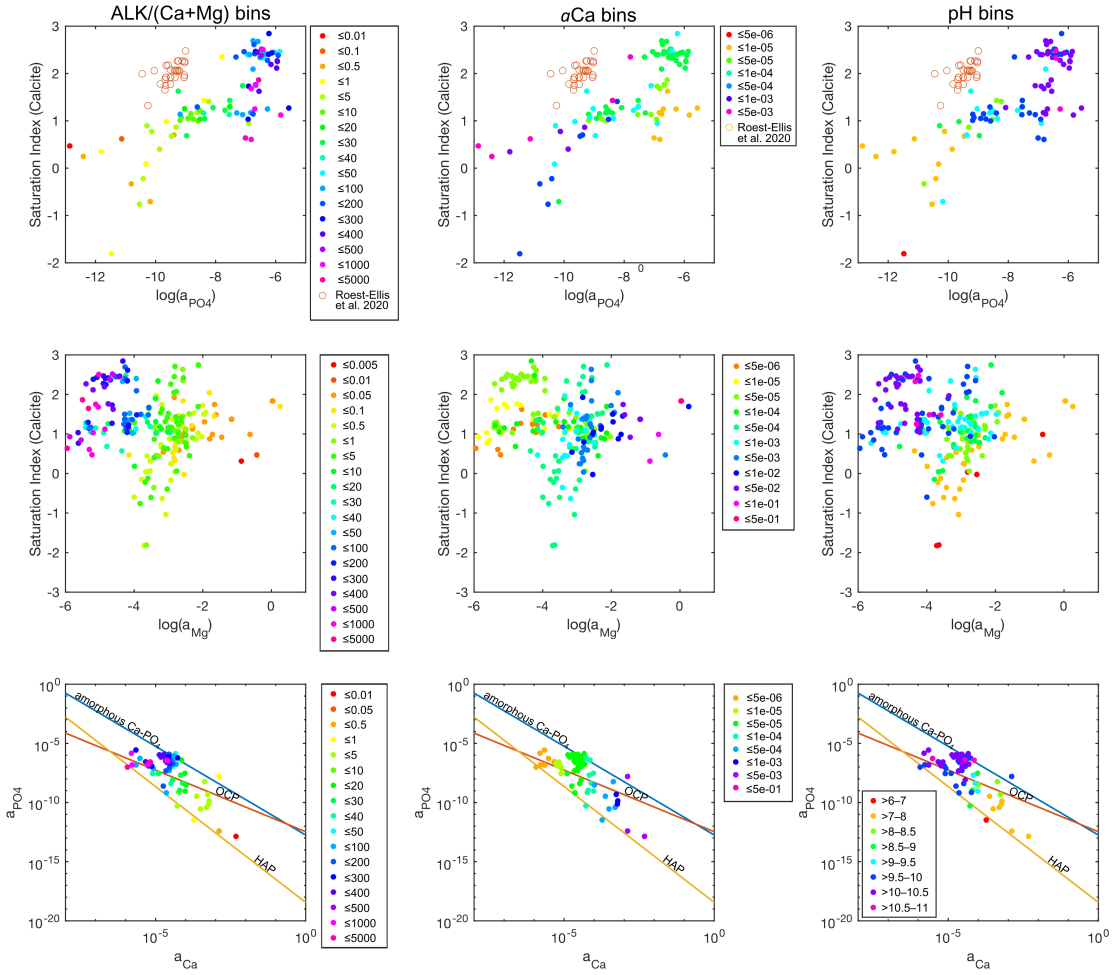


Figure 4.6: Saturation index of calcite *vs* log10($a_{PO_4^{3-}}$) and log10($a_{Mg^{2+}}$) (first and second rows, respectively), and $a_{PO_4^{3-}}$ vs $a_{Ca^{2+}}$ and solubility lines for various Ca-PO_4 phases (third row). Colour-coding according to ALK/(Ca+Mg) (first column), $a_{Ca^{2+}}$ (middle column) and pH (third column).

In line with previous studies on the effects of ΣPO_4 on $CaCO_3$ precipitation, Roest-Ellis et al. (2021) [124] have shown that even relatively low concentrations of ΣPO_4 (above ∼12 µM) can severely inhibit spontaneous $CaCO_3$ nucleation, allowing a significant increase in supersaturation at $SI_{cal} \approx 1.65$ and above. Their data

are also shown in Fig. 4.6, upper row, for comparison with the natural alkaline lake waters dataset. At the extreme end of high $a_{PO_4^{3-}}$ in Fig. 4.6, nearly two orders of magnitude higher than in their experiments, lie some natural alkaline lake waters samples from Last Chance and Goodenough lakes in Canada, with reported high ΣPO_4 values. Although this extreme end may imply a possible connection between high dissolved ΣPO_4 concentrations and high $CaCO_3$ supersaturation, it is important to consider some caveats and alternative explanations, addressed further below.

Combining the constraint of CBE$\leq$10% with the total amount of samples reporting ΣPO_4 concentration the total dataset becomes further reduced, and only lakes from Brazil, Canada, Egypt, Kenya, South Africa, Tanzania and the United States remain. Still, it is visible that increasing $a_{PO_4^{3-}}$ broadly correlates with increasing SI_{cal}. The two leftmost "tails" may represent well two general initial state endmembers of a spectrum with low $a_{PO_4^{3-}}$. From a very low SI_{cal} (lower "tail") starting from waters with relatively lower pH, increasing $a_{PO_4^{3-}}$ correlates with SI_{cal} ramping up rapidly (Fig. 4.6). Interestingly, it is also visible that this overall trend correlates generally well with increasing ALK/(Ca+Mg). Following along the upper "tail" the same trend of increasing SI_{cal} with $a_{PO_4^{3-}}$ is visible, although the increase in SI_{cal} is gentler. This may be a limiting effect in natural waters, associated with a certain SI_{cal} (and $a_{Ca^{2+}}$) threshold, whereby higher $[Ca^{2+}]$ with higher ΣPO_4 will favour apatite precipitation instead. Regardless, the two trends converge at SI_{cal} = ~1–1.3, corresponding to an average $[Ca^{2+}] \approx 0.2$ mmol/kg, and $a_{PO_4^{3-}}$ between ~10^{-9}–10^{-8}, which corresponds to an average dissolved ΣPO_4 = ~0.07 mmol/kg (N = 11). The upper right end comprises samples from only two locations, Last Chance and Goodenough lakes in British Columbia, Canada, which are in the range of hyperalkaline Na-CO_3-(SO_4)-Cl waters with pH > 9.5. These ephemeral and perennial lakes, respectively, lie less than 0.5 km apart and are fed by groundwaters that drain through basalts, glaciofluvial deposits and other sedimentary rocks (Hirst 1995 [100]). The recharge zones and hydraulic head are probably more effective in replenishing the aquifer and maintaining a relatively fresher groundwater flux to

the lakes than in arid plains/rain shadow areas. These lakes are also influenced by freezing and thawing cycles, whereby a "salting out" effect occurs in winter and melting of ice returns fresh water to the lakes by springtime (Hirst 1995 [100]). These processes in turn might be contributing factors preventing [Ca^{2+}] to be completely depleted in these two very close locations, compared to other hyperalkaline lake waters such as the Wadi Natrun and Lake Magadi, for example.

Therefore, the available data suggests that what may allow excessively high $CaCO_3$ supersaturation (*i.e.*, $SI_{cal} \geq 2$) to be reached is a convergence of factors. Inhibitors, of which PO_4^{3-} is probably amongst the most significant, allow supersaturation by absorbing onto existing crystal surfaces and nucleating clusters, increasing the interfacial free energy and consequently the critical free energy barrier (discussed in Chapter 5), therefore decreasing the rate of precipitation (Mucci 1986 [116]; Sumner and Grotzinger 1996 [125]). But this factor alone seems to approach a plateau in most natural alkaline waters surveyed, at $SI_{cal} = \sim 1$–1.3. This may suggest that higher [Ca^{2+}] cannot be sustained by prolonged times with higher ΣPO_4, even at higher DIC and ALK levels. The maximum ΣPO_4 concentration is $\approx$ 40 mmol/kg under more conservative [Ca^{2+}] average values (5–6 mmol/kg) taken from the present dataset (N = 232, *i.e.*, removing [Ca^{2+}] values <LD and still adopting CBE$\leq$10%). Conversely, very high $CaCO_3$ supersaturations, such as indicated in Last Chance and Goodenough lakes, may be a phenomenon associated with a very specific set of circumstances, namely a combination of the presence of inhibitors with a constant supply of relatively fresher groundwaters/runoff waters, freeze-thaw cycle (which these two lakes are strongly influenced by; Hirst 1995 [100]) and favourable lithologies/regional geology.

Still, the dataset also clearly shows that total dissolved phosphate concentration in turn can increase substantially under high pH and DIC and limited Ca^{2+} supply, as suggested in earlier studies (*e.g.*, Talling et al. 1973 [88]) and more recently highlighted by Toner and Catling (2020) [94]. This is indicated in Fig. 4.6, lower row, showing the solubilities of HAP, OCP and ACP as functions of $a_{Ca^{2+}}$ and $a_{PO_4^{3-}}$.

Under progressively lower $a_{Ca^{2+}}$ (towards the left), $a_{PO_4^{3-}}$ may increase in solution before crossing the HAP solubility threshold. Interestingly, these calculations indicate that ΣPO_4 concentration in solution is also controlled by less stable phosphate solid phases, as previous workers have already pointed out in their investigations (*e.g.*, Van Cappellen 1991 [20]; Gunnars et al. 2004 [122]).

4.4.3 Mg^{2+} interactions with $CaCO_3$ in alkaline lake waters

With respect to [Mg^{2+}] (as $a_{Mg^{2+}}$), there is surprisingly a large scatter, suggesting at first glance that it does not exert a dominant inhibitory effect on $CaCO_3$ supersaturation in alkaline lake waters (Fig. 4.6, middle row). However, at confined pH ranges there is an indication that increasing [Mg^{2+}] does correlate with increasing SI_{cal} (Fig. 4.6, middle row, rightmost panel). For values of pH ≤ 7 the effect seems more prominent, that is, more [Mg^{2+}] generally correlates with a steeper increase in SI_{cal}. The effect seems to become somewhat attenuated within the range of $8 \leq$ pH < 9, and above this pH value there is no clear correlation.

Still, the difficulty in establishing a clear-cut and strong role of Mg^{2+} in influencing or inhibiting $CaCO_3$ precipitation in natural alkaline lakes can be further illustrated in Fig. 4.7. In this case, the same data that was shown in Fig. 4.4 is plotted against ranked Mg/Ca molal ratios, and again a significant spread in the ratio values is observed. It can be seen that lower ratios generally tend to cover the whole sampled range between the saturations of MHC and amorphous $CaCO_3$ phases, although a trend of higher Mg/Ca ratios emerges at Ca^{2+} activities between $10^{\breve{}3.95} \leq a_{Ca^{2+}} \leq \sim 10^{-5.55}$ (Fig. 4.7A). This is more likely simply reflecting the normal evaporation process, though, whereby the ensuing precipitation of calcium carbonate phases draws down Ca^{2+} from solution, thereby proportionally increasing the Mg/Ca ratio as a result.

In the evolving trajectory towards evaporitic soda brines, some lakes clearly reach higher Mg/Ca ratios (Mg/Ca >5, but predominantly between 10 and 50) and are also closer to the saturation of Mg-CO_3 phases (Fig. 4.7B). Some of these lakes

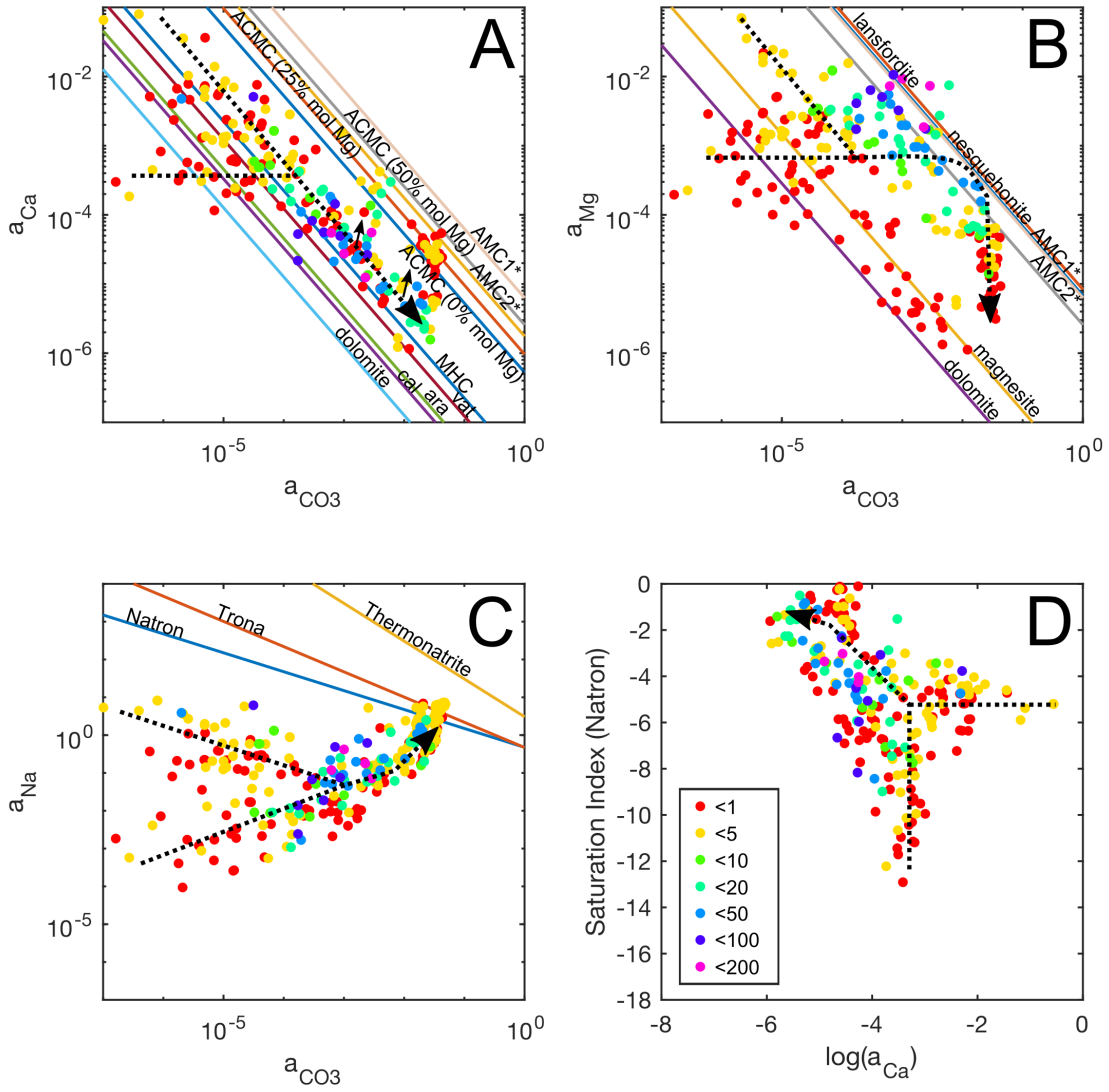


Figure 4.7: Activity and saturation index diagrams for 281 water samples whose CBE≤10%. (A) Activity of calcium ($a_{Ca^{2+}}$) *vs* activity of CO_3^{2-} ($a_{CO_3^{2-}}$) and solubility lines for various Ca-Mg-CO_3 crystal and amorphous phases. (B) $a_{Mg^{2+}}$ vs $a_{CO_3^{2-}}$ and solubility lines for various Mg-(Ca)-CO_3 phases. (C) a_{Na^+} vs $a_{CO_3^{2-}}$ and solubility lines for various Na-CO_3 minerals. (D) SI of natron versus $\log_{10}(a_{Ca^{2+}})$. Samples are colour-coded according to Mg/Ca molal ratio intervals, shown in panel D.

include East Basin (Australia); Goodenough (Canada); Qinghai (China); Baga Nuur, Bor-Khag Nuur, Ikh-Gashun Nuur, Khyargas Nuur (Mongolia); Khilganta (Russia); Big Soda, Pyramid, Walker (United States); and Van (Turkey). However, the extreme end of samples, with the highest pH, alkalinity and DIC values, comprising the hyperalkaline lakes Last Chance and Goodenough, is also within the lower range of Mg/Ca ratios. This might therefore suggest their chemistry is unfavourable for

the precipitation of Mg-CO_3 mineral phases (Fig. 4.7B). On one hand, this might reflect the dilution due to relatively fresher groundwater supply or related to thawing during springtime (Hirst 1995 [100]), or a combination of both processes. On the other hand, it is also relevant to highlight that dissolved SiO_2 plays an additional and important role in influencing the general chemical evolution of alkaline lakes (*e.g.*, Chase et al. 2020 [78]) and particularly in establishing a ceiling to Mg^{2+} concentrations, thereby indirectly controlling maximum Mg/Ca ratios. According to Tutolo and Tosca (2018) [28], the concentration of $SiO_{2(aq)}$ in alkaline lakes is, in turn, "controlled by (1) solubility constraints applied to amorphous silica saturation, (2) silica uptake by mineral surfaces and (3) the precipitation of Mg-silicates". Nevertheless, the primary availability of $SiO_{2(aq)}$ in alkaline lakes is constrained by the surrounding bedrock geology, which will inherently contribute with the dissolved load, thereby setting the initial conditions for the ensuing evolution of underfilled, evaporative basins (Fig. 4.5). In summary, $SiO_{2(aq)}$ availability likely has an effect on the observed variability of Mg/Ca ratios. An exhaustive analysis of the relations between $SiO_{2(aq)}$, Mg^{2+} and Ca^{2+} is however outside the scope of the present contribution. Thus, a combination of conditions needs to be factored in, taking into account the surrounding geology, climate, topography gradient and distance from recharge zones (therefore affecting hydraulic head and groundwater fluid flow), etc (Fig. 4.5).

In this respect, the plot shown in Fig. 4.7B is however useful in pointing out possible different geochemical and environmental controls in modern lakes that may be more conducive to the precipitation of Mg-CO_3 minerals at ambient conditions, as well as for their preservation. In turn, Fig. 4.7C also shows that low Mg/Ca cover the whole range of the compositional space towards the saturation of Na-carbonate phases, with higher ratios concentrating before the saturation of natron is reached, at the intersection of the two lines, and decreasing again as Na-carbonate saturation is approached. This probably reflects the point where the saturation of Mg-CO_3 phases are reached and Mg^{2+} is also drawn down from solution, decreasing the Mg/Ca ratio again before Na-CO_3 mineral saturation is reached. However, it

should be noted that the lowering in the Mg/Ca ratio may be reflecting the specific combination of factors discussed above for the Last Chance and Goodenough lakes, since the samples approaching natron/trona saturation are dominated by samples from these two lakes.

Finally, the plot of natron saturation index (SI_{natron}) *vs* $\log(a_{Ca^{2+}})$ illustrates a similar trend in an alternative way (Fig. 4.7D), with Mg/Ca ratios decreasing again once SI_{natron} gets closer to saturation ($SI_{natron} \rightarrow 0$). This in turn seems to highlight the main role of the evaporative pathway in influencing the natural increase followed by the decline in Mg/Ca ratios as the main pattern in the evolution of alkaline lakes, however bearing in mind the same caveat pointed out above.

4.4.4 Constraints on calcium concentration from ΣPO_4 levels and vice-versa in alkaline lakes

Considering the data discussed above, the observations that aqueous ΣPO_4 concentrations generally correlate with DIC in alkaline lakes, as well as observations made by Fukushi and Matsumiya (2018) [1], Ingalls et al. (2020) [31] and Toner and Catling (2020) [94], it is possible to define some constraints on dissolved Ca^{2+} concentrations in these environments. If $CaCO_3$ precipitation effectively removes aqueous Ca^{2+}, this in turn may largely prevent Ca-phosphate precipitation. It is therefore conceivable that this may correspond to an important factor controlling maximum phosphate concentrations that can be maintained in alkaline solutions.

Furthermore, if metastable precursor phases control Ca-phosphate concentrations in addition to $CaCO_3$, as shown by the present survey and highlighted in Fig. 4.6, with simple geochemical calculations it is possible to point to the key role of Ca^{2+} in modulating ΣPO_4 concentrations in alkaline lake waters. As an exercise, we can initially assume the average value of $a_{Ca^{2+}} = 0.0056$ (calculated from our database, excluding samples whose CBE>10% and those with undetected [Ca^{2+}] values) and use this value to constrain the solubility of Ca-phosphates at a given pH value. Combining these constraints, and assuming that OCP, a likely precursor of apatite, represents a reasonable upper limit on ΣPO_4 concentrations (Van Cappellen

1991 [20]; Gunnars et al. 2004 [122]), as also shown in Fig. 4.6 (bottom) we can demonstrate a clear inverse relationship between [Ca^{2+}] and ΣPO_4. The solubility of OCP (K_{OCP}) is given by (Tung et al. 1988 [68]; see also Chapter 2, eqn. 2.32):

$$K_{OCP} = (a_{Ca^{2+}})^4 \cdot (a_{H^+}) \cdot (a_{PO_4^{3-}})^3 \tag{4.2}$$

where $K_{OCP} = 10^{-48.4}$. The parameters above permit recovery of individual phosphate species concentrations that will be in equilibrium in a given range of pH and [Ca^{2+}] values, based on the following additional equilibrium relations (Chapter 2, eqn. 2.33, 2.34 and 2.35):

$$H_3PO_4 \longrightarrow H^+ + H_2PO_4^- \quad , \quad K_{1P} = \frac{a_{H^+} \times a_{H_2PO_4^-}}{a_{H_3PO_4}} \tag{4.3}$$

$$H_2PO_4^- \longrightarrow H^+ + HPO_4^{2-} \quad , \quad K_{2P} = \frac{a_{H^+} \times a_{HPO_4^{2-}}}{a_{H_2PO_4^-}} \tag{4.4}$$

$$HPO_4^{2-} \longrightarrow H^+ + PO_4^{3-} \quad , \quad K_{3P} = \frac{a_{H^+} \times a_{PO_4^{3-}}}{a_{HPO_4^{2-}}} \tag{4.5}$$

where K_{1P}, K_{2P}, and K_{3P} refer to the first, second and third thermodynamic dissociation constants of H_3PO_4, respectively. Briefly, the activity coefficients and ionisation constants are functions of the solution ionic strength and can be determined for single electrolyte solutions (*e.g.*, NaCl) using the Pitzer ion interaction model equations (*e.g.*, Pitzer 1987 [54]; Millero and Pierrot 1998 [126]; Tosca et al. 2011 [105]). Here, the activity coefficients for H^+, H_3PO_4, $H_2PO_4^-$, HPO_4^{2-}, and PO_4^{3-} were determined for the average alkaline lake assuming of [Na^+] = 706 mmolal, [Cl^-] = 535 mmolal, and the ionic strength = 1134 mmolal, using the Pitzer model equations and the parameters determined by Hershey et al. (1989) [51]. Once these have been calculated, the dissociation constants were determined for this specific set of conditions. Details of the calculations are given in Chapter 2 and the values used are shown in Table 2.2.

With this system constrained we observe, similar to Toner and Catling (2020) [94], that lower calcium concentrations allow high-pH solutions to maintain significant concentrations of ΣPO_4 in solution, and vice-versa (Fig. 4.8A). Fig. 4.8B-D shows phosphate speciation as a function of OCP solubility in a large pH range and with $[Ca^{2+}]$ = 1, 0.1 and 0.01 mmol/kg, respectively. This figure shows that the main species predicted in solution are $H_2PO_4^-$ and HPO_4^{2-} at pH>8, and total PO_4 concentration can be 100s mmol/kg high in the pH range ∼8–9 (Fig. 4.8A). At lower $[Ca^{2+}]$ values, theoretical ΣPO_4 concentration can be considerably higher at higher pH, >1 mol/kg, similar to the findings of Toner and Catling (2020) [94], whereas the contribution of PO_4^{3-} species to total ΣPO_4 increases significantly at pH>10 (Fig. 4.8B-D). In summary, this species likely exert a strong influence in $CaCO_3$ inhibition/precipitation as discussed above in light of known carbonate precipitation kinetics. This exercise also shows that ΣPO_4 in solution can reach values above several millimolal levels at relatively low $[Ca^{2+}]$ (Fig. 4.8A), and that at pH>10 HPO_4^{2-} and PO_4^{3-} are the dominant species in solution (Fig. 4.8B-D).

However, it is worth highlighting that the presence of other dissolved ions such as Mg^{2+} can contribute with further complex interactions by increasing the dehydration energy (Nielsen 1984 [127]), as pointed out above. Conversely, an experimental study by Bischoff 1968 [128] found that calcite nucleation rates tend to increase with increasing ionic strength, as a function of the square root of the latter one. As the author suggested, ionic strength- mediated nucleation may result from the decreased interfacial free energy barriers (Chapter 5), favouring the movement of reactants across the double layer. Thus, these competing effects potentially affect the rate of Ca^{2+} removal from solution. This implies that the equilibrium relations between Ca-PO_4 modelled here might represent a lower boundary to both Ca^{2+} and ΣPO_4 concentrations that can co-exist at any given pH value. More importantly though, is that at high alkalinities but lower pH values (see, for example, Fig. 3.2, both Ca^{2+} and ΣPO_4 can co-exist as dissolved phases in proportionally higher concentrations, as shown in Fig. 4.8A.

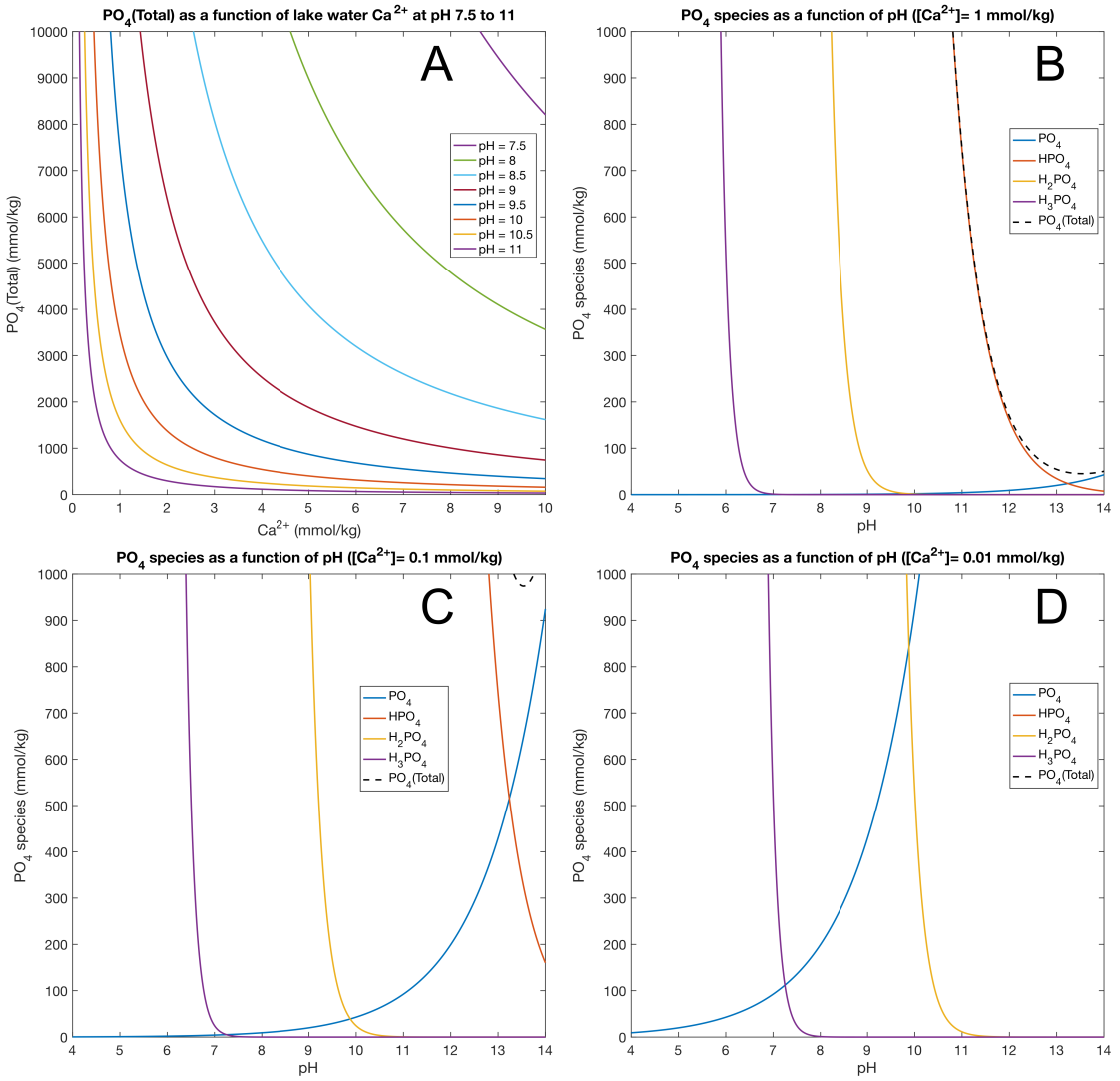


Figure 4.8: (A) ΣPO_4 as a function of pH and $[Ca^{2+}]$, assuming the conditions explained in the text for a hypothetical alkaline lake composition with average values calculated from the database and using dissociation constants and activity coefficients shown in Table 2.2 (Chapter 2). (B) Speciation of ΣPO_4 calculated as explained in the preceding lines, for $[Ca^{2+}] = 1$ mmol/kg. (C) Same as in (B), but for $[Ca^{2+}] = 0.1$ mmol/kg. (D) Same as before, but considering $[Ca^{2+}] = 0.01$ mmol/kg.

4.5 Conclusions

The present compilation of fluid chemistry from modern alkaline lakes and the thermodynamic calculations contribute to expand our understanding about the underlying chemical controls favouring $CaCO_3$ supersaturation and affecting $CaCO_3$ precipitation in these environments. Regardless of the inherent uncertainties regarding the Mg/Ca ratios variations pointed out above, the observations consistently

indicate that phosphate plays a dominant inhibitory role on $CaCO_3$ precipitation and in sustaining its supersaturation, compared to Mg^{2+}. The latter influence's as a strong inhibitor is less clear, as it is observed that its proportion only increases at the expense of Ca^{2+} draw down during progressive evaporation and $CaCO_3$ precipitation. These extended results in turn confirm that $CaCO_3$ supersaturation is a general trait in alkaline lakes (roughly 80% of all alkaline lakes assessed) maintained between the saturation states of monohydrocalcite and amorphous Ca-Mg-carbonate (ACMC) phases by the presence of inhibitors. This condition is likely conducive of non-traditional precipitation pathways involving metastable intermediate precursors such as MHC, which may influence fabric development and are more indiscriminate towards trace element incorporation. The fact that some waters have become extensively depleted in $[Ca^{2+}]$ explains why the remaining ∼20% of alkaline lakes *apparently* are not saturated with respect to $CaCO_3$ phases, even though low and undetectable $[Ca^{2+}]$ can in principle contribute to $CaCO_3$ supersaturation. In the case of limited or depleted $[Ca^{2+}]$, ΣPO_4 concentrations can reach several 10s–100s millimoles, as shown in a number of soda lakes. The present geochemical calculations also show that ΣPO_4 in the order of a few moles/kg with $[Ca^{2+}] \approx 5$ mmol/kg and pH ∼9 are theoretically possible. In line with other studies, this suggests alkaline lakes might have been one favourable aqueous environment enabling high concentrations of soluble phosphate in the early Earth, predating the emergence of life.

4.6 Summary and Future Outlook

A final caveat worth highlighting is that lakes are highly dynamic systems, because among other factors they are extremely susceptible to seasonality. Therefore, sampling and fluid analysis will reflect the season of the year as well as interannual variability. This assessment did not aim at looking at the level of internal variance within each individual lake but aimed instead at addressing the broader general patterns that may consistently emerge from an extended analysis of the thermodynamic properties of alkaline lake waters. Likewise, variations with depth

arising from lake stratification and an established chemocline, which can cause redox gradients and therefore concentration gradients, are not accounted for in this large compilation, since most studies report only "total" lake concentrations. In all these respects, it is clear that this study necessarily builds on many previous works, and therefore assumes that sample collection and analysis, characterisation of the lacustrine environments and their classification as alkaline lakes are not contentious issues. Future work should therefore aim to expand the current database and improve the present calculations, ideally providing refined experimental data as well.

5

Merging Crystal Growth Theory and Experimental Approaches to Investigate Precipitation in the Phosphate-Carbonate Systems

5.1 Introduction

The observations made in the preceding chapters set the main motivation for the present study. Here, the mechanisms of homogeneous and heterogeneous nucleation of $CaCO_3$ minerals of relevance to sedimentary Earth's surface environments are investigated, focusing on the roles of the relevant inhibitor ΣPO_4 and supersaturation. To address the effects of these parameters on carbonate nucleation, growth and fabric development in alkaline solution conditions likely to have existed in ancient marine and lacustrine environments, a dynamic chem-stat (constant) composition experiment was employed.

The results unequivocally show that concentrations of a few tens of micromoles ΣPO_4 are enough to exert a strong inhibitory effect on $CaCO_3$ growth and nucleation, thereby sustaining elevated supersaturations ($\Omega_{calcite} \approx 70$–$100$) during heterogenous nucleation experiments and decreasing growth rate, as in numerous studies before

(*e.g.*, Mucci 1986 [116]; Burton and Walter 1990 [117]; Dove and Hochella 1993 [118]; Lin and Singer 2006 [35]). Finally, the effects of supersaturation driving fabric development are also reviewed.

The combined observations in this study provide support to other investigations indicating that characteristic carbonate mineral textures preserved in the rock record, such radiaxial fibrous calcites and spherulitic aggregates, often crystallise by particle attachment and agglomeration. Since these mechanisms require supersaturation, and the latter requires compounds that inhibit crystallisation (barring conditions such as rapid CO_2 degassing, where supersaturation is reached 'instantaneously' and locally), these crystal morphologies may be used as a qualitative index of saturation level and/or inhibitor concentration. However, other conditions such as the one just mentioned (rapid degassing, or a non-steady flux) have to be ruled out with the presentation of additional and independent evidence.

5.2 Methodology and Experimental Design

5.2.1 General experimental conditions

All solutions were prepared with deionised water (resistivity 18.2 $M\Omega \cdot cm$) in plasticware previously cleaned in acid (4% HNO_3) and deionised water baths for at least a couple of days in each. The following reagents were used: Na_2CO_3 (Sigma-Aldrich, 99.5%), $NaHCO_3$ (Sigma-Aldrich, 99.5%), NaCl (Sigma-Aldrich, 99.5%), 1 molal NaOH stock solution from NaOH pellets (Sigma-Aldrich, 98%), 0.1 molal NaH_2PO_4 stock solution from NaH_2PO_4 powder (Acros Organics, 99%), $MgCl_2$ (Sigma-Aldrich, 1 M), $CaCl_2$ (Sigma-Aldrich, 1 M), $(NH_4)_2CO_3$ (Sigma-Aldrich, $\geq$99.5%) and NH_4Cl (Sigma-Aldrich, $\geq$99.5%). The initial concentrations of the experimental solutions are indicated the following sub-sections.

5.2.2 Free-drift experiments

Free-drift experiments (Gruzensky 1967 [129]) were originally set to produce seed material for the constant composition experiments. This method is well-established

and produces supersaturated solutions reasonably rapidly (days to few weeks), whereby it is possible to obtain pure and highly crystalline calcite (Gruzensky 1967 [129]; Reeder et al. 1990 [130]). However, it comes with the main setback that it is not generally possible to determine the degree of supersaturation with precision (Blue et al. 2017 [44]). These experiments were henceforth only used to produce internal reference calcite for X-ray diffraction (XRD) pattern comparisons and to assess homogeneity of crystal seeds within a given experiment. Surface area measured by the KBr-BET method (De Kanel and Morse 1978 [113]), in a Micromeritics TriStar II Plus surface area and porosity analyser with N_2 gas, at a temperature of –195.85^{o}C at the Department of Chemistry, University of Oxford. The surface area of these synthetically produced calcite crystals was determined to be 0.010 m^2 $g^{\breve{}1}$ on average. This surface area was too low for the purposes of use of the material as seeds in subsequent experiments. Therefore, commercial $CaCO_3$ powder (Acros®), whose surface area was measured as being 1.441 m^2 $g^{\breve{}1}$, was used as seed material instead.

Solutions were prepared by mixing 80 mmol/kg $CaCl_2$ with 1.2 mol/kg NH_4Cl and a small amount of ΣPO_4 (40 μmol/kg) to slow the nucleation reaction in a beaker containing 400 mL deionised water. Then, 25 g of $(NH_4)_2CO_3$ were placed on top of a watch glass sitting on top of the beaker, in a sealed box. Thus, the internal atmosphere would become saturated in CO_2 during the spontaneous decomposition of $(NH_4)_2CO_3$, promoting the diffusion of CO_2 into the solution, thereby increasing its DIC and saturation with respect to $CaCO_3$. Experiments were run for ∼30–35 days.

5.2.3 Constant Composition Experiments

The constant composition experiments are essentially a chemostat technique (Mucci and Morse 1983 [33]; Mucci 1986 [116]; Beck et al. 2013 [131]), which is based on the simultaneous injection of two titrants in equal amounts by an auto-titrator system (902 Titrando®, Metrohm). The mixture of the two titrants needs to reproduce the exact composition of the WS, plus an excess in calcium and carbonate

alkalinity to compensate for the magnesian calcite precipitation (Mucci 1986 [116]). These experiments were performed under different inhibitor concentrations (total phosphate, referred to as ΣPO_4) at constant supersaturation in the presence of calcite crystal seeds. The experiments aimed to test how these parameters may affect overall precipitation rates, and face-specific growth rates, which in turn controls crystalline morphology of the carbonate overgrowths. The pH and $[Ca^{2+}]$ of the solutions were monitored with a pH and an ISE, respectively. The pH-metre was calibrated against NIST-traceable buffers (Orion®, Thermo Scientific) with pH 4, 7 and 10. The potentials measured with the Ca^{2+} ISE were converted to concentrations, following calibration curves for each experiment, based on the measurement of four internal standard solutions with $[Ca^{2+}]$ = 2, 5, 10 and 20 mmol/kg.

Under these experimental conditions, the precipitation of carbonate material is carried out in an open system reactor (maintaining atmospheric pressure and fluxes in and out of the vessel, according to titration rate), thereby allowing the maintenance of a constant state of disequilibrium. This state is sustained in the working solution by holding constant the a_{H^+} (pH) and pCO_2, permitting the $CO_3^{2\breve{}}$ concentration to be kept constant throughout the experiment, as well as the concentration of Ca^{2+}. Following Mucci and Morse (1983) [33] and Mucci (1986) [116], the pH and dissolved inorganic carbon (DIC) are maintained by addition of excess carbonate alkalinity in the form of $HCO_3^{\breve{}}$ and $CO_3^{2\breve{}}$ from a mixed $NaHCO_3$-Na_2CO_3-electrolytes solution, whereas Ca^{2+} is supplied from an independent $CaCl_2$ solution. The WS was stirred at a constant rate of 250 rpm for homogeneity and kept at a temperature of 21 ± 1.5°C. Some experiments were run for several hours after the observed induction (nucleation) time, in order to observe if mineralogical changes of the material crystallised from solution might occur within longer time frames. Table 5.1 gives a summary of the general conditions maintained in these experiments.

The saturation state of the solution (Ω) with respect to the solid phase (calcite, in this case) was defined in eqn. 2.1 in chapter 2, shown here again for clarity as:

$$\Omega = IAP/Ksp \tag{5.1}$$

Where IAP is the ion activity product and *Ksp* is the solubility product (for calcite, $10^{\check{}8.48}$ at 25^{o}C, Plummer and Busenberg 1982 [59]). There is an inherent uncertainty in the precise determination of saturation states, because they directly depend on the *Ksp*. The latter is theoretically or more often experimentally determined, but in any case it depends on the conditions assumed, whether it was calculated from standard Gibbs free energies of formation (in turn, themselves determined experimentally) or determined directly from experiments. The same applies to the IAP values, which depend on the model used to estimate activities and activity coefficients. As a result, the value of Ω itself is model-dependent. Therefore, the values indicated on Table 5.1 reflect a sensitivity analysis, encompassing the range of greater likelihood considered in the present experiments.

Table 5.1: Typical solution composition of a constant composition experiment.

Parameter	**Concentration (millimolal)**
Na^+	100
Mg^{2+}	50
Ca^{2+}	10
Cl^-	210
ΣPO_4	0; 0.025; 0.050
DIC	10
ALK	13
Ionic strength	285
Additional constraints	
Ω	70–100
pH	8.8
$\Sigma_{cations}$ (meq/kg)	220
Σ_{anions} (meq/kg)	223
Charge balance error (%)	–0.8

5.2.4 Solid sample characterisation and *in situ* monitoring

5.2.4.1 X-ray diffractometry

Solid samples were analysed with a PANalytical Empyrean X-ray diffractrometer with a Co-Kα radiation source at 40 kV and 40 mA current, and the mineralogy was identified using the ICCD (International Centre for Diffraction Data) Powder Diffraction File-4+ database and the reference intensity ratio method (Snyder and Bish 1989 [132]) in the HighScore® software (Malvern Pananalytical; Degen et al. 2014 [133]).

5.2.4.2 Scanning electron microscopy with energy dispersive X-ray spectrometry (SEM-EDS)

Analyses were performed at the Sir William Dunn School of Pathology, University of Oxford. For this purpose, solid samples were Au-coated preceding the investigation under the electron microscope. The microscopic investigation used a Zeiss Sigma 300 field emission electron gun operated at 2 kV accelerating voltage and 15 µm aperture, equipped with a Ultim Extreme EDS for chemical quantification of selected spots in the solid samples.

5.2.4.3 *In situ* Raman spectroscopy

In situ Raman spectra were collected during a few selected experiments, using a Tornado HyperFlux PRO Plus spectrometer with collection of 12 scans averaged over 120 s intervals, and the data were processed using the Panorama Pro software (LabCognition GmbH).

5.3 Results

5.3.1 Free-drift experiments

These experiments tend to yield well-formed calcite crystals in a few days to weeks, after which the solids should approximate equilibrium with the bulk solution. However, running the experiments for 30 days shows that the formation of larger crystals is still occurring at the expenses of smaller crystals, which in turn reveal

clear signs of ongoing dissolution (Fig. 5.1). The heterogeneity in grain size, as well as the porosity created by dissolution, precluded the use of these calcite crystals as seeds. However, they provided useful calcite reference material for comparison with X-ray diffraction patterns of samples from constant composition experiments (Fig. 5.5).

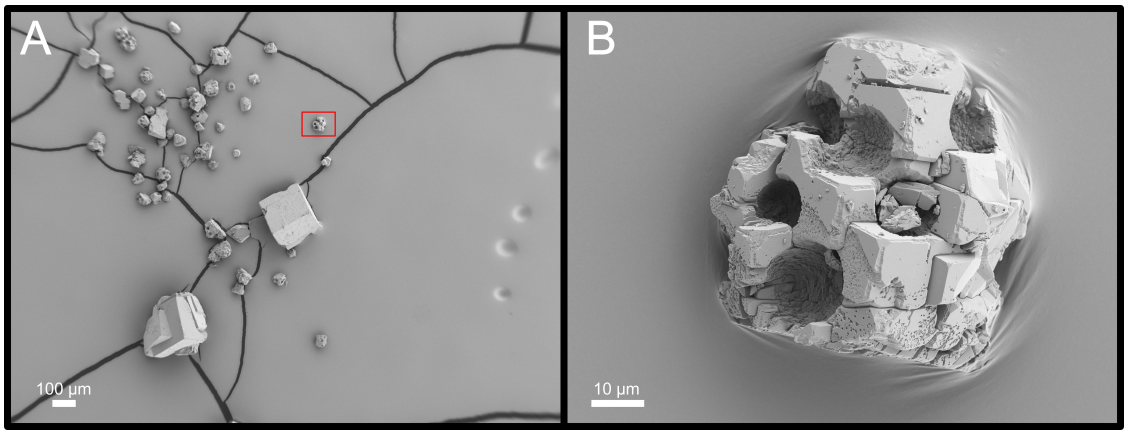


Figure 5.1: Calcite crystals grown from free-drift experiments. A: general view, illustrating heterogeneity in grain size. B: close view of a smaller grain in A, revealing clear patterns of dissolution, likely at the expenses of growth of larger crystals.

5.3.2 Constant Composition experiments

Constant composition experiments required several tests to calibrate the conditions and at least a few replicates of the same conditions were ran again, spaced in time, to assess reproducibility (Fig. 5.2). As indicated in Table 5.1, the chemical conditions were not changed, only the concentration of ΣPO_4. Control experiments were run without any ΣPO_4 and further experiments had ΣPO_4 concentrations of 25 and 50 μmol/kg (Fig. 5.3), respectively. All these experiments contained the commercial calcite powder introduced into the flow reactor at the onset of each experimental run, whereby one of the goals was to observe heterogeneous growth at the surface of the seeds. However, it was soon observed that spontaneous, homogeneous nucleation would always occur, the induction time following a clear dependence on ΣPO_4 concentration. The introduction of seeds to those control experiments without any ΣPO_4 immediately triggered nucleation from the bulk

solution, whereas the same did not occur in any of those experiments containing ΣPO_4 (Fig. 5.3).

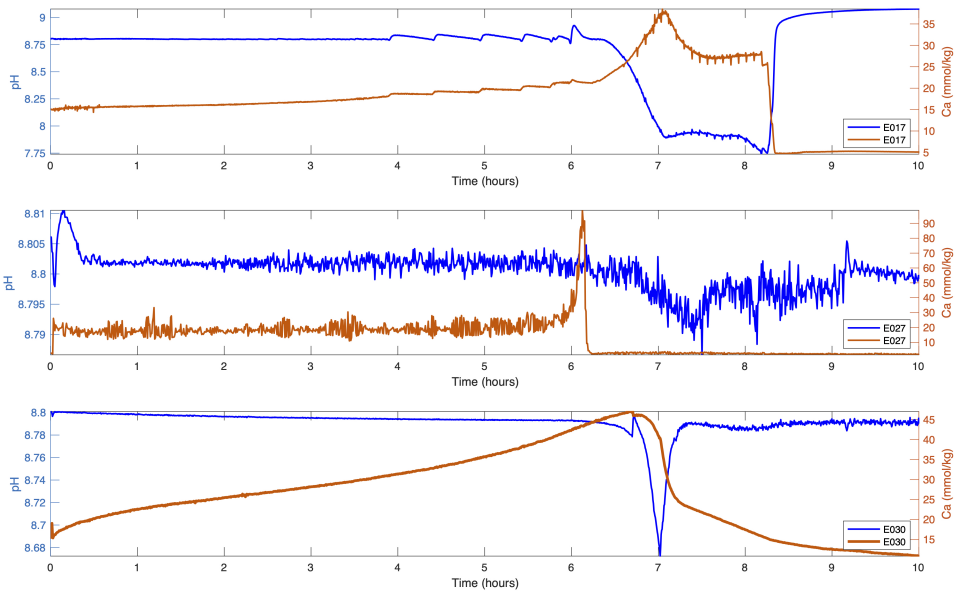


Figure 5.2: Variation of pH and $[Ca^{2+}]$ with time in three constant composition replicating the same solution conditions of heterogeneous (crystal seed) growth, eventually reaching a point of homogeneous (spontaneous) nucleation. Solution compositions (for full details, see also Table 5.1): Ω = 70–100, DIC = 10 mmol/kg, ΣPO_4 = 25 μmol/kg, $[Ca^{2+}]$ = 10 mmol/kg, pH = 8.8.

Also, control experiments without ΣPO_4 and left to run for several hours after spontaneous nucleation showed a variety of $CaCO_3$ polymorphs, including vaterite, aragonite and calcite, (*e.g.*, E016, Fig. 5.5). An equivalent "blank" experiment was terminated after 1.5 hour elapsed, or as soon as nucleation started, because the goal was precisely to observe the spontaneous precipitation of $CaCO_3$ at the onset of the experiment as observed previously, only aragonite and calcite were identified (*e.g.*, E033, Fig. 5.5).

Experiments containing 25 μmol/kg ΣPO_4 also had interesting results. For example, experiment E027 was stopped in 24 h, despite homogeneous nucleation occurring after the first 7.5 hours. Therefore, any amorphous precursors and/or metastable crystal phases nucleated at this stage had roughly 16.5 hours to recrystallise into more stable phases such as calcite. Conversely, experiment E017 ran for longer

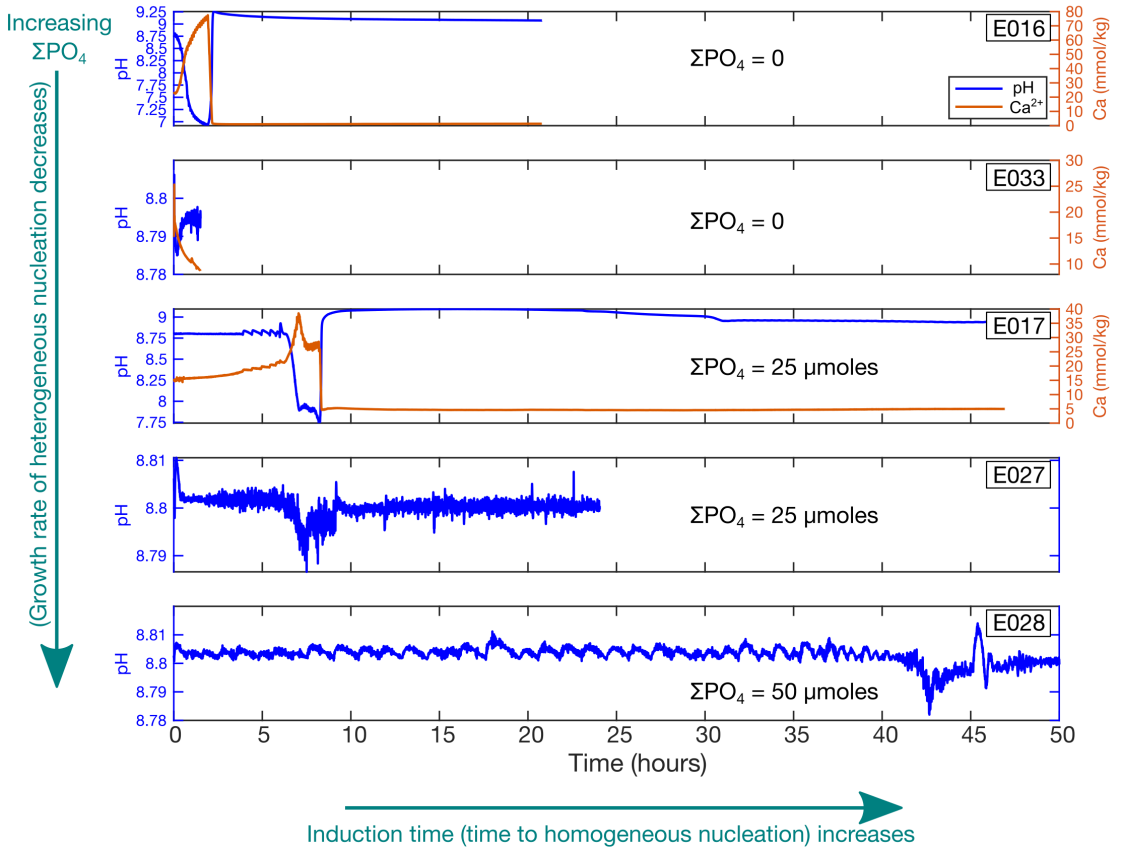


Figure 5.3: The three topmost experiments show the variation in pH (blue) and Ca concentration (light brown; as measured with the Ca ion selective electrode – Ca ISE). The two lowermost experiments show only pH as a function of time, because Ca concentration could not be measured following intermittent problems with the Ca ISE. Experiments E033 and E027 are replicate experiments of E016 and E017, respectively.

(∼40 h) after homogeneous nucleation was observed within about 7–7.5 hours as well. The X-ray data of samples from this experiment showed higher degree of crystallinity than the samples from experiment E027, suggesting that changes from metastable phases to more stable phases are achieved relatively quickly in solution, in a matter of several hours to a couple of days. Fig. 5.5 shows X-ray diffractogram patterns of these and other selected experiments for comparison. Fig. 5.4 shows a comparison of the material products from the experiments above, the EDS spectra and their chemical composition, detailed in Table 5.2.

Finally, experiments with higher ΣPO_4 concentration (= 50 μmol/kg) could maintain the same supersaturation level, under heterogeneous growth conditions, for greater

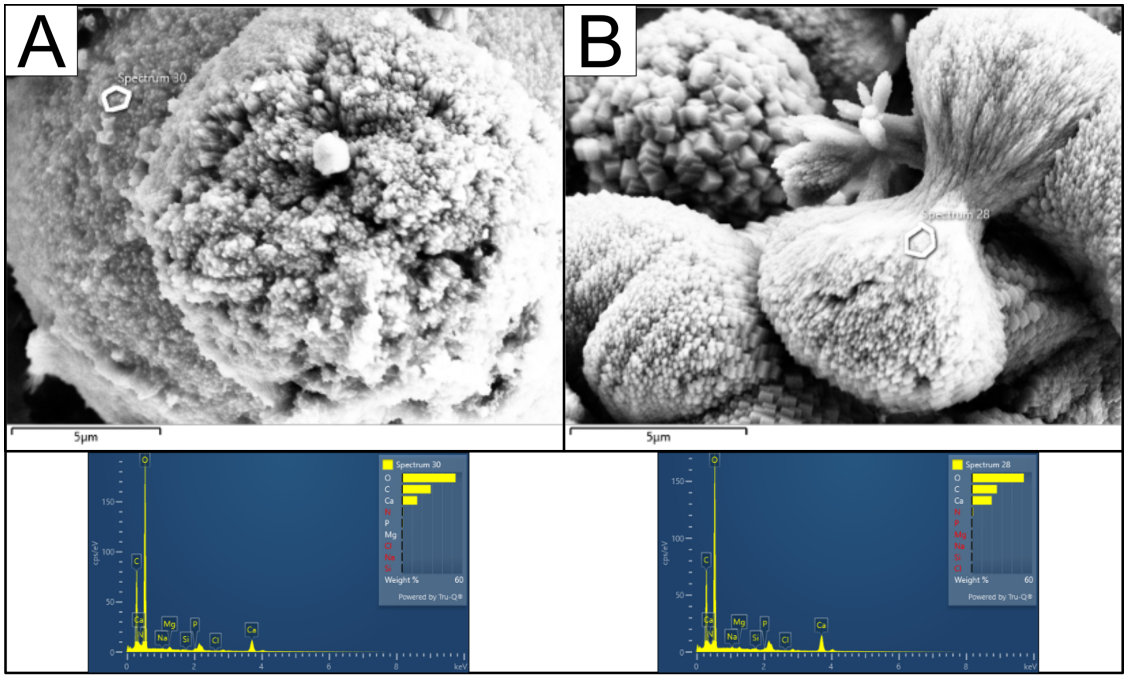


Figure 5.4: A: Likely monohydrocalcite (MHC) (?) or hydrated $CaCO_3$ phase from experiment E027. The experiment was terminated ~16.5 hours after induction time, and the homogeneously nucleated particles may not have had time to develop full crystallinity. B: Calcitic dumbbell formed after induction time in experiment E017, which lasted for 40 hours after this nucleation "event" (Fig. 5.3 in the main text).

Table 5.2: Chemical composition of solid sample from constant composition experiment E027 (Fig. 5.4), based on spectra collected by EDS, as described in the text. Stoichiometric calculations assuming an ideal $CaCO_3$ formula unit.

Spectrum 30	Wt%	Wt% Sigma	Gfw (g/mol)	Conc. (mmol/kg)	Stoichiometry (assuming 1:1Ca [$CaCO_3$])
C	28.69	0.26	12.01	23888	**6.3**
N	0.86	0.32	14.0067		
O	53.59	0.3	16	33494	**8.8**
Na	0.16	0.05	22.98977		
Mg	0.55	0.04	24.305	226	**0.06**
Si	0.04	0.04	28.0855		
P	0.73	0.07	30.97376	236	**0.06**
Cl	0.18	0.06	35.453		
Ca	15.2	0.22	40.078	3793	**1**
Total	100				1Ca:0.1Mg:6C:9O

intervals of time, of which experiment E028 is an example (Fig.5.5). The results from some replicate experiments were not recorded due to error in the real-time data transfer from the autotitrator and saving to the computer, but similar trends were observed. The visible growth at the surface of the commercial calcite seeds

during experimental run E028 is illustrated in Fig. 5.6, in which the original seeds are also shown for comparison. At this high value of supersaturation (Ω_{calcite} = 70–100) and following the induction time, as illustrated in Fig. 5.3, the formation of wheat sheaf/dumbbells/spherulitic aggregates by homogeneous nucleation would overwhelm growth by heterogeneous nucleation at the seeds' surfaces (Fig. 5.7).

5.4 Discussion

5.4.1 Evidence from Constant Composition Experiments of Kinetic Inhibition and Sustained Supersaturation of $CaCO_3$ by ΣPO_4

As shown in the Results section and illustrated in Fig. 5.3, the presence of incremental amounts of ΣPO_4 allows the maintenance of an oscillatory dynamical system kept at disequilibrium conditions under constant composition and high supersaturation for extended time (*e.g.*, experiment E028). The oscillation arises because of the combination of two factors: the natural behaviour of the system, whereby the pH tends to decrease as a result of $CaCO_3$ precipitation and growth, and the regular addition of the titrant solutions to compensate for the deviations from the constant composition. This results in a transient steady-state equilibrium, until nucleation occurs. Intriguingly, repeated experimental observations revealed that the pattern can only be maintained for so long, before a "collapse" occurs, leading eventually to spontaneous nucleation of calcium carbonate, despite the presence of inhibitors. Abrupt increase in the rate of titrant addition and visual inspection of the WS in the reactor - which suddenly becomes "milky" (Fig. 5.8) - are taken as indication that spontaneous nucleation occurred in all these cases.

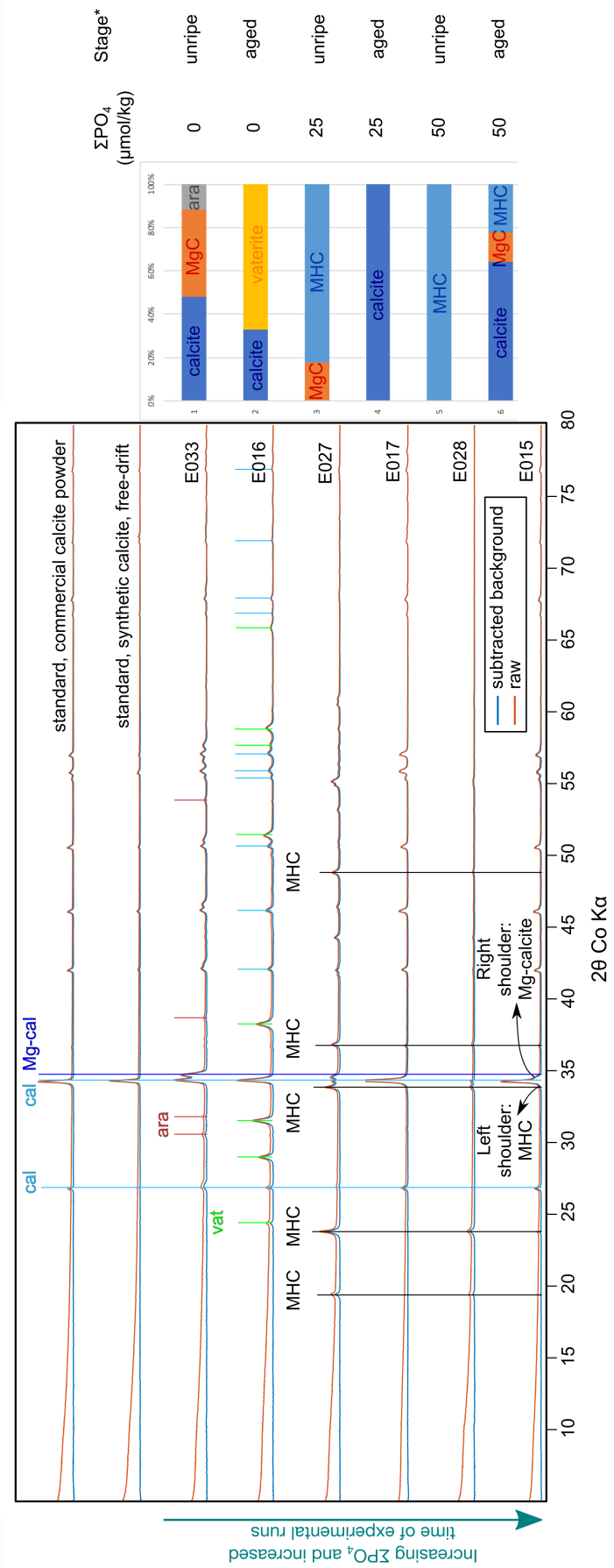


Figure 5.5: Typical X-ray diffractograms of samples from free-drift and constant composition experiments (E015–E033). A commercial $CaCO_3$ powder (Acros®) and the calcite seeds from one free-drift experiment are shown at the top, as calcite standards for comparison with the constant composition material products. **cal**: calcite; **Mg-cal**: magnesian calcite; **ara**: aragonite; vat: vaterite; **MHC**: monohydrocalcite. The bar diagram to the right indicates the relative proportion of $CaCO_3$ mineral phases from semi-quantitative XRD analysis. *Stage of solution after nucleation: aged indicates the experiment was run for several hours after nucleation, whereas unripe means the experiment was stopped soon after or a little after nucleation was observed. Colour bars refer to the characteristic diffraction peaks of the respective minerals: light blue, calcite; dark blue, Mg-calcite; green, vaterite; brown, aragonite; black, MHC.

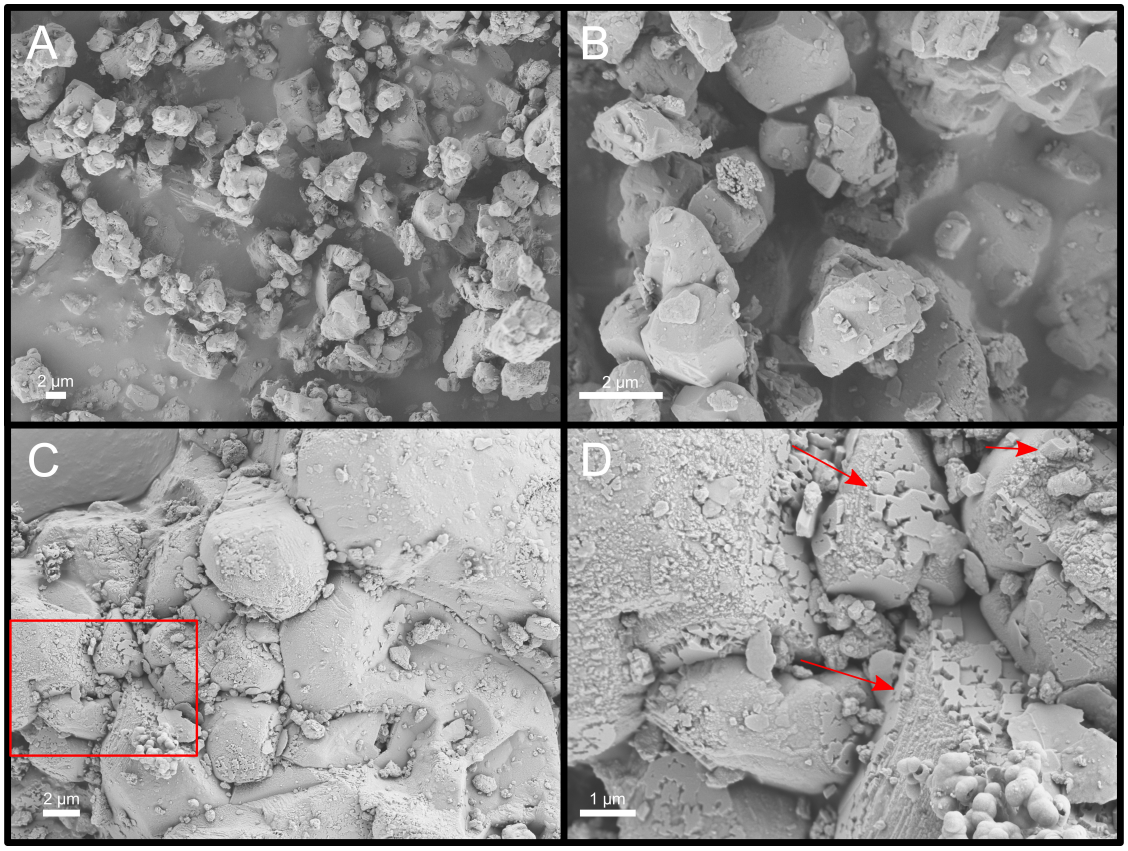


Figure 5.6: A: Calcite "seeds" from commercial $CaCO_3$ powder, added at the beginning of constant composition experiments in order to investigate heterogeneous precipitation. B: closer detail of seeds, showing generally smooth surface facets at this scale. C: nucleation on seed material, produced during experiment run E028, sustained with supersaturation ($\Omega_{calcite}$) = 70–100 and Mg/Ca = 5 for >40 hours, with ΣPO_4 = 50 μmol/kg. D: detail of area shown in C, highlighting the 2-D to 3-D growth at the surface of the seeds (red arrows). The remainder of the precipitates after the induction time at ~42 hours was essentially composed of MHC (see also diffractogram in Fig. 5.5).

The *in situ* Raman spectra obtained from experiment E028 ($\Omega_{calcite}$ = 70–100, Mg/Ca = 5, ΣPO_4 = 50 μmol/kg, pH = 8.8, [DIC] = 10 mmol/kg), shown in Fig. 5.9, gives additional support to the interpretation that nucleation invariably occurred, even when pH shifts/excursions are of lesser magnitude, such as in the case of this experiment. It visibly captures the initial introduction of the calcite seeds at the beginning of the experiment, at t = 0 seconds, shown as a peak in the absorption wavenumber of $CaCO_3$ (calcite), at ~1086 cm^{-1}. It also clearly shows a long and continuous hump stretching across the whole length of the experiment and comprising the absorption wavenumber interval between ~1068–1086 cm^{-1}.

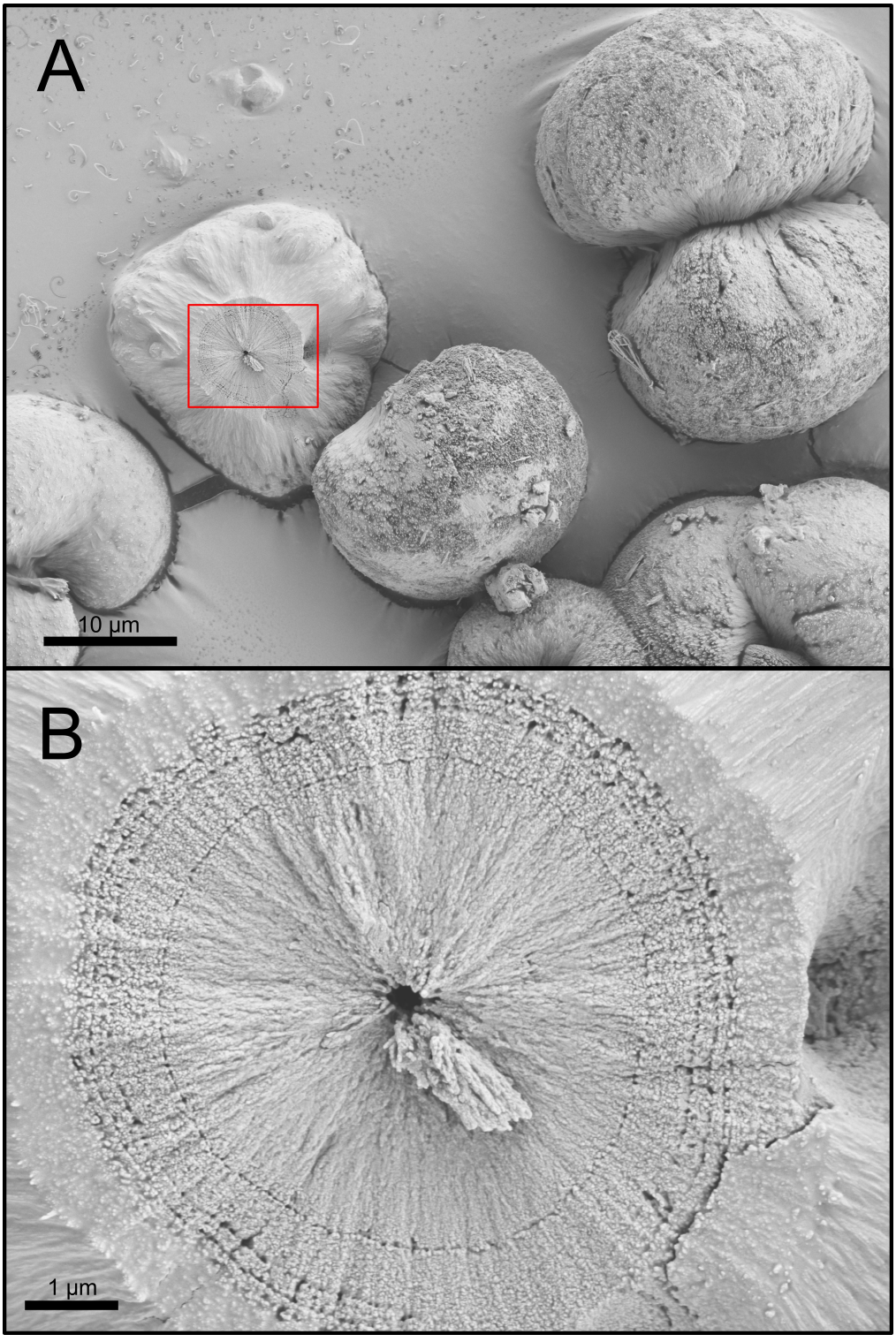
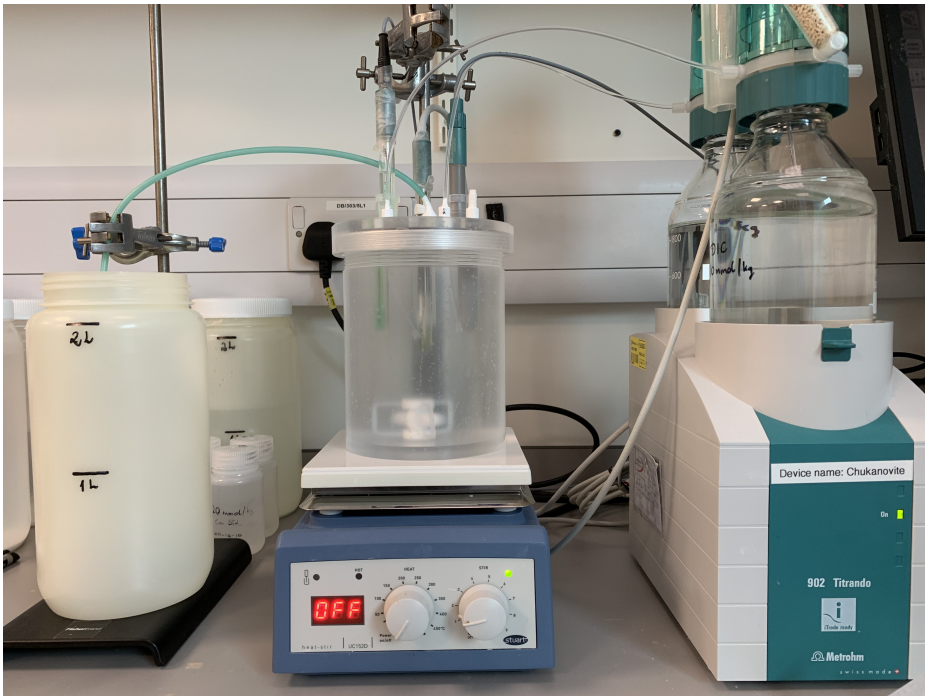
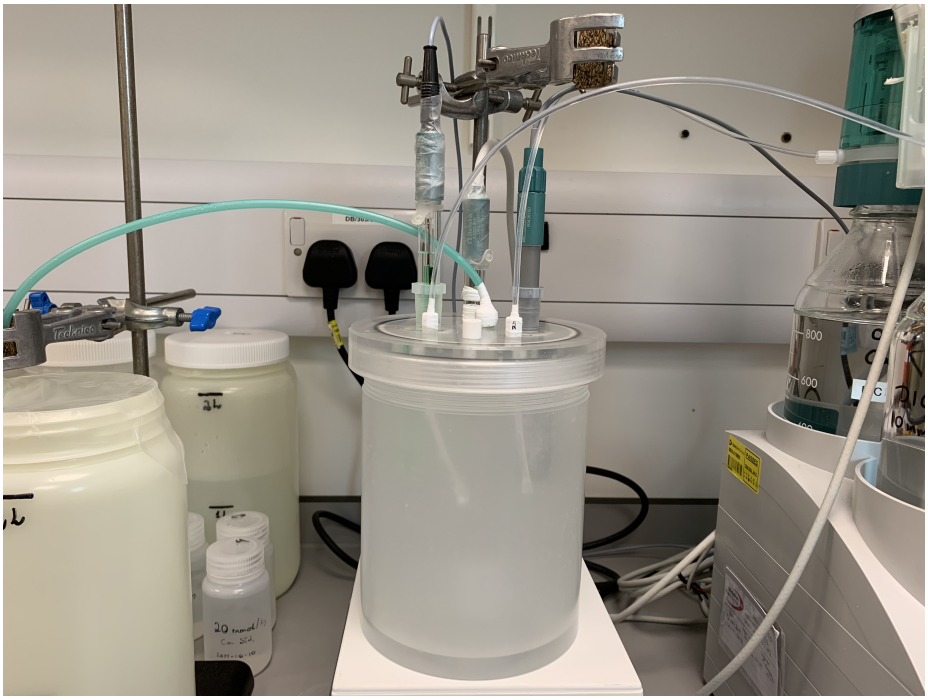


Figure 5.7: A: Overview of "dumbbells" / spherulitic aggregates nucleated from supersaturated solution ($\Omega_{calcite}$=70–100), under experimental conditions equivalent to experiment E028 (shown also in Fig. 5.3, Fig. 5.5 and Fig. 5.6). B: Cut showing detail of spherulite core, revealing its fibrous and polycrystalline structure.



(a) Initial experimental conditions of experiment E017. WS is evidently clear and transparent in the reactor vessel (centre).



(b) Experiment E017 WS after spontaneous nucleation (also evident from the clear drop in pH values and rise in titration rate), with turbid and "milky" appearance.

Figure 5.8: A typical constant composition experimental setup. Working solution (WS is in place in the reactor (centre of the figure). Autotitrator and titrant solutions are seen on the right, and the outlet for solution overflow is seen on the left.

At this high supersaturation this likely reflects the concurrent existence of several aqueous carbonate ion (–CO_3) complex species (*e.g.*, $CO_3^{2\breve{}}$ and $CaCO_3{}^0$) as well as multiple co-existing calcium carbonate phases (*e.g.*, ACMC, ACC, –CO_3 complexes, monohydrocalcite) (Montes-Hernandez and Renard 2016 [134]; Purgstaller et al. 2016 [43]; Borromeo et al. 2017 [135]; Purgstaller et al. 2017 [136]; Konrad et al. 2018 [137]; Purgstaller et al. 2019 [107]). Approaching the end of the experiment, spontaneous nucleation occurs, as indicated by the pH drop and the Raman shift producing a peak at ∼1068 cm^{-1} (MHC, *e.g.*, Purgstaller et al. 2017 [136]), as well as by the solid products observed under the SEM (Fig. 5.7) and their XRD patterns (Fig. 5.5), reflecting 100% MHC.

With regards to crystal growth resulting from nucleation on the calcite seed material, following Mucci (1986) [116], the number of moles (M_{CaCO_3}) of $CaCO_3$ precipitated on the surface of the crystal seeds and the rate of precipitation can be determined in accordance to these relations:

$$M_{CaCO_3} = \frac{(W_i \times ALK_i) + (W_t \times ALK_t) - ((2 \times W_t + W_i) \times ALK_f)}{2000} \tag{5.2}$$

and

$$R(mole \cdot hr^{-1}m^{-2}) = \frac{(W_t \times ALK_t) - (2 \times W_t \times ALK_f)}{2000 \times t \times W_{seed} \times A_{BET}} \tag{5.3}$$

Where W_i is the weight in kg of the initial solution, W_t is the weight of titrant solution added, W_{seed} is the weight in grams of the seed material, ALK_i and ALK_f are the alkalinity of the initial and final solution (considering the time preceding spontaneous nucleation in solution), respectively, given in mol/kg, and A_{BET} is the calcite seed surface area. The 2000 in the denominator is a factor to convert units of meq/kg to mol/kg and therefore if ALK is already given in mol/kg this factor can be removed from both equations.

The measured values and the relations assumed in these equations allow the estimation of the numbers shown in Table 5.3.

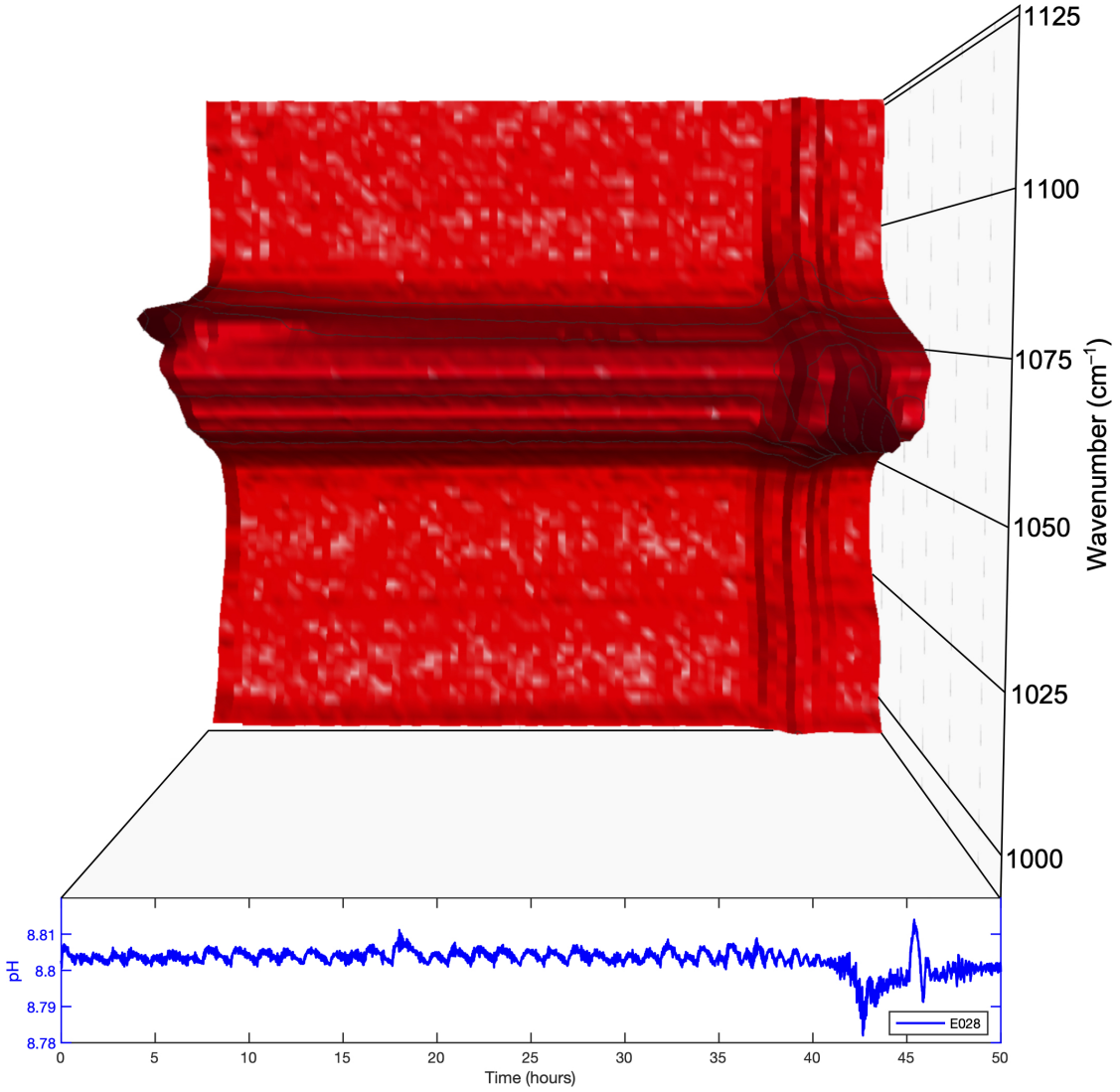


Figure 5.9: Raman spectra and pH variation with time of experiment E028.

Interestingly, the interfacial free energy between calcite and water is known to be relatively high, a fundamental fact that has been also attributed to contribute to its tendency to crystallise via amorphous precursors, whose interfacial energies are lower (Bruno et al. 2013 [138]). This aspect will be discussed in greater detail in the next sections.

Additionally, although it has long been known that many compounds inhibit $CaCO_3$ precipitation, it becomes unequivocally clear in these experiments that minimum concentrations of ΣPO_4 suffice to strongly inhibit calcite and aragonite precipitation, as demonstrated in other studies (Reddy 1977 [32]; De Kanel and Morse 1978 [113];

Table 5.3: The effect of orthophosphate as inhibiting seeded growth (heterogeneous nucleation) of calcite. Three replicate experiments, shown in Fig. 5.3, and a fourth experiment with double the amount of ΣPO_4, showing reproducibility of the overall conditions and the effects of higher ΣPO_4 on growth rate, when all other conditions are maintained the same.

Exp #	pCO_2	ΣPO_4 (μmole/kg)	log(Ω–1)	pH	ALK (mmole/kg)	t (hours)*	Wt (kg)	Rate (mole·hr^{-1}·m^{-2})	M_{CaCO_3} (mmoles)
E017	atmospheric	25	1.99	8.8	13.5	6.2	0.02	1.7×10^{-3}	15.2
E027	atmospheric	25	1.99	8.8	13.5	6.2	0.021	1.8×10^{-3}	16.0
E030	atmospheric	25	1.99	8.8	13.5	6.2	0.022	1.9×10^{-3}	16.7
E028	atmospheric	50	1.99	8.8	13.5	40	0.01	1.3×10^{-4}	7.6

* hours of experimental run until the point of spontaneous nucleation

Mucci 1986 [116]; Burton and Walter 1990 [117]; Dove and Hochella 1993 [118]; Gratz and Hillner 1993 [34]; Lin and Singer 2006 [35]; Roest-Ellis et al. 2020 [124]). As already mentioned, modern alkaline lakes are often supersaturated with respect to calcite and aragonite (Fukushi and Matsumyia 2018 [1]; chapter 4) and also tend to have high ΣPO_4 (Jellison et al. 1993 [30]; Nielsen and DePaolo 2013 [139]; Ingalls et al. 2020 [31]; Toner and Catling 2020 [94]). Furthermore, since sustained supersaturation requires the presence of compounds that interfere or inhibit precipitation, taken at face value these observations seem to strongly suggest that ΣPO_4 is a relevant contributor influencing $CaCO_3$ mineralisation pathways via intermediate precursors in natural environments. This increases the critical energy of nucleation of stable calcite (discussed in detailed below) and permits sufficiently supersaturated solutions that can reach the saturation of metastable phases.

The combined effects of supersaturation and ΣPO_4 on calcite growth rates can be illustrated with an experimentally observed relationship. By fitting experimental data of variable orthophosphate concentration and calcite supersaturation levels, Mucci (1986)[116] could establish an empirical equation for determination of calcite growth rate in solutions with 35 per mil salinity (artificial seawater) and within a pCO_2 range between 0.032–0.310%:

$$log_{Rate} = -15.76 - 1.45 \times log(PO_4^{3-}) + 3.17 \times log(\Omega - 1) \tag{5.4}$$

Under the conditions constrained in his experiments, a clear effect of orthophosphate concentration on the growth rate of calcite crystal seeds can be observed, whereby the higher the $PO_4^{3\breve{}}$ concentration the lower the overall growth, regardless of

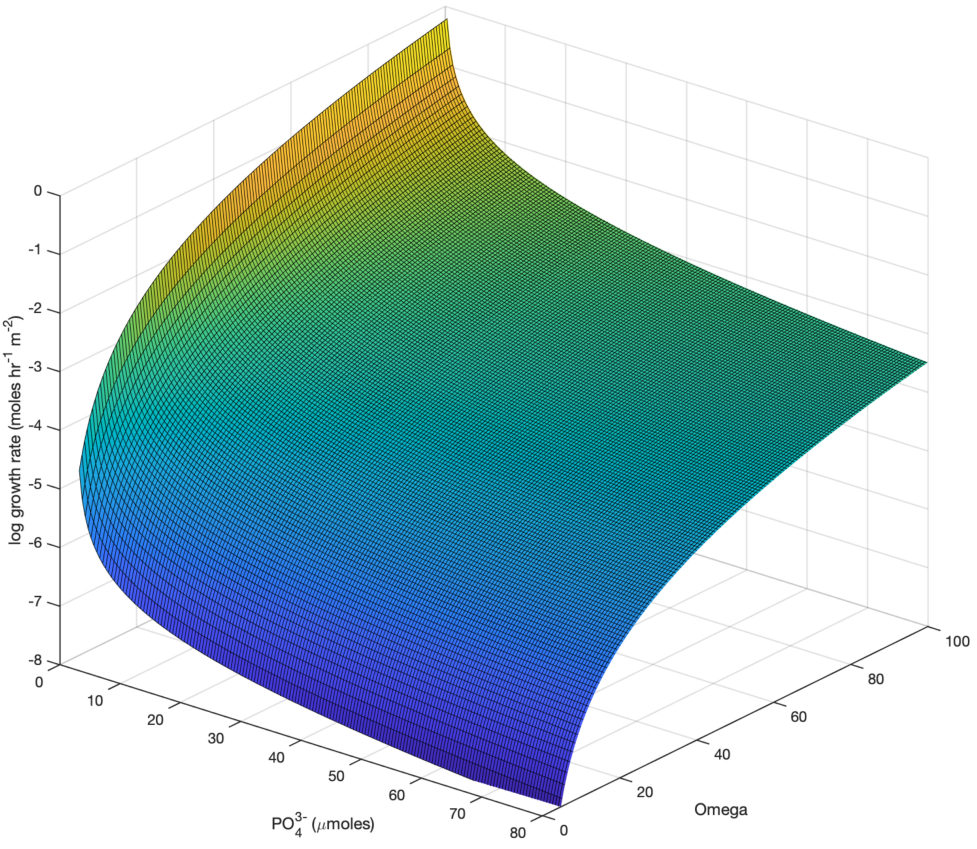


Figure 5.10: Logarithmic of calcite crystal growth rate (z-axis) with variable PO_4^{3-} concentration (x-axis) and calcite supersaturation level (y-axis). Increasing supersaturation accelerates the growth rate, since it increases the driving force for precipitation. However, increasing orthophosphate in solution causes the opposite effect, counterbalancing to some extent the effect of elevated supersaturations. Orthophosphate cannot increase indefinitely though, whereby the cost to be paid would be the precipitation of phosphate phases (amorphous or crystalline), drawing Ca^{2+} down from solution, thereby preventing further precipitation of $CaCO_3$ (*e.g.*, Toner and Catling, 2020 [94]).

increasing supersaturation (Fig. 5.10). Mucci (1986)[116] highlighted though that the empirically derived equation is of limited application to systems of greater complexity involving other inhibitors, such as organic matter, for example. This last point is important because it emphasises how natural systems, comprised of multiple interacting and dependent variables, behave in more complex ways as a result of small perturbations to the varying inputs and the interactions within the borders of the system itself. Even so, justifiable assumptions can allow us to constrain lower

and upper boundaries to a certain investigated phenomenon with some confidence, for example constraining the role of a single inhibitor and observing the stepwise evolution of conditions with additional inhibitors in solution (*e.g.*, Mucci 1986 [116]; see also discussion in Chapter 4).

Nevertheless, with respect to relatively simple and well-constrained systems the observations taken from the experimental results shown in Table 5.3 reveal that the estimated rates of precipitation lie very close in their respective orders of magnitude to the rates that one would predict using eqn. 5.4 proposed by Mucci (1986)[116]. In the latter case the rates would be 8.63×10^{-4} and 3.16×10^{-4} for the conditions given in Table 5.3, or about the same orders of magnitude than the rates estimated in the current experiments. This suggests that the small differences between the solution matrices used in this study and in Mucci's study (artificial seawater), predominantly related to differences in ionic strength, likely do not exert any significant difference. Thus, eqn. 5.4 should still yield valid approximations under the present experimental conditions of Ω_{calcite}, ΣPO_4 and ionic strength as well.

5.4.2 Thermodynamics of Nucleation from Aqueous Solutions at Low Temperatures

At this point it is useful to provide a brief review of the theoretical principles regarding the free energy changes of crystal nucleation and growth, which find support in the overall experimental results. These concepts are of utmost relevance because they outline a logical framework for understanding the factors involved and for predicting the outcomes of these processes, which can in turn be investigated experimentally. Therefore, they will be introduced with a discussion focusing on the observations derived from the constant composition experiments, which provide a very illustrative picture and a nice fit to the theory describing mineral nucleation and growth. The goal is to show that experimental observations and theory match and together support the hypothesis that $CaCO_3$ minerals tend to nucleate and/or grow via metastable intermediate phases from supersaturated solutions, which is of great

relevance to our understanding of natural aqueous systems and the interpretation of the sedimentary rock record.

5.4.2.1 Seeded experiments, heterogeneous and homogeneous nucleation

Interestingly, the introduction of the $CaCO_3$ crystal seeds in a supersaturated solution without ΣPO_4 (despite the presence of Mg^{2+} in the initial Mg/Ca ratio 5:1), as in the control experiments, caused an instantaneous disturbance leading to overall homogeneous precipitation, as well as growth at the surfaces of the seeds (heterogeneous precipitation) (Fig. 5.3). This clearly demonstrates that the presence of ΣPO_4 in concentration of a few tens of micromole units (*e.g.*, 25–50 μmol/kg as in constant composition experiments) has a greater inhibitory effect to $CaCO_3$ polymorph phases such as calcite, aragonite and vaterite than Mg^{2+} alone under these conditions, which was present in concentrations three orders of magnitude higher.

The disturbance caused at the onset of such experiments by the introduction of the seeds, mentioned in the preceding lines, followed immediately by instantaneous precipitation, may be linked to the lower interfacial free energy between the solid crystal substrate and the solvated cluster phases in solution (Van Cappellen 1991 [20]; De Yoreo and Vekilov, 2003 [21]). Without a stronger inhibitor in solution, such as ΣPO_4, that would adsorb onto these clusters, the kinetic barrier to new crystal nucleation is proportionally lower, favouring nucleation and precipitation under a certain threshold and at higher supersaturations (Van Cappellen 1991 [20]). The process of nucleation on foreign surfaces has been extensively documented in the literature, and was reviewed extensively by De Yoreo and Vekilov (2003)[21]. Here the process is briefly discussed, as it relates to the outcomes observed in the constant composition experiments.

In the case of heterogeneous precipitation, anisotropy arising from pre-existing crystallographic orientation of the substrate mineral is expected to variably affect the overall interfacial free energy (sometimes called interfacial tension or surface free energy) between the crystal and the solution, and hence the morphology of

the growing crystal(s) (*e.g.*, Van Cappellen 1991 [20]; Bruno et al. 2013 [138]; Fultz 2020 [140]). A perfectly smooth surface corresponds in reality to an idealised theoretical construct, whereupon heterogeneous nucleation would behave exactly as a two-dimensional analogue of homogeneous nucleation (Van Cappellen 1991 [20]). This follows because under this assumption the movement of adsorbed ions is fully stochastic and the likelihood of forming clusters is the same everywhere on the surface. However, just as mentioned above, real crystals and their surfaces contain irregularities of various kinds, such as structural defects (*e.g.*, surface steps/ledges/kinks; Fig. 1.2) or chemical impurities, all of which will variably influence the nucleation process on their surfaces (Van Cappellen 1991 [20]; Morse et al. 2007 [26]). This "contingency" effect has therefore implications for the development of crystal morphology, because, to some extent, the initial state of the pre-existing substrate, along with other factors such as solution composition and degree of saturation, will influence the ensuing nucleation pathways (*e.g.*, Dove and Hochella 1993 [118]).

Nevertheless, if the degree of supersaturation is high enough, in a heterogenous system the surfaces of the substrate have a greater likelihood of becoming fully saturated and covered with ions and clusters. Eventually, at higher supersaturation states, the number of homogeneous nucleation sites in the bulk solution will supersede the increasingly limited sites available at the pre-existing surfaces, whereupon the overall process of homogeneous nucleation will dominate, even in the presence of foreign surfaces (Nielsen and Christoffersen 1982 [141]; Nielsen and Toft 1984 [142]; Steefel and Van Cappellen 1990 [143]; Van Cappellen 1991 [20]) (Fig. 5.11). Minerals with a relatively moderate to high interfacial free energy (σ), such as calcite, having a $\sigma \approx$ 210-412 mJ/m^2 (Bruno et al. 2013 [138]; Sun et al. 2015 [144]), the surface reaction-controlled process of heterogeneous nucleation completely outcompetes homogeneous nucleation at lower supersaturations, requiring instead elevated supersaturations to shift this trend (Van Cappellen 1991 [20]). Furthermore, as pointed out above, at very high supersaturations and without the presence of inhibitors such as ΣPO_4, the interfacial free energy potential is basically the same as

the pure mineral phase and water (that is, comparatively lower with respect to the same mineral phase containing inhibiting species at its surfaces) and homogeneous nucleation will soon dominate over growth on existing surfaces. This explains the behaviour observed in the constant composition experiments that ran without ΣPO_4, whereby the introduction of the crystal seeds at the beginning of the runs immediately induced spontaneous nucleation (Fig. 5.3). It also explains the observation that homogeneous nucleation occurs even under prescribed "seeded growth" conditions, once the rate of transport to the surfaces of the growing seed material becomes lower than the rate of transport to and growth of the new nucleating clusters elsewhere in the solution.

5.4.2.2 Nucleation and growth

Slightly different formulations to derive the size or radius of the critical nucleus and the critical free energy of nucleation exist in the literature. Nonetheless, they all are based on the same principles, varying precisely on whether the radius or the number of clusters are considered (*e.g.*, Nielsen 1984 [127]; Steefel and Van Cappellen 1990 [143]; Van Cappellen 1991 [20]; Lasaga 1998 [145]; De Yoreo and Vekilov 2003 [21]; Fultz 2020 [140]). Here, we follow Nielsen's (1984) [127] and Van Cappellen's (1991) [20] formulation, based on the number of clusters nucleating from a solution. For homogeneous nucleation:

$$\Delta G_{bulk} = k_b T ln(S) \tag{5.5}$$

$$\Delta G_{surf} = \sigma A \tag{5.6}$$

$$\Delta G = (-n\Delta G_{bulk} + \Delta G_{surf}) \cdot N_A \tag{5.7}$$

$$A = \alpha a^2 n^{2/3} \tag{5.8}$$

$$a = (v_m/\eta N_A)^{1/3} \tag{5.9}$$

$$S = (\Omega)^{1/\eta} \tag{5.10}$$

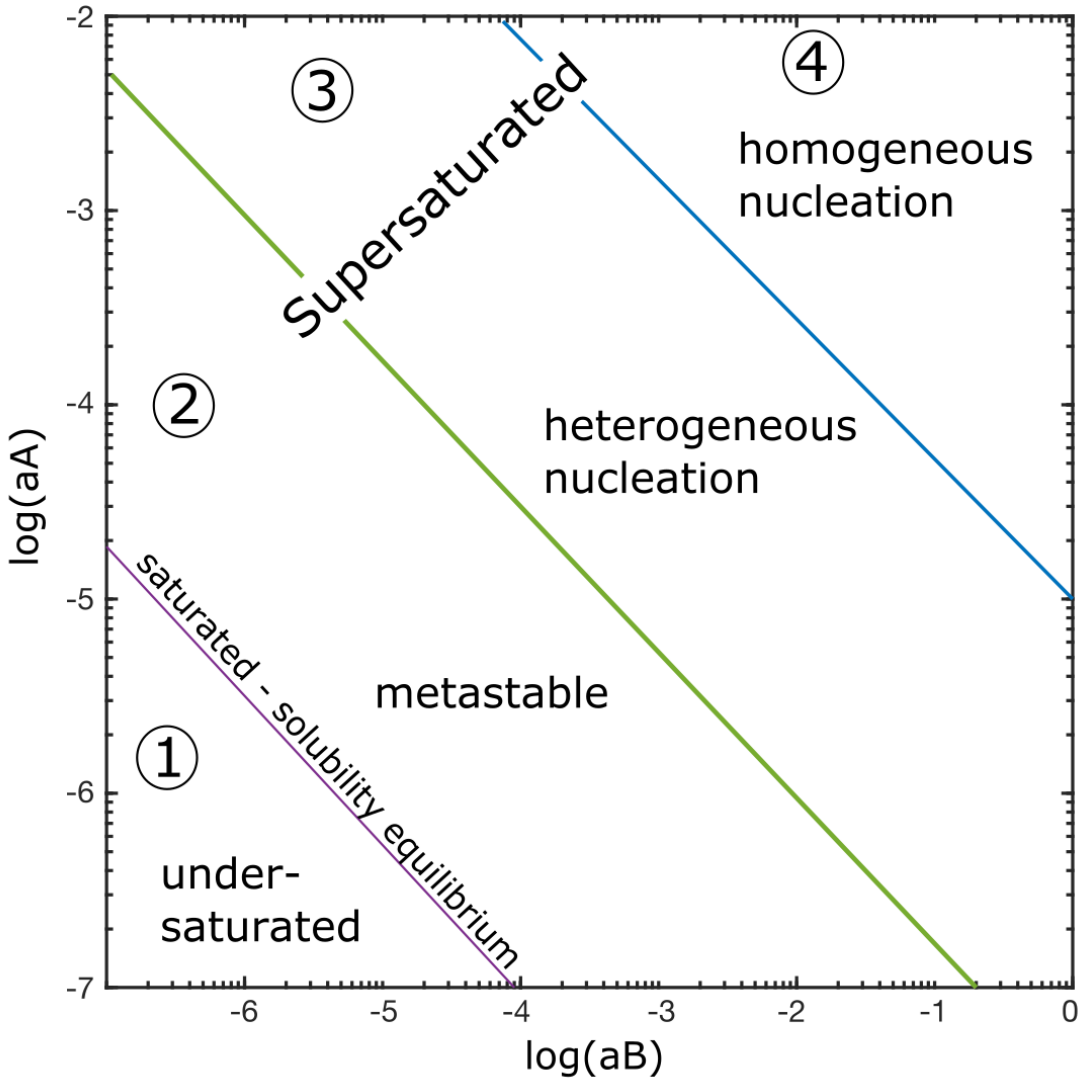


Figure 5.11: Arbitrary x–y values simply to highlight the logarithmic scales and for guidance in their visualisation. After Nielsen and Toft (1984) [142].

Where k_b is the Boltzmann's constant (1.380649×10^{-23} J·K$^{\breve{}1}$), T is the absolute temperature, σ corresponds to the interfacial free energy, A is the area of the interface between the two phases, α is a factor that depends on the shape of the nucleating crystal (for spherical geometry, $\alpha = 4.84$), n corresponds to the number of ions in the crystal, and S is the normalised saturation ratio. The variable "a" is the mean ionic diameter of the nucleating mineral (Nielsen 1984 [127]), and depends on v_m, the molar volume of the mineral (for calcite, $v_m = V \times N_A = 36.9340 \times 10^{\breve{}6} m^3 \cdot mol^{\breve{}1}$, *i.e.*, the volume per molecule, $V = 61.331 \times 10^{\breve{}30}$ m^3 times N_A, the Avogadro's constant) and η, the number of ions per formula unit of the mineral. The critical

number of clusters (n*) required to cross the critical free energy of formation (ΔG*) corresponds to the maximum of the function ΔG (eqn. 5.7), and therefore can be found by equating its derivative to zero. Finally, it also depends on the number β, which is a factor related to the shape of the clusters (Van Cappellen 1991 [20]):

$$\beta = (2\alpha/3)^3 \tag{5.11}$$

$$n^* = \beta(a^2\sigma/k_bT)^3(1/(lnS)^3) \tag{5.12}$$

$$\Delta G^* = \beta/2(a^2\sigma/k_bT)^3(k_bT/(lnS)^2)\cdot N_A \tag{5.13}$$

$$r = 2V\sigma/\Delta\mu \tag{5.14}$$

Where r corresponds to the critical radius of nucleation, given in meters (De Yoreo and Vekilov 2003 [21]). On the other hand, for heterogeneous nucleation the following expressions hold, considering the surface island model (Van Cappellen 1991 [20]):

$$A_{ex} = 2\pi rh = 2(\pi a^3)^{1/2}h^{1/2}n^{1/2} \tag{5.15}$$

$$n^* = \beta'(a^2\sigma/k_bT)^2(1/(lnS)^2) \tag{5.16}$$

$$\beta' = \pi(h/a) \tag{5.17}$$

$$\Delta G^* = \beta'/(a^2\sigma/k_bT)^2(k_bT/(lnS))\cdot N_A \tag{5.18}$$

$$r = (3Vn^*/2\pi)^{1/3} \tag{5.19}$$

Where r is again the critical radius (of heterogeneous nucleation) and h is the height of the surface island disk which, according to considerations regarding crystal structure, it follows that it must have dimensions that agree with the lattice dimensions of the nucleating mineral (Van Cappellen 1991 [20]). Therefore, for most

common minerals reasonable values of h are likely in the range of a few ångstroms to a few tens of ångstroms (Van Cappellen 1991 [20]), and is taken here as h = 5 Å. The interfacial free energy σ of the surface cluster in eqns. 5.16 and 5.18 is more correctly denoted as σ_{cw}, where the subscript cw stands for cluster-water contact, but in the present study it is considered a valid approximation to the σ value initially applied for homogeneous nucleation such as in eqn. 5.6. There are a few assumptions implied behind this consideration, but for extended discussions the reader is referred for example to the texts of Van Cappellen (1991) [20], De Yoreo and Vekilov (2003) [21] and Fultz (2020) [140].

The surface island model for heterogeneous nucleation introduced above was chosen for comparison in Fig. 5.12 instead of another alternative, the half-sphere model, because of the 2-D and 3-D growth pattern observed at the surface of the calcite seeds, which seemed to match its theoretical description. Briefly, whenever the bonding between the precipitating particles and the surface of the substrate is strong, the clusters will tend to spread out on this surface and form thin surface islands (Van Cappellen 1991 [20]). A special case that describes this condition is precisely the formation of a new nucleating mineral on the existing surface of another mineral of the same kind (Van Cappellen 1991 [20]).

However, it is relevant to illustrate the half-sphere model for heterogeneous nucleation/growth, where it will be assumed that the new cluster-substrate interface has a more favourable energetics (*i.e.*, lower barrier or energy cost) than the cluster-solution interface. In this case, considering the half-sphere model (Steefel and Van Cappellen 1990 [143]; Van Cappellen 1991 [20]):

$$n^* = (2\pi/3)(a^2\sigma/k_bT)^3(1/(lnS)^3) \tag{5.20}$$

$$\Delta G^* = (\pi/3)(a^2\sigma/k_bT)^3(k_bT/(lnS)^2) \cdot N_A \tag{5.21}$$

Table 5.4 shows a comparison between the energetics, the critical cluster size and critical radii of homogeneous and heterogeneous nucleation, which are also

compared in Fig. 5.12 for the values chosen in the table. The ΔG_{surf} always comprises a positive quantity, that is, it corresponds to a mandatory energy penalty for nucleation to proceed, because energy is required in order to create an interface (De Yoreo and Vekilov 2003 [21]; Fultz 2020 [140]). Therefore, if ΔG_{bulk} is positive, nucleation cannot occur because σ is always a positive number. Using force field calculations Bruno et al. (2013) [138] estimated the interfacial free energy of the calcite {1014} face/water contact to be 412 ± 20 mJ/m^2, indeed a high value which alone and without requiring inhibitors sets a high threshold for the spontaneous precipitation of calcite (Fig. 5.12A; Table 5.4). In a different study, Sun et al. (2015)[144] have estimated that the hydrated surface energy of calcite with 7% $MgCO_3$, that is, forming from solutions of present-day seawater composition with Mg/Ca = 5.2, is 350 mJ/m^2, still significantly elevated compared to its polymorph aragonite, whose corresponding σ = 280 mJ/m^2, or to ACC with σ = 14-25 mJ/m^2 (Sun et al. 2015 [144]; Henzler et al. 2018 [50]).

This discussion and the estimated σ values pointed out above shed light on the empirical observations and theoretical formulations showing that metastable and more soluble phases such as ACC are very unlikely to form as a precursor phase at low supersaturations, because, just like the interfacial free energy (σ), the ΔG_{bulk} will also be a positive quantity, thereby rendering the total free energy (ΔG) a monotonically increasing quantity. Conversely, at higher supersaturation values the formation of the metastable phase becomes more favourable, because the interfacial free energy is comparatively lower than that for the corresponding stable phase, resulting in the formation of end-member stable calcite via a series of phase transitions described as Ostwald step rule (Lasaga 1998 [145]). This can be clearly visualised following the derivation of the total free energy function, where it is shown that the critical energy of nucleation scales with the cube of the interfacial free energy, but is only decreased with the square power of the bulk free energy of the solution (*i.e.*, $\Delta G^* \approx \sigma^3 / lnS^2$).

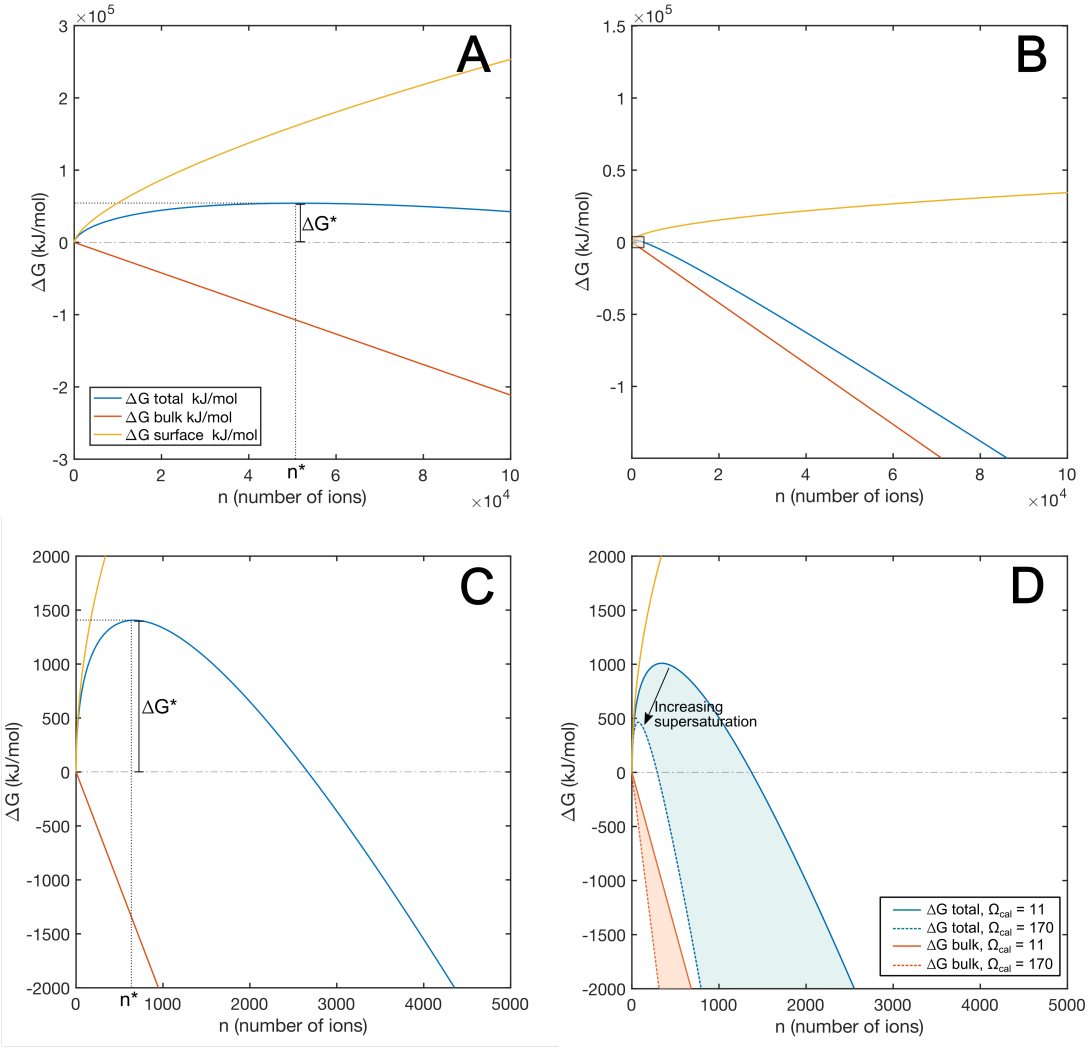


Figure 5.12: Comparison of values of critical free energies for nucleation of calcite under different saturation states (A=B=C≠D); for conditions similar to seawater (A–C), for reference, and for a wider saturation state range of relevance to alkaline waters of general interest (D), and under homogeneous (A) and heterogeneous (B–D) growth. A. Free energy of formation of spherical clusters under homogeneous nucleation, considering a saturation state of calcite ($\Omega_{calcite}$) = 5.5, that is, close to seawater values. B: Free energy of formation based on the model of surface island disc clusters under heterogeneous nucleation, also considering $\Omega_{calcite}$=5.5. Observe the dramatic reduction in the critical energy and in the number of clusters necessary for precipitation. Note the y-axis scale was reduced by half compared to A, in order to make the curves reasonably visible but still comparable to the previous picture. C: Detail of the small and barely visible square shown adjacent to the y-axis in B, highlighting in a more suitable scale the critical energy and the critical number of clusters for heterogeneous nucleation. Same saturation conditions as in A and B ($\Omega_{calcite}$=5.5). D: Plot of calculated total free energies, ΔG_{bulk} and $\Delta G_{surface}$ for a wider range of supersaturations, of general relevance to alkaline waters, from $\Omega_{calcite}$=11 to $\Omega_{calcite}$=170. The change in $\Delta G_{surface}$ is not visible in this scale.

Table 5.4: Illustration of some values of ΔG^* and n* with respect to variable saturation state of calcite ($\Omega_{calcite}$), calculated in the plots shown in Fig. 5.12, according to explanations in the text, at T = 25°C. For the surface islands model, the height (h) of a disk of 5 ångstroms was assumed.

$[Ca^{2+}]$ (mmol / kg)	[DIC] (mmol / kg)	pH	$\Omega_{calcite}$	Homogeneous ΔG^* (kJ/mol)	nucleation n*	r (m)[1]	Heterogeneous (surface islands ΔG^* (kJ/mol)	nucleation model) n*	r (m)[1]	Heterogeneous (half-sphere ΔG^* (kJ/mol)	nucleation model) n*	r (m)[1]
10	2	8.2	5.5	54207	51391	1.44E–8	1406	666	2.69E–9	3380	3204	4.54E–9
0.1	100	9	10.7	27955	19032	1.04E–8	1009	344	2.16E–9	1743	1187	3.26E–9
10	10	8.8	81.2	8124	2982	5.58E–9	544	100	1.43E–9	506	186	1.76E–9
1	100	9.5	170.2	5951	1869	4.78E–9	465	73	1.29E–9	371	117	1.51E–9

[1]For both homogeneous and heterogeneous nucleation the critical radius of nucleation (r, in metres) can also be given by the expression $r = 2V\sigma/\Delta\mu$ (*e.g.*, Fultz 2020 [140]); however, the interfacial free energies will be different, thereby changing the respective critical radii of nucleation.

As a general approximation, given that supersaturations are high enough (order of SI $\geq$ 1.5-2, which scales with lnS $\geq$ 1.73-2.3), ACC will form first, and then recrystallisation via dissolution-reprecipitation may follow via MHC, vaterite, aragonite and finally to calcite (*e.g.*, Sun et al. 2015 [144]; Myszka et al. 2019 [146]). However, the pathways to crystallisation can be different and more complex than this simplified picture might imply. For example, as Blue et al. (2017) [44] have pointed out, variable Mg^{2+} concentrations will affect the solubility of aragonite, whereby higher concentrations make it less soluble than calcite. Furthermore, dissolved phosphate may in turn also increase the interfacial free energy and act to stabilise clusters and inhibit the precipitation of vaterite and aragonite (*e.g.*, Mucci 1986 [116]; Myszka et al. 2019 [146]), leading to the transformation of the precursor phases into final calcite, without an aragonitic intermediate, for example.

As an example, these same principles above can be used to make predictions delineating the energetic requirements and phase transformations among the various $CaCO_3$ polymorphs. Unfortunately, as yet there are great uncertainties or no estimations at all for reasonable values of vaterite and MHC surface energies (Sun et al. 2015 [144]), so arbitrary values between aragonite (Sun et al. 2015 [144]) and ACC (Henzler et al. 2018 [50]) surface energies are considered here for illustrative purposes (Table 5.5), assuming the proposition of Sun et al. (2015) [144] that the surface energies of $CaCO_3$ phases must be ordered according to the sequence ACC $<$ vaterite $<$ aragonite–calcite. However, at supersaturation levels commonly found in alkaline lakes (Chapter 4), with $SI_{calcite}$ values $\approx$ 1-2 or $\Omega_{calcite} \approx$ 10-100, and assuming pure ACC with solubility constant of $10^{-6.277}$ (Purgstaller et al. 2019 [107]) and σ between 14-25 mJ/m^2 estimated from relatively simple experimental electrolyte solution mixtures of $NaCO_3$ and $CaCl_2$ (Henzler et al. 2018 [50]), ACC is rendered an unlikely intermediate precursor phase, as pointed out above. On the other hand, in complex electrolyte solutions containing inhibitors such as phosphate these relations may be changed. Thus, even though MHC σ value is not clearly established, from the data discussed in Chapter 4 and the preceding considerations MHC is deemed the most likely precursor phase of calcite in alkaline lakes.

Under the conditions shown in Table 5.5 and illustrated in Fig. 5.13, calculations indicate that calcite may form via ACC only at $\Omega_{calcite}$ values > 180, or $SI_{calcite}$ > 2.25, otherwise ACC is energetically unfavourable. The point worth highlighting is that given sufficiently high supersaturation levels, ACC becomes unambiguously the most energetically favourable $CaCO_3$ phase to form, otherwise MHC is more likely the predominant precursor.

Table 5.5: Comparison of results of calculations of critical cluster/nucleus size and critical free energy of nucleation of different $CaCO_3$ phases, for given values of $\Omega_{calcite}$, assuming a = 3.13×10^{-10} m, $\alpha = 4.84$, and solubility constants at T = 25^oC.

		calcite	**aragonite**	**vaterite**	**MHC**	**ACC**		
σ **(mJ/m²)**		350	280	200	100	20		
Ksp		$10^{-8.48(a)}$	$10^{-8.34(a)}$	$10^{-7.91(b)}$	$10^{-7.65(b)}$	$10^{-6.277(c)}$		
$\Omega_{calcite}$	226	3279	1898	1066	183	150	ΔG^*	**kJ/mol**
		977	601	419	84	701	n^*	
$\Omega_{calcite}$	215	3339	1935	1091	188	204	ΔG^*	**kJ/mol**
		1003	619	434	88	1105	n^*	
$\Omega_{calcite}$	188	3511	2042	1167	203	672	ΔG^*	**kJ/mol**
		1082	670	480	99	6631	n^*	
$\Omega_{calcite}$	161	3728	2176	1264	223	205084	ΔG^*	**kJ/mol**
		1184	738	541	114	35358753	n^*	

[a] Plummer and Busenberg (1982) [59]. [b] Fukushi and Matsumiya (2018) [1].
[c] Purgstaller et al. (2019) [107].

Interestingly, in a different study on heterogeneous nucleation Zhu et al. 2021 [147] have estimated that an incorporation of only 0.9% of sulphate during nucleation of $CaCO_3$ on quartz particles increased the interfacial free energy of additional $CaCO_3$ nanoparticles by 11-15%, a substantial increment causing as a result an increase in the critical energy barrier as well (eqns. 5.6, 5.7 and 5.13). The same authors emphasise the underestimated impact of anion incorporation on $CaCO_3$ precipitation, which go in line with the observations highlighting here the correlation between high dissolved ΣPO_4 concentration and high $CaCO_3$ supersaturation in alkaline lakes, where sulphate is generally not excessively high but phosphate on the other hand may be the most relevant anion increasing the surface energy. Some exceptions to this may certainly exist, such as the Last Chance lake in Canada, which is a Na-CO_3-SO_4-Cl lake, thus containing relatively high sulphate concentrations. However, sulphate exists in about the same order of magnitude as phosphate in

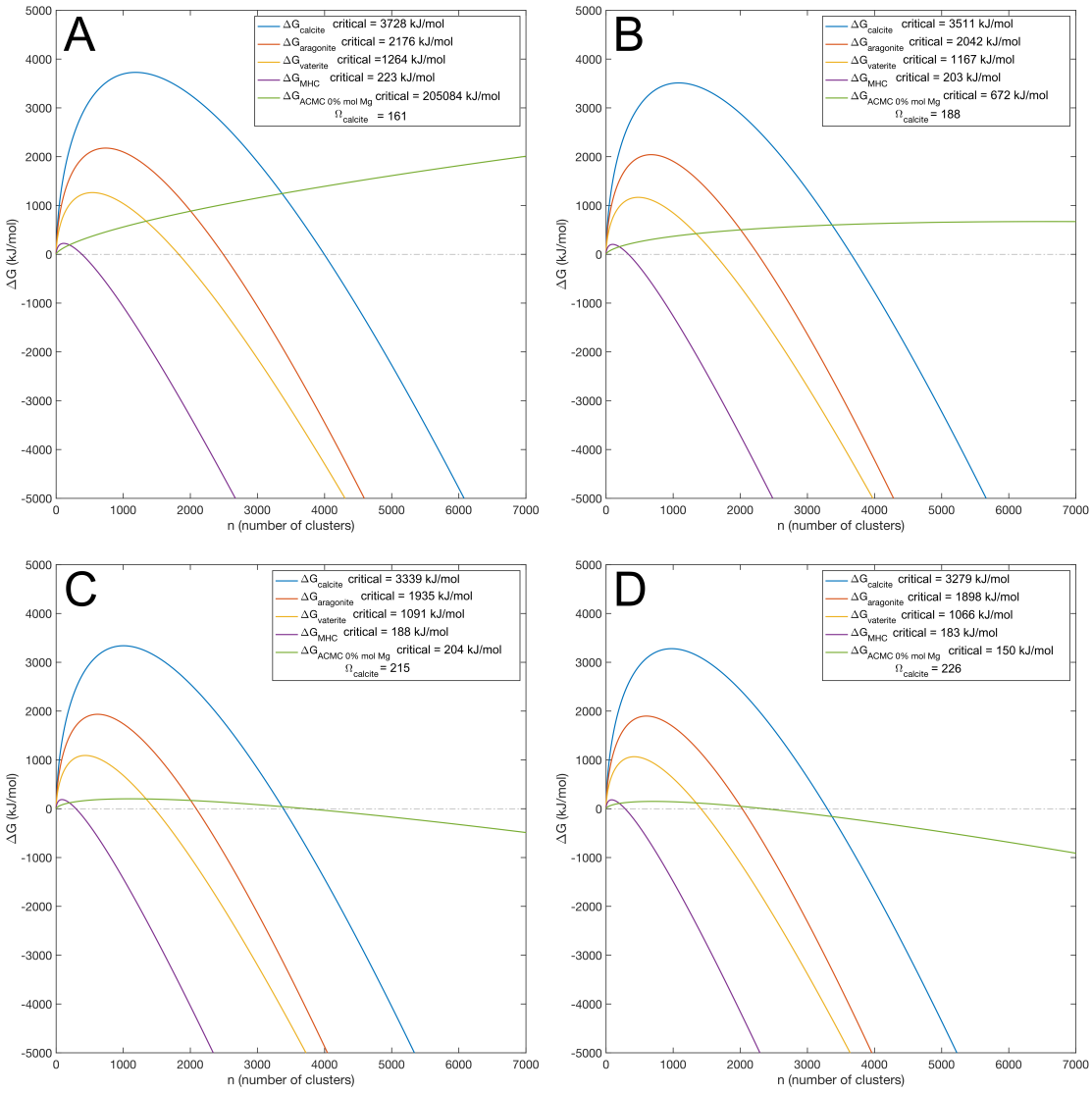


Figure 5.13: Calculations of critical free energy of nucleation (ΔG^*) and critical cluster size (n^*) of different $CaCO_3$ polymorphs, with reference to different $\Omega_{calcite}$, in accordance with data shown in Table 5.5. Observe that, for the conditions assumed, calcite has always the highest ΔG^* an MHC the lowest, until $\Omega_{calcite} > 215$, when ACC becomes the energetically most favourable $CaCO_3$ phase.

the case of this lake, whereas phosphate data are not available for other lakes that have reported higher sulphate concentrations, as in some lakes in Bolivia, Chad, Inner Mongolia in China, Western Mongolia, and in the United States. Therefore, a complete comparative evaluation of their relative effective roles as inhibitors in natural lake waters at their respective naturally occurring average proportions cannot be done at this point. Nevertheless, experimental results have already

pointed out that phosphate is a more effective inhibitor of calcite crystal growth than sulphate, requiring comparatively lower concentrations (about two orders of magnitude less phosphate) to yield the same reduction in the rates of calcite growth (Meyer 1984 [115]). Finally, the sum of these observations suggest, in turn, that it is highly likely that calcite precipitation in alkaline environments predominantly forms via metastable intermediates, where MHC is probably the main intermediate, crystallising after dissolution and reprecipitation processes (Rodriguez-Navarro et al. 2016 [2]) and following Ostwald step rule.

5.5 Conclusions

The preceding observations can be schematically summarised in Figure 5.14. The axes values are arbitrary, the purpose being simply to qualitatively represent the products of the different experimental conditions. At low supersaturation the crystals will grow slowly by ion-by-ion attachment, normally under heterogeneous precipitation regime whereby an existing interface will contribute to decrease the energy of nucleation. At high supersaturation and under the effect of an additive or inhibiting agent, heterogeneous nucleation can be sustained for some time, favouring 2-D and 3-D growth at the surface of the solid carbonate phase. This was clearly observed in the constant composition experiments with up to 50 μmol/kg ΣPO_4. Higher supersaturations will favour direct nucleation from solution, triggering crystallisation by particle attachment and agglomeration (Lewis et al. 2015 [47]). Fibrous radiating crystals (addressed in the next chapter) are an example reflecting heterogeneous nucleation at high supersaturation, whereas the dumbbell- or spherulitic-shaped morphotypes reflect homogeneous nucleation by particle agglomeration under higher supersaturation (Fig. 5.14).

The aggregated particles may be initially comprised of the corresponding metastable $CaCO_3$ phases that will be favourable at higher supersaturations. However, the recrystallisation process can occur in a matter of hours to days, producing more stable calcite crystals. Importantly, the larger initial texture of the aggregate may

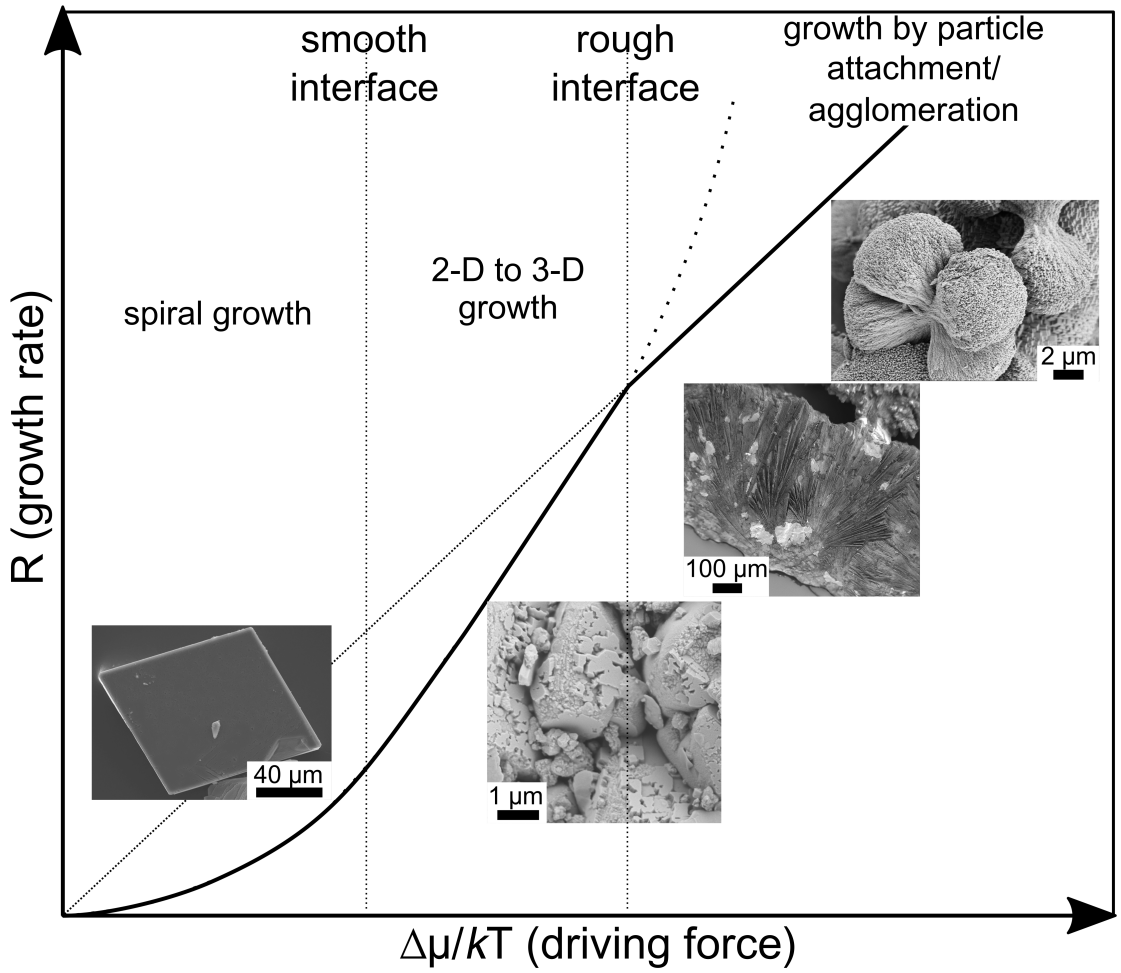


Figure 5.14: Schematic representation of the effects of increasing supersaturation on rates of crystal growth and morphology development in arbitrary x–y axes' scales. After Sunagawa (2007) [148], Shiraki and Brantley (1995) [149] Jiang and Tosca (2020) [150] and various other sources, with observations from the present study.

be preserved in this process, which can still be regarded as a proxy for the conditions of precipitation.

These experimental observations clearly bear implications for interpretations of the sedimentary record, specifically concerning non-skeletal carbonate deposits. For example, based on the preceding paragraphs, particle morphology (as well as mineralogy) may provide a qualitative to semi-quantitative guideline on which we may be able to set at least coarse boundaries with respect to pH, alkalinity, saturation state and rates of precipitation. This is something geologists have been applying for decades, as discussed in Chapter 1, but now these interpretations

are likely to become more fine-tuned and more evidence-based because of recent progress in theoretical and experimental work, which was also the goal of the present study.

Of course, any interpretation of the sedimentary record carries additional complications, because chemical sedimentary rocks may be comprised of phases that were not all formed as a mineral association during the progressive evolution of the same parent fluid. In other words, rocks may represent multiple successive and superimposing events, sometimes overprinting and completely obliterating the primary textures, and these can all be witnesses of complex geological events and later fluids. Thus, whether one is interested in the reconstruction of ancient environments or in trying to understand diagenesis and its impacts on the physical properties of sedimentary rocks (*e.g.*, porosity and permeability), it is certainly critical to be aware of these caveats. In any case, detailed petrographic and geochemical characterisation of mineral phases will be most useful if underpinned by a strong and reliable characterisation of the mineralogy itself as well as the geology, sedimentology, stratigraphy and the broader tectonic context of a given sedimentary basin.

6

Non-skeletal Carbonate Deposits as Physicochemical Recorders of Aqueous Carbonate Chemistry: A Case Study from the Barra Velha Formation

6.1 Chapter Summary

This chapter introduces a main geological problem residing in the challenges to understand both the broader global context and the local conditions of deposition of a vast volume of continental (lacustrine) carbonate rocks during the break-up of western Gondwana, in the Early Cretaceous. These rocks have little parallel in the geological rock record, in the sense that their main building blocks consist of nonskeletal calcite crystals with unusual morphologies, covering a vast geographic extent and volume in several sedimentary basins in the present-day South Atlantic. As the rock record becomes scarcer and/or increasingly subjected to alteration and metamorphism, a better understanding of these "younger" Cretaceous rocks and of the conditions of their deposition may in turn provide insights for investigations of other and more ancient nonskeletal carbonate rocks, particularly Archaean and Proterozoic carbonates. The chapter continues with a substantial discussion on our

current understanding of the kinetics of precipitation of calcium carbonate minerals, addressing some knowledge gaps and illustrating how an improved knowledge may help to constrain the conditions of their deposition. In this context, this chapter provides the backdrop and motivation for the work developed in the preceding chapters, focussing on the thermodynamics and kinetic theories relevant to understand calcium carbonate precipitation in saline and alkaline solutions, the geochemical modelling of natural alkaline lakes, and experiments on carbonate mineral precipitation.

This chapter was published in very similar form and content in the journal *Geochimica et Cosmochimica Acta* (Pietzsch et al. 2022 [151]). Supplementary material accompanying the published version is provided as an appendix, along with some additional datasets and discussion.

6.2 Introduction

The Lower Cretaceous rifting and breakup of Gondwana gave birth to one of the largest dominantly non-marine depositional systems in Earth's history. As rifting propagated along the South Atlantic margin, incipient grabens and their sedimentary fill transitioned to regionally extensive basins with the onset of thermal subsidence (Bate et al. 2001 [152]; Karner and Gambôa 2007 [153]; Torsvik et al. 2009 [154]; Kukla et al. 2018 [155]). Along the Brazilian margin of the South Atlantic rift system, much of the ensuing sedimentation (or "sag" deposits) took place during the Barremian to Early Aptian (Tedeschi et al. 2017 [156]; Gomes et al. 2020 [157]; Lima et al. 2020 [158]). In distal portions of the Santos and Campos basins of offshore Brazil, this phase featured prolific carbonate deposition (termed "Pre-salt", used here to denote units stratigraphically below a thick capping unit of anhydrite and halite-dominated marine evaporites, *e.g.*, Karner and Gambôa 2007 [153]). Palaeogeographic reconstructions (Chaboureau et al. 2013 [159]; Szatmari and Milani 2016 [160]), ostracod assemblages (Poropat and Colin 2012 [161]), the lack of marine fauna (Thompson et al. 2015 [162]; Muniz and Bosence 2015 [163]; Sabato

Ceraldi and Green 2017 [164]), and unusually thick accumulations of fascicular optic and radiaxial fibrous calcite often associated with Mg-silicate clays (Moreira et al. 2007 [165]; Wright 2012 [166]) reflect a non-marine carbonate depositional environment that was, at least at times, characterised by high alkalinity and pH $\geq$ 8.5 (Moreira et al. 2007 [165]; Wright and Barnett 2015 [18]; Tosca and Wright 2018 [167]). Carbonate deposition was abruptly terminated with extensive evaporite deposition along the central segment of the South Atlantic (Dias 2005 [168]; Moreira et al. 2007 [165]; Winter et al. 2007 [169]; Tedeschi et al. 2017 [156]; Rodriguez et al. 2018 [170]), before marine conditions were eventually established through continued spreading and subsidence (Kukla et al. 2018 [155]; Tedeschi et al. 2020 [171]).

The chemical controls on the formation and diagenesis of Pre-salt carbonates of the Santos Basin are poorly understood because these deposits have comparatively few modern or ancient analogues. Although biological influences may have played a role, the generation of non-marine carbonates is strongly influenced by depositional chemistry. From this point of view, the unusual calcite fabrics of the Pre-salt sag-phase carbonates of the Santos Basin also offer an opportunity to better understand dominantly chemical controls on carbonate sedimentation, in particular for systems that lack a skeletal carbonate factory. For example, before the emergence of metazoan calcification thought to have occurred in the Ediacaran (Knoll 2003 [172]), carbonate deposition through much of the Precambrian was strongly influenced by abiotic chemical processes (and to varying degrees, by the interactions between microbial communities and local environments) (Grotzinger and James 2000 [7]; Cantine et al. 2020 [173]). Extensive seafloor cements, composed of aragonite crystal fans, and unusual fibrous morphologies of calcite, speak to strong chemical influences on fabric development that have fundamentally shifted over the course of Archaean through Proterozoic Earth history (Grotzinger and James 2000 [7]; Sumner and Grotzinger 2000 [8]).

Observations from modern natural environments and laboratory experiments (*e.g.*, Barge et al. 2014 [174]; Toner and Catling 2020 [94]) provide a platform to investigate and to understand the influence of aqueous chemistry on depositional processes. However, applying this information to deep time is not straightforward. This is because the products of geological processes represent an inverse problem, which carry multiple alternative solutions to the boundary conditions governing depositional processes. In addition, sedimentary successions of increasing stratigraphic age typically become less complete, and also more likely to have been overprinted by metamorphism. Nevertheless, the rock record sometimes yields exceptionally well-preserved examples where the influence of some geochemical parameters outweighs several others. It is in this spirit that we propose that a detailed understanding of the geochemical processes that influenced mineral formation in Pre-salt carbonate depositional environments can underpin the development of new facies models that integrate both sedimentology and chemistry. Specifically, this endeavour may in turn open up windows into important aspects of climate dynamics during a key transition in Cretaceous Earth history (Wright 2022 [175]; Pietzsch 2021 [176]). More importantly though, the knowledge obtained from these investigations can in its own right contribute with potentially useful insights to our understanding of other periods of time whose geological record is more sparsely preserved or inexistent.

Observation of modern environments also inform us that carbonate deposition from alkaline lacustrine environments typically commences from a chemical state of high supersaturation with respect to $CaCO_3$. However, the mechanisms in past environments that led to sustained $CaCO_3$ supersaturation, which in turn governed calcium carbonate deposition and fabric development, are not well understood. Because $CaCO_3$ supersaturation, by definition, requires the modification or inhibition of $CaCO_3$ precipitation pathways, the production of carbonate from alkaline lakes must therefore be closely associated with the accumulation of compounds that inhibit or otherwise influence the kinetics of carbonate mineralisation. Consistent with this expectation, previous work has long indicated that of the compounds

known to inhibit $CaCO_3$ precipitation, phosphate strongly suppresses the nucleation of calcite and aragonite (Reddy 1977 [32]; De Kanel and Morse 1978 [113]; Meyer 1984 [115]; Burton and Walter 1990 [117]; Dove and Hochella 1993 [118]), and considerably slows the growth of pre-existing carbonate minerals (Mucci 1986 [116]). These combined effects may result in progressive increases in supersaturation until the formation of amorphous $CaCO_3$ precursors is triggered. For example, in the highly alkaline Mono Lake, a number of authors have suggested that the high supersaturation with respect to calcite ($\Omega_{\text{Calcite}} > 20$) might be maintained as a result of the inhibitory effect of dissolved reactive phosphate (> 400 μM) (Jellison et al. 1993 [30]; Nielsen and DePaolo 2013 [139]). Under these conditions, minimal carbonate precipitation occurs in the water column at Mono Lake, yet carbonate sediments can host significant carbonate-associated phosphate (CAP). These sediments can in turn preserve P/Ca ratios that are proportional to the ratio in the original solution from which they precipitated (Ingalls et al. 2020 [31]). Nevertheless, the mechanisms by which aqueous P may influence the carbonate chemistry and sedimentary fabrics generated from alkaline lakes, and how these processes may in turn regulate P budgets, are poorly understood. This is because few datasets are available which interrogate carbonate-associated phosphorus in dominantly non-skeletal carbonate depositional environments.

Therefore, the first goal of our study is to propose a geological system that may be a suitable testing ground candidate to evaluate if and how given physicochemical conditions observed in modern alkaline environments and emulated in experiments may have equivalently occurred in the past and may have left signs of preservation in the rock record. Our second goal is to test the hypothesis that dissolved phosphate may have additionally played a role in shaping the evolution of carbonate chemistry and fabric development of carbonate sediments deposited in the Santos Basin. To test these hypotheses, we have undertaken a detailed investigation of the Lower Cretaceous alkaline lake carbonate deposits from the BVF, offshore southeastern Brazil, focusing on the relationship between carbonate-associated P and other chemostratigraphic, sedimentological and mineralogical data. We combine these

data with aqueous geochemical constraints to ask: Could P have influenced non-skeletal $CaCO_3$ precipitation and sustained high supersaturation? Did P accumulate in bottom or pore waters during carbonate deposition, and if so, do these carbonate rocks provide an accessible record of P cycling?

6.3 Study Area and Geological Background

The Lower Cretaceous "Pre-salt" interval of the Santos Basin does not crop out on land, and so the well-documented carbonate reservoir rocks occur in the distal part of this offshore basin, along the southeastern margin of Brazil. Although rift-related Pre-salt deposits have been known in the adjacent Campos Basin to the north since the early 1980s (*e.g.*, Bertani and Carozzi 1985a [177];b [178]), these unusual carbonate rocks and associated deposits have become the target of intense studies from industry and academia for much of the last decade, as a result of initial discoveries in 2007 of giant oil reservoirs in the Santos Basin (Carminatti et al. 2008 [179]).

The Santos Basin was formed during the final stages of the break-up of Gondwana, which led to the formation of the southern domain of the South Atlantic Ocean and to other extensional basins such as Campos Basin, and their conjugate Namibe and Kwanza basins offshore southwest Africa. The basin is limited in its northern part by the adjacent Campos Basin and in its southern part by the Pelotas Basin. The formation of the Pre-salt deposits, common in all these basins, was constrained in the south by the volcanic lineament of the Walvis Ridge and the Rio Grande Rise, which served as barriers for the direct inflow of seawater from the southernmost Atlantic Ocean (Thompson et al. 2015 [162]; Sabato Ceraldi and Green 2017 [164]). Further to the north of these basins, additional Pre-salt basins were forming, such as the Espírito Santo and Cabinda basins, in the Brazilian and African margins, respectively.

Due to their economic importance, the Campos, Santos, and Kwanza basins are by far the most extensively studied along the South Atlantic margins of South America

and Africa (*e.g.*, Bate et al. 2001 [152]; Dias 2005 [168]; Moreira et al. 2007 [165]; Winter et al. 2007 [169]; Terra et al. 2010 [180]; Wright 2012 [166]; Buckley et al. 2015 [181]; Muniz and Bosence 2015 [163]; Wright and Barnett 2015 [18]; Alvarenga et al. 2016 [182]; Armelenti et al. 2016 [183]; Saller et al. 2016 [184]; Szatmari and Milani 2016 [160]; Herlinger et al. 2017 [185]; Teboul et al. 2017 [186]; Tedeschi et al. 2017 [156]; Chafetz et al. 2018 [187]; Tosca and Wright 2018 [167]; Tutolo and Tosca 2018 [28]; Lima and De Ros 2019 [188]; Mercedes-Martín et al. 2019 [189]; Teboul et al. 2019 [190]; Gomes et al. 2020 [157]; Wright and Barnett 2020 [191]). Beginning with early studies dating back to the mid-2000s along the Brazilian margin, different models have been proposed to explain the extensive deposition of the post-rift (or "sag" tectonic phase) carbonates found throughout these basins. The carbonates themselves display distinct and unique morphology, facies, and stratigraphy; they lack marine fossils, and are accompanied by atypical authigenic and diagenetic mineral associations. In addition, a nonmarine ostracod fossil record, radiogenic strontium and stable carbon and oxygen isotopic data, the presence of Mg-silicate clay mineral deposits (sometimes completely dissolved and/or replaced) – and unusual calcite morphologies (fascicular crusts and spherulites) all favour deposition within continental lacustrine settings in isolation from the sea (*e.g.*, Wright 2012 [166]; Wright and Barnett 2015 [18]; Saller et al. 2016 [184]; Sabato Ceraldi and Green 2017 [164]; Tedeschi et al. 2017 [156]; Pietzsch et al. 2018 [192]; Tosca and Wright 2018 [167]; Lima and De Ros 2019 [188]; Mercedes-Martín et al. 2019 [189]; Pietzsch et al. 2020 [193]). In the Santos Basin, most studies have focussed on the Barra Velha Formation (BVF), comprising the main reservoir rocks, and whose bulk makeup consists mostly of unusual non-skeletal carbonate deposits. These in turn are extensively distributed throughout these basins in both thickness and stratigraphic extent (*i.e.*, the predominantly shrubby and spherulitic carbonates).

Previous work on the Santos, Campos, and Kwanza basin carbonates has favoured a strong biotic control on the production of distinct carbonate textures and rocks more generally (*e.g.*, Dias 2005 [168]; Terra et al. 2010 [180]; Saller et al. 2016

[184]; Chafetz et al. 2018 [187]). However, although the preservation of biotic influences is subject to taphonomic factors and so are difficult to completely rule out, most geochemical and sedimentological evidence implies that abiotic factors may be capable of explaining the precipitation of the non-skeletal carbonate fabrics representing the dominant carbonate textures found in these basins, and more specifically in the Barra Velha Fm (*e.g.*, Wright 2012 [166]; Wright and Barnett 2015 [18]; Herlinger et al. 2017 [185]; Pietzsch et al. 2018 [192]; Lima and De Ros 2019 [188]; Mercedes-Martín et al. 2019 [189]; Pietzsch et al. 2020 [193]).

In spite of the general consensus towards generally alkaline and evaporitic conditions controlling the inorganic precipitation of the carbonates and associated minerals found in these basins, the specific chemistry and mechanisms are not fully understood. For example, hydrothermalism (*e.g.*, fuelled by heat associated with mantle serpentinization), and seepage influx of marine-derived $CaCl_2$-bearing hydrothermal brines through the Walvis Ridge–Rio Grande Rise barrier have been invoked to explain some of unusual mineral associations such as Mg-silicates and dawsonite, as well as some temperature data estimated from clumped isotope measurements (*e.g.*, Pinto et al. 2017 [194]; Farias et al. 2019 [195]; Lima et al. 2020 [158]). However, fluids predominantly derived from these sources and a dominantly hydrothermal control on $CaCO_3$ production in this lacustrine depositional setting are not clearly supported by radiogenic strontium isotopes or unambiguous clumped isotope data (Dias 1998 [196]; Tedeschi 2017 [197]; Pietzsch et al. 2018 [192]; Farias et al. 2019 [195]; Lima et al. 2020 [158]).

Recently, in an effort to understand the processes dictating non-skeletal carbonate production in the Santos Basin, Wright and Barnett (2020) [191] showed that, in a single >225m-thick section, fascicular crusts of outward-radiating fibrous calcite (or "shrubs") represented a dominant lithofacies building block and 65% of this component occurred *in situ*, whereas the remainder was physically re-worked. These authors found no evidence for an aragonitic precursor, which suggests that these shrubs may not have undergone extensive recrystallisation and/or neomorphism.

Low-Mg calcite pseudomorphs after high-Mg calcite or aragonitic precursors have been interpreted in sediments at least as old as 2.7 Ga (Sumner and Grotzinger, 1996a [12]; 2000 [8]). This in turn reinforces previous suggestions that this material likely preserves the original chemical composition related to the environment of deposition (in spite of not necessarily preserving primary clumped isotope values, likely to be modified as a result of solid-state reactions; *cf.* Stolper and Eiler 2015 [198]; Winkelstern and Lohmann 2016 [199]). At the same time, the intimate association of dolomite and Mg-silicate clays, in combination with an apparent Mg-calcite shrub precursor, indicates the presence of an aragonitic inhibitor, because aragonite precipitation is known to be kinetically favoured under the estimated relatively high Mg/Ca ratios.

Together, these observations indicate a depositional setting involving an extensive and productive non-skeletal inorganic carbonate factory, largely controlled by the physical and chemical conditions of the environment. In turn, the solution chemistry involved in their precipitation was likely to have been controlled through interaction with the surrounding lithologies (including crystalline bedrock), climate, and tectonics. This unusual set of circumstances, evidently rare in the geological record, establishes these relatively well-preserved carbonates as suitable candidates for further exploring conditions relevant to non-marine environments present on the ancient Earth. As pointed out in the introduction, the general physicochemical conditions occurring in certain modern systems such as in those alkaline lakes surveyed by Toner and Catling (2020) [94] are often used in a somewhat "actualistic sense" (*cf.* Romano, 2015 [200]) to infer processes that may have had a role in similar settings on the early Earth. However, it is unclear if such conditions could have indeed been established repeatedly and/or systematically across other periods of time in Earth's history. It is therefore necessary to find evidence preserved in the geologic record indicating how relevant such scenarios might have been. It is in this sense we believe that this interesting geological system may be a suitable testing ground to investigate such assumptions. This last point is also emphasised by the fact that the conditions in which this extensive carbonate system was sustained

seem to reflect a predominantly abiotically-driven carbonate production, as opposed to carbonate factories strongly controlled by carbonate producing skeletal organisms, as it has been the case in marine settings through most of the Phanerozoic (*e.g.*, Grotzinger, 1990 [9]; James and Jones, 2015 [201]).

6.4 Material and Methods

The present study is based on carbonate rocks retrieved from a core comprising 198.1m of uninterrupted cored interval across the upper Barra Velha Fm, which occupies a stratigraphic position above the Intra-Alagoas unconformity (*e.g.*, Moreira et al. 2007 [165]). The core comes from the same area studied by de Paula Faria et al. (2017) [202], Sartorato (2018) [203] and Gomes et al. (2020) [157] (well #3 in the case of the latter) (Fig. 6.1).

6.4.1 Optical Petrography

Standard petrographic analysis to characterise microfabrics and diagenetic features in the present study is based on a subset of 489 thin sections used by Gomes et al. (2020) [157], following their criteria and classification scheme. Thin sections were stained with a solution of Alizarin Red-S and potassium ferricyanide (*cf.* Friedman, 1959 [204]) to aid the identification of carbonate minerals.

6.4.2 Bulk Rock Geochemistry

Bulk rock slabs or plugs taken from the core underwent the same preparation protocols for bulk rock geochemical analyses by ICP-OES and ICP-MS as described in Pietzsch et al. (2018) [192]. Briefly, chemical analyses of 691 different individual samples, comprising 489 with detailed petrography and additional 202 interspersed samples, were determined in an Elan DRC II Perkin Elmer ICP-MS and in an Optima 7300 DV Perkin Elmer ICP-OES in order to measure the elemental abundance of Na, Mg, Al, Si, P, K, Ca, Ti, Mn, Fe, Rb, Sr, and Ba. Here, however, we focus our attention only on the elements central to our discussion for the present study, *i.e.*, Ca, Mg, Si and P. Additional 279 duplicate samples corresponding to those depths

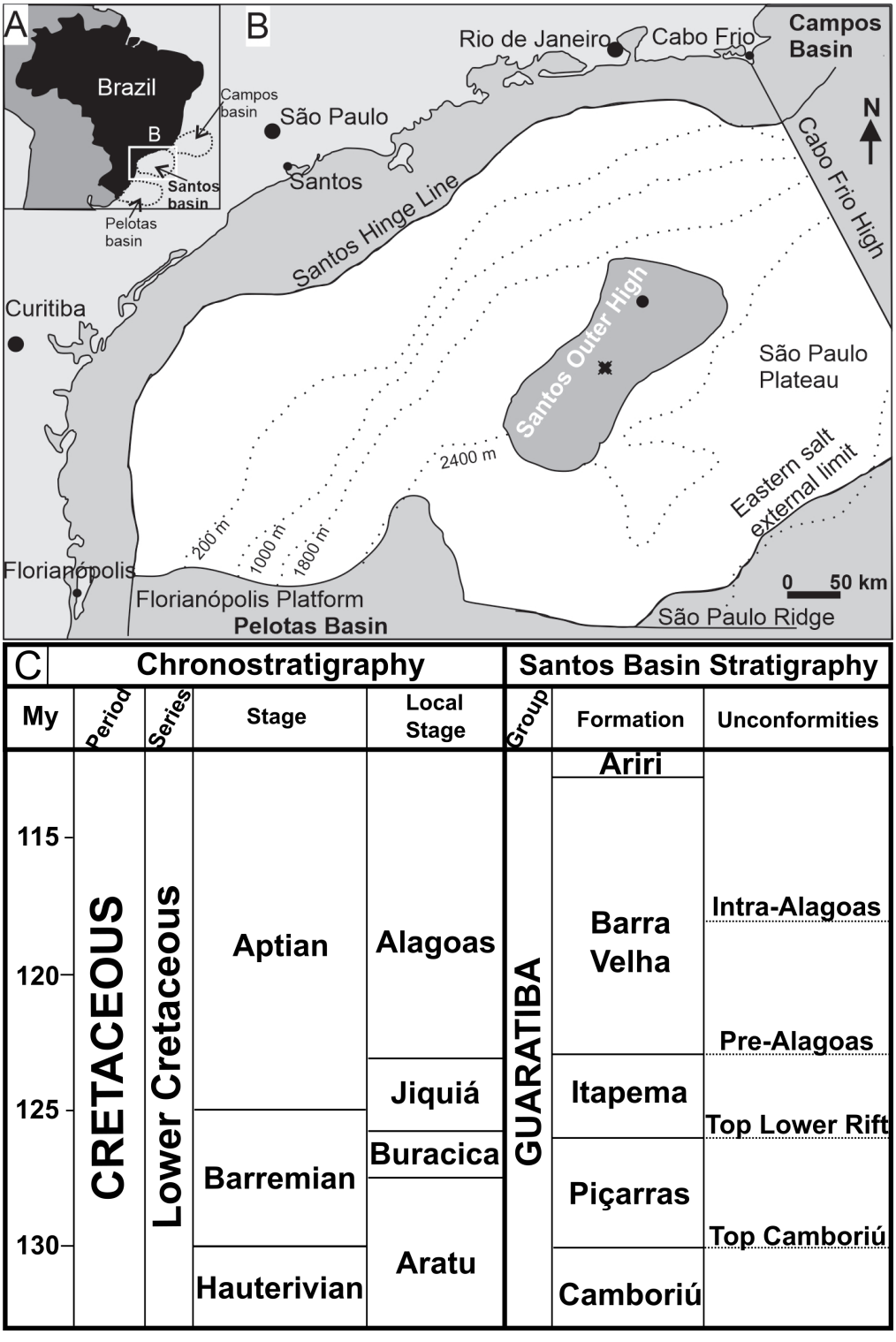


Figure 6.1: Map and stratigraphic chart of the study area, after from Gomes et al. (2020) [157] and Moreira et al. (2007) [165], respectively. A: general view of the investigated region, with a highlight of the Santos Basin along the southeastern Brazilian margin (white rectangle). The adjacent basins of Pelotas, to the south, and Campos, to the north, are also indicated. B: detail of the Santos Basin, emphasising the outer high, where the wells investigated in this study are located. The black X and the black circle correspond respectively to the locations of wells #3 and S10, set approximately 75 km apart, detailed in the text. C: Lower Cretaceous stratigraphic chart for the Santos Basin.

with previous petrographic descriptions were re-collected in order to account for the natural variability of the population. Finally, 130 random laboratory replicates from this global set were generated, for quality control purposes. The final number of samples analysed was thus 1100. The average distance between the slabs or plugs taken from the 200-metre continuous cored interval was 20-30 cm. Detection limits were 0.01% for major elements (as oxides) and better than 50 ppm for minor/trace elements.

Additionally, small chunks of 125 sidewall core rock samples from well S10, addressed in previous studies (Pietzsch et al. 2018 [192]; 2020 [193]) were also analysed for phosphorus following the procedure above. The well S10 is located *ca.* 75 km to the northeast of the main well (well #3) being addressed in this study (Fig. 6.1).

6.4.3 EPMA

A total of 10 samples, eight corresponding to those with bulk rock analyses and two additional new samples, were selected for detailed EPMA. The analyses aimed to characterise the chemical composition and P concentration of the different textural elements and minerals that comprise the bulk framework of various lithofacies (including spherulites and shrubs) following the classification of Gomes et al. (2020) [157] and the potentially diagenetic minerals (different phases of dolomite, as well as quartz, magnesite and calcite cement). For these analyses, the samples were carbon-coated using an EMITECH K950X coater. The analyses were performed in a JEOL JXA-8230 instrument containing an array of five wavelength dispersive X-ray spectrometry (WDS) detectors with the analysing crystals LDE1, LDE2, TAP, PET/L-H and LiF/L-H. Each of these crystals allows the diffraction and consequently the detection of different wavelength ranges, corresponding to different elements present in the spotted area, covering from the Kα ines of B to the Lα lines of U. The instrument is also equipped with an additional EDS JEOL detector which was used to aid in the analyses. In all cases the analytical conditions of the instrument were ran with a voltage of 15 kV, current of 5 nA, and 10 μm spot size whereas the acquisition time varied between 10–30 s per element, according to its

expected abundance. A total of 18 different standards, including calcite, siderite, dolomite, apatite, barite, olivine, feldspars, fluorite and glass, were used for the purpose of calibrating the instrument for the detection of the following elements: Ca, Mg, Si, Al, P, S, Mn, Fe, Sr, Ba, La, Ce, and Pb. Detection limits averaged 100 ppm for all elements.

6.4.4 SEM with EDS and XRD

Further mineralogical mapping of additional 24 (22 new plus two also with EPMA) thin sections, QEMSCAN and powder XRD analyses were also performed. Chemical and mineralogical maps of 24 thin sections were obtained using QEMSCAN 650 automated mineralogical mapping equipment (FEI Company) with accelerating voltage of 15 kV and 10 μm spot size. The mineralogical maps show the spatial distribution of mineral phases and the relationship between them, and their abundances were quantified as percentage of area or percentage of mass (considering the theoretical density of minerals). Percentages lower than 0.01% were not considered.

Mineral identification and quantification (bulk) of 679 samples from the 691 total with bulk rock analysis were determined using a D8 Advance X-ray diffractometer (Bruker), employing Cu-Kα radiation with 40 kV accelerating voltage, 40 mA filament current, step size of $0.02^o 2\Theta$, from 5 to $70^o\Theta$. Qualitative identification of the bulk mineralogy was performed using Jade 9 software (Materials Data Inc.) and from the mineral data bank PDF-2 (International Centre for Diffraction Data). Quantitative analyses were done using the Rietveld method (Young 1995 [205]) with the aid of the TOPAS software (Bruker).

6.4.5 Bulk Rock Stable Isotope Analyses ($\delta^{13}C$ and $\delta^{18}O$)

A total of 502 different samples were collected from the core, corresponding to different depths, averaging *ca.* 40 cm distance between sampling sites. Before analysis, all samples followed the cleaning protocol for oil extraction and salt removal as described in Pietzsch et al. (2018) [192]. Afterwards, the isotopic

analyses of around 30 μg of powder per sample were carried out on a Kiel IV preparation unit for CO_2 extraction from the reaction with orthophosphoric acid at $\sim 75^o$C, coupled to a dual-inlet mode isotope ratio mass spectrometer (IRMS) Delta V Plus. Every batch of *ca.* 30 samples was intercalated with the analysis of a standard (NBS-19) and additional replicate measurements of samples, and the analytical reproducibility for δ^{13}C and for δ^{18}O was better than 0.05‰ and 0.10‰, respectively. The values are reported in the conventional delta notation in parts per thousand related to the Vienna Pee Dee Belemnite (VPDB) standard.

Because the measured $\delta^{18}O_{VPDB}$ reflects bulk rock with different proportions of calcite and dolomite, the measured $\delta^{18}O_{VPDB}$ values need be corrected to take in consideration the different fractionation factors between CO_2 and the carbonate mineral resulting from the reaction with phosphoric acid. The correction used here considers the relative abundances of calcite and dolomite in each sample and the fractionation factors between CO_2–calcite and CO_2–dolomite at $\sim 75^o$C, the temperature of the reaction with the orthophosphoric acid during the analytical procedure. To account for the fractionation at this temperature we use the fractionation factor between CO_2–calcite estimated by Swart et al. (1991) [206] and a second-order polynomial interpolation of the fractionation factors between CO_2–dolomite estimated at different temperatures by Rosenbaum and Sheppard (1986) [207]. We report here both the measured and the corrected $\delta^{18}O_{VPDB}$ values. A brief review of definitions and conventions used in stable isotope geochemistry and details of the aforementioned calculations are given in appendix A at the end of this chapter.

6.4.6 Radiogenic Strontium-Isotope Ratio Analyses

Additionally, 71 samples and 10 more individual aliquots taken from this set consisting of 71 original powdered samples were analysed for their $^{87}Sr/^{86}Sr$ ratios. Approximately 1 mg of sample powder was digested in weak acetic acid (0.5 mol L^{-1}) in SavillexTM tubes in order to avoid leaching of ^{87}Sr and Rb from non-carbonate phases. The samples were centrifuged, and the supernatant collected, after which

they were dried and dissolved in HNO_3 (18%). This was followed by separation of Sr from the eluent in Teflon chromatographic columns filled with cationic exchange resin (Biorad AG-50W-X8 100–200 mesh). The collected solutions were analysed in a NEPTUNE multicollector inductively coupled plasma mass spectrometer (MC-ICP-MS) in static mode. The resulting $^{87}Sr/^{86}Sr$ ratios were determined based on approximately 100 measurements and were normalised assuming a $^{88}Sr/^{86}Sr$ ratio = 0.1194. The external reproducibility of the $^{87}Sr/^{86}Sr$ measurements was determined with the analysis of the NBS-987 standard, yielding an average 0.710248 ± 0.000019 (2SD).

6.4.7 Statistical Analyses

The bulk mineralogical and chemical results were assessed in terms of basic descriptive statistics, and the microanalytical results were evaluated with multivariate data analyses using PCA. Fundamental principles are covered in many textbooks (*e.g.*, Reyment and Savazzi 1999 [208]; Varmuza and Filzmoser 2009 [209]). Briefly, the PCA corresponds to a method of dimension reduction employing linear transformations following matrix operations, thereby producing new variables – the principal components, that are uncorrelated with each other – each of which accounting for a decreasing amount of the total variance of the dataset (Pietzsch et al. 2010 [210]; Filzmoser and Todorov 2011 [211]). The PCA transformation of the EPMA results produced new scores (representing the contribution of each sample to each principal component) and variable loadings (the contribution of each variable, represented as vectors of the elements, in this case, to each principal component). The EPMA data were also assessed with aid of code generated boxplots implemented in the ggplot2 tool written in R language, aiming to highlight differences in the compositional variability among groups of distinct minerals (calcite, dolomite and quartz) and of different fabrics with respect to single individual elements such as phosphorus (as ΣPO_4). Prior to statistical treatment, undetected values were replaced by a random value between zero and the respective limit of detection of a given element (see supplement).

Statistical treatment of raw data based on correlation and/or covariance of two or more dependent variables consisting of compositional data is subjected to biases due to the unit-sum constraint or closure effect, thoroughly discussed by Aitchison (1986) [212]. For the present purpose, the centred-log ratio transformation (CLR) is considered a useful treatment for compositional data, helping to mitigate the fixed sum constraint (Aitchison 1986 [212]; Pietzsch et al. 2018 [192]).

6.5 Results

6.5.1 Lithofacies Characteristics

The predominant facies documented in the studied well are characterised by variable amounts of three petrographic components that we and others interpret as having originally formed in situ (Gomes et al. 2020 [157]): (1) mud comprised of fine-grained components such as microcrystalline calcite and clay minerals, (2) calcite spherulites (spherical or sub-spherical outward-radiating aggregates of fibrous calcite) and (3) calcite shrubs (upward-radiating aggregates of fibrous calcite with optical properties resembling both fascicular optic and radiaxial fibrous varieties). Additionally, grainstones often occur and can be comprised of reworked particles made by all three components. These components have been extensively documented in the South Atlantic Pre-salt basins, but there are divergent classification attempts and interpretations in terms of the processes involved in their formation. Here, to leverage previous petrographic and sedimentological analyses of these rocks, we follow the Gomes et al. (2020) [157] classification, who worked on the same set of samples used in the present study. Fig. 6.2 shows a selection of representative samples found in well #3, among shrubstones, spherulitestones, a mudstone and a packstone. It is noteworthy that bioclasts – represented by ostracod shells and/or phosphatic fragments – could be observed in 24 out of 174 thin sections (*i.e.*, 13.8%) coming from the upper interval between $\sim$ 10 and $\sim$ 70 m. In the remainder of studied well (from $\sim$ 70 to 203 m), bioclasts were observed in 15 out of 382 thin sections (*i.e.*, 4% of the total for this interval).

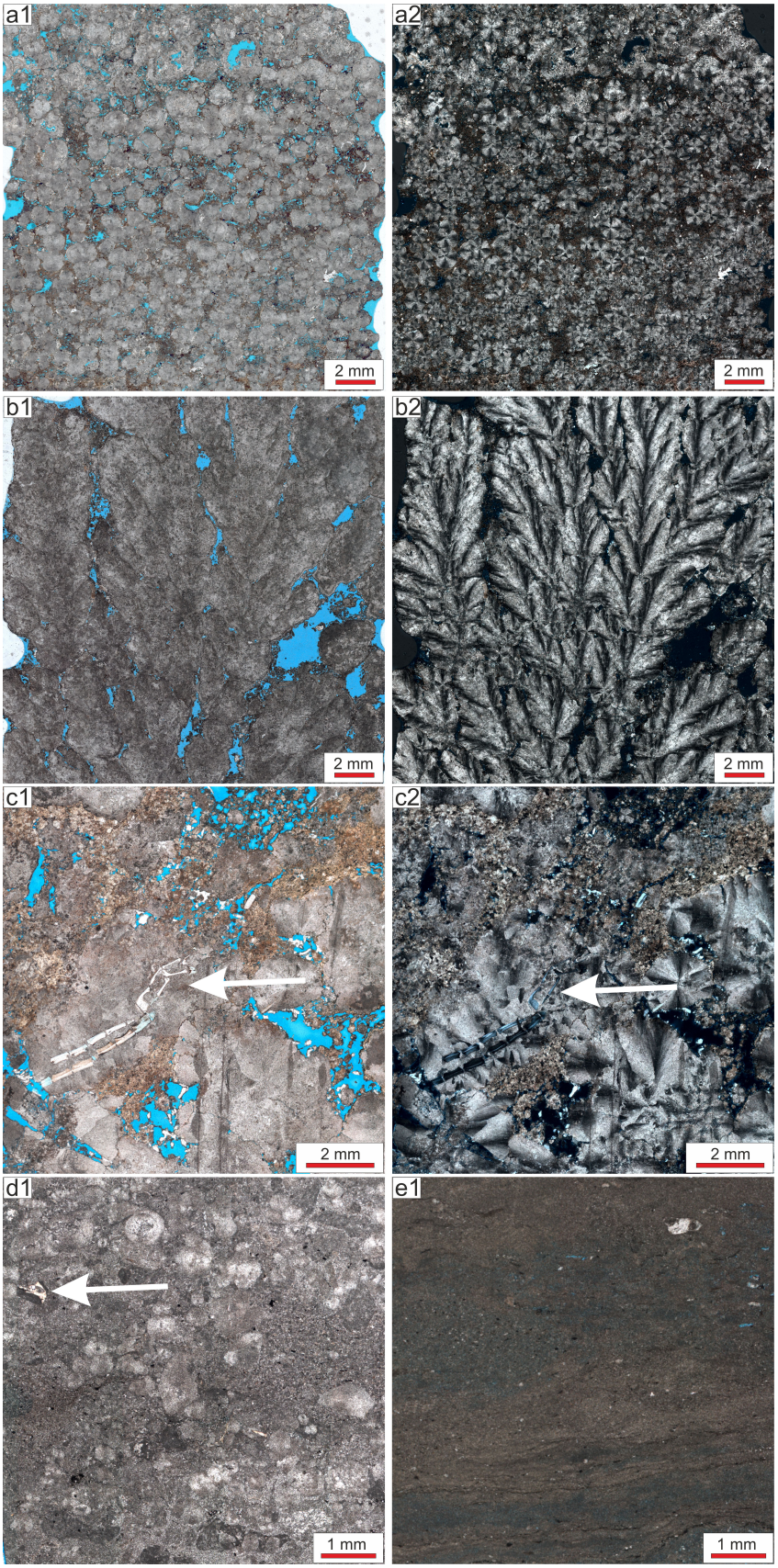


Figure 6.2: (Caption next page.)

Figure 6.2: (Previous page.) Main lithofacies investigated in this study, following the classification in Gomes et al. (2020). (a) spherulitestone, comprising calcite spherulites and rhombohedral and anhedral dolomites with inter-particle porosity. (b) shrubstone, comprising fascicular-optic calcite crust with framework porosity. (c) spherulitic shrubstone, comprising fascicular-optic shrubs, calcite spherulites and rhombohedral and anhedral dolomites with inter-particle porosity. White arrow shows phosphatic particle. (d) intraclastic packstone with inter-particle porosity. White arrow shows phosphatic particle. (e) mudstone, comprised of alternating layers rich in detrital grains and dolomite and calcitic-rich layers. Image pairs from (a)–(c) correspond to parallel polarisers (PPL) and crossed polarisers (XP), respectively, whereas (d) and (e) are PPL only. All thin sections were impregnated with blue epoxy resin to highlight the porosity.

6.5.2 Bulk Rock Geochemistry, Mineralogy, Facies and Phosphorus Association

In order to efficiently assess the bulk rock geochemistry data with respect to calcium and magnesium concentrations, the results were compared with the mineralogical data acquired through XRD measurements. Calcite and dolomite mineral compositions were assumed, in a simplified first order approach, to represent pure stoichiometric phases. CaO and MgO concentrations can be readily calculated with the formula:

$$C_i = x_j({}^{AM_i}/_{MM_j}) + x_z({}^{AM_i}/_{MM_z}) + ... + x_n({}^{AM_i}/_{MM_n}) \tag{6.1}$$

where C_i represents the element (or oxide) concentration, x_j, x_z and x_n represent the fraction of mineral j, z and n, respectively, which contain the element (or oxide) i, AM_i is the atomic mass (or formula weight) of element (or oxide) i, and MM_j, MM_z and MM_n correspond to the formula weight of mineral j, z and n, respectively, which contain the element (or oxide) i.

This approach can be useful in carbonate sections where either calcite and/or dolomite are the main sources of Ca and Mg. This can be readily seen plotting the measured values of Ca and Mg with ICP-OES versus the calculated values based on mineralogical composition from XRD measurements. These plots are shown in Fig. 6.3. The ternary diagrams, in turn, show facies and bulk rock phosphorus concentration and how they are distributed among the three predominant minerals, calcite, dolomite and quartz (Fig. 6.4a and 6.4b).

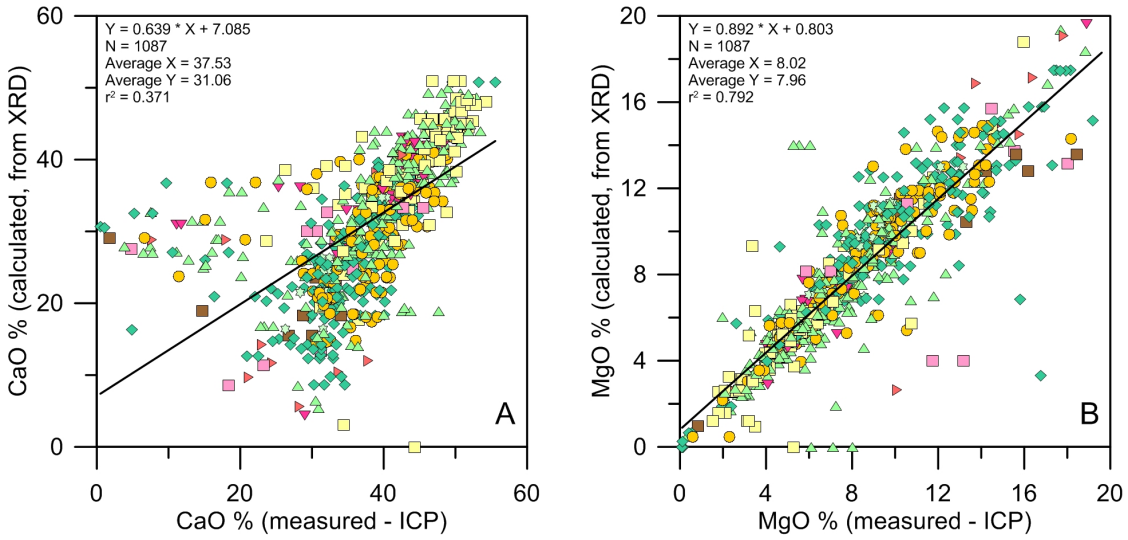


Figure 6.3: A: crossplots showing CaO calculated from mineralogy data determined by X-ray diffraction (XRD) vs CaO concentration measured by ICP-OES in bulk rock; B: same plot for MgO data.

6.5.3 Stratigraphic Variability in Bulk Rock Phosphorus Association

The profile of P concentration with depth, mineralogy and facies distribution is shown in Fig. 6.5. Phosphorus concentrations are visibly very high in the upper interval, between ~ 0–74 m. A histogram reveals that the P concentration measured in 489 unique individual samples, plus 279 re-collected duplicate samples and an additional 202 different interspersed plugs collected among the 489 described samples and 130 laboratory replicates measured for quality control, totalling 1100 results, shows a log-normal distribution strongly skewed to the right (supplementary Figs. B.1a and B.1b). Supplementary Table B.1 shows the median concentration of P (as well as calculated ΣPO_4) and of calcite, dolomite and quartz calculated for each facies, based on 768 samples (489 unique individual samples plus their 279 corresponding recollected duplicates). Evaluating the distribution of the whole set of 1100 samples for outliers, estimated from the lower and upper bounds of the interquartile range (3^{rd} quartile minus 1^{st} quartile), indicates that this set contains 118 outlier values, corresponding to >216 ppm P (or >662 ppm ΣPO_4). The histogram in supplementary Fig. B.1c shows the distribution with the outlier values removed. Considering this, the median concentration of P (as well as ΣPO_4, calcite,

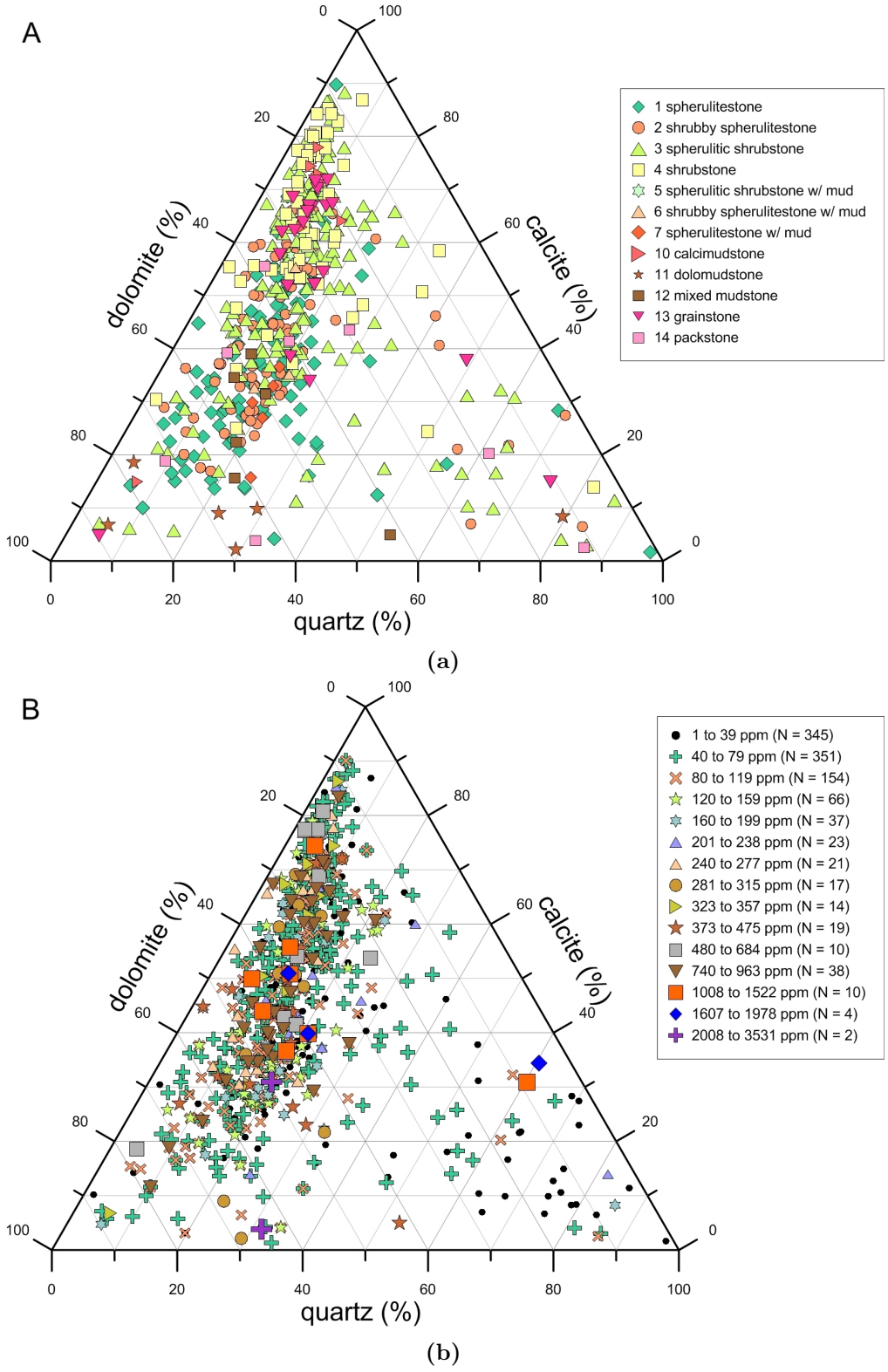


Figure 6.4: A: ternary diagram of calcite vs. dolomite vs. quartz content – vs. facies; B: ternary diagram of calcite vs. dolomite vs. quartz content – vs. phosphorus concentration.

dolomite and quartz) was determined for each group of facies. These results are shown in supplementary Table B.2. Tables B.3 and B.4 show the same estimations based only on those samples with P > LD, for comparison.

The medians of calcium concentrations determined from the ICP-OES data and calculated from XRD data, assuming stoichiometric calcite and dolomite, as well as P/(Ca+Mg) ratios based on the measured and calculated values, are shown for comparison. It can be seen that the median values agree fairly well, both for calcium and magnesium concentrations determined by ICP-OES and estimated from mineralogy. Accordingly, the P/(Ca+Mg) ratios calculated employing these two different sources agree with $p < .01$ and a Pearson coefficient between 0.878–0.996. This independently suggests that phosphorus is predominantly associated with these two minerals. Bulk rock phosphorus concentrations according to facies are shown in Fig. 6.6a-6.6b, which include all samples, outliers inclusive, corresponding to data from the interval above $\sim$ 74 m and the lower interval, respectively.

6.5.4 Bulk Rock δ^{13}C and δ^{18}O Data

High-resolution $\delta^{13}C_{VPDB}$ and $\delta^{18}O_{VPDB}$ profiles are plotted in Fig. 6.5, together with bulk rock phosphorus content, radiogenic strontium isotopes, mineralogy, and facies distribution. The measured $\delta^{13}C_{VPDB}$ and $\delta^{18}O_{VPDB}$ values vary from -1.71 to 3.54‰ and from -4.57 to 6.63‰, with average $\delta^{13}C_{VPDB} = 1.58 \pm 0.69$‰ and $\delta^{18}O_{VPDB} = 1.21 \pm 0.99$‰ (N = 502), respectively, across the entire range of the studied interval. Corrected $\delta^{18}O_{VPDB}$ values (plotted in Fig. 6.5) range between -4.57 and 5.66‰, averaging 0.77 ± 1.02‰ (N = 497). Because of the high-frequency variation which can be seen in this high-resolution sample set, some of which might result from the effects of diagenesis, the data were further processed applying nine points running average filter. This smoothing of the data resulted in recalculated $\delta^{13}C_{VPDB}$ and $\delta^{18}O_{VPDB}$ values varying from 0.33 to 2.75‰ and from -0.50 to 3.23‰, respectively, with average $\delta^{13}C_{VPDB}$ and $\delta^{18}O_{VPDB}$ values of 1.62 ± 0.52‰ and 1.21 ± 0.67‰(thick red line in the $\delta^{18}O_{VPDB}$ profile; Fig. 6.5), respectively (N = 502). The latter values are based on the measured raw bulk rock

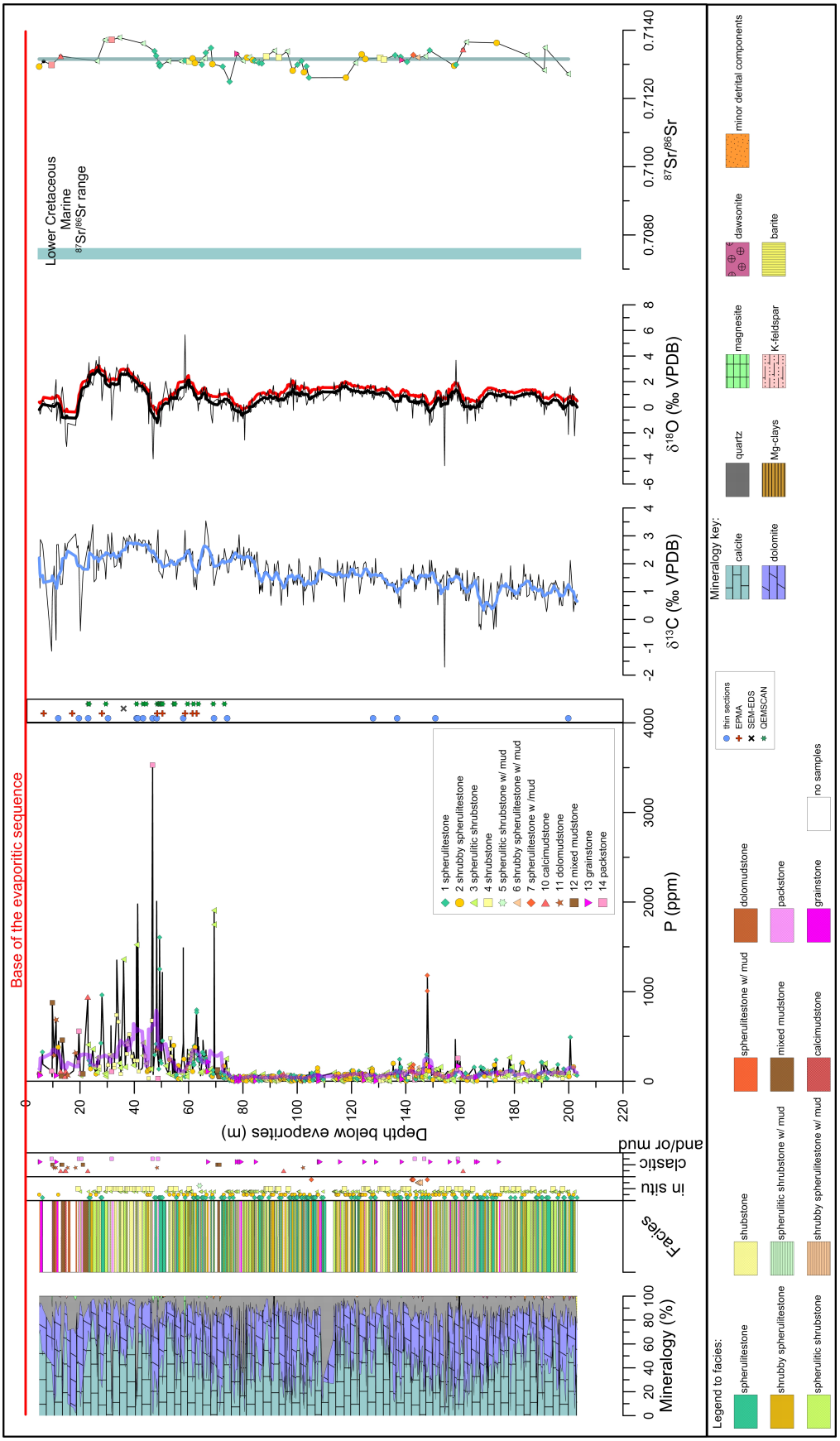


Figure 6.5: (Caption next page.)

Figure 6.5: (Previous page.) Detailed well profile, showing well mineralogy, facies, bulk rock phosphorus concentration profile, $\delta^{13}C_{VPDB}$, $\delta^{18}O_{VPDB}$ and $^{87}Sr/^{86}Sr$ profiles. Thick purple and blue lines in the bulk rock phosphorus and $\delta^{13}C_{VPDB}$ represent the nine-points running average of those respective results. Red and black lines in the $\delta^{18}O_{VPDB}$ profiles correspond to nine-points running average applied to the measured bulk rock $\delta^{18}O_{VPDB}$ values and to the $\delta^{18}O_{VPDB}$ after correction accounting for different acid fractionation factors resulting from calcite and dolomite present in different proportions in bulk rock samples, as explained in the text. After the nine-points running average filter is applied the P concentrations in the upper 74m vary closer to the average bulk rock P concentration for that interval, ∼300 ppm. Thinner straight greyish line in the middle of the $^{87}Sr/^{86}Sr$ profile represent its average value throughout this section, and the thicker line to its left shows the range of marine carbonate $^{87}Sr/^{86}Sr$ values reported for the Lower Cretaceous.

$\delta^{18}O_{VPDB}$ (uncorrected for different acid fractionation factors between CO_2-calcite and CO_2-dolomite, as explained above). If the smoothing is applied to the corrected $\delta^{18}O_{VPDB}$ (black lines) the values vary between −1.21 and 2.91‰, average = 0.78 ± 0.72‰ (N = 497; thick black line in the $\delta^{18}O_{VPDB}$ profile; Fig. 6.5).

6.5.5 $^{87}Sr/^{86}Sr$ Ratios

The results of measured $^{87}Sr/^{86}Sr$ ratios in 71 samples are also shown in Fig. 6.5, plotted according to facies. The $^{87}Sr/^{86}Sr$ values vary from 0.71249 to 0.71378, which average = 0.71315 (middle line crossing the $^{87}Sr/^{86}Sr$ profile). For comparison, the $^{87}Sr/^{86}Sr$ range reported in corresponding Lower Cretaceous marine carbonates is also indicated. The distribution of $^{87}Sr/^{86}Sr$ ratio values according to facies is shown in appendix B (supplementary Fig. B.3).

6.5.6 Selected EPMA, and Elemental Map Images (QEMSCAN, EPMA and SEM-EDS)

EPMA data were collected from shrubs and crusts, spherulites, euhedral and saddle dolomites and other cements, and the BSE images indicating the analysed spots, as well as an SEM sample image, are shown in Fig. 6.7–6.9. The first sample analysed is from 6.59m depth, a predominantly calcimudstone sample containing some calcitic crust layers developing into shrubs, as well as some spherulites. Fig. 6.7 shows some backscattered electron images indicating the spots where data was collected in these spherulites and crusts, as well as in dolomites. A backscattered

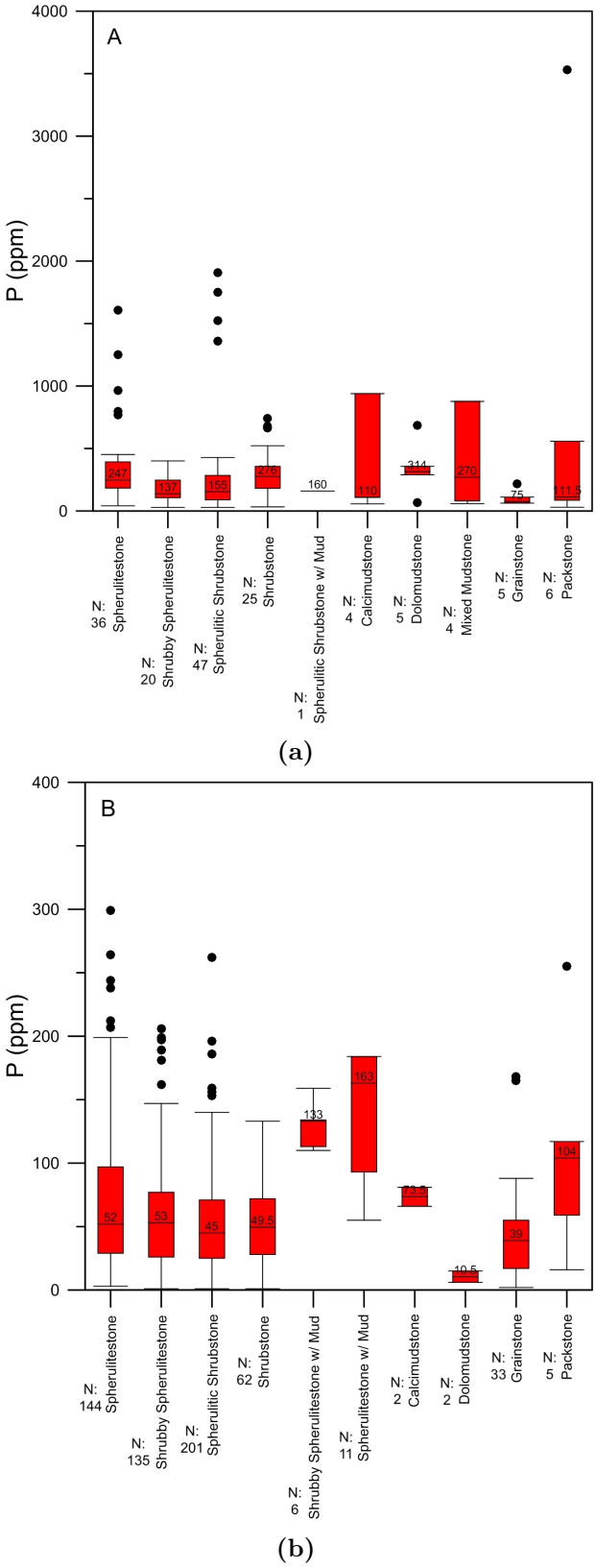


Figure 6.6: A: boxplots of bulk rock P concentration distribution per facies, upper 74 m; B: boxplots of bulk rock P concentration distribution per facies, lower interval below 74 m. Median values and number of samples in each facies group are indicated.

electron image and compositional maps acquired with SEM-EDS on sample from 36.04m depth are shown in Fig. 6.8. This sample corresponds to a spherulitic shrubstone after the classification of Gomes et al. (2020). The individual maps of the elements Ca, Mg, Si, Sr, P, Fe, S are indicated in Fig. 6.8A–F. Another sample, from 59.64m and corresponding to a shrubby spherulitestone was surveyed with QEMSCAN, providing a mineralogical map shown in Fig. 6.9.

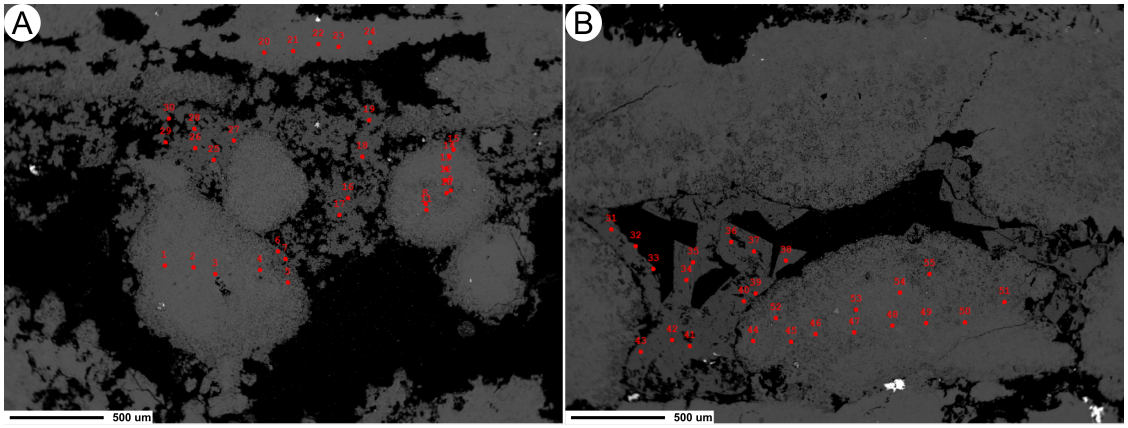


Figure 6.7: Backscattered electron (BSE) images of areas in sample from 6.59m, selected for EPMA.

6.6 Data Interpretation

6.6.1 Depositional Setting and Diagenetic Conditions According to Petrographic Data

Whilst the main non-skeletal calcium carbonate components comprising the bulk of the Barra Velha Fm (shrubs and spherulites) are authigenic minerals, a number of studies suggest the shrubs correspond to primary lake-bottom precipitation, whereas the spherulitic calcites are likely to be very early diagenetic products (Fig. 6.2a). The former commonly display interstitial growth-framework porosity, show variable and random incorporation of detrital particles, and are often observed to have grown *in situ*, as implied by their crystal elongation perpendicular to sub-perpendicular to the substrate (Fig. 6.2b; Herlinger et al. 2017 [185]; Gomes et al. 2020 [157]; Wright and Barnett 2020 [191]). Under conventional polarising microscope they morphologically resemble $CaCO_3$ minerals known to have formed in a range of

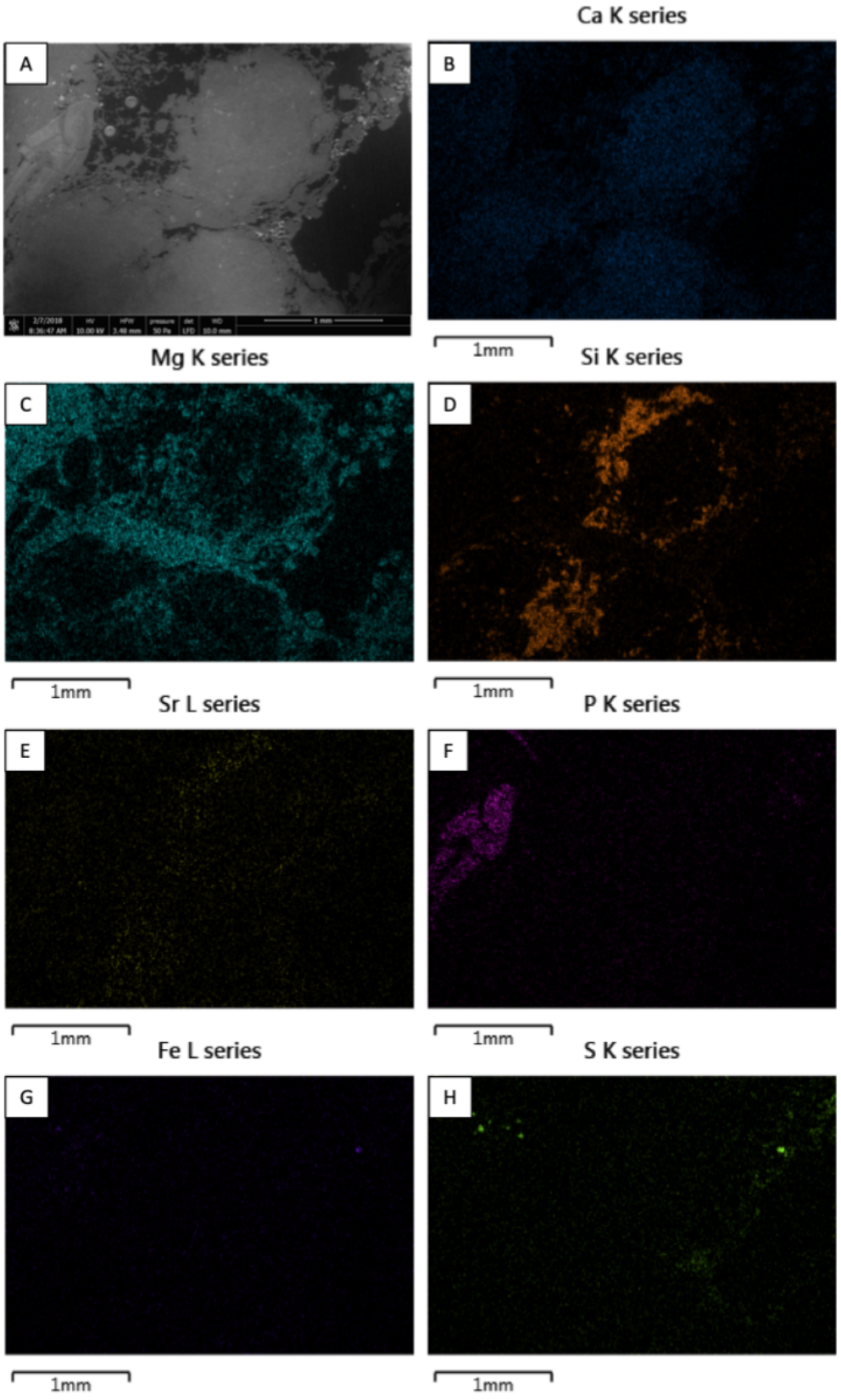


Figure 6.8: BSE and SEM-EDS compositional maps of sample from 36.04m.

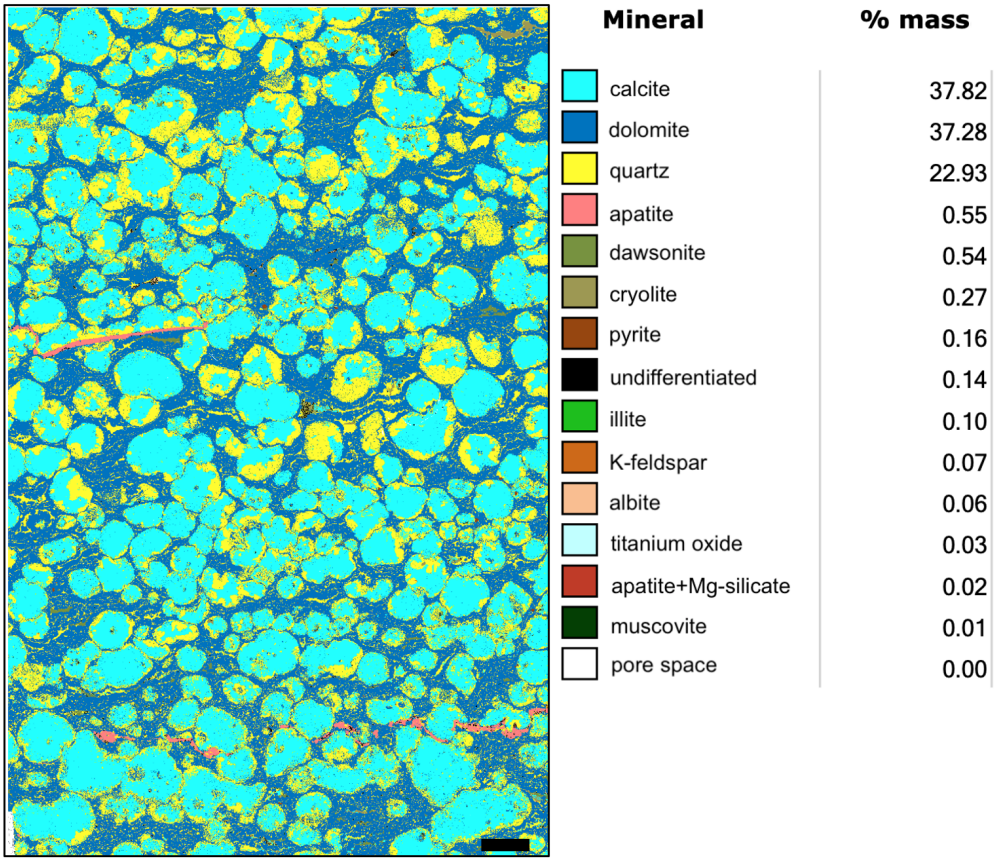


Figure 6.9: QEMSCAN images of samples from 59.64m, corresponding to a shrubby spherulitestones. Observe sub-millimetric occurrences of apatite layers at the base of dissolved spherulites. The black bar on the lower right corresponds to 1mm.

Recent non-marine environments (*e.g.*, Della Porta 2015 [27]; Richter et al. 2015 [213]; Jones 2017 [40]).

The early diagenetic origin of the calcite spherulites, and by inference, of most lithotypes predominantly composed of spherulitic aggregates, has been recently thoroughly addressed by Lima and De Ros (2019) [188], Gomes et al. (2020) [157] and Wright and Barnett (2020) [191]. However, there have also been suggestions that at least some occurrences of the spherulites are primary, in which case they may have grown close to the sediment-water interface (Chafetz et al. 2018 [187]; Gomes et al. 2020 [157]; Mercedes-Martín et al. 2022 [214]). These examples typically either replace and displace the laminated Mg-silicate clay matrices, which frequently appear wrapping the spherulites due to compaction, or occur in units lacking such a matrix (Lima and De Ros 2019 [188]; Wright and Barnett 2020

[191]). In the latter case, congruent matrix dissolution may have occurred in some instances, as suggested by the existence of aligned lamellae composed of small platy aggregates of dolomite, which in turn sometimes occur with remnants of Mg-silicate clays and in other cases without their presence (Wright and Barnett 2020 [191]). Visible silicification, in some circumstances, may be an early diagenetic product also deriving from the dissolution of the pre-existing matrix. There are yet other instances in which transitional forms between spherulites and the upward-radiating fibrous aggregates occur (Fig. 6.2c), further supporting interpretations that both textures formed very early and in the depositional environment or close to depositional conditions (Lima and De Ros 2019 [188]).

Although it still remains a fundamental challenge to set hard boundaries between strictly depositional and diagenetic histories (*e.g.*, Swart 2015 [215]; De Boever et al. 2017 [216]), the studies above suggest it seems reasonable to assume that these textural elements may reflect the general geochemical conditions of their depositional setting. In this case, they likely reflect conditions of precipitation more closely related to the primary lake fluids, rather than from extensively modified pore fluid chemistries. Hence, these elements (shrubs and spherulites) are addressed as primary deposits throughout the remainder of the text.

6.6.2 Observations from Bulk Rock Geochemistry, Mineralogy, Facies and Phosphorus Association

The plots of Ca (measured) *vs* Ca (calculated) and Mg (measured) *vs* Mg (calculated) do indicate that the approximation between bulk chemistry and mineralogy is reasonable in the case considered here (Fig. 6.3). Moreover, they indicate where the approximation is poorer, highlighting samples where either the assumption of purity is considerably incorrect or where other phases contributing with these elements might be present. Fig. 6.3A shows that the Ca concentration calculated from XRD data results in underestimation of total Ca, compared to measured Ca concentration. This stems from assuming ideal stoichiometric proportions for calcite and dolomite, indicating that these minerals deviate from stoichiometric phases, and

that dolomite is possibly more calcic than assumed. In the case of Mg (Fig. 6.3B), it is particularly interesting because the correlation is significantly high, strongly suggesting that most Mg determined via ICP-OES is derived from dolomite and to some extent from Mg-calcite. This can be considered to be a good approximation, because from XRD measurements just a few samples indicated the presence of magnesite, another source of Mg, and the well is nearly devoid of Mg-silicate clays, as also shown by the XRD data.

Dolomite content may be variable within a given facies, but shrubby facies clearly tend to have less dolomite and are predominantly composed of calcite (Fig. 6.4a). Spherulitic facies tend to have a wider range in both dolomite and quartz content but compared with the shrubby facies generally have greater proportion of dolomite as well as quartz (Fig. 6.4a). This is probably a reflection of the association between spherulitic growth within a former laminated Mg-silicate clay matrix or an amorphous precursor of similar composition, which may have been congruently dissolved in some instances, yielding both dolomite and quartz as products, as some studies and petrographic evidence suggest (*e.g.*, Lima and De Ros 2019 [188]; Gomes et al. 2020 [157]; Wright and Barnett 2020 [191]).

The ternary diagram in Fig. 6.4b, in turn, shows bulk phosphorus concentration ranges according to mineralogy. A large number of the analysed samples contain below 200 ppm P ($\sim$ 6.5 mmol/kg P), and they have variable calcite, dolomite and quartz content. However, a considerable number of samples with high P concentration is mostly comprised of calcite and dolomite, normally with higher calcite content, associated with the predominance of the shrubby facies. These can typically have P concentrations >480 ppm, but can also reach concentrations >1008 ppm P (Fig. 6.4b).

To summarise, the bulk rock data suggests that calcite and dolomite host essentially the entire range of P concentrations, whereas quartz hosts usually the very lowest concentrations. Very high phosphorus probably is related to bioclasts in some

instances, but in these cases phosphatic grains are typically associated with shrubby and/or spherulitic carbonate facies composed predominantly of calcite and dolomite.

6.6.3 Considerations on the Stratigraphic Variability in Bulk Rock Phosphorus

Based on the preceding evaluation of outliers of P concentrations in bulk rock, the 95% confidence interval (CI) of the P concentrations corresponding to both the outlier and non-outlier groups were calculated (CI = 387.9–689.1 ppm and 57.9–67.5 ppm, respectively), and a Student's t test for comparing the mean values between these two groups was performed. The outlier range has mean = 538.5 ppm, std dev = 497.1 and median = 348 ppm (N = 118), and the non-outlier range has mean = 62.7 ppm, std dev = 45.6 and median = 54 ppm (N = 982). Considering the one-tailed distribution, the mean of the outlier group is higher than the mean of the non-outlier group, and the difference between these two groups is statistically significant at $p < .005$.

Hence, if the "non-outlier" group could be considered to be of "normal" P content in Pre-salt samples, the values according to facies should correspond approximately to those shown in supplementary Table B.2. Facies considered to correspond to primary deposits – in other words, containing textural elements considered to closely reflect formation in the surface environment or during early diagenesis close to the sediment/lake bottom interface – thus show median P concentrations $\sim$ 50–56 ppm or $\sim$ 1.6–1.8 mmol/kg (facies 1–4, *i.e.*, shrubstones and spherulitestones). Facies containing mud typically have higher phosphorus concentration, although the number of samples is considerably smaller as well (5.5% of samples in this set; supplementary Table B.2). However, it is important to highlight here that these outliers do not correspond to analytical artefacts, and the sole purpose of identifying them is to shed light on the background concentration of P in the studied section.

If the outliers are considered, and the groups are simply separated in the upper and lower intervals at $\sim$ 74 m according to phosphorus concentration, the difference between the means of these two are significant at $p < .005$ when comparing, for

example, the facies shrubstone above and below that depth (for reference, shrubstone mean [P] = 300.4 and 49.9 ppm [$\sim$ 9.7 and $\sim$ 1.6 mmol/kg P] and median [P] = 276 and 49.5 ppm [$\sim$ 8.9 and $\sim$ 1.6 mmol/kg P], above and below 74 m, respectively) (Fig. 6.6a and 6.6b). The interval above shows median P concentrations from $\sim$ 5.1–8.9 mmol/kg, whereas the interval below shows median P concentrations from $\sim$ 1.5–1.7 mmol/kg, again for shrubstones and spherulitestones, and muddy facies can have both higher and lower median values than this (Table 6.1). Dolomudstones have the highest median values in the whole interval (9.3 mmol/kg), but are represented by only seven samples in 768. A single packstone sample reaches the highest absolute P abundance (114 mmol/kg, or 3531 ppm P) (Fig. 6.5), but this may be related to reworking and to accumulation of phosphatic bioclasts, as observed in thin section.

To summarise, there is a contrasting difference in P concentration in the upper and the lower intervals, where the former contains considerably higher P concentrations. As observed before, calcite and dolomite minerals alone likely account for most of the P content. Although high bulk P concentrations may be attributed in some cases to accumulation of phosphatic bioclasts, primary shrubstone and spherulitestone facies predominantly composed of non-skeletal calcite tend to be correlated with high P content in the upper 74m of the studied interval compared to the remainder of the succession.

6.6.4 Bulk Rock Stable Isotopes and $^{87}Sr/^{86}Sr$ Ratio

Based on the smoothing of the stable isotope data, variations in $\delta^{13}C_{VPDB}$ and $\delta^{18}O_{VPDB}$ higher than those standard deviation values presented earlier are likely meaningful and representative of overall changes in the carbonate-lake water system, reflected in the carbonate samples. Boxplots with the distribution of the measured $\delta^{13}C_{VPDB}$ and $\delta^{18}O_{VPDB}$ values according to facies are shown in the supplementary material (supplementary Fig. B.2). In these cases, it can also be observed that there is a statistically significant difference ($p < .01$) between both the $\delta^{13}C_{VPDB}$ and $\delta^{18}O_{VPDB}$values of spherulitestones and shrubstones, in which the latter tend to have higher values. A possible explanation for this difference is that the shrubstones

Table 6.1: Median values, samples below 74 metres (below upper zone) and samples above 74 m (in parentheses).

Facies category*	[P] mmol/kg	[ΣPO_4] mmol/kg	dolomite %	quartz %	calcite %	[Ca]meas[a] mmol/kg	[Ca]min[b] mmol/kg	[Mg]meas[a] mmol/kg	[Mg]dol[c] mmol/kg	P/(Ca+Mg)meas[a] mmol/mol	P/(Ca+Mg)min[b] mmol/mol	N samples
1	1.68 (7.43)	1.12 (4.97)	45.5 (43.1)	13.5 (15.9)	34.4 (39.4)	6175 (5878)	5900 (6272)	2299 (2747)	2467 (2336)	198 (861)	201 (863)	144 (42)
2	1.71 (4.42)	1.14 (2.96)	41.4 (29.5)	13.6 (11.8)	42.9 (57.5)	6850 (6840)	6536 (7341)	2185 (2128)	2246 (1600)	189 (493)	195 (495)	135 (22)
3	1.45 (5.07)	0.97 (3.39)	29.4 (24.5)	13.2 (7.8)	51.3 (64.5)	7138 (7507)	6721 (7770)	1603 (1576)	1593 (1331)	166 (558)	175 (557)	201 (48)
4	1.60 (8.91)	1.07 (5.96)	24.1 (26.4)	8.4 (6.8)	62.9 (63.5)	8094 (7900)	7592 (7778)	1217 (1438)	1308 (1432)	172 (954)	180 (968)	62 (25)
5	(5.17)	(3.46)	(32)	(10.4)	(57.6)	(7190)	(7491)	(2128)	(1735)	(554)	(560)	0 (1)
6	4.29	2.87	42.7	17	34.6	5960	5774	2068	2317	535	531	6 (0)
7	5.26	3.52	51.1	19.8	29.2	5605	5690	2322	2773	664	622	11 (0)
10	2.37 (3.55)	1.59 (2.38)	49.4 (19.9)	11.1 (6.3)	39.5 (73.3)	6809 (7757)	6630 (8398)	2566 (1039)	2679 (1079)	253 (404)	255 (375)	2 (4)
11	0.34 (10.14)	0.23 (6.78)	12.2 (68.1)	79.5 (22.9)	8.4 (9.0)	2291 (4364)	1496 (4593)	1555 (3648)	661 (3694)	88 (1265)	157 (1223)	2 (5)
12	(2.62)	(1.75)	(52.7)	(19.4)	(22.4)	(5359)	(5096)	(3309)	(2860)	(302)	(329)	0 (9)
13	1.26 (2.42)	0.84 (1.62)	25.1 (24.0)	9.0 (9.3)	57.8 (66.8)	7654 (7645)	7140 (7970)	1413 (1326)	1364 (1301)	139 (270)	148 (261)	33 (5)
14	3.36 (3.60)	2.25 (2.41)	37.3 (50.2)	9.2 (27.6)	39.2 (18.9)	6359 (4856)	5941 (4609)	2632 (2838)	2024 (2724)	373 (468)	422 (491)	5 (6)

* Category legend: (1) spherulitestone; (2) shrubby spherulitestone; (3) spherulitic shrubstone; (4) shrubstone; (5) spherulitic shrubstone w/ mud; (6) shrubby spherulitestone w/ mud; (7) spherulitestone w/ mud; (10) calcimudstone; (11) dolomudstone; (12) mixed mudstone; (13) grainstone; (14) packstone. [a] median values of concentrations measured by ICP-OES.
[b] median values of concentrations calculated from mineralogical data (calcite + dolomite). [c] median values of concentrations calculated from dolomite content.

formed during intervals of greater aridification. However, this would imply more concentrated brines, whereby both $CaCO_3$ supersaturation driving its precipitation and greater concentration of other ions, exerting an inhibitory effect on $CaCO_3$ precipitation, could be likely alternative and non-exclusive scenarios. This is discussed in more detail below.

The $^{87}Sr/^{86}Sr$ ratio varies 0.00129 in this given set of samples from well #3, and all the values are still considerably radiogenic, implying an important contribution from fluids draining the continental crust. The observed range of values is also in agreement with what has been documented in other studies in different sectors of the Santos Basin as well as in the Campos Basin (Dias 1998 [196]; Tedeschi 2017 [197]; Pietzsch et al. 2018 [192]; Farias et al. 2019 [195]; Lima et al. 2020 [158]). For reference, typical mantle and basaltic $^{87}Sr/^{86}Sr$ values are ∼0.703–0.704 and Aptian marine carbonate values are lower than ∼0.7075, whereas typical continental crust values are ≥0.713 (*e.g.*, Elderfield 1986 [217]; Banner 2004 [218]; Bodin et al. 2015 [219]).

6.6.5 Interpretation of Compositional Data from Elemental Map Images (QEMSCAN and SEM-EDS) and Microanalytical Data (EPMA)

6.6.5.1 Microanalytical Data, Compositional and Mineralogical Maps

Microanalytical data and compositional maps indicate that phosphorus is associated with bioclastic material and as more finely-disseminated Ca-phosphate crystals and/or cements. For example, Fig. 6.8 shows SEM-EDS compositional maps from a selected area in spherulitic shrubstone sample from 36.04m depth. This sample was selected to evaluate the phosphorus distribution in samples containing bioclasts, since this thin section shows the presence of some of them, one of which is clearly visible in the left corner of the backscattered electron image. The compositional mapping reveals that phosphorus in this sample is particularly concentrated in the bioclast (Fig. 6.8F).

In contrast to Fig. 6.8, Fig. 6.9 provides microtextural evidence that phosphate was likely concentrated in the pore waters during diagenesis, which may have occurred soon after deposition. This example shows one selected QEMSCAN image, made on a thin section of a sample corresponding to the depth 59.64m. It corresponds to a shrubby spherulitestone, following the classification of Gomes et al. (2020) [157]. This sample was selected to compare the bulk rock P measurements with the phosphate concentration (calculated as a function of apatite, in turn estimated with the QEMSCAN analysis). Apatite is approximated with the formula $Ca_5(PO_4)_3OH$ to retrieve the equivalent P concentration derived from the QEMSCAN determination of the apatite content (originally determined with QEMSCAN, based on the X-ray spectra collected with four energy dispersive X-ray spectrometers and their comparison against its large database of known spectra). The sample has equivalent bulk rock P = 156 ppm. However, its apatite content estimated by QEMSCAN is 0.55%, yielding P = 1074 ppm from QEMSCAN. In the case of this sample the presence of apatite is unambiguous, as it occurs in preferential sub-millimetric layers likely associated with the dissolution of previous carbonate phases (spherulites, with apatite layers in pink) (Fig. 6.9).

6.6.5.2 Interpretation of Microanalytical Data Results

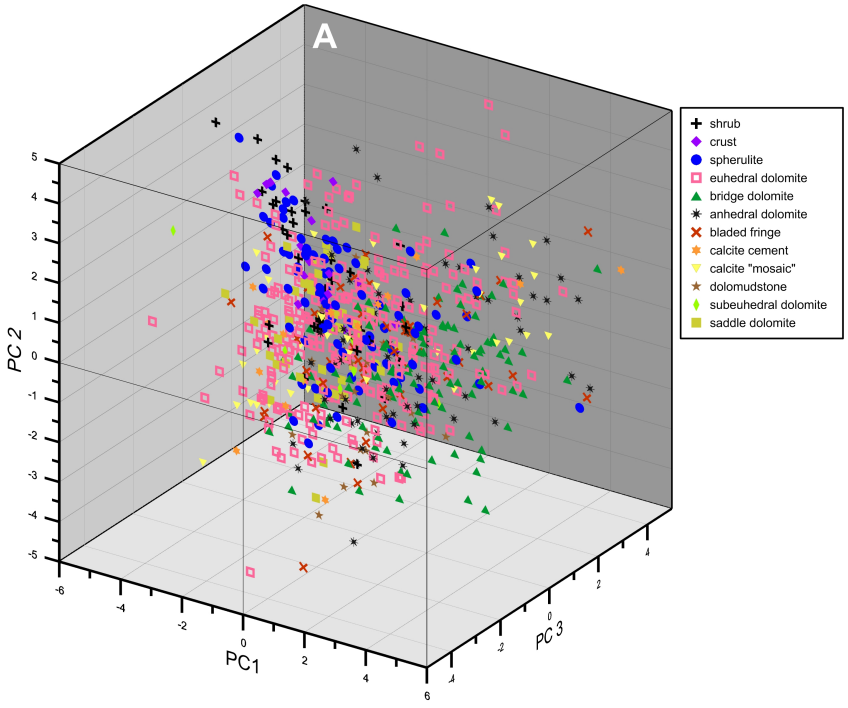
The EPMA measurements have the advantage over stepped acid digestion protocols that they do not depend on variable dissolution times resulting from nonstoichiometric carbonate phases. The latter can potentially induce incorrect estimates related to the element concentrations and the phases to which they belong to. Yet it may be difficult to extract patterns and assess the distribution and association of the elements in such a large data set. To explore and compare trace element data from EPMA, the elements P, Ba, Fe, Mn, Ce, La, Sr, Pb and S were normalised to the concentration total and followed then centred-log ratio transformation (Aitchison 1986 [212]). The major elements were not considered in this exercise in order to avoid discrepancies arising from size effects; hence only elements with similar concentration ranges were compared. Identified magnesite and quartz minerals

were not considered because of their far less frequent occurrence and also to avoid additional discrepancies arising from comparison between ratios where Ca is a trace element. A principal component analysis with these data was run, based on the variance-covariance matrix data. The results are shown in Table 6.2. The first three principal components (PCs) account for ∼50% of the explained variance, and the sum of the first three eigenvalues alone account for all the nine variables represented. Hence only the first three PCs are retained, and their graphical representations are shown in Fig. 6.10a–6.10b.

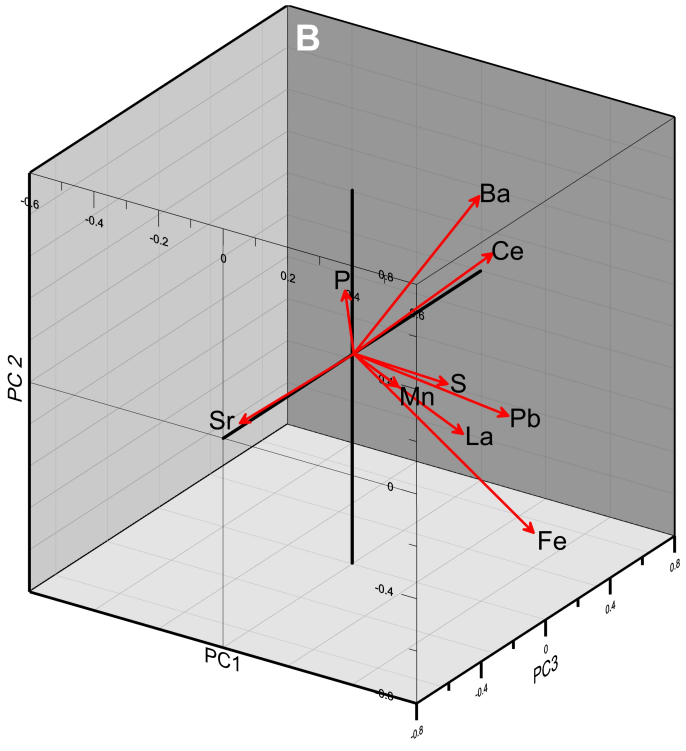
Table 6.2: Principal component loadings as variances accounted for the trace elements (magnesite and quartz minerals removed).

	PC 1	PC 2	PC 3	PC 4	PC 5	PC 6	PC 7	PC 8	PC 9
Ba	1.30%	17.50%	32.20%	2.50%	0.20%	0.70%	5.40%	30.50%	9.70%
P	8.30%	36.10%	38.40%	5.70%	1.10%	0.20%	3.80%	0.00%	6.40%
La	14.80%	1.80%	0.70%	17.00%	56.80%	0.00%	8.80%	0.20%	0.00%
Fe	27.20%	27.80%	0.70%	38.30%	0.20%	2.40%	1.70%	0.00%	1.80%
Mn	1.70%	0.80%	0.10%	21.40%	1.30%	30.90%	35.90%	7.10%	0.90%
Sr	7.20%	8.60%	2.70%	2.00%	0.20%	0.40%	2.10%	0.30%	76.50%
Ce	3.70%	6.70%	24.20%	1.20%	0.60%	0.20%	5.70%	53.20%	4.60%
S	12.40%	0.30%	1.00%	3.30%	25.50%	17.90%	35.00%	4.50%	0.10%
Pb	23.40%	0.40%	0.00%	8.70%	14.20%	47.30%	1.60%	4.20%	0.20%
Eigenvalue	4.7197	2.7882	2.1545	2.0784	1.8784	1.8047	1.6582	1.3055	0.9686
% variance	24.38	14.41	11.13	10.74	9.7	9.32	8.57	6.74	5
Cumulative % variance	24.38	38.79	49.92	60.66	70.36	79.69	88.25	95	100

This statistical analysis shows that Ba, Ce and P tend to have a closer relation, whereas S, Pb and La form a second more closely associated group (Table 6.2; Fig. 6.10b). Iron, Mn and Sr tend to follow individual patterns, more distinctly separated from other associations. The less-pronounced association of Mn with the other trace elements may imply a comparatively less selective and more homogeneous distribution within carbonate phases, although there is a tendency for Mn to co-vary with Fe. Sr is distinct from these relationships and this might reflect a preferential phase association, as yet unclear. In turn, the closer association among P, Ce and Ba (Fig. 6.10b) could reflect the existence of micro inclusions within the carbonate minerals and may indicate that some phosphorus comes from apatite, since Ba and Ce are often highly enriched in apatite minerals (*e.g.*, Shimura et al. 2014 [220]). However, the association is not extensive, suggesting that some phosphorus may be instead bound to the carbonate lattice, or that apatite micro inclusions



(a)



(b)

Figure 6.10: EPMA trace element data PCA results. Shown are the first three principal components. A: 3-D plot of the scores of each sample with respect to the first three principal components. These scores correspond to transformations of the original data (element concentration per sample), now reflecting the contribution of each sample to each principal component, which are in turn independent from each other. B: 3-D plot of the loadings, showing the contributions of each variable to each principal component. The vectors also allow to graphically represent the correlation trends among the variables.

vary substantially in composition, because P does not always co-vary strongly with Ba and Ce (Table 6.2; Fig. 6.10b). Interestingly, Fig. 6.10a–6.10b suggests that spherulites and calcite crusts tend to be relatively enriched in Ce and Ba as compared to other carbonate phases analysed. On the other hand, Fe tends to be concentrated in some specific dolomite types, such as 'bridge' dolomites (supplementary Fig. B.5), whereas other types of dolomite, such as euhedral dolomite, tend to have a uniform distribution, suggesting that they do not discriminate against specific compositions. This may suggest that they generally formed from fluid compositions that would often reflect the host rock composition or that were usually close to the primary conditions of deposition. Similarly, the broader association among Fe, Pb, La and S in Fig. 6.10b could be indicative of micro inclusions of reduced mineral phases such as pyrite.

When these data are grouped by depth and fabric in boxplot diagrams (supplementary Fig. B.5–B.7) some of these associations and tendencies become more visible. The boxplots for iron confirm the tendency for this element to be more concentrated in specific types of dolomite, such as bridge dolomites (sub-millimetric elongate dolomites following the orientation of what may have previously been Mg-silicate clays) and those found in the dolomudstone facies, potentially suggesting distinct processes involved in their formation. Primary or secondary calcite fabrics, however, tend to be depleted in Fe (supplementary Fig. B.5). It also becomes clear, for example, that not all spherulites, shrubs and crusts are enriched in Ba and Ce, but this is particularly true of sample from 11.99 m. Shrubs and spherulites from lower depths are not strictly enriched and different from other textures. Thus, the compositional variation more likely reflects changes in primary fluid composition/source with evolution of the lake or as a result of burial related mechanism, rather than an inherent feature related to the generation of once specific depositional or diagenetic fabric. Despite this, the data may still reflect preferential incorporation in these textural elements, since co-occurring minerals/fabrics at the same depth do not show corresponding enrichment in Ba and Ce. The same boxplots for phosphorus concentration calculated as ΣPO_4 (Fig. 6.11) reveal a

similar pattern as that of Ba and Ce in shrubs, crusts and spherulites analysed in the upper samples (samples 6.59 and 11.99 m), which suggests that some phosphorus likely occurs as apatite micro inclusions in these textures indeed. Furthermore, as indicated in Fig. 6.11, the median ΣPO_4 values are relatively high in different carbonate mineral textures in two of the uppermost samples analysed. The median values are particularly higher in crusts, shrubs and spherulitic calcite minerals interpreted here to have formed as primary to early diagenetic deposits, and roughly vary between 1000 and 2000 ppm (10.5–21.1 mmol/kg). In turn, the average P/(Ca + Mg) molar ratio values based on EPMA data for these three calcite textures are 1.45 ± 0.98, 1.13 ± 0.97 and 1.09 ± 0.90 mmol/mol, respectively, varying from as low as 0.01 to 4.80 mmol/mol in measured spots within shrubs (Table B.8).

In summary, our computational statistical approach shows that phosphorus, potentially as phosphate, occurs in several hundreds of ppm to a few thousands of ppm in the analysed carbonate minerals, comprised of calcites and dolomites with different textures. However, P tends to have higher concentrations in calcite crusts, shrubs, and spherulites, and is comparatively more concentrated in samples from the upper portion of the stratigraphy, among the ten thin sections analysed (Fig. 6.11 and Table B.8). Iron, a known inhibitor of calcium carbonate nucleation (Sumner and Grotzinger 1996b [125]), occurs in relatively low concentrations in these primary textures, particularly compared with some dolomite morphologies, which may correspond to different stages of diagenesis. It often co-varies with other indicators of more reduced conditions (Table 6.2), and their relative lower abundances suggest such conditions may not have been predominant.

6.7 Discussion

6.7.1 Concentration and Distribution of P in Pre-Salt Carbonates

Based on bulk rock results, phosphorus shows striking variations in concentration through the upper part of the studied well (Fig. 6.5). Although our data reveal clear

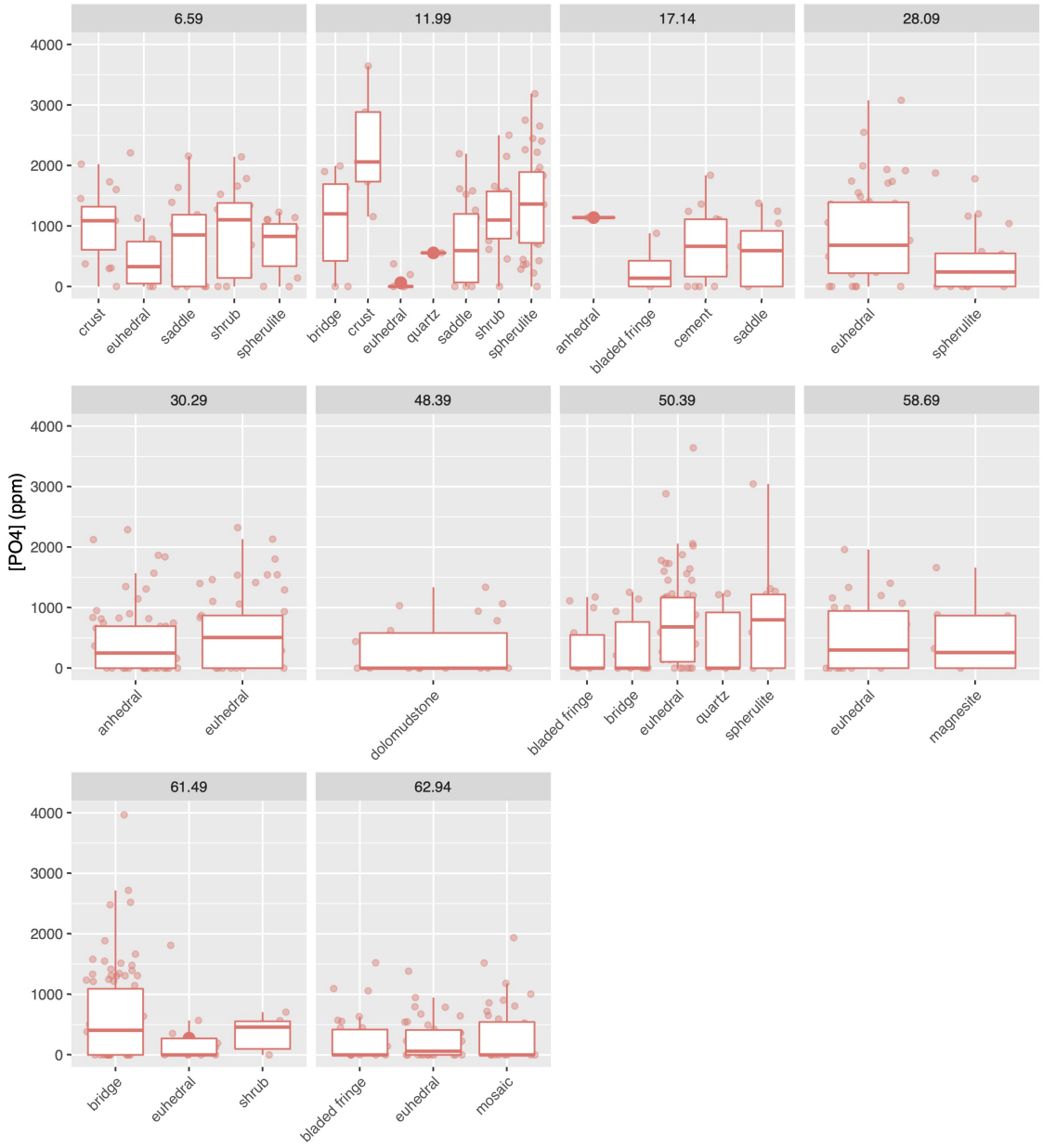


Figure 6.11: Boxplots of EPMA ΣPO_4 data grouped according to different textural elements and carbonate mineral (predominantly calcite or dolomite, but also magnesite) or quartz, from 10 individual thin section, each corresponding to a particular depth, as indicated in the figure.

stratigraphic trends in P concentration, we caution here that bulk rock analyses alone cannot provide definitive information as to the mineralogical hosts of P and its ultimate origins. Indeed, our data document spatial variability in P at the millimetre scale, which in turn can lead to unavoidable heterogeneity in sample processing for bulk rock analysis. Nevertheless, our data do clearly show that P

is associated with both skeletal and non-skeletal components. For example, our petrographic analysis shows that the upper stratigraphic interval – showing high P concentration – also hosts a greater abundance of fish bones and other phosphatic remnants.

Although phosphatic bioclasts represent an important pool of sedimentary P, our data also indicate that much carbonate-associated P is not associated with phosphatic bioclasts. For example, boxplots of ΣPO_4 data from microanalyses (Fig. 6.11) indicate that shrubby and spherulitic components composed of fibrous calcite tend to have higher phosphorus concentration than later diagenetic calcite cements. These data also indicate that crusts/shrubs and spherulites tend to have higher median values in the shrubby spherulitestones (*sensu* Gomes et al. 2020 [157]) (supplementary Fig. B.8). In turn, in the "pure" spherulitestone facies the trend is not so clear, although both spherulites and euhedral dolomites have generally higher concentrations than other fabrics in this same facies. Hence, the primary calcitic components (shrubs, crusts, spherulites) may have either formed under higher phosphorus concentrations in solution or may simply lend themselves to better preservation of solid phase P concentrations by sequestering it more preferentially than other carbonate phases, such as dolomite. This could also either suggest that modified solutions involved in silicification and in dolomitisation did not contain as much P, that could have removed P from primary carbonate phases, and/or that phosphate is not as readily accommodated in the dolomite structure relative to calcite.

Our data also show that some phosphorus correlates with Ba and Ce, which is more compatible with an apatite mineral host for P rather than a carbonate lattice-bound host (*e.g.*, Shimura et al. 2014 [220]). This implies that apatite micro inclusions could be responsible for the high ΣPO_4 content observed in these textural elements in the analysed upper samples. Although physical breakdown or disarticulation of phosphatic skeletal grains and occlusion into growing calcite cannot be completely ruled out at this time, physical comminution is unlikely to produce particles below

the beam spot size of the EPMA (*i.e.*, <10 microns). Therefore, we interpret this distinct pool of P as dominantly authigenic in origin, resulting from *in situ* co-precipitation of Ca-CO_3-PO_4, and not associated with fragments of phosphatic bioclasts.

It is critical to stress at this point that bulk rock geochemical analyses or even microanalytical techniques such as EPMA cannot on their own resolve between inorganic and organic P phases that might be present in minute amounts as intraparticle material. However, combining multiple techniques, beginning with basic petrography and aided by stable carbon isotopes and screening with microanalytical tools (SEM-EDS, EPMA, and QEMSCAN) it may be possible to provide a rough, bird's-eye view of the distribution of the elements. Particularly when they occur in mineral phases of their own and can be visible under the microscope (*e.g.*, apatite) this becomes less ambiguous. Furthermore, some of the microanalytical tools, such as EPMA, combined with improved statistical data analyses such as unsupervised PCA used in this study or supervised learning algorithms such as random forest and artificial neural networks, all of which are at the heart of modern machine learning (ML), may become able to place stronger constraints on phase-specific relationships (*e.g.*, da Silva et al. 2021 [221]; Sun et al. 2022 [222]; Acosta-Góngora et al. 2022 [223]). These microanalytical and statistical techniques combined can be relatively less time-consuming and less expensive as well, thus helping to mitigate this problem. Alternatively, selective extraction (*e.g.*, Guilbaud et al. 2020 [224]) and non-destructive analyses such as the detection of specific spectra resting on X-ray absorption near-edge structure (XANES) (*e.g.*, Ingall et al. 2011 [225]; Richardson et al. 2022 [226]) and/or solid-state nuclear magnetic resonance (NMR) spectroscopy (Mason et al. 2007 [227]; 2011 [228]; Phillips et al. 2016 [229]) can better resolve between these different phase relations. In any case, refinement of the investigation attempting to more clearly disentangle between inorganic- and organic-bound P phases should proceed employing some of these techniques that can be more diagnostic of specific P phases.

Assuming the EPMA P data reflect essentially inorganic phosphate, the elevated P concentrations of primary calcitic textures (specifically P/(Ca + Mg) ratios) lie within the range reported by Ingalls et al. (2020) [31] for non-marine carbonate minerals from several alkaline lake deposits spanning the Recent to the Eocene. These authors showed that P/Ca ratios in carbonates precipitated in these environments can be up to three orders of magnitude higher than in marine carbonates, and they report P/Ca values ranging from 0.432 ± 0.019 in the Searles Lake to 13.995 ± 0.794 in the Pleistocene Wilson Creek Formation. Marine carbonate P/Ca ratios reported in that study vary between 0.003 to 0.184 mmol/mol, encompassing biogenic coral aragonites, ooids and inorganic cements composed of aragonite, calcite or dolomite. Taken conservatively, the ratios determined in our study are ∼two- to five-fold higher than for the Eocene Green River Formation. If the P/(Ca + Mg) ratios of the Barra Velha Formation carbonates correspond to values inherited from the surficial environment of deposition, they represent a potential additional proxy for the alkalinity condition in the palaeo-lake(s), as suggested by Ingalls et al. (2020) [31] for more recent carbonate deposits. Specifically, our data lie well above the threshold of P/Ca > 0.5 mmol/mol which was suggested by Ingalls et al. (2020) [31] to limit $[Ca^{2+}]/ALK_T < 0.75$ (where ALK_T is total alkalinity), consistent with their hypothesis that high alkalinity promotes enhanced phosphate concentrations in lake bottom and sediment pore waters.

To what extent do relatively high P/Ca ratios in carbonates reflect proportionally high P/Ca ratios in their parent fluids? Büttner et al. (2020) [230] have shown that modern stromatolites forming in association with low-ΣPO_4 freshwater seeps on the coast of Cape Recife, South Africa can concentrate P in crusts of Ca-phosphate mineral phases colonised by microbial communities, including cyanobacteria. Indeed, as discussed above, biological influences on pre-salt carbonate precipitation and early diagenesis cannot be entirely ruled out. However, intervals comprised of upward fibrous-radiating textures ('shrubs') more characteristic of inorganic growth may best reflect the overall fluid composition rather than an artefact arising from biological activity during early diagenesis. Furthermore, as addressed above and

below, the broader depositional environment was characterised by prevailing alkaline and evaporitic conditions in a continental endorheic basin, as opposed to freshwaters springs on coastal areas, and thus more closely resembles the lacustrine environments addressed in Ingalls et al. (2020) [31] and Toner and Catling's (2020) [94] studies.

A remaining consideration is the degree to which diagenesis may have influenced the concentration and distribution of P in Pre-salt carbonates. To address this, we begin with trace elemental relationships with P, noting in particular enrichment of Ba, Ce, P and Sr. We infer that these elements are primarily incorporated in the carbonate phase or in apatite because available petrography and geochemical data indicate that sulphate concentrations were relatively low in lake waters (in contrast to the ocean) (*e.g.*, Wright and Barnett 2015 [18]); this, in turn, may have limited barite formation. Elevated Sr and Ba concentrations in high-Mg calcite are compatible with limited diagenetic recrystallisation, which typically decreases the concentrations of these elements in calcite (*e.g.*, Brand and Veizer 1980 [231]; Joseph et al. 2013 [232]). These data are consistent with previous studies which document limited, if any, diagenetic recrystallisation within the Barra Velha Fm (*e.g.*, Wright and Barnett 2020 [191]), and also with our EPMA data showing that calcitic crusts, shrubs, and spherulites are composed of high Mg-calcite (defined as >4 mol% $MgCO_3$; Stanley et al. 2002 [233]; Appelo and Postma 2004 [234]), with average $MgCO_3$ = 11.67, 6.60 and 7.00 mol%, respectively and maximum $MgCO_3$ = 23.03, 11.52 and 27.97 mol%, respectively.

Further suggestion of limited diagenetic recrystallisation comes from high Sr/Ca ratios (or Sr/(Ca+Mg) ratio, whose average and median values ≈3) in primary calcitic textures as well as probable early diagenetic dolomite (supplementary Table B.8). For comparison, the average Sr/Ca ratio in modern aragonites formed from seawater is 10.62 mmol/mol and calcite is 1.88 mmol/mol (Joseph et al. 2013 [232]). This may be an additional indication of overall preservation of primary carbonate textures formed under high concentrations of Sr, and/or the formation of later

phases mostly under fluid buffered conditions, where secondary carbonate minerals formed predominantly inheriting the composition of the host carbonate rocks.

It is worth underscoring that Ba, Ce, and ΣPO_4 do also vary somewhat in their concentrations among some calcite and dolomite phases. More specifically, when compared against mineralogy and morphology and grouped by depth, the observed differences point toward a possible link with stratigraphy, where higher concentrations of these elements occur in primary textures in the upper portions of the succession (Fig. 6.11 and supplementary Figs. B.6–B.7). Whether these elemental trends reflect unaltered syn-sedimentary precipitates capturing original lake water chemistry change with time or post depositional modification is difficult to disentangle. However, as discussed above, the high concentrations of some elements such as Sr, Ba, P, Ce in calcite mineral fabrics regarded primary textures, such as shrubs and crusts and spherulites (or eventually very early diagenetic in the latter case), suggest that they faithfully preserve their primary composition.

6.7.2 Pre-Salt Chemostratigraphy and the Broader Context During Carbonate Deposition

The $\delta^{13}C_{VPDB}$, $\delta^{18}O_{VPDB}$ and $^{87}Sr/^{86}Sr$ show consistent trends across a broad spatial/geographical extent in turn suggesting that these carbonates dominantly record the isotopic composition of their depositional environments rather than localised diagenetic processes (Fig. 6.12). Several possible competing and alternative mechanisms may have affected the isotopic fractionation between lake waters and the precipitated mineral phases during the formation of these carbonates. Although it may not be the final word and it is still based on interpretation of data, Pietzsch et al. 2020 [193] favoured a predominantly "equilibrated" DIC pool with atmospheric CO_2 (even though it does not necessarily follow that the solid $CaCO_3$ phase had to precipitate in strict chemical and/or isotopic equilibrium with the fluid phase). Furthermore, these correlations, consistent across a *ca.* 75 km distance between wells, further suggest that either the carbonates were formed from the same well-mixed lake waters, or from lake bodies that were at least in hydraulic communication.

Alternatively, completely isolated lakes enclosed within similar bedrock geology country rocks and within the same climatic zone might have followed similar pathways with respect to the evolution of their waters, even at slightly different times. However, this seems more unlikely, given the isotopic data discussed herein.

Stratigraphic correlation across the basin also indicates that lake waters may have remained close to chemical equilibrium with ambient atmospheric CO_2, and that climatic conditions oscillated between arid and humid, in turn controlling the balance between net evaporation and precipitation. For example, based on carbon-isotope stratigraphy the wells investigated in our study can be tentatively correlated with composite marine sections (Wissler et al. 2003 [235]; Herrle et al. 2015 [236]; Pietzsch et al. 2020 [193]), and these correspond to the zones indicated as BVF I to BVF IV (Barra Velha Fm I–IV; Fig. 6.12). Within this overall correlation, smaller cycles are also indicated across the upper Barra Velha Fm, which have been previously interpreted as different lake stages reflecting climatic oscillations, potentially affecting lake level (Fig. 6.12; Pietzsch et al. 2020 [193]). It is worth noting that the overall $\delta^{13}C_{VPDB}$ values are the heaviest across interval BVF III (supplementary Fig. B.4A), and that the $\delta^{18}O_{VPDB}$ values corresponding to lake stages 11/10 (Fig. 6.12), associated with a higher abundance of shrubstone facies, are the heaviest in both studied wells (1.92 ± 0.83‰and 1.59 ± 0.41‰, wells #3 and S10, respectively). In fact, $\delta^{18}O_{VPDB}$ values from the upper Barra Velha Fm carbonates as a whole are characteristically heavier than corresponding $\delta^{18}O_{VPDB}$ observed in diagenetically unaltered marine calcite, and heavier than marine carbonates from the late Barremian to the earliest Aptian from the Tethys palaeo ocean (Clarke and Jenkyns 1999 [237]; Menegatti et al. 1998 [238]; Föllmi et al 2006 [239]). This consideration remains valid even after accounting for dolomite content and applying the correction for different fractionation factors according to mineralogy, described earlier. Together, these isotopically enriched $\delta^{13}C_{VPDB}$ and $\delta^{18}O_{VPDB}$ values and their subtle oscillation in concert high $^{87}Sr/^{86}Sr$ ratios likely reflect lake waters that were isolated from co-eval marine waters and periodically subjected to evaporative concentration and relative freshening.

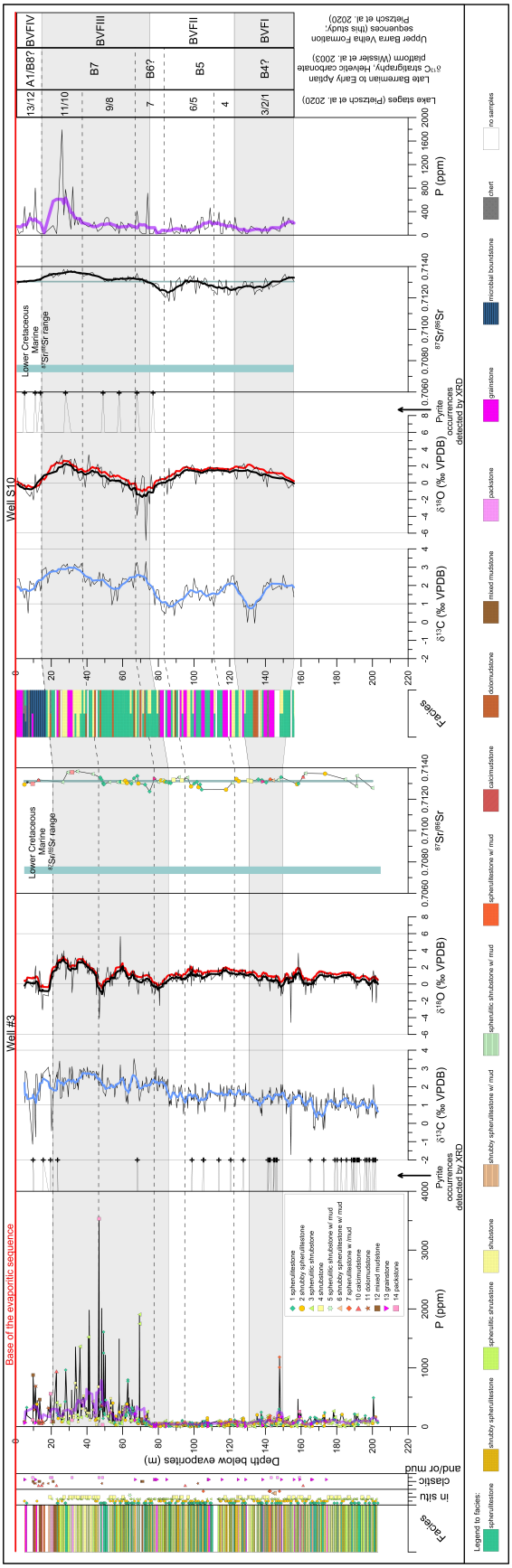


Figure 6.12: (Caption next page.)

Figure 6.12: (Previous page.) Correlation between well #3 detailed in the present study and well S10 detailed elsewhere (Pietzsch et al. 2018 [192]; 2020 [193]). New P concentration data in well S10 were acquired for the present study. Curves and colours are the same as those shown in Fig. 6.5. Pyrite occurrences detected by XRD are also shown for both wells. The light grey areas highlight the correlation between the two wells, based on stable isotopes. These grey areas are based on the correlation with the carbon-isotope curve of marine sections shown in Pietzsch et al. (2020) [193], and are henceforth designated as BVF sequences I–IV; lake units shown by the latter authors are also included for guidance, as well as additional stratigraphic information based on $\delta^{13}C_{VPDB}$ of a marine platform in the Swiss Alps (from Wissler et al. 2003 [235]).

Whether the ultimate origins of the fluids discharging into the lake(s) system might in part be derived from seawater originally infiltrating through crustal rocks (*e.g.*, Farias et al. 2019 [195]), this is not possible to disentangle with the $^{87}Sr/^{86}Sr$ data alone. The radiogenic strontium isotope data do however consistently imply that, although the contribution of fluids leaching mafic rocks was likely also important (*e.g.*, Wright 2012 [166]), there existed a relevant contribution of fluids leaching felsic rocks, which probably superseded the former by up to four orders of magnitude (Pietzsch et al. 2018 [192]). Regardless of the primary nature of the fluids (*e.g.*, whether marine or meteoric), the data suggests that these would have become significantly modified as they reacted with the crust. In this case, calcium may not have been provided in disproportionately high concentrations to the lake basin(s).

6.7.3 Geochemical Constraints on Non-Skeletal Carbonate Precipitation from a Cretaceous Alkaline Lake

Together, our analytical data indicate that primary calcitic textures are intimately associated with levels of P that tend to be higher than P concentrations reported in both biogenic and abiotic marine carbonates (Ingalls et al. 2020 [31]). These data strongly support the presence of P (presumably as ΣPO_4) in Santos Basin waters at the time of sedimentation, although complexities with P incorporation during growth preclude meaningful estimates of corresponding ΣPO_4 concentrations. Here we return to our motivating question: how might aqueous ΣPO_4 have influenced non-skeletal carbonate precipitation in the Pre-salt system? We first discuss evidence for two key geochemical features common to many Barra Velha depositional systems:

high Mg/Ca and high supersaturation. We then consider the role of dissolved phosphate in light of this evidence, and finally discuss some processes which may have promoted enhanced sedimentary P concentrations as we have documented above.

6.7.3.1 Evidence for High Mg/Ca During $CaCO_3$ Deposition

The origins of the fascicular calcite crusts/shrubs and the spherulites documented in the South Atlantic Pre-salt system have captivated several authors over the last few years, many of whom have emphasised that these fabrics reflect distinct primary to early diagenetic lacustrine carbonate chemistry (*e.g.*, Wright 2012 [166]; Wright and Barnett 2015 [18]; Lima and De Ros 2019 [188]; Mercedes-Martín et al. 2019 [189]; Gomes et al. 2020 [157]; Wright and Barnett 2020 [191]). In particular, the unusual and extensive occurrence of authigenic Mg-silicate minerals further indicates that the solutions from which these minerals precipitated was characterised by high Mg/Ca ratios (Wright 2012 [166]; Tosca and Wright 2018 [167]; Tutolo and Tosca 2018 [28]). From a mass balance perspective, the widespread deposition of authigenic Mg-silicates indicates that aqueous Mg^{2+} concentrations may have been relatively high in the parent fluid. This is because each mole of Mg-silicate (assuming an ideal talc or stevensite composition) requires three moles of Mg^{2+} from the corresponding fluid. For comparison, present-day seawater [Mg^{2+}] contains roughly 50 mmol/kg (Zeebe and Wolf-Gladrow 2001 [72]), whereas an average alkaline lake would contain five-fold less than that, based on the present compilation discussed in Chapter 4. Anyhow, in order to fill pore spaces on the scale observed in the Pre-salt sediments comparatively high dissolved Mg^{2+} concentrations would have been required.

Additional constraints on Mg/Ca arise from the mineralogy, microtexture, and morphology of the fibrous calcite components themselves. Petrographic evidence for primary aragonite precipitation has yet to be conclusively documented in the Barra Velha Fm (Wright and Barnett 2020 [191]). The fibrous morphology of the calcite itself is understood to result from growth rate anisotropy of different calcite

crystal surfaces, which is strongly controlled by solution chemistry (Folk 1974 [240]; Davis et al. 2000 [25]; Richter et al. 2011 [16]). Previous work has shown that the incorporation of foreign cations into growing calcite crystals is in turn controlled by the surface structural differences among calcite crystal faces (Paquette and Reeder 1990 [241]; Paquette and Reeder 1995 [242]; Davis et al. 2000 [25]; Davis et al. 2004 [243]; Hong et al. 2016 [244]). As a result, different cation and anion components are taken up in different configurations and at different rates on to growing calcite surfaces, which strongly controls relative growth rates and therefore crystal morphology. Experiments investigating the role of Mg^{2+} uptake onto growing calcite surfaces have shown that Mg^{2+} incorporation leads to inhibitory effects and the accumulation of lattice strain at positive and negative edges of {104} faces; this in turn leads to the development of new {010} faces and elongation of the calcite crystal habit along the *c*-axis (Davis et al. 2004 [243]). Together, these constraints support the inference that Mg/Ca was relatively high during $CaCO_3$ growth, and that Mg^{2+} was commonly present at concentrations that would have directed the growth morphology of calcite toward fibrous forms, perhaps via the mechanism suggested by Davis et al. (2004) [243].

6.7.3.2 Evidence for High $CaCO_3$ Supersaturation

The morphology of calcite crystals that construct the dominant depositional components of the Barra Velha Formation indicates that in addition to high Mg/Ca, $CaCO_3$ precipitation occurred in association with high supersaturation states with respect to calcite. First, calcitic components of the Barra Velha Fm are dominantly composed of fibrous calcite in either upward-radiating polycrystalline aggregates or spherulitic aggregates (*e.g.*, Gomes et al. 2020 [157]; Wright and Barnett 2020 [191]). These aggregates are characterised by low-angle (or non-crystallographic) branching between individual crystals, which is a distinctive characteristic of so-called spherulitic growth. Experimental and theoretical investigations of crystal growth indicate that spherulitic growth requires very high relative supersaturations. For example, in an experimental investigation of the crystal growth of plagioclase

feldspar, Lofgren (1974) [245] observed that the morphology of the growing crystals evolved in response to changes in the degree of undercooling (or supersaturation, expressed as the difference in temperature between the equilibrium temperature and that of crystal growth) of the melt. With increases in undercooling, plagioclase crystals evolved from tabular or euhedral lamellar forms to skeletal morphologies produced when growth rates were fastest at edges and corners. With further undercooling dendritic crystalline morphologies were produced, and only the highest levels of undercooling generated spherulitic aggregates.

The development of classical growth theory has further clarified the conditions required for dendritic and spherulitic crystal growth and helps reconcile experimental results such as those reported by Lofgren (1974) [245] and many others. Briefly, classical growth theory successfully predicts that at low supersaturation, crystal growth proceeds through a so-called spiral growth mechanism (Lasaga 1998 [145]). This mechanism generates euhedral crystals with atomically smooth interfaces. At supersaturations above a critical threshold, nucleation on the crystal surface becomes energetically favourable, and the formation and growth of 2-dimensional nuclei takes over as the dominant growth mechanism (Lasaga 1998 [145]). Under this growth regime, 2-D surface nucleation is most favourable at the edges or corners of growing crystals. These 2-D nuclei thus advance inward to the centre of the growth face, a process which commonly produces hopper-type or skeletal crystal morphologies, also with atomically smooth interfaces (Lasaga 1998 [145]). As supersaturation increases further beyond a second critical threshold, a transition to aggregation-based growth occurs. Above this threshold, three-dimensional nucleation (or particle aggregation) occurs at the interface where local supersaturation is highest (Lasaga 1998 [145]; Sunagawa 2005 [148]). In general, this growth mechanism leads to inherent instability at the growing interface with crystalline morphology determined by the interplay between component transport and the kinetics of the growing interface (*e.g.*, Gránásy et al. 2005 [246]). In addition, this growth regime is also associated with a transition from atomically smooth to atomically rough interfaces, reflecting a shift in the mechanism of crystal growth at the molecular scale. It is

above this critical supersaturation that dendritic and spherulitic morphologies are produced.

Kinetic theory further predicts that this "roughening transition", and therefore the onset of spherulitic growth, occurs with increasing supersaturation (that is, greater free energy changes associated with growth) and is associated with smaller differences in bonding characteristics between solution and the growing interface (Lasaga 1998 [145]). In other words, phases with low surface energy will display atomically disordered and therefore rough surfaces upon growth whereas phases with higher surface energy will display surfaces with ordered and therefore atomically smooth atomic-scale characteristics. Indeed, Monte Carlo simulations of the atomic structure of growing interfaces support these relationships, and have de-lineated the roughening transition in terms of supersaturation and bonding characteristics (Xiao et al. 1988 [247]; Xiao et al. 1990 [248]).

These theoretical predictions are in turn consistent with observations of growing calcite surfaces as a function of supersaturation. For example, atomic force microscopy (AFM) was used to show that at low levels of supersaturation (*i.e.*, $\Omega_{\text{calcite}} <$ 2-10 at low Mg/Ca, where $\Omega_{\text{calcite}} = (a_{Ca^{2+}} * a_{CO_3{}^{2-}})/\text{Ksp}$), calcite growth proceeds via the screw dislocation mechanism on (10-14) surfaces (Rodriguez-Navarro et al. 2016 [2]). With increasing supersaturation (*e.g.*, above $\Omega_{\text{calcite}} = 3$; Rodriquez-Navarro et al. 2016 [2]) 2-D nucleation has been observed. One recent AFM-based study showed that calcite growth beyond 2-D nucleation (taking place at $\Omega_{\text{calcite}} > 122$) involves the production of ACC nanoparticles which then diffuse along the interface and attach to kink sites exposed at the surface (Rodriguez-Navarro et al. 2016 [2]). Restructuring and fusion of the ACC nanoparticles with the calcite substrate facilitates continued growth of the calcite crystal. Indeed, the low surface energy of ACC (Rodriguez-Navarro et al. 2016 [2]) and high supersaturations required for this growth mechanism are consistent with predictions from kinetic theory, as discussed above. This ACC-mediated growth mechanism may, in fact, be characteristic of calcite growth above the "roughening transition" and therefore

inherent in the production of spherulitic calcite structures like those dominating the Barra Velha Formation. In addition, these observations open the possibility that growth above the roughening transition may carry distinctive trace element and isotopic signatures. For example, ACC is known to be relatively indiscriminate toward the incorporation of trace elements such as Sr^{2+} (Littlewood et al. 2017 [249]), and elevated Sr^{2+} content, such as observed in Barra Velha Formation carbonates, may be in part result from ACC recrystallisation, and/or from Sr^{2+} accumulation in parent waters.

A final constraint on supersaturation states associated with $CaCO_3$ precipitation arises from the apparent co-precipitation of Mg-silicate and $CaCO_3$ from the same fluid. Mg-silicate minerals are important authigenic components in Pre-salt sediments, and their presence constrains pH to $\geq$ 8.5 (Tosca et al. 2011 [250]; Tutolo and Tosca 2018 [28]; Baldermann et al. 2018 [251]). In addition, petrographic evidence indicates that Mg-silicates and Mg-calcite grew in intimate contact with one another, likely from the same fluid (*e.g.*, Wright and Barnett 2015 [18]; Herlinger et al. 2017 [185]; Lima and De Ros 2019 [188]; Wright and Barnett 2020 [191]). This relationship requires that total alkalinity (ALK_T) of the waters must have been equal to or greater than 2*[Ca^{2+}] in order for pH to remain high enough to precipitate Mg-silicate (Al-Droubi et al. 1980 [38]; Strauss and Tosca 2020 [252]); this consideration finds additional support in the P/(Ca + Mg) data discussed above. In addition, stratigraphic correlation across the basin also indicates that lake waters may have remained close to chemical equilibrium with ambient atmospheric CO_2 (Pietzsch et al. 2020 [193]; Fig. 6.12). Thus, if we assume that the lake maintained chemical equilibrium with ambient atmospheric pCO_2, we may derive coarse constraints on carbonate chemistry associated with Mg-silicate/Mg-calcite deposition from Barra Velha Formation lake water. Using conservative values on early Barremian pCO_2 values derived from stomatal indices ($\sim$600-1100 ppm CO_2) (Haworth et al. 2006 [253]), through chemical equilibrium relationships we conclude that $\Omega_{calcite}$ must have been higher than 14-45 and likely

within the range of 100-180, consistent with transitions to aggregation-based growth taking place at ACC saturation of $\Omega_{calcite}$ ~122, as discussed above.

6.7.3.3 The Potential Role of ΣPO_4 in Influencing Non-Skeletal Carbonate Precipitation in the Barra Velha Formation

Overall, mineralogical, textural, and geochemical constraints from primary to early diagenetic calcitic constituents indicate that aragonite nucleation and growth was inhibited, yet $CaCO_3$ supersaturation was likely very high. Additionally, the general absence of finely particulate (micritic) $CaCO_3$ in the shrubby and spherulitic facies indicates that nucleation of $CaCO_3$ from the water column was also inhibited. Kinetic inhibitors reduce the rate of new crystal nucleation, principally because they increase the surface free energy of nucleation by adsorbing onto clusters of dissolved species that would have become crystal nuclei (Sumner and Grotzinger 1996b [125], and references therein). This, in turn, results in preferential growth of crystals in/on existing substrates where the kinetic barrier to solid phase $CaCO_3$ formation is lower. Thus, despite high supersaturation, precipitation was maintained mostly at the surfaces of existing crystals, favouring growth.

Collectively, these observations suggest that a kinetic inhibitor of aragonite precipitation played a major role in carbonate sedimentation, likely sustaining high carbonate saturation state, suppressing the nucleation of new $CaCO_3$, and favouring calcite precipitation as growth on available solid substrates continued. Although a number of compounds are known to inhibit $CaCO_3$ nucleation and/or growth, we hypothesise that aqueous ΣPO_4 is perhaps the most effective compound in this regard (but need not be the only one; *e.g.*, Mercedes-Martín et al. 2016 [36]), in particular in systems dominated by non-skeletal carbonate precipitation. Furthermore, even though Mg^{2+} was likely present in much higher concentration than ΣPO_4, it has been demonstrated that the latter produces a significantly stronger inhibitory effect than the former (Gratz and Hillner 1993 [34]).

For the Pre-salt system of the Barra Velha Fm, we envisage that aqueous ΣPO_4 sharply reduced the nucleation and growth rate of aragonite and calcite (*e.g.*,

Mucci 1986 [116]; Dove and Hochella 1993 [118]), in turn permitting non-traditional precipitation pathways perhaps involving metastable intermediates. This general kinetic effect, in turn, would be expected to result in a progressive increase in carbonate alkalinity as carbonate burial decreases. This increase in carbonate alkalinity (and pH), is likely to have magnified the inhibition effect of ΣPO_4, which is known to be sensitive to pH, establishing a positive feedback between ΣPO_4 and alkalinity (*e.g.*, Burton and Walter 1990 [117]; Lin and Singer 2006 [35]). In fact, a recent experimental study of the effects of dissolved phosphate on $CaCO_3$ nucleation from seawater-derived solutions showed that at Mg/Ca = 5.6, nucleation of $CaCO_3$ did not occur until $\Omega_{calcite} = 80$ and perhaps higher (Roest-Ellis et al. 2021 [124]), consistent with geochemical considerations described above, and with the overall lack of finely crystalline $CaCO_3$ in some intervals of the Barra Velha Formation. Given strong evidence that dissolved phosphate may have played a role in modifying sedimentation and fabric development of Barra Velha Formation carbonates, what processes might have promoted enhanced phosphate concentrations in pore or bottom waters?

6.7.3.4 Processes Leading to Sedimentary P Enrichment within the Barra Velha Formation

Phosphorus cycling in lacustrine systems is driven by complex interactions between inorganic and biotic processes, but also by climate (*e.g.*, Boström et al. 1988 [254]). While our data cannot uniquely constrain the nature of P cycling in the Barra Valha lacustrine system, in combination with geochemical considerations they highlight processes potentially responsible for variations in P deposition and for enhanced P concentrations bound in skeletal and non-skeletal components identified toward the upper interval of our succession. First, the high P and relative enrichment in bioclasts we observe toward the upper portion of the stratigraphy may reflect initially enhanced phosphate availability in the water column (and possible eutrophication) which favoured expansion and restructuring of lake biota. However, although Wright and Barnett (2020) [191] interpreted enhanced phosphatic bioclast deposition as a signal of lake water freshening, this same interval is dominated by

depositional components that reflect high alkalinity and evaporative concentration (*i.e.*, predominance of shrubstones, followed by spherulitestones, which in turn often occur in association with Mg-silicates requiring high pH to precipitate, and somewhat high stable isotope values). In addition, previous work has shown that the diversity and abundance of ostracods – dominated by a halotolerant genus – tend to decrease upwards across the Barra Velha Fm (*e.g.*, Pietzsch et al. 2018 [192]), suggesting that conditions became progressively less tolerable for these animals. Together, these observations indicate that lake water chemistry was highly variable, where periods of faunal colonisation and phosphate skeletonization were punctuated by sporadic eutrophication, and increasing alkalinity and evaporation, ultimately favouring high mortality rates.

It has also been suggested (*e.g.*, Wright and Barnett 2020 [191]) that primary productivity may not have been significant for an extensive part of the depositional history, based on circumstantial observations indicating a lack of fossilised bacterial remnants as well as on work suggesting that high alkalinity may hinder adequate cell physiology maintenance (Konhauser 2009 [255]). These interpretations are complemented by indications that productivity levels were likely variable in the Pre-salt lake(s), possibly becoming higher in the upper metres of the Barra Velha Fm (Wright and Barnett 2020 [191]; Pietzsch et al. 2020 [193]). However, it is generally acknowledged that modern alkaline lakes are currently among the most productive environments on the planet (*e.g.*, Chase et al. 2021 [78]). Therefore, it is also possible that the primary productivity in such a Pre-salt lake (or lakes) may not have been as restricted as initially considered. For example, recent work by Azerêdo et al. (2021) [256] reported for the first time the presence of fossils of charophyte algae found in samples of laminated spherulitic mudstones of the Barra Velha Formation. Charophytes are multicellular algae that thrive in fresh to hyperalkaline waters (Soulié-Märsche and García, 2015). Nevertheless, from Azerêdo et al.'s (2021) [256] work the stratigraphic position where the fossils were documented is not clear; if they were found in the last tens of metres of the Barra Velha Fm it would simply reinforce current interpretations suggesting its uppermost

part may have resumed to relatively fresher and more tolerable conditions. However, regardless of the possibility of relatively high primary productivity, it seems that conditions for extensive preservation of organic material in the Barra Velha lake(s) may not have been favoured, as discussed herein. For instance, daily or seasonal lake water overturn might have prevented meromixis and the development of a permanent chemocline, and thus lake bottom waters might not have developed permanent anoxia. This would in turn favour remineralisation of the organic matter (OM) and prevent its preservation.

In turn, enhanced P supply to lake waters, and potentially eutrophication, carry some specific consequences for carbonate and phosphate water column and pore water geochemistry. For instance, enhanced primary production in the near surface would have in turn driven enhanced respiration of organic matter, which, depending on the dominant metabolic pathway, would have strongly influenced carbonate and phosphate mineral stability. For example, aerobic respiration in the water column or sediments is accompanied by increases in DIC but not alkalinity, ultimately resulting in a decrease in $CaCO_3$ saturation state (Zeebe and Wolf-Gladrow 2001 [72]; Soetaert et al. 2007 [257]). With increased biological O_2 demand in response to enhanced primary production, deeper waters may have been occasionally driven to anoxia, a condition which might have been stable for extended periods depending on the physical processes sustaining stratification (Boehrer and Schulze 2008 [258]). Anaerobic respiration, however, may also have been accompanied by decreases in $CaCO_3$ saturation at depth if ambient concentrations of SO_4 and sedimentary Fe were limited, which would have increased the relative importance of methanogenesis (which decreases Ω_{calcite}) relative to microbial SO_4- and Fe-reduction (which increase Ω_{calcite}). Overall, however, evidence for pervasive anoxia in the water column and/or sediments during Barra Velha Fm deposition is limited. The OM content in thin sections is low, and the $\delta^{13}C_{\text{VPDB}}$ values do not generally reflect extensive remineralisation of OM or microbial metabolisms involving sulphate reduction or methanogenesis. Additionally, although pyrite tends to be a common accessory mineral observed in thin sections, occurring as euhedral and framboidal crystals

a few microns to several tens of microns in size, only traces could be detected by XRD, in just 8.8% of the samples (60 out of 679). Furthermore, these occurrences are not predominantly associated with the high P levels (Figs. 6.5 and 6.12). These observations may indicate that the high P levels could be associated with lower depositional rates and a proportionally higher P flux to the sediments at this interval.

Alternatively, these considerations suggest that enhanced supply of phosphate may have forced much of the water column and underlying sediment pore waters to become more corrosive to Ca-carbonates and phosphates than surface waters. This would have been a direct consequence of the decay of organic matter, locally decreasing the pH. These waters would also be expected to be rich in dissolved phosphate because phosphorus hosted in OM is efficiently mined during respiration; this may have been supplemented by anoxic conditions if and when they developed, because anoxia is understood to result in sediment P regeneration to the water column (Ingall et al. 1993 [259]; Ingall and Jahnke 1994 [260]). Aside from OM-bound ΣPO_4 and redox-dependent P regeneration, phosphatic skeletal components may have played an important role in cycling P between lake water and sediment pore waters as lake water chemistry fluctuated. As discussed above, aerobic or anaerobic organic matter remineralisation, or both, would have locally driven pH downward as DIC would have been produced while conserving total alkalinity (Soetaert et al. 2007 [257]). As a consequence, phosphatic bioclast dissolution may have been favoured, therefore returning phosphate to pore/lake water. In fact, our microanalytical data indicate that phosphorus tends to occur in higher concentration in spherulitic and shrubby calcite crystals in samples towards the top of the succession, in turn suggesting that P cycling was probably very efficient in removing P from proximal sinks (*e.g.*, bioclasts and/or organic matter) back to solution. Lake mixing and overturn, perhaps on daily, seasonal, yearly or decadal timescales (Boehrer and Schultze 2008 [258]) would have resupplied surface waters with these nutrients.

However, although not the only process capable of driving large scale changes in P cycling, evaporative concentration may have played an important role in shifting the degree of internal P recycling and the permanent P sinks within the Barra Velha system. For example, it is widely understood that if the water column or dilute inflow was associated with relatively high $ALK_T/(Ca + Mg)$ ratios, further increases in evaporation would then drive increases in pH due to residual alkalinity left after carbonate mineral formation (Al-Droubi et al. 1980 [38]). Toner and Catling (2019 [261]; 2020 [94]) have documented that alkaline lakes are often accompanied by high dissolved ΣPO_4 concentrations because carbonate mineral precipitation removes Ca which otherwise would promote the precipitation of relatively insoluble Ca-phosphate minerals. However, although enhanced ΣPO_4 concentrations may result as a *consequence* of high alkalinity, they may also serve as an important *contributing factor* to high alkalinity itself. ΣPO_4 is a strong inhibitor of $CaCO_3$ nucleation and growth, which would have decreased the $CaCO_3$ precipitation flux and therefore the dominant process removing alkalinity from the lake. This may have been associated with a positive feedback given that the inhibition effect of ΣPO_4 is known to increase in magnitude with increasing pH. In fact, in a recent evaluation of modern alkaline lake geochemistry, Fukushi and Matsumiya (2018) [1] noted that Ca^{2+}, Mg^{2+} and CO_3^{2+} concentrations in alkaline lakes are poised at saturation with respect to metastable solid carbonate phases, including amorphous Ca and/or Mg-carbonate. Together, the data compiled by Fukushi and Matsumiya (2018) [1], Toner and Catling (2020) [94] and Ingalls et al. (2020) [31] are consistent with the inference that $CaCO_3$ supersaturation, a key characteristic of alkaline lakes in general, must be sustained in part through kinetic inhibition of $CaCO_3$ nucleation and/or growth.

Finally, periods of high alkalinity (and perhaps high salinity) may have, in turn, carried important consequences for P and N cycling. For instance, high pH shifts chemical equilibria of dissolved nitrogen species such that large fractions of NH_4^+ produced in bottom waters and sediments would exist as toxic and volatile NH_3 (Jellison et al. 1993 [30]; Clarisse et al. 2019 [262]). The processes of ammonia

poisoning and volatilisation are widely recognised to generate significant deficits in fixed nitrogen in many alkaline lake systems (Clarisse et al. 2019 [262]). Similarly, high salinity could also have been important in reducing the capacity of nitrogen fixers to keep up with nitrogen demand relative to phosphorus (Herbst 1998 [263]). If nitrogen became limiting, dissolved P would be expected to increase in the lake, which may be recorded in the enhanced P contents of authigenic $CaCO_3$ formed in response to these conditions (Figures 6.11 and 6.12). As a consequence, potential attenuation in primary production, deriving from N limitation, may have resulted in substantial inorganic P deposition in $CaCO_3$ and as phosphate minerals. Although these processes may have been important at times, they do not preclude other potential perturbations to P cycling in the Barra Velha system. However, the hypotheses outlined above are consistent with petrographic data, our sedimentary P data presented above, as well as general geochemical considerations. For example, if N isotopes can be further investigated in residual organic matter preserved in the Barra Velha Fm deposits, they may provide clues as to whether large isotopic fractionations arising from the dissociation of NH_4^+ and subsequent volatilisation of NH_3 occurred under the inferred high pH values (*e.g.*, Stüeken et al. 2015 [264]). These hypotheses are also testable with further detailed modelling and further constraints on the concentration, distribution and speciation of both P and N in Barra Velha Formation sediments.

6.8 Conclusions

Our study provided new sedimentologic and geochemical evidence for non-skeletal carbonate minerals as important hosts of phosphorus in a dynamic alkaline lake setting established in the Early Cretaceous. Based on this dataset, as well as on theoretical considerations and experimental observations reported in the literature, we find support to earlier suggestions that this environment supported conditions for prolonged saturation and precipitation of $CaCO_3$. Here we suggest it was maintained by feedbacks between supersaturation itself, high alkalinity, and dissolved phosphate. Sedimentary geochemical data indicate that phosphate concentrations through time,

reflected in bioclastic and authigenic P pools, were likely modulated by changes in lake water level, productivity, turnover and possibly in the supply of Ca^{2+} ions to the lake water. Release of P from particulate organic matter and bioclasts, as a result of microbial activity in either aerated or anaerobic conditions, may have promoted an increase in phosphate in solution, which may have been further enhanced by increased alkalinity and evaporation. The latter may have been a strong factor favouring phosphate build up in solution. Under these conditions, productivity may have decreased relatively, as dissolved N instead of P would likely have become limiting. This increase in phosphate under higher alkalinity probably carried additional impacts on calcium carbonate precipitation through pH-dependent inhibition mechanisms. This seems to have changed the dynamics of $CaCO_3$ precipitation, which are reflected in the more pronounced accumulation of shrubstone and spherulitestone facies associated with higher P content in two wells considered in this study. Whilst at this point it was not entirely possible to constrain with absolute confidence the ultimate source of sedimentary P, the possible mechanisms involving cycling of organic matter or inorganic enrichment of phosphate in the lake have been thoroughly highlighted. Further studies will be needed to narrow down the most likely sources of phosphorus to this environment.

The considerations regarding the geochemical and isotopic composition of the two main calcite morphologies discussed in this chapter, along with the observations and discussion in the previous chapters, can help to shed some light on their mechanisms of precipitation. The "shrubs" seem to unambiguously represent heterogeneous growth, facilitated by a pre-existing interface between a substrate and the fluid from which they grew, thereby reducing the energetic barrier for their growth. The spherulites may have formed either as a result of homogeneous nucleation (which would imply high supersaturation, thereby also implying inhibiting compounds) or following nucleation and growth in a concentrated fluid or some (colloidal) matrix. Fluids concentrated in Si and saturated with respect to Mg-silicate clays have been shown to decrease the induction time of carbonate precipitation and even inducing spherical $CaCO_3$ morphologies (Tutolo and Tosca 2018 [28]). In this case,

it seems that SiO_2 and ΣPO_4 might have competing effects on $CaCO_3$ nucleation and growth, something that requires to be further explored. However, this latter condition would also suggest high $CaCO_3$ supersaturation, since a solution close to or above Mg-silicate clays' saturation would imply a pH $\geq$8.5. This reasoning suggests therefore that shrubs might have precipitated under comparatively lower saturation or lower inhibiting compound concentrations, since the energetic constraints are also lower, and spherulites might have required higher saturation states to form. It is important to highlight that the *bulk* isotopic composition of shrubs and spherulites might accommodate an opposite interpretation (Appendix B). However, this might also be related to kinetic effects involving the formation of metastable precursors, rather than directly reflecting the isotopic fractionation during the precipitation of calcite crystals forming directly and strictly close to equilibrium conditions.

The observations reported here may help to guide new investigations into the mechanisms of non-skeletal carbonate deposition, both in non-marine and marine environments, as well as in the time preceding the emergence of biomineralising organisms (*i.e.*, the Precambrian). Furthermore, abiotically-driven geochemical processes required for the concentration of soluble phosphorus in surface environments may not have been difficult to attain on the early Earth, as noted by recent studies of alkaline lakes (Ingalls et al. 2020 [31]; Toner and Catling 2020 [94]) and suggested here for this Cretaceous setting. Importantly, however, our data shed light on geochemical feedbacks that would have influenced the evolution of alkaline systems across other periods of Earth's history, and provide a framework for understanding just how widely alkalinity and P concentrations might have fluctuated in dominantly abiotic sedimentary systems. Finally, given its relatively good preservation, absence of metamorphism or alteration due to uplift and weathering, this sedimentary system may be yet a relevant testing ground for probing these ideas further, as well as the behaviour of other geochemical proxies under fewer overlapping long-term geological processes.

6.9 Addendum

The data discussed here has potentially interesting implications for the vast lacustrine carbonate deposits found in the Lower Cretaceous basins in the South Atlantic Ocean. The sheer size of these deposits preserved in the sedimentary basins along the margins of Brazil and western Africa together has been seen as a seeming conundrum, which indeed requires explanation. They have often been regarded as gigantic deposits that required 'huge' amounts of Ca^{2+}, Mg^{2+} and SiO_2 to form (*e.g.*, Lima and De Ros 2019 [188]), implying anomalously high fluxes of these elements, thereby requiring some unique condition at that time, and therefore outstanding questions remains unanswered: How might these deposits have accumulated? Were they necessarily driven by some unique or unparalleled condition in the geological history of the planet?

It may be a correct statement that the deposits are generally thick and extend for large geographical areas. However, it is evident that such statements are required to be grounded in physical and therefore more quantitative estimates. In this sense, it may be a useful exercise to consider a first order approximation, starting by ignoring later extra basinal fluids that may or may not have contributed to the present mass and volume of carbonate rocks preserved in place in any of these basins.

Accordingly, we may consider a few coarse constraints, specifically focussing on the Santos Basin Barra Velha Fm carbonate system. The area of the basin is 352,000 km^2, and we could conservatively assume the average thickness/calcium carbonate content in the BVF to be 50 m (Gomes et al. 2020 [157]) and (also excluding Mg-silicate clays, silica/chert, dolomite, pores and other minor components), then

The volume of rock $V_r = 1760 \times 10^{10}$ m^3

This estimate is clearly strongly dependent on assumptions from sparse published data that do not provide a clear picture of the real volume of carbonate rock alone contained in the Santos Basin and comprising the Barra Velha Fm, which also contains other lithotypes/minerals and variable porosity.

Considering the calcium atomic number = 40.078 g/mol and the gram-formula weight of $CaCO_3$ = 100.086 g/mol, then assuming this volume of rock is comprised of 100% $CaCO_3$, in other words it contains Ca^{2+} and CO_3^{2-} in the proportion 1:1, therefore it contains 400 g Ca/kg rock.

Total calcium in this volume of rock: $[Ca^{2+}]$ = (400 g/kg) × (1/40.078 mol/g) = 10 moles Ca/kg rock.

Considering now the density of calcite = 2709 kg/m^3

$\rho = M_r/V_r \therefore M_r = V_r \times \rho \therefore (1760 \times 10^{10}\ m^3) \times (2709\ kg/m^3) \therefore M_r = 4.768 \times 10^{16}$ kg

Where V_r and M_r are the volume and mass of rock, respectively, of carbonates of the BVF.

Under the above assumptions, the total $[Ca^{2+}]$ in the BVF = (10 moles Ca/kg rock) × (4.768 × 10^{16} kg) = 4.768 × 10^{17} moles.

If the lake waters had 7.9 mmol Ca/L (Caspian Sea concentration, the largest modern endorheic lake, and also close to the modern alkaline lake waters average (Chapter 4), from experimental results and the theory and calculations discussed in Chapter 5):

$\therefore V_{lakewater}$ = (4.768× 10^{17} moles Ca) / (7.9 × 10^{-3} moles Ca/L) = 6.03 × 10^{19} L.

This would have been the volume of water that would ever have been required to precipitate the BVF carbonates in their entirety, across the entire time span of their deposition. It is easy to see that if Ca^{2+} concentration was higher than this, less water would have been required. For comparison, the present volume of the Caspian Sea, the largest existing endorheic lake in the world, is 78,200 km^3, or 78.2 × 10^{15} L (Meybeck 1995 [265]). This is three orders of magnitude less than the amount of water calculated above needed to precipitate the BVF carbonates. If we consider the BVF thickness as 300 m (of pure carbonate) and covering the entire Santos Basin, which is more likely an overestimation, the figure above increases

six-fold, to 3.62×10^{20} L, now four orders of magnitude greater than the current Caspian Sea water volume. Therefore, considering these assumptions, significant quantities of water would have been likely required to precipitate the BVF at any given time, considering the time span of its deposition, roughly from three to 10 million years (*e.g.*, Pietzsch et al. 2018 [192]).

Finally, considering the assumptions above, and the volume of water of 6.03×10^{19} L filling homogeneously the entirety of the basin (which is certainly inaccurate, but may be considered as a rough first-order approximation for the purposes of our exercise here), the average water depth of this "single Santos Basin lake" would be equal to 171 kilometres, compared to an average water depth of 211 metres in the Caspian Sea (maximum depth = 1025 m). Of course, this calculated average depth is absolutely unrealistic, since these assumptions are an oversimplification and assume a hypothetical basin geometry entirely and homogeneously filled with carbonates. Therefore, they ignore several other factors that could have influenced differently the evolution of the lake(s), such as variable basin topography and compartmentalisation, resulting in separate and different lakes at any given time, variation through time in Ca^{2+} concentration levels (steady-state and non-steady-states), seasonality, aridification, humidification, and sustained supersaturation resulting from inhibitory effects, such as what happens in the present in many complex and saturated solutions, such as the seawater and saline/alkaline lakes in general. Even so, these approximations are useful in the sense that they may steer additional investigations regarding the potential effects of all these factors and their broader implications if any for the changing hydrological cycle regime during the time of deposition of the BVF.

Still, this reasoning can be extended further to make a more realistic scenario of basin filling during time intervals, also ignoring the uncertainties associated with the duration of the time and cycles of deposition of the BVF. For the sake of the exercise, if we assume the entire deposition took 10 million years, and that every 50,000 years the water filling the space of this basin with hypothetically ideal

geometry was completely renewed, then the average depth and volume of water filling in the entire basin at each interval of 50 thousand years would be 856 metres and 3.02×10^{17} L, respectively. This is still a volume of water 10 times larger than that of the Caspian Sea, being re-cycled and existing continuously for 200 cycles of 50 thousand years. Therefore, whilst the *concentration* of elements such as Ca^{2+} required to create the BVF may not have been anything like anomalous, the *fluxes of water* required to transport the elements were likely high. However, it is worth pointing out again that this exercise places a likely maximum volume of water ever required to form the BVF. It is not meant to claim that the calculated volume accurately reflects the real amount of water involved in the transport of elements and thus in the deposition of the BVF. As helpful as this exercise is, the caveats mentioned earlier should all be considered.

A similar reasoning can be applied to the evaporitic salt layer on top of the Barra Velha Fm. If they are predominantly derived from marine waters, one may assume seawater compositions compatible with that expected for the Cretaceous, and take the relative proportions of anhydrite and halite and the average thickness of the evaporites. Then, the amount of seawater inflow to the basin can be estimated.

6.10 Directions of Future Work

Despite unparalleled advances in analytical techniques for chemical and mineralogical characterisation of solid materials, it is clear that we still rely on good petrographic characterisation of a rock sample. Not all calcites and dolomites are the same in one hand specimen or even in a single thin section, and often their different crystal textures and morphologies reflect different stages of (pore) fluid evolution and crystallisation. Detailed petrographic work coupled with advanced geochemical techniques can generate excellent quality data. Together with new computational tools, algorithms and modern programming languages, geochemical and mineralogical investigations can benefit greatly from the "big data" transformation, revealing hidden compositional patterns in the crystalline phases. This may

therefore contribute to the making of new hypotheses regarding fluid evolution and potentially about different pathways of crystallisation in sedimentary basins. These combined tools and skills can improve our ability to distinguish different processes in sedimentary basins and bring new insights to understand better the stages of evolution of sedimentary rocks. Thus, a more complete picture of the geological evolution of sedimentary basins and, ultimately, of Earth surface processes through time, from the moment of deposition to burial diagenesis, can be built.

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7 Conclusions

7.1 Concluding Remarks

This work explored the geochemistry of alkaline lakes with a special focus on the carbonate and phosphate subsystems. In this pursuit, the present work contributed with a modification and an expansion of the code thermo_phrqpitz.tdat, which builds on theoretical thermodynamic and aqueous geochemical framework originally developed by Kenneth Pitzer and many others (Chapter 2). The ensuing results therefore permitted the explicit incorporation of available Pitzer models to treat the dissociation of phosphoric acid under high ionic strength and high alkalinity conditions, coupling it to the carbonic acid subsystem. This allowed the present work to explore the coupled behaviour of Ca-phosphate and Ca-carbonate mineral phases under high ionic strength and pH solutions. As a consequence, this treatment allows better predictions of maximum ΣPO_4 under given Ca^{2+} concentrations and vice-versa in alkaline lakes brines and high pH (Chapters 2–4).

The present work has also shown that the majority of all alkaline lakes are significantly supersaturated with respect to $CaCO_3$ minerals, specifically calcite, one of the most common sedimentary minerals and frequently used for investigations attempting to reconstruct the composition of ancient Earth's oceans, lakes and

atmosphere (Chapter 4). Roughly 80% of all alkaline lakes possess $0 < SI_{cal} < 2.9$. The remaining ∼20% are likely limited or depleted in Ca^{2+} and therefore the precipitation of $CaCO_3$ mineral phases cannot occur extensively. These are soda lakes whose waters are approaching saturation in Na-carbonate phases. Although this observation is not necessarily new (it has been emphasised at least since the seminal work of Hardie and Eugster in 1970 [90]), it is to the best of the author's knowledge the first time a global survey and major quantification of the saturation state of alkaline lakes has been made.

According to theoretical calculations shown in Chapter 4, these $CaCO_3$ supersaturated lakes can concentrate substantially high proportions of ΣPO_4, but mostly approaching the ceiling limit of $\Sigma PO_4 \approx$ 2-3 mol/kg at pH ≈ 9 and $[Ca^{2+}] \approx$ 4-5 mmol/kg. However, based on a more conservative estimate of the available data from natural alkaline lakes the average dissolved $[Ca^{2+}]$ tends to be in the order of ∼5 mmol/kg, and the maximum ΣPO_4 at this $[Ca^{2+}]$ concentration is likely lower than shown by calculations by ∼two orders of magnitude, ≈ 40 mmol/kg at pH ∼9–9.5. Some modern lakes can show higher ΣPO_4 concentrations, but on specific circumstances such as lower $[Ca^{2+}]$. The fact that ΣPO_4 does not seem to be usually higher than ∼40 mmol/kg may reflect the high productivity documented in these systems. In this case, high phosphate concentrations (as well as bioavailable nitrogen) are sequestered by photosynthesising organisms, thereby maintaining lower levels of ΣPO_4 then predicted by theoretical calculations. Conversely, ammonia volatilisation, a phenomenon that may occur as a result of high alkalinity in some lakes, may result in nitrogen becoming the main limiting factor to productivity, thereby allowing dissolved phosphate levels to increase as they may not be efficiently mined from lake waters. Alternatively, above this average ΣPO_4 threshold the sediments may also become a sink at very high phosphate and moderate to high calcium levels, precipitating as insoluble apatite minerals at such high alkalinity and pH values. Nevertheless, assuming that high productivity is the main cause of maximum $\Sigma PO_4 \approx$ 40 mmol/kg in modern alkaline lakes then, as theoretical calculations and experiments suggest, alkaline lakes in the early Earth may have

been indeed suitable for prebiotic chemistry conditions requiring available and concentrated phosphate levels.

The preceding remarks, as well as the supporting experimental investigations and modelling, in turn, have also unambiguously shown that small concentrations of ΣPO_4 of $\geq$25 μmol/kg maintain supersaturation ratios (Ω) $\approx$ 70-100 (Chapter 5). This is a strong evidence in support of the hypothesis that alkaline lakes maintain prolonged high supersaturations, despite the drive towards precipitation, as a result of inhibitor concentrations. Data from the present constant composition experiments closely match predictions estimated by using the equation $log_{Rate} = -15.76 - 1.45 \times log(PO_4^{3-}) + 3.17 \times log(\Omega - 1)$, that Mucci (1986) [116] derived from fitting his experimental data. Consequently, rates of $CaCO_3$ precipitation tend to be decreased with increasing ΣPO_4, although this effect may be counterbalanced by rates of evaporation. That is, if the lake does not maintain a water balance, the continuing evaporation is likely a forcing that works towards balancing or cancelling the effect of inhibitors. Put simply, without water the solids are all that is left. In other words, increasing ionic strength, and hence ion concentration, will tend to favour final solid products, counterbalancing the effect of inhibition. More importantly, however, is the fact that sustained supersaturation favours the crystallisation involving the formation of clusters of intermediate hydrated and metastable phases, which require lower interfacial free energy to form and which tend to incorporate impurities more indiscriminately. In other words, this potentially induces both heterogeneous or homogeneous precipitation via formation of intermediate amorphous precursors or metastable monohydrocalcite, depending on the saturation level. This is in consonance with a number of recent studies that have pointed in similar direction (*e.g.*, Blue et al. (2017)[44], Henzler et al. (2018)[50], Myszka et al. (2019)[146], Koishi et al. (2019)[266], Mergelsberg et al. (2020)[267]). The formation of aragonite is potentially prevented, and the precursor phases likely recrystallise very early into vaterite and finally into calcite. This is likely the predominant pathway leading to the final precipitation of $CaCO_3$ as

calcite, via dehydration or dissolution of precursors and reprecipitation, in many alkaline lakes.

The sum of these observations implies that MHC should be overwhelmingly the main precursor of the end product calcite forming in alkaline lakes. This carries further implications for investigations of the geological record attempting to reconstruct the chemical evolution of the planetary surface from non-skeletal carbonates. The main reason for this is that K_d's (distribution coefficients) and isotopic fractionation factors often assume values determined for "thermodynamically ideal" calcite, *i.e.*, direct precipitation of calcite formed in equilibrium conditions. In this sense, it seems important to experimentally pursue a better understanding of how MHC behaves with respect to the aforementioned parameters. Thus, future attempts to constrain the geochemical scenarios of formation of ancient lake deposits may see significant progress.

The experimental work has also shown that particle morphology (as well as mineralogy), specifically concerning non-skeletal carbonate crystals, can provide a semi-quantitative guideline on which we may be able to set at least coarse constraints with respect to pH, alkalinity, saturation state and rates of precipitation. Even though this has been a long tradition among geologists, now these interpretations are becoming more evidence-based and fine-tuned, benefiting from recent progress in theoretical and experimental work, which was also the goal of the present study. Thus, bearing in mind the caveats concerning late diagenetic events that may always completely obliterate any original fabrics, depending on the geological history of a given basin, in general morphology can be diagnostic of overall fluid conditions. For instance, taking the main textures investigated in this study, fibrous radiating crystals ("shrubs") and dumbbell- or spherulitic-shaped ("spherulites") morphotypes may be interpreted as reflecting heterogeneous nucleation at high supersaturation and homogeneous nucleation by particle agglomeration under even higher supersaturation, respectively.

The present work also highlights that the conversion of the metastable phases to the more stable ones, calcite in this case, can occur in a matter of hours. Additionally, it is confirmed that a few tens of micromoles of ΣPO_4 suppress aragonite precipitation, even at Mg/Ca ratios equivalent to the ratio in present-day seawater, where aragonite precipitation is considered to be favoured ("aragonite sea"). In modern oceans ΣPO_4 is roughly in the range of 3–4 μmol/kg, mainly because of substantial uptake by primary producers in the photic zone (Holland 1984 [6]). This may have implications for the interpretation of the ancient sedimentary record and their environments of precipitation, where supersaturation, Mg/Ca ratios and ΣPO_4 were likely variable. Could the absence or lesser amount of aragonite during "calcite seas" alternatively reflect higher ΣPO_4 concentrations and $CaCO_3$ supersaturations, rather than necessarily lower Mg/Ca ratios in the corresponding time intervals? Presently, it seems that alternative hypotheses to this "standard model" may not be completely ruled out and should be investigated. However, this assessment does not take into account the role of biomineralising organisms and their physiology, whose intracellular microenvironment is kept in disequilibrium with the surroundings, thereby permitting them to precipitate metastable phases (*e.g.*, Schoeppler et al. 2021 [46]). Different organisms, therefore, cope with different strategies and can regulate intracellular Mg/Ca and ΣPO_4 to suit their demands, adding further complications to these interpretations, and were outside of the scope of the present study.

Chapter 6 brought together the knowledge gained with fine-grained theoretical and experimental work on geochemistry with that from basin-wide geological investigation involving sedimentology and facies analysis, attempting to bridge a gap regarding the investigation of the mineralogy and geochemistry of ancient sedimentary deposits. It contributed with new datasets and a computational analysis regarding the variability of trace components in the main carbonate mineral constituents of the Barra Velha Fm carbonate rocks. The computational analysis, supported by careful petrographic characterisation and microanalytical data acquisition (Chapter 6 and Appendix B), provides a solid foundation to

investigate minor and trace element variability in different carbonate mineral textures, including phosphorus. In turn, these procedures likely provide a robust framework to investigate minor and trace element partitioning between different mineral textures and phases, mineral formation in the context of fluid evolution, and diagenesis. Based on the analysis of these datasets, P/(Ca + Mg) ratios estimated from EPMA data obtained in the main calcite textures, in combination with additional proxies, allow estimations of alkalinity and calcite saturation state of lake waters. The average P/(Ca + Mg) molar ratio values for carbonate crusts, "shrubs" and the "spherulites" in the upper part of the analysed interval are 1.45 ± 0.98, 1.13 ± 0.97 and 1.09 ± 0.90 mmol/mol, respectively. These values may suggest the waters from which these calcite minerals precipitated had $[Ca^{2+}]/ALK_T<0.75$. These data together permit the inference that lake waters had $\Omega_{calcite} > 14–45$ and possibly within the range of 100–180. This last chapter also implemented an improved calculation to determine the individual oxygen isotopic composition of calcite and dolomite in mixed carbonate mineral samples deriving from bulk rock analysis. This likely allows more accurate estimates of isotopic variability in this system for further chemostratigraphic studies. The results and the interpretations discussed in this and the preceding chapters ultimately allow one to make coarse estimations about the maximum volume of water likely required for the deposition of the Barra Velha Fm carbonates, which might have been in the order of $\sim 6 \times 10^{19}$ L, or *three orders of magnitude larger* than the *current* Caspian Sea water volume of 78.2×10^{15} L. Therefore, a large volume of water should have flown through and across the basin, from the catchment areas and through the subsurface and to the atmosphere via evaporation, during the time spanning the deposition of the BVF, estimated to have lasted from three to 10 million years. This raises additional questions about what implications could this have had for the global climate and hydrological cycle during this period of time.

Finally, these observations, deriving from the investigation of the geologic record together with the knowledge developed in the previous chapters about the chemistry of alkaline lakes and the mechanisms of calcium carbonate precipitation, may close a

gap regarding the compositional variation in trace elements incorporated in different mineral textures. In line with other experimental studies, it is suggested that saturation state, partly influenced by inhibitors (both, in turn, affecting growth rate) results in different mechanisms of precipitation, through intermediate metastable precursor phases that are more indiscriminate towards the incorporation of trace elements, thereby affecting the final crystalline products. Therefore, this caveat echoes other studies that highlight the importance of taking cautionary measures and avoid the direct interpretation of past fluid compositions from the chemical composition of mineral and rock materials. When looking at the ancient rock record, it still remains a challenge to differentiate between equilibrium and kinetic processes in the frozen products of crystallisation from long-gone fluids. Therefore, these limitations have to be considered in any study investigating ancient sedimentary rocks, and a word of caution should be uttered when directly interpreting past fluid compositions from the chemical composition of mineral and rock materials. As a rule of thumb, equilibrium conditions during the precipitation of carbonate minerals in most natural environments are likely more the exception than the rule.

7.2 Summary and Future outlook

The combined effort brought together in this study points to a clearer picture, whereby inhibitors play a decisive role in influencing supersaturation in alkaline environments. This, in turn, favours the formation of metastable intermediates that can develop unusual crystal textures and which can incorporate amounts of trace elements that depart from predictions assuming equilibrium precipitation. On the other hand, the concentration of the inhibitors themselves is controlled by complex multi-phase relations as predicted by classical thermodynamic principles, that is, the solubility and the free energy of formation of the most stable phases. In other words, even when metastable phases form first, amorphous Ca-phosphates are still more stable phases compared to metastable and amorphous Ca-carbonate phases. Thus, the concentration of the dissolved inhibitor (phosphate, in this case) will be controlled by the concentration of the corresponding ion pair (Ca^{2+}, in this case),

setting limits to its upper levels in solution. Simply, although concentrations of species and saturation of minerals can be higher than purely predicted by simple thermodynamics (*i.e.*, standard Gibbs free energies of formation), there is no contradiction or violation because complex electrolyte solutions reach more stable but transient configurations ("local equilibrium"). Upper thresholds to concentration levels of dissolved species that are allowed in solution are still governed by the more stable among the metastable phases that may form. It is just that other energetic factors have to be considered, such as the energies of dehydration or those related to the relative bond strengths involving multiple ion-pairs. Thus, hydrated phases whose interfacial energy with the solution is comparatively lower than the corresponding crystalline phase are much more likely to form first in saturated media. This all has important implications in the case of investigating the possible chemical scenarios and inhibitor concentrations from long-gone fluids when interpreting the rock record, for example from ancient non-skeletal carbonates deposits. If these physicochemical principles are assumed to be the main ones involved in the precipitation of ancient carbonate rocks and ruling out other atypical processes on the surface, such as anomalous heat and pressure gradients, thereby affecting solubility relations, it may still be possible to reconstruct a reasonably accurate picture of past surface conditions.

Likewise, these observations can be potentially relevant to investigations of natural and synthetic crystals as well as biominerals. Understanding the mechanisms of precipitation of such an array of materials and how their attributes relate to the properties of the surrounding media is a recurring shared goal among these fields. For instance, studies aiming to understand evolutionary adaptations and different strategies of biomineralising organisms in response to environmental stress often rest on the geochemistry and mineralogy of modern and fossil shells to interpret past and present environmental change. This depends on some knowledge about the steps implicated in biomineralisation, often involving amorphous and metastable precursor phases. As a result, biominerals will also carry with them different

geochemical characteristics from what directly precipitated calcite or aragonite would be expected to have.

Lastly, regarding the BVF carbonates, Chapter 6 closed showing there is still room for improvement in our current understanding of their environment of deposition and specifically regarding sources of phosphorus and its phase-specific relationships. Unambiguously disentangling between inorganic- and organic-bound P trapped as inclusions or structurally associated with the carbonate minerals has, for instance, the potential to provide insights into redox conditions of the palaeolake(s). In this respect, further investigations may find additional benefits in the development and implementation of further machine learning algorithms coupled with traditional microanalytical tools, or the use of more specific analyses, such as selective extraction, P *K*-edge XANES and solid-state NMR spectroscopy. These same implementations may yield fruitful results to the investigation of other non-skeletal carbonate deposits elsewhere. This chapter also closed indicating that, to the best of this author's knowledge, experimental studies specifically investigating the potentially antagonistic effects of dissolved silica and phosphate on $CaCO_3$ nucleation and growth have not been undertaken. Thus, there is a further need to explore this gap in our knowledge.

Appendices

A

Appendix A

A.1 Review of definitions in stable isotope geochemistry and details of calculations used in chapter 6

Basic considerations about isotope mixing, isotope fractionation during acid reaction, and corrections of $\delta^{18}O_{VPDB,bulk}$ values measured in bulk carbonate mineral samples. The calculations used here are already well-established and follow those provided in many different sources, some examples of which can be found in Hayes (2004) [268], Sharp (2007) [269] and Hoefs (2015) [270].

(1) Definition of fractionation factor for an equilibrium isotopic reaction at some given temperature between two species or substances, A and B, exchanging isotopes in reactions of the kind A $\Leftrightarrow B$

$$\alpha_{A-B} = \frac{R_A}{R_B} \tag{A.1}$$

(2) Where R is the ratio between the heavy to the light isotope, for example oxygen isotopes in CO_2 gas:

$$R_{CO_2} = \frac{^{18}O}{^{16}O} \tag{A.2}$$

(3) And also:

$$\alpha_{A-B} = \frac{1 + \frac{\delta_A}{1000}}{1 + \frac{\delta_B}{1000}} \tag{A.3}$$

(4) Where, following the original definition of McKinney et al. (1950) [271], δ corresponds to:

$$\delta = (\frac{R_{sample}}{R_{std}} - 1) \times 1000 \tag{A.4}$$

(5) Where R_{std} is the isotopic ratio in the standard material. Rearranging (eqn. A.3) we have:

$$\therefore \alpha_{A-B} = \frac{\delta_A + 1000}{\delta_B + 1000} \tag{A.5}$$

Now, it is possible to derive an expression for the determination of the acid fractionation factor during the dissolution of a bulk sample composed of a mixture of carbonate minerals, for example calcite plus dolomite. From simple isotopic mass-balance:

$$\delta_\Sigma = f_{cal} \cdot \delta_{cal} + f_{dol} \cdot \delta_{dol} \tag{A.6}$$

And hence

$$\delta\Sigma = (1 - f_{dol}) \cdot \delta_{cal} + f_{dol} \cdot \delta_{dol} \tag{A.7}$$

From (eqn. A.1) and (eqn. A.2) it follows that:

$$\alpha_{CO_2(acid)-carb(meas)} = \frac{(^{18}O/^{16}O)_{CO_2(acid)}}{(^{18}O/^{16}O)_{carb(meas)}} \tag{A.8}$$

Where "$carb_{(meas)}$" refers to the isotopic ratio in any given carbonate mineral (*e.g.*, calcite or dolomite) being measured. Based on (eqn. A.5) and (eqn. A.6), we have:

$$\alpha_{CO_2(acid)-carb(meas)} = \frac{\delta^{18}O_{CO_2(acid)VPDB} + 1000}{\delta^{18}O_{carb(meas)VPDB} + 1000} \quad (A.9)$$

Which is the fractionation produced between a carbonate mineral sample and the CO_2 gas liberated during the reaction with orthophosphoric acid, at some given temperature T (in Kelvin). If the CO_2 produced during the acid reaction is assumed to occur with the mineral calcite, the fractionation $\alpha_{(\mathrm{CO2(acid)\text{-}carb(meas)})}$ is equal to $\alpha_{(\mathrm{CO2(acid)\text{-}cal})}$, and the δ^{18}O value of the CO_2 gas released during this reaction can be calculated by rearranging equation A.9 above:

$$\delta^{18}O_{CO_2(acid)VPDB} = \alpha_{CO_2(acid)-carb(meas)} \times (\delta^{18}O_{carb(meas)VPDB} + 1000) - 1000 \quad (A.10)$$

The final, corrected, value of the bulk sample can now be recalculated from the δ^{18}O value of the CO_2 gas, the fractionation between CO_2 gas and calcite and dolomite, and the original δ^{18}O value measured in the bulk sample, combining equations A.7 and A.10:

$$\begin{aligned}\delta^{18}O_{bulk(corrected)VPDB} = f_{cal}(\frac{\delta^{18}O_{CO_2(acid)VPDB} + 1000}{\alpha_{CO_2(acid)-cal}} - 1000) \\ + (1 - f_{cal})(\frac{\delta^{18}O_{CO_2(acid)VPDB} + 1000}{\alpha_{CO_2(acid)-dol}} - 1000)\end{aligned} \quad (A.11)$$

The values of f_{cal} and f_{dol} must be corrected for their relative abundances, *i.e.*, assuming that they sum up to 100% carbonate in the sample. Swart et al., (1991) [206] determined the acid fractionation between CO_2 and low-Mg calcites for a range of temperatures, whilst Rosenbaum and Sheppard (1986) [207] determined the acid fractionation between CO_2 and dolomite at 25, 50 and 100^{o}C. The fractionation factors experimentally determined by these authors and followed in the present study are given in Table A.1.

A second-order polynomial function was used to interpolate the fractionation factors between CO_2 – dolomite determined at different temperatures by Rosenbaum and Sheppard (1986) [207]. This enabled the calculation of the fractionation factor at

Table A.1: Oxygen isotope fractionation between CO_2 and dolomite (DOL) and calcite (CAL), as a result of reaction with orthophosphoric acid, for specific temperatures.

T(°C)	**DOL (R & S, 1986)**	**CAL (Swart et al. 1991)**
25	1.01178	1.01025
50	1.01039	1.00924
75	nd	1.00853
90	nd	1.00821
100	1.00913	

75^oC, the temperature of the acid reaction during the analyses of the carbonate samples used in the present study. The polynomial function is given by:

$$Y = 4.053^{-7} \cdot X^2 - 8.6 \cdot 10^{-5} + 1.014 \tag{A.12}$$

Yielding a fractionation factor (α) between CO_2–dolomite at 75^oC equal to ∼1.00951. This was the value assumed for $\alpha_{(CO_2(acid)-dol)}$, used in equation A.11 above, allowing to finally provide a corrected value for the $\delta^{18}O$ measured in the bulk carbonate samples ($\delta^{18}O_{bulk(corrected)VPDB}$).

B

Appendix B

B.1 Statistical summaries of bulk rock geochemical and mineralogical data

A total of 489 individual thin section samples from core #3 were classified leveraging previous work (Gomes et al. 2020 [157]). All these samples with petrographic description were analysed by ICP-MS, following the methods in Pietzsch et al. (2018) [192]. Additionally, as detailed in the main text, 279 samples were re-collected with the intent to create duplicate samples from the same depth (and lithofacies). This corresponds to 768 analytical samples with corresponding petrographic description and facies characterisation. An additional 202 different interspersed plugs were collected among these 489 described samples. Finally, 130 laboratory replicates were generated, for quality control, totalling 1100 results. From this total number of analyses, 439 samples had P concentrations below the limit of detection of the method (LD <50 ppm), or ca. 40% of the total number. The relative number is the same if only the 768 samples with description are considered, in which 306 samples analysed were below the limit of detection for P. To account for these "empty" values, a random integer between 0 and the limit of detection was generated for each of these samples. This alternative is common practice and the topic is discussed

in the literature of compositional data analysis at some length (*e.g.*, Yunker et al. 2005 [272]; Martín-Fernández and Thió-Henestrosa 2006 [273]).

Whilst this procedure might be deemed an artificial expansion of the set of samples with detectable concentrations of P, the actual analytical data correspond to the set of all measured samples, whether the analytical values are above or below the detection limit. Furthermore, the fact that P was below the limit of detection does not necessarily mean these samples contain no P at all, it simply means the method did not allow the detection of P that may be present in very low concentrations. Thus, if a statistic is applied to the set that contains only detected values, it may push the values of the sample, whose aim is to be an estimator of the population, to higher values, leading to a potential overestimation of the latter.

To take a practical example, following the procedure described in the main text to estimate outliers and the range of P values that may more closely approximate to a "background" level in the studied interval, considering the set consisting only of detected P levels (N = 661), there are thus 70 outliers and the non-outlier range is 50–302 ppm. This upper threshold is higher than the value of 216 ppm P considered in the main text, which was based on the whole set of 1100 analyses, with "empty" values being replaced as described above. This permits a more conservative approach towards the estimation of central tendency values of the population and therefore the subsequent statistical analyses followed this procedure. Tables S1 and S2 show the median values of P, ΣPO_4, Ca, Mg, calcite, dolomite and quartz according to facies categories, considering the total of 768 samples with description and removing the outliers from this set, respectively. For comparison, Tables S3 and S4 in turn consider only those samples with values of P above the limit of detection (>LD) of the method.

Whilst the profiles of bulk rock P values in Figs. 6.5 and 6.12 in the main text show only the samples with detected values, being true to the analytical results within their limitations, and potentially highlighting some stratigraphic variations, the remainder of the text considered the approach described above.

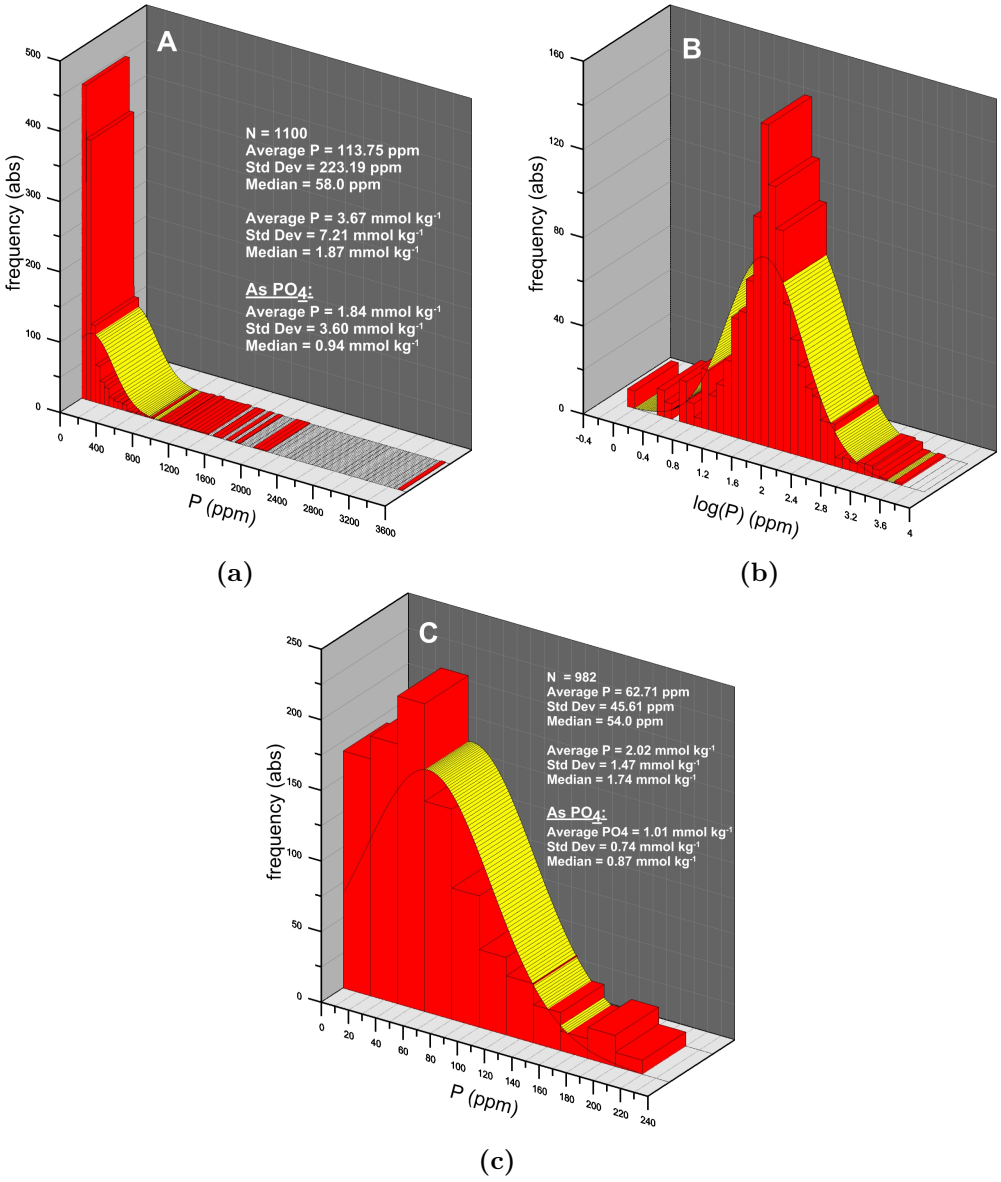


Figure B.1: Total number of bulk rock analyses (ICP-MS), the range of P concentration, and the central tendency values of total P in the analysed samples. A: histogram of phosphorus concentration [P] data, all analysed samples (with replicates) considered; B: histogram of [P] - all data, logarithm of data in (A); C: histogram of [P] - no outliers. For convenience, data are indicated in ppm units, as reported from ICP-MS measurements, and in units of mmol kg^{-1}. ΣPO_4 concentration considers measured total phosphorus (P) as phosphate (ΣPO_4).

B.2 Additional chemostratigraphic data

Stable isotope ratios provide additional context for the origin of P in these carbonates. Both the $\delta^{13}C$ and $\delta^{18}O$ values tend to show a relative increase towards the top of the section. The $^{87}Sr/^{86}Sr$ ratios also show considerably radiogenic values. All

Table B.1: Median values according to facies, from 768 samples across the entire studied interval – 489 originals (with facies description) plus 279 duplicate samples.

Facies category*	[P] mmol/kg	[ΣPO_4] mmol/kg	dolomite %	quartz %	calcite %	[Ca]meas[a] mmol/kg	[Ca]min[b] mmol/kg	[Mg]meas[a] mmol/kg	[Mg]dol[c] mmol/kg	P/(Ca+Mg)meas[a] mmol/mol	P/(Ca+Mg)min[b] mmol/mol	N samples
1	2.08	1.39	45.2	14.2	35	6144	5947	2384	2450	244	248	186
2	1.84	1.23	41.2	13.5	44	6850	6631	2185	2235	204	208	157
3	1.71	1.14	28.5	12.1	53.4	7229	6883	1591	1547	194	203	249
4	2.07	1.38	24.6	7.6	63.5	8073	7681	1277	1334	221	229	87
5	5.17	3.46	32	10.4	57.6	7190	7491	2128	1735	554	560	1
6	4.29	2.87	42.7	17	34.6	5960	5774	2068	2317	535	531	6
7	5.26	3.52	51.1	19.8	29.2	5605	5690	2322	2773	664	622	11
10	3.07	2.05	20.2	7	68.5	7673	7941	1049	1098	352	339	6
11	9.33	6.24	66.4	28.2	8.4	4102	4435	3421	3600	1240	1161	7
12	2.62	1.75	52.7	19.4	22.4	5359	5096	3309	2860	302	329	9
13	1.4	0.94	25.1	9.3	62.2	7649	7575	1411	1364	155	157	38
14	3.55	2.38	37.3	27	29.8	5564	4996	2632	2024	433	506	11

* Category legend: (1) spherulitestone; (2) shrubby spherulitestone; (3) spherulitic shrubstone; (4) shrubstone; (5) spherulitic shrubstone w/ mud; (6) shrubby spherulitestone w/ mud; (7) spherulitestone w/ mud; (10) calcimudstone; (11) dolomudstone; (12) mixed mudstone; (13) grainstone; (14) packstone.
[a] median values of concentrations measured by ICP-OES. [b] median values of concentrations calculated from mineralogical data (calcite + dolomite).
[c] median values of concentrations calculated from dolomite content.

Table B.2: Median values, after removing outliers estimated from lower and upper bounds of interquartile range (3_{rd} quartile minus 1^{st} quartile; values above 216 ppm P, or 6.97 mmol/kg P). Outliers were estimated based on a set of 1100 measurements. The results in the table reflect only samples with detailed petrographic description.

Facies category*	[P] mmol/kg	[ΣPO_4] mmol/kg	dolomite %	quartz %	calcite %	[Ca]meas[a] mmol/kg	[Ca]min[b] mmol/kg	[Mg]meas[a] mmol/kg	[Mg]dol[c] mmol/kg	P/(Ca+Mg)meas[a] mmol/mol	P/(Ca+Mg)min[b] mmol/mol	N samples
1	1.78	1.19	45.5	14	34.4	6104	5904	2376	2471	209	212	157
2	1.81	1.21	41.3	13.5	43.8	6883	6613	2177	2240	200	204	151
3	1.61	1.08	28.7	13	52.2	7158	6769	1595	1556	184	194	229
5	5.17	3.46	32	10.4	57.6	7190	7491	2128	1735	554	560	1
6	4.29	2.87	42.7	17	34.6	5960	5774	2068	2317	535	531	6
7	4.46	2.98	51.1	19.8	29.2	5571	5690	2380	2773	560	526	9
10	2.62	1.75	20.1	6.7	72.9	7745	8370	1045	1088	298	276	5
11	0.48	0.32	12.2	79.5	8.4	3215	1496	2512	661	85	225	3
12	2.13	1.43	58.5	19.4	22.4	5359	5411	3532	3175	240	248	7
13	1.4	0.94	25.1	9.3	62.2	7649	7575	1411	1364	155	157	38
14	3.07	2.05	33.3	27.6	20.3	5518	3836	2332	1808	391	543	8

* Category legend: (1) spherulitestone; (2) shrubby spherulitestone; (3) spherulitic shrubstone; (4) shrubstone; (5) spherulitic shrubstone w/ mud; (6) shrubby spherulitestone w/ mud; (7) spherulitestone w/ mud; (10) calcimudstone; (11) dolomudstone; (12) mixed mudstone; (13) grainstone; (14) packstone.
[a] median values of concentrations measured by ICP-OES. [b] median values of concentrations calculated from mineralogical data (calcite + dolomite).
[c] median values of concentrations calculated from dolomite content.

Table B.3: Median values according to facies, based only on samples >LD for P (N = 462).

Facies category*	[P] mmol/kg	[ΣPO_4] mmol/kg	dolomite %	quartz %	calcite %	[Ca]meas[a] mmol/kg	[Ca]min[b] mmol/kg	[Mg]meas[a] mmol/kg	[Mg]dol[c] mmol/kg	P/(Ca+Mg)meas[a] mmol/mol	P/(Ca+Mg)min[b] mmol/mol	N samples
1	3.58	2.4	50.1	15	33.9	6071	6105	2586	2718	414	406	112
2	2.52	1.68	41.4	13.5	44.3	6812	6671	2231	2246	278	282	97
3	2.84	1.9	29.8	10.2	54.7	7344	7075	1704	1614	314	327	136
4	2.78	1.86	26.6	8.6	61	7893	7533	1413	1442	298	309	54
5	5.17	3.46	32	10.4	57.6	7190	7491	2128	1735	554	560	1
6	4.29	2.87	42.7	17	34.6	5960	5774	2068	2317	535	531	6
7	5.26	3.52	51.1	19.8	29.2	5605	5690	2322	2773	664	622	11
10	3.07	2.05	20.2	7	68.5	7673	7941	1049	1098	352	339	6
11	10.14	6.78	68.1	22.9	9	4364	4593	3648	3694	1265	1223	5
12	2.62	1.75	52.7	19.4	22.4	5359	5096	3309	2860	302	329	9
13	2.03	1.36	25.1	9	66.3	7762	7988	1413	1364	222	217	16
14	3.65	2.44	37.3	27	20.3	5564	4052	2632	2024	445	600	9

* Category legend: (1) spherulitestone; (2) shrubby spherulitestone; (3) spherulitic shrubstone; (4) shrubstone; (5) spherulitic shrubstone w/ mud; (6) shrubby spherulitestone w/ mud; (7) spherulitestone w/ mud; (10) calcimudstone; (11) dolomudstone; (12) mixed mudstone; (13) grainstone; (14) packstone.
[a] median values of concentrations measured by ICP-OES. [b] median values of concentrations calculated from mineralogical data (calcite + dolomite).
[c] median values of concentrations calculated from dolomite content.

Table B.4: Median values according to facies, after removing 70 outliers estimated from lower and upper bounds of interquartile range (3rd quartile minus 1st quartile; values above 302 ppm P, or 9.75 mmol/kg P) considering all sample measurements >LD for P (N = 661; with and without petrographic description). Median values below in turn were calculated for samples with petrographic characterisation (N = 418) within this larger data set.

Facies category*	[P] mmol/kg	[ΣPO_4] mmol/kg	dolomite %	quartz %	calcite %	[Ca]meas[a] mmol/kg	[Ca]min[b] mmol/kg	[Mg]meas[a] mmol/kg	[Mg]dol[c] mmol/kg	P/(Ca+Mg)meas[a] mmol/mol	P/(Ca+Mg)min[b] mmol/mol	N samples
1	3.23	2.16	50.8	15.5	33.1	6008	6064	2586	2757	376	366	99
2	2.49	1.66	42.7	13.5	44.4	6850	6750	2231	2314	274	274	93
3	2.78	1.86	29.8	10.1	53.6	7333	6971	1686	1617	308	323	127
4	2.6	1.74	27.7	8.8	59.6	7865	7458	1429	1504	280	290	46
5	5.17	3.46	32	10.4	57.6	7190	7491	2128	1735	554	560	1
6	4.29	2.87	42.7	17	34.6	5960	5774	2068	2317	535	531	6
7	4.46	2.98	51.1	19.8	29.2	5571	5690	2380	2773	560	526	9
10	2.62	1.75	20.1	6.7	72.9	7745	8370	1045	1088	298	276	5
11	5.73	3.83	64.7	25.8	9.4	5424	4454	3450	3512	646	719	2
12	2.13	1.43	58.5	19.4	22.4	5359	5411	3532	3175	240	248	7
13	2.03	1.36	25.1	9	66.3	7762	7988	1413	1364	222	217	16
14	3.55	2.38	29.4	27	20.3	5564	3621	2632	1593	433	681	7

* Category legend: (1) spherulitestone; (2) shrubby spherulitestone; (3) spherulitic shrubstone; (4) shrubstone; (5) spherulitic shrubstone w/ mud; (6) shrubby spherulitestone w/ mud; (7) spherulitestone w/ mud; (10) calcimudstone; (11) dolomudstone; (12) mixed mudstone; (13) grainstone; (14) packstone.
[a] median values of concentrations measured by ICP-OES. [b] median values of concentrations calculated from mineralogical data (calcite + dolomite).
[c] median values of concentrations calculated from dolomite content.

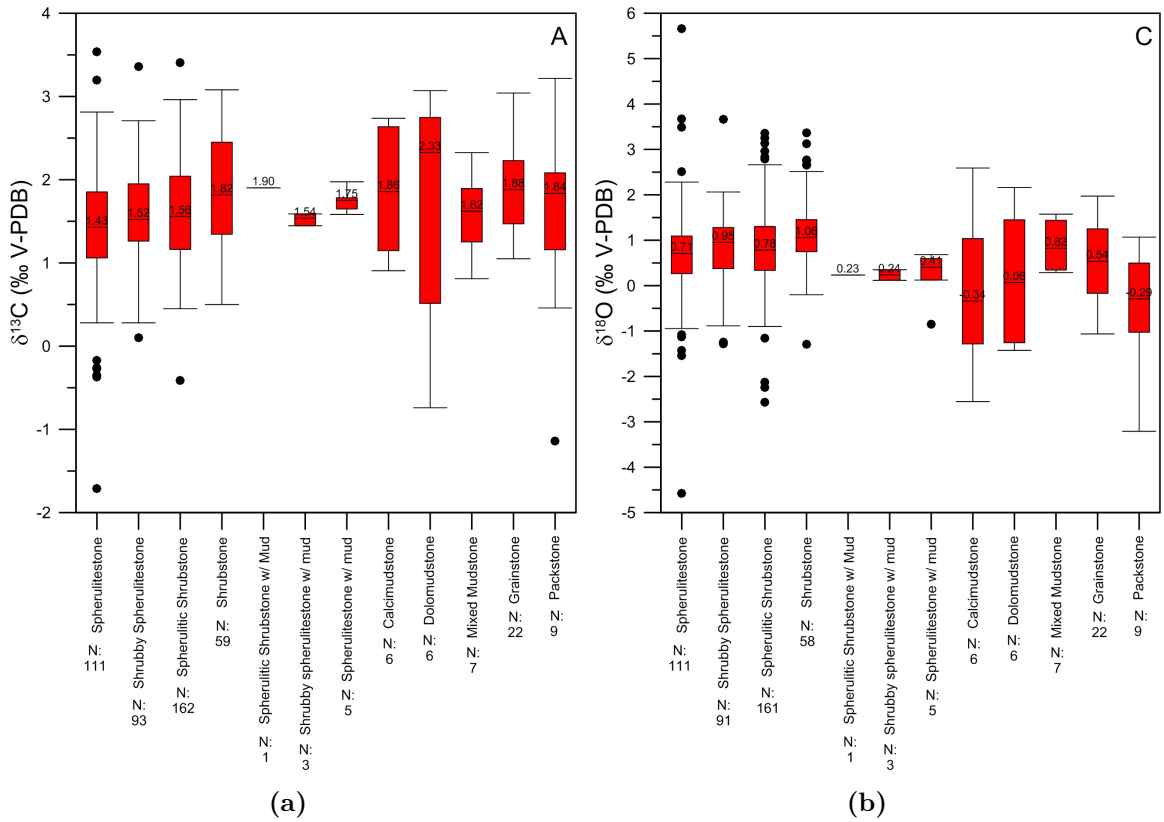


Figure B.2: A: boxplots of bulk rock $\delta^{13}C$ values distribution per facies; B: boxplots of bulk rock $\delta^{18}O$ values distribution per facies. Median values are indicated in the centre of each box, and number of samples (N) are shown close to each class designation.

these trends are reproduced across a broad spatial/geographical extent in two wells set *ca.* 75 km apart from each other, as shown in Fig. 6.12.

The $\delta^{18}O_{VPDB}$ values are typically high (*i.e.*, with a reported upper BVF average based on measured bulk rock $\delta^{18}O_{VPDB}$ of 1.13 ± 1.19‰ (N = 140), after diagenetically altered samples were removed; Pietzsch et al. 2020 [193]). Considering the corrected $\delta^{18}O_{VPDB}$ values of 126 samples belonging to that set, the average $\delta^{18}O_{VPDB}$ of the upper BVF in well S10 is 0.73 ± 1.14‰. The values are very close to the average $\delta^{18}O_{VPDB}$ value reported above in well #3 of 1.21 ± 0.67‰, N = 502 (or 0.78 ± 0.72‰, N = 497, if the corrected $\delta^{18}O_{VPDB}$ values are considered), and are in fact identical if the standard deviation of the entire set of samples analysed in this study is taken into account. Fig. B.4A and Fig. 6.8B compare the average $\delta^{13}C_{VPDB}$ and $\delta^{18}O_{VPDB}$ between the units in the two wells indicated in Fig. 6.12. Table S6 shows a summary of the data plotted in Fig B.4A–B.4B. These average

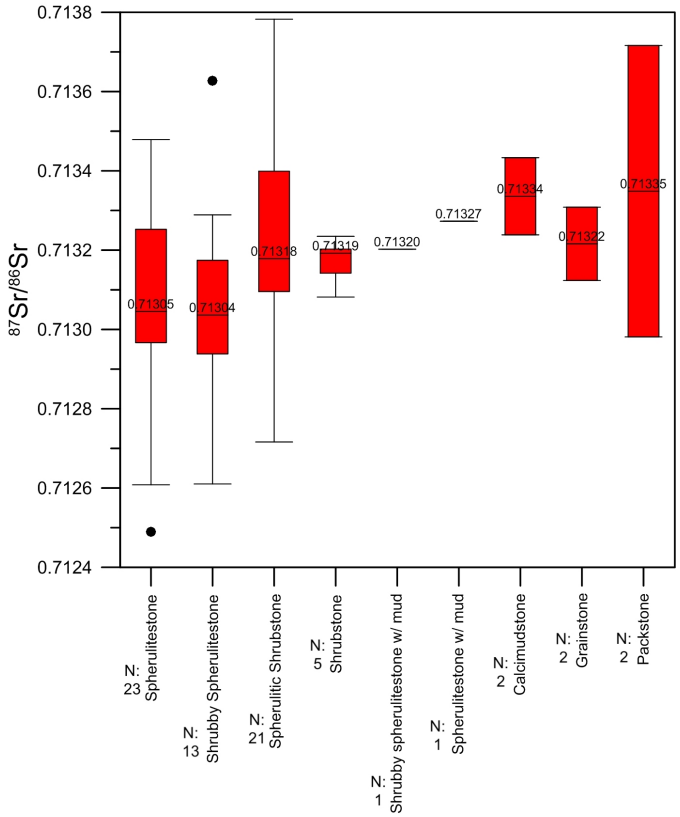


Figure B.3: Boxplot of bulk rock $^{87}Sr/^{86}Sr$ values distribution per facies. Median values are indicated in the centre of each box, and number of samples (N) are shown close to each class designation.

values are based on the smoothed $\delta^{13}C_{VPDB}$ and $\delta^{18}O_{VPDB}$ data shown in Fig. 6.12 (main text, black curves, in the case of $\delta^{18}O_{VPDB}$).

It can be seen from Fig. B.4A that all intervals are statistically identical between the two wells in terms of their average $\delta^{13}C_{VPDB}$ values. It is also possible to observe an overall increase in the $\delta^{13}C_{VPDB}$ values from BVF I to BVF III, followed by a fall in the uppermost interval, BVF IV (also, Fig. 6.12). Similarly, to the average $\delta^{13}C_{VPDB}$ values, all four intervals can be considered identical between the two wells in terms of their average $\delta^{18}O_{VPDB}$ values and the respective standard deviations (Fig. B.4B). Fig. B.4C compares the $^{87}Sr/^{86}Sr$ ratio between corresponding units in the two wells, also indicated in Table B.6. It is noteworthy that the bulk rock phosphorus profile from well S10 also shows a similar increase in P concentration towards the top, associated with the shrubstone facies as well (the fascicular crusts in the study by Pietzsch et al. 2020 [193]; Table B.7; Fig. B.4D).

Although the BVF III interval (Fig. 6.12 and Fig. B.4) has average $\delta^{18}O_{VPDB}$ values that are slightly lower than the BVF II interval below (Fig. 6.12 and Fig. B.4), it is important to highlight that this unit, similarly to the others, is composed of smaller segments (indicated as lake stages 7–11, Fig. 6.12) reaching the highest values in both studied wells (1.92 ± 0.83‰ and 1.59 ± 0.41‰, wells #3 and S10, respectively). Additionally, if facies are compared individually in terms of their $\delta^{13}C_{VPDB}$ and corrected $\delta^{18}O_{VPDB}$ values, shrubstones tend to possess higher values than other primary facies (Fig. B.2A and Fig. B.2B).

Table B.5: Summary of average $\delta^{13}C_{VPDB}$ and $\delta^{18}O_{VPDB}$ values per sequence in each well, based on the smoothed data shown in Fig. 6.12 (the smoothed $\delta^{18}O_{VPDB}$ in turn are based on the correction applied to the measured bulk rock $\delta^{18}O_{VPDB}$ values, which accounts for different phosphoric acid fractionation factors between CO_2-calcite and CO_2-dolomite).

Sequence	**well #3**				**well S10**			
	$\delta^{13}C_{VPDB}$ (‰)	N	$\delta^{18}O_{VPDB}$ (‰)	N	$\delta^{13}C_{VPDB}$ (‰)	N	$\delta^{18}O_{VPDB}$ (‰)	N
BVF IV	1.80 ± 0.39	23	–0.19 ± 0.48	22	1.90 ± 0.21	14	–0.44 ± 0.36	12
BVF III	2.24 ± 0.26	155	0.98 ± 1.04	154	2.45 ± 0.35	57	0.49 ± 1.10	47
BVF II	1.54 ± 0.15	125	1.04 ± 0.28	125	1.49 ± 0.35	43	0.91 ± 0.75	43
BVF I	1.38 ± 0.17	56	0.53 ± 0.36	54	1.60 ± 0.48	29	0.95 ± 0.48	24

Table B.6: Summary of average $^{87}Sr/^{86}Sr$ values per sequence in each well, (based on the measured values in well #3 and smoothed data in well S10, as shown in Fig. 6.12).

Sequence	**well #3**		**well S10**	
	$^{87}Sr/^{86}Sr$	N	$^{87}Sr/^{86}Sr$	N
BVF IV	0.71306 ± 0.00013	4	0.71308 ± 0.00006	13
BVF III	0.71318 ± 0.00026	32	0.71336 ± 0.00012	53
BVF II	0.71305 ± 0.00024	17	0.71276 ± 0.00022	43
BVF I	0.71322 ± 0.00010	9	0.71286 ± 0.00024	29

Table B.7: Summary of average P values per sequence in each well, (based on smoothed data in both wells, as shown in Fig. 6.12).

Sequence	**well #3**		**well S10**	
	P (ppm)	N	P (ppm)	N
BVF IV	234 ± 78	22	200 ± 53	11
BVF III	259 ± 170	155	235 ± 151	48
BVF II	55 ± 13	125	130 ± 53	42
BVF I	115 ± 57	56	123 ± 48	24

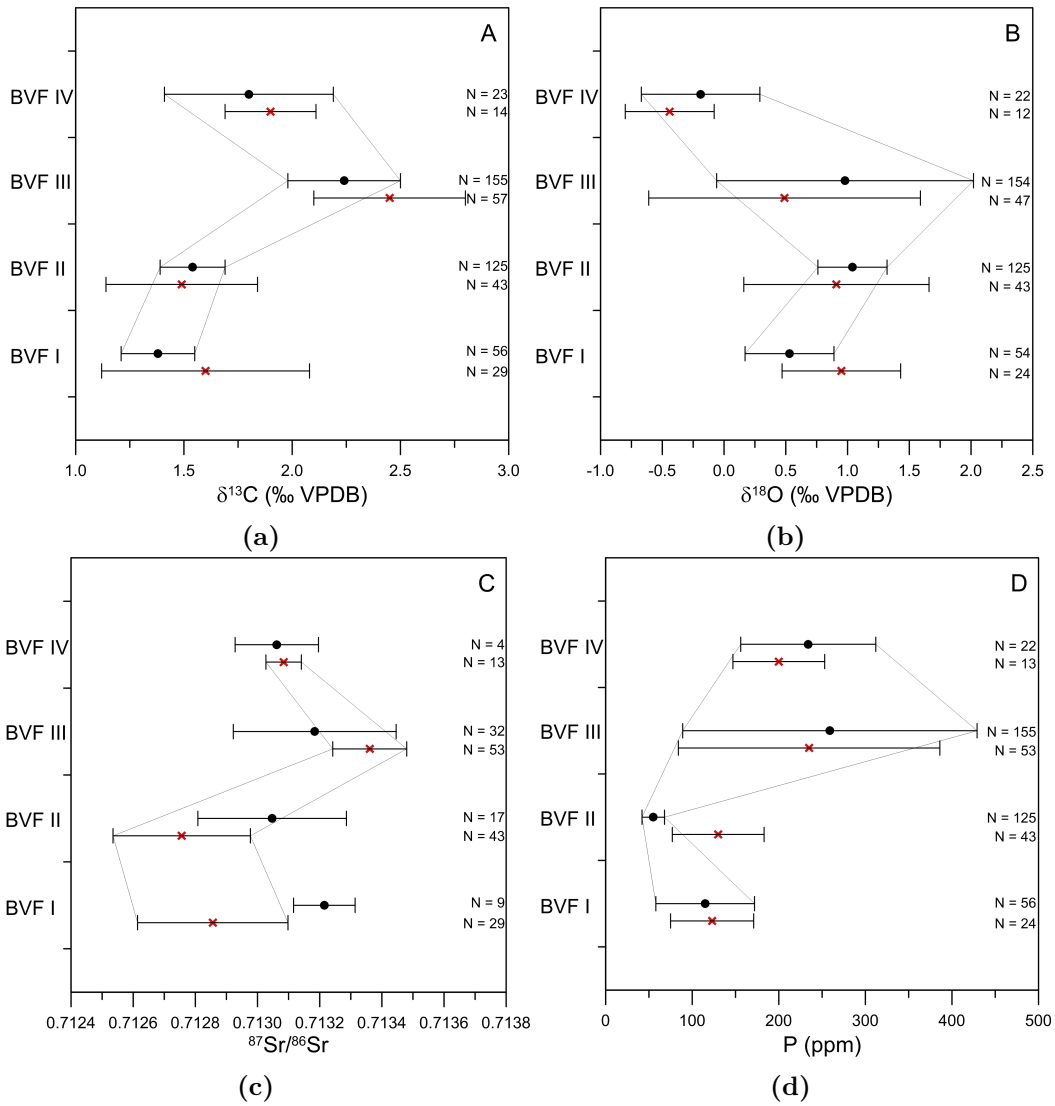


Figure B.4: Averaged values of key components across the four BVF units shown in Fig. 6.12. All the averaged values are based on the recalculated 9-point moving average values indicated by the bold lines in the $\delta^{13}C_{VPDB}$, $\delta^{18}O_{VPDB}$, $^{87}Sr/^{86}Sr$, and phosphorus profiles, except for the $^{87}Sr/^{86}Sr$ ratio in well #3, which contains fewer and sparser results. (A): comparison of average $\delta^{13}C_{VPDB}$ values and corresponding standard deviations per unit, between well #3 (black circles) and well S10 (red crosses). (B): comparison of average $\delta^{18}O_{VPDB}$ values and corresponding standard deviations per unit between well #3 and well S10. (C): comparison of average $^{87}Sr/^{86}Sr$ values and corresponding standard deviations per unit between well #3 and well S10. (D): comparison of average bulk rock phosphorus content and corresponding standard deviations per unit between well #3 and well S10.

B.3 Statistical summary of EPMA data

This section presents graphical summaries and a table compiling the main statistical results regarding other trace elements briefly discussed in chapter 6, according to

the mineral textures and phases, as well as according to facies.

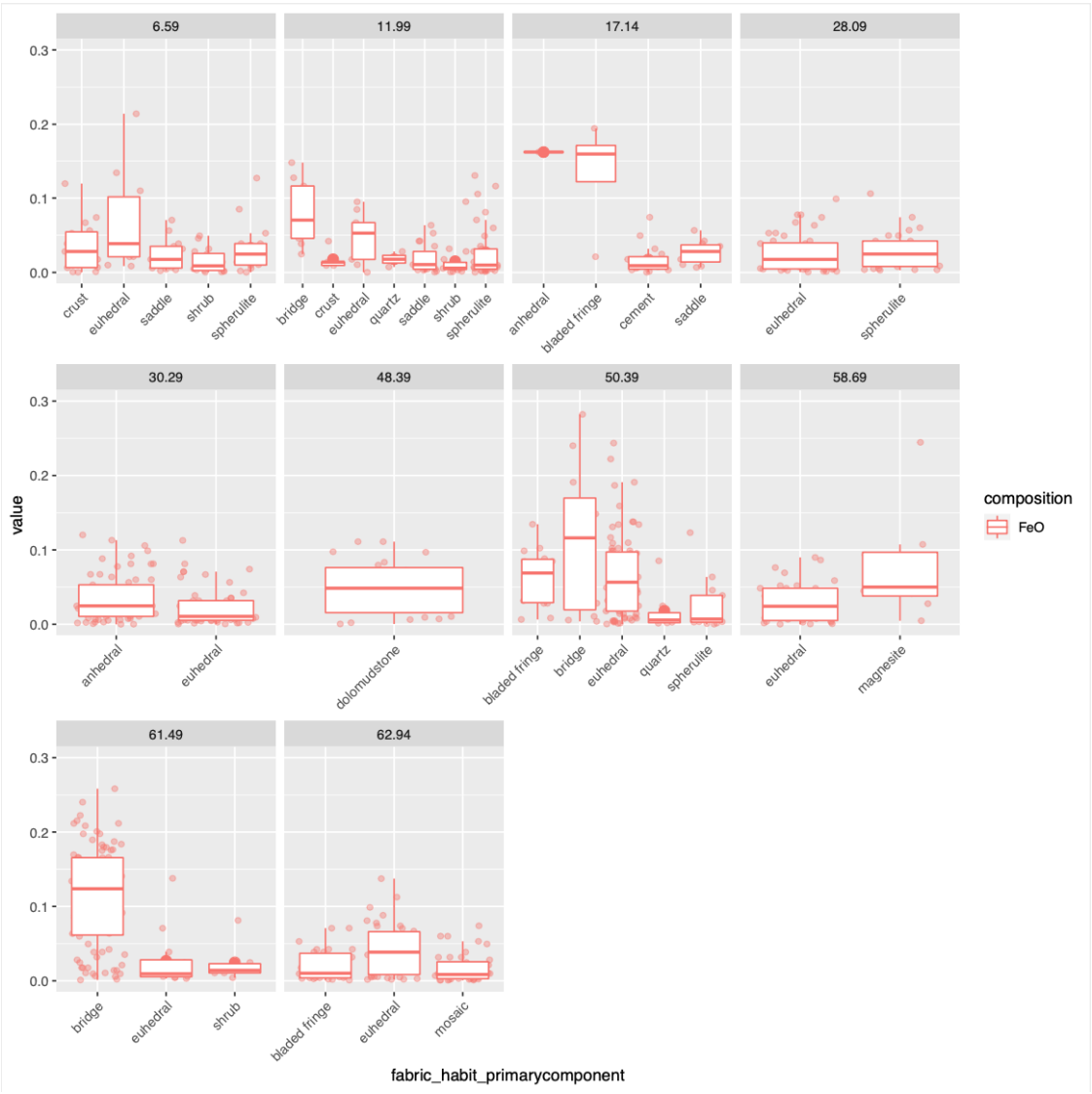


Figure B.5: Boxplots of EPMA FeO data grouped according to different textural elements and carbonate mineral (calcite or dolomite), from each individual thin section corresponding to a particular sample from a given depth (indicated on the top of each diagram). Values are in wt%.

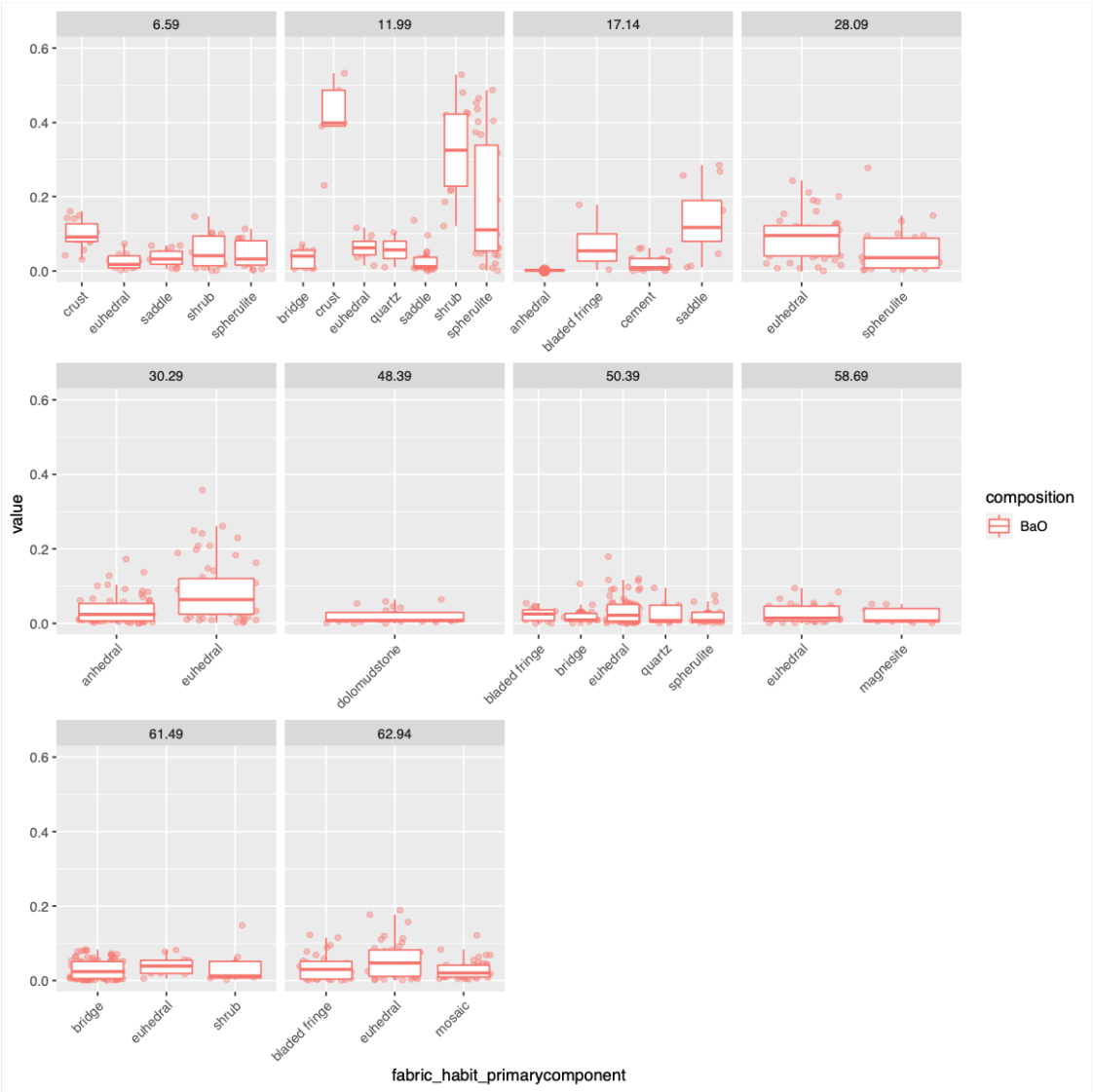


Figure B.6: Boxplots of EPMA BaO data grouped according to different textural elements and carbonate mineral (calcite or dolomite), from each individual thin section corresponding to a particular sample from a given depth (indicated on the top of each diagram). Values are in wt%.

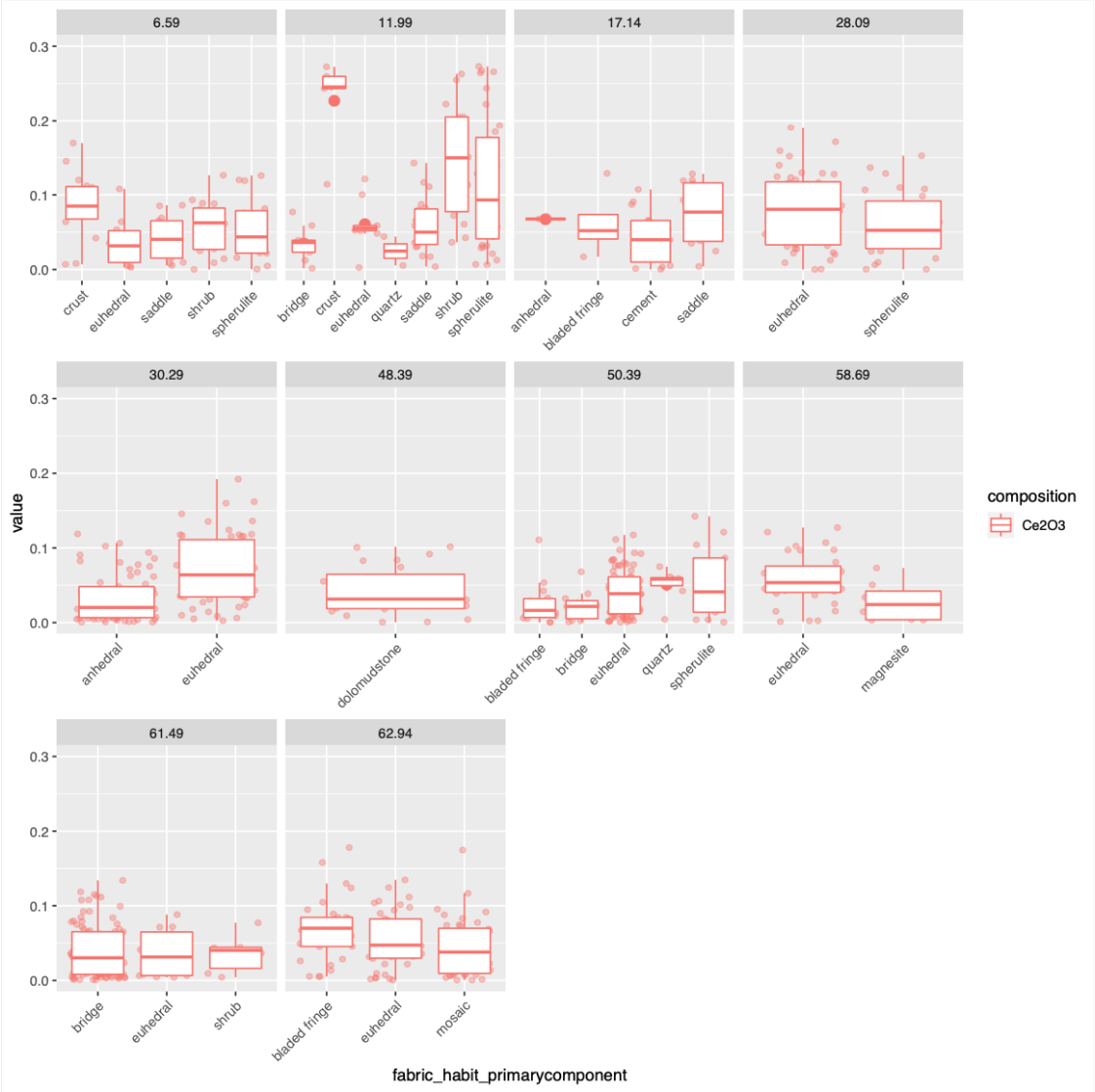


Figure B.7: Boxplots of EPMA Ce_2O_3 data grouped according to different textural elements and carbonate mineral (calcite or dolomite), from each individual thin section corresponding to a particular sample from a given depth (indicated on the top of each diagram). Values are in wt%.

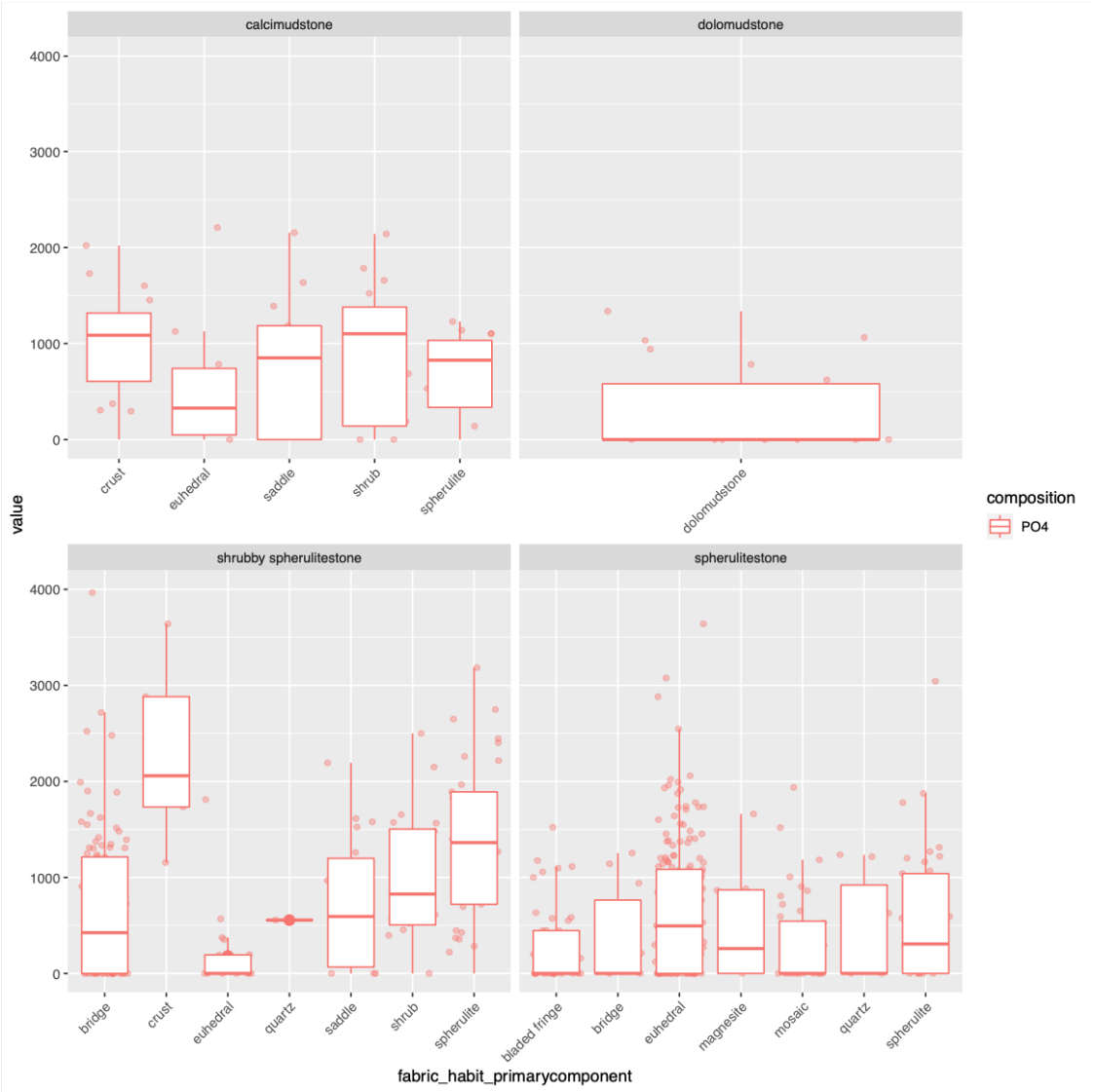


Figure B.8: Boxplots of EPMA ΣPO_4 data grouped by facies and discriminating different carbonate mineralogies and mineral textures. Values are in ppm.

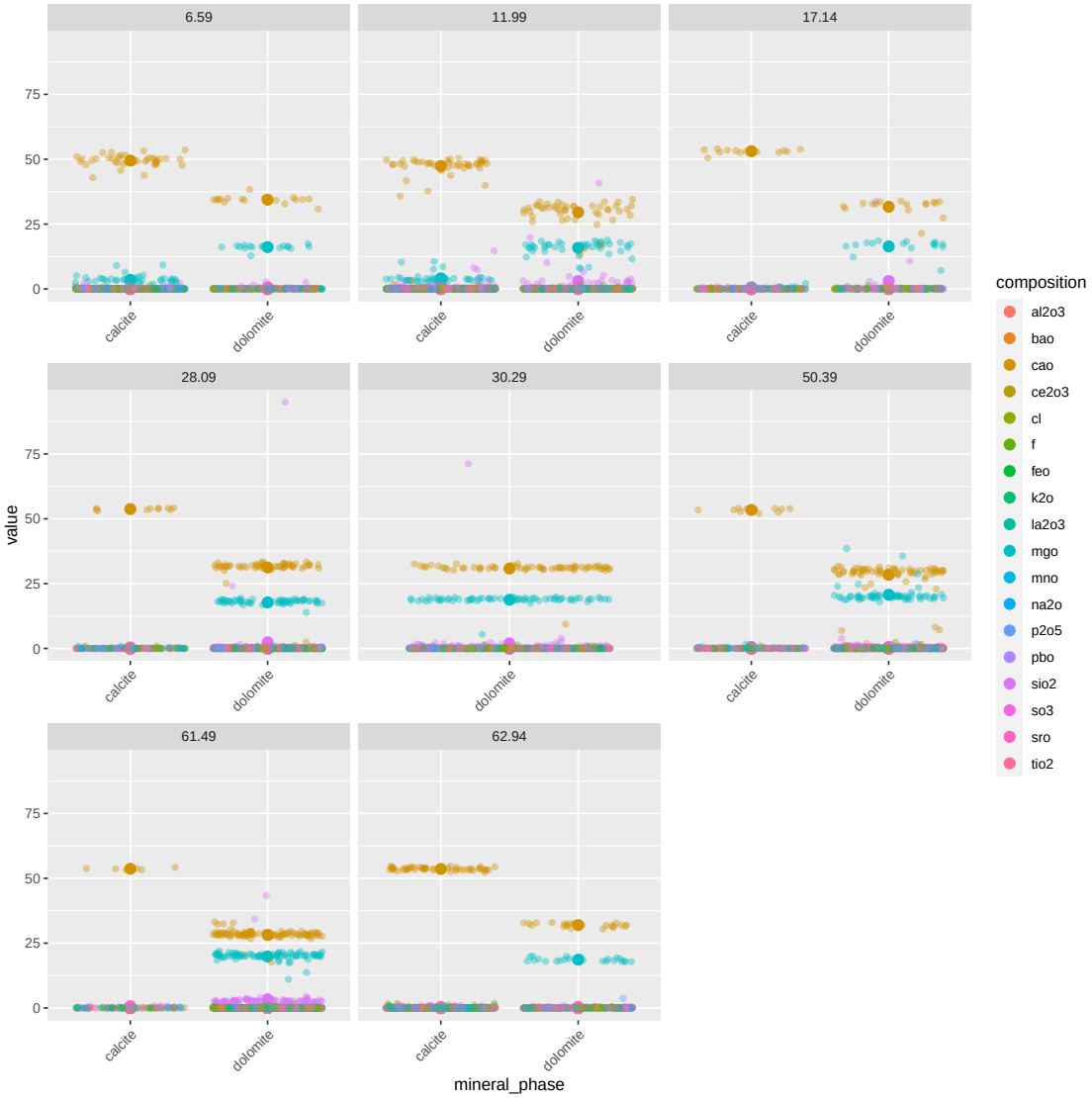


Figure B.9: EPMA compositional data grouped by depth and carbonate mineral (calcite or dolomite). Values are in ppm.

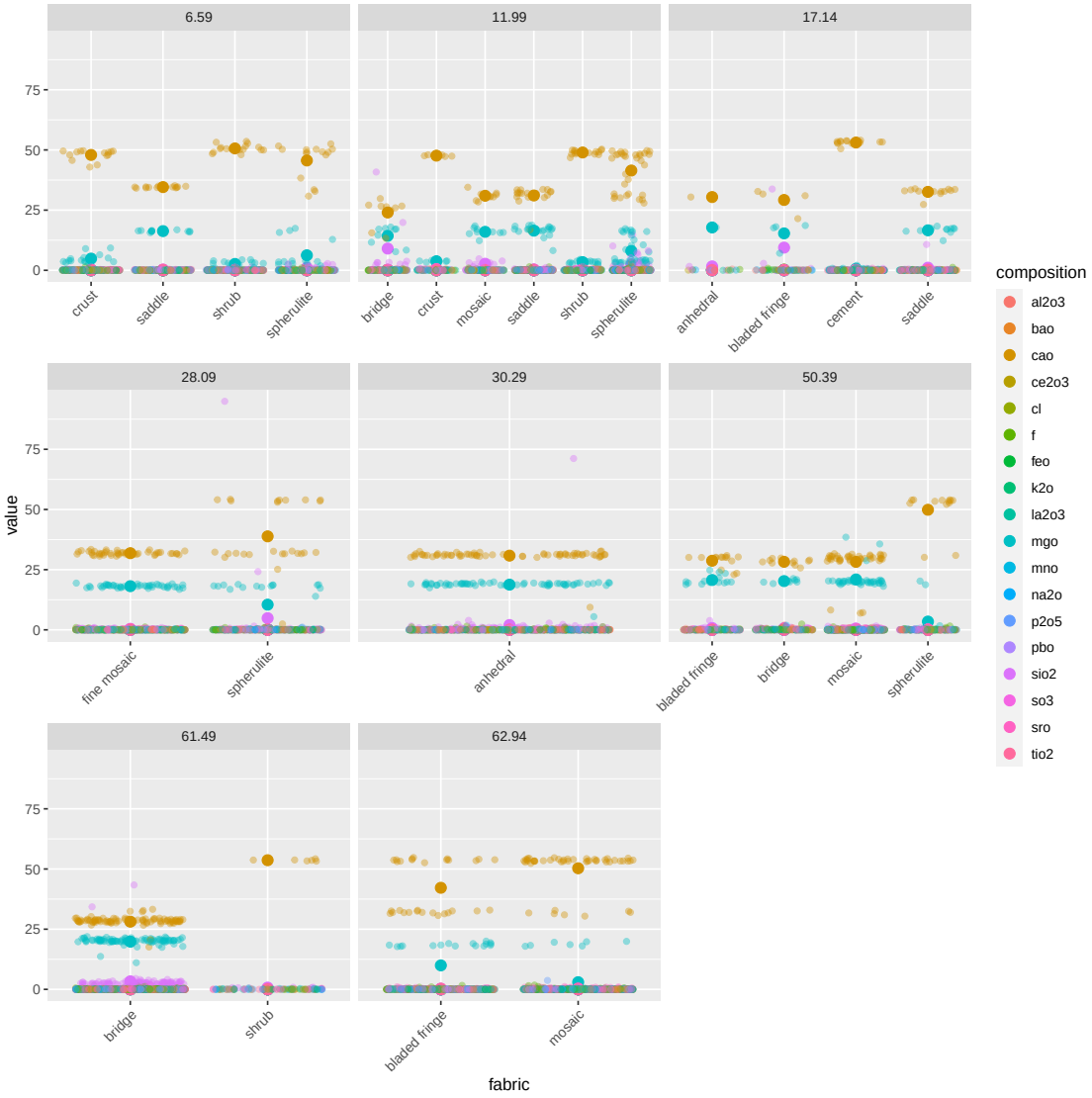


Figure B.10: EPMA compositional data grouped by depth and main textural constituents. Values are in ppm.

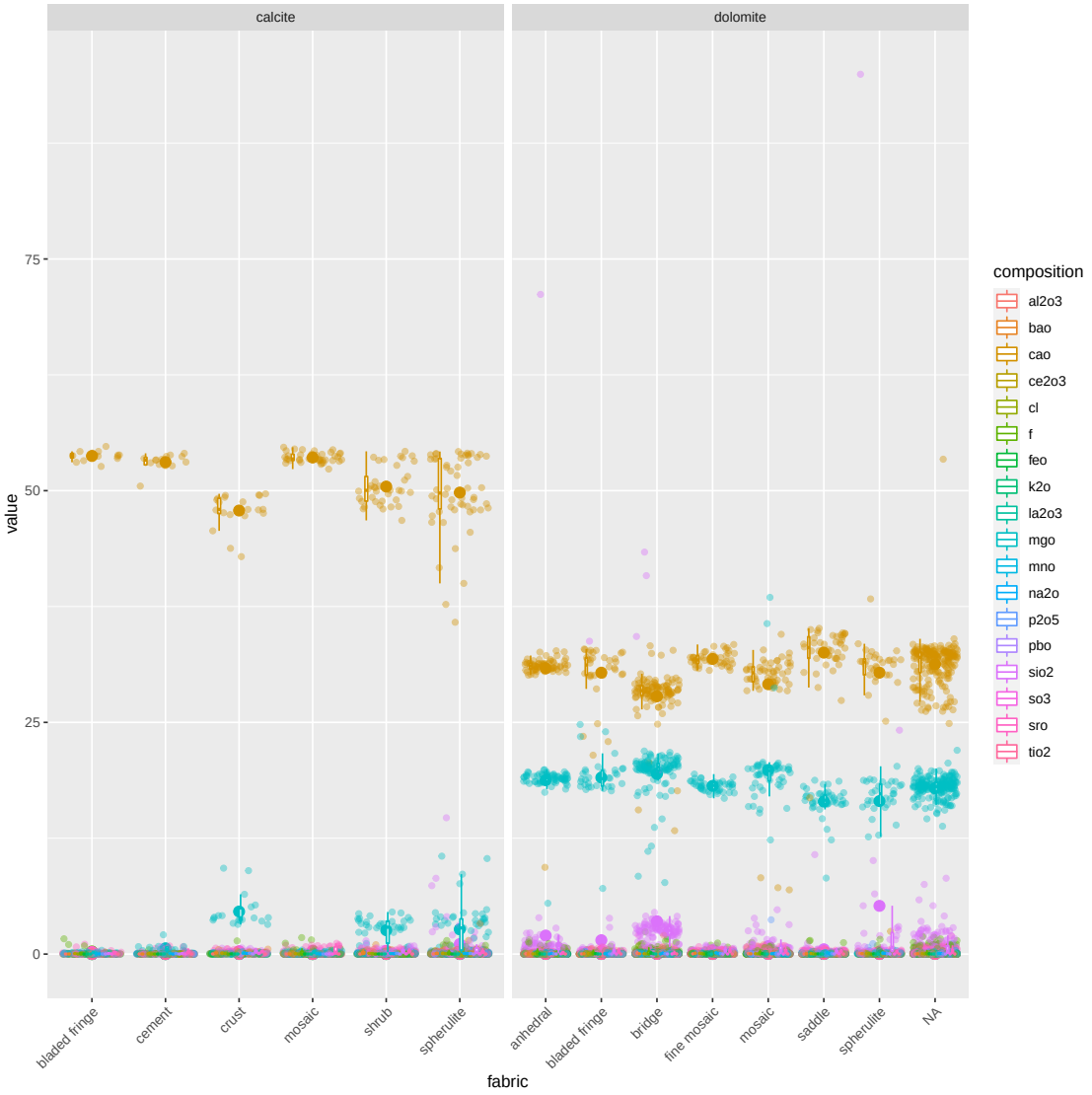


Figure B.11: EPMA compositional data grouped by carbonate mineral (calcite and dolomite) and their main textural constituents. Boxplots of the compositional variability are also shown (with decreased size, to highlight the individual sampled spots/analyses). Values are in ppm.

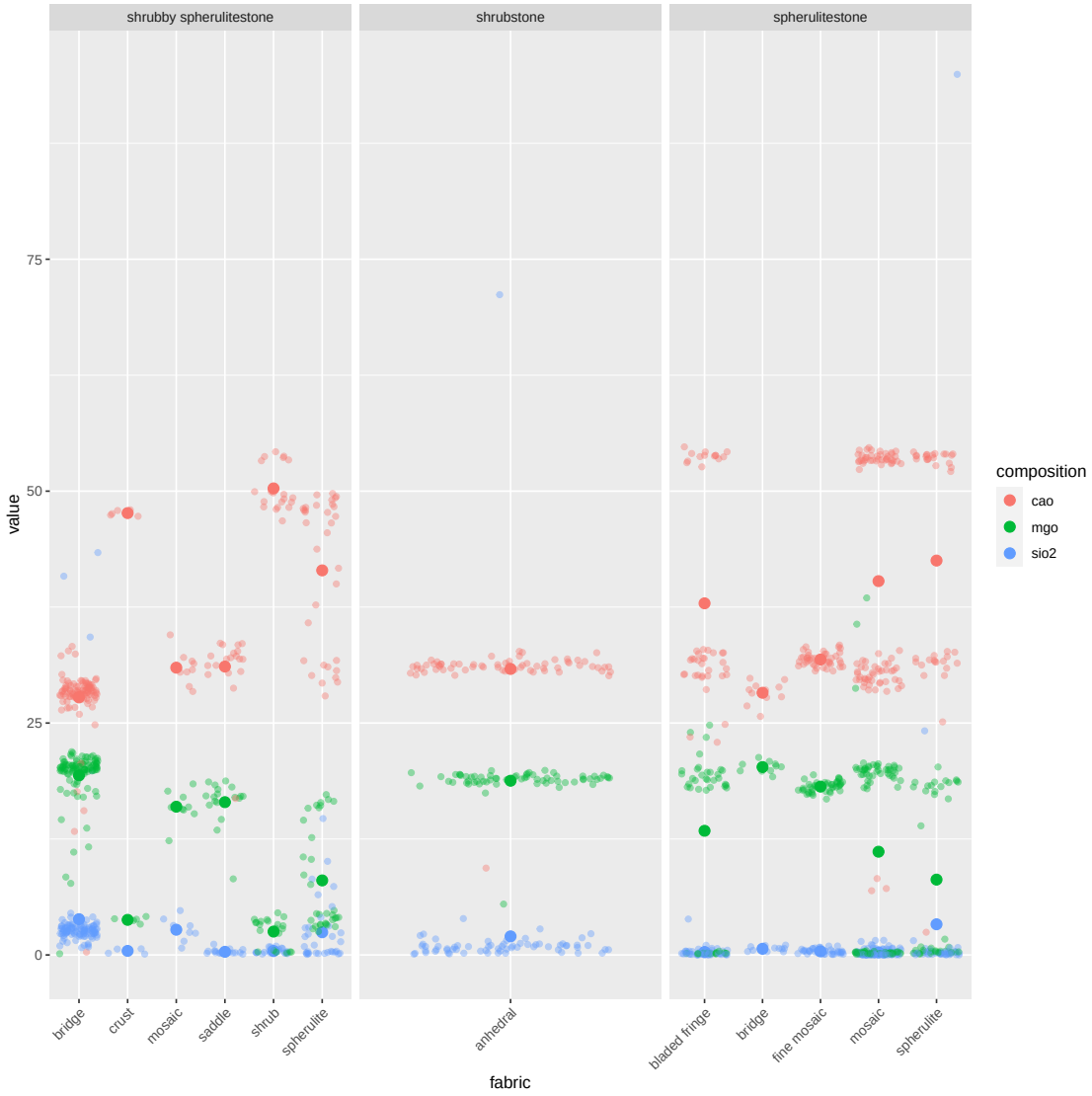


Figure B.12: EPMA compositional data (filtered for CaO, MgO and SiO_2 only) grouped according to main "primary facies" and their main textural constituents analysed. Values are in ppm.

Table B.8: Summary statistics of EPMA trace element ratios and calculated mol% of relevant carbonate phases, according to the type of mineral texture analysed.

		calcite, shrub	calcite, crust	calcite, spheru-lite	dolomite, spheru-lite	dolomite, euhedral	dolomite, bridge	dolomite, anhedral	calcite, bladed fringe	dolomite, bladed fringe	calcite, cement	calcite, mosaic	dolomud-stone	dolomite, sub-euhedral	dolomite, saddle	magne-site
Sr/(Ca+Mg)	Avrg =	3.17	2.97	2.42	2.47	3.03	1.34	1.3	2.37	2.86	2.76	3.76	1.58	3.58	2.99	1.32
mmol/mol	Std Dev =	1.58	1.63	1.8	1.25	2.5	1.65	1.02	3.21	1.9	2.81	3.91	0.81	1.54	1.17	3.51
	Median =	2.94	2.54	2.31	2.3	2.61	0.74	1.23	1.2	2.83	2.38	2.13	1.79	3.01	2.86	0.05
	Max =	6.78	6.51	7.42	5.66	19.64	7.62	3.24	10.74	7.2	8.95	11.76	3.56	6.04	5.6	10.01
	Min =	0.33	0.97	0.02	0.13	0	0	0	0	0	0	0.01	0.18	1.77	0.43	0.01
	N =	37	20	55	32	269	111	66	14	34	15	40	23	7	44	8
Mg/(Ca+Mg)	Avrg =	0.07	0.12	0.07	0.42	0.45	0.49	0.46	0	0.46	0.02	0.01	0.47	0.45	0.41	0.99
mol/mol	Std Dev =	0.04	0.04	0.07	0.05	0.06	0.03	0.01	0	0.05	0.01	0	0.01	0.02	0.02	0.01
	Median =	0.07	0.1	0.07	0.43	0.44	0.5	0.46	0	0.45	0.01	0.01	0.47	0.45	0.41	1
	Max =	0.12	0.23	0.28	0.48	0.89	0.54	0.47	0.01	0.6	0.05	0.01	0.49	0.48	0.45	1
	Min =	0.01	0.08	0	0.18	0.02	0.37	0.43	0	0.32	0	0	0.46	0.43	0.39	0.98
	N =	37	20	55	32	269	111	66	14	34	15	40	23	7	44	8
P/(Ca+Mg)	Avrg =	1.13	1.45	1.09	1.79	0.7	0.84	0.5	0.29	0.36	0.81	0.4	0.41	7.41	0.81	0.59
mmol/mol	Std Dev =	0.97	0.98	0.9	3.75	1.11	1.3	0.57	0.33	0.47	0.61	0.49	0.47	19.16	0.84	0.65
	Median =	1.08	1.26	0.96	0.86	0.4	0.44	0.27	0.14	0.11	0.73	0.14	0.13	0.13	0.65	0.27
	Max =	4.8	4.08	3.75	19.88	13.47	10.35	2.35	1.16	1.65	2.02	2.1	1.44	50.85	4.58	1.72
	Min =	0.01	0.06	0.04	0	0	0	0.01	0.02	0.01	0.02	0.01	0.01	0	0	0.05
	N =	37	20	55	32	269	111	66	14	34	15	40	23	7	44	8
Mn/Sr	Avrg =	0.54	0.77	3.42	1.31	4.19	2.61	2.11	23.04	8.73	171.58	6.96	2.53	0.24	0.81	15.04
mol/mol	Std Dev =	0.59	0.51	9.55	1.96	35.11	6.59	5.46	71.76	46.72	645.72	18.38	3.52	0.42	0.5	33.71
	Median =	0.33	0.79	0.71	0.78	0.4	0.33	0.2	0.43	0.16	0.47	0.24	0.98	0.04	0.74	1.62
	Max =	2.5	1.86	58.48	10.18	534.78	45.85	28.5	271.15	272.81	2505.13	82.77	15.43	1.16	2.98	97.32
	Min =	0.01	0	0.03	0.12	0	0.01	0	0.04	0	0.08	0	0.36	0.02	0.13	0.01
	N =	37	20	55	32	269	111	66	14	34	15	40	23	7	44	8
La/(Ca+Mg)	Avrg =	0.13	0.12	0.12	0.23	0.11	0.17	0.09	0.08	0.08	0.15	0.13	0.1	0.05	0.11	0.13
mmol/mol	Std Dev =	0.16	0.14	0.13	0.62	0.14	0.57	0.12	0.1	0.1	0.16	0.13	0.13	0.09	0.13	0.1
	Median =	0.06	0.05	0.05	0.05	0.05	0.05	0.04	0.05	0.04	0.06	0.05	0.05	0.01	0.06	0.13
	Max =	0.53	0.43	0.53	3.56	0.72	5.91	0.52	0.33	0.42	0.48	0.44	0.47	0.25	0.47	0.26
	Min =	0	0	0	0.01	0	0	0	0.02	0	0	0	0.02	0	0	0.02
	N =	37	20	55	32	269	111	66	14	34	15	40	23	7	44	8
Ce/(Ca+Mg)	Avrg =	0.63	0.76	0.74	0.38	0.34	0.25	0.19	0.38	0.33	0.27	0.29	0.28	0.35	0.36	0.19
mmol/mol	Std Dev =	0.61	0.52	1.37	0.27	0.25	0.24	0.19	0.24	0.27	0.22	0.24	0.22	0.12	0.23	0.21
	Median =	0.45	0.62	0.41	0.29	0.31	0.19	0.13	0.37	0.3	0.26	0.24	0.2	0.32	0.36	0.14
	Max =	3.01	1.75	10.04	0.92	1.16	1.37	0.7	0.82	1.05	0.68	1.1	0.71	0.52	0.92	0.65
	Min =	0	0.04	0	0	0	0	0	0.03	0	0	0	0	0.18	0.02	0.02
	N =	37	20	55	32	269	111	66	14	34	15	40	23	7	44	8
Ba/(Ca+Mg)	Avrg =	1.23	1.19	1.23	0.4	0.37	0.71	0.23	0.18	0.26	0.15	0.2	0.13	0.19	0.4	0.14
mmol/mol	Std Dev =	1.44	1.05	3.3	0.35	0.37	5.58	0.25	0.27	0.25	0.15	0.17	0.15	0.26	0.47	0.16
	Median =	0.67	0.72	0.41	0.35	0.27	0.15	0.13	0.05	0.21	0.06	0.14	0.06	0.05	0.24	0.04
	Max =	6.91	3.65	24.16	1.78	2.26	58.99	1.1	0.84	1.12	0.41	0.82	0.46	0.61	1.87	0.34
	Min =	0.01	0.21	0.01	0.01	0	0	0	0.01	0	0	0.03	0	0.01	0	0.01
	N =	37	20	55	32	269	111	66	14	34	15	40	23	7	44	8
Fe/(Ca+Mg)	Avrg =	0.24	0.45	0.33	0.74	0.57	1.71	0.5	0.15	0.8	0.25	0.25	0.75	0.29	0.44	1.26
mmol/mol	Std Dev =	0.31	0.44	0.42	1	0.6	1.65	0.47	0.19	0.86	0.3	0.28	0.54	0.26	0.86	1.56

Continuation of Table B.8

		calcite, shrub	calcite, crust	calcite, spherulite	dolomite, spherulite	dolomite, euhedral	dolomite, bridge	dolomite, anhedral	calcite, bladed fringe	dolomite, bladed fringe	calcite, cement	calcite, mosaic	dolomudstone	dolomite, subeuhedral	dolomite, saddle	magnesite
	Median =	0.13	0.25	0.14	0.45	0.38	1.71	0.33	0.07	0.52	0.13	0.12	0.76	0.24	0.24	0.67
	Max =	1.4	1.71	1.74	5.41	3.87	15.4	2.29	0.61	4.06	1.09	1.07	1.62	0.81	5.75	4.95
	Min =	0.01	0.01	0	0	0	0.02	0	0.01	0.05	0	0.01	0.01	0.08	0.01	0.07
	N =	37	20	55	32	269	111	66	14	34	15	40	23	7	44	8
Fe/Mn	Avrg =	1.86	2.39	0.5	0.49	8.04	16.17	6.16	0.35	6.67	0.27	0.53	0.48	1.79	0.26	15.72
mol/mol	Std Dev =	6.96	7.99	1.54	0.47	76.96	28.75	12.19	0.63	19.4	0.29	0.72	0.42	1.67	0.59	16.88
	Median =	0.18	0.24	0.16	0.29	0.51	6.92	1.67	0.14	1.31	0.15	0.26	0.43	2.15	0.14	8.93
	Max =	37.75	35.7	11.45	1.79	1218.18	249.27	66.3	2.41	93.8	0.82	3.77	1.68	4.53	3.97	40.08
	Min =	0	0	0.01	0	0	0.04	0	0.03	0.1	0	0.02	0.01	0.06	0	0.48
	N =	37	20	55	32	269	111	66	14	34	15	40	23	7	44	8
Pb/(Ca+Mg)	Avrg =	0.08	0.13	0.08	0.14	0.08	0.13	0.07	0.13	0.07	0.04	0.09	0.08	0.06	0.11	0.11
mmol/mol	Std Dev =	0.11	0.13	0.1	0.27	0.09	0.45	0.08	0.13	0.08	0.05	0.11	0.11	0.07	0.1	0.09
	Median =	0.04	0.09	0.03	0.05	0.04	0.04	0.04	0.05	0.04	0.03	0.04	0.03	0.04	0.07	0.09
	Max =	0.42	0.41	0.34	1.52	0.44	4.72	0.35	0.44	0.31	0.21	0.42	0.38	0.2	0.42	0.26
	Min =	0	0	0	0	0	0	0	0.01	0	0	0	0	0	0	0.02
	N =	37	20	55	32	269	111	66	14	34	15	40	23	7	44	8
CaCO3	Avrg =	92.95	87.83	92.6	57.44	54.8	50.73	54.04	99.19	53.37	97.98	98.99	52.63	54.46	58.39	0.59
mol%	Std Dev =	3.57	4.17	6.6	5.38	5.61	2.49	0.83	0.45	4.88	1.2	0.6	1.07	1.71	1.77	0.56
	Median =	92.17	89.47	92.26	56.33	55.4	50.33	53.93	99.41	54.43	98.04	99.22	52.61	54.79	58.41	0.47
	Max =	99.04	91.24	99.68	81.81	98.06	61.02	56.52	99.65	68.08	99.54	99.75	54.26	56.33	61.18	1.94
	Min =	87.95	76.59	71.8	51.43	11.44	46.02	52.62	98.2	39.76	94.29	98.03	50.63	52.14	54.51	0.19
	N =	37	20	55	32	269	111	66	14	34	15	40	23	7	44	8
MgCO3	Avrg =	6.6	11.67	7	42.05	44.72	48.92	45.75	0.49	46.21	1.61	0.54	46.94	45.1	41.06	99.13
mol%	Std Dev =	3.51	4.22	6.5	5.34	5.61	2.62	0.84	0.19	4.92	1.18	0.26	1.06	1.79	1.83	1.04
	Median =	7.38	10.14	7.28	43.22	44.08	49.36	45.84	0.45	45.2	1.26	0.51	46.87	44.64	40.81	99.42
	Max =	11.52	23.03	27.97	48.13	88.42	53.02	47.24	1.04	59.78	5.41	1.14	48.91	47.53	45.31	99.65
	Min =	0.55	8.19	0.25	17.91	1.64	35.98	43.39	0.31	31.26	0.33	0.1	45.34	43.04	38.19	96.57
	N =	37	20	55	32	269	111	66	14	34	15	40	23	7	44	8
SrCO3	Avrg =	0.32	0.3	0.24	0.25	0.3	0.13	0.13	0.24	0.29	0.27	0.37	0.16	0.36	0.3	0.13
mol%	Std Dev =	0.16	0.16	0.18	0.12	0.25	0.16	0.1	0.32	0.19	0.28	0.39	0.08	0.15	0.12	0.35
	Median =	0.29	0.25	0.23	0.23	0.26	0.07	0.12	0.12	0.28	0.24	0.21	0.18	0.3	0.29	0
	Max =	0.67	0.65	0.74	0.56	1.93	0.75	0.32	1.06	0.71	0.88	1.16	0.35	0.6	0.56	0.99
	Min =	0.03	0.1	0	0.01	0	0	0	0	0	0	0	0.02	0.18	0.04	0
	N =	37	20	55	32	269	111	66	14	34	15	40	23	7	44	8
FeCO3	Avrg =	0.02	0.04	0.03	0.07	0.06	0.17	0.05	0.02	0.08	0.03	0.02	0.07	0.03	0.04	0.13
mol%	Std Dev =	0.03	0.04	0.04	0.1	0.06	0.16	0.05	0.02	0.09	0.03	0.03	0.05	0.03	0.09	0.15
	Median =	0.01	0.03	0.01	0.05	0.04	0.17	0.03	0.01	0.05	0.01	0.01	0.08	0.02	0.02	0.07
	Max =	0.14	0.17	0.17	0.54	0.38	1.5	0.23	0.06	0.4	0.11	0.11	0.16	0.08	0.57	0.49
	Min =	0	0	0	0	0	0	0	0	0.01	0	0	0	0.01	0	0.01
	N =	37	20	55	32	269	111	66	14	34	15	40	23	7	44	8
MnCO3	Avrg =	0.11	0.17	0.12	0.19	0.12	0.04	0.03	0.07	0.05	0.11	0.07	0.2	0.05	0.21	0.02
mol%	Std Dev =	0.08	0.11	0.08	0.13	0.15	0.12	0.04	0.04	0.05	0.04	0.05	0.11	0.07	0.1	0.03
	Median =	0.08	0.18	0.1	0.15	0.08	0.02	0.02	0.06	0.05	0.11	0.07	0.16	0.02	0.2	0.01
	Max =	0.27	0.39	0.43	0.63	1.64	1.21	0.22	0.14	0.25	0.18	0.18	0.58	0.21	0.49	0.08
	Min =	0	0	0.01	0.03	0	0	0	0.02	0	0.03	0	0.07	0.01	0.05	0
	N =	37	20	55	32	269	111	66	14	34	15	40	23	7	44	8

C

Appendix C

C.1 Data from well #3 used to plot Figures 6.5 and 6.12 in Chapter 6. Corrected $\delta^{18}O_{bulk}$ uses the correction procedures explained in the text and whose calculations are detailed in this Appendix. $^{87}Sr/^{87}Sr$ ratios are given as measured (*i.e.*, not corrected for age and Rb content), since previous work has shown that corrections tend to cause negligible change in these values for samples belonging to the Barra Velha Formation (Tedeschi 2017 [197]; Pietzsch et al. 2018 [192]).

Table C: Data from well #3 used to plot **Figures 6.5** and **6.12** in Chapter 6. Corrected $\delta^{18}O_{bulk}$ uses the correction procedures explained in the text and whose calculations are detailed in this Appendix. $^{86}Sr/^{87}Sr$ ratios are given as measured (*i.e.*, not corrected for age and Rb content), since previous work has shown that corrections tend to cause little change in these values for samples belonging to the Barra Velha Formation (Tedeschi 2017; Pietzsch et al. 2018).

depth (m) below salt	Facies*	Lake units	Sequences	$\delta^{13}C$ (V-PDB)	$\delta^{13}C$ (1σ - ‰)	$\delta^{13}C$ 9-points moving avg	$\delta^{18}O$ (V-PDB)	$\delta^{18}O$ (1σ - ‰)	$\delta^{18}O$ 9-points moving avg	**Corrected $\delta^{18}O_{bulk}$ (V-PDB)**	$\delta^{18}O$ 9-points moving avg (of the corrected $\delta^{18}O_{bulk}$ values)	$^{87}Sr/^{86}Sr$	Std Dev	P (ppm)	P 9-points moving avg
4.99	2	13/12		2.06	0.05	2.21	0.19	0.05	0.40	-0.08	-0.19	0.71294	0.00001	83	137
5.24	13			1.12	0.06	1.65	-0.34	0.05	0.34	-0.54	-0.11			75	132
5.39	13		**BVF IV**	2.87	0.01	1.53	-0.25	0.02	0.41	-0.51	-0.05			63	256
6.19	1			2.70	0.05	1.58	1.01	0.05	0.51	0.57	0.23			326	261
6.59	0			2.30	0.06	1.32	1.39	0.07	0.78			0.71309	0.00002		
9.54	14			-1.14	0.04	1.39	0.01	0.03	0.67	-0.38	0.08	0.71298	0.00000	113	311
9.79	12			0.81	0.04	1.57	0.87	0.05	0.79	0.29	0.12			877	349
10.44	11			1.92	0.04	1.39	1.16	0.03	0.69	0.31	0.04			289	355
11.19	11			-0.74	0.05	1.22	2.94	0.07	0.81	2.16	0.21			684	322
11.39	13			2.68	0.03	1.11	-0.78	0.05	0.92	-1.06	0.33			63	337
11.99	2			2.69	0.03	1.54	0.72	0.06	0.86	0.26	0.28			379	331
12.84	10			1.25	0.08	1.72	-1.08	0.08	0.50	-1.28	-0.03	0.71324	0.00006	109	245
13.14	12			1.25	0.05	1.79	2.03	0.03	0.06	1.06	-0.41			58	222
13.49	12			1.26	0.05	2.18	2.44	0.05	-0.32	1.57	-0.79			459	153
14.49	10			2.74	0.04	2.22	-0.58	0.03	-0.28	-0.76	-0.83			57	181
14.74	10			2.47	0.04	2.21	-2.35	0.04	-0.34	-2.56	-0.86			111	140
15.09	12			2.51	0.04	2.36	-2.83	0.03	-0.14	-3.08	-0.67			74	152
15.49	11			2.74	0.07	2.45	-0.42	0.08	-0.35	-1.26	-0.82			66	207
18.39	11			3.07	0.03	2.27	-0.49	0.04	-0.38	-1.43	-0.85			314	164
18.89	0			2.57	0.05	2.01	0.19	0.06	-0.11	0.04	-0.65			11	167
19.29	4			2.65	0.04	1.92	0.71	0.07	0.31	0.35	-0.28			216	163

Table C: *Continued*

depth (m) below salt	Facies*	Lake units	Sequences	$\delta^{13}C$ (V-PDB)	$\delta^{13}C$ (1σ - ‰)	$\delta^{13}C$ 9-points moving avg	$\delta^{18}O$ (V-PDB)	$\delta^{18}O$ (1σ - ‰)	$\delta^{18}O$ 9-points moving avg	**Corrected $\delta^{18}O_{bulk}$ (V-PDB)**	$\delta^{18}O$ 9-points moving avg (of the corrected $\delta^{18}O_{bulk}$ values)	$^{87}Sr/^{86}Sr$	Std Dev	P (ppm)	P 9-points moving avg
19.59	14			2.08	0.04	1.93	0.19	0.08	0.95	-0.29	0.35			558	260
20.14	3			-0.42	0.05	1.91	2.20	0.04	1.27	1.30	0.74			65	297
20.49	14	11/10		0.46	0.04	1.88	1.84	0.04	1.74	1.07	1.29			86	288
21.09	12			1.62	0.04	1.80	1.41	0.06	1.98	0.82	1.52			81	301
22.89	10		**BVF III**	2.64	0.03	1.80	2.89	0.03	2.13	2.59	1.67			939	297
22.99	3			2.55	0.04	1.87	2.49	0.06	2.37	2.25	1.93			407	251
23.29	1			2.81	0.05	2.29	3.74	0.07	2.32	3.49	1.98			230	283
23.54	0			1.84	0.05	2.39	2.32	0.05	2.40	2.09	2.12			128	291
23.74	1			2.59	0.03	2.37	2.07	0.03	2.69	1.74	2.44			182	291
23.89	2			2.71	0.04	2.36	2.33	0.05	2.76	2.06	2.51			139	198
24.69	3			3.41	0.05	2.29	1.82	0.04	2.88	1.71	2.63			357	182
25.19	3			1.35	0.04	2.17	2.57	0.02	2.80	2.33	2.55			155	172
25.94	2			1.45	0.03	2.24	4.00	0.04	3.02	3.66	2.76			81	175
26.24	3			2.51	0.04	2.22	3.49	0.05	3.10	3.25	2.86	0.71310	0.00005	100	173
26.54	3			1.95	0.03	2.20	3.61	0.03	3.20	3.36	2.91			264	205
26.79	3			1.74	0.04	2.07	3.00	0.03	3.13	2.79	2.78			141	272
27.09	0			2.41	0.05	2.14	4.26	0.05	3.23	3.97	2.87			156	264
27.14	4			2.45	0.04	2.14	2.84	0.04	3.06	2.65	2.71			164	261
27.74	1			2.49	0.03	2.20	3.20	0.03	2.94	2.51	2.58			425	270
28.09	1			2.31	0.06	2.27	1.22	0.05	2.86	0.51	2.51			963	274
29.14	3			1.97	0.04	2.32	3.44	0.04	2.79	3.13	2.41	0.71372	0.00004	86	289
29.49	3			1.44	0.06	2.39	2.48	0.04	2.29	2.26	1.86			54	284
30.29	4			3.06	0.02	2.37	2.40	0.03	2.13	2.08	1.69			181	270
30.99	4			2.56	0.03	2.30	2.94	0.04	1.99	2.67	1.58			294	239
31.34	3			2.15	0.07	2.26	2.34	0.06	2.22	1.92	1.87			281	214

Table C: *Continued*

depth (m) below salt	Facies*	Lake units	Sequences	$\delta^{13}C$ (V-PDB)	$\delta^{13}C$ (1σ - ‰)	$\delta^{13}C$ 9-points moving avg	$\delta^{18}O$ (V-PDB)	$\delta^{18}O$ (1σ - ‰)	$\delta^{18}O$ 9-points moving avg	**Corrected $\delta^{18}O_{bulk}$ (V-PDB)**	$\delta^{18}O$ 9-points moving avg (of the corrected $\delta^{18}O_{bulk}$ values)	$^{87}Sr/^{86}Sr$	Std Dev	P (ppm)	P 9-points moving avg
31.64	14			3.11	0.05	2.31	-0.24	0.05	2.19	-1.03	1.83	0.71372	0.00003	110	279
32.39	0			2.24	0.03	2.38	1.42	0.04	2.24	1.18	1.86			32	295
32.64	4			1.87	0.04	2.29	1.88	0.05	2.15	1.51	1.76			152	292
33.44	4			1.93	0.04	2.21	3.33	0.03	2.17	3.13	1.77			740	268
34.14	4			2.45	0.06	2.30	3.12	0.02	2.22	2.75	1.83			664	388
34.49	3			2.04	0.04	2.27	2.99	0.03	2.63	2.49	2.28	0.71378	0.00004	201	393
34.79	3			2.30	0.04	2.30	1.56	0.02	2.84	1.23	2.46			150	437
35.04	4			1.82	0.04	2.42	3.14	0.03	2.94	2.77	2.57			81	454
36.04	3			2.96	0.07	2.50	2.81	0.06	2.98	2.45	2.59			1360	417
36.64	3			2.82	0.06	2.49	3.41	0.05	2.93	2.97	2.55			159	398
36.99	3			2.50	0.03	2.60	3.32	0.03	2.89	2.84	2.55			425	434
37.24	4			2.93	0.03	2.66	2.76	0.05	2.98	2.47	2.63			305	448
37.54	4			2.68	0.04	2.75	3.72	0.03	2.96	3.36	2.61			407	459
37.69	0			2.39	0.04	2.71	2.64	0.03	2.99	2.39	2.66			496	343
38.14	4			3.02	0.03	2.74	2.68	0.07	2.77	2.51	2.47			522	352
39.09	4			2.82	0.03	2.74	2.31	0.03	2.61	1.88	2.33			275	474
39.64	3			2.67	0.03	2.69	2.98	0.05	2.45	2.66	2.19			179	465
39.74	0			2.57	0.07	2.69	3.13	0.05	2.33	2.83	2.10			323	640
40.24	4			3.08	0.04	2.75	1.37	0.04	2.33	1.25	2.09			234	597
40.79	3			2.53	0.05	2.72	1.87	0.03	2.19	1.66	1.94			1522	555
41.09	4			2.47	0.04	2.72	1.36	0.04	2.16	1.13	1.94			231	572
41.24	0			2.70	0.03	2.74	2.67	0.02	2.06	2.55	1.85			1978	583
41.64	4			2.88	0.05	2.71	2.56	0.04	1.91	2.35	1.68			112	569
42.89	0			2.72	0.04	2.65	1.46	0.08	1.89	1.17	1.65			142	555
43.19	3			2.85	0.00	2.65	2.05	0.00	1.80	1.86	1.56	0.71361	0.00000	428	399

Table C: *Continued*

depth (m) below salt	Facies*	Lake units	Sequences	$\delta^{13}C$ (V-PDB)	$\delta^{13}C$ (1σ - ‰)	$\delta^{13}C$ 9-points moving avg	$\delta^{18}O$ (V-PDB)	$\delta^{18}O$ (1σ - ‰)	$\delta^{18}O$ 9-points moving avg	**Corrected $\delta^{18}O_{bulk}$ (V-PDB)**	$\delta^{18}O$ 9-points moving avg (of the corrected $\delta^{18}O_{bulk}$ values)	$^{87}Sr/^{86}Sr$	Std Dev	P (ppm)	P 9-points moving avg
43.99	4			2.82	0.04	2.69	2.07	0.05	1.58	1.86	1.29			277	377
44.34	3			2.36	0.04	2.69	1.76	0.03	1.54	1.27	1.22			196	172
44.75	2			2.56	0.04	2.67	1.19	0.05	1.36	0.96	1.03			106	175
45.10	2			2.49	0.02	2.62	1.07	0.04	1.36	0.85	1.04			123	235
45.30	4			2.85	0.03	2.53	-0.62	0.04	0.87	-1.29	0.47			33	579
45.74	2			2.67	0.05	2.46	2.33	0.04	0.30	1.97	-0.18			135	557
46.14	3			2.72	0.04	2.45	0.95	0.05	0.17	0.65	-0.32			137	568
46.39	4			2.23	0.05	2.39	1.41	0.05	0.11	1.20	-0.42			677	602
46.74	14			2.03	0.01	2.42	-2.30	0.06	0.07	-3.21	-0.54			3531	628
46.94	0	9/8		2.26	0.04	2.46	-3.10	0.03	0.10	-4.04	-0.54			75	628
47.44	1			2.23	0.04	2.36	0.56	0.04	-0.19	0.04	-0.85	0.71339	0.00005	294	628
48.09	1			2.04	0.03	2.24	0.67	0.05	-0.23	0.01	-0.90	0.71325	0.00004	416	792
48.39	11			2.75	0.03	2.18	0.72	0.06	-0.50	-0.18	-1.21			357	742
48.74	14			3.22	0.06	2.13	-0.32	0.06	-0.31	-1.28	-0.96			30	372
49.04	1			1.73	0.04	2.04	-0.32	0.05	0.15	-0.82	-0.46	0.71303	0.00005	137	414
49.29	1			1.70	0.00	2.07	0.63	0.00	0.33	0.15	-0.23	0.71295	0.00000	1607	400
49.64	1			1.63	0.02	2.09	-1.08	0.06	0.36	-1.54	-0.15	0.71297	0.00003	228	363
49.99	1			1.61	0.05	2.00	-0.56	0.06	0.28	-0.95	-0.16			201	350
50.39	1			1.48	0.03	1.88	1.09	0.05	0.50	0.46	0.14			452	400
51.59	3			2.50	0.04	1.92	2.16	0.01	0.65	2.04	0.34			173	416
52.59	3			2.22	0.06	1.97	0.91	0.03	0.57	0.79	0.29	0.71310	0.00004	84	244
52.99	2			1.87	0.05	2.00	-0.01	0.05	0.79	-0.29	0.52			240	263
53.29	4			2.16	0.00	2.06	1.65	0.00	0.93	1.45	0.69			480	247
53.59	4			2.11	0.02	2.11	1.07	0.02	1.04	0.91	0.80			276	224
54.14	3			2.13	0.03	2.05	-0.09	0.04	0.97	-0.24	0.69			63	213

Table C: *Continued*

depth (m) below salt	Facies*	Lake units	Sequences	$\delta^{13}C$ (V-PDB)	$\delta^{13}C$ (1σ - ‰)	$\delta^{13}C$ 9-points moving avg	$\delta^{18}O$ (V-PDB)	$\delta^{18}O$ (1σ - ‰)	$\delta^{18}O$ 9-points moving avg	**Corrected $\delta^{18}O_{bulk}$ (V-PDB)**	$\delta^{18}O$ 9-points moving avg (of the corrected $\delta^{18}O_{bulk}$ values)	$^{87}Sr/^{86}Sr$	Std Dev	P (ppm)	P 9-points moving avg
54.54	2			1.94	0.02	1.96	0.88	0.02	1.06	0.47	0.66			401	211
54.69	3			2.10	0.02	1.99	0.71	0.02	1.15	0.63	0.78			52	204
54.94	0			1.93	0.08	1.97	2.06	0.05	1.12	1.44	0.69			244	153
55.29	4			2.01	0.05	1.97	1.52	0.05	1.09					73	133
55.54	1			1.43	0.00	1.98	1.78	0.00	1.27	1.07	0.68			70	153
56.24	2			2.11	0.00	2.12	0.77	0.00	1.91	0.51	1.34			174	114
56.84	3			1.93	0.03	2.12	1.34	0.02	1.98	0.82	1.41			28	123
57.14	3			2.18	0.06	2.17	0.87	0.06	1.96	0.56	1.52	0.71310	0.00004	88	104
58.24	2			2.22	0.05	2.20	1.47	0.07	2.02	0.88	1.55			247	113
58.69	1			3.20	0.02	2.32	6.63	0.02	2.00	5.66	1.59	0.71311	0.00005	49	123
59.04	3			2.06	0.02	2.37	1.37	0.04	2.17	1.12	1.75			130	135
59.29	3			2.36	0.06	2.44	1.91	0.04	2.29	1.65	1.91			79	165
59.64	2			2.34	0.05	2.46	2.01	0.04	2.41	1.72	2.03			156	194
59.94	3			2.52	0.06	2.47	1.61	0.04	2.47	1.36	2.12			153	199
60.24	4			2.50	0.05	2.38	2.31	0.06	1.99	2.00	1.68	0.71308	0.00005	287	206
60.54	3			2.55	0.07	2.31	2.45	0.05	1.99	2.20	1.65			298	215
60.79	3			2.36	0.04	2.18	1.95	0.07	1.96	1.69	1.59	0.71315	0.00005	346	249
61.04	3			2.32	0.00	2.08	2.03	0.00	1.92	1.68	1.53			295	274
61.49	2			2.45	0.02	1.92	2.30	0.01	1.89	1.67	1.49	0.71317	0.00006	109	346
61.74	1			1.38	0.03	1.86	1.36	0.02	1.74	0.87	1.34			208	348
62.09	1			1.16	0.04	1.82	1.62	0.03	1.50	1.09	1.06			393	342
62.39	2			1.52	0.00	1.79	1.64	0.00	1.39	1.17	0.91	0.71304	0.00000	381	346
62.94	1			1.06	0.05	1.74	1.32	0.04	1.23	1.04	0.75			796	331
63.24	1			1.95	0.02	1.67	1.03	0.04	1.05	0.62	0.61			302	330
63.54	1			2.14	0.03	1.76	0.29	0.03	1.09	-0.30	0.67			247	318

Table C: *Continued*

depth (m) below salt	Facies*	Lake units	Sequences	$\delta^{13}C$ (V-PDB)	$\delta^{13}C$ (1σ - ‰)	$\delta^{13}C$ 9-points moving avg	$\delta^{18}O$ (V-PDB)	$\delta^{18}O$ (1σ - ‰)	$\delta^{18}O$ 9-points moving avg	**Corrected $\delta^{18}O_{bulk}$ (V-PDB)**	$\delta^{18}O$ 9-points moving avg (of the corrected $\delta^{18}O_{bulk}$ values)	$^{87}Sr/^{86}Sr$	Std Dev	P (ppm)	P 9-points moving avg
63.74	0			2.14	0.00	1.90	0.95	0.00	1.11	0.34	0.68			386	303
63.99	5			1.90	0.03	1.98	0.58	0.03	1.10	0.23	0.67			160	297
64.29	3			1.76	0.02	2.13	0.70	0.03	1.21	0.42	0.74			94	242
64.59	3			2.24	0.05	2.22	1.72	0.04	1.17	1.39	0.73	0.71308	0.00005	106	237
64.89	1			2.35	0.00	2.38	1.78	0.00	1.33	1.21	0.92	0.71299	0.00000	257	237
65.19	1			2.24	0.00	2.52	1.51	0.00	1.46	1.08	1.05			325	206
65.64	1			2.42	0.05	2.63	2.30	0.03	1.46	1.64	1.06			300	212
65.94	3			2.83	0.00	2.64	0.72	0.00	1.52	0.56	1.11	0.71318	0.00000	254	217
66.34	1			3.54	0.04	2.61	1.74	0.05	1.36	1.38	0.89	0.71334	0.00010	253	212
66.64	2			3.36	0.03	2.61	2.10	0.03	1.08	1.53	0.62			106	189
67.29	13			2.89	0.00	2.53	0.55	0.00	1.01	0.29	0.52			216	162
67.94	3			1.92	0.00	2.40	1.25	0.00	0.85	0.89	0.39			138	341
68.24	1			1.93	0.05	2.29	0.25	0.04	0.93	-0.54	0.40	0.71348	0.00005	59	327
68.79	2			2.33	0.00	2.16	-0.66	0.00	0.84	-1.24	0.29	0.71301	0.00000	54	306
69.09	1			1.55	0.05	1.98	0.86	0.06	0.84	0.21	0.28			81	300
69.39	3			1.21	0.00	1.90	0.88	0.00	0.84	0.47	0.23			1906	287
70.64	12			1.89	0.05	1.93	1.42	0.05	0.81	0.65	0.18			126	282
71.09	12			2.33	0.03	1.96	0.88	0.03	0.86	0.34	0.28			66	294
71.39	12			1.79	0.00	1.98	2.14	0.00	1.02	1.44	0.46			56	297
72.04	1			2.13	0.00	2.05	0.51	0.00	0.99	-0.17	0.46			100	315
72.54	1			2.20	0.00	2.11	1.03	0.00	0.99	0.50	0.47	0.71294	0.00000	88	117
72.94	2			2.18	0.00	2.09	0.64	0.00	1.03	0.32	0.56			170	108
73.19	1			2.55	0.05	2.02	0.78	0.05	1.07	0.42	0.63			76	104
73.84	3			2.19	0.02	2.06	0.65	0.03	1.04	0.14	0.61			250	104
74.19	3			1.77	0.04	2.08	0.86	0.04	1.03	0.55	0.63			117	96

Table C: *Continued*

depth (m) below salt	Facies*	Lake units	Sequences	$\delta^{13}C$ (V-PDB)	$\delta^{13}C$ (1σ - ‰)	$\delta^{13}C$ 9-points moving avg	$\delta^{18}O$ (V-PDB)	$\delta^{18}O$ (1σ - ‰)	$\delta^{18}O$ 9-points moving avg	**Corrected $\delta^{18}O_{bulk}$ (V-PDB)**	$\delta^{18}O$ 9-points moving avg (of the corrected $\delta^{18}O_{bulk}$ values)	$^{87}Sr/^{86}Sr$	Std Dev	P (ppm)	P 9-points moving avg
74.54	3			1.66	0.03	2.09	1.75	0.03	0.91	1.48	0.54			51	92
74.84	3			1.73	0.06	2.12	1.26	0.04	0.93	1.02	0.54			30	76
75.09	1			2.17	0.00	2.09	1.89	0.00	0.80	1.19	0.37	0.71249	0.00000	57	71
75.44	2			2.24	0.05	2.08	0.40	0.10	0.77	0.04	0.33			27	47
75.74	3			2.30	0.00	2.13	0.00	0.00	0.75	-0.31	0.30			46	40
76.19	2			2.48	0.05	2.23	0.78	0.10	0.59	0.31	0.12			26	38
76.44	1			2.25	0.05	2.30	-0.42	0.10	0.39	-1.13	-0.13			36	40
77.19	3			2.12	0.05	2.39	0.38	0.10	0.22	-0.14	-0.24			36	37
77.49	3			2.18	0.05	2.37	0.73	0.10	0.19	0.24	-0.28			48	36
77.89	13	7		2.58	0.00	2.31	0.33	0.00	0.21	-0.17	-0.26	0.71331	0.00000	39	36
78.14	3			2.34	0.05	2.24	-0.59	0.10	0.10	-1.16	-0.38			48	37
78.59	13			3.04	0.00	2.23	0.37	0.00	0.09	0.15	-0.36			26	38
79.09	13			2.05	0.05	2.28	0.14	0.10	0.09	-0.27	-0.32			16	40
79.49	13			1.77	0.00	2.26	0.21	0.00	-0.19	-0.18	-0.63			48	39
79.84	3			1.79	0.05	2.20	-0.27	0.10	-0.20	-0.78	-0.62			38	39
80.04	3			2.18	0.00	2.21	-0.51	0.00	-0.09	-0.90	-0.48	0.71311	0.00000	40	36
80.34	2			2.60	0.05	2.14	0.40	0.10	-0.11	0.22	-0.50			53	38
80.64	3			1.97	0.00	2.20	-1.82	0.00	-0.09	-2.57	-0.46			43	43
80.89	3			2.09	0.05	2.24	0.26	0.10	-0.08	-0.10	-0.44			37	43
81.29	2			2.39	0.00	2.25	0.40	0.00	-0.02	0.15	-0.40			20	46
81.94	3			2.44	0.05	2.27	0.16	0.10	0.04	-0.08	-0.33			48	45
82.29	3			2.56	0.05	2.21	0.36	0.10	0.10	0.13	-0.27	0.71321	0.00005	60	46
82.49	3			2.10	0.00	2.21	0.30	0.00	0.37	-0.02	0.02			46	48
82.74	3			1.88	0.00	2.22	0.25	0.00	0.42	-0.40	0.04			71	54
83.09	2			2.42	0.05	2.21	0.08	0.10	0.48	-0.31	0.05			29	59

Table C: *Continued*

depth (m) below salt	Facies*	Lake units	Sequences	$\delta^{13}C$ (V-PDB)	$\delta^{13}C$ (1σ - ‰)	$\delta^{13}C$ 9-points moving avg	$\delta^{18}O$ (V-PDB)	$\delta^{18}O$ (1σ - ‰)	$\delta^{18}O$ 9-points moving avg	**Corrected $\delta^{18}O_{bulk}$ (V-PDB)**	$\delta^{18}O$ 9-points moving avg (of the corrected $\delta^{18}O_{bulk}$ values)	$^{87}Sr/^{86}Sr$	Std Dev	P (ppm)	P 9-points moving avg
83.34	3			2.02	0.05	2.11	0.88	0.10	0.54	0.74	0.06			63	58
83.64	2			2.02	0.05	2.07	0.64	0.10	0.54	0.07	0.05	0.71313	0.00005	57	56
83.94	3			2.17	0.00	2.10	0.73	0.00	0.59	0.10	0.10			95	54
84.24	1			2.31	0.05	2.07	0.92	0.10	0.66	0.26	0.17	0.71310	0.00005	61	50
84.49	3			1.52	0.00	1.90	0.73	0.00	0.78	-0.03	0.27			44	51
84.84	13			2.15	0.05	1.81	0.35	0.10	0.88	0.02	0.31			39	49
85.19	3			2.42	0.00	1.70	0.76	0.00	0.97	0.42	0.40	0.71307	0.00000	28	48
85.89	1			1.57	0.00	1.60	0.85	0.00	1.05	0.29	0.49	0.71305	0.00000	37	41
86.09	1			0.92	0.05	1.46	1.14	0.10	1.06	0.52	0.52			34	43
86.34	1		**BVF II**	1.23	0.05	1.48	1.78	0.10	1.06	1.12	0.57			45	43
86.59	3			1.04	0.05	1.43	1.48	0.10	1.09	0.86	0.60			49	42
86.94	1			1.28	0.05	1.35	1.46	0.10	1.08	0.96	0.60	0.71303	0.00004	32	44
87.24	3			0.99	0.05	1.41	0.99	0.10	1.13	0.51	0.69			77	44
87.59	2			1.68	0.00	1.53	0.75	0.00	1.14	0.44	0.75			49	41
87.94	3			1.72	0.00	1.61	0.58	0.00	1.11	0.26	0.77			30	42
88.14	3			1.73	0.05	1.67	0.69	0.10	1.08	0.40	0.76			42	43
88.59	4			2.12	0.05	1.69	1.32	0.10	0.99	1.12	0.69	0.71323	0.00005	36	41
88.84	4			1.99	0.00	1.67	1.25	0.00	1.01	1.07	0.68			12	38
89.19	4			1.98	0.00	1.60	1.47	0.00	1.01	1.30	0.66			50	39
89.59	1			1.57	0.05	1.56	1.22	0.10	1.14	0.77	0.75			55	42
89.94	3			1.41	0.00	1.50	0.67	0.00	1.33	0.32	0.89			15	43
90.24	4			0.84	0.05	1.49	1.14	0.10	1.25	0.46	0.84			52	41
90.54	2			1.06	0.00	1.44	0.78	0.00	1.19	0.20	0.78			57	44
90.79	2			1.32	0.00	1.42	1.70	0.00	1.11	1.07	0.69			58	40
91.24	2			1.20	0.05	1.46	2.38	0.10	1.08	1.70	0.69			56	40

Table C: *Continued*

depth (m) below salt	Facies*	Lake units	Sequences	$\delta^{13}C$ (V-PDB)	$\delta^{13}C$ (1σ - ‰)	$\delta^{13}C$ 9-points moving avg	$\delta^{18}O$ (V-PDB)	$\delta^{18}O$ (1σ - ‰)	$\delta^{18}O$ 9-points moving avg	**Corrected $\delta^{18}O_{bulk}$ (V-PDB)**	$\delta^{18}O$ 9-points moving avg (of the corrected $\delta^{18}O_{bulk}$ values)	$^{87}Sr/^{86}Sr$	Std Dev	P (ppm)	P 9-points moving avg
91.59	3			2.00	0.00	1.54	0.68	0.00	1.14	0.68	0.78	0.71340	0.00000	13	45
91.99	3			1.60	0.00	1.65	0.70	0.00	1.10	0.49	0.79			38	42
92.29	3			1.76	0.05	1.69	0.68	0.10	1.07	0.48	0.77			20	47
92.59	4			1.97	0.05	1.65	0.95	0.10	0.93	0.80	0.65			55	45
92.94	4			2.10	0.00	1.58	1.22	0.00	0.80	1.10	0.53			58	45
93.19	4			1.82	0.05	1.47	0.79	0.10	0.84	0.63	0.50	0.71320	0.00005	19	51
93.44	1			1.47	0.05	1.42	0.51	0.10	0.97	0.02	0.56			103	56
93.84	2			0.96	0.00	1.38	0.45	0.00	1.09	-0.01	0.64			40	59
94.14	1			0.51	0.00	1.33	1.20	0.00	1.19	0.54	0.66			57	58
94.44	2			1.07	0.05	1.24	1.04	0.10	1.17	0.47	0.60			67	58
95.04	10			1.15	0.05	1.13	1.85	0.10	1.17	1.04	0.55			81	59
95.34	2	6/5		1.37	0.00	1.15	1.82	0.00	1.28	1.13	0.65			53	56
95.64	2			1.50	0.00	1.27	1.79	0.00	1.37	1.04	0.73			41	54
96.24	3			1.28	0.00	1.41	1.04	0.00	1.51	0.53	0.88	0.71338	0.00000	57	54
96.49	3			0.82	0.00	1.48	0.87	0.00	1.74	0.22	1.08			36	54
96.74	4			1.73	0.00	1.56	1.46	0.00	1.70	0.89	1.06			73	45
96.99	1			1.98	0.00	1.56	1.24	0.00	1.78	0.75	1.13			19	44
97.44	1			1.78	0.05	1.53	2.48	0.10	1.60	1.86	0.99			55	42
97.74	1			1.74	0.05	1.55	3.14	0.10	1.78	2.28	1.13			69	43
98.04	2			1.80	0.05	1.60	1.48	0.10	1.90	0.82	1.26			1	42
98.34	2			1.38	0.05	1.57	2.56	0.10	2.07	1.79	1.39	0.71282	0.00005	41	37
98.59	1			1.25	0.00	1.51	0.16	0.00	2.02	-0.25	1.36			25	40
98.84	1			1.48	0.00	1.45	2.63	0.00	1.82	1.82	1.19			66	39
99.14	2			1.29	0.05	1.43	1.98	0.10	1.59	1.34	1.04			25	36
99.49	1			1.42	0.00	1.48	2.97	0.00	1.57	2.14	1.08			31	42

Table C: *Continued*

depth (m) below salt	Facies*	Lake units	Sequences	$\delta^{13}C$ (V-PDB)	$\delta^{13}C$ (1σ - ‰)	$\delta^{13}C$ 9-points moving avg	$\delta^{18}O$ (V-PDB)	$\delta^{18}O$ (1σ - ‰)	$\delta^{18}O$ 9-points moving avg	**Corrected $\delta^{18}O_{bulk}$ (V-PDB)**	$\delta^{18}O$ 9-points moving avg (of the corrected $\delta^{18}O_{bulk}$ values)	$^{87}Sr/^{86}Sr$	Std Dev	P (ppm)	P 9-points moving avg
99.74	1			1.43	0.00	1.54	0.78	0.00	1.47	0.41	1.00			50	43
100.04	1			1.22	0.00	1.55	0.70	0.00	1.62	0.40	1.12	0.71299	0.00000	45	42
100.34	3			1.63	0.00	1.54	1.08	0.00	1.46	0.90	1.01			44	40
100.59	3			2.18	0.00	1.58	1.30	0.00	1.41	1.19	0.96			50	43
100.94	2			2.00	0.00	1.48	1.67	0.00	1.31	1.07	0.89			53	41
101.24	2			1.28	0.05	1.49	1.51	0.10	1.51	0.83	1.06			12	41
101.59	1			1.44	0.05	1.47	1.17	0.10	1.67	0.80	1.19	0.71310	0.00006	50	39
101.89	1			1.62	0.00	1.41	1.54	0.00	1.61	0.94	1.11			53	37
102.24	11			0.51	0.00	1.31	2.02	0.00	1.54	1.45	1.01			15	36
102.54	2			1.52	0.05	1.23	2.59	0.10	1.47	1.98	0.96	0.71277	0.00006	45	36
102.79	1			1.01	0.05	1.22	2.19	0.10	1.52	1.54	1.02			25	40
103.44	1			1.13	0.00	1.28	0.49	0.00	1.53	0.17	1.01	0.71294	0.00000	32	38
103.74	1			1.26	0.05	1.29	0.70	0.10	1.52	0.32	0.98			40	39
104.04	1			1.28	0.05	1.38	1.04	0.10	1.45	0.65	0.91			50	47
104.29	1			1.24	0.00	1.31	1.91	0.00	1.29	1.36	0.77	0.71261	0.00000	49	45
104.64	2			1.92	0.00	1.27	1.26	0.00	1.11	0.69	0.63			36	47
105.19	7			1.75	0.00	1.26	1.45	0.00	1.20	0.68	0.71			58	50
105.39	1			1.29	0.00	1.31	1.41	0.00	1.36	0.78	0.82			90	56
105.79	1			0.92	0.05	1.31	1.12	0.10	1.35	0.73	0.82			21	57
106.04	1			0.63	0.00	1.36	0.63	0.00	1.39	0.27	0.84			50	68
106.34	1			1.08	0.05	1.29	1.32	0.10	1.38	0.90	0.86			55	69
106.69	1			1.70	0.00	1.32	2.08	0.00	1.38	1.30	0.91			97	69
107.24	3			1.24	0.05	1.43	0.99	0.10	1.39	0.69	0.96			57	65
107.49	2			1.71	0.00	1.56	2.27	0.00	1.44	1.56	1.04			147	69
107.74	2			1.33	0.00	1.65	1.16	0.00	1.56	0.82	1.13			44	69

Table C: *Continued*

depth (m) below salt	Facies*	Lake units	Sequences	$\delta^{13}C$ (V-PDB)	$\delta^{13}C$ (1σ - ‰)	$\delta^{13}C$ 9-points moving avg	$\delta^{18}O$ (V-PDB)	$\delta^{18}O$ (1σ - ‰)	$\delta^{18}O$ 9-points moving avg	**Corrected $\delta^{18}O_{bulk}$ (V-PDB)**	$\delta^{18}O$ 9-points moving avg (of the corrected $\delta^{18}O_{bulk}$ values)	$^{87}Sr/^{86}Sr$	Std Dev	P (ppm)	P 9-points moving avg
108.04	13			1.99	0.00	1.73	1.42	0.00	1.54	1.16	1.14			60	66
108.29	13			2.23	0.05	1.73	1.48	0.10	1.37	1.25	1.05			55	58
108.59	13			2.15	0.05	1.76	1.60	0.10	1.47	1.37	1.13			57	57
108.99	1			1.40	0.05	1.75	1.71	0.10	1.51	1.14	1.17			46	51
109.44	3			1.82	0.00	1.78	1.15	0.00	1.57	1.00	1.23			30	54
109.64	1			1.73	0.05	1.71	0.59	0.10	1.54	0.50	1.20			25	54
113.34	3			1.47	0.05	1.60	1.89	0.10	1.53	1.33	1.18			47	56
113.59	3			1.64	0.00	1.60	2.63	0.00	1.47	1.96	1.14			95	53
113.94	3			1.62	0.00	1.62	1.65	0.00	1.48	1.33	1.15			68	57
114.19	3			1.37	0.05	1.61	1.14	0.10	1.58	0.89	1.24			65	58
114.49	2			1.19	0.00	1.58	1.45	0.00	1.60	1.12	1.24			75	58
114.79	2			2.13	0.00	1.62	1.03	0.00	1.62	0.96	1.30			28	59
115.19	2			1.65	0.00	1.64	1.76	0.00	1.56	1.28	1.27			83	54
115.54	3			1.70	0.05	1.69	2.12	0.10	1.63	1.79	1.35			34	54
115.84	13			1.47	0.00	1.60	0.71	0.00	1.68	0.46	1.40			27	55
116.14	3			1.83	0.00	1.61	2.12	0.00	1.73	1.89	1.45			55	56
116.39	3			1.83	0.05	1.53	2.02	0.10	1.90	1.72	1.57			52	59
116.69	3			2.01	0.00	1.57	2.30	0.00	1.92	2.00	1.62			71	56
117.39	4			0.63	0.05	1.56	1.60	0.10	1.89	1.38	1.57			74	61
117.74	2			1.26	0.05	1.58	1.93	0.10	2.01	1.59	1.68			78	63
117.94	2			1.35	0.00	1.59	2.55	0.00	1.93	2.02	1.59	0.71261	0.00000	56	63
118.44	3			2.07	0.05	1.58	1.92	0.10	1.94	1.72	1.56			55	70
118.79	2			1.58	0.05	1.52	1.84	0.10	1.83	1.35	1.43			78	72
119.34	2			1.68	0.00	1.64	1.84	0.00	1.82	1.41	1.39			51	77
119.54	2			1.93	0.00	1.72	1.37	0.00	1.85	1.13	1.39			52	76

Table C: *Continued*

depth (m) below salt	Facies*	Lake units	Sequences	$\delta^{13}C$ (V-PDB)	$\delta^{13}C$ (1σ - ‰)	$\delta^{13}C$ 9-points moving avg	$\delta^{18}O$ (V-PDB)	$\delta^{18}O$ (1σ - ‰)	$\delta^{18}O$ 9-points moving avg	**Corrected $\delta^{18}O_{bulk}$ (V-PDB)**	$\delta^{18}O$ 9-points moving avg (of the corrected $\delta^{18}O_{bulk}$ values)	$^{87}Sr/^{86}Sr$	Std Dev	P (ppm)	P 9-points moving avg
119.94	1			1.72	0.05	1.81	2.11	0.10	1.73	1.47	1.32			118	74
120.29	3			1.49	0.00	1.78	1.31	0.00	1.65	0.83	1.25			86	74
120.54	2			1.71	0.00	1.81	1.51	0.00	1.68	0.96	1.30			116	74
120.84	2			1.99	0.05	1.78	2.21	0.10	1.68	1.64	1.29			74	81
121.14	1			2.10	0.00	1.66	1.48	0.00	1.71	1.40	1.28			40	85
121.44	3			1.82	0.05	1.61	1.21	0.10	1.65	1.04	1.23	0.71304	0.00004	55	81
122.44	3			1.88	0.05	1.61	2.04	0.10	1.66	1.83	1.25			77	79
122.74	1			1.34	0.05	1.58	1.88	0.10	1.63	1.33	1.23			112	75
122.99	2	4		0.91	0.00	1.56	1.62	0.00	1.54	1.05	1.17			84	74
123.44	2			1.25	0.05	1.55	1.60	0.10	1.55	1.03	1.16			86	78
123.74	2			1.49	0.00	1.58	1.39	0.00	1.59	0.95	1.19	0.71329	0.00000	70	80
123.94	2			1.46	0.00	1.60	1.24	0.00	1.56	0.78	1.16			75	81
124.29	2			1.83	0.05	1.67	1.41	0.10	1.53	1.14	1.13			67	74
124.59	4			2.01	0.05	1.75	1.59	0.10	1.50	1.30	1.12			73	72
124.84	13			2.01	0.05	1.79	1.54	0.10	1.50	1.27	1.15			79	70
125.09	2			2.07	0.05	1.81	1.81	0.10	1.52	1.55	1.19	0.71315	0.00005	79	66
125.34	4			2.01	0.00	1.82	1.59	0.00	1.51	1.09	1.22			52	59
125.64	4			1.64	0.05	1.80	1.31	0.10	1.55	0.98	1.26			63	67
125.94	4			1.55	0.00	1.72	1.65	0.00	1.64	1.30	1.32			68	67
126.24	3			1.74	0.00	1.71	1.53	0.00	1.61	1.28	1.26			34	74
126.54	3			1.52	0.05	1.65	1.17	0.10	1.58	1.03	1.21			17	71
126.79	3			1.68	0.05	1.57	1.76	0.10	1.51	1.57	1.16			140	70
127.09	1			1.30	0.05	1.54	2.40	0.10	1.50	1.79	1.14			75	65
127.64	2			1.87	0.05	1.61	1.26	0.10	1.59	0.72	1.19			137	65
127.94	3			1.58	0.00	1.59	1.59	0.00	1.61	1.17	1.19			52	67

Table C: *Continued*

depth (m) below salt	Facies*	Lake units	Sequences	$\delta^{13}C$ (V-PDB)	$\delta^{13}C$ (1σ - ‰)	$\delta^{13}C$ 9-points moving avg	$\delta^{18}O$ (V-PDB)	$\delta^{18}O$ (1σ - ‰)	$\delta^{18}O$ 9-points moving avg	**Corrected $\delta^{18}O_{bulk}$ (V-PDB)**	$\delta^{18}O$ 9-points moving avg (of the corrected $\delta^{18}O_{bulk}$ values)	$^{87}Sr/^{86}Sr$	Std Dev	P (ppm)	P 9-points moving avg
128.19	2			1.22	0.05	1.59	0.94	0.10	1.61	0.59	1.19			42	71
128.54	1			1.38	0.05	1.59	1.20	0.10	1.53	0.83	1.11			20	59
128.84	1			2.19	0.05	1.63	2.48	0.10	1.39	1.70	1.03			71	56
129.14	13			1.58	0.00	1.60	1.65	0.00	1.34	1.30	1.03			51	45
129.44	3			1.50	0.00	1.58	1.24	0.00	1.30	1.07	1.01			51	47
130.59	4			1.69	0.03	1.58	1.00	0.03	1.37	0.86	1.07	0.71319	0.00005	30	51
131.14	4			1.66	0.01	1.60	1.12	0.02	1.44	1.01	1.16			54	58
131.54	4	3/2/1		1.60	0.00	1.47	0.81	0.00	1.41	0.75	1.16			35	61
131.94	4			1.39	0.04	1.46	1.28	0.03	1.36	1.01	1.13	0.71314	0.00006	73	61
132.34	3		**BVF I**	1.26	0.00	1.44	1.51	0.00	1.39	1.10	1.14			78	61
132.74	3			1.49	0.03	1.39	1.91	0.03	1.38	1.63	1.11			77	58
133.04	3			1.10	0.00	1.35	2.17	0.00	1.39	1.67	1.08			96	63
133.24	4			1.44	0.04	1.30	1.17	0.06	1.45	1.05	1.06			55	81
133.59	2			1.33	0.03	1.25	1.52	0.04	1.46	1.15	1.01			52	82
133.89	3			1.23	0.00	1.25	0.95	0.00	1.38	0.61	0.90			2	85
135.09	3			1.34	0.03	1.22	1.18	0.02	1.19	0.78	0.68			97	85
135.39	2			1.09	0.00	1.26	1.33	0.00	0.98	0.57	0.54			199	83
135.74	3			0.96	0.00	1.20	1.36	0.00	0.95	0.56	0.47			80	88
136.09	1			1.29	0.02	1.11	0.86	0.02	0.85	0.09	0.43	0.71327	0.00005	110	85
136.29	2			1.24	0.02	1.07	0.17	0.03	0.90					76	112
136.84	2			1.42	0.00	0.96	0.24	0.00	0.96	-0.32	0.48			77	119
137.14	1			0.88	0.00	1.05	0.93	0.00	0.93	0.38	0.44			101	102
137.39	3			0.55	0.03	1.10	0.61	0.02	0.90	0.38	0.45			23	99
137.69	1			0.84	0.03	1.11	1.42	0.03	0.96	0.81	0.50			244	97
138.09	1			0.41	0.00	1.12	1.73	0.00	1.11	1.11	0.61	0.71322	0.00000	162	101

Table C: *Continued*

depth (m) below salt	Facies*	Lake units	Sequences	$\delta^{13}C$ (V-PDB)	$\delta^{13}C$ (1σ - ‰)	$\delta^{13}C$ 9-points moving avg	$\delta^{18}O$ (V-PDB)	$\delta^{18}O$ (1σ - ‰)	$\delta^{18}O$ 9-points moving avg	**Corrected $\delta^{18}O_{bulk}$ (V-PDB)**	$\delta^{18}O$ 9-points moving avg (of the corrected $\delta^{18}O_{bulk}$ values)	$^{87}Sr/^{86}Sr$	Std Dev	P (ppm)	P 9-points moving avg
138.29	1			1.84	0.00	1.12	1.08	0.00	1.25	0.34	0.77			45	102
138.64	13			1.40	0.04	1.17	1.06	0.05	1.31	0.70	0.86	0.71312	0.00007	53	99
138.94	4			1.43	0.04	1.25	1.42	0.05	1.38	1.03	0.90			88	101
139.24	4			1.34	0.03	1.30	1.48	0.03	1.33	1.04	0.88			112	80
139.44	3			1.40	0.04	1.43	1.49	0.03	1.28	1.18	0.85			91	69
139.89	4			1.30	0.00	1.37	1.46	0.00	1.26	1.17	0.87			77	68
140.19	2			1.28	0.03	1.37	1.28	0.02	1.29	0.74	0.89			33	83
140.44	1			1.32	0.00	1.39	0.99	0.00	1.25	0.58	0.82	0.71307	0.00000	63	89
140.79	1			1.53	0.03	1.43	1.30	0.03	1.19	0.83	0.75			56	94
141.09	4			1.29	0.01	1.46	0.86	0.02	1.00	0.58	0.52			43	99
141.39	3			1.45	0.01	1.54	1.37	0.03	0.98	0.88	0.46			186	111
141.69	2			1.56	0.00	1.51	1.02	0.00	0.94	0.37	0.44			136	114
142.19	7			1.78	0.01	1.49	0.98	0.03	0.93	0.41	0.44			163	113
142.54	7			1.65	0.02	1.46	-0.22	0.03	0.92	-0.85	0.43			138	112
142.79	7			1.97	0.00	1.44	1.21	0.00	0.96	0.60	0.44	0.71327	0.00000	184	109
143.19	3			1.00	0.01	1.40	0.93	0.02	0.87	0.60	0.36			53	96
143.29	14			1.16	0.00	1.40	0.89	0.00	0.86	0.50	0.36			59	94
143.49	3			1.31	0.02	1.38	1.26	0.03	0.82	0.75	0.33			42	93
143.69	1			1.09	0.00	1.34	1.19	0.00	0.94	0.71	0.45			24	91
143.99	2			1.11	0.00	1.28	0.57	0.00	0.88	0.18	0.42			69	77
144.34	6			1.54	0.08	1.33	0.94	0.04	0.85	0.35	0.38	0.71320	0.00005	113	86
144.59	6			1.59	0.00	1.37	0.65	0.00	0.90	0.12	0.42			159	86
144.79	3			1.32	0.02	1.42	0.78	0.03	0.80	0.23	0.34			119	86
145.04	3			1.43	0.03	1.52	0.74	0.03	0.82	0.31	0.39			59	90
145.34	6			1.45	0.00	1.59	0.59	0.00	0.93	0.24	0.45			134	97

Table C: *Continued*

depth (m) below salt	Facies*	Lake units	Sequences	$\delta^{13}C$ (V-PDB)	$\delta^{13}C$ (1σ - ‰)	$\delta^{13}C$ 9-points moving avg	$\delta^{18}O$ (V-PDB)	$\delta^{18}O$ (1σ - ‰)	$\delta^{18}O$ 9-points moving avg	**Corrected $\delta^{18}O_{bulk}$ (V-PDB)**	$\delta^{18}O$ 9-points moving avg (of the corrected $\delta^{18}O_{bulk}$ values)	$^{87}Sr/^{86}Sr$	Std Dev	P (ppm)	P 9-points moving avg
145.69	1			1.52	0.03	1.59	1.38	0.03	0.97	0.89	0.51			56	98
145.94	3			1.76	0.00	1.58	0.32	0.00	0.91	0.05	0.44			41	88
146.19	2			1.95	0.04	1.56	1.41	0.02	0.90	1.12	0.45			57	96
146.54	1			1.77	0.02	1.56	1.53	0.03	0.92	0.78	0.43			139	123
146.79	14			1.48	0.03	1.57	1.32	0.02	0.93	0.86	0.44			117	239
147.19	3			1.58	0.00	1.56	0.13	0.00	0.86	-0.54	0.18	0.71323	0.00000	72	245
147.39	2			1.06	0.03	1.60	0.69	0.01	0.74					189	245
147.69	1			1.43	0.02	1.52	0.91	0.02	0.63	0.34	0.15			299	257
147.94	7			1.58	0.00	1.56	0.65	0.00	0.40	0.12	-0.10			1181	249
148.49	2			1.39	0.01	1.57	0.75	0.02	0.21	0.30	-0.29			113	237
148.79	1			2.13	0.02	1.56	-0.70	0.01	0.24	-1.43	-0.40	0.71341	0.00006	38	239
149.14	13			1.30	0.02	1.63	0.36	0.01	0.27	-0.17	-0.28			165	232
149.49	0			2.12	0.02	1.67	-0.48	0.01	0.35	-1.19	-0.18			64	208
149.99	2			1.53	0.02	1.67	-0.38	0.02	0.48	-0.89	-0.07			16	84
150.24	3			1.46	0.02	1.65	0.39	0.02	0.50	-0.10	-0.06			87	87
150.49	3			1.69	0.02	1.47	0.93	0.02	0.66	0.46	0.15			127	86
150.89	2			1.84	0.03	1.45	1.67	0.01	0.73	1.25	0.23			79	71
151.14	2			1.61	0.04	1.32	1.77	0.03	0.95	1.17	0.45			70	73
151.54	3			1.16	0.02	1.31	0.93	0.03	1.10	0.36	0.59			136	89
151.79	3			0.52	0.03	1.30	0.78	0.02	1.24	0.44	0.71			29	86
152.04	3			1.08	0.03	1.27	0.95	0.01	1.26	0.54	0.73			35	81
152.34	2			1.00	0.03	1.24	1.52	0.01	1.17	0.82	0.64			80	74
152.69	3			1.43	0.02	1.24	0.92	0.02	1.12	0.38	0.62			156	72
152.94	3			1.33	0.03	0.92	1.73	0.02	0.50	0.99	0.07			65	58
153.29	4			1.45	0.02	0.99	1.08	0.01	0.61	0.59	0.14			80	55

Table C: *Continued*

depth (m) below salt	Facies*	Lake units	Sequences	$\delta^{13}C$ (V-PDB)	$\delta^{13}C$ (1σ - ‰)	$\delta^{13}C$ 9-points moving avg	$\delta^{18}O$ (V-PDB)	$\delta^{18}O$ (1σ - ‰)	$\delta^{18}O$ 9-points moving avg	**Corrected $\delta^{18}O_{bulk}$ (V-PDB)**	$\delta^{18}O$ 9-points moving avg (of the corrected $\delta^{18}O_{bulk}$ values)	$^{87}Sr/^{86}Sr$	Std Dev	P (ppm)	P 9-points moving avg
153.59	3			1.54	0.02	1.00	0.89	0.02	0.73	0.47	0.23			16	55
153.89	2			1.61	0.01	1.09	1.24	0.01	0.71	0.96	0.22			51	48
154.29	1			-1.71	0.14	1.11	-4.57	0.09	0.77	-4.57	0.30			10	43
154.59	2			1.19	0.03	1.14	1.69	0.03	0.65	1.10	0.23			2	45
154.94	3			1.19	0.01	1.15	2.07	0.01	0.69	1.37	0.29			38	42
155.19	3			1.74	0.02	1.13	1.30	0.02	0.75	0.71	0.32			13	52
155.44	0			1.68	0.03	1.09	1.51	0.01	0.72	1.05	0.27			111	50
155.84	4			1.55	0.04	1.43	0.65	0.02	1.42	0.40	0.89			80	55
156.24	13			1.58	0.02	1.44	1.44	0.01	1.33	1.14	0.83			58	63
156.54	3			1.33	0.01	1.46	1.46	0.01	1.19	0.76	0.82			105	63
156.79	3			1.26	0.02	1.43	0.90	0.01	1.27	0.47	0.85			32	74
156.94	3			1.32	0.02	1.40	1.74	0.02	1.28	0.99	1.14			53	69
157.19	2			1.33	0.03	1.43	0.90	0.01	1.70	0.56	1.21			77	71
157.54	3			1.32	0.03	1.43	0.85	0.02	1.77					39	79
157.84	2			1.47	0.04	1.48	1.98	0.02	1.72	1.30	1.14	0.71296	0.00009	114	96
158.14	1			1.44	0.03	1.52	1.61	0.02	1.94	0.96	1.27			66	111
158.49	1			1.85	0.03	1.56	4.41	0.03	1.89	3.67	1.37	0.71299	0.00005	99	109
158.79	4			1.52	0.03	1.52	2.05	0.02	1.86	1.08	1.28			130	115
159.14	14			1.84	0.03	1.50	1.00	0.03	1.81	0.45	1.23			255	116
159.44	13			1.55	0.04	1.52	2.89	0.03	1.65	1.97	1.11			168	106
159.74	3			1.68	0.04	1.47	1.31	0.01	1.51	1.31	1.01			31	106
160.24	4			1.03	0.03	1.39	0.65	0.01	1.06	0.26	0.57			133	97
160.54	3			1.15	0.02	1.34	0.38	0.01	0.90	0.06	0.44			45	88
160.84	2			1.66	0.03	1.21	0.56	0.03	0.96	0.22	0.48			29	70
161.14	10			0.91	0.04	1.11	0.31	0.03	0.75	0.08	0.30	0.71343	0.00011	66	53

Table C: *Continued*

depth (m) below salt	Facies*	Lake units	Sequences	$\delta^{13}C$ (V-PDB)	$\delta^{13}C$ (1σ - ‰)	$\delta^{13}C$ 9-points moving avg	$\delta^{18}O$ (V-PDB)	$\delta^{18}O$ (1σ - ‰)	$\delta^{18}O$ 9-points moving avg	**Corrected $\delta^{18}O_{bulk}$ (V-PDB)**	$\delta^{18}O$ 9-points moving avg (of the corrected $\delta^{18}O_{bulk}$ values)	$^{87}Sr/^{86}Sr$	Std Dev	P (ppm)	P 9-points moving avg
161.44	3			1.14	0.04	1.12	0.37	0.01	0.55	-0.31	0.02			19	51
161.74	3			1.07	0.04	1.12	0.61	0.01	0.56	-0.12	0.02			45	42
162.04	1			0.69	0.02	1.06	1.58	0.02	0.66	0.82	0.08			90	41
162.34	3			0.67	0.03	0.97	1.01	0.01	0.66	0.42	0.04	0.71365	0.00009	21	40
162.59	2			1.76	0.02	0.98	-0.51	0.02	0.70	-1.28	0.05			10	37
162.94	2			1.01	0.03	1.00	0.71	0.02	0.69	0.31	0.07			50	40
163.19	3			0.66	0.02	1.04	1.30	0.02	0.67	0.54	0.07			37	36
163.49	3			0.83	0.04	1.15	0.58	0.03	0.60	-0.11	0.01			26	44
163.79	3			0.99	0.04	1.22	0.67	0.02	0.43	0.22	-0.15			34	43
164.29	3			1.33	0.00	1.17	0.29	0.00	0.58	-0.20	0.06			46	47
164.64	4			1.43	0.02	1.22	0.42	0.01	0.53	-0.06	0.01			14	42
165.19	1			1.70	0.03	1.32	0.91	0.02	0.49	0.27	0.02			157	43
165.64	1			1.26	0.02	1.40	-0.54	0.02	0.44	-1.08	-0.02			11	49
165.94	13			1.29	0.03	1.26	0.89	0.01	0.46	0.67	0.00			45	51
166.29	2			1.49	0.01	1.09	0.28	0.01	0.54	-0.17	0.09			5	57
166.59	13			1.54	0.02	0.89	0.94	0.02	0.55	0.61	0.09			50	73
166.94	1			1.53	0.00	0.78	0.11	0.00	0.53	-0.47	0.04			77	64
166.99	1			-0.26	0.10	0.80	0.83	0.05	0.76	0.41	0.26			58	78
167.34	1			-0.17	0.10	0.70	1.01	0.05	0.79	0.59	0.27			95	80
167.64	1			-0.37	0.10	0.56	0.55	0.05	0.90	-0.04	0.41			158	85
168.29	1			0.71	0.10	0.45	0.67	0.05	0.97	-0.13	0.45			74	91
168.64	1			1.45	0.10	0.33	1.57	0.05	1.14	0.87	0.65			143	89
168.99	2			0.40	0.10	0.51	1.18	0.05	1.25	0.78	0.75			57	94
169.54	0			0.17	0.00	0.61	1.23	0.00	1.36	1.05	0.84			56	96
169.99	1			0.59	0.10	0.62	1.54	0.05	1.43	0.99	0.95			100	79

Table C: *Continued*

depth (m) below salt	Facies*	Lake units	Sequences	$\delta^{13}C$ (V-PDB)	$\delta^{13}C$ (1σ - ‰)	$\delta^{13}C$ 9-points moving avg	$\delta^{18}O$ (V-PDB)	$\delta^{18}O$ (1σ - ‰)	$\delta^{18}O$ 9-points moving avg	**Corrected $\delta^{18}O_{bulk}$ (V-PDB)**	$\delta^{18}O$ 9-points moving avg (of the corrected $\delta^{18}O_{bulk}$ values)	$^{87}Sr/^{86}Sr$	Std Dev	P (ppm)	P 9-points moving avg
170.29	3			0.45	0.10	0.55	1.66	0.05	1.51	1.31	1.04			58	91
171.34	2			1.32	0.10	0.45	1.81	0.05	1.51	1.30	1.10			106	76
171.69	1			0.80	0.10	0.37	2.00	0.05	1.49	1.41	1.07			110	96
172.39	1			-0.35	0.10	0.43	1.24	0.05	1.45	0.98	1.00			4	97
172.69	2			0.10	0.10	0.52	1.32	0.05	1.41	0.69	0.96			181	95
173.04	2			0.55	0.10	0.58	1.58	0.05	1.40	1.35	0.97			11	98
173.24	1			-0.27	0.10	0.59	0.99	0.05	1.40	0.52	0.98			238	98
173.49	2			0.70	0.10	0.69	0.89	0.05	1.30	0.41	0.91	0.71363	0.00005	69	95
173.79	2			1.36	0.10	0.87	1.16	0.05	1.29	0.69	0.90			78	101
174.39	13			1.05	0.10	0.99	1.62	0.05	1.28	1.40	0.94			88	86
174.79	2			1.41	0.10	1.07	1.83	0.05	1.22	1.34	0.87			99	94
175.24	3			1.66	0.10	1.20	1.10	0.05	1.23	0.77	0.89			87	79
175.54	4			1.27	0.10	1.22	1.15	0.05	1.30	0.94	0.98			54	78
176.49	3			1.14	0.10	1.19	1.23	0.05	1.32	1.05	1.03			53	99
176.84	4			1.31	0.10	1.29	1.03	0.05	1.25	0.69	0.88			81	104
177.14	4			0.92	0.10	1.21	1.07	0.05	1.17	0.74	0.80			98	111
177.44	3			0.82	0.10	1.18	1.50	0.05	1.19	1.23	0.81			67	112
178.19	3			1.14	0.10	1.13	1.34	0.05	1.18	1.07	0.79			262	115
178.59	1			1.93	0.10	1.10	1.00	0.05	1.18	0.09	0.78			139	112
178.99	3			0.71	0.10	1.05	1.13	0.05	1.20	0.65	0.79			159	111
179.34	3			1.41	0.10	1.02	1.29	0.05	1.18	0.87	0.76			93	110
179.64	4			0.82	0.10	1.01	1.03	0.05	1.13	0.72	0.73			83	103
179.94	3			0.87	0.10	1.03	1.21	0.05	1.10	0.92	0.70			30	81
180.24	1			0.79	0.10	0.91	1.24	0.05	1.12	0.79	0.79			68	66
180.84	3			0.72	0.10	0.96	0.84	0.05	1.17	0.52	0.83			89	70

Table C: *Continued*

depth (m) below salt	Facies*	Lake units	Sequences	$\delta^{13}C$ (V-PDB)	$\delta^{13}C$ (1σ - ‰)	$\delta^{13}C$ 9-points moving avg	$\delta^{18}O$ (V-PDB)	$\delta^{18}O$ (1σ - ‰)	$\delta^{18}O$ 9-points moving avg	**Corrected $\delta^{18}O_{bulk}$ (V-PDB)**	$\delta^{18}O$ 9-points moving avg (of the corrected $\delta^{18}O_{bulk}$ values)	$^{87}Sr/^{86}Sr$	Std Dev	P (ppm)	P 9-points moving avg
181.24	4			0.72	0.10	0.93	1.12	0.05	1.19	0.91	0.86			1	83
181.54	4			1.27	0.10	1.06	1.07	0.05	1.22	0.79	0.86			64	76
182.04	3			0.85	0.10	1.14	1.17	0.05	1.26	0.90	0.90			6	75
182.54	1			1.18	0.10	1.23	1.59	0.05	1.28	1.05	0.92			199	77
183.04	2			1.18	0.10	1.24	1.40	0.05	1.35	1.16	1.00			206	79
183.49	3			1.98	0.10	1.26	1.30	0.05	1.33	0.72	0.98			18	86
183.79	2			1.54	0.10	1.30	1.60	0.05	1.33	1.30	0.99			22	83
184.24	3			1.63	0.00	1.35	1.44	0.00	1.37	0.92	1.04			88	85
184.59	3			0.81	0.07	1.38	1.44	0.05	1.36	1.23	1.06	0.71327	0.00007	107	71
185.49	3			0.89	0.10	1.36	0.96	0.05	1.34	0.78	1.04			64	53
185.84	3			1.63	0.10	1.25	1.07	0.05	1.36	0.85	1.09			34	63
186.19	3			1.35	0.10	1.15	1.54	0.05	1.33	1.37	1.07			27	63
186.69	4			1.41	0.10	1.06	1.46	0.05	1.37	1.22	1.11			72	59
186.94	4			0.97	0.10	1.08	1.27	0.05	1.31	0.98	1.02			47	50
187.29	3			0.98	0.10	1.16	1.48	0.05	1.35	1.20	1.03			105	48
187.64	3			0.68	0.10	1.12	1.28	0.05	1.36	1.07	1.05			26	53
187.94	1			0.81	0.10	1.10	1.87	0.05	1.26	1.28	0.92			50	51
188.29	1			1.03	0.10	1.04	0.88	0.05	1.16	0.39	0.79			24	67
188.94	2			1.61	0.10	1.02	1.27	0.05	1.21	0.93	0.79			44	84
189.24	3			1.23	0.10	1.07	1.19	0.05	1.19	0.97	0.79			84	77
189.59	3			1.21	0.10	1.09	0.65	0.05	1.04	0.27	0.60			7	84
189.94	1			0.87	0.00	1.07	0.57	0.00	0.91	0.03	0.50			212	100
190.29	1			0.78	0.10	0.99	1.74	0.05	0.84	0.95	0.43			207	102
190.59	3			1.42	0.10	0.86	1.29	0.05	0.78	1.18	0.36			42	101
190.99	3			0.81	0.10	0.84	-0.14	0.05	0.73	-0.59	0.28	0.71283	0.00005	88	102

Table C: *Continued*

depth (m) below salt	Facies*	Lake units	Sequences	$\delta^{13}C$ (V-PDB)	$\delta^{13}C$ (1σ - ‰)	$\delta^{13}C$ 9-points moving avg	$\delta^{18}O$ (V-PDB)	$\delta^{18}O$ (1σ - ‰)	$\delta^{18}O$ 9-points moving avg	**Corrected $\delta^{18}O_{bulk}$ (V-PDB)**	$\delta^{18}O$ 9-points moving avg (of the corrected $\delta^{18}O_{bulk}$ values)	$^{87}Sr/^{86}Sr$	Std Dev	P (ppm)	P 9-points moving avg
191.29	3			0.67	0.10	0.85	0.75	0.05	0.75	0.34	0.30	0.71349	0.00004	196	110
191.84	1			0.28	0.10	0.90	0.27	0.05	0.78	-0.19	0.33			39	100
192.14	1			0.44	0.10	0.95	0.68	0.05	0.69	0.27	0.30			31	87
192.64	1			1.12	0.10	0.94	0.78	0.05	0.66	0.25	0.25			98	93
193.49	3			1.28	0.10	0.96	0.84	0.05	0.83	0.46	0.45			80	92
193.79	3			1.31	0.10	1.04	0.81	0.05	0.87	0.27	0.51			123	78
194.29	4			1.24	0.10	1.13	0.95	0.05	0.96	0.69	0.58			84	95
194.59	3			1.33	0.10	1.21	1.01	0.05	0.98	0.72	0.57			102	102
194.89	3			0.96	0.10	1.14	1.38	0.05	0.96	1.25	0.55			79	98
195.14	3			1.40	0.10	1.09	1.10	0.05	0.95	0.84	0.53			69	99
195.99	1			1.13	0.10	1.02	1.12	0.05	0.95	0.47	0.53			185	95
196.34	2			1.14	0.10	0.94	0.85	0.05	0.88	0.20	0.44			94	93
196.59	3			0.51	0.10	0.84	0.56	0.05	0.81	0.08	0.33			67	86
196.94	3			0.82	0.10	0.89	0.79	0.05	0.80	0.29	0.28			89	92
197.24	3			0.65	0.10	0.86	0.76	0.05	0.72	0.24	0.16			87	99
197.49	3			0.49	0.10	0.84	0.38	0.05	0.60	-0.16	0.03			69	85
197.79	4			0.50	0.10	0.84	0.31	0.05	0.63	-0.20	0.10			31	84
198.14	1			1.37	0.10	0.88	1.29	0.05	0.43	0.78	-0.14			139	86
198.44	1			1.13	0.10	0.91	0.43	0.05	0.49	-0.22	-0.06			129	82
198.94	3			0.96	0.10	1.07	0.05	0.05	0.62	-0.70	0.09			58	127
199.64	3			1.12	0.10	1.20	1.12	0.05	0.68	0.82	0.17			90	136
199.89	3			0.84	0.10	1.25	-1.23	0.05	0.79	-2.13	0.31	0.71272	0.00005	79	147
200.19	2			1.13	0.10	1.20	1.34	0.05	0.79	1.03	0.33			53	149
200.59	1			2.12	0.10	1.11	1.88	0.05	0.87	1.60	0.47			491	152
200.94	1			1.62	0.10	1.07	0.94	0.05	0.72	0.51	0.30			154	154

Table C: *Continued*

depth (m) below salt	Facies*	Lake units	Sequences	$\delta^{13}C$ (V-PDB)	$\delta^{13}C$ (1σ - ‰)	$\delta^{13}C$ 9-points moving avg	$\delta^{18}O$ (V-PDB)	$\delta^{18}O$ (1σ - ‰)	$\delta^{18}O$ 9-points moving avg	**Corrected $\delta^{18}O_{bulk}$ (V-PDB)**	$\delta^{18}O$ 9-points moving avg (of the corrected $\delta^{18}O_{bulk}$ values)	$^{87}Sr/^{86}Sr$	Std Dev	P (ppm)	P 9-points moving avg
201.39	0			0.99	0.10	1.01	1.32	0.05	0.63	1.08	0.16			134	146
201.49	1			0.90	0.10	1.01	1.22	0.05	0.88	0.99	0.47			149	145
201.79	2			0.28	0.10	1.00	1.22	0.05	0.82	1.01	0.40			162	157
202.14	3			0.65	0.10	0.84	-1.35	0.05	0.67	-2.25	0.23			74	109
202.54	0			0.52	0.10	0.71	0.32	0.05	0.63	-0.36	0.19			21	101
203.09	1			0.90	0.10	0.65	1.03	0.05	0.49	0.64	0.01			67	95

*Facies (according to Gomes et al. 2020) codes: 0 – not described; 1 – spherulitestone; 2 – shrubby spherulitestone; 3 – spherulitic shrubstone; 4 – shrubstone; 5 – spherulitic shrubstone with mud; 6 – shrubby spherulitestone with mud; 7 – spherulitestone with mud; 10 – calcimudstone; 11 – dolomudstone; 12 – mixed mudstone; 13 – grainstone; 14 – packstone.

D

Appendix D

D.1 Mineralogical and bulk rock chemical data from well #3 used to plot Figures 6.4, 6.5 and 6.12 in Chapter 6.

Table D: Mineralogical and bulk rock chemical data from well #3 used to plot **Figures 6.4, 6.5** and **6.12** in Chapter 6.

depth (m) below salt	Facies *	Lake units	Sequences	dolomite	quartz	calcite	py-rite	mag-nesite	Mg-clays	K-felds	clays + micas	ba-rite	daws-onite	fluo-rite	tuni-site	cryo-lite	CaO (%,ICP-OES)	MgO (%,ICP-OES)	SiO_2 (%,ICP-OES)
4.99	2	13/12		25.95	5.34	68.71											48.84	5.6	5.85
5.24	13			18.93	9.27	71.80											42.53	3.94	8.59
5.39	13		**BVF IV**	26.15	5.34	68.51											42.87	4.93	5
6.19	1			41.10	8.51	50.39											40.65	7.94	8.76
6.59	0			NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
9.54	14			29.35	27.03	43.62											32.14	6.08	26.19
9.79	12			52.71	12.67	34.62	TR										33.3	9.71	11.09
10.44	11			68.08	22.92	9.00											37.83	15.31	4.22
11.19	11			77.19	4.25	18.56											24.47	13.21	22.79
11.39	13			26.82	9.32	63.86											43.07	5.54	8.39
11.99	2			39.68	16.51	43.81											33.72	8.1	16.45
12.84	10			20.06	5.26	73.63				1.50							43.43	4.04	4.88
13.14	12			4.51	95.49	0.00											1.8	1	>90
13.49	12			42.01	52.96	5.03											14.72	7.77	51.7
14.49	10			17.23	4.81	77.96											52.08	4.37	4.02
14.74	10			19.71	7.41	72.88											43.57	4.19	7.49
15.09	12			22.94	7.31	67.76				1.99							41.23	4.83	7.88
15.49	11			61.37	28.77	9.86	TR										23	12.91	26.67
18.39	11			66.35	28.15	2.06		3.44									21.16	15.46	26.42
18.89	0			13.39	13.32	73.29											46.2	2.66	13.46
19.29	4			27.71	26.42	45.87											33.73	5.59	28.56
19.59	14			40.29	18.27	41.44	TR										33.33	8.38	15.64
20.14	3			88.44	4.37	7.19											30.91	17.49	4.8
20.49	14	11/10		71.83	9.30	18.87											31.2	14.91	8.74

Table D: *Continued*

depth (m) below salt	Facies *	Lake units	Sequences	dolomite	quartz	calcite	py-rite	mag-nesite	Mg-clays	K-felds	clays + micas	ba-rite	daws-onite	fluo-rite	tuni-site	cryo-lite	CaO (%,ICP -OES)	MgO (%,ICP -OES)	SiO_2 (%,ICP -OES)
21.09	12			49.12	19.35	31.53											30.5	9.79	19.55
22.89	10		BVF III	27.52	9.59	62.89											38.95	5.52	8.91
22.99	3			22.25	6.58	71.17											42.09	4.68	6.14
23.29	1			23.41	8.01	68.58											43.46	5.07	7.68
23.54	0			19.28	18.14	62.58	TR										40.35	4.32	16.67
23.74	1			32.12	5.90	61.98											44.91	6.27	5.78
23.89	2			26.28	4.92	68.80											44.14	5.52	4.54
24.69	3			11.06	2.60	86.34											50.68	2.86	2.43
25.19	3			24.42	2.50	73.08											48.87	5.15	2.12
25.94	2			30.99	10.88	58.13											40.35	5.88	12.22
26.24	3			10.38	57.32	32.30											18.47	2.05	57.43
26.54	3			24.46	7.63	67.91											44.87	5.52	7.37
26.79	3			17.05	19.53	63.42											36.62	3.86	19.61
27.09	0			29.21	2.44	68.35											44.53	6.62	2.09
27.14	4			18.55	5.05	76.40											46.37	4.14	4.79
27.74	1			66.12	6.92	26.96											35.53	13.82	6.44
28.09	1			63.37	13.24	23.39											33.03	13.56	13.39
29.14	3			31.08	1.58	67.34											48.68	6.67	1.43
29.49	3			22.24	3.00	74.76											44.53	5.01	3.12
30.29	4			28.35	12.25	59.40											45.41	6.98	11.15
30.99	4			26.53	4.31	69.16											46.98	5.74	3.72
31.34	3			38.40	10.72	50.88											38.18	8.11	10.2
31.64	14			11.60	85.82	2.58											4.85	2.73	89.26
32.39	0			24.47	3.22	72.31											51.3	6.3	3.11
32.64	4			33.95	10.86	55.19											40.56	7.31	10.5

Table D: *Continued*

depth (m) below salt	Facies *	Lake units	Sequences	dolomite	quartz	calcite	py-rite	mag-nesite	Mg-clays	K-felds	clays + micas	ba-rite	daws-onite	fluo-rite	tuni-site	cryo-lite	CaO (%,ICP -OES)	MgO (%,ICP -OES)	SiO_2 (%,ICP -OES)
33.44	4			19.73	4.18	76.09											48.81	4.63	3.53
34.14	4			33.81	12.15	54.04											39.7	7	11.01
34.49	3			42.26	17.90	39.84											35.88	9.07	17.19
34.79	3			26.77	21.30	51.93											37.11	6.07	20.84
35.04	4			32.58	13.95	53.47											39.2	7.09	12.39
36.04	3			34.13	10.14	55.73											39.55	7.19	9.67
36.64	3			34.44	25.08	40.48											32.83	7.99	26.82
36.99	3			47.26	4.71	48.03											38.71	9.76	4.56
37.24	4			26.24	12.24	61.52											40.61	5.94	12.43
37.54	4			32.53	12.00	55.47											40.76	7.71	11.7
37.69	0			22.98	8.15	68.87											42.85	5.08	7.72
38.14	4			16.40	2.86	80.74											49.14	4.14	2.87
39.09	4			43.10	1.40	55.50											43.99	9.35	1.39
39.64	3			31.25	4.93	63.82											42.43	7.05	4.97
39.74	0			29.07	3.59	67.34											46.27	6.79	3.41
40.24	4			12.01	2.74	85.25											50.13	2.99	2.69
40.79	3			8.74	60.35	30.91											43.03	7.33	8.24
41.09	4			4.35	81.74	13.91											48.82	3.42	4.09
41.24	0			5.08	60.49	34.43											41.03	7.22	4.54
41.64	4			19.98	10.82	69.20											43.22	4.32	10.86
42.89	0			28.16	4.40	67.44											44.87	6.23	4.22
43.19	3			17.66	10.24	72.10											44.03	4.24	10.22
43.99	4			20.72	4.71	74.57											48.92	4.75	4.11
44.34	3			46.85	6.40	46.75											40.62	9.88	6.11
44.75	2			21.89	7.87	70.24											45.24	5.24	7.45

Table D: *Continued*

depth (m) below salt	Facies *	Lake units	Sequences	dolomite	quartz	calcite	py-rite	mag-nesite	Mg-clays	K-felds	clays + micas	ba-rite	daws-onite	fluo-rite	tuni-site	cryo-lite	CaO (%,ICP-OES)	MgO (%,ICP-OES)	SiO_2 (%,ICP-OES)
45.10	2			20.62	7.04	72.34											43.08	4.7	6
45.30	4			67.55	1.97	30.48											36.47	14.38	2.07
45.74	2			35.90	4.45	59.65											40.16	7.78	3.99
46.14	3			27.05	12.86	60.09											39.38	6.27	12.7
46.39	4			20.89	1.65	77.46											46.03	4.69	1.36
46.74	14			62.84	30.63	3.74		2.79									23.26	15.52	30.2
46.94	0	9/8		60.59	32.31	1.27		5.83									18.75	15.78	31.44
47.44	1			43.21	19.28	37.51											29.31	8.69	18.79
48.09	1			47.17	28.53	22.58		1.72									25.26	10.8	26.27
48.39	11			87.23	5.93	6.84											28.28	17.76	5.12
48.74	14			60.10	28.24	0.00		11.66									18.42	18.86	26.76
49.04	1			42.90	17.52	39.58											35.12	9.7	17.62
49.29	1			38.73	20.71	39.39							1.17				31.23	8.16	20.08
49.64	1			39.33	18.22	42.45											33.66	8.47	17.81
49.99	1			32.09	15.68	49.06		3.17									38.44	8.64	15.98
50.39	1			47.66	24.87	25.97								1.50			28.9	10.5	23.24
51.59	3			11.40	3.93	84.67											52.96	3	4.22
52.59	3			12.50	4.09	83.41											50.02	2.94	3.98
52.99	2			26.71	6.93	66.36											45.28	7	8.35
53.29	4			18.89	3.72	77.39											50.14	4.4	3.32
53.59	4			16.21	6.00	77.79											52.48	4.14	5.73
54.14	3			14.72	5.06	80.22											48.86	3.87	4.87
54.54	2			37.55	12.72	49.73											38.11	7.9	11.28
54.69	3			7.75	3.81	87.05						1.39					48.92	1.99	3.27
54.94	0			54.82	14.57	30.61											31.7	11.25	13.43

Table D: *Continued*

depth (m) below salt	Facies *	Lake units	Sequences	dolomite	quartz	calcite	py-rite	mag-nesite	Mg-clays	K-felds	clays + micas	ba-rite	daws-onite	fluo-rite	tuni-site	cryo-lite	CaO (%,ICP -OES)	MgO (%,ICP -OES)	SiO_2 (%,ICP -OES)
55.29	4			0.00	0.00	0.00											44.3	5.26	9.74
55.54	1			59.76	18.07	22.17											29.68	12.8	16.5
56.24	2			24.74	9.46	65.80											46.77	5.78	9.45
56.84	3			42.04	22.00	35.96											33.78	8.99	20.57
57.14	3			27.21	15.12	57.67											42.46	6.73	16.13
58.24	2			52.66	14.45	32.89											37.58	11.85	13.23
58.69	1			15.14	53.65	0.00		31.21									4.92	16.45	52.25
59.04	3			23.76	6.53	69.71											44.67	5.41	6.77
59.29	3			23.77	11.15	65.08											47.92	4.97	7.17
59.64	2			27.58	6.34	66.08											43.52	6.05	6.35
59.94	3			24.32	7.29	68.39											41.73	4.71	6.54
60.24	4			28.85	7.63	63.52											42.95	6.21	7.51
60.54	3			23.15	7.80	69.05											43.12	6.23	7.98
60.79	3			24.60	10.20	65.20											41.25	5.45	9.62
61.04	3			34.02	6.46	59.52											42.11	6.68	6.69
61.49	2			52.65	18.99	28.36											30.1	11.12	17.58
61.74	1			38.38	24.42	37.20											28.88	8.2	23.67
62.09	1			53.47	1.75	44.78											38.52	10.96	1.6
62.39	2			41.19	14.53	44.28											38.03	9.91	15.34
62.94	1			26.96	4.34	68.70											47.61	6.28	3.88
63.24	1			35.57	15.93	48.50											36.06	7.8	14.67
63.54	1			49.96	15.94	32.92		1.18									32.22	11.02	14.45
63.74	0			52.37	16.04	30.03		1.56									33.33	12.84	17.34
63.99	5			31.97	10.42	57.61											40.32	6.71	10.05
64.29	3			26.88	4.26	68.86											42.91	5.48	3.89

Table D: *Continued*

depth (m) below salt	Facies *	Lake units	Sequences	dolomite	quartz	calcite	py-rite	mag-nesite	Mg-clays	K-felds	clays + micas	ba-rite	daws-onite	fluo-rite	tuni-site	cryo-lite	CaO (%,ICP-OES)	MgO (%,ICP-OES)	SiO_2 (%,ICP-OES)
64.59	3			29.81	11.84	58.35											39.84	6.43	11.83
64.89	1			45.24	23.64	31.12											32.89	11.55	20.81
65.19	1			38.49	13.69	47.82											32.38	9.84	14.07
65.64	1			45.68	32.61	21.71											24.28	9.37	32.03
65.94	3			15.34	4.55	80.11											48.73	3.75	4.31
66.34	1			30.91	15.62	53.47											36.37	7.45	18.43
66.64	2			45.03	21.23	31.22		2.52									29.65	10.66	20.69
67.29	13			23.97	9.28	66.75											43.98	6.81	8.81
67.94	3			31.67	14.75	53.58											39.53	7.22	15.33
68.24	1			60.77	24.56	13.46	TR	1.21									25.42	13.38	23.51
68.79	2			50.21	16.77	33.02											32.41	11.12	17.84
69.09	1			53.82	17.34	26.60											32.14	11.61	17.26
69.39	3			36.21	12.11	50.13											35.59	7.52	13.22
70.64	12			62.15	22.20	15.65											26.78	13.28	21.26
71.09	12			47.76	13.24	39.00											35.09	10.08	12.39
71.39	12			58.52	19.10	22.38											33.99	12.14	16.43
72.04	1			59.75	14.76	25.49											31.56	13.9	13.62
72.54	1			48.88	10.23	40.89											34.89	10.09	8.99
72.94	2			27.98	15.23	56.79											37.01	6.53	12.7
73.19	1			31.33	15.54	53.13											38.43	7.14	16.44
73.84	3			48.79	8.01	43.20											35.5	9.62	8.11
74.19	3			28.15	13.16	58.69											42.22	6.48	16.83
74.54	3			24.48	8.94	66.58											44.78	5.84	9.48
74.84	3			22.65	8.34	69.01											47.4	3.67	4
75.09	1			58.70	18.48	22.82											40.05	7.37	16.03

Table D: *Continued*

depth (m) below salt	Facies *	Lake units	Sequences	dolomite	quartz	calcite	py-rite	mag-nesite	Mg-clays	K-felds	clays + micas	ba-rite	daws-onite	fluo-rite	tuni-site	cryo-lite	CaO (%,ICP -OES)	MgO (%,ICP -OES)	SiO_2 (%,ICP -OES)
75.44	2			34.60	8.01	57.39											43.29	8.81	8.75
75.74	3			28.19	11.05	60.76											49.73	5	6.12
76.19	2			39.71	17.36	42.93											38.84	9.23	16.47
76.44	1			58.77	20.41	20.82											31.82	13.8	17.28
77.19	3			41.26	23.38	35.36											36.51	10.27	20.25
77.49	3			39.44	21.44	39.12											35.53	9.54	23.85
77.89	13	7		41.59	19.88	38.53											34.69	9.88	22.15
78.14	3			24.53	58.86	16.61											11.09	3.35	69.35
78.59	13			21.16	8.10	70.74											47.65	6.36	8.4
79.09	13			10.91	74.11	14.98											11.12	2.41	76.96
79.49	13			35.43	12.75	51.82											36.53	7.19	12.15
79.84	3			18.91	64.38	16.71											16.62	4.66	62.41
80.04	3			14.66	63.70	21.64											17.2	3.49	66.5
80.34	2			18.11	4.94	76.95											47.5	6.5	8.52
80.64	3			10.91	86.04	3.05											3.88	2.33	84.74
80.89	3			32.70	13.97	53.33											43.89	6.54	11.96
81.29	2			24.16	7.10	68.74											42.35	7.56	5.96
81.94	3			21.53	12.36	66.11											46.36	5.67	8.78
82.29	3			21.10	9.97	68.93											42.51	5.71	7.87
82.49	3			28.64	12.96	58.40											40.5	7.48	11.57
82.74	3			64.00	5.00	31.00											43.78	4.95	8.06
83.09	2			14.27	63.93	21.80											15.11	3.67	64.24
83.34	3			13.09	9.00	77.91											43.43	3.29	8.55
83.64	2			53.93	8.94	37.13											37.89	13.45	9.85
83.94	3			56.00	14.00	30.00											33.29	12.82	11.27

Table D: *Continued*

depth (m) below salt	Facies *	Lake units	Sequences	dolomite	quartz	calcite	py-rite	mag-nesite	Mg-clays	K-felds	clays + micas	ba-rite	daws-onite	fluo-rite	tuni-site	cryo-lite	CaO (%,ICP -OES)	MgO (%,ICP -OES)	SiO_2 (%,ICP -OES)
84.24	1			58.00	14.00	28.00											33.78	13.77	9.03
84.49	3			14.59	81.35	4.06											6.5	3.32	81.11
84.84	13			31.24	6.74	62.02											44.36	7.5	6.65
85.19	3			31.99	9.95	58.06											39.86	8.34	10.22
85.89	1			45.16	21.15	33.69											30.92	11.56	18.78
86.09	1			54.12	15.59	30.29											30.3	12.69	19.54
86.34	1		BVF II	59.81	12.22	27.97											32.58	14.19	13.12
86.59	3			56.90	12.12	30.98											34.34	12.74	14.68
86.94	1			41.54	19.92	38.54											33.35	8.37	19.32
87.24	3			43.02	11.97	45.01											36.13	10.18	11.87
87.59	2			27.73	11.54	60.73											39.08	6.13	12.36
87.94	3			30.06	7.00	62.94											41.44	7.25	7.23
88.14	3			26.93	9.16	63.91											42.03	5.49	8.77
88.59	4			19.91	3.68	76.41											46.62	4.94	3.09
88.84	4			17.44	2.29	80.27											46.8	4.23	1.45
89.19	4			17.14	2.85	80.01											48.46	3.95	2.64
89.59	1			36.82	21.91	41.27											34.44	7.78	21.99
89.94	3			32.99	10.38	56.63											43.45	7.65	10.09
90.24	4			57.19	17.76	25.05											31.18	11.81	17.01
90.54	2			47.00	21.70	31.30											30.14	9.45	21.19
90.79	2			56.24	14.71	29.05											31.97	11.72	19.78
91.24	2			67.00	4.00	29.00											38.33	12.38	6.85
91.59	3			0.00	12.49	52.18										35.33	41.6	8.73	11.81
91.99	3			20.28	9.90	69.82											44.81	4.56	9.74
92.29	3			18.77	7.34	73.89											50.32	4.46	7.39

Table D: *Continued*

depth (m) below salt	Facies *	Lake units	Sequences	dolomite	quartz	calcite	py-rite	mag-nesite	Mg-clays	K-felds	clays + micas	ba-rite	daws-onite	fluo-rite	tuni-site	cryo-lite	CaO (%,ICP-OES)	MgO (%,ICP-OES)	SiO_2 (%,ICP-OES)
92.59	4			14.36	4.84	80.80											49.88	3.65	4.65
92.94	4			11.70	5.43	82.87											50.88	2.86	4.9
93.19	4			14.88	10.55	74.57											46.19	3.41	8.71
93.44	1			44.76	11.62	43.62											41.37	10.66	11.28
93.84	2			41.37	13.78	44.85											33.32	14.87	7.43
94.14	1			64.07	7.00	28.93											38.85	14.93	6.62
94.44	2			53.63	9.28	37.09											38.64	11.95	8.75
95.04	10			78.35	6.66	14.99											33.74	17.58	5.71
95.34	2	6/5		59.59	16.34	24.07											35.7	13.69	15.25
95.64	2			68.20	11.70	20.10											36.08	15.34	8.63
96.24	3			48.10	8.40	43.50											38.94	10.52	8.75
96.49	3			36.80	45.70	17.50											29.11	9.86	25.59
96.74	4			51.60	12.30	36.10											34.39	10.49	12.16
96.99	1			42.85	15.97	41.18											36.11	9.33	16.1
97.44	1			57.55	9.99	32.46											39.05	11.53	7.38
97.74	1			80.00	10.00	10.00											31.67	16.42	6.75
98.04	2			53.39	20.80	25.81											30.84	11.5	19.23
98.34	2			65.41	17.60	16.99											31.4	17.6	9.06
98.59	1			36.46	13.05	50.49											41.2	7.67	8.74
98.84	1			72.20	12.79	15.01	TR										32.98	16.28	12.14
99.14	2			56.32	15.16	28.52											32.29	16.33	5.58
99.49	1			79.86	5.85	14.29											34.07	15.99	5.08
99.74	1			33.34	12.18	54.48											40.9	6.96	7.57
100.04	1			28.00	9.00	63.00											44.29	6.37	6.48
100.34	3			15.00	20.00	65.00											47.14	4.84	3.22

Table D: *Continued*

depth (m) below salt	Facies *	Lake units	Sequences	dolomite	quartz	calcite	py-rite	mag-nesite	Mg-clays	K-felds	clays + micas	ba-rite	daws-onite	fluo-rite	tuni-site	cryo-lite	CaO (%,ICP-OES)	MgO (%,ICP-OES)	SiO_2 (%,ICP-OES)
100.59	3			11.13	2.06	86.81											46.21	3.38	2.44
100.94	2			49.91	20.18	29.91											32.96	11.23	20.26
101.24	2			63.16	9.91	26.93											39.13	9.85	15.99
101.59	1			31.61	16.03	52.36											41.32	8.25	8.56
101.89	1			56.07	9.57	34.36											38.16	11.04	10.5
102.24	11			12.18	79.46	8.36											7.66	2.3	78.21
102.54	2			59.80	3.91	36.29											39	12.54	4.92
102.79	1			57.27	14.27	28.46											33.89	11.65	13.85
103.44	1			28.72	11.88	59.40											43.53	7.2	11.54
103.74	1			35.80	8.89	55.31											41.02	7.17	9.69
104.04	1			36.38	10.22	53.40											39.13	7.39	9.22
104.29	1			42.49	24.09	33.42											30.83	8.46	23.38
104.64	2			46.50	20.44	33.06											31.2	9.57	20.53
105.19	7			59.43	24.77	15.80	TR										26.27	12.09	20.12
105.39	1			51.29	21.17	27.54	TR										35.25	12.3	18.59
105.79	1			35.11	12.14	52.75											44.02	6.87	12.1
106.04	1			33.23	12.21	54.56											39.2	6.67	13.07
106.34	1			37.99	11.14	50.87											42.55	8.16	10.46
106.69	1			71.95	11.44	16.61											32.93	14.96	11.7
107.24	3			26.00	16.49	57.51											43.17	5.87	16.24
107.49	2			65.72	9.92	24.36											35.39	15	11.29
107.74	2			29.90	15.58	54.52											42.38	6.5	15.09
108.04	13			24.35	8.73	66.92											48.42	5.51	9.88
108.29	13			21.31	8.48	70.21											48.29	4.79	8.05
108.59	13			21.59	11.49	66.92											47.06	4.74	10.89

Table D: *Continued*

depth (m) below salt	Facies *	Lake units	Sequences	dolomite	quartz	calcite	py-rite	mag-nesite	Mg-clays	K-felds	clays + micas	ba-rite	daws-onite	fluo-rite	tuni-site	cryo-lite	CaO (%,ICP-OES)	MgO (%,ICP-OES)	SiO_2 (%,ICP-OES)
108.99	1			26.21	55.53	18.26											18.39	4.89	60.3
109.44	3			2.20	86.40	11.40											7.57	0.36	86.85
109.64	1			2.94	68.74	28.32											9.72	0.49	84.52
113.34	3			37.10	36.25	26.65											27.06	7.14	36.46
113.59	3			63.71	7.60	28.69											40.04	13.29	5.69
113.94	3			25.65	23.02	51.33	TR										40.22	6.37	13.07
114.19	3			24.13	6.11	69.76											48.94	5.23	4.81
114.49	2			31.59	8.61	59.80											46.37	6.61	7.6
114.79	2			2.19	70.32	27.49											15.91	0.57	71.43
115.19	2			42.65	13.59	43.76											39.21	8.85	13.14
115.54	3			31.68	5.63	62.69											49.4	6.66	4.94
115.84	13			13.19	48.99	37.82											28.32	3.91	36.39
116.14	3			22.61	3.96	73.43											50.73	4.82	4.33
116.39	3			29.06	4.77	66.17											48.74	5.79	4.56
116.69	3			27.56	10.42	62.02											46.49	5.84	9.25
117.39	4			21.41	3.73	74.86											50.32	4.84	3.26
117.74	2			32.53	9.35	58.12											47.09	8.55	5.65
117.94	2			49.06	10.35	40.59											28.62	7.62	33.29
118.44	3			19.68	4.19	76.13											51.81	4.56	3.86
118.79	2			45.85	8.59	45.56											42.08	10.89	6.75
119.34	2			41.08	9.03	49.89											44.64	8.46	8.83
119.54	2			21.28	13.31	65.41											48.74	4.38	10.94
119.94	1			60.27	7.93	31.80											40.19	10.87	7.6
120.29	3			45.30	9.17	45.53											43.5	8.47	9.52
120.54	2			48.66	14.58	36.76	TR										36.63	10.34	14.88

Table D: *Continued*

depth (m) below salt	Facies *	Lake units	Sequences	dolomite	quartz	calcite	py-rite	mag-nesite	Mg-clays	K-felds	clays + micas	ba-rite	daws-onite	fluo-rite	tuni-site	cryo-lite	CaO (%,ICP-OES)	MgO (%,ICP-OES)	SiO_2 (%,ICP-OES)
120.84	2			53.87	8.88	37.25											40.41	10.72	8.25
121.14	1			8.57	1.76	89.67											55.56	2.3	1.57
121.44	3			15.84	6.80	77.36											50.01	3.49	5.27
122.44	3			20.97	3.43	75.60											43.34	8.77	3.96
122.74	1			50.81	10.34	38.85											40.69	9.85	10.66
122.99	2	4		49.80	15.55	34.65											37.53	12.48	12.28
123.44	2			51.32	14.10	34.58											37.1	10.8	14.26
123.74	2			38.40	15.10	46.50											38.62	8.05	14.92
123.94	2			40.42	14.98	44.60											40.54	8.25	15.2
124.29	2			25.51	9.61	64.88											45.25	5.53	9.14
124.59	4			26.58	11.78	61.64											45.22	5.8	10.71
124.84	13			25.14	9.02	65.84											47.93	5.42	8.11
125.09	2			24.03	10.01	65.96											45.41	4.92	8.58
125.34	4			26.21	49.32	24.47											37.82	9.77	16.19
125.64	4			28.04	16.71	55.25											37.37	5.47	14.63
125.94	4			30.26	17.53	52.21											43.74	4.3	7.09
126.24	3			21.98	15.58	62.44											42.06	4.55	14.37
126.54	3			10.82	23.30	65.88											40.44	2.79	28.27
126.79	3			18.96	2.09	78.95											46.87	5.58	4.39
127.09	1			58.31	6.10	35.59											41.05	12.56	6.09
127.64	2			44.81	19.87	35.32	TR										34.15	9.36	21.24
127.94	3			39.36	8.60	52.04											37.98	8.19	7.66
128.19	2			31.09	13.39	55.52											39.48	6.43	11.7
128.54	1			32.62	13.54	53.84											39.34	6.54	11.49
128.84	1			66.14	18.57	15.29											29.42	13.41	18.2

Table D: *Continued*

depth (m) below salt	Facies *	Lake units	Sequences	dolomite	quartz	calcite	py-rite	mag-nesite	Mg-clays	K-felds	clays + micas	ba-rite	daws-onite	fluo-rite	tuni-site	cryo-lite	CaO (%,ICP-OES)	MgO (%,ICP-OES)	SiO_2 (%,ICP-OES)
129.14	13			33.60	8.59	57.81											40.28	7	6.84
129.44	3			16.62	7.16	76.22											50.68	4.06	5.65
130.59	4			14.40	1.30	84.30											52.85	3.24	1.55
131.14	4			7.30	34.20	58.50											47.28	2.55	13.68
131.54	4	3/2/1		5.60	7.50	86.90											46.77	3.46	6.44
131.94	4			25.90	6.40	67.70											46.81	6.1	6.97
132.34	3		**BVF I**	36.90	12.60	50.50											40.31	7.47	15.84
132.74	3			26.60	9.50	63.90											45.07	8.5	7.06
133.04	3			48.90	6.50	44.60											42.23	11.97	4.9
133.24	4			12.00	3.70	84.30											51.97	2.37	3.32
133.59	2			37.30	3.50	59.20											48.19	6.85	4.49
133.89	3			16.40	52.40	31.20											23.26	3.59	54.77
135.09	3			37.30	11.10	51.60											40.14	7.72	11.8
135.39	2			66.70	15.70	17.60											32.12	15.63	13.72
135.74	3			54.30	34.40	11.30											24.57	12.62	33.5
136.09	1			69.50	13.50	17.00											31.34	15.29	16.18
136.29	2			0.00	0.00	0.00											36.44	9.67	17.5
136.84	2			47.00	17.50	35.50											37.09	9.08	19.06
137.14	1			47.20	16.00	36.80											34.9	9.69	17.88
137.39	3			22.70	8.00	69.30											45.62	4.72	9.61
137.69	1			57.40	8.70	33.90											36.85	11.57	10.52
138.09	1			51.20	20.20	28.60											31.3	10.58	20.47
138.29	1			39.80	46.40	12.20		1.60									16.37	7.36	57.43
138.64	13			30.90	17.00	52.10											41.9	6.37	16.56
138.94	4			39.00	5.30	55.70											43.48	8.95	6.22

Table D: *Continued*

depth (m) below salt	Facies *	Lake units	Sequences	dolomite	quartz	calcite	py-rite	mag-nesite	Mg-clays	K-felds	clays + micas	ba-rite	daws-onite	fluo-rite	tuni-site	cryo-lite	CaO (%,ICP-OES)	MgO (%,ICP-OES)	SiO_2 (%,ICP-OES)
139.24	4			42.60	4.70	52.70											42.65	7.9	5.23
139.44	3			29.70	6.00	64.30											48.29	6.18	6.08
139.89	4			28.90	5.70	65.40											45.51	6.14	6.07
140.19	2			50.20	9.80	40.00											41.32	9.48	7.12
140.44	1			39.50	6.70	53.80											44.79	8.09	7.29
140.79	1			43.70	9.20	47.10											39.74	8.85	8.92
141.09	4			23.70	16.20	60.10											26.29	3.57	48.12
141.39	3			41.30	17.60	41.10	TR										35.37	7.98	19.62
141.69	2			54.50	18.20	27.30											33.16	11.77	20.59
142.19	7			47.20	19.80	33.00	TR										32.22	10.32	22.98
142.54	7			51.90	21.10	27.00	TR										28.35	10.48	23.1
142.79	7			51.10	17.60	29.20	TR			2.10							31.24	9.92	19.35
143.19	3			28.40	14.40	57.20											44.38	6.17	9.36
143.29	14			37.30	7.10	55.60											42.71	7.32	6.42
143.49	3			43.40	17.10	39.50											37.55	7.75	17.03
143.69	1			42.80	13.00	44.20											38.01	8.74	12.9
143.99	2			34.90	13.50	51.60											40.89	7.15	14.58
144.34	6			50.40	17.00	32.60											32.94	11.9	19
144.59	6			42.70	21.00	34.60	TR			1.70							33.9	9.71	22.41
144.79	3			48.50	14.00	37.50											35.84	10.08	15.41
145.04	3			35.50	18.70	45.80	TR										36.38	7.87	19.16
145.34	6			32.30	12.30	55.40	TR										39.78	6.96	14.34
145.69	1			44.80	12.30	42.90											37.72	9.16	12.56
145.94	3			22.10	19.70	57.00		1.20									40.65	5.02	20.27
146.19	2			25.80	10.80	58.60	TR			3.80			1.00				40	5.34	16.35

Table D: *Continued*

depth (m) below salt	Facies *	Lake units	Sequences	dolomite	quartz	calcite	py-rite	mag-nesite	Mg-clays	K-felds	clays + micas	ba-rite	daws-onite	fluo-rite	tuni-site	cryo-lite	CaO (%,ICP-OES)	MgO (%,ICP-OES)	SiO_2 (%,ICP-OES)
146.54	1			66.70	13.60	19.70	TR										32.51	14.73	14.6
146.79	14			18.30	61.40	20.30											30.69	13.3	20.62
147.19	3			56.90	18.10	25.00											29.14	12.01	18.97
147.39	2			0.00	0.00	0.00											40.11	8.35	12.46
147.69	1			51.10	12.90	36.00											35.44	10.48	14.48
147.94	7			44.30	19.10	36.60											31.43	9.54	19.5
148.49	2			41.80	8.10	50.10											40.81	8.57	8.2
148.79	1			49.80	34.10	16.10											26.16	12.16	31.32
149.14	13			40.80	25.30	33.90											33.53	9.17	24.67
149.49	0			56.00	23.50	20.50											30.02	13.45	22.02
149.99	2			23.00	55.90	21.10											20.7	5.94	51.14
150.24	3			42.65	16.62	40.73											36.15	9.15	15.92
150.49	3			41.00	15.90	43.10											36.76	9.03	15.17
150.89	2			41.40	5.00	53.60											43.08	9.08	5.36
151.14	2			56.30	9.90	33.80											36.76	12.32	9.93
151.54	3			48.10	18.20	33.70											35.36	10.59	18.33
151.79	3			24.60	30.40	45.00											34.32	5.77	27.4
152.04	3			29.70	30.00	40.30											33.64	6.93	28.08
152.34	2			57.80	19.80	22.40											32.51	12.65	19.48
152.69	3			43.76	21.27	34.97											34.61	9.38	21.52
152.94	3			64.80	15.00	20.20											31.66	14.25	15.22
153.29	4			43.30	14.10	42.60											39.29	9.71	13.67
153.59	3			35.85	18.16	45.99											38.44	8.56	18.15
153.89	2			16.20	43.20	40.60											29.3	3.96	41.22
154.29	1			0.00	98.90	1.10											0.5	0.12	>90

Table D: *Continued*

depth (m) below salt	Facies *	Lake units	Sequences	dolomite	quartz	calcite	py-rite	mag-nesite	Mg-clays	K-felds	clays + micas	ba-rite	daws-onite	fluo-rite	tuni-site	cryo-lite	CaO (%,ICP-OES)	MgO (%,ICP-OES)	SiO_2 (%,ICP-OES)
154.59	2			9.90	83.60	6.50											6.63	2.03	85.42
154.94	3			26.70	62.90	10.40											14.86	5.76	65.28
155.19	3			27.90	54.00	18.10											20.41	6.78	53.63
155.44	0			44.60	5.60	49.80											43.35	10.17	6.18
155.84	4			24.30	5.10	70.60											49.94	5.71	5.5
156.24	13			29.00	8.70	62.30											45.57	6.94	8.98
156.54	3			64.50	11.00	24.50											34.91	13.41	11.15
156.79	3			35.90	18.50	45.60											39.78	7.77	16.8
156.94	3			70.70	8.90	20.40											35.49	15.13	8.92
157.19	2			30.70	12.30	57.00											44.42	7.24	11.07
157.54	3			NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	44.2	8.08	7.91
157.84	2			54.90	21.50	23.60											31.63	11.41	20.35
158.14	1			54.40	18.30	27.30											33.69	12.1	17.17
158.49	1			69.30	8.20	22.50											27.49	18.59	11.19
158.79	4			86.00	10.11	0.00				2.36		1.53					34.41	14.24	7.3
159.14	14			51.60	9.20	39.20											35.66	9.86	9.34
159.44	13			89.70	5.50	4.80											28.96	18.4	5.68
159.74	3			0.00	60.30	12.50										27.20	15.22	6.02	57.4
160.24	4			36.50	8.60	54.90											38.32	7.23	8.62
160.54	3			31.10	5.40	63.50											25.33	10.21	32.92
160.84	2			30.50	14.40	55.10											42.2	6.59	13.87
161.14	10			20.40	15.50	64.10											42.63	4.13	15.62
161.44	3			22.80	67.30	9.90											12.79	5.39	65.51
161.74	3			50.10	33.70	16.20											42.9	6.1	5.1
162.04	1			69.10	11.80	19.10											33.4	14.57	12.37

Table D: *Continued*

depth (m) below salt	Facies *	Lake units	Sequences	dolomite	quartz	calcite	py-rite	mag-nesite	Mg-clays	K-felds	clays + micas	ba-rite	daws-onite	fluo-rite	tuni-site	cryo-lite	CaO (%,ICP-OES)	MgO (%,ICP-OES)	SiO_2 (%,ICP-OES)
162.34	3			48.90	20.50	30.60											33.26	10.28	19.43
162.59	2			27.90	65.10	7.00											11.48	7.22	67.74
162.94	2			30.80	23.80	45.40											36.43	6.89	24.55
163.19	3			64.10	18.90	17.00											30.75	13.88	20.13
163.49	3			46.60	34.00	19.40											26.61	10.25	33.39
163.79	3			38.00	18.00	44.00											36.85	8.42	18.49
164.29	3			44.10	13.00	42.90											36.72	9.37	13.49
164.64	4			45.80	6.50	47.70											41.51	9.82	6.96
165.19	1			54.40	16.10	28.50	TR						1.00				33.5	11.02	17.76
165.64	1			45.60	19.10	35.30											34.67	9.82	19.18
165.94	13			20.30	12.30	67.40											44.41	4.49	12.46
166.29	2			38.00	18.00	44.00											35.42	7.6	16.83
166.59	13			28.20	17.30	54.50											39.87	5.95	16.36
166.94	1			50.10	16.80	33.10											33.01	10.16	16.77
166.99	1			29.08	33.31	37.61											29.89	6.49	32.13
167.34	1			34.73	20.07	45.20											36.85	7.43	19.02
167.64	1			44.99	26.48	28.53											30.83	9.97	25.37
168.29	1			66.44	19.94	13.62											28.53	14.48	20.15
168.64	1			67.66	5.49	25.42							1.43				34.31	14.05	6.52
168.99	2			33.51	18.22	48.27											37.56	7.01	16.79
169.54	0			6.00	66.50	27.50											16.99	1.53	69.05
169.99	1			50.10	9.10	38.10				1.00			1.70				36.24	10.04	9.52
170.29	3			28.70	19.90	51.40											38.44	6.31	20.82
171.34	2			48.00	8.60	43.40											36.94	9.45	7.84
171.69	1			48.90	19.70	31.40											29.3	9.16	18.46

Table D: *Continued*

depth (m) below salt	Facies *	Lake units	Sequences	dolomite	quartz	calcite	py-rite	mag-nesite	Mg-clays	K-felds	clays + micas	ba-rite	daws-onite	fluo-rite	tuni-site	cryo-lite	CaO (%,ICP-OES)	MgO (%,ICP-OES)	SiO_2 (%,ICP-OES)
172.39	1			23.40	12.90	63.70											39.2	4.67	11.37
172.69	2			53.41	18.32	28.27	TR										31.11	10.87	18.07
173.04	2			14.00	39.80	46.20											30.64	3.01	40.76
173.24	1			42.30	11.00	45.30							1.40				38.8	9.12	11.42
173.49	2			39.20	21.40	39.40											35.56	8.2	21.04
173.79	2			41.29	14.02	44.69											38.2	8.73	14.88
174.39	13			21.00	7.40	71.60											44.31	4.54	6.95
174.79	2			44.80	10.80	44.40											38.67	10.06	11.19
175.24	3			31.20	7.10	61.70											45.3	7.33	6.86
175.54	4			14.00	35.30	50.70											34.64	3.38	33.61
176.49	3			15.50	17.60	66.90											42.41	3.53	18.57
176.84	4			30.90	12.20	56.90											42.43	6.95	12.65
177.14	4			24.88	26.85	48.27											34.7	5.27	28.54
177.44	3			25.30	8.90	65.80											44.16	5.47	8.91
178.19	3			25.16	8.38	66.46											45.54	5.61	9.11
178.59	1			60.53	33.89	4.12							1.46				22.5	12.73	35.24
178.99	3			40.10	18.40	41.50	TR										36.55	8.63	19.41
179.34	3			36.20	16.10	47.70											38.68	7.8	16.37
179.64	4			28.40	11.80	59.80											40.38	6.07	10.96
179.94	3			24.70	16.90	58.40											43.4	5.35	15.72
180.24	1			39.79	14.05	45.07	TR						1.90				39.31	8.85	13.75
180.84	3			29.65	10.08	60.27											45.69	6.38	8.02
181.24	4			20.00	8.10	71.90											47.92	4.16	6.85
181.54	4			26.00	8.80	65.20											45.75	5.33	7.72
182.04	3			24.20	14.30	61.50											43.48	5.03	12.33

Table D: *Continued*

depth (m) below salt	Facies *	Lake units	Sequences	dolomite	quartz	calcite	py-rite	mag-nesite	Mg-clays	K-felds	clays + micas	ba-rite	daws-onite	fluo-rite	tuni-site	cryo-lite	CaO (%,ICP-OES)	MgO (%,ICP-OES)	SiO_2 (%,ICP-OES)
182.54	1			47.10	15.20	37.70	TR										35.74	8.85	13.74
183.04	2			23.10	8.10	68.80											46.95	5.4	7.19
183.49	3			51.50	13.50	35.00											37.49	10.68	12.13
183.79	2			26.34	9.38	59.44									4.84		43.75	5.21	9.42
184.24	3			45.52	14.39	40.09											39.68	6.99	9.77
184.59	3			18.80	15.60	65.60											43.77	4.08	14.55
185.49	3			17.70	3.80	78.50	TR										48.77	3.44	4.86
185.84	3			19.00	16.80	64.20											41.26	4.17	17.1
186.19	3			12.40	27.30	60.30											38.46	2.87	27.56
186.69	4			23.90	4.60	71.50											45.7	4.97	4.31
186.94	4			27.25	9.85	62.90											41.08	5.07	8.82
187.29	3			25.67	9.13	62.15									3.50		42.02	5.35	8.77
187.64	3			19.30	11.90	68.80											46.01	4.1	12.55
187.94	1			49.50	19.00	31.50											31.91	9.84	19.43
188.29	1			44.40	12.60	43.00	TR										36.9	8.84	13.4
188.94	2			31.70	9.10	59.20											43.41	6.77	9.71
189.24	3			21.00	8.10	70.90	TR										45	4.56	7.96
189.59	3			32.50	16.10	51.40											37.04	6.67	14.76
189.94	1			43.45	19.27	34.66	TR			2.62							34.56	9.18	20.89
190.29	1			59.04	23.69	13.38	TR		3.89								24.54	11.3	23.41
190.59	3			11.50	1.80	86.70											51.85	2.27	3.71
190.99	3			33.60	28.40	38.00											32.75	6.6	27.16
191.29	3			35.15	16.08	47.20	TR			1.57							35.53	6.66	16.63
191.84	1			38.68	17.58	42.24	TR			1.50							33.92	7.32	18.31
192.14	1			34.55	16.26	47.77	TR			1.42							36.65	6.89	17.49

Table D: *Continued*

depth (m) below salt	Facies *	Lake units	Sequences	dolomite	quartz	calcite	py-rite	mag-nesite	Mg-clays	K-felds	clays + micas	ba-rite	daws-onite	fluo-rite	tuni-site	cryo-lite	CaO (%,ICP-OES)	MgO (%,ICP-OES)	SiO_2 (%,ICP-OES)
192.64	1			43.20	19.10	35.00	TR			2.70							32.15	8.77	20.14
193.49	3			34.40	12.20	53.40											41.85	7.44	11.45
193.79	3			50.00	9.90	40.10											38.29	10.25	9.38
194.29	4			22.50	15.60	60.40							1.50				40.8	5.03	15.32
194.59	3			28.10	6.70	65.20											46.05	5.81	6.52
194.89	3			12.30	5.50	82.20											48.66	2.91	5.46
195.14	3			23.40	13.50	63.10											43.44	5.1	13.38
195.99	1			45.47	32.26	22.27	TR										27.22	9.63	31.36
196.34	2			54.10	19.50	26.40											32.07	10.78	18.54
196.59	3			40.00	20.00	40.00											33.56	7.92	17.51
196.94	3			45.20	11.90	42.90	TR										37.83	8.82	10.87
197.24	3			45.60	14.96	39.44											35.02	8.22	12.58
197.49	3			45.76	17.44	36.80											33.53	7.99	15.85
197.79	4			41.90	20.80	37.30											34.34	7.98	18.23
198.14	1			39.56	20.18	35.82	TR		2.89				1.55				30.28	7.48	18.1
198.44	1			52.97	18.42	26.09	TR		2.52								31.44	11.16	20.45
198.94	3			71.82	6.78	21.40											36.44	14.3	7.86
199.64	3			25.29	18.21	56.50											38.06	5.09	16.98
199.89	3			84.03	9.76	6.21											30.54	16.95	8.99
200.19	2			26.32	12.85	56.98	TR						3.85				38.41	4.71	11.59
200.59	1			21.68	23.19	52.24	TR			1.41			1.48				34.47	4.25	22.62
200.94	1			38.96	12.79	48.25											38.48	7.29	12.16
201.39	0			19.39	21.88	58.73	TR										39.39	4.55	21.38
201.49	1			18.26	22.01	57.63	TR						2.10				39.29	4.22	20.39
201.79	2			16.22	22.20	59.34	TR		2.24								36.54	3.45	22.76

Table D: *Continued*

depth (m) below salt	Facies *	Lake units	Sequences	dolomite	quartz	calcite	py-rite	mag-nesite	Mg-clays	K-felds	clays + micas	ba-rite	daws-onite	fluo-rite	tuni-site	cryo-lite	CaO (%,ICP-OES)	MgO (%,ICP-OES)	SiO_2 (%,ICP-OES)
202.14	3			77.02	17.15	5.83											28	15.33	16.92
202.54	0			58.62	17.06	24.32											31.55	11.02	15.69
203.09	1			28.56	5.92	43.08						22.44					31.16	5.18	6.2

*Facies (according to Gomes et al. 2020) codes: 0 – not described; 1 – spherulitestone; 2 – shrubby spherulitestone; 3 – spherulitic shrubstone; 4 – shrubstone; 5 – spherulitic shrubstone with mud; 6 – shrubby spherulitestone with mud; 7 – spherulitestone with mud; 10 – calcimudstone; 11 – dolomudstone; 12 – mixed mudstone; 13 – grainstone; 14 – packstone.

NA: not analysed.

TR: traces detected.

E

Appendix E

E.1 Data from well S10 used to plot Figure 6.12 in Chapter 6. Corrected $\delta^{18}O_{bulk}$ uses the correction procedures explained in the text and whose calculations are detailed in this Appendix A. Data originally published in Pietzsch et al. (2018) [192] and Pietzsch et al. (2020) [193], except for corrected $\delta^{18}O_{bulk}$ values, P concentrations, Barra Velha Formation sequence divisions and running average data.

Table E: Data from well S10 used to plot **Figure 6.12** in Chapter 6. Corrected $\delta^{18}O_{bulk}$ uses the correction procedures explained in the text and whose calculations are detailed in this Appendix. Data originally published in Pietzsch et al. (2018) and Pietzsch et al. (2020), except for corrected $\delta^{18}O_{bulk}$ values, P concentrations, Barra Velha Formation sequence divisions and running average data.

depth (m) below salt	lake units (Pietzsch et al. 2020)	Sequences	$\delta^{13}C$ (VPDB) (Pietzsch et al. 2020)	$\delta^{13}C$ (1σ, ‰)	$\delta^{13}C$ 9-points moving avg	$\delta^{18}O$ (VPDB) (Pietzsch et al. 2020)	$\delta^{18}O$ (1σ, ‰)	$\delta^{18}O$ 9-points moving avg	**Corrected $\delta^{18}O_{bulk}$ (VPDB)**	$\delta^{18}O$ 9-points moving avg (of the corrected $\delta^{18}O_{bulk}$)	$^{87}Sr/^{86}Sr$ (measured; Pietzsch et al. 2018)	Std Dev	$^{87}Sr/^{86}Sr$ (initial, calculated; Pietzsch et al. 2018)	$^{87}Sr/^{86}Sr$ 9-point moving avg (based on measured values)	P (ppm)	P 9-points moving avg
1.00	13		2.35	0.02	1.93	0.90	0.03	0.14	0.59	-0.17	0.712880	0.000010	0.712879	0.713030	110	147
2.00			2.36	0.02	1.90	-0.36	0.02	0.00	-0.53	-0.33	0.713020	0.000020	0.713019	0.713020	25	141
3.00		**BVF IV**	1.93	0.02	1.70	0.18	0.03	-0.11	-0.09	-0.51	0.713040	0.000010	0.713039	0.713030	56	141
4.00			1.69	0.03	1.77	-0.36	0.03	-0.28	-0.63	-0.59	0.713080	0.000050	0.713078	0.713040	57	176
5.00			1.30	0.03	1.80	0.33	0.03	-0.33	-0.19	-0.75	0.713130	0.000010	0.713121	0.713040	488	176
6.00			1.76	0.03	1.77	-0.71	0.03	-0.55	-1.12	-0.70	0.712970	0.000010	0.712969	0.713060	109	174
7.00			0.49	0.02	1.70	-0.74	0.03	-0.31			0.713090	0.000030	0.713085	0.713070		
8.00	12		2.25	0.02	1.71	-1.45	0.03	-0.43	-1.63	-0.78	0.713070	0.000020	0.713069	0.713090	386	287
9.00			2.06	0.02	1.77	-0.73	0.03	-0.54	-1.08	-0.78						
10.00			2.12	0.02	1.82	-1.12	0.04	-0.53	-2.06	-0.62	0.713090	0.000010	0.713088	0.713090	94	248
11.00			1.69	0.02	1.94	1.81	0.02	-0.56	1.00	-0.45	0.713100	0.000010	0.713074	0.713110	803	276
12.00			2.03	0.01	2.20	-0.86	0.04	-0.37	-1.18	-0.04	0.713170	0.000040	0.713160	0.713150	72	234
13.00			2.25	0.02	2.29	-1.38	0.03	-0.32			0.713130	0.000010	0.713118	0.713160		
14.00			1.69	0.02	2.29	0.38	0.04	0.00	-0.11	0.40	0.713100	0.000010	0.713092	0.713200	25	204
15.00	11	**BVF III**	2.84	0.03	2.34	-0.91	0.02	0.55								
16.00			2.90	0.03	2.47	0.90	0.03	0.37	0.82	0.89	0.713390	0.000020	0.713389	0.713340	25	41
17.00			2.99	0.02	2.56	-0.96	0.04	0.65								
18.00			2.12	0.02	2.61	2.17	0.03	1.17			0.713450	0.000020	0.713446	0.713410		
19.00			2.59	0.02	2.72	3.76	0.04	1.47			0.713580	0.000020	0.713575	0.713460		
20.00			2.82	0.03	2.74	0.26	0.03	1.99			0.713570	0.000010	0.713568	0.713470		
21.00			2.85	0.03	2.77	1.64	0.01	2.02	1.32	1.23	0.713290	0.000010	0.713290	0.713530	164	576

Table E: *Continued*

depth (m) below salt	lake units (Pietzsch et al. 2020)	Sequences	$\delta^{13}C$ (VPDB) (Pietzsch et al. 2020)	$\delta^{13}C$ (1σ, ‰)	$\delta^{13}C$ 9-points moving avg	$\delta^{18}O$ (VPDB) (Pietzsch et al. 2020)	$\delta^{18}O$ (1σ, ‰)	$\delta^{18}O$ 9-points moving avg	**Corrected $\delta^{18}O_{bulk}$ (VPDB)**	$\delta^{18}O$ 9-points moving avg (of the corrected $\delta^{18}O_{bulk}$)	$^{87}Sr/^{86}Sr$ (measured; Pietzsch et al. 2018)	Std Dev	$^{87}Sr/^{86}Sr$ (initial, calculated; Pietzsch et al. 2018)	$^{87}Sr/^{86}Sr$ 9-point moving avg (based on measured values)	P (ppm)	P 9-points moving avg
23.00			2.73	0.02	2.78	3.26	0.02	2.39	2.58	1.37	0.713510	0.000010	0.713510	0.713520	25	610
24.00			2.63	0.02	2.89	3.08	0.04	2.34	2.31	1.81	0.713400	0.000010	0.713399	0.713560	560	610
26.00	10		3.07	0.03	2.90	3.83	0.02	2.32	3.30	1.91	0.713600	0.000010	0.713600	0.713570	1792	610
27.00			3.14	0.01	2.90	1.18	0.02	2.63	0.99	2.14	0.713820	0.000010	0.713819	0.713590	341	537
28.00			3.03	0.01	2.89	2.36	0.02	2.58	2.27	2.24	0.713480	0.000010	0.713428	0.713630	778	631
29.00			3.18	0.02	2.94	1.72	0.02	2.58			0.713800	0.000040	0.713796	0.713640		
30.00			2.62	0.03	2.98	3.52	0.03	2.52			0.713630	0.000030	0.713626	0.713670		
31.00			2.82	0.03	2.97	3.11	0.02	2.20	2.81	2.04	0.713750	0.000010	0.713748	0.713670	101	384
32.00			2.79	0.03	2.96	1.14	0.03	2.13	0.81	1.81	0.713690	0.000010	0.713689	0.713650	823	377
33.00			3.16	0.02	2.98	3.29	0.04	1.96	2.87	1.49	0.713600	0.000030	0.713600	0.713670	168	302
34.00			3.05	0.02	2.92	2.49	0.02	1.93	2.22	1.51	0.713640	0.000010	0.713639	0.713620	303	289
35.00			2.98	0.04	2.86	0.98	0.04	1.51	0.79	1.20	0.713650	0.000010	0.713649	0.713600	176	276
36.00			3.02	0.02	2.82	0.53	0.03	1.59	0.27	1.26	0.713640	0.000010	0.713640	0.713570	289	281
37.00			3.22	0.03	2.73	0.89	0.03	1.66	0.37	1.33	0.713620	0.000010	0.713619	0.713560	251	208
38.00	9		2.58	0.02	2.63	1.39	0.04	1.40	1.21	1.10	0.713390	0.000020	0.713389	0.713560	197	206
39.00			2.16	0.03	2.52	-0.23	0.03	1.31	-0.55	0.97	0.713430	0.000010	0.713426	0.713550	179	198
41.00			2.46	0.04	2.44	3.85	0.03	1.48	3.33	1.13	0.713490	0.000020	0.713489	0.713520	139	185
42.00			1.94	0.02	2.41	1.73	0.04	1.70	1.45	1.28	0.713590	0.000010	0.713590	0.713490	171	163
43.00			2.27	0.03	2.26	1.00	0.05	1.88	0.78	1.45	0.713630	0.000020	0.713629	0.713450	152	147
44.00			2.05	0.04	2.27	1.63	0.06	1.77	1.06	1.27	0.713490	0.000010	0.713489	0.713430	226	142
46.00			2.25	0.04	2.29	2.51	0.03	1.75	2.21	1.26	0.713390	0.000010	0.713386	0.713380	61	153
47.00			2.74	0.03	2.27	2.55	0.02	1.38	1.63	0.93	0.713380	0.000010	0.713380	0.713340	90	171
48.00			1.93	0.03	2.30	2.46	0.02	1.19	1.89	0.74	0.713230	0.000050	0.713225	0.713280	108	184
49.00			2.65	0.02	2.31	0.40	0.02	1.25	-0.37	0.81	0.713210	0.000030	0.713205	0.713230	155	185

Table E: *Continued*

depth (m) below salt	lake units (Pietzsch et al. 2020)	Sequences	$\delta^{13}C$ (VPDB) (Pietzsch et al. 2020)	$\delta^{13}C$ (1σ, ‰)	$\delta^{13}C$ 9-points moving avg	$\delta^{18}O$ (VPDB) (Pietzsch et al. 2020)	$\delta^{18}O$ (1σ, ‰)	$\delta^{18}O$ 9-points moving avg	**Corrected $\delta^{18}O_{bulk}$ (VPDB)**	$\delta^{18}O$ 9-points moving avg (of the corrected $\delta^{18}O_{bulk}$)	$^{87}Sr/^{86}Sr$ (measured; Pietzsch et al. 2018)	Std Dev	$^{87}Sr/^{86}Sr$ (initial, calculated; Pietzsch et al. 2018)	$^{87}Sr/^{86}Sr$ 9-point moving avg (based on measured values)	P (ppm)	P 9-points moving avg
50.00			2.34	0.04	2.19	-0.40	0.04	1.28	-0.66	0.81	0.713030	0.000010	0.713019	0.713190	271	177
51.00			2.29	0.03	2.09	0.55	0.03	1.10	0.41	0.58	0.713120	0.000010	0.713114	0.713170	301	191
52.00			2.20	0.02	2.00	-0.01	0.03	0.90	-0.26	0.41	0.713050	0.000010	0.713049	0.713160	293	189
53.00			2.38	0.04	1.91	1.57	0.02	0.72	1.38	0.21	0.713210	0.000030	0.713209	0.713160	162	200
54.00	8		0.93	0.03	1.85	1.92	0.04	0.74	1.07	0.30	0.713050	0.000010	0.713050	0.713150	149	184
55.00			1.33	0.03	1.81	0.87	0.04	0.88			0.713290	0.000010	0.713281	0.713170		
56.00			1.93	0.35	1.82	0.76	0.04	0.75	0.10	0.24	0.713280	0.000010	0.713277	0.713190	74	165
57.00			1.14	0.03	1.84	0.84	0.04	0.86	0.13	0.25	0.713210	0.000010	0.713205	0.713210	193	144
58.00			2.10	0.04	1.83	0.55	0.02	0.79	0.10	0.26	0.713140	0.000010	0.713138	0.713190	25	133
59.00			1.97	0.02	1.97	0.84	0.03	0.61	0.39	0.07	0.713210	0.000010	0.713190	0.713240	224	140
60.00			2.40	0.02	2.07	-0.59	0.03	0.50	-1.13	-0.06	0.713310	0.000020	0.713303	0.713210	198	143
61.00			2.34	0.03	2.12	0.98	0.04	0.45							127	148
62.00			2.36	0.03	2.20	0.90	0.06	0.26	0.46	-0.27	0.713060	0.000010	0.713060	0.713220	76	141
63.00			2.19	0.03	2.29	0.33	0.04	0.31	-0.16	-0.22	0.713390	0.000040	0.713389	0.713230	203	152
64.00			2.20	0.03	2.44	-0.10	0.03	-0.14	-0.34	-0.66	0.713110	0.000010	0.713109	0.713270	166	173
65.00			2.37	0.02	2.44	0.34	0.04	-0.14	-0.12	-0.87	0.713190	0.000010	0.713189	0.713240	120	159
66.00			1.86	0.03	2.46	-0.95	0.03	-0.12	-1.74	-0.65	0.713350	0.000010	0.713349	0.713240	128	147
67.00	7		2.94	0.03	2.45	1.02	0.02	-0.04	0.57	-0.63	0.713200	0.000010	0.713199	0.713220	127	142
68.00			3.27	0.02	2.57	-3.23	0.03	-0.77	-3.89	-1.38	0.713560	0.000040	0.713487	0.713200	413	122
69.50			2.43	0.02	2.56	-0.57	0.05	-0.81	-1.51	-1.44	0.713060	0.000010	0.713059	0.713200	68	183
71.00			2.55	0.03	2.49	1.22	0.05	-1.02	0.85	-1.71	0.713260	0.000010	0.713259	0.713170	25	172
72.00			2.24	0.02	2.50	1.57	0.04	-0.77	0.64	-1.41	0.712890	0.000010	0.712888	0.713120	25	178
73.00			3.31	0.03	2.39	-6.22	0.06	-0.95	-6.87	-1.59	0.713180	0.000010	0.713175	0.713060	25	165
74.00			2.10	0.02	2.13	-0.45	0.03	-0.57	-0.89	-1.19	0.713090	0.000020	0.713088	0.712990	714	127

Table E: *Continued*

depth (m) below salt	lake units (Pietzsch et al. 2020)	Sequences	$\delta^{13}C$ (VPDB) (Pietzsch et al. 2020)	$\delta^{13}C$ (1σ, ‰)	$\delta^{13}C$ 9-points moving avg	$\delta^{18}O$ (VPDB) (Pietzsch et al. 2020)	$\delta^{18}O$ (1σ, ‰)	$\delta^{18}O$ 9-points moving avg	**Corrected $\delta^{18}O_{bulk}$ (VPDB)**	$\delta^{18}O$ 9-points moving avg (of the corrected $\delta^{18}O_{bulk}$)	$^{87}Sr/^{86}Sr$ (measured; Pietzsch et al. 2018)	Std Dev	$^{87}Sr/^{86}Sr$ (initial, calculated; Pietzsch et al. 2018)	$^{87}Sr/^{86}Sr$ 9-point moving avg (based on measured values)	P (ppm)	P 9-points moving avg
75.00			1.75	0.03	2.06	-1.58	0.05	-0.52	-2.52	-1.09	0.712910	0.000010	0.712906	0.712980	25	127
76.00			1.89	0.03	1.97	1.33	0.06	-0.61	0.97	-1.17	0.712940	0.000020	0.712918	0.712930		
77.00			1.97	0.02	1.85	-0.58	0.04	-0.64	-1.12	-1.16	0.712680	0.000020	0.712662	0.712890	25	127
78.00		**BVF II**	0.93	0.03	1.55	0.19	0.03	0.03	-0.25	-0.43	0.712920	0.000010	0.712902	0.712790	105	127
79.00			1.77	0.02	1.37	-0.12	0.02	0.25	-0.60	-0.26	0.712920	0.000010	0.712918	0.712670	69	41
80.00			1.75	0.02	1.29	0.34	0.03	0.27	0.11	-0.13	0.712850	0.000020	0.712848	0.712600	25	46
81.00			1.16	0.02	1.17	1.34	0.02	0.39	0.77	-0.05	0.712500	0.000010	0.712499	0.712470	25	54
82.00			0.63	0.02	1.07	-0.20	0.04	0.44	-0.38	0.00	0.712300	0.000010	0.712299	0.712520	25	84
84.00	6		0.46	0.03	1.10	1.52	0.02	0.44	0.70	0.01	0.712020	0.000010	0.712018	0.712460	25	80
85.00			1.07	0.03	0.94	-1.38	0.04	0.67	-1.40	0.21	0.712260	0.000010	0.712258	0.712340	70	75
86.00			0.76	0.02	0.88	2.36	0.04	0.80	1.74	0.32	0.711770	0.000010	0.711768	0.712360	114	79
87.00			1.07	0.01	0.85	-0.11	0.03	0.80	-0.73	0.29	0.713120	0.000020	0.713117	0.712450	297	79
88.00			1.19	0.02	0.87	0.19	0.02	1.03	-0.13	0.47	0.712400	0.000010	0.712397	0.712460	67	97
89.00			0.34	0.03	0.96	1.97	0.03	1.03	1.19	0.52	0.711810	0.000010	0.711807	0.712560	25	101
90.00			1.23	0.03	1.05	1.53	0.05	1.40	1.13	0.88	0.713040	0.000030	0.713027	0.712670	67	112
92.00			0.93	0.04	1.19	1.28	0.01	1.37	0.53	0.91	0.713300	0.000010	0.713298	0.712790	25	102
93.00			0.74	0.03	1.24	1.92	0.04	1.58	1.24	1.15	0.712430	0.000010	0.712429	0.712810	186	81
94.00			1.29	0.03	1.26	1.48	0.02	1.79	1.08	1.36	0.712940	0.000010	0.712938	0.712920	58	76
95.00	5		1.91	0.04	1.38	1.97	0.04	1.83	1.88	1.46	0.713210	0.000030	0.713204	0.713070	168	81
96.00			2.03	0.03	1.51	2.11	0.03	1.88	2.00	1.54	0.712870	0.000020	0.712868	0.713110	25	81
97.00			1.52	0.02	1.62	1.77	0.04	1.75	1.45	1.46	0.713310	0.000010	0.713309	0.713000	106	88
98.00			1.38	0.02	1.74	2.05	0.04	1.74	1.74	1.49	0.713400	0.000010	0.713398	0.713100	25	94
99.00			1.38	0.04	1.73	2.40	0.04	1.65	2.13	1.44	0.713160	0.000010	0.713157	0.713060	67	91
100.00			2.40	0.03	1.67	1.94	0.05	1.65	1.79	1.42	0.713410	0.000010	0.713408	0.713050	65	106

Table E: *Continued*

depth (m) below salt	lake units (Pietzsch et al. 2020)	Sequences	$\delta^{13}C$ (VPDB) (Pietzsch et al. 2020)	$\delta^{13}C$ (1σ, ‰)	$\delta^{13}C$ 9-points moving avg	$\delta^{18}O$ (VPDB) (Pietzsch et al. 2020)	$\delta^{18}O$ (1σ, ‰)	$\delta^{18}O$ 9-points moving avg	**Corrected $\delta^{18}O_{bulk}$ (VPDB)**	$\delta^{18}O$ 9-points moving avg (of the corrected $\delta^{18}O_{bulk}$)	$^{87}Sr/^{86}Sr$ (measured; Pietzsch et al. 2018)	Std Dev	$^{87}Sr/^{86}Sr$ (initial, calculated; Pietzsch et al. 2018)	$^{87}Sr/^{86}Sr$ 9-point moving avg (based on measured values)	P (ppm)	P 9-points moving avg
101.00			1.90	0.02	1.61	0.12	0.04	1.59	-0.18	1.34	0.712260	0.000030	0.712259	0.713060	94	136
102.00			1.85	0.03	1.62	1.81	0.02	1.58	1.48	1.34	0.713300	0.000010	0.713296	0.713060	241	135
103.00			1.17	0.02	1.69	0.72	0.03	1.49	0.67	1.26	0.712600	0.000010	0.712596	0.713030	25	145
104.00			1.41	0.01	1.70	1.90	0.03	1.43	1.70	1.18	0.713100	0.000010	0.713096	0.712970	303	153
105.00			1.51	0.02	1.57	1.60	0.02	1.45	1.31	1.20	0.713010	0.000010	0.713006	0.712900	299	197
106.00			1.58	0.04	1.51	1.72	0.05	1.60	1.39	1.35	0.713270	0.000010	0.713266	0.712930	95	202
107.00			2.02	0.04	1.40	1.23	0.01	1.61	1.06	1.38	0.713140	0.000010	0.713137	0.712830	116	203
108.00			1.50	0.03	1.47	1.80	0.03	1.78	1.40	1.51	0.712640	0.000020	0.712636	0.712790	137	220
109.00			1.15	0.03	1.51	2.12	0.03	1.74	1.96	1.47	0.712780	0.000020	0.712776	0.712800	465	229
110.00			1.39	0.04	1.56	1.50	0.04	1.76	1.18	1.50	0.712490	0.000010	0.712487	0.712800	140	199
111.00			0.91	0.03	1.57	1.93	0.04	1.68	1.77	1.44	0.712480	0.000010	0.712476	0.712730	250	191
113.00	4		1.77	0.04	1.52	2.20	0.02	1.75	1.80	1.50	0.712200	0.000010	0.712199	0.712640	171	208
114.00			1.73	0.04	1.57	1.52	0.03	1.70	1.37	1.49	0.713150	0.000010	0.713143	0.712700	391	203
115.00			1.97	0.02	1.70	1.82	0.02	1.67	1.53	1.46	0.713020	0.000010	0.713016	0.712630	25	171
116.00			1.67	0.03	1.77	0.98	0.03	1.68	0.88	1.45	0.712700	0.000010	0.712697	0.712600	25	183
117.00			1.58	0.03	1.95	1.87	0.02	1.63	1.61	1.41	0.712320	0.000040	0.712319	0.712640	265	169
118.00			1.93	0.04	2.03	1.32	0.00	1.63	1.27	1.40	0.713150	0.000020	0.713149	0.712680	91	158
119.00			2.38	0.03	2.07	1.91	0.02	1.64	1.70	1.36	0.712180	0.000010	0.712176	0.712620	185	148
120.00			1.97	0.03	2.10	1.56	0.02	1.55	1.14	1.23	0.712230	0.000040	0.712227	0.712530	242	158
121.00			2.51	0.03	2.11	1.51	0.03	1.68	1.41	1.35	0.712780	0.000010	0.712775	0.712500	124	163
122.00	3		2.55	0.04	2.09	2.21	0.02	1.73	1.69	1.39	0.712570	0.000010	0.712566	0.712540	71	136
123.00			2.04	0.21	1.97	1.55	0.52	1.91	0.97	1.50	0.712660	0.000010	0.712641	0.712530	303	139
124.00		**BVF I**	2.25	0.03	1.80	1.00	0.04	1.93	0.40	1.48	0.712170	0.000010	0.712138	0.712620	117	121
125.00			1.74	0.03	1.58	2.22	0.03	1.83	1.97	1.41	0.712460	0.000010	0.712455	0.712670	67	97

Table E: *Continued*

depth (m) below salt	lake units (Pietzsch et al. 2020)	Sequences	$\delta^{13}C$ (VPDB) (Pietzsch et al. 2020)	$\delta^{13}C$ (1σ, ‰)	$\delta^{13}C$ 9-points moving avg	$\delta^{18}O$ (VPDB) (Pietzsch et al. 2020)	$\delta^{18}O$ (1σ, ‰)	$\delta^{18}O$ 9-points moving avg	**Corrected $\delta^{18}O_{bulk}$ (VPDB)**	$\delta^{18}O$ 9-points moving avg (of the corrected $\delta^{18}O_{bulk}$)	$^{87}Sr/^{86}Sr$ (measured; Pietzsch et al. 2018)	Std Dev	$^{87}Sr/^{86}Sr$ (initial, calculated; Pietzsch et al. 2018)	$^{87}Sr/^{86}Sr$ 9-point moving avg (based on measured values)	P (ppm)	P 9-points moving avg
127.00			1.44	0.02	1.41	2.28	0.02	1.78	1.96	1.40	0.712640	0.000010	0.712636	0.712670	25	93
128.00			0.82	0.03	1.22	2.94	0.03	1.74	2.29	1.43	0.713040	0.000010	0.713027	0.712720	113	104
129.00			0.91	0.02	1.10	2.11	0.04	1.84	1.51	1.43	0.713050	0.000010	0.713045	0.712750	25	75
130.00			-0.02	0.03	0.84	0.68	0.03	2.12	0.51	1.52	0.712680	0.000010	0.712678	0.712760	25	68
131.00	2		0.93	0.03	0.77	1.05	0.02	2.16			0.712760	0.000010	0.712755	0.712750		
132.00			0.86	0.01	0.74	1.83	0.03	2.08	1.33	1.32	0.712980	0.000020	0.712974	0.712740	153	86
133.00			0.99	0.02	0.80	2.49	0.02	1.94			0.712980	0.000010	0.712972	0.712670		
134.00			-0.07	0.04	0.92	3.45	0.03	1.73			0.712210	0.000010	0.712201	0.712640		
135.00			1.06	0.04	1.14	2.64	0.02	1.78	1.89	1.21	0.712440	0.000010	0.712439	0.712700	92	105
137.00			1.18	0.03	1.27	1.54	0.03	1.62	1.02	0.90	0.712550	0.000010	0.712541	0.712730	106	93
138.00			1.32	0.03	1.41	1.63	0.03	1.60	1.22	0.88	0.712390	0.000020	0.712388	0.712680	25	83
139.00			2.00	0.03	1.56	0.27	0.02	1.55	0.13	1.02	0.712740	0.000010	0.712734	0.712680	102	88
140.00			1.95	0.02	1.77	1.15	0.04	1.36	1.02	1.02	0.713260	0.000010	0.713259	0.712730	150	92
141.00			2.18	0.02	1.87	-0.44	0.05	1.19	-0.52	0.89	0.713020	0.000040	0.713017	0.712790	25	89
142.00	1		2.06	0.02	1.94	1.69	0.03	1.25	1.35	0.85	0.712540	0.000010	0.712539	0.712860	82	87
143.00			2.39	0.02	2.07	2.01	0.03	1.17	1.74	0.74	0.712950	0.000010	0.712949	0.712960	119	123
144.00			1.76	0.04	2.10	1.74	0.03	1.19	1.32	0.65	0.712700	0.000020	0.712699	0.713050	128	127
148.00			1.99	0.02	2.09	1.10	0.04	1.11	0.73	0.52	0.712940	0.000040	0.712935	0.713040	62	124
149.00			1.77	0.03	2.07	2.14	0.02	1.14			0.713160	0.000010	0.713072	0.713080		
150.00			2.57	0.03	2.07	0.83	0.02	0.99	0.65	0.52	0.713350	0.000010	0.713322	0.713160	316	177
151.00			2.22	0.03	1.95	0.53	0.03	0.75	0.22	0.42	0.713510	0.000010	0.713507	0.713180	137	190
152.00			1.86	0.02	1.98	0.35	0.04	0.63			0.713220	0.000020	0.713203	0.713240		
153.00			1.98	0.02	1.98	-0.13	0.04	0.56	-0.66	0.23	0.713370	0.000010	0.713292	0.713280	292	228
155.00			2.06	0.02	2.01	0.31	0.03	0.30	-0.18	0.05	0.713260	0.000020	0.713249	0.713300	182	228

Table E: *Continued*

depth (m) below salt	lake units (Pietzsch et al. 2020)	Sequences	$\delta^{13}C$ (VPDB) (Pietzsch et al. 2020)	$\delta^{13}C$ (1σ, ‰)	$\delta^{13}C$ 9-points moving avg	$\delta^{18}O$ (VPDB) (Pietzsch et al. 2020)	$\delta^{18}O$ (1σ, ‰)	$\delta^{18}O$ 9-points moving avg	**Corrected $\delta^{18}O_{bulk}$ (VPDB)**	$\delta^{18}O$ 9-points moving avg (of the corrected $\delta^{18}O_{bulk}$)	$^{87}Sr/^{86}Sr$ (measured; Pietzsch et al. 2018)	Std Dev	$^{87}Sr/^{86}Sr$ (initial, calculated; Pietzsch et al. 2018)	$^{87}Sr/^{86}Sr$ 9-point moving avg (based on measured values)	P (ppm)	P 9-points moving avg
156.00			1.38	0.02	1.90	-0.11	0.02	0.19	-0.46	-0.09	0.713070	0.000010	0.713069	0.713290	212	206

F

Appendix F

F.1 Same data as in Table C, but including all raw isotopic and P data not used to plot Figures, with duplicate/triplicate sample measurements. Samples in red correspond to those with thin sections analysed in the electron microprobe.

Table F: Same data as in Table C, but including all raw isotopic and P data not used to plot Figures, with duplicate/triplicate sample measurements. Samples in red correspond to those with thin sections analysed in the electron microprobe.

Depth (m)	$\delta^{13}C$ (VPDB)	$\delta^{13}C$ (1σ, ‰)	$\delta^{18}O$ (VPDB)	$\delta^{18}O$ (1σ, ‰)	$^{87}Sr/^{86}Sr$	std error	abs error	Ratio 85/87	P (ppm), raw values	P (ppm), "zero" values replaced
4.99	2.06	0.05	0.19	0.05	0.71294	0.00210	0.00001	110.08837	83	83
5.24	1.12	0.06	-0.34	0.05					75	75
5.39	2.87	0.01	-0.25	0.02					63	63
6.19	2.70	0.05	1.01	0.05					326	326
6.29									188	188
6.59	2.30	0.06	1.39	0.07	0.71309	0.00070	0.00002	19.04993		
9.54	-1.14	0.04	0.01	0.03	0.71298	0.00110	0.00000	139.82397	113	113
9.74									51	51
9.79	0.81	0.04	0.87	0.05					877	877
10.44	1.92	0.04	1.16	0.03					289	289
11.19	-0.74	0.05	2.94	0.07					684	684
11.39	2.68	0.03	-0.78	0.05					63	63
11.99	2.69	0.03	0.72	0.06					379	379
12.09									445	445
12.84	1.25	0.08	-1.08	0.08	0.71324	0.00410	0.00006	50.77688	109	109
12.94									94	94
13.14	1.25	0.05	2.03	0.03					58	58
13.49	1.26	0.05	2.44	0.05					459	459
14.49	2.74	0.04	-0.58	0.03					57	57
14.74	2.47	0.04	-2.35	0.04					111	111
15.09	2.51	0.04	-2.83	0.03					74	74
15.49	2.74	0.07	-0.42	0.08					66	66
17.14										
17.59									115	115
18.39	3.07	0.03	-0.49	0.04					314	314
18.89	2.57	0.05	0.19	0.06						11
19.04										12
19.29	2.65	0.04	0.71	0.07					216	216
19.59	2.08	0.04	0.19	0.08					558	558
20.14	-0.42	0.05	2.20	0.04					65	65
20.49	0.46	0.04	1.84	0.04					86	86
21.09	1.62	0.04	1.41	0.06					81	81
22.89	2.64	0.03	2.89	0.03					939	939
22.99	2.55	0.04	2.49	0.06					407	407
23.29	2.81	0.05	3.74	0.07					230	230
23.54	1.84	0.05	2.32	0.05					128	128
23.74	2.59	0.03	2.07	0.03					182	182
23.89	2.71	0.04	2.33	0.05					139	139

Table F: *Continued*

Depth (m)	$\delta^{13}C$ (VPDB)	$\delta^{13}C$ (1σ, ‰)	$\delta^{18}O$ (VPDB)	$\delta^{18}O$ (1σ, ‰)	$^{87}Sr/^{86}Sr$	std error	abs error	Ratio 85/87	P (ppm), raw values	P (ppm), "zero" values replaced
24.69	3.41	0.05	1.82	0.04					357	357
25.19	1.35	0.04	2.57	0.02					155	155
25.94	1.45	0.03	4.00	0.04					81	81
26.09									222	222
26.24	2.51	0.04	3.49	0.05	0.71310	0.00100	0.00005	8.05880	100	100
26.54	1.95	0.03	3.61	0.03					264	264
26.79	1.74	0.04	3.00	0.03					141	141
27.09	2.41	0.05	4.26	0.05					156	156
27.14	2.45	0.04	2.84	0.04					164	164
27.74	2.49	0.03	3.20	0.03					425	425
28.09	2.31	0.06	1.22	0.05					963	963
29.14	1.97	0.04	3.44	0.04	0.71372	0.00090	0.00004	6.53610	86	86
29.49	1.44	0.06	2.48	0.04					54	54
29.49									78	78
30.29	3.06	0.02	2.40	0.03					181	181
30.39									245	245
30.99	2.56	0.03	2.94	0.04					294	294
31.34	2.15	0.07	2.34	0.06					281	281
31.39									619	619
31.64	3.11	0.05	-0.24	0.05	0.71372	0.00090	0.00003	17.69220	110	110
32.39	2.24	0.03	1.42	0.04						32
32.64	1.87	0.04	1.88	0.05					152	152
32.64									188	188
33.44	1.93	0.04	3.33	0.03					740	740
33.54									1352	1352
34.14	2.45	0.06	3.12	0.02					664	664
34.49	2.04	0.04	2.99	0.03	0.71378	0.00100	0.00004	7.98240	201	201
34.79	2.30	0.04	1.56	0.02					150	150
34.94									272	272
35.04	1.82	0.04	3.14	0.03					81	81
35.99									1113	1113
35.99									1348	1348
36.04	2.96	0.07	2.81	0.06					1360	1360
36.64	2.82	0.06	3.41	0.05					159	159
36.89									289	289
36.99	2.50	0.03	3.32	0.03					425	425
37.24	2.93	0.03	2.76	0.05					305	305
37.54	2.68	0.04	3.72	0.03					407	407
37.69	2.39	0.04	2.64	0.03					496	496
38.14	3.02	0.03	2.68	0.07					522	522

Table F: *Continued*

Depth (m)	$\delta^{13}C$ (VPDB)	$\delta^{13}C$ (1σ, ‰)	$\delta^{18}O$ (VPDB)	$\delta^{18}O$ (1σ, ‰)	$^{87}Sr/^{86}Sr$	std error	abs error	Ratio 85/87	P (ppm), raw values	P (ppm), "zero" values replaced
39.09	2.82	0.03	2.31	0.03					275	275
39.64	2.67	0.03	2.98	0.05					179	179
39.74	2.57	0.07	3.13	0.05					323	323
40.24	3.08	0.04	1.37	0.04					234	234
40.69									162	162
40.79	2.53	0.05	1.87	0.03					1522	1522
41.09	2.47	0.04	1.36	0.04					231	231
41.24	2.70	0.03	2.67	0.02					1978	1978
41.64	2.88	0.05	2.56	0.04					112	112
42.89	2.72	0.04	1.46	0.08					142	142
43.04									160	160
43.19									285	285
43.19	2.85	0.04	2.05	0.06	0.71361	0.00090	0.00006	6.74465	428	428
43.99	2.82	0.04	2.07	0.05					277	277
44.34	2.36	0.04	1.76	0.03					196	196
44.75	2.56	0.04	1.19	0.05					106	106
45.10	2.49	0.02	1.07	0.04					123	123
45.25									122	122
45.30	2.85	0.03	-0.62	0.04						33
45.74	2.67	0.05	2.33	0.04					135	135
45.89									100	100
46.14	2.72	0.04	0.95	0.05					137	137
46.39	2.23	0.05	1.41	0.05					677	677
46.74	2.03	0.01	-2.30	0.06					3531	3531
46.94	2.26	0.04	-3.10	0.03					75	75
47.44	2.23	0.04	0.56	0.04	0.71339	0.00120	0.00005	7.48900	294	294
48.09	2.04	0.03	0.67	0.05	0.71325	0.00070	0.00004	8.92170	416	416
48.24									2008	2008
48.39	2.75	0.03	0.72	0.06					357	357
48.49										2
48.74	3.22	0.06	-0.32	0.06						30
49.04	1.73	0.04	-0.32	0.05	0.71303	0.00070	0.00005	6.04450	137	137
49.29									1251	1251
49.29	1.70	0.04	0.63	0.04	0.71295	0.00080	0.00005	7.53400	1607	1607
49.64	1.63	0.02	-1.08	0.06	0.71297	0.00130	0.00003	10.60920	228	228
49.99	1.61	0.05	-0.56	0.06					201	201
50.34									1214	1214
50.39	1.48	0.03	1.09	0.05					452	452
51.59	2.50	0.04	2.16	0.01					173	173
51.69									143	143

Table F: *Continued*

Depth (m)	$\delta^{13}C$ (VPDB)	$\delta^{13}C$ (1σ, ‰)	$\delta^{18}O$ (VPDB)	$\delta^{18}O$ (1σ, ‰)	$^{87}Sr/^{86}Sr$	std error	abs error	Ratio 85/87	P (ppm), raw values	P (ppm), "zero" values replaced
52.59	2.22	0.06	0.91	0.03	0.71310	0.00090	0.00004	7.91640	84	84
52.99	1.87	0.05	-0.01	0.05					240	240
53.04									234	234
53.29									357	357
53.29	2.16	0.03	1.65	0.03					480	480
53.59	2.11	0.02	1.07	0.02					276	276
53.99									176	176
54.14	2.13	0.03	-0.09	0.04					63	63
54.54	1.94	0.02	0.88	0.02					401	401
54.69	2.10	0.02	0.71	0.02					52	52
54.94	1.93	0.08	2.06	0.05					244	244
54.94									181	181
55.29	2.01	0.05	1.52	0.05					73	73
55.39									69	69
55.39									68	68
55.39									97	97
55.54										41
55.54	1.43	0.05	1.78	0.04					70	70
56.24										28
56.24	2.11	0.08	0.77	0.06					174	174
56.84	1.93	0.03	1.34	0.02						28
57.14	2.18	0.06	0.87	0.06	0.71310	0.00080	0.00004	5.52240	88	88
58.04									427	427
58.04									1485	1485
58.04									590	590
58.24	2.22	0.05	1.47	0.07					247	247
58.69	3.20	0.02	6.63	0.02	0.71311	0.00090	0.00005	6.37630		49
58.94									50	50
59.04	2.06	0.02	1.37	0.04					130	130
59.29	2.36	0.06	1.91	0.04					79	79
59.29									50	50
59.59									356	356
59.59									189	189
59.64	2.34	0.05	2.01	0.04					156	156
59.64									146	146
59.94	2.52	0.06	1.61	0.04					153	153
59.94									151	151
60.24	2.50	0.05	2.31	0.06	0.71308	0.00095	0.00005	7.13815	287	287
60.24									285	285
60.54	2.55	0.07	2.45	0.05					298	298

Table F: *Continued*

Depth (m)	$\delta^{13}C$ (VPDB)	$\delta^{13}C$ (1σ, ‰)	$\delta^{18}O$ (VPDB)	$\delta^{18}O$ (1σ, ‰)	$^{87}Sr/^{86}Sr$	std error	abs error	Ratio 85/87	P (ppm), raw values	P (ppm), "zero" values replaced
60.54									232	232
60.64									242	242
60.79	2.36	0.04	1.95	0.07	0.71315	0.00070	0.00005	5.23770	346	346
60.99									349	349
61.04									256	256
61.04	2.32	0.04	2.03	0.03					295	295
61.49	2.45	0.02	2.30	0.01	0.71317	0.00080	0.00006	3.57490	109	109
61.74	1.38	0.03	1.36	0.02					208	208
61.74									181	181
62.09	1.16	0.04	1.62	0.03					393	393
62.09									183	183
62.14									355	355
62.14									347	347
62.14									415	415
62.39									373	373
62.39	1.52	0.03	1.64	0.02	0.71304	0.00120	0.00013	4.73660	381	381
62.94	1.06	0.05	1.32	0.04					796	796
62.94									768	768
63.24	1.95	0.02	1.03	0.04					302	302
63.24									247	247
63.49									475	475
63.49									487	487
63.54	2.14	0.03	0.29	0.03					247	247
63.54									230	230
63.74									323	323
63.74	2.14	0.04	0.95	0.05					386	386
63.99	1.90	0.03	0.58	0.03					160	160
64.29	1.76	0.02	0.70	0.03					94	94
64.39									61	61
64.39									115	115
64.59	2.24	0.05	1.72	0.04	0.71308	0.00090	0.00005	6.77340	106	106
64.89									218	218
64.89	2.35	0.03	1.78	0.02	0.71299	0.00100	0.00007	5.23400	257	257
65.19									315	315
65.19	2.24	0.05	1.51	0.04					325	325
65.29									212	212
65.29									456	456
65.64	2.42	0.05	2.30	0.03					300	300
65.79									329	329
65.94									222	222

Table F: *Continued*

Depth (m)	$\delta^{13}C$ (VPDB)	$\delta^{13}C$ (1σ, ‰)	$\delta^{18}O$ (VPDB)	$\delta^{18}O$ (1σ, ‰)	$^{87}Sr/^{86}Sr$	std error	abs error	Ratio 85/87	P (ppm), raw values	P (ppm), "zero" values replaced
65.94	2.83	0.01	0.72	0.04	0.71318	0.00075	0.00006	5.08585	254	254
66.34	3.54	0.04	1.74	0.05	0.71334	0.00070	0.00010	4.26490	253	253
66.34									235	235
66.39									290	290
66.39									166	166
66.39									347	347
66.64	3.36	0.03	2.10	0.03					106	106
67.29									111	111
67.29	2.89	0.02	0.55	0.03					216	216
67.39									85	85
67.39									108	108
67.69										45
67.94									125	125
67.94									89	89
67.94	1.92	0.03	1.25	0.02					138	138
68.24	1.93	0.05	0.25	0.04	0.71348	0.00085	0.00005	5.07975	59	59
68.49										22
68.79									52	52
68.79	2.33	0.03	-0.66	0.03	0.71301	0.00155	0.00005	12.45505	54	54
68.84										2
69.09	1.55	0.05	0.86	0.06					81	81
69.09									122	122
69.34									112	112
69.34									124	124
69.39									1749	1749
69.39	1.21	0.03	0.88	0.04					1906	1906
69.64									93	93
70.34									62	62
70.34									131	131
70.64	1.89	0.05	1.42	0.05					126	126
70.64									119	119
71.09	2.33	0.03	0.88	0.03					66	66
71.39									51	51
71.39	1.79	0.02	2.14	0.05					56	56
71.49									80	80
71.49										3
71.49										31
72.04									77	77
72.04	2.13	0.02	0.51	0.03					100	100
72.49										13

Table F: *Continued*

Depth (m)	$\delta^{13}C$ (VPDB)	$\delta^{13}C$ (1σ, ‰)	$\delta^{18}O$ (VPDB)	$\delta^{18}O$ (1σ, ‰)	$^{87}Sr/^{86}Sr$	std error	abs error	Ratio 85/87	P (ppm), raw values	P (ppm), "zero" values replaced
72.49									51	51
72.54										40
72.54	2.20	0.03	1.03	0.02	0.71294	0.00115	0.00005	7.05660	88	88
72.94									65	65
72.94	2.18	0.02	0.64	0.03					170	170
73.19	2.55	0.05	0.78	0.05					76	76
73.19										32
73.84	2.19	0.02	0.65	0.03					250	250
74.04										35
74.04										22
74.19	1.77	0.04	0.86	0.04					117	117
74.44										26
74.44										15
74.54	1.66	0.03	1.75	0.03					51	51
74.84	1.73	0.06	1.26	0.04						30
74.84										16
75.09										8
75.09	2.17	0.01	1.89	0.02	0.71249	0.00120	0.00004	10.50790	57	57
75.34										35
75.34										42
75.44	2.24	0.05	0.40	0.10						27
75.44										21
75.74										5
75.74	2.30	0.05	0.00	0.10						46
75.94										35
75.94										49
76.19	2.48	0.05	0.78	0.10						26
76.19										21
76.19										14
76.44	2.25	0.05	-0.42	0.10						36
76.89										14
76.89										5
77.19	2.12	0.05	0.38	0.10						36
77.19										17
77.29										44
77.29										4
77.49	2.18	0.05	0.73	0.10						48
77.49										42
77.89										17
77.89										6

Table F: *Continued*

Depth (m)	$\delta^{13}C$ (VPDB)	$\delta^{13}C$ (1σ, ‰)	$\delta^{18}O$ (VPDB)	$\delta^{18}O$ (1σ, ‰)	$^{87}Sr/^{86}Sr$	std error	abs error	Ratio 85/87	P (ppm), raw values	P (ppm), "zero" values replaced
77.89	2.58	0.05	0.33	0.10	0.71331	0.00080	0.00005	5.23640		39
77.99										2
77.99										19
78.14	2.34	0.05	-0.59	0.10						48
78.14										26
78.59										12
78.59	3.04	0.05	0.37	0.10						26
78.79										43
78.79										41
78.79										9
79.09	2.05	0.05	0.14	0.10						16
79.09										3
79.49										33
79.49	1.77	0.05	0.21	0.10						48
79.59										16
79.59										42
79.84	1.79	0.05	-0.27	0.10						38
79.84										24
80.04										11
80.04										24
80.04	2.18	0.05	-0.51	0.10	0.71311	0.00130	0.00005	12.75790		40
80.34	2.60	0.05	0.40	0.10					53	53
80.34										12
80.49										29
80.49										15
80.64										13
80.64	1.97	0.05	-1.82	0.10						43
80.89	2.09	0.05	0.26	0.10						37
80.89										14
81.29										19
81.29	2.39	0.05	0.40	0.10						20
81.29										2
81.49					0.71320	0.00110	0.00004	8.78450	50	50
81.64										21
81.64									57	57
81.94	2.44	0.05	0.16	0.10						48
82.19										6
82.19									54	54
82.29	2.56	0.05	0.36	0.10	0.71321	0.00070	0.00005	4.84810	60	60
82.49										38

Table F: *Continued*

Depth (m)	$\delta^{13}C$ (VPDB)	$\delta^{13}C$ (1σ, ‰)	$\delta^{18}O$ (VPDB)	$\delta^{18}O$ (1σ, ‰)	$^{87}Sr/^{86}Sr$	std error	abs error	Ratio 85/87	P (ppm), raw values	P (ppm), "zero" values replaced
82.49	2.10	0.05	0.30	0.10						46
82.74										6
82.74										22
82.74	1.88	0.05	0.25	0.10					71	71
83.09	2.42	0.05	0.08	0.10						29
83.34	2.02	0.05	0.88	0.10					63	63
83.34										6
83.54										1
83.54										8
83.64	2.02	0.05	0.64	0.10	0.71313	0.00100	0.00005	6.26483	57	57
83.64										11
83.94									58	58
83.94									57	57
83.94	2.17	0.05	0.73	0.10					95	95
84.24	2.31	0.05	0.92	0.10	0.71310	0.00120	0.00005	7.60010	61	61
84.24										5
84.34										16
84.34										31
84.49										43
84.49	1.52	0.05	0.73	0.10						44
84.84	2.15	0.05	0.35	0.10						39
84.84										7
84.94										14
84.94										46
84.94									53	53
85.19										20
85.19	2.42	0.05	0.76	0.10	0.71307	0.00095	0.00005	8.80000		28
85.79										24
85.79										4
85.89										3
85.89	1.57	0.05	0.85	0.10	0.71305	0.00080	0.00004	7.23845		37
86.09	0.92	0.05	1.14	0.10						34
86.09										27
86.34	1.23	0.05	1.78	0.10						45
86.59	1.04	0.05	1.48	0.10						49
86.59										25
86.84										14
86.84										23
86.94	1.28	0.05	1.46	0.10	0.71303	0.00100	0.00004	7.28010		32
86.94										7

Table F: *Continued*

Depth (m)	$\delta^{13}C$ (VPDB)	$\delta^{13}C$ (1σ, ‰)	$\delta^{18}O$ (VPDB)	$\delta^{18}O$ (1σ, ‰)	$^{87}Sr/^{86}Sr$	std error	abs error	Ratio 85/87	P (ppm), raw values	P (ppm), "zero" values replaced
87.24	0.99	0.05	0.99	0.10					77	77
87.24										43
87.59										32
87.59	1.68	0.05	0.75	0.10						49
87.69									54	54
87.94										19
87.94	1.72	0.05	0.58	0.10						30
88.14	1.73	0.05	0.69	0.10						42
88.14										34
88.59	2.12	0.05	1.32	0.10	0.71323	0.00090	0.00005	5.96320		36
88.59										8
88.69										47
88.69										48
88.84										11
88.84	1.99	0.05	1.25	0.10						12
89.19										10
89.19	1.98	0.05	1.47	0.10						50
89.19										49
89.59	1.57	0.05	1.22	0.10					55	55
89.84									68	68
89.84									65	65
89.94										10
89.94	1.41	0.05	0.67	0.10						15
90.14									55	55
90.14										3
90.24	0.84	0.05	1.14	0.10					52	52
90.54										10
90.54	1.06	0.05	0.78	0.10					57	57
90.54										44
90.79									52	52
90.79	1.32	0.05	1.70	0.10					58	58
91.24	1.20	0.05	2.38	0.10					56	56
91.59										1
91.59	2.00	0.05	0.68	0.10	0.71340	0.00080	0.00007	8.84850		13
91.69									73	73
91.69										38
91.99										36
91.99	1.60	0.05	0.70	0.10						38
91.99										20
92.29	1.76	0.05	0.68	0.10						20

Table F: *Continued*

Depth (m)	$\delta^{13}C$ (VPDB)	$\delta^{13}C$ (1σ, ‰)	$\delta^{18}O$ (VPDB)	$\delta^{18}O$ (1σ, ‰)	$^{87}Sr/^{86}Sr$	std error	abs error	Ratio 85/87	P (ppm), raw values	P (ppm), "zero" values replaced
92.29										15
92.59	1.97	0.05	0.95	0.10					55	55
92.59										28
92.64										45
92.64										33
92.94										6
92.94	2.10	0.05	1.22	0.10					58	58
93.19	1.82	0.05	0.79	0.10	0.71320	0.00080	0.00005	6.76305		19
93.19										14
93.19										4
93.29									109	109
93.29										17
93.44	1.47	0.05	0.51	0.10					103	103
93.44									88	88
93.84										22
93.84										33
93.84	0.96	0.05	0.45	0.10						40
93.94									84	84
93.94									65	65
94.14										47
94.14	0.51	0.05	1.20	0.10					57	57
94.44	1.07	0.05	1.04	0.10					67	67
94.79										9
94.79										38
95.04	1.15	0.05	1.85	0.10					81	81
95.14									69	69
95.14									63	63
95.14									61	61
95.34										23
95.34	1.37	0.05	1.82	0.10					53	53
95.64										26
95.64	1.50	0.05	1.79	0.10						41
95.94									54	54
96.09										28
96.09										6
96.24										35
96.24	1.28	0.05	1.04	0.10	0.71338	0.00110	0.00005	5.30140	57	57
96.49										27
96.49	0.82	0.05	0.87	0.10						36
96.49										5

Table F: *Continued*

Depth (m)	$\delta^{13}C$ (VPDB)	$\delta^{13}C$ (1σ, ‰)	$\delta^{18}O$ (VPDB)	$\delta^{18}O$ (1σ, ‰)	$^{87}Sr/^{86}Sr$	std error	abs error	Ratio 85/87	P (ppm), raw values	P (ppm), "zero" values replaced
96.74										47
96.74	1.73	0.05	1.46	0.10					73	73
96.99										16
96.99	1.98	0.05	1.24	0.10						19
97.14										17
97.14										4
97.44	1.78	0.05	2.48	0.10					55	55
97.44									55	55
97.74	1.74	0.05	3.14	0.10					69	69
97.74									63	63
97.74									54	54
97.94										32
97.94										3
98.04	1.80	0.05	1.48	0.10						1
98.34	1.38	0.05	2.56	0.10	0.71282	0.00090	0.00005	5.85550		41
98.34										21
98.59										9
98.59	1.25	0.05	0.16	0.10						25
98.84										16
98.84									51	51
98.84	1.48	0.05	2.63	0.10					66	66
98.94										27
98.94										43
99.14	1.29	0.05	1.98	0.10						25
99.14										9
99.49										26
99.49	1.42	0.05	2.97	0.10						31
99.74										19
99.74	1.43	0.05	0.78	0.10						50
99.84										14
99.84										40
99.84										38
100.04										24
100.04	1.22	0.05	0.70	0.10	0.71299	0.00090	0.00005	5.39380		45
100.34										31
100.34	1.63	0.05	1.08	0.10						44
100.59										17
100.59	2.18	0.05	1.30	0.10					50	50
100.74										31
100.74										21

Table F: *Continued*

Depth (m)	$\delta^{13}C$ (VPDB)	$\delta^{13}C$ (1σ, ‰)	$\delta^{18}O$ (VPDB)	$\delta^{18}O$ (1σ, ‰)	$^{87}Sr/^{86}Sr$	std error	abs error	Ratio 85/87	P (ppm), raw values	P (ppm), "zero" values replaced
100.94										48
100.94										49
100.94	2.00	0.05	1.67	0.10					53	53
101.09										29
101.09										27
101.24	1.28	0.05	1.51	0.10						12
101.24										6
101.59	1.44	0.05	1.17	0.10	0.71310	0.00070	0.00006	4.19940		50
101.59										46
101.74										17
101.74										26
101.89										29
101.89										15
101.89	1.62	0.05	1.54	0.10					53	53
102.24										6
102.24	0.51	0.05	2.02	0.10						15
102.54	1.52	0.05	2.59	0.10	0.71277	0.00073	0.00006	5.26097		45
102.54										14
102.64										37
102.64									60	60
102.79	1.01	0.05	2.19	0.10						25
102.79										4
103.09										36
103.44										21
103.44										25
103.44	1.13	0.05	0.49	0.10	0.71294	0.00070	0.00005	5.52710		32
103.74	1.26	0.05	0.70	0.10						40
103.74										36
103.94										21
103.94										10
104.04	1.28	0.05	1.04	0.10						50
104.04										16
104.29										19
104.29	1.24	0.05	1.91	0.10	0.71261	0.00080	0.00004	8.78160		49
104.44									73	73
104.44									99	99
104.44									95	95
104.64										5
104.64	1.92	0.05	1.26	0.10						36
105.19									55	55

Table F: *Continued*

Depth (m)	$\delta^{13}C$ (VPDB)	$\delta^{13}C$ (1σ, ‰)	$\delta^{18}O$ (VPDB)	$\delta^{18}O$ (1σ, ‰)	$^{87}Sr/^{86}Sr$	std error	abs error	Ratio 85/87	P (ppm), raw values	P (ppm), "zero" values replaced
105.19	1.75	0.05	1.45	0.10					58	58
105.39									77	77
105.39	1.29	0.05	1.41	0.10					90	90
105.79	0.92	0.05	1.12	0.10						21
105.79										9
105.94										31
105.94										46
105.94										17
106.04										35
106.04	0.63	0.05	0.63	0.10						50
106.34	1.08	0.05	1.32	0.10					55	55
106.34										40
106.69									63	63
106.69	1.70	0.05	2.08	0.10					97	97
106.99										10
106.99										26
107.04										12
107.04										13
107.24	1.24	0.05	0.99	0.10					57	57
107.34										34
107.34									61	61
107.34									55	55
107.49									107	107
107.49	1.71	0.05	2.27	0.10					147	147
107.74										4
107.74	1.33	0.05	1.16	0.10						44
108.04										4
108.04	1.99	0.05	1.42	0.10					60	60
108.29	2.23	0.05	1.48	0.10					55	55
108.29										42
108.44									51	51
108.44									78	78
108.44										6
108.59	2.15	0.05	1.60	0.10					57	57
108.59										42
108.99	1.40	0.05	1.71	0.10						46
108.99										33
109.44										8
109.44	1.82	0.05	1.15	0.10						30
109.64	1.73	0.05	0.59	0.10						25

Table F: *Continued*

Depth (m)	$\delta^{13}C$ (VPDB)	$\delta^{13}C$ (1σ, ‰)	$\delta^{18}O$ (VPDB)	$\delta^{18}O$ (1σ, ‰)	$^{87}Sr/^{86}Sr$	std error	abs error	Ratio 85/87	P (ppm), raw values	P (ppm), "zero" values replaced
109.64										22
113.34	1.47	0.05	1.89	0.10						47
113.34										19
113.34										19
113.59									93	93
113.59	1.64	0.05	2.63	0.10					95	95
113.94									57	57
113.94	1.62	0.05	1.65	0.10					68	68
114.04									76	76
114.04									53	53
114.19	1.37	0.05	1.14	0.10					65	65
114.19										31
114.49									75	75
114.49									72	72
114.49	1.19	0.05	1.45	0.10					75	75
114.79										26
114.79	2.13	0.05	1.03	0.10						28
114.94									54	54
114.94									67	67
115.14									51	51
115.14									73	73
115.19									65	65
115.19	1.65	0.05	1.76	0.10					83	83
115.54	1.70	0.05	2.12	0.10						34
115.54										27
115.84										23
115.84	1.47	0.05	0.71	0.10						27
115.99										19
115.99									53	53
116.14										3
116.14	1.83	0.05	2.12	0.10					55	55
116.14										19
116.39	1.83	0.05	2.02	0.10					52	52
116.39										4
116.69										3
116.69	2.01	0.05	2.30	0.10					71	71
117.14										45
117.14										41
117.24										2
117.24									97	97

Table F: *Continued*

Depth (m)	$\delta^{13}C$ (VPDB)	$\delta^{13}C$ (1σ, ‰)	$\delta^{18}O$ (VPDB)	$\delta^{18}O$ (1σ, ‰)	$^{87}Sr/^{86}Sr$	std error	abs error	Ratio 85/87	P (ppm), raw values	P (ppm), "zero" values replaced
117.39	0.63	0.05	1.60	0.10					74	74
117.74	1.26	0.05	1.93	0.10					78	78
117.74										15
117.74										33
117.94										34
117.94	1.35	0.05	2.55	0.10	0.71261	0.00090	0.00004	8.86730	56	56
118.44	2.07	0.05	1.92	0.10					55	55
118.44									50	50
118.54									98	98
118.54									71	71
118.79	1.58	0.05	1.84	0.10					78	78
118.79									51	51
118.79										20
118.99									76	76
118.99									74	74
119.34										43
119.34	1.68	0.05	1.84	0.10					51	51
119.39										34
119.39										39
119.54										23
119.54	1.93	0.05	1.37	0.10					52	52
119.94	1.72	0.05	2.11	0.10					118	118
119.94									94	94
120.19									76	76
120.19									91	91
120.19									54	54
120.29									84	84
120.29	1.49	0.05	1.31	0.10					86	86
120.54									106	106
120.54	1.71	0.05	1.51	0.10					116	116
120.69									68	68
120.69									71	71
120.84	1.99	0.05	2.21	0.10					74	74
120.84									59	59
121.14										22
121.14										32
121.14	2.10	0.05	1.48	0.10						40
121.44	1.82	0.05	1.21	0.10	0.71304	0.00107	0.00004	12.39627	55	55
121.44										17
121.54										2

Table F: *Continued*

Depth (m)	$\delta^{13}C$ (VPDB)	$\delta^{13}C$ (1σ, ‰)	$\delta^{18}O$ (VPDB)	$\delta^{18}O$ (1σ, ‰)	$^{87}Sr/^{86}Sr$	std error	abs error	Ratio 85/87	P (ppm), raw values	P (ppm), "zero" values replaced
121.54										28
122.14										22
122.14										36
122.44	1.88	0.05	2.04	0.10					77	77
122.44									55	55
122.64									67	67
122.64									60	60
122.64										11
122.74	1.34	0.05	1.88	0.10					112	112
122.74									112	112
122.99									56	56
122.99	0.91	0.05	1.62	0.10					84	84
123.44	1.25	0.05	1.60	0.10					86	86
123.44									77	77
123.74									68	68
123.74	1.49	0.05	1.39	0.10	0.71329	0.00100	0.00004	12.17780	70	70
123.84										45
123.84									68	68
123.84									55	55
123.94									64	64
123.94	1.46	0.05	1.24	0.10					75	75
124.24									70	70
124.24									57	57
124.29	1.83	0.05	1.41	0.10					67	67
124.29										10
124.59	2.01	0.05	1.59	0.10					73	73
124.59									62	62
124.84	2.01	0.05	1.54	0.10					79	79
124.84										15
124.84									58	58
124.99										9
124.99									74	74
125.09	2.07	0.05	1.81	0.10	0.71315	0.00090	0.00005	5.29190	79	79
125.09									72	72
125.34										45
125.34	2.01	0.05	1.59	0.10					52	52
125.64	1.64	0.05	1.31	0.10					63	63
125.64										37
125.94										36
125.94	1.55	0.05	1.65	0.10					68	68

Table F: *Continued*

Depth (m)	$\delta^{13}C$ (VPDB)	$\delta^{13}C$ (1σ, ‰)	$\delta^{18}O$ (VPDB)	$\delta^{18}O$ (1σ, ‰)	$^{87}Sr/^{86}Sr$	std error	abs error	Ratio 85/87	P (ppm), raw values	P (ppm), "zero" values replaced
125.94										10
126.24										25
126.24	1.74	0.05	1.53	0.10						34
126.54	1.52	0.05	1.17	0.10						17
126.54										7
126.64										17
126.64									60	60
126.79	1.68	0.05	1.76	0.10					140	140
126.79										27
126.84										37
126.84										21
126.84									61	61
127.09	1.30	0.05	2.40	0.10					75	75
127.09									72	72
127.64	1.87	0.05	1.26	0.10					137	137
127.64									90	90
127.64									111	111
127.94										12
127.94	1.58	0.05	1.59	0.10					52	52
127.99									53	53
127.99									76	76
128.19	1.22	0.05	0.94	0.10						42
128.19										34
128.54	1.38	0.05	1.20	0.10						20
128.54										8
128.59										25
128.59										34
128.84	2.19	0.05	2.48	0.10					71	71
128.84										35
129.14										25
129.14	1.58	0.05	1.65	0.10					51	51
129.14										2
129.44										38
129.44	1.50	0.05	1.24	0.10					51	51
129.49									60	60
129.49									55	55
129.49										50
130.59	1.69	0.03	1.00	0.03	0.71319	0.00080	0.00005	6.30770		30
130.59										2
131.14	1.66	0.01	1.12	0.02					54	54

Table F: *Continued*

Depth (m)	$\delta^{13}C$ (VPDB)	$\delta^{13}C$ (1σ, ‰)	$\delta^{18}O$ (VPDB)	$\delta^{18}O$ (1σ, ‰)	$^{87}Sr/^{86}Sr$	std error	abs error	Ratio 85/87	P (ppm), raw values	P (ppm), "zero" values replaced
131.14										48
131.24									50	50
131.24										38
131.39										35
131.39										20
131.54										20
131.54										5
131.54	1.60	0.02	0.81	0.01						35
131.94	1.39	0.04	1.28	0.03	0.71314	0.00075	0.00006	4.78565	73	73
131.94										45
132.34									71	71
132.34	1.26	0.03	1.51	0.04					78	78
132.74	1.49	0.03	1.91	0.03					77	77
132.74										9
133.04									81	81
133.04	1.10	0.04	2.17	0.04					96	96
133.09									64	64
133.09									50	50
133.09									53	53
133.24	1.44	0.04	1.17	0.06					55	55
133.24										10
133.49									56	56
133.49									57	57
133.59	1.33	0.03	1.52	0.04					52	52
133.59										46
133.89										1
133.89	1.23	0.03	0.95	0.03						2
134.14									53	53
134.14									53	53
134.14										39
134.29									55	55
134.29										48
135.09	1.34	0.03	1.18	0.02					97	97
135.09									60	60
135.39									197	197
135.39	1.09	0.02	1.33	0.02					199	199
135.49									57	57
135.49										23
135.74									66	66
135.74	0.96	0.04	1.36	0.03					80	80

Table F: *Continued*

Depth (m)	$\delta^{13}C$ (VPDB)	$\delta^{13}C$ (1σ, ‰)	$\delta^{18}O$ (VPDB)	$\delta^{18}O$ (1σ, ‰)	$^{87}Sr/^{86}Sr$	std error	abs error	Ratio 85/87	P (ppm), raw values	P (ppm), "zero" values replaced
135.74									62	62
136.09	1.29	0.02	0.86	0.02	0.71327	0.00105	0.00005	6.55600	110	110
136.09									97	97
136.29	1.24	0.02	0.17	0.03					76	76
136.29									60	60
136.39									130	130
136.39									124	124
136.49									53	53
136.84									82	82
136.84	1.42	0.01	0.24	0.02					77	77
137.14									85	85
137.14	0.88	0.02	0.93	0.02					101	101
137.14									55	55
137.39	0.55	0.03	0.61	0.02						23
137.39										10
137.49									133	133
137.49									116	116
137.69	0.84	0.03	1.42	0.03					244	244
137.69									104	104
137.94									180	180
137.94									194	194
138.09									138	138
138.09									154	154
138.09	0.41	0.03	1.73	0.04	0.71322	0.00070	0.00004	5.50030	162	162
138.29										37
138.29	1.84	0.03	1.08	0.03						45
138.64	1.40	0.04	1.06	0.05	0.71312	0.00077	0.00007	4.48277	53	53
138.64										20
138.94	1.43	0.04	1.42	0.05					88	88
138.94									70	70
139.24	1.34	0.03	1.48	0.03					112	112
139.24									63	63
139.34									79	79
139.34									79	79
139.34									80	80
139.44	1.40	0.04	1.49	0.03					91	91
139.44									85	85
139.59									73	73
139.59									50	50
139.89									70	70

Table F: *Continued*

Depth (m)	$\delta^{13}C$ (VPDB)	$\delta^{13}C$ (1σ, ‰)	$\delta^{18}O$ (VPDB)	$\delta^{18}O$ (1σ, ‰)	$^{87}Sr/^{86}Sr$	std error	abs error	Ratio 85/87	P (ppm), raw values	P (ppm), "zero" values replaced
139.89	1.30	0.04	1.46	0.04					77	77
140.19	1.28	0.03	1.28	0.02						33
140.19										1
140.44										45
140.44										12
140.44	1.32	0.03	0.99	0.03	0.71307	0.00090	0.00004	8.77630	63	63
140.54										44
140.54										22
140.79	1.53	0.03	1.30	0.03					56	56
140.79									51	51
141.09	1.29	0.01	0.86	0.02						43
141.09										40
141.39	1.45	0.01	1.37	0.03					186	186
141.39									153	153
141.59									92	92
141.59									91	91
141.59									102	102
141.69									120	120
141.69	1.56	0.03	1.02	0.05					136	136
142.19	1.78	0.01	0.98	0.03					163	163
142.19									128	128
142.54	1.65	0.02	-0.22	0.03					138	138
142.54									93	93
142.64									123	123
142.64									105	105
142.79									183	183
142.79	1.97	0.02	1.21	0.04	0.71327	0.00090	0.00006	5.99665	184	184
142.79									183	183
143.19	1.00	0.01	0.93	0.02					53	53
143.19										31
143.29										16
143.29	1.16	0.01	0.89	0.02					59	59
143.49	1.31	0.02	1.26	0.03						42
143.49										32
143.69										18
143.69	1.09	0.03	1.19	0.03						24
143.99									58	58
143.99									60	60
143.99	1.11	0.02	0.57	0.03					69	69
144.34	1.54	0.08	0.94	0.04	0.71320	0.00070	0.00005	5.85220	113	113

Table F: *Continued*

Depth (m)	$\delta^{13}C$ (VPDB)	$\delta^{13}C$ (1σ, ‰)	$\delta^{18}O$ (VPDB)	$\delta^{18}O$ (1σ, ‰)	$^{87}Sr/^{86}Sr$	std error	abs error	Ratio 85/87	P (ppm), raw values	P (ppm), "zero" values replaced
144.34									110	110
144.39									121	121
144.39									87	87
144.59									133	133
144.59	1.59	0.04	0.65	0.05					159	159
144.69									150	150
144.69									125	125
144.79	1.32	0.02	0.78	0.03					119	119
144.79									95	95
144.79									119	119
145.04	1.43	0.03	0.74	0.03					59	59
145.04										48
145.34									133	133
145.34	1.45	0.04	0.59	0.02					134	134
145.69	1.52	0.03	1.38	0.03					56	56
145.69										43
145.79									90	90
145.79									68	68
145.94										23
145.94										21
145.94	1.76	0.02	0.32	0.02						41
146.19	1.95	0.04	1.41	0.02					57	57
146.19									51	51
146.54	1.77	0.02	1.53	0.03					139	139
146.54									108	108
146.59									72	72
146.59									84	84
146.79	1.48	0.03	1.32	0.02					117	117
146.79									104	104
147.19									58	58
147.19										48
147.19	1.58	0.01	0.13	0.02	0.71323	0.00085	0.00006	6.20940	72	72
147.39	1.06	0.03	0.69	0.01					189	189
147.39									125	125
147.49									90	90
147.49										31
147.69	1.43	0.02	0.91	0.02					299	299
147.69									264	264
147.94									1008	1008
147.94	1.58	0.02	0.65	0.02					1181	1181

Table F: *Continued*

Depth (m)	$\delta^{13}C$ (VPDB)	$\delta^{13}C$ (1σ, ‰)	$\delta^{18}O$ (VPDB)	$\delta^{18}O$ (1σ, ‰)	$^{87}Sr/^{86}Sr$	std error	abs error	Ratio 85/87	P (ppm), raw values	P (ppm), "zero" values replaced
148.49	1.39	0.01	0.75	0.02					113	113
148.54										12
148.79	2.13	0.02	-0.70	0.01	0.71341	0.00120	0.00006	11.16150		38
149.14	1.30	0.02	0.36	0.01					165	165
149.49	2.12	0.02	-0.48	0.01					64	64
149.99	1.53	0.02	-0.38	0.02						16
150.24	1.46	0.02	0.39	0.02					87	87
150.29									62	62
150.49	1.69	0.02	0.93	0.02					127	127
150.89	1.84	0.03	1.67	0.01					79	79
150.89									67	67
151.09										33
151.14	1.61	0.04	1.77	0.03					70	70
151.54	1.16	0.02	0.93	0.03					136	136
151.79	0.52	0.03	0.78	0.02						29
152.04	1.08	0.03	0.95	0.01						35
152.09										32
152.34	1.00	0.03	1.52	0.01					80	80
152.69	1.43	0.02	0.92	0.02					156	156
152.94	1.33	0.03	1.73	0.02					65	65
152.99									69	69
152.99									62	62
153.29	1.45	0.02	1.08	0.01					80	80
153.59	1.54	0.02	0.89	0.02						16
153.89	1.61	0.01	1.24	0.01					51	51
153.99										9
154.29	-1.71	0.14	-4.57	0.09						10
154.59	1.19	0.03	1.69	0.03						2
154.69									81	81
154.94	1.19	0.01	2.07	0.01						38
155.19	1.74	0.02	1.30	0.02						13
155.44	1.68	0.03	1.51	0.01					111	111
155.44										33
155.64									58	58
155.84	1.55	0.04	0.65	0.02					80	80
156.24	1.58	0.02	1.44	0.01					58	58
156.54	1.33	0.01	1.46	0.01					105	105
156.59									94	94
156.79	1.26	0.02	0.90	0.01						32
156.94	1.32	0.02	1.74	0.02					53	53

Table F: *Continued*

Depth (m)	$\delta^{13}C$ (VPDB)	$\delta^{13}C$ (1σ, ‰)	$\delta^{18}O$ (VPDB)	$\delta^{18}O$ (1σ, ‰)	$^{87}Sr/^{86}Sr$	std error	abs error	Ratio 85/87	P (ppm), raw values	P (ppm), "zero" values replaced
157.19	1.33	0.03	0.90	0.01					77	77
157.29									79	79
157.54	1.32	0.03	0.85	0.02						39
157.54										2
157.84	1.47	0.04	1.98	0.02	0.71296	0.00130	0.00009	5.54680	114	114
158.14	1.44	0.03	1.61	0.02					66	66
158.24									466	466
158.49	1.85	0.03	4.41	0.03	0.71299	0.00090	0.00005	6.92140	99	99
158.79	1.52	0.03	2.05	0.02					130	130
159.14	1.84	0.03	1.00	0.03					255	255
159.24									102	102
159.44	1.55	0.04	2.89	0.03					168	168
159.74	1.68	0.04	1.31	0.01						31
160.04									219	219
160.04									204	204
160.09									135	135
160.24	1.03	0.03	0.65	0.01					133	133
160.54	1.15	0.02	0.38	0.01						45
160.84	1.66	0.03	0.56	0.03						29
160.94										9
161.14	0.91	0.04	0.31	0.03	0.71343	0.00110	0.00011	3.85960	66	66
161.44	1.14	0.04	0.37	0.01						19
161.74	1.07	0.04	0.61	0.01						45
161.79										29
162.04	0.69	0.02	1.58	0.02					90	90
162.04									81	81
162.34	0.67	0.03	1.01	0.01	0.71365	0.00100	0.00009	4.33680		21
162.59	1.76	0.02	-0.51	0.02						10
162.69									54	54
162.94	1.01	0.03	0.71	0.02						50
163.19	0.66	0.02	1.30	0.02						37
163.49	0.83	0.04	0.58	0.03						26
163.54										1
163.79	0.99	0.04	0.67	0.02						34
164.29										1
164.29	1.33	0.03	0.29	0.02						46
164.34										29
164.64	1.43	0.02	0.42	0.01						14
165.14										45
165.19	1.70	0.03	0.91	0.02					157	157

Table F: *Continued*

Depth (m)	$\delta^{13}C$ (VPDB)	$\delta^{13}C$ (1σ, ‰)	$\delta^{18}O$ (VPDB)	$\delta^{18}O$ (1σ, ‰)	$^{87}Sr/^{86}Sr$	std error	abs error	Ratio 85/87	P (ppm), raw values	P (ppm), "zero" values replaced
165.64	1.26	0.02	-0.54	0.02						11
165.94	1.29	0.03	0.89	0.01						45
166.04									52	52
166.29	1.49	0.01	0.28	0.01						5
166.59	1.54	0.02	0.94	0.02						50
166.69										27
166.94									69	69
166.94	1.53	0.01	0.11	0.01					77	77
166.99	-0.26	0.10	0.83	0.05					58	58
167.19									86	86
167.34	-0.17	0.10	1.01	0.05					95	95
167.64	-0.37	0.10	0.55	0.05					158	158
168.29	0.71	0.10	0.67	0.05					74	74
168.44									99	99
168.64	1.45	0.10	1.57	0.05					143	143
168.99	0.40	0.10	1.18	0.05					57	57
169.44									108	108
169.54										47
169.54	0.17	0.10	1.23	0.05					56	56
169.99	0.59	0.10	1.54	0.05					100	100
170.29	0.45	0.10	1.66	0.05					58	58
170.44										8
170.64									51	51
171.34	1.32	0.10	1.81	0.05					106	106
171.59									89	89
171.69	0.80	0.10	2.00	0.05					110	110
172.39	-0.35	0.10	1.24	0.05						4
172.69	0.10	0.10	1.32	0.05					181	181
172.79									59	59
172.79									92	92
173.04	0.55	0.10	1.58	0.05						11
173.24	-0.27	0.10	0.99	0.05					238	238
173.49	0.70	0.10	0.89	0.05	0.71363	0.00130	0.00005	7.78810	69	69
173.79	1.36	0.10	1.16	0.05					78	78
173.94									102	102
174.39	1.05	0.10	1.62	0.05					88	88
174.79	1.41	0.10	1.83	0.05					99	99
174.94									51	51
175.24	1.66	0.10	1.10	0.05					87	87
175.54	1.27	0.10	1.15	0.05					54	54

Table F: *Continued*

Depth (m)	$\delta^{13}C$ (VPDB)	$\delta^{13}C$ (1σ, ‰)	$\delta^{18}O$ (VPDB)	$\delta^{18}O$ (1σ, ‰)	$^{87}Sr/^{86}Sr$	std error	abs error	Ratio 85/87	P (ppm), raw values	P (ppm), "zero" values replaced
175.54										47
175.94									147	147
176.14									78	78
176.49	1.14	0.10	1.23	0.05					53	53
176.74									91	91
176.84	1.31	0.10	1.03	0.05					81	81
177.14	0.92	0.10	1.07	0.05					98	98
177.44	0.82	0.10	1.50	0.05					67	67
177.74									87	87
178.19	1.14	0.10	1.34	0.05					262	262
178.59	1.93	0.10	1.00	0.05					139	139
178.59									113	113
178.69									191	191
178.99	0.71	0.10	1.13	0.05					159	159
179.34	1.41	0.10	1.29	0.05					93	93
179.64	0.82	0.10	1.03	0.05					83	83
179.89									85	85
179.94	0.87	0.10	1.21	0.05						30
180.24	0.79	0.10	1.24	0.05					68	68
180.54									117	117
180.84	0.72	0.10	0.84	0.05					89	89
181.14										4
181.14									88	88
181.24	0.72	0.10	1.12	0.05						1
181.54	1.27	0.10	1.07	0.05					64	64
182.04	0.85	0.10	1.17	0.05						6
182.29										2
182.54	1.18	0.10	1.59	0.05					199	199
183.04	1.18	0.10	1.40	0.05					206	206
183.39										29
183.49	1.98	0.10	1.30	0.05						18
183.79	1.54	0.10	1.60	0.05						22
184.24										5
184.24	1.63	0.10	1.44	0.05					88	88
184.49										29
184.59	0.81	0.07	1.44	0.05	0.71327	0.00110	0.00007	6.10245	107	107
185.49	0.89	0.10	0.96	0.05					64	64
185.84	1.63	0.10	1.07	0.05						34
185.94									63	63
186.19	1.35	0.10	1.54	0.05						27

Table F: *Continued*

Depth (m)	$\delta^{13}C$ (VPDB)	$\delta^{13}C$ (1σ, ‰)	$\delta^{18}O$ (VPDB)	$\delta^{18}O$ (1σ, ‰)	$^{87}Sr/^{86}Sr$	std error	abs error	Ratio 85/87	P (ppm), raw values	P (ppm), "zero" values replaced
186.69	1.41	0.10	1.46	0.05					72	72
186.89										5
186.94	0.97	0.10	1.27	0.05						47
187.29	0.98	0.10	1.48	0.05					105	105
187.29									86	86
187.64	0.68	0.10	1.28	0.05						26
187.94	0.81	0.10	1.87	0.05						50
188.04										9
188.29	1.03	0.10	0.88	0.05						24
188.59										24
188.94	1.61	0.10	1.27	0.05						44
188.99									72	72
189.24	1.23	0.10	1.19	0.05					84	84
189.59	1.21	0.10	0.65	0.05						7
189.94									95	95
189.94	0.87	0.10	0.57	0.05					212	212
189.99										23
190.29	0.78	0.10	1.74	0.05					207	207
190.59	1.42	0.10	1.29	0.05						42
190.99	0.81	0.10	-0.14	0.05	0.71283	0.00110	0.00005	4.29850	88	88
191.19										28
191.29	0.67	0.10	0.75	0.05	0.71349	0.00070	0.00004	6.60330	196	196
191.84	0.28	0.10	0.27	0.05						39
192.14	0.44	0.10	0.68	0.05						31
192.64	1.12	0.10	0.78	0.05					98	98
193.39									61	61
193.39									114	114
193.49	1.28	0.10	0.84	0.05					80	80
193.79	1.31	0.10	0.81	0.05					123	123
194.29	1.24	0.10	0.95	0.05					84	84
194.39									85	85
194.59	1.33	0.10	1.01	0.05					102	102
194.89	0.96	0.10	1.38	0.05					79	79
195.14	1.40	0.10	1.10	0.05					69	69
195.59									125	125
195.99	1.13	0.10	1.12	0.05					185	185
196.34	1.14	0.10	0.85	0.05					94	94
196.34									70	70
196.59	0.51	0.10	0.56	0.05					67	67
196.69										33

Table F: *Continued*

Depth (m)	$\delta^{13}C$ (VPDB)	$\delta^{13}C$ (1σ, ‰)	$\delta^{18}O$ (VPDB)	$\delta^{18}O$ (1σ, ‰)	$^{87}Sr/^{86}Sr$	std error	abs error	Ratio 85/87	P (ppm), raw values	P (ppm), "zero" values replaced
196.94	0.82	0.10	0.79	0.05					89	89
197.24	0.65	0.10	0.76	0.05					87	87
197.49	0.49	0.10	0.38	0.05					69	69
197.69										41
197.79	0.50	0.10	0.31	0.05						31
198.14	1.37	0.10	1.29	0.05					139	139
198.44	1.13	0.10	0.43	0.05					129	129
198.89									84	84
198.89									74	74
198.94	0.96	0.10	0.05	0.05					58	58
199.29										30
199.29									63	63
199.64	1.12	0.10	1.12	0.05					90	90
199.89	0.84	0.10	-1.23	0.05	0.71272	0.00070	0.00005	5.24490	79	79
199.99									73	73
200.19	1.13	0.10	1.34	0.05					53	53
200.59	2.12	0.10	1.88	0.05					491	491
200.94	1.62	0.10	0.94	0.05					154	154
201.39	0.99	0.10	1.32	0.05					134	134
201.49	0.90	0.10	1.22	0.05					149	149
201.79	0.28	0.10	1.22	0.05					162	162
202.14	0.65	0.10	-1.35	0.05					74	74
202.54	0.52	0.10	0.32	0.05						21
203.09	0.90	0.10	1.03	0.05					67	67

G

Appendix G

G.1 Aqueous chemistry database of alkaline lake waters compiled from the published literature, as well as corresponding results from calculations described in chapters 2 and 3, and investigated in detail in chapter 4.

The table is divided in 11 parts, containing the results of geochemical calculations encompassing the most relevant physicochemical parameters determined for the systems addressed in the present study, i.e., alkaline lakes and the carbonate-phosphate subsystems. Original references, location/area/geology (when available), ion activities, activity coefficients, mineral saturation states, free concentrations of the main species and other physical parameters are indicated. The complete database is stored and available on github.com under the repository "raphapietzsch/alkaline_lakes".

Table G. part 1: Aqueous chemistry database of alkaline lake waters compiled from published literature, as well as corresponding results from calculations described in chapters 2 and 3, and investigated in detail in chapter 4.

Sequence # (sample #)	Reference	Original_source	sample_name	Lake
1	Fukushi and Matsumyia (2018)	Wen and He (1999)	1	Duikou
2	Fukushi and Matsumyia (2018)	Wen and He (1999)	2	ErquanjingII
3	Fukushi and Matsumyia (2018)	Wen and He (1999)	3	Kulun
4	Fukushi and Matsumyia (2018)	Li et al. (2009)	4	Qinghai
5	Fukushi and Matsumyia (2018)	Yang and Williams (2003); Arp et al. (1998)	5	Huhejilin or Huhejaran
6	Fukushi and Matsumyia (2018)	Arp et al. (1998)	6	Nuoertu
7	Fukushi and Matsumyia (2018)	Yang and Williams (2003)	7	Sumujilin-S
8	Fukushi and Matsumyia (2018)	Yang and Williams (2003)	8	Sumujilin-N
9	Fukushi and Matsumyia (2018)	Yang (2006)	9	Yabulai 11
10	Fukushi and Matsumyia (2018)	Baatar et al. (2017)	10	Oigon
11	Fukushi and Matsumyia (2018)	Baatar et al. (2017)	11	Telmen
12	Fukushi and Matsumyia (2018)	Baatar et al. (2017)	12	Tsegeen
13	Fukushi and Matsumyia (2018)	Isupov et al. (2012)	13	Shaazgai
14	Fukushi and Matsumyia (2018)	Namsaraev et al. (2010)	14	Khilganta
15	Fukushi and Matsumyia (2018)	Reimer et al. (2009); Kazmierczak and Kempe (2003)	15	Van
16	Fukushi and Matsumyia (2018)	Dongarra et al. (1983); Aiuppa et al. (2007)	16	Specchio di Venere
17	Fukushi and Matsumyia (2018)	Last (1992)	17	East Basin
18	Fukushi and Matsumyia (2018)	Coshell et al. (1998)	18	Richmond
19	Fukushi and Matsumyia (2018)	Coshell et al. (1998)	19	Walyungup
20	Fukushi and Matsumyia (2018)	Connell and Dreiss (1995); Bischoff et al. (1993)	20	Mono
21	Fukushi and Matsumyia (2018)	Gosselin (1997)	21	Wilkinson
22	Fukushi and Matsumyia (2018)	Cloern et al. (1983)	22	Big Soda
23	Fukushi and Matsumyia (2018)	Iwama et al. (1997)	23	Pyramid
24	Fukushi and Matsumyia (2018)	Cooper and Koch (1984); Benson et al. (1991)	24	Walker
25	Guerreiro et al. (2019)	Guerreiro et al. (2019)	1	Nhecolandia
26	Guerreiro et al. (2019)	Guerreiro et al. (2019)	2	Nhecolandia
27	Guerreiro et al. (2019)	Guerreiro et al. (2019)	3	Nhecolandia
28	Guerreiro et al. (2019)	Guerreiro et al. (2019)	4	Nhecolandia
29	Guerreiro et al. (2019)	Guerreiro et al. (2019)	5	Nhecolandia
30	Guerreiro et al. (2019)	Guerreiro et al. (2019)	6	Nhecolandia
31	Guerreiro et al. (2019)	Guerreiro et al. (2019)	7	Nhecolandia
32	Guerreiro et al. (2019)	Guerreiro et al. (2019)	8	Nhecolandia
33	Guerreiro et al. (2019)	Guerreiro et al. (2019)	9	Nhecolandia
34	Guerreiro et al. (2019)	Guerreiro et al. (2019)	10	Nhecolandia
35	Guerreiro et al. (2019)	Guerreiro et al. (2019)	11	Nhecolandia
36	Guerreiro et al. (2019)	Guerreiro et al. (2019)	12	Nhecolandia

Table G. part 1: *Continued*

Sequence # (sample #)	Reference	Original_source	sample_name	Lake
37	Guerreiro et al. (2019)	Guerreiro et al. (2019)	13	Nhecolandia
38	Guerreiro et al. (2019)	Guerreiro et al. (2019)	14	Nhecolandia
39	Guerreiro et al. (2019)	Guerreiro et al. (2019)	15	Nhecolandia
40	Guerreiro et al. (2019)	Guerreiro et al. (2019)	16	Nhecolandia
41	Guerreiro et al. (2019)	Guerreiro et al. (2019)	17	Nhecolandia
42	Shvartsev et al. (2014)	Shvartsev et al. (2014)	1	Shaazgai Nuur
43	Shvartsev et al. (2014)	Shvartsev et al. (2014)	2	Shaazgai Nuur
44	Shvartsev et al. (2014)	Shvartsev et al. (2014)	3	Shaazgai Nuur
45	Shvartsev et al. (2014)	Shvartsev et al. (2014)	4	Shaazgai Nuur
46	Shvartsev et al. (2014)	Shvartsev et al. (2014)	5	Shaazgai Nuur
47	Shvartsev et al. (2014)	Shvartsev et al. (2014)	6	Shaazgai Nuur
48	Shvartsev et al. (2014)	Shvartsev et al. (2014)	7	Shaazgai Nuur
49	Shvartsev et al. (2014)	Shvartsev et al. (2014)	8	Khara-Us Nuur
50	Shvartsev et al. (2014)	Shvartsev et al. (2014)	9	Khara-Us Nuur
51	Shvartsev et al. (2014)	Shvartsev et al. (2014)	10	Khyargas Nuur
52	Shvartsev et al. (2014)	Shvartsev et al. (2014)	11	Khyargas Nuur
53	Shvartsev et al. (2014)	Shvartsev et al. (2014)	12	Khyargas Nuur
54	Shvartsev et al. (2014)	Shvartsev et al. (2014)	13	Airag Nuur 1
55	Shvartsev et al. (2014)	Shvartsev et al. (2014)	14	Airag Nuur 2
56	Shvartsev et al. (2014)	Shvartsev et al. (2014)	15	Ureg Nuur
57	Shvartsev et al. (2014)	Shvartsev et al. (2014)	16	Ulgijn Nuur
58	Shvartsev et al. (2014)	Shvartsev et al. (2014)	17	SangijnDalai Nuur 1
59	Shvartsev et al. (2014)	Shvartsev et al. (2014)	18	Dergen Nuur
60	Shvartsev et al. (2014)	Shvartsev et al. (2014)	19	Tsokhor Nuur
61	Shvartsev et al. (2014)	Shvartsev et al. (2014)	20	Ikh-Gashun Nuur
62	Shvartsev et al. (2014)	Shvartsev et al. (2014)	21	Uvs Nuur
63	Shvartsev et al. (2014)	Shvartsev et al. (2014)	22	Baga Nuur 1
64	Shvartsev et al. (2014)	Shvartsev et al. (2014)	23	Bor-Khag Nuur
65	Shvartsev et al. (2014)	Shvartsev et al. (2014)	24	Baga Nuur 2
66	Chase et al. (2020)	Darragi & Tardy (1987)	1	Lake Yoa
67	Chase et al. (2020)	Darragi & Tardy (1987)	2	Lake Yoa
68	Chase et al. (2020)	Darragi & Tardy (1987)	3	Lake Yoa
69	Chase et al. (2020)	Darragi & Tardy (1987)	6	Lake Yoa
70	Chase et al. (2020)	Darragi & Tardy (1987)	9	Lake Yoa
71	Chase et al. (2020)	Darragi & Tardy (1987)	4	Lake Yoa
72	Chase et al. (2020)	Darragi & Tardy (1987)	5	Lake Yoa
73	Chase et al. (2020)	Darragi & Tardy (1987)	7	Lake Yoa
74	Chase et al. (2020)	Darragi & Tardy (1987)	8	Lake Yoa

Table G. part 1: *Continued*

Sequence # (sample #)	Reference	Original_source	sample_name	Lake
75	Chase et al. (2020)	Darragi & Tardy (1987)	11	Lake Yoa
76	Chase et al. (2020)	Darragi & Tardy (1987)	13	Lake Yoa
77	Chase et al. (2020)	Darragi & Tardy (1987)	14	Lake Yoa
78	Chase et al. (2020)	Darragi & Tardy (1987)	16	Lake Yoa
79	Chase et al. (2020)	Darragi & Tardy (1987)	17	Lake Yoa
80	Chase et al. (2020)	Darragi & Tardy (1987)	10	Lake Yoa
81	Chase et al. (2020)	Darragi & Tardy (1987)	12	Lake Yoa
82	Chase et al. (2020)	Darragi & Tardy (1987)	15	Lake Yoa
83	Chase et al. (2020)	Darragi & Tardy (1987)	18	Lake Yoa
84	Chase et al. (2020)	Darragi & Tardy (1987)	19	Lake Yoa
85	Chase et al. (2020)	Darragi & Tardy (1987)	20	Lake Yoa
86	Chase et al. (2020)	Deocampo (2005)	95_11	Mti Moja Eastern Lake Spring
87	Chase et al. (2020)	Deocampo (2005)	95_12	Mti Moja Eastern Lake Spring
88	Chase et al. (2020)	Deocampo (2005)	96_13	Mti Moja Eastern Lake Spring
89	Chase et al. (2020)	Deocampo (2005)	97_21	Mti Moja Eastern Lake Spring
90	Chase et al. (2020)	Deocampo (2005)	97_22	Mti Moja Eastern Lake Spring
91	Chase et al. (2020)	Deocampo (2005)	97_23	Mti Moja Eastern Lake Spring
92	Chase et al. (2020)	Deocampo (2005)	99_52	Lake Makat Eastern Lake Margin
93	Chase et al. (2020)	Deocampo (2005)	99_6	Munge stream Eastern Lake Margin
94	Chase et al. (2020)	Deocampo (2005)	95_2	95GN1
95	Chase et al. (2020)	Deocampo (2005)	95_3	95GMWP
96	Chase et al. (2020)	Deocampo (2005)	95_5	95NGSH
97	Chase et al. (2020)	Deocampo (2005)	96_1	96GN2
98	Chase et al. (2020)	Deocampo (2005)	96_10	96NGP
99	Chase et al. (2020)	Deocampo (2005)	96_11	96NGW
100	Chase et al. (2020)	Deocampo (2005)	96_12	96GRE
101	Chase et al. (2020)	Deocampo (2005)	99_8	Ngoitokitok-Gorigor Wetlands
102	Chase et al. (2020)	Deocampo (2005)	99_57	Gorigor west culvert
103	Chase et al. (2020)	Deocampo (2005)	99_60	Gorigor south culvert
104	Chase et al. (2020)	Deocampo (2005)	99_62	Gorigor noth culvert
105	Chase et al. (2020)	Deocampo (2005)	95_4	95ZIKID(Lerai Stream and Wetlands)
106	Chase et al. (2020)	Deocampo (2005)	95_6	95LER(Lerai Stream and Wetlands)
107	Chase et al. (2020)	Deocampo (2005)	96_2	96LER(Lerai Stream and Wetlands)
108	Chase et al. (2020)	Deocampo (2005)	97_15	Gor-Lake (Lerai Stream and Wetlands)
109	Chase et al. (2020)	Deocampo (2005)	99_7	lerai x-ing (Lerai Stream and Wetlands)
110	Chase et al. (2020)	Deocampo (2005)	99_53	Gorigor Lake
111	Chase et al. (2020)	Deocampo (2005)	99_59	Lerai Hippo pool Culvert
115	Chase et al. (2020)	Deocampo (2005)	99_13	Jangwani warm spring Lake Eyasi Basin (E Margin)

Table G. part 1: *Continued*

Sequence # (sample #)	Reference	Original_source	sample_name	Lake
116	Chase et al. (2020)	Deocampo (2005)	99_16	Jangwani warm spring Lake Eyasi Basin (E Margin)
117	Chase et al. (2020)	Deocampo (2005)	99_26	Jangwani warm spring Lake Eyasi Basin (E Margin)
118	Chase et al. (2020)	Deocampo (2005)	97_8	Jangwani hot spring Lake Eyasi Basin (E Margin)
119	Chase et al. (2020)	Deocampo (2005)	99_30	Jangwani hot spring Lake Eyasi Basin (E Margin)
120	Chase et al. (2020)	Deocampo (2005)	99_23	Lake Eyasi Basin (E Margin)
121	Chase et al. (2020)	Deocampo (2005)	99_24	Lake Eyasi Basin (E Margin)
125	Chase et al. (2020)	Deocampo (2005)	99_10	Kisimangeda
126	Chase et al. (2020)	Deocampo (2005)	99_11	Kisimangeda
127	Chase et al. (2020)	Deocampo (2005)	99_12	Kisimangeda
128	Chase et al. (2020)	Deocampo (2005)	99_18	Kisimangeda
129	Chase et al. (2020)	Deocampo (2005)	99_20	Kisimangeda
130	Chase et al. (2020)	Deocampo (2005)	99_21	Kisimangeda
131	Chase et al. (2020)	Deocampo (2005)	99_22	Kisimangeda
132	Chase et al. (2020)	Deocampo (2005)	99_28	Kisimangeda
133	Chase et al. (2020)	Deocampo (2005)	99_29	Kisimangeda
134	Chase et al. (2020)	Deocampo (2005)	99_31	Cyperus Swamp
135	Chase et al. (2020)	Deocampo (2005)	99_32	Cyperus Swamp
136	Chase et al. (2020)	Deocampo (2005)	99_34	Cyperus Swamp
137	Chase et al. (2020)	Deocampo (2005)	99_35	Cyperus Swamp
138	Chase et al. (2020)	Deocampo (2005)	99_38	Kisimangeda
139	Chase et al. (2020)	Servant-Vildary & Roux (1990)	BAL1	Ballivian
140	Chase et al. (2020)	Servant-Vildary & Roux (1990)	RAM5	Ramaditas
141	Chase et al. (2020)	Servant-Vildary & Roux (1990)	VER2	Laguna verde
142	Chase et al. (2020)	Servant-Vildary & Roux (1990)	HED3	Hedionda
143	Chase et al. (2020)	Servant-Vildary & Roux (1990)	PUJ5	Pujio
144	Chase et al. (2020)	Servant-Vildary & Roux (1990)	PUR4	Puripica
145	Chase et al. (2020)	Servant-Vildary & Roux (1990)	HON3	Honda
146	Chase et al. (2020)	Servant-Vildary & Roux (1990)	CHI4	Chiar Kkota
147	Chase et al. (2020)	Servant-Vildary & Roux (1990)	CAN3	Canapa
148	Chase et al. (2020)	Servant-Vildary & Roux (1990)	CHU3	Chullucani
149	Chase et al. (2020)	Servant-Vildary & Roux (1990)	CHU2	Chulluncani
150	Chase et al. (2020)	Servant-Vildary & Roux (1990)	CLD4	Laguna Colorada
151	Chase et al. (2020)	Servant-Vildary & Roux (1990)	CLD33	Laguna Colorada
152	Chase et al. (2020)	Servant-Vildary & Roux (1990)	CAL19	Cachi Laguna
153	Chase et al. (2020)	Servant-Vildary & Roux (1990)	PAG22	Pastos Grandes: Central lake
154	Chase et al. (2020)	Servant-Vildary & Roux (1990)	PAG40	Pastos Grandes: Central lake
155	Chase et al. (2020)	Servant-Vildary & Roux (1990)	PAG30	Pastos Grandes: Central lake
156	Chase et al. (2020)	Servant-Vildary & Roux (1990)	PAG44	Pastos Grandes: Central lake

Table G. part 1: *Continued*

Sequence # (sample #)	Reference	Original_source	sample_name	Lake	
157	Chase et al. (2020)	Servant-Vildary & Roux (1990)	PAG48	Pastos Grandes: Central lake	
158	Chase et al. (2020)	Servant-Vildary & Roux (1990)	PAG69	Pastos Grandes: W-N Lake	
159	Chase et al. (2020)	Servant-Vildary & Roux (1990)	PAG72	Pastos Grandes: W-N Lake	
160	Chase et al. (2020)	Servant-Vildary & Roux (1990)	PAG74	Pastos Grandes: W-N Lake	
161	Chase et al. (2020)	Servant-Vildary & Roux (1990)	PAG73	Pastos Grandes: W-N Lake	
162	Chase et al. (2020)	Servant-Vildary & Roux (1990)	PAG75	Pastos Grandes: W-N Lake	
163	Chase et al. (2020)	Servant-Vildary & Roux (1990)	PAG77	Pastos Grandes: W-N Lake	
164	Chase et al. (2020)	Servant-Vildary & Roux (1990)	PAG81	Eastern lake	
165	Chase et al. (2020)	Servant-Vildary & Roux (1990)	PAG83	Eastern lake	
166	Chase et al. (2020)	Servant-Vildary & Roux (1990)	PAG96	Eastern lake	
167	Chase et al. (2020)	Servant-Vildary & Roux (1990)	PAG124	Eastern lake	
168	Chase et al. (2020)	Servant-Vildary & Roux (1990)	PAG115	Eastern lake	
169	Chase et al. (2020)	Risacher & Fritz (1991)	1	Laguna Colorada	
170	Chase et al. (2020)	Risacher & Fritz (1991)	2	Laguna Colorada	
171	Chase et al. (2020)	Risacher & Fritz (1991)	3	Laguna Colorada	
172	Chase et al. (2020)	Risacher & Fritz (1991)	4	Laguna Colorada	
173	Chase et al. (2020)	Risacher & Fritz (1991)	5	Laguna Colorada	
174	Chase et al. (2020)	Risacher & Fritz (1991)	6	Laguna Colorada	
175	Chase et al. (2020)	Risacher & Fritz (1991)	7	Laguna Colorada	
176	Chase et al. (2020)	Risacher & Fritz (1991)	TUR SL	Lake Turguiri	
177	Chase et al. (2020)	Risacher & Fritz (1991)	CHU SL	Chulluncani	
178	Chase et al. (2020)	Risacher & Fritz (1991)	PAG SL	Pastos Grandes	
179	Chase et al. (2020)	Risacher & Fritz (1991)	CAL SL	Cachi Laguna	
180	Chase et al. (2020)	Risacher & Fritz (1991)	KAR SL	Kara	
181	Chase et al. (2020)	Risacher & Fritz (1991)	CAP SL	Capina	
182	Chase et al. (2020)	Risacher & Fritz (1991)	CLD SL	Laguna Colorada	
183	Chase et al. (2020)	Risacher & Fritz (1991)	LAG SL	Lagunillas	
184	Chase et al. (2020)	Risacher & Fritz (1991)	CHA SL	Challviri	
185	Chase et al. (2020)	Risacher & Fritz (1991)	HND SL	Honda Sur	
186	Chase et al. (2020)	Risacher & Fritz (1991)	PUR SL	Puripica	
187	Chase et al. (2020)	Risacher & Fritz (1991)	VER SL	Laguna Verde	
188	Chase et al. (2020)	Risacher & Fritz (1991)	COL SL	Collpa	
189	Chase et al. (2020)	Risacher & Fritz (1991)	HDS SL	Hedionda Sur	
190	Chase et al. (2020)	Risacher & Fritz (1991)	TOT SL	Totoral	
191	Chase et al. (2020)	Risacher & Fritz (1991)	CAT SL	Catalcito	
192	Chase et al. (2020)	Risacher & Fritz (1991)	BUS SL	Bush	
193	Chase et al. (2020)	Risacher & Fritz (1991)	PEL SL	Pelada	
194	Chase et al. (2020)	Risacher & Fritz (1991)	LOR SL		0.00

Table G. part 1: *Continued*

Sequence # (sample #)	Reference	Original_source	sample_name	Lake
195	Chase et al. (2020)	Risacher & Fritz (1991)	LUR SL	Luriques
196	Chase et al. (2020)	Risacher & Fritz (1991)	CHL SL	Chojllas
197	Chase et al. (2020)	Risacher & Fritz (1991)	COR SL	Coruto
199	Chase et al. (2020)	Reimer et al. (2009)	2 Gessner (1957)	Lake Van
200	Chase et al. (2020)	Reimer et al. (2009)	3 Irion (1973)	Lake Van
201	Chase et al. (2020)	Reimer et al. (2009)	4 Kempe (1977)	Lake Van
202	Chase et al. (2020)	Reimer et al. (2009)	5 Schweizer (1975)	Lake Van
203	Chase et al. (2020)	Reimer et al. (2009)	6 Kempe (1977)	Lake Van
204	Chase et al. (2020)	Reimer et al. (2009)	7 Tugrul et al. (1984)	Lake Van
205	Chase et al. (2020)	Reimer et al. (2009)	1989 - 5m	Lake Van
206	Chase et al. (2020)	Reimer et al. (2009)	1989 - 50m	Lake Van
207	Chase et al. (2020)	Reimer et al. (2009)	1989 - 400m	Lake Van
208	Chase et al. (2020)	Fussmann et al. (2020)	0	Lake Neusiedl
209	Chase et al. (2020)	Badaut & Risacher (1983)	CAN	Bolivian Salar Canapa
210	Chase et al. (2020)	Badaut & Risacher (1983)	HON	Bolivian Salar Honda
211	Chase et al. (2020)	Badaut & Risacher (1983)	RAM	Bolivian Salar Ramadita
212	Chase et al. (2020)	Badaut & Risacher (1983)	PUJ	Bolivian Salar Pujio
213	Chase et al. (2020)	Badaut & Risacher (1983)	BAL	Bolivian Salar Ballivian
214	Chase et al. (2020)	Badaut & Risacher (1983)	HED	Bolivian Salar Hedionda
215	Chase et al. (2020)	Badaut & Risacher (1983)	CHI	Bolivian Salar Chiar-Khota
216	Chase et al. (2020)	Badaut & Risacher (1983)	CHU	Bolivian Salar Chulluncani
217	Chase et al. (2020)	Badaut & Risacher (1983)	PGS	Bolivian Salar Pastos Grandes-South
218	Chase et al. (2020)	Badaut & Risacher (1983)	PGC	Bolivian Salar Pastos Grandes-Center
219	Chase et al. (2020)	Badaut & Risacher (1983)	a	Bolivian Saline Lakes
220	Chase et al. (2020)	Badaut & Risacher (1983)	b	Bolivian Saline Lakes
221	Chase et al. (2020)	Badaut & Risacher (1983)	c	Bolivian Saline Lakes
222	Chase et al. (2020)	Badaut & Risacher (1983)	d	Bolivian Saline Lakes
223	Chase et al. (2020)	Badaut & Risacher (1983)	e	Bolivian Saline Lakes
224	Chase et al. (2020)	Badaut & Risacher (1983)	f	Bolivian Saline Lakes
225	Chase et al. (2020)	Power et al. (2009)	A	Como Lake
226	Chase et al. (2020)	Power et al. (2009)	B	W of Como Lake
227	Chase et al. (2020)	Power et al. (2009)	C	Wetland
228	Chase et al. (2020)	Power et al. (2009)	D	N playa wetland
229	Chase et al. (2020)	Power et al. (2009)	E	N playa spring
230	Chase et al. (2020)	Power et al. (2009)	F	Groundwater well from southern playas (2005)
232	Chase et al. (2020)	Power et al. (2009)	G	SE playa (2005)
234	Chase et al. (2020)	Power et al. (2009)	H	Isolated wetland
235	Chase et al. (2020)	Power et al. (2009)	I	Grassland transect

Table G. part 1: *Continued*

Sequence # (sample #)	Reference	Original_source	sample_name	Lake
236	Chase et al. (2020)	Power et al. (2009)	J	Atlin Lake
237	Chase et al. (2020)	Power et al. (2009)	K	Atlin Lake Inlet (mouth)
238	Chase et al. (2020)	Power et al. (2009)	L	Atlin Lake inlet (wetland)
239	Chase et al. (2020)	Power et al. (2009)	M	Wetland E of S Playas
240	Chase et al. (2020)	Power et al. (2009)	N	Pine Creek
241	Chase et al. (2020)	Power et al. (2009)	O	Monarch Mt spring
242	Chase et al. (2020)	Power et al. (2009)	P	Monarch Mt pond
243	Chase et al. (2020)	Power et al. (2009)	Q	Monarch mt SE pond
244	Chase et al. (2020)	Power et al. (2014)	Spring	Spring
245	Chase et al. (2020)	Power et al. (2014)	Groundwater well	Groundwater well
246	Chase et al. (2020)	Power et al. (2014)	Mound water	Mound water
247	Chase et al. (2020)	Power et al. (2014)	Isolated pond	Isolated pond
248	Chase et al. (2020)	Power et al. (2014)	Wetland (N lobe)	Wetland (N lobe)
249	Chase et al. (2020)	Power et al. (2014)	Wetland(S lobe)	Wetland(S lobe)
250	Chase et al. (2020)	Zorz et al. (2019)	Deer Lake (2015)	Deer Lake
251	Chase et al. (2020)	Zorz et al. (2019)	Deer Lake (2017)	Deer Lake
252	Chase et al. (2020)	Zorz et al. (2019)	Probe Lake (2015)	Probe Lake
253	Chase et al. (2020)	Zorz et al. (2019)	Probe Lake (2017)	Probe Lake
254	Chase et al. (2020)	Zorz et al. (2019)	Good Enough (2015)	Good Enough
255	Chase et al. (2020)	Zorz et al. (2019)	Good Enough (2017)	Good Enough
256	Chase et al. (2020)	Zorz et al. (2019)	Last Chance (2015)	Last Chance Lake
257	Chase et al. (2020)	Zorz et al. (2019)	Last Chance (2017)	Last Chance Lake
258	Chase et al. (2020)	Renaut (1993)	ML-1-88	Milk Lake
259	Chase et al. (2020)	Renaut (1993)	ML-11-90	Milk Lake
260	Chase et al. (2020)	Renaut (1993)	MK-3-89	Milk Lake
261	Chase et al. (2020)	Renaut (1993)	ML-2-90	Milk Lake
262	Chase et al. (2020)	Renaut (1993)	ML-5-90	Milk Lake
263	Chase et al. (2020)	Renaut (1993)	ML-7-88	Milk Lake
264	Chase et al. (2020)	Renaut (1993)	ML-16-90	Milk Lake
265	Chase et al. (2020)	Renaut (1993)	ML-5-89	Milk Lake
266	Chase et al. (2020)	Renaut (1993)	Little Milk	Little Milk Lake
267	Chase et al. (2020)	Renaut (1993)	Slime	Slime Lake
268	Chase et al. (2020)	Renaut (1993)	Alberta 1	Alberta 1 Lake
269	Chase et al. (2020)	Renaut (1993)	Alberta 2	Alberta 2 Lake
271	Chase et al. (2020)	Phillips and Van Denburgh (1971)	1b	Lake Abert E shore(Jan 1959)
272	Chase et al. (2020)	Phillips and Van Denburgh (1971)	1c	Lake Abert E shore(Apr 1961)
274	Chase et al. (2020)	Phillips and Van Denburgh (1971)	1e	Lake Abert E shore(Sept 1961)
275	Chase et al. (2020)	Phillips and Van Denburgh (1971)	1f	Lake Abert E shore (Jan 1962)

Table G. part 1: *Continued*

Sequence # (sample #)	Reference	Original_source	sample_name	Lake
278	Chase et al. (2020)	Phillips and Van Denburgh (1971)	1i	Lake Abert E shore (June 1962)
283	Chase et al. (2020)	Phillips and Van Denburgh (1971)	3b	Lake Abert SE shore (Aug 1956)
284	Chase et al. (2020)	Phillips and Van Denburgh (1971)	3c	Lake Abert SE shore (Oct 1957)
285	Chase et al. (2020)	Phillips and Van Denburgh (1971)	3d	Lake Abert SE shore (Nov 1958)
287	Chase et al. (2020)	Phillips and Van Denburgh (1971)	16a	Summer Lake
288	Chase et al. (2020)	Phillips and Van Denburgh (1971)	16d	Summer Lake
289	Chase et al. (2020)	Phillips and Van Denburgh (1971)	16f	Summer Lake
290	Chase et al. (2020)	Phillips and Van Denburgh (1971)	21c	Goose Lake E shore
291	Chase et al. (2020)	Phillips and Van Denburgh (1971)	21g	Goose Lake E shore
292	Chase et al. (2020)	Phillips and Van Denburgh (1971)	22d	Goose Lake W shore
293	Chase et al. (2020)	Phillips and Van Denburgh (1971)	23a	Goose Lake S end
294	Chase et al. (2020)	Phillips and Van Denburgh (1971)	23b	Goose Lake S end
295	Chase et al. (2020)	Phillips and Van Denburgh (1971)	23c	Goose Lake S end
296	Chase et al. (2020)	Phillips and Van Denburgh (1971)	31d	Silver Lake
297	Chase et al. (2020)	Phillips and Van Denburgh (1971)	31e	Silver Lake
298	Chase et al. (2020)	Phillips and Van Denburgh (1971)	34b	Harney Lake
299	Chase et al. (2020)	Phillips and Van Denburgh (1971)	37b	Crump Lake W shore
300	Chase et al. (2020)	Phillips and Van Denburgh (1971)	38b	Hart Lake NW shore
301	Chase et al. (2020)	Phillips and Van Denburgh (1971)	40b	Deep Creek
302	Chase et al. (2020)	Phillips and Van Denburgh (1971)	41a	Honey Creek
303	Chase et al. (2020)	Rawson and Moore (1944)	Little Manitou	Little Manitou
304	Chase et al. (2020)	Rawson and Moore (1944)	Big Quill	Big Quill
306	Chase et al. (2020)	Rawson and Moore (1944)	Manito	Manito
307	Chase et al. (2020)	Rawson and Moore (1944)	Redberry	Redberry
308	Chase et al. (2020)	Rawson and Moore (1944)	Bitter	Bitter
309	Chase et al. (2020)	Rawson and Moore (1944)	Antelope	Antelope
310	Chase et al. (2020)	Rawson and Moore (1944)	Basin	Basin
311	Chase et al. (2020)	Rawson and Moore (1944)	Stoney (Humboldt)	Stoney (Humboldt)
313	Chase et al. (2020)	Rawson and Moore (1944)	Lenore	Lenore
314	Chase et al. (2020)	Rawson and Moore (1944)	Fishing	Fishing
315	Chase et al. (2020)	Rawson and Moore (1944)	Wakaw	Wakaw
316	Chase et al. (2020)	Rawson and Moore (1944)	Last Mountain	Last Mountain
317	Chase et al. (2020)	Rawson and Moore (1944)	Margo	Margo
319	Chase et al. (2020)	Rawson and Moore (1944)	Carlyle	Carlyle
320	Chase et al. (2020)	Rawson and Moore (1944)	Round (P.A.)	Round (P.A.)
321	Chase et al. (2020)	Rawson and Moore (1944)	Echo	Echo
322	Chase et al. (2020)	Rawson and Moore (1944)	Jackfish	Jackfish
323	Chase et al. (2020)	Rawson and Moore (1944)	Kenosee	Kenosee

Table G. part 1: *Continued*

Sequence # (sample #)	Reference	Original_source	sample_name	Lake	
325	Chase et al. (2020)	Rawson and Moore (1944)	Kenderdine	Kenderdine	
329	Chase et al. (2020)	Rawson and Moore (1944)	Wilson	Wilson	
330	Chase et al. (2020)	Rawson and Moore (1944)	Edward's	Edward's	
331	Chase et al. (2020)	Rawson and Moore (1944)	Round (Qu'App.)	Round (Qu'App.)	
332	Chase et al. (2020)	Rawson and Moore (1944)	Good Spirit	Good Spirit	
333	Chase et al. (2020)	Rawson and Moore (1944)	Clearwater	Clearwater	
334	Chase et al. (2020)	Rawson and Moore (1944)	Murray	Murray	
335	Chase et al. (2020)	Rawson and Moore (1944)	Birch	Birch	
336	Chase et al. (2020)	Rawson and Moore (1944)	Christopher	Christopher	
337	Chase et al. (2020)	Rawson and Moore (1944)	Emma	Emma	
338	Chase et al. (2020)	Rawson and Moore (1944)	Sturgeon	Sturgeon	
340	Chase et al. (2020)	Rawson and Moore (1944)	Pelletier	Pelletier	
341	Chase et al. (2020)	Rawson and Moore (1944)	Greenwater	Greenwater	
342	Chase et al. (2020)	Rawson and Moore (1944)	Brightsand	Brightsand	
343	Chase et al. (2020)	Rawson and Moore (1944)	Madge	Madge	
345	Chase et al. (2020)	Rawson and Moore (1944)	Little Loon	Little Loon	
346	Chase et al. (2020)	Rawson and Moore (1944)	Deep	Deep	
347	Chase et al. (2020)	Rawson and Moore (1944)	Turtle	Turtle	
348	Chase et al. (2020)	Rawson and Moore (1944)	Halkett	Halkett	
349	Chase et al. (2020)	Rawson and Moore (1944)	Meeting	Meeting	
352	Chase et al. (2020)	Rawson and Moore (1944)	Namekus	Namekus	
353	Chase et al. (2020)	Rawson and Moore (1944)	Waskesiu	Waskesiu	
356	Chase et al. (2020)	Whitehead and Feth (1961)	117	Little Borax Lake, Lake Country	
357	Chase et al. (2020)	Whitehead and Feth (1961)	344	Little Borax Lake, Lake Country	
358	Chase et al. (2020)	Whitehead and Feth (1961)	393	Big Borax Lake	
359	Chase et al. (2020)	Whitehead and Feth (1961)	455	Mono Lake	
361	Chase et al. (2020)	Whitehead and Feth (1961)	447	Saddlebag Lake	
368	Chase et al. (2020)	Whitehead and Feth (1961)	456	Hot Spring, Black Point	
370	Chase et al. (2020)	Whitehead and Feth (1961)	1092	Big Washoe Lake	
371	Chase et al. (2020)	Whitehead and Feth (1961)	1157	Big Washoe Lake	
372	Chase et al. (2020)	Whitehead and Feth (1961)	1090	Little Washoe Lake	
373	Chase et al. (2020)	Whitehead and Feth (1961)	804	Big Soda Lake	
374	Chase et al. (2020)	Whitehead and Feth (1961)	921	Pyramid Lake	
375	Chase et al. (2020)	Whitehead and Feth (1961)	944		0
376	Chase et al. (2020)	Whitehead and Feth (1961)	945		0
377	Chase et al. (2020)	Whitehead and Feth (1961)	935	Walker Lake (N end)	
378	Chase et al. (2020)	Whitehead and Feth (1961)	936	Walker Lake (S end)	
381	Chase et al. (2020)	Whitehead and Feth (1961)	805		0

Table G. part 1: *Continued*

Sequence # (sample #)	Reference	Original_source	sample_name	Lake	
382	Chase et al. (2020)	Whitehead and Feth (1961)	1089	Closed-basin sump, Lyon Country	
383	Chase et al. (2020)	Whitehead and Feth (1961)	533	Abert Lake	
384	Chase et al. (2020)	Whitehead and Feth (1961)	724	Abert Lake	
385	Chase et al. (2020)	Whitehead and Feth (1961)	725	spring, E shore Abert Lake	
386	Chase et al. (2020)	Whitehead and Feth (1961)	691	Great Salt Lake	
387	Chase et al. (2020)	Whitehead and Feth (1961)	689	hot spring, Box Elder County	
388	Chase et al. (2020)	Whitehead and Feth (1961)	690	hot spring, Box Elder County	
389	Chase et al. (2020)	Whitehead and Feth (1961)	961	Locomotive Spring, Box Elder County	
390	Chase et al. (2020)	Whitehead and Feth (1961)	W-78		0
392	Chase et al. (2020)	Whitehead and Feth (1961)	1186	Weber River	
393	Chase et al. (2020)	Whitehead and Feth (1961)	1187	Bear River	
394	Chase et al. (2020)	Whitehead and Feth (1961)	1188	Jordan River	
395	Chase et al. (2020)	Whitehead and Feth (1961)	W-54		0
396	Chase et al. (2020)	Whitehead and Feth (1961)	692	brine, US Highway 40, Bonneville salt flats	
397	Chase et al. (2020)	Fritz et al. (1993)	ALBT	Albert, Hamlin	
398	Chase et al. (2020)	Fritz et al. (1993)	ALK2	Alkali, Sargent	
399	Chase et al. (2020)	Fritz et al. (1993)	ALKA	Alkaline, Kidder	
400	Chase et al. (2020)	Fritz et al. (1993)	ANTE	Antelope, Sask	
401	Chase et al. (2020)	Fritz et al. (1993)	AROM	Aroma, Sask	
402	Chase et al. (2020)	Fritz et al. (1993)	BASI	Basin, Sask	
403	Chase et al. (2020)	Fritz et al. (1993)	BITI	Bitter, Day CO.	
404	Chase et al. (2020)	Fritz et al. (1993)	BITT	Bitter, Sask	
405	Chase et al. (2020)	Fritz et al. (1993)	BOUC	Boucher, Sask	
406	Chase et al. (2020)	Fritz et al. (1993)	BQUI	Big Quill, Sask	
408	Chase et al. (2020)	Fritz et al. (1993)	COLD	Coldwater, McIntosh Co	
409	Chase et al. (2020)	Fritz et al. (1993)	COON	Coon, Nelson Co	
410	Chase et al. (2020)	Fritz et al. (1993)	DEAD	Deadmoose, Sask	
411	Chase et al. (2020)	Fritz et al. (1993)	DEVI	Devils, Ramsey Co	
412	Chase et al. (2020)	Fritz et al. (1993)	ECKL	Eckelson, Barnes Co	
413	Chase et al. (2020)	Fritz et al. (1993)	ECOT	E. Coteau, Sask	
414	Chase et al. (2020)	Fritz et al. (1993)	EDEV	E. Devils, Ramsey Co.	
415	Chase et al. (2020)	Fritz et al. (1993)	ELBW	Elbow, Benson Co.	
416	Chase et al. (2020)	Fritz et al. (1993)	ESTU	E. Stump, Nelson Co.	
417	Chase et al. (2020)	Fritz et al. (1993)	FIFE	Fife, Sask	
418	Chase et al. (2020)	Fritz et al. (1993)	FISH	Fishing, Sask	
419	Chase et al. (2020)	Fritz et al. (1993)	FREE	Free People, Benson Co.	
420	Chase et al. (2020)	Fritz et al. (1993)	GEOR	George, Kidder Co.	
421	Chase et al. (2020)	Fritz et al. (1993)	HAZL	Hazelden, Day Co.	

Table G. part 1: *Continued*

Sequence # (sample #)	Reference	Original_source	sample_name	Lake
422	Chase et al. (2020)	Fritz et al. (1993)	HERM	Herman, Lake Co.
423	Chase et al. (2020)	Fritz et al. (1993)	HORS	Horseshoe, Eddy Co.
424	Chase et al. (2020)	Fritz et al. (1993)	HUMB	Humbolt, Sask
425	Chase et al. (2020)	Fritz et al. (1993)	ISOB	Isabel, Kidder Co.
426	Chase et al. (2020)	Fritz et al. (1993)	LENO	Lenore, Sask
427	Chase et al. (2020)	Fritz et al. (1993)	LONG	Long, Benson Co.
428	Chase et al. (2020)	Fritz et al. (1993)	MADI	Madison, Lake Co.
429	Chase et al. (2020)	Fritz et al. (1993)	MANI	Manito, Sask
430	Chase et al. (2020)	Fritz et al. (1993)	MEDI	Medicine, Codington
431	Chase et al. (2020)	Fritz et al. (1993)	MISS	Mission Bay, Benson Co.
432	Chase et al. (2020)	Fritz et al. (1993)	MOON	Moon, Barnes Co.
433	Chase et al. (2020)	Fritz et al. (1993)	MUSK	Muskiki, Sask
434	Chase et al. (2020)	Fritz et al. (1993)	NBLA	N. Blaine, Sask
435	Chase et al. (2020)	Fritz et al. (1993)	NORD	Norden, Hamlin Co.
436	Chase et al. (2020)	Fritz et al. (1993)	OAKW	Oakwood, Brookings Co.
437	Chase et al. (2020)	Fritz et al. (1993)	OPUN	Opuntia, Sask
439	Chase et al. (2020)	Fritz et al. (1993)	POIN	Poinsett, Hamlin Co.
440	Chase et al. (2020)	Fritz et al. (1993)	PORT	Porter, Sask
441	Chase et al. (2020)	Fritz et al. (1993)	RABB	Rabbit, Sask
442	Chase et al. (2020)	Fritz et al. (1993)	REDB	Rederry, Sask
443	Chase et al. (2020)	Fritz et al. (1993)	REFL	Reflex, Sask
444	Chase et al. (2020)	Fritz et al. (1993)	ROSL	Roslyn Pond, Day Co.
445	Chase et al. (2020)	Fritz et al. (1993)	ROU1	Round, Benson Co.
446	Chase et al. (2020)	Fritz et al. (1993)	ROU2	Round, McHenry Co.
447	Chase et al. (2020)	Fritz et al. (1993)	ROY	Roy Marshall Co.
448	Chase et al. (2020)	Fritz et al. (1993)	SAYE	Sayer, Sask
449	Chase et al. (2020)	Fritz et al. (1993)	SBLA	S. Blaine, Sask
450	Chase et al. (2020)	Fritz et al. (1993)	SHIN	Shinbone, Benson Co.
451	Chase et al. (2020)	Fritz et al. (1993)	SPRG	Spring, Benson Co.
452	Chase et al. (2020)	Fritz et al. (1993)	SPRT	Sprintwood, Stutsman Co.
453	Chase et al. (2020)	Fritz et al. (1993)	STI2	Stink, Stutsman Co.
454	Chase et al. (2020)	Fritz et al. (1993)	STIN	Stink, Benson Co.
455	Chase et al. (2020)	Fritz et al. (1993)	TRAM	Tramping, Sask
456	Chase et al. (2020)	Fritz et al. (1993)	TWIN	Twin, Benson Co.
457	Chase et al. (2020)	Fritz et al. (1993)	WAKA	Wakaw, Sask
458	Chase et al. (2020)	Fritz et al. (1993)	WALD	Waldea, Sask
459	Chase et al. (2020)	Fritz et al. (1993)	WAUB	Waubay, Day Co.
460	Chase et al. (2020)	Fritz et al. (1993)	WHIT	Whiteshore, Sask

Table G. part 1: *Continued*

Sequence # (sample #)	Reference	Original_source	sample_name	Lake
461	Chase et al. (2020)	Fritz et al. (1993)	WILL	Willowbunch, Sask
462	Chase et al. (2020)	Fritz et al. (1993)	WSTU	W. Stump, Nelson Co.
473	Chase et al. (2020)	Mohamed et al. (2014)	3	Lower Lake, Wadi El Raiyan
474	Chase et al. (2020)	Mohamed et al. (2014)	7	Lower Lake, Wadi El Raiyan
475	Chase et al. (2020)	Mohamed et al. (2014)	9	Lower Lake, Wadi El Raiyan
476	Chase et al. (2020)	Mohamed et al. (2014)	12	Lower Lake, Wadi El Raiyan
477	Chase et al. (2020)	Mohamed et al. (2014)	15	Lower Lake, Wadi El Raiyan
478	Chase et al. (2020)	Mohamed et al. (2014)	16	Lower Lake, Wadi El Raiyan
479	Chase et al. (2020)	Mohamed et al. (2014)	17	Lower Lake, Wadi El Raiyan
480	Chase et al. (2020)	Mohamed et al. (2014)	18	Lower Lake, Wadi El Raiyan
481	Chase et al. (2020)	Mohamed et al. (2014)	19	Lower Lake, Wadi El Raiyan
482	Chase et al. (2020)	Mohamed et al. (2014)	20	Lower Lake, Wadi El Raiyan
483	Chase et al. (2020)	Mohamed et al. (2014)	21	Lower Lake, Wadi El Raiyan
484	Chase et al. (2020)	Mohamed et al. (2014)	22	Lower Lake, Wadi El Raiyan
485	Chase et al. (2020)	Mohamed et al. (2014)	23	Lower Lake, Wadi El Raiyan
486	Chase et al. (2020)	Mohamed et al. (2014)	32	Upper Lake, Wadi El Raiyan
487	Chase et al. (2020)	Mohamed et al. (2014)	33	Upper Lake, Wadi El Raiyan
488	Chase et al. (2020)	Mohamed et al. (2014)	34	Upper Lake, Wadi El Raiyan
489	Chase et al. (2020)	Mohamed et al. (2014)	35	Upper Lake, Wadi El Raiyan
490	Chase et al. (2020)	Mohamed et al. (2014)	36	Upper Lake, Wadi El Raiyan
522	Hirst (1995)	Hirst (1995)	GE Spring	Goodenough Lake (March)
523	Hirst (1995)	Hirst (1995)	LSZ 1A	Goodenough Lake (March)
524	Hirst (1995)	Hirst (1995)	LSZ 1B	Goodenough Lake (March)
525	Hirst (1995)	Hirst (1995)	GET1	Goodenough Lake (March)
526	Hirst (1995)	Hirst (1995)	C.LAKE	Goodenough Lake (March)
527	Hirst (1995)	Hirst (1995)	GE SITE2	Goodenough Lake (May)
528	Hirst (1995)	Hirst (1995)	GE SITE3	Goodenough Lake (May)
529	Hirst (1995)	Hirst (1995)	GE SITE4	Goodenough Lake (May)
530	Hirst (1995)	Hirst (1995)	GE SITE5	Goodenough Lake (May)
531	Hirst (1995)	Hirst (1995)	LSZ 1	Goodenough Lake (August)
532	Hirst (1995)	Hirst (1995)	LSZ 1A	Goodenough Lake (August)
533	Hirst (1995)	Hirst (1995)	LSZ 2	Goodenough Lake (August)
534	Hirst (1995)	Hirst (1995)	LSZ 3	Goodenough Lake (August)
535	Hirst (1995)	Hirst (1995)	LSZ 3A	Goodenough Lake (August)
536	Hirst (1995)	Hirst (1995)	LSZ 5	Goodenough Lake (August)
537	Hirst (1995)	Hirst (1995)	GET2	Goodenough Lake (August)
538	Hirst (1995)	Hirst (1995)	GET5	Goodenough Lake (August)
539	Hirst (1995)	Hirst (1995)	GE LAKE	Goodenough Lake (August)

Table G. part 1: *Continued*

Sequence # (sample #)	Reference	Original_source	sample_name	Lake
540	Hirst (1995)	Hirst (1995)	GE/SSITE1	Goodenough Lake (September)
541	Hirst (1995)	Hirst (1995)	GESITEA	Goodenough Lake (September)
542	Hirst (1995)	Hirst (1995)	GESITEB	Goodenough Lake (September)
543	Hirst (1995)	Hirst (1995)	T2P3	Goodenough Lake (September)
544	Hirst (1995)	Hirst (1995)	T4P3	Goodenough Lake (September)
545	Hirst (1995)	Hirst (1995)	GELAKE1	Goodenough Lake (September)
546	Hirst (1995)	Hirst (1995)	GELAKE2	Goodenough Lake (September)
547	Hirst (1995)	Hirst (1995)	GE/SW	Goodenough Lake (September)
548	Hirst (1995)	Hirst (1995)	GET7	Goodenough Lake (September)
549	Hirst (1995)	Hirst (1995)	T7SEEP	Goodenough Lake (September)
550	Hirst (1995)	Hirst (1995)	L.SEEPPIT	Goodenough Lake (September)
551	Hirst (1995)	Hirst (1995)	GE/SS.W.	Goodenough Lake (September)
552	Hirst (1995)	Hirst (1995)	GECORE3	Goodenough Lake (September)
553	Hirst (1995)	Hirst (1995)	GECORE6	Goodenough Lake (September)
554	Hirst (1995)	Hirst (1995)	GE/SLAKE	Goodenough Lake (September)
555	Hirst (1995)	Hirst (1995)	LCA1	Last Chance Lake
556	Hirst (1995)	Hirst (1995)	LCA2	Last Chance Lake
557	Hirst (1995)	Hirst (1995)	LC ESKER	Last Chance Lake
558	Hirst (1995)	Hirst (1995)	LC FAR END	Last Chance Lake
559	Hirst (1995)	Hirst (1995)	LC/M LAKE	Last Chance Lake
560	Hirst (1995)	Hirst (1995)	LC SPRING	Last Chance Lake
561	Hirst (1995)	Hirst (1995)	LC LAKE	Last Chance Lake
562	Hirst (1995)	Hirst (1995)	LCP1	Last Chance Lake
563	Hirst (1995)	Hirst (1995)	P1-SURF	Last Chance Lake
564	Hirst (1995)	Hirst (1995)	P1-LOW	Last Chance Lake
565	Hirst (1995)	Hirst (1995)	LCP2	Last Chance Lake
566	Hirst (1995)	Hirst (1995)	LCA3 SP	Last Chance Lake
567	Hirst (1995)	Hirst (1995)	LCA3	Last Chance Lake
568	Hirst (1995)	Hirst (1995)	LCP3 M.P.	Last Chance Lake
569	Hirst (1995)	Hirst (1995)	LCP4	Last Chance Lake
570	Hirst (1995)	Hirst (1995)	LCA5 W.P.	Last Chance Lake
571	Hirst (1995)	Hirst (1995)	LC ?SP	Last Chance Lake
572	Hirst (1995)	Hirst (1995)	CHASM SP	Misc.
573	Hirst (1995)	Hirst (1995)	61 CREEK (MAY)	Misc.
574	Hirst (1995)	Hirst (1995)	OSOR 1	Misc.
575	Hirst (1995)	Hirst (1995)	OSOR 2	Misc.
576	Hirst (1995)	Hirst (1995)	LBLC	Misc.
577	Hirst (1995)	Hirst (1995)	61 MILE CREEK	Misc.

Table G. part 1: *Continued*

Sequence # (sample #)	Reference	Original_source	sample_name	Lake
578	Ashton & Schoeman (1983)	Ashton & Schoeman (1983)	inflow	Pretoria Salt Pan
579	Ashton & Schoeman (1983)	Ashton & Schoeman (1983)	0.00	Pretoria Salt Pan
580	Ashton & Schoeman (1983)	Ashton & Schoeman (1983)	0.25	Pretoria Salt Pan
581	Ashton & Schoeman (1983)	Ashton & Schoeman (1983)	0.50	Pretoria Salt Pan
582	Ashton & Schoeman (1983)	Ashton & Schoeman (1983)	1.00	Pretoria Salt Pan
583	Ashton & Schoeman (1983)	Ashton & Schoeman (1983)	1.50	Pretoria Salt Pan
584	Ashton & Schoeman (1983)	Ashton & Schoeman (1983)	2.00	Pretoria Salt Pan
585	Ashton & Schoeman (1983)	Ashton & Schoeman (1983)	2.50	Pretoria Salt Pan
586	Eugster (1970)	Eugster (1970)	M17.3	Lake Magadi
587	Eugster (1970)	Eugster (1970)	M17.4	Lake Magadi
588	Eugster (1970)	Eugster (1970)	M30A	Lake Magadi
589	Eugster (1970)	Eugster (1970)	M30B	Lake Magadi
590	Eugster (1970)	Eugster (1970)	M30C	Lake Magadi
591	Eugster (1970)	Eugster (1970)	M35	Lake Magadi
592	Eugster (1970)	Eugster (1970)	M39	Lake Magadi
593	Eugster (1970)	Eugster (1970)	M65	Lake Magadi
594	Eugster (1970)	Eugster (1970)	M68	Lake Magadi
595	Eugster (1970)	Eugster (1970)	M69	Lake Magadi
596	Eugster (1970)	Eugster (1970)	M80	Lake Magadi
597	Eugster (1970)	Eugster (1970)	M87B	Lake Magadi
598	Eugster (1970)	Eugster (1970)	M91	Lake Magadi
599	Eugster (1970)	Eugster (1970)	M218	Lake Magadi
600	Eugster (1970)	Eugster (1970)	M RLH	Lake Magadi
601	Eugster (1970)	Eugster (1970)	Natron A	Lake Magadi
602	Eugster (1970)	Eugster (1970)	Natron B	Lake Magadi
603	Jones, Eugster, Rettig (1977)	Jones, Eugster, Rettig (1977)	Little Magadi Lake, M507	Lake Magadi
604	Jones, Eugster, Rettig (1977)	Jones, Eugster, Rettig (1977)	Little Magadi Lake, M1016	Lake Magadi
605	Jones, Eugster, Rettig (1977)	Jones, Eugster, Rettig (1977)	M520	Lake Magadi
606	Jones, Eugster, Rettig (1977)	Jones, Eugster, Rettig (1977)	M535	Lake Magadi
607	Jones, Eugster, Rettig (1977)	Jones, Eugster, Rettig (1977)	M536	Lake Magadi
608	Jones, Eugster, Rettig (1977)	Jones, Eugster, Rettig (1977)	M538	Lake Magadi
609	Jones, Eugster, Rettig (1977)	Jones, Eugster, Rettig (1977)	M540	Lake Magadi
610	Jones, Eugster, Rettig (1977)	Jones, Eugster, Rettig (1977)	M557	Lake Magadi
611	Jones, Eugster, Rettig (1977)	Jones, Eugster, Rettig (1977)	M664	Lake Magadi
612	Jones, Eugster, Rettig (1977)	Jones, Eugster, Rettig (1977)	M710	Lake Magadi
613	Jones, Eugster, Rettig (1977)	Jones, Eugster, Rettig (1977)	M1028	Lake Magadi
614	Jones, Eugster, Rettig (1977)	Jones, Eugster, Rettig (1977)	M1029	Lake Magadi
615	Imhoff et al. (1979)	Imhoff et al. (1979)	Gabara	Gabara

Table G. part 1: *Continued*

Sequence # (sample #)	Reference	Original_source	sample_name	Lake
616	Imhoff et al. (1979)	Imhoff et al. (1979)	Hamara	Hamara
617	Imhoff et al. (1979)	Imhoff et al. (1979)	Zugm	Zugm
618	Imhoff et al. (1979)	Imhoff et al. (1979)	Gaar	Gaar
619	Imhoff et al. (1979)	Imhoff et al. (1979)	Muluk	Muluk
620	Imhoff et al. (1979)	Imhoff et al. (1979)	Rizunia	Rizunia
621	Melack & Kilham (1974)	Melack & Kilham (1974)	Nakuru	Nakuru
622	Melack & Kilham (1974)	Melack & Kilham (1974)	Elmenteita	Elmenteita
623	Melack & Kilham (1974)	Melack & Kilham (1974)	Magad	Magad
624	Melack & Kilham (1974)	Melack & Kilham (1974)	Manyara	Manyara

Table G. part 2: Aqueous chemistry database of alkaline lake waters compiled from published literature, as well as corresponding results from calculations described in chapters 2 and 3, and investigated in detail in chapter 4.

Sequence # (sample #)	area	geology	country	Temp (°C)
1	China (North Hebei)	unidentified	China	
2	China (North Hebei)	unidentified	China	
3	China (North Hebei)	unidentified	China	
4	China (Tibet)	unidentified	China	
5	China (Inner-Mongolia)	unidentified	China	
6	China (Inner-Mongolia)	unidentified	China	17.8
7	China (Inner-Mongolia)	unidentified	China	
8	China (Inner-Mongolia)	unidentified	China	
9	China (Inner-Mongolia)	unidentified	China	
10	Western Mongolia	unidentified	Mongolia	19
11	Western Mongolia	unidentified	Mongolia	
12	Western Mongolia	unidentified	Mongolia	
13	Northwestern Mongolia	unidentified	Mongolia	
14	Russia (Sourtheastarn Transbaikalia)	unidentified	Russia	
15	Turkey (eastern Anatolia)	metamorphic & volcanics	Turkey	
16	Italy (Pantelleria Island)	unidentified	Italy	26.2
17	Southern Australia	unidentified	Australia	
18	Western Australia	unidentified	Australia	
19	Western Australia	unidentified	Australia	
20	United States (California)	complex (granite, volcanics, sedimentary)	United States	12.8
21	United States (Nebraska)	unidentified	United States	15.1
22	United States (Nevada)	volcanics	United States	
23	United States (Nevada)	volcanics	United States	9.2
24	United States (Nevada)	volcanics	United States	
25	Central-West Brazil	unidentified	Brazil	38.7
26	Central-West Brazil	unidentified	Brazil	38.3
27	Central-West Brazil	unidentified	Brazil	32.2
28	Central-West Brazil	unidentified	Brazil	41.3
29	Central-West Brazil	unidentified	Brazil	34.7
30	Central-West Brazil	unidentified	Brazil	35
31	Central-West Brazil	unidentified	Brazil	42.3
32	Central-West Brazil	unidentified	Brazil	28
33	Central-West Brazil	unidentified	Brazil	36.1
34	Central-West Brazil	unidentified	Brazil	38
35	Central-West Brazil	unidentified	Brazil	31.2
36	Central-West Brazil	unidentified	Brazil	36

Table G. part 2: *Continued*

Sequence # (sample #)	area	geology	country	Temp (°C)
37	Central-West Brazil	unidentified	Brazil	34.3
38	Central-West Brazil	unidentified	Brazil	32
39	Central-West Brazil	unidentified	Brazil	36
40	Central-West Brazil	unidentified	Brazil	35.3
41	Central-West Brazil	unidentified	Brazil	33.8
42	Western Mongolia	unidentified	Mongolia	
43	Western Mongolia	unidentified	Mongolia	
44	Western Mongolia	unidentified	Mongolia	
45	Western Mongolia	unidentified	Mongolia	
46	Western Mongolia	unidentified	Mongolia	
47	Western Mongolia	unidentified	Mongolia	
48	Western Mongolia	unidentified	Mongolia	
49	Western Mongolia	unidentified	Mongolia	
50	Western Mongolia	unidentified	Mongolia	
51	Western Mongolia	unidentified	Mongolia	
52	Western Mongolia	unidentified	Mongolia	
53	Western Mongolia	unidentified	Mongolia	
54	Western Mongolia	unidentified	Mongolia	
55	Western Mongolia	unidentified	Mongolia	
56	Western Mongolia	unidentified	Mongolia	
57	Western Mongolia	unidentified	Mongolia	
58	Western Mongolia	unidentified	Mongolia	
59	Western Mongolia	unidentified	Mongolia	
60	Western Mongolia	unidentified	Mongolia	
61	Western Mongolia	unidentified	Mongolia	
62	Western Mongolia	unidentified	Mongolia	
63	Western Mongolia	unidentified	Mongolia	
64	Western Mongolia	unidentified	Mongolia	
65	Western Mongolia	unidentified	Mongolia	
66	Chad	unidentified	Chad	
67	Chad	unidentified	Chad	
68	Chad	unidentified	Chad	
69	Chad	unidentified	Chad	
70	Chad	unidentified	Chad	
71	Chad	unidentified	Chad	
72	Chad	unidentified	Chad	
73	Chad	unidentified	Chad	
74	Chad	unidentified	Chad	

Table G. part 2: *Continued*

Sequence # (sample #)	area	geology	country	Temp (°C)
75	Chad	unidentified	Chad	
76	Chad	unidentified	Chad	
77	Chad	unidentified	Chad	
78	Chad	unidentified	Chad	
79	Chad	unidentified	Chad	
80	Chad	unidentified	Chad	
81	Chad	unidentified	Chad	
82	Chad	unidentified	Chad	
83	Chad	unidentified	Chad	
84	Chad	unidentified	Chad	
85	Chad	unidentified	Chad	
86	Tanzania	volcanics	Tanzania	26
87	Tanzania	volcanics	Tanzania	16
88	Tanzania	volcanics	Tanzania	22
89	Tanzania	volcanics	Tanzania	19
90	Tanzania	volcanics	Tanzania	19
91	Tanzania	volcanics	Tanzania	17
92	Tanzania	volcanics	Tanzania	18
93	Tanzania	volcanics	Tanzania	17
94	Tanzania	volcanics	Tanzania	24
95	Tanzania	volcanics	Tanzania	24
96	Tanzania	volcanics	Tanzania	22
97	Tanzania	volcanics	Tanzania	19
98	Tanzania	volcanics	Tanzania	24
99	Tanzania	volcanics	Tanzania	22
100	Tanzania	volcanics	Tanzania	27
101	Tanzania	volcanics	Tanzania	24
102	Tanzania	volcanics	Tanzania	19
103	Tanzania	volcanics	Tanzania	21
104	Tanzania	volcanics	Tanzania	
105	Tanzania	volcanics	Tanzania	17
106	Tanzania	volcanics	Tanzania	19
107	Tanzania	volcanics	Tanzania	19
108	Tanzania	volcanics	Tanzania	18
109	Tanzania	volcanics	Tanzania	17
110	Tanzania	volcanics	Tanzania	18
111	Tanzania	volcanics	Tanzania	19
115	Tanzania	volcanics	Tanzania	36

Table G. part 2: *Continued*

Sequence # (sample #)	area	geology	country	Temp (°C)
116	Tanzania	volcanics	Tanzania	
117	Tanzania	volcanics	Tanzania	22
118	Tanzania	volcanics	Tanzania	48
119	Tanzania	volcanics	Tanzania	45
120	Tanzania	volcanics	Tanzania	
121	Tanzania	volcanics	Tanzania	24
125	Tanzania	volcanics	Tanzania	
126	Tanzania	volcanics	Tanzania	
127	Tanzania	volcanics	Tanzania	21
128	Tanzania	volcanics	Tanzania	21
129	Tanzania	volcanics	Tanzania	23
130	Tanzania	volcanics	Tanzania	19.5
131	Tanzania	volcanics	Tanzania	24
132	Tanzania	volcanics	Tanzania	21
133	Tanzania	volcanics	Tanzania	26
134	Tanzania	volcanics	Tanzania	22
135	Tanzania	volcanics	Tanzania	23
136	Tanzania	volcanics	Tanzania	
137	Tanzania	volcanics	Tanzania	19
138	Tanzania	volcanics	Tanzania	21
139	Bolivia	unidentified	Bolivia	5
140	Bolivia	unidentified	Bolivia	1
141	Bolivia	unidentified	Bolivia	2
142	Bolivia	volcanic & sedimentary	Bolivia	8
143	Bolivia	unidentified	Bolivia	1
144	Bolivia	unidentified	Bolivia	4
145	Bolivia	intermediate volcanics (dacite)	Bolivia	6
146	Bolivia	unidentified	Bolivia	8
147	Bolivia	unidentified	Bolivia	6
148	Bolivia	intermediate volcanics (dacite)	Bolivia	5
149	Bolivia	intermediate volcanics (dacite)	Bolivia	8
150	Bolivia	intermediate volcanics (dacite)	Bolivia	6
151	Bolivia	intermediate volcanics (dacite)	Bolivia	10
152	Bolivia	intermediate volcanics (dacite)	Bolivia	21
153	Bolivia	intermediate volcanics (dacite)	Bolivia	1
154	Bolivia	intermediate volcanics (dacite)	Bolivia	4
155	Bolivia	intermediate volcanics (dacite)	Bolivia	6
156	Bolivia	intermediate volcanics (dacite)	Bolivia	5

Table G. part 2: *Continued*

Sequence # (sample #)	area	geology	country	Temp (°C)
157	Bolivia	intermediate volcanics (dacite)	Bolivia	5
158	Bolivia	intermediate volcanics (dacite)	Bolivia	5
159	Bolivia	intermediate volcanics (dacite)	Bolivia	10
160	Bolivia	intermediate volcanics (dacite)	Bolivia	1
161	Bolivia	intermediate volcanics (dacite)	Bolivia	1
162	Bolivia	intermediate volcanics (dacite)	Bolivia	10
163	Bolivia	intermediate volcanics (dacite)	Bolivia	10
164	Bolivia	intermediate volcanics (dacite)	Bolivia	10
165	Bolivia	intermediate volcanics (dacite)	Bolivia	15
166	Bolivia	intermediate volcanics (dacite)	Bolivia	10
167	Bolivia	intermediate volcanics (dacite)	Bolivia	10
168	Bolivia	intermediate volcanics (dacite)	Bolivia	7
169	Bolivia	intermediate volcanics (dacite)	Bolivia	6
170	Bolivia	intermediate volcanics (dacite)	Bolivia	4.5
171	Bolivia	intermediate volcanics (dacite)	Bolivia	5
172	Bolivia	intermediate volcanics (dacite)	Bolivia	5
173	Bolivia	intermediate volcanics (dacite)	Bolivia	5
174	Bolivia	intermediate volcanics (dacite)	Bolivia	10
175	Bolivia	intermediate volcanics (dacite)	Bolivia	6
176	Bolivia	intermediate volcanics (dacite)	Bolivia	12
177	Bolivia	intermediate volcanics (dacite)	Bolivia	5
178	Bolivia	intermediate volcanics (dacite)	Bolivia	5
179	Bolivia	intermediate volcanics (dacite)	Bolivia	25
180	Bolivia	intermediate volcanics (dacite)	Bolivia	5
181	Bolivia	intermediate volcanics (dacite)	Bolivia	6
182	Bolivia	intermediate volcanics (dacite)	Bolivia	6
183	Bolivia	intermediate volcanics (dacite)	Bolivia	8
184	Bolivia	intermediate volcanics (dacite)	Bolivia	3
185	Bolivia	intermediate volcanics (dacite)	Bolivia	5.5
186	Bolivia	intermediate volcanics (dacite)	Bolivia	4
187	Bolivia	intermediate volcanics (dacite)	Bolivia	5
188	Bolivia	intermediate volcanics (dacite)	Bolivia	5
189	Bolivia	intermediate volcanics (dacite)	Bolivia	5
190	Bolivia	intermediate volcanics (dacite)	Bolivia	2.8
191	Bolivia	intermediate volcanics (dacite)	Bolivia	4
192	Bolivia	intermediate volcanics (dacite)	Bolivia	8.8
193	Bolivia	intermediate volcanics (dacite)	Bolivia	6.2
194	Bolivia	intermediate volcanics (dacite)	Bolivia	0

Table G. part 2: *Continued*

Sequence # (sample #)	area	geology	country	Temp (°C)
195	Bolivia	intermediate volcanics (dacite)	Bolivia	0.7
196	Bolivia	intermediate volcanics (dacite)	Bolivia	5
197	Bolivia	intermediate volcanics (dacite)	Bolivia	2.5
199	Turkey (eastern Anatolia)	metamorphic & volcanics	Turkey	
200	Turkey (eastern Anatolia)	metamorphic & volcanics	Turkey	
201	Turkey (eastern Anatolia)	metamorphic & volcanics	Turkey	
202	Turkey (eastern Anatolia)	metamorphic & volcanics	Turkey	
203	Turkey (eastern Anatolia)	metamorphic & volcanics	Turkey	
204	Turkey (eastern Anatolia)	metamorphic & volcanics	Turkey	
205	Turkey (eastern Anatolia)	metamorphic & volcanics	Turkey	
206	Turkey (eastern Anatolia)	metamorphic & volcanics	Turkey	
207	Turkey (eastern Anatolia)	metamorphic & volcanics	Turkey	
208	Austria	sedimentary	Austria	
209	Bolivia	intermediate volcanics (dacite)	Bolivia	
210	Bolivia	intermediate volcanics (dacite)	Bolivia	
211	Bolivia	intermediate volcanics (dacite)	Bolivia	
212	Bolivia	intermediate volcanics (dacite)	Bolivia	
213	Bolivia	intermediate volcanics (dacite)	Bolivia	
214	Bolivia	intermediate volcanics (dacite)	Bolivia	
215	Bolivia	intermediate volcanics (dacite)	Bolivia	
216	Bolivia	intermediate volcanics (dacite)	Bolivia	
217	Bolivia	intermediate volcanics (dacite)	Bolivia	
218	Bolivia	intermediate volcanics (dacite)	Bolivia	
219	Bolivia	intermediate volcanics (dacite)	Bolivia	
220	Bolivia	intermediate volcanics (dacite)	Bolivia	
221	Bolivia	intermediate volcanics (dacite)	Bolivia	
222	Bolivia	intermediate volcanics (dacite)	Bolivia	
223	Bolivia	intermediate volcanics (dacite)	Bolivia	
224	Bolivia	intermediate volcanics (dacite)	Bolivia	
225	0	unidentified	Canada	
226	0	unidentified	Canada	
227	0	unidentified	Canada	
228	0	unidentified	Canada	
229	0	unidentified	Canada	
230	0	unidentified	Canada	
232	0	unidentified	Canada	
234	0	unidentified	Canada	
235	0	unidentified	Canada	

Table G. part 2: *Continued*

Sequence # (sample #)	area	geology	country	Temp (°C)
236	0	unidentified	Canada	
237	0	unidentified	Canada	
238	0	unidentified	Canada	
239	0	unidentified	Canada	
240	0	unidentified	Canada	
241	0	unidentified	Canada	
242	0	unidentified	Canada	
243	0	unidentified	Canada	
244	0	unidentified	Canada	
245	0	unidentified	Canada	
246	0	unidentified	Canada	
247	0	unidentified	Canada	
248	0	unidentified	Canada	
249	0	unidentified	Canada	
250	0	unidentified	Canada	
251	0	unidentified	Canada	
252	0	unidentified	Canada	
253	0	unidentified	Canada	
254	Canada	basaltic*	Canada	
255	Canada	basaltic*	Canada	
256	Canada	basaltic*	Canada	
257	Canada	basaltic*	Canada	
258	0	unidentified	Canada	
259	0	unidentified	Canada	
260	0	unidentified	Canada	
261	0	unidentified	Canada	
262	0	unidentified	Canada	
263	0	unidentified	Canada	
264	0	unidentified	Canada	
265	0	unidentified	Canada	
266	0	unidentified	Canada	
267	0	unidentified	Canada	
268	Canada	unidentified	Canada	
269	Canada	unidentified	Canada	
271	United States	basaltic	United States	
272	United States	basaltic	United States	13.33
274	United States	basaltic	United States	
275	United States	basaltic	United States	0.56

Table G. part 2: *Continued*

Sequence # (sample #)	area	geology	country	Temp (°C)
278	United States	basaltic	United States	18.89
283	United States	basaltic	United States	21.67
284	United States	basaltic	United States	6.67
285	United States	basaltic	United States	
287	0	unidentified	United States	
288	0	unidentified	United States	1.67
289	0	unidentified	United States	25.56
290	0	unidentified	United States	
291	0	unidentified	United States	18.89
292	0	unidentified	United States	27.78
293	0	unidentified	United States	22.22
294	0	unidentified	United States	17.22
295	0	unidentified	United States	21.67
296	0	unidentified	United States	12.78
297	0	unidentified	United States	
298	0	unidentified	United States	
299	0	unidentified	United States	16.67
300	0	unidentified	United States	15
301	0	unidentified	United States	18.33
302	0	unidentified	United States	22.22
303	0	unidentified	Canada	
304	0	unidentified	Canada	
306	0	unidentified	Canada	
307	0	unidentified	Canada	
308	0	unidentified	Canada	
309	0	unidentified	Canada	
310	0	unidentified	Canada	
311	0	unidentified	Canada	
313	0	unidentified	Canada	
314	0	unidentified	Canada	
315	0	unidentified	Canada	
316	0	unidentified	Canada	
317	0	unidentified	Canada	
319	0	unidentified	Canada	
320	0	unidentified	Canada	
321	0	unidentified	Canada	
322	0	unidentified	Canada	
323	0	unidentified	Canada	

Table G. part 2: *Continued*

Sequence # (sample #)	area	geology	country	Temp (°C)
325	0	unidentified	Canada	
329	0	unidentified	Canada	
330	0	unidentified	Canada	
331	0	unidentified	Canada	
332	0	unidentified	Canada	
333	0	unidentified	Canada	
334	0	unidentified	Canada	
335	0	unidentified	Canada	
336	0	unidentified	Canada	
337	0	unidentified	Canada	
338	0	unidentified	Canada	
340	0	unidentified	Canada	
341	0	unidentified	Canada	
342	0	unidentified	Canada	
343	0	unidentified	Canada	
345	0	unidentified	Canada	
346	0	unidentified	Canada	
347	0	unidentified	Canada	
348	0	unidentified	Canada	
349	0	unidentified	Canada	
352	0	unidentified	Canada	
353	0	unidentified	Canada	
356	USA (California)	metasedimentary	United States	
357	USA (California)	metasedimentary	United States	
358	USA (California)	metasedimentary	United States	
359	USA (California)	complex (granite, volcanics, sedimentary)	United States	16.67
361	0	unidentified	United States	
368	0	unidentified	United States	62.22
370	0	complex (rhyolitic flows, volcanics, intrusives, sedimentary)	United States	
371	0	complex (rhyolitic flows, volcanics, intrusives, sedimentary)	United States	
372	0	complex (rhyolitic flows, volcanics, intrusives, sedimentary)	United States	17.22
373	USA (California)	volcanic	United States	
374	USA (California)	volcanic	United States	16.67
375	0	unidentified	United States	
376	0	unidentified	United States	
377	USA (California)	volcanic	United States	
378	USA (California)	volcanic	United States	
381	0	unidentified	United States	

Table G. part 2: *Continued*

Sequence # (sample #)	area	geology	country	Temp (°C)
382	0	unidentified	United States	
383	USA (Oregon)	basaltic	United States	6.67
384	USA (Oregon)	basaltic	United States	18.33
385	0	unidentified	United States	0
386	USA (California)	complex (igneous, metamorphic, sedimentary)	United States	8.89
387	0	unidentified	United States	47.78
388	0	unidentified	United States	56.67
389	0	unidentified	United States	16.11
390	0	unidentified	United States	60
392	0	unidentified	United States	2.78
393	0	unidentified	United States	1.67
394	0	unidentified	United States	10
395	0	unidentified	United States	
396	0	unidentified	United States	
397	0	unidentified	United States	
398	0	unidentified	United States	
399	0	unidentified	United States	
400	0	unidentified	Canada	
401	0	unidentified	Canada	
402	0	unidentified	Canada	
403	0	unidentified	United States	
404	0	unidentified	Canada	
405	0	unidentified	Canada	
406	0	unidentified	Canada	
408	0	unidentified	United States	
409	0	unidentified	United States	
410	0	unidentified	Canada	
411	0	unidentified	United States	
412	0	unidentified	United States	
413	0	unidentified	Canada	
414	0	unidentified	United States	
415	0	unidentified	United States	
416	0	unidentified	United States	
417	0	unidentified	Canada	
418	0	unidentified	Canada	
419	0	unidentified	United States	
420	0	unidentified	United States	
421	0	unidentified	United States	

Table G. part 2: *Continued*

Sequence # (sample #)	area	geology	country	Temp (°C)
422	0	unidentified	United States	
423	0	unidentified	United States	
424	0	unidentified	Canada	
425	0	unidentified	United States	
426	0	unidentified	Canada	
427	0	unidentified	United States	
428	0	unidentified	United States	
429	0	unidentified	United States	
430	0	unidentified	United States	
431	0	unidentified	United States	
432	0	unidentified	United States	
433	0	unidentified	Canada	
434	0	unidentified	Canada	
435	0	unidentified	United States	
436	0	unidentified	United States	
437	0	unidentified	Canada	
439	0	unidentified	United States	
440	0	unidentified	Canada	
441	0	unidentified	Canada	
442	0	unidentified	Canada	
443	0	unidentified	Canada	
444	0	unidentified	United States	
445	0	unidentified	United States	
446	0	unidentified	United States	
447	0	unidentified	United States	
448	0	unidentified	Canada	
449	0	unidentified	Canada	
450	0	unidentified	United States	
451	0	unidentified	United States	
452	0	unidentified	United States	
453	0	unidentified	United States	
454	0	unidentified	United States	
455	0	unidentified	Canada	
456	0	unidentified	United States	
457	0	unidentified	Canada	
458	0	unidentified	Canada	
459	0	unidentified	United States	
460	0	unidentified	Canada	

Table G. part 2: *Continued*

Sequence # (sample #)	area	geology	country	Temp (°C)
461	0	unidentified	Canada	
462	0	unidentified	United States	
473	Egypt	sedimentary (limestones, shales, evaporites)	Egypt	30.4
474	Egypt	sedimentary (limestones, shales, evaporites)	Egypt	31.4
475	Egypt	sedimentary (limestones, shales, evaporites)	Egypt	31.1
476	Egypt	sedimentary (limestones, shales, evaporites)	Egypt	32.7
477	Egypt	sedimentary (limestones, shales, evaporites)	Egypt	29.8
478	Egypt	sedimentary (limestones, shales, evaporites)	Egypt	29
479	Egypt	sedimentary (limestones, shales, evaporites)	Egypt	30.3
480	Egypt	sedimentary (limestones, shales, evaporites)	Egypt	29.9
481	Egypt	sedimentary (limestones, shales, evaporites)	Egypt	29.9
482	Egypt	sedimentary (limestones, shales, evaporites)	Egypt	30.7
483	Egypt	sedimentary (limestones, shales, evaporites)	Egypt	30.6
484	Egypt	sedimentary (limestones, shales, evaporites)	Egypt	28.6
485	Egypt	sedimentary (limestones, shales, evaporites)	Egypt	28.9
486	Egypt	sedimentary (limestones, shales, evaporites)	Egypt	27.2
487	Egypt	sedimentary (limestones, shales, evaporites)	Egypt	29.7
488	Egypt	sedimentary (limestones, shales, evaporites)	Egypt	32.4
489	Egypt	sedimentary (limestones, shales, evaporites)	Egypt	27.6
490	Egypt	sedimentary (limestones, shales, evaporites)	Egypt	30
522	Canada	basaltic*	Canada	4.5
523	Canada	basaltic*	Canada	0
524	Canada	basaltic*	Canada	0
525	Canada	basaltic*	Canada	0
526	Canada	basaltic*	Canada	0
527	Canada	basaltic*	Canada	7
528	Canada	basaltic*	Canada	7
529	Canada	basaltic*	Canada	7
530	Canada	basaltic*	Canada	7
531	Canada	basaltic*	Canada	16
532	Canada	basaltic*	Canada	17.9
533	Canada	basaltic*	Canada	18
534	Canada	basaltic*	Canada	16
535	Canada	basaltic*	Canada	18.8
536	Canada	basaltic*	Canada	22.4
537	Canada	basaltic*	Canada	12
538	Canada	basaltic*	Canada	15
539	Canada	basaltic*	Canada	17

Table G. part 2: *Continued*

Sequence # (sample #)	area	geology	country	Temp (°C)
540	Canada	basaltic*	Canada	7
541	Canada	basaltic*	Canada	7
542	Canada	basaltic*	Canada	7
543	Canada	basaltic*	Canada	7
544	Canada	basaltic*	Canada	7
545	Canada	basaltic*	Canada	7
546	Canada	basaltic*	Canada	7
547	Canada	basaltic*	Canada	16.5
548	Canada	basaltic*	Canada	11
549	Canada	basaltic*	Canada	13
550	Canada	basaltic*	Canada	9
551	Canada	basaltic*	Canada	11
552	Canada	basaltic*	Canada	11
553	Canada	basaltic*	Canada	14
554	Canada	basaltic*	Canada	12
555	Canada	basaltic*	Canada	0
556	Canada	basaltic*	Canada	0
557	Canada	basaltic*	Canada	0
558	Canada	basaltic*	Canada	0
559	Canada	basaltic*	Canada	18
560	Canada	basaltic*	Canada	11.8
561	Canada	basaltic*	Canada	16
562	Canada	basaltic*	Canada	11.5
563	Canada	basaltic*	Canada	11.5
564	Canada	basaltic*	Canada	11.5
565	Canada	basaltic*	Canada	11
566	Canada	basaltic*	Canada	8
567	Canada	basaltic*	Canada	15
568	Canada	basaltic*	Canada	20
569	Canada	basaltic*	Canada	11
570	Canada	basaltic*	Canada	16
571	Canada	basaltic*	Canada	11
572	Canada	basaltic*	Canada	7
573	Canada	basaltic*	Canada	7
574	Canada	basaltic*	Canada	18
575	Canada	basaltic*	Canada	17
576	Canada	basaltic*	Canada	15
577	Canada	basaltic*	Canada	15.5

Table G. part 2: *Continued*

Sequence # (sample #)	area	geology	country	Temp (°C)
578	South Africa	unidentified	South Africa	25
579	South Africa	unidentified	South Africa	25
580	South Africa	unidentified	South Africa	25
581	South Africa	unidentified	South Africa	25
582	South Africa	unidentified	South Africa	25
583	South Africa	unidentified	South Africa	25
584	South Africa	unidentified	South Africa	25
585	South Africa	unidentified	South Africa	25
586		unidentified	Kenya	28
587		unidentified	Kenya	26
588		unidentified	Kenya	31
589		unidentified	Kenya	26
590		unidentified	Kenya	27
591		unidentified	Kenya	52
592		unidentified	Kenya	34
593		unidentified	Kenya	34
594		unidentified	Kenya	36
595		unidentified	Kenya	41
596		unidentified	Kenya	27
597		unidentified	Kenya	26
598		unidentified	Kenya	39
599		unidentified	Kenya	
600		unidentified	Kenya	
601		unidentified	Kenya	
602		unidentified	Kenya	
603		unidentified	Kenya	
604		unidentified	Kenya	
605		unidentified	Kenya	
606		unidentified	Kenya	
607		unidentified	Kenya	
608		unidentified	Kenya	
609		unidentified	Kenya	
610		unidentified	Kenya	
611		unidentified	Kenya	
612		unidentified	Kenya	
613		unidentified	Kenya	
614		unidentified	Kenya	
615		unidentified	Egypt	

Table G. part 2: *Continued*

Sequence # (sample #)	area	geology	country	Temp (°C)
616		unidentified	Egypt	
617		unidentified	Egypt	
618		unidentified	Egypt	
619		unidentified	Egypt	
620		unidentified	Egypt	
621		unidentified	Kenya	
622		unidentified	Kenya	
623		unidentified	Tanzania	
624		unidentified	Tanzania	

Table G. part 3: Aqueous chemistry database of alkaline lake waters compiled from published literature, as well as corresponding results from calculations described in chapters 2 and 3, and investigated in detail in chapter 4.

Sequence # (sample #)	pH	Carbonate alkalinity mmol/kg as CaCO3	Na+ mmol/kg	K+ mmol/kg	Mg++ mmol/kg	Ca++ mmol/kg	Cl- mmol/kg	SO4-- mmol/kg	ΣPO4 mmol/kg	SiO2(aq) mmol/kg	CO3-- (DIC) mmol/kg
1	9.4	9.878	100	1.00E-06	13	0.23	97	7.5	1.00E-12	1.00E-09	16
2	9.3	11.91	120	1.00E-06	8.3	0.18	93	7.7	1.00E-12	1.00E-09	20
3	9.6	32.58	160	1.00E-06	3.1	0.08	93	3.9	1.00E-12	1.00E-09	49
4	9.23	11.58	170	3.9	35	0.3	170	24	1.00E-12	1.00E-09	19
5	10.46	441.6	1900	91	4.7	0.21	830	130	1.00E-12	1.00E-09	460
6	10	339.4	1600	120	6.4	0.31	820	120	1.00E-12	1.00E-09	380
7	10.54	485.9	2200	110	6.3	0.19	1200	160	1.00E-12	1.00E-09	500
8	10.64	645.3	3400	110	3.6	0.19	1200	290	1.00E-12	1.00E-09	660
9	9.7	22.29	250	7.2	12	0.1	190	27	1.00E-12	1.00E-09	31
10	9.02	15.76	320	1.00E-06	31	1.2	240	59	1.00E-12	1.00E-09	27
11	9.06	11.72	67	1.00E-06	16	0.74	43	16	1.00E-12	1.00E-09	21
12	9.07	9.13	150	1.00E-06	18	1.2	110	28	1.00E-12	1.00E-09	16
13	9.28	40.38	220	2.3	0.59	0.21	130	7.8	1.00E-12	1.00E-09	67
14	9.8	20.53	640	1.00E-06	64	0.23	480	130	1.00E-12	1.00E-09	25
15	9.7	110.5	340	14	4.4	0.1	160	25	1.00E-12	1.00E-09	150
16	9	35.73	280	10	5.2	0.15	230	7	1.00E-12	1.00E-09	63
17	9.15	21.46	720	15	50	0.81	840	4.6	1.00E-12	1.00E-09	33
18	9.1	6.041	24	0.46	7	0.64	24	1.8	1.00E-12	1.00E-09	11
19	9.1	5.581	92	1.8	23	0.32	100	4.9	1.00E-12	1.00E-09	9.8
20	9.8	391.8	1500	45	1.7	0.1	640	140	1.00E-12	1.00E-09	460
21	10.04	221.6	1000	193	1.3	0.08	470	220	1.00E-12	1.00E-09	250
22	9.7	48.29	350	7.9	6	0.12	180	58	1.00E-12	1.00E-09	66
23	9.39	11.42	58	1.00E-06	7.2	0.21	59	1.7	1.00E-12	1.00E-09	19
24	9.45	23.87	130	4.2	5.6	0.27	63	21	1.00E-12	1.00E-09	38
25	9.4	10.75	39.4	6.106	0.09493	0.422	14.4	0.01493	0.001568	1.00E-09	18.39
26	9.8	7.407	11.92	5.777	0.01693	0.1059	1.056	0.04786	5.23E-04	1.00E-09	11.35
27	9.6	3.714	6.246	1.644	0.01694	0.1543	0.2889	0.1156	1.00E-12	1.00E-09	6.2
28	10.1	4.368	6.988	2.26	0.01198	0.1493	0.6117	0.02017	0.004394	1.00E-09	6.038
29	10	3.19	4.411	2.44	0.03264	0.0952	0.07364	0.01746	1.00E-12	1.00E-09	4.626
30	9.7	17.66	16.89	2.002	0.008258	0.1037	14.82	0.02058	1.00E-12	1.00E-09	27.2
31	10.1	11.13	14.5	2.157	0.04378	0.3817	2.602	0.1728	0.05659	1.00E-09	14.98
32	9.3	6.269	10.22	2.927	0.009914	0.2077	0.9543	0.2848	0.04895	1.00E-09	11.22
33	9.1	5.26	9.346	3.595	0.01115	0.1876	0.7759	0.08612	0.01506	1.00E-09	9.788
34	9.7	17.96	38.67	4.285	0.02477	0.1352	8.77	0.06653	0.002927	1.00E-09	27.65
35	9.3	3.134	51.75	7.388	0.3694	0.3106	4.872	0.7982	0.3829	1.00E-09	5.552
36	10	1.692	2.271	1.361	0.102	0.1358	0.07931	3.97E-03	5.23E-04	1.00E-09	2.481

Table G. part 3: *Continued*

Sequence # (sample #)	pH	Carbonate alkalinity mmol/kg as CaCO3	Na+ mmol/kg	K+ mmol/kg	Mg++ mmol/kg	Ca++ mmol/kg	Cl- mmol/kg	SO4-- mmol/kg	ΣPO4 mmol/kg	SiO2(aq) mmol/kg	CO3-- (DIC) mmol/kg
37	9.6	8.37	13.01	5.392	0.01817	0.1322	0.8948	0.1695	0.06213	1.00E-09	13.73
38	10	20.51	71.69	10.76	0.01649	0.07949	37.72	0.06363	0.08758	1.00E-09	27.41
39	9.8	5.245	10.13	2.491	0.01115	0.1237	0.4984	0.01484	0.003243	1.00E-09	8.113
40	10.2	1.425	3.363	1.567	0.01694	0.1025	0.2153	3.97E-03	1.00E-12	1.00E-09	1.93
41	9.2	5.776	10.74	2.619	0.03842	0.249	0.6202	0.04275	0.002824	1.00E-09	10.56
42	9.4	27.38	213.2	0.6362	0.5322	0.1018	159.4	5.738	1.00E-12	0.2086	43.64
43	9.4	31.2	224.7	0.5844	0.4496	0.1487	206.9	4.923	1.00E-12	0.1819	49.04
44	10.3	60.68	230.6	1.881	0.6542	0.1488	151.7	6.962	1.00E-12	0.3258	69.25
45	10.2	64.46	258.7	2.158	0.6942	0.1981	173.9	7.274	1.00E-12	0.4476	75.18
46	10.1	59.87	239	2.109	0.6539	0.1487	160.3	5.574	1.00E-12	0.4976	72.24
47	10.2	63.43	235.4	2.16	0.6131	0.1735	152.7	6.557	1.00E-12	0.5059	74.25
48	10.2	62.92	204.8	2.086	0.6138	0.1737	124.1	5.602	1.00E-12	0.4867	74.04
49	9.7	15.4	74.85	1.203	3.005	0.2995	48.59	5.76	1.00E-12	1.229	22.96
50	10	16.19	69.6	1.075	2.47	0.5992	45.11	5.282	1.00E-12	1.304	21.5
51	9.8	26.58	109.8	6.278	10.22	0.9461	59.95	21.17	1.00E-12	0.4733	36.9
52	9.8	25.19	78.11	5.137	9.785	2.244	47.52	12.51	1.00E-12	0.4707	35.44
53	9.6	23.71	83.08	5.34	10.52	1.097	35.78	20.32	1.00E-12	0.4489	35.99
54	9.1	18.63	363.7	2.197	7.679	0.3942	209.6	70.72	1.00E-12	0.03287	31.61
55	9.6	14.59	56.02	3.481	5.723	1.898	25.07	13.76	1.00E-12	0.2132	22.61
56	9	9.001	24.27	1.281	17.39	0.2199	18.08	13.45	1.00E-12	1.00E-09	16.47
57	9.1	55.16	191.3	0.4577	3.559	2.109	61.7	23.29	1.00E-12	0.1986	96.23
58	9.5	49.2	935.7	107.3	14.57	0.2865	624.5	191.6	1.00E-12	0.06848	66.75
59	9.9	27.22	59.87	4.375	7.737	0.3494	19.47	12.13	1.00E-12	1.00E-09	37.32
60	9.3	51.69	1289	36.99	10.34	0.3759	249.9	511.9	1.00E-12	0.1175	74.16
61	9.8	41.87	292.5	15.78	13.91	4.933	168.4	61.9	1.00E-12	1.00E-09	54.91
62	9.4	13.83	220.2	1.574	14.46	9.906	159	45.76	1.00E-12	0.3849	21.37
63	9.1	15.41	84.48	1.253	3.127	0.2994	54.07	5.674	1.00E-12	0.218	27.61
64	9.2	83.98	344	7.737	25.38	2.458	175.1	49.24	1.00E-12	1.00E-09	136.4
65	9	287.3	1722	23.55	75.97	4.779	1120	182.2	1.00E-12	1.00E-09	433
66	7	0.332	1.19	0.18	0.26	0.18	0.16	0.29	1.00E-12	0.31	0.8
67	6.8	0.3032	1.98	0.22	0.27	0.42	1.1	0.63	1.00E-12	0.27	0.8
68	7.1	0.4316	2.03	0.59	0.18	0.6	0.46	0.98	1.00E-12	0.62	1
69	7.9	0.8337	6.45	0.61	0.19	0.35	1.56	1.51	1.00E-12	0.73	1.7
70	9.7	2.183	30.72	2.42	0.25	0.2	1	10.82	1.00E-12	0.39	3.4
71	6.9	0.6006	2.42	0.31	0.68	0.9	0.98	1.15	1.00E-12	0.45	1.5
72	7.1	0.651	4.62	0.26	1.45	0.8	1.88	2.43	1.00E-12	0.4	1.5
73	7.1	1.175	6.75	0.88	2.25	0.7	1.38	3.58	1.00E-12	1.08	2.7
74	7.1	0.9143	8.25	0.66	1.25	1.65	4.93	3.44	1.00E-12	0.32	2.1

Table G. part 3: *Continued*

Sequence # (sample #)	pH	Carbonate alkalinity mmol/kg as CaCO3	Na+ mmol/kg	K+ mmol/kg	Mg++ mmol/kg	Ca++ mmol/kg	Cl- mmol/kg	SO4-- mmol/kg	ΣPO4 mmol/kg	SiO2(aq) mmol/kg	CO3-- (DIC) mmol/kg
75	9.3	8.098	115	7.43	0.11	0.5	23.33	27.22	1.00E-12	1.06	13.8
76	9.7	61.72	712	58.8	0.11	0.12	204.9	134.8	1.00E-12	2.99	82.8
77	9.9	97.53	1130	81.29	0.12	0.12	292.1	241.8	1.00E-12	5.58	117.5
78	9.7	314	2990	176	1.00E-09	1.00E-09	1065	378.3	1.00E-12	9.52	375.9
79	9.7	338.9	3240	191.5	1.00E-09	1.00E-09	1116	436	1.00E-12	9.15	403.5
80	10.3	13.34	72.5	6.98	0.52	0.17	12.17	1.25	1.00E-12	2.04	16.3
81	7.9	17.68	122.5	13.4	0.16	0.52	62.74	13.02	1.00E-12	3.18	35.7
82	9.8	433.5	2720	127.6	0.06	0.07	1002	206.5	1.00E-12	5.49	504.8
83	10	509	3900	222.6	0.08	0.15	618.7	691.5	1.00E-12	21.64	562.1
84	9.7	282.6	4440	198.5	0.1	0.3	639	914.5	1.00E-12	19.56	338.6
85	9.8	458	6003	555.5	0.06	0.18	2049	1203	1.00E-12	17.48	552.5
86	8.5	0.8088	2.6	0.4	0.3	0.1	0.7	0.04	1.00E-12	0.8	1.6
87	9.4	5.504	32.6	5.4	0.1	0.1	7.9	1.4	1.00E-12	1.6	9.5
88	9.4	2.68	13.4	2.3	0.02	0.1	2.7	0.6	1.00E-12	1.4	4.7
89	8.4	1.359	4.3	0.7	0.8	0.5	0.7	0.03	1.00E-12	1.4	2.7
90	8.8	1.499	6.6	0.4	0.1	0.7	1	0.2	1.00E-12	2.6	2.9
91	9.9	30.71	110	21.2	4.1	0.3	18	4.3	1.00E-12	4.9	42.3
92	9.8	16.31	117	9.5	0.04	0.1	19.6	5.8	1.00E-12	0.9	23.7
93	8.1	1.19	2.5	0.1	0.2	0.8	0.1	0.02	1.00E-12	0.4	2.4
94	8.5	2.935	0.7	0.2	0.2	0.6	0.04	0.02	1.00E-12	0.4	5.8
95	8.5	2.282	4.1	0.7	1.4	1.8	0.8	0.01	1.00E-12	1.1	4.5
96	7.6	0.8582	1.1	0.3	0.5	0.4	0.3	0.1	1.00E-12	0.8	1.8
97	7.6	2.388	3.2	1.2	1	0.7	0.7	0.1	1.00E-12	1	5
98	7.4	0.9723	0.1	0.1	0.4	0.5	0.2	0.1	1.00E-12	1.1	2.1
99	7.7	2.369	10.1	1.5	4.5	0.5	1	1.00E-06	1.00E-12	1.6	4.9
100	8	3.259	1.7	0.4	2.3	1.6	0.4	0.01	1.00E-12	1.7	6.6
101	7.9	0.8327	0.6	0.3	0.3	0.4	0.2	0.8	1.00E-12	0.9	1.7
102	7.8	1.313	2.4	0.3	0.5	0.7	0.1	0.02	1.00E-12	0.6	2.7
103	7	1.165	2.2	0.3	0.4	0.7	0.1	0.01	1.00E-12	0.6	2.8
104	7.1	1.164	1.8	0.3	0.5	0.8	0.2	0.02	1.00E-12	0.5	2.7
105	9.7	5.227	40.97	3.3	0.2	0.4	4.7	1.8	1.00E-12	1.1	8.2
106	7.2	0.6648	0.3	0.1	0.5	0.7	0.1	1.00E-06	1.00E-12	0.7	1.5
107	7	0.6233	0.5	0.2	0.6	0.8	0.1	1.00E-06	1.00E-12	0.9	1.5
108	9.2	6.848	31	1.3	0.4	0.3	3.2	1.3	1.00E-12	4.1	12.4
109	7.1	0.7314	0.5	0.1	0.4	0.5	0.1	1.00E-06	1.00E-12	0.5	1.7
110	9.7	4.249	35	3.6	0.2	0.2	3.4	1.7	1.00E-12	0.6	6.7
111	8	2.962	9	1	1.1	0.9	0.6	0.2	1.00E-12	1	6
115	9	4.014	45.3	1.00E-06	1.00E-09	1.00E-09	16.8	0.9	1.00E-12	0.6	7.5

Table G. part 3: *Continued*

Sequence # (sample #)	pH	Carbonate alkalinity mmol/kg as CaCO3	Na+ mmol/kg	K+ mmol/kg	Mg++ mmol/kg	Ca++ mmol/kg	Cl- mmol/kg	SO4-- mmol/kg	ΣPO4 mmol/kg	SiO2(aq) mmol/kg	CO3-- (DIC) mmol/kg
116	9.5	7.889	137	0.02	0.7	0.1	63.8	3	1.00E-12	0.2	12.7
117	7.6	7.162	53.2	1.00E-06	0.8	0.04	20.1	0.5	1.00E-12	0.7	14.9
118	9.6	20.07	272	2.33	1.00E-09	0.8	221	8.8	1.00E-12	4.2	29.3
119	9.4	18.69	330	0.1	0.7	1.00E-09	163	8.3	1.00E-12	0.6	30
120	9.6	6.688	123	1.00E-06	0.4	0.1	65.6	2.9	1.00E-12	0.2	10.4
121	9.5	6.938	113	1.00E-06	0.4	0.1	61	2.9	1.00E-12	0.2	11.2
125	7.4	3.399	12.5	0.1	1.4	1	4.2	0.1	1.00E-12	0.7	7.3
126	7.6	6.406	86.6	0.02	1.1	0.6	33.8	0.5	1.00E-12	0.6	13.3
127	8.2	7.762	62.6	0.03	1.5	0.4	6.7	0.3	1.00E-12	0.5	15.5
128	8.3	6.35	53.1	0.01	4.7	0.6	15.5	0.1	1.00E-12	0.3	12.6
129	8.4	1.87	8.3	0.02	6.9	1.00E-09	3	0.4	1.00E-12	0.8	3.7
130	7.8	1.805	7.8	1.00E-06	7.2	0.5	3.1	0.2	1.00E-12	0.9	3.7
131	7.7	2.856	4.4	0.04	10.1	0.7	1.8	0.1	1.00E-12	1.5	5.9
132	7.4	1.258	4.6	0.03	7.1	0.6	2	0.4	1.00E-12	1	2.7
133	7.9	1.326	6.9	0.02	4.4	0.3	3.1	0.2	1.00E-12	0.9	2.7
134	7.2	1.692	6.2	1.00E-06	0.8	0.4	1.5	0.3	1.00E-12	0.8	3.8
135	8.4	3.405	39.4	0.01	5.6	2.4	8.6	15.3	1.00E-12	0.6	6.7
136	8	5.539	23.6	0.02	0.8	0.6	5.8	1	1.00E-12	1.00E-09	11.2
137	7.5	1.463	6.2	0.04	1.1	1.1	2.5	0.1	1.00E-12	1	3.1
138	7.8	6.207	43.4	0.02	0.8	0.6	13.5	0.2	1.00E-12	0.7	12.7
139	8.18	1.139	591	43.5	24.9	29.9	620	59.4	1.00E-12	0.9	2.2
140	8.15	0.6654	330	26.3	13.4	34.2	392	32	1.00E-12	1.48	1.3
141	8.72	1.5	196	7.88	10.8	5.44	182	24	1.00E-12	1.02	2.8
142	8.5	2.233	885	53.7	26.7	13	693	186	1.00E-12	0.983	4.1
143	8.85	1.462	435	26.1	8.64	9.98	400	45	1.00E-12	0.933	2.6
144	8.52	1.701	415	44	11.3	11.6	430	48.5	1.00E-12	0.735	3.2
145	8.28	0.9735	293	25.3	5.76	4.99	290	27.1	1.00E-12	1.13	1.9
146	8.05	1.916	900	63.9	46.9	33.4	1090	42.5	1.00E-12	1.23	3.7
147	9.18	0.3486	156	5.42	1.4	1.62	63.4	52.8	1.00E-12	1.12	0.6
148	8.8	7.97	1310	327	78.2	18.2	1240	277	1.00E-12	0.783	13
149	10.2	2.163	101	46	2.18	4.99	55.5	45.4	1.00E-12	0.667	2.6
150	8.4	7.398	1770	109	37.2	6.48	1830	61.1	1.00E-12	1.63	13.4
151	8.5	2.856	865	54	15.7	2.57	831	62.3	1.00E-12	1.16	5.3
152	10.38	80.92	460	73	6.03	0.06	128	38.6	1.00E-12	5.75	90.4
153	9.35	0.2282	19.6	1.1	0.45	0.61	19.7	0.75	1.00E-12	1.37	0.4
154	8.52	0.9013	403	26.1	10.9	8.98	470	4.84	1.00E-12	1.13	1.7
155	8.05	0.7529	196	12.8	5.43	4.99	227	2.6	1.00E-12	0.617	1.5
156	7.4	2.255	1480	101	4.53	27.4	1730	13.2	1.00E-12	0.733	4.6

Table G. part 3: *Continued*

Sequence # (sample #)	pH	Carbonate alkalinity mmol/kg as CaCO3	Na+ mmol/kg	K+ mmol/kg	Mg++ mmol/kg	Ca++ mmol/kg	Cl- mmol/kg	SO4-- mmol/kg	ΣPO4 mmol/kg	SiO2(aq) mmol/kg	CO3-- (DIC) mmol/kg
157	7.2	6.011	4480	363	143	77.3	5470	25.6	1.00E-12	1.12	12
158	8.42	1.134	174	13.6	3.7	4.99	204	2.76	1.00E-12	1.3	2.2
159	6.95	0.7382	3.48	0.42	0.83	1.27	2.54	1.09	1.00E-12	1.33	1.8
160	8.15	1.161	170	10.2	5.68	4.74	190	3.15	1.00E-12	2.1	2.3
161	7.85	0.9799	15.2	1.23	2.28	0.82	16.9	1.35	1.00E-12	1.08	2
162	8.35	0.8724	196	14.8	5.43	4.99	234	3.18	1.00E-12	1.15	1.7
163	7.91	2.351	2000	128	49.4	37.4	2420	30.4	1.00E-12	1.22	4.5
164	9.62	0.02965	1.82	0.11	0.13	0.15	1.78	0.15	1.00E-12	0.567	0.05
165	7.46	2.476	3350	165	51.4	41.1	3770	35.1	1.00E-12	1.18	4.9
166	8.92	0.2611	3.7	0.32	0.31	0.31	4.23	0.05	1.00E-12	0.8	0.5
167	6.95	2.044	3520	251	105	59.4	4330	33.8	1.00E-12	0.6	4.2
168	7.5	3.299	4000	3520	85.6	62.3	4450	33.1	1.00E-12	1.12	6.6
169	8.76	0.2581	8.48	0.58	0.27	0.34	6.59	0.99	1.00E-12	1.01	0.5
170	8.78	0.3637	18.4	1.19	0.56	0.48	15.8	1.7	1.00E-12	0.983	0.7
171	8.88	0.6376	47.8	2.32	1.53	1.52	43.9	3.79	1.00E-12	1.36	1.2
172	8.92	0.7056	113	6.27	1.98	1.6	106	8.59	1.00E-12	1.04	1.3
173	9.1	2.597	350	21.4	5.88	2.99	335	26.8	1.00E-12	1.27	4.4
174	8.52	2.866	865	54	15.7	2.57	831	62.3	1.00E-12	1.16	5.3
175	8.4	7.402	1770	109	37.6	6.48	1830	67.1	1.00E-12	1.63	13.4
176	8.31	0.6528	3.38	0.58	4.43	0.53	1.53	0.69	1.00E-12	0.625	1.3
177	8.8	7.97	1310	327	78.2	18.2	1240	277	1.00E-12	0.783	13
178	7.2	6.011	4480	363	143	77.3	5460	25.6	1.00E-12	1.12	12
179	10.05	588.9	4000	910	0.12	0.15	1610	373	1.00E-12	7.2	656.1
180	9.4	6.736	134	7.16	2.74	0.09	116	2.17	1.00E-12	1.13	11
181	8.6	2.698	370	37.3	10.7	20	487	1.00E-06	1.00E-12	1.22	5
182	8.4	7.402	1770	109	37.6	6.46	1830	67.1	1.00E-12	1.63	13.4
183	9.8	0.06379	2.08	0.85	0.11	0.94	0.61	1.63	1.00E-12	1.24	0.1
184	8.34	0.9824	313	9.72	10.1	10.9	330	24.9	1.00E-12	1.39	1.9
185	9.5	106.5	2160	66.5	0.05	0.1	1420	242	1.00E-12	2.37	135.4
186	8.52	1.701	415	44	11.3	11.6	430	48.5	1.00E-12	0.735	3.2
187	8.48	4.329	870	35	47.7	19.3	873	102	1.00E-12	0.942	7.9
188	10.81	134.5	744	32.2	0.13	0.18	188	4.93	1.00E-12	2.5	140.4
189	10.6	84.83	548	43	0.26	0.41	189	17.3	1.00E-12	3.16	91
190	10.3	0.3072	3.93	0.01	0.03	0.44	0.52	0.47	1.00E-12	1.64	0.4
191	9.1	2.659	144	8.06	0.35	1.43	136	7.5	1.00E-12	1.56	4.7
192	8.3	3.33	1100	25.4	6.71	15.1	966	109	1.00E-12	1.07	6.3
193	9.1	3.024	229	28.9	3.25	6.76	161	54.8	1.00E-12	0.655	5.2
194	7.8	31.67	3620	946	360	3.79	5040	272	1.00E-12	0.105	60.9

Table G. part 3: *Continued*

Sequence # (sample #)	pH	Carbonate alkalinity mmol/kg as CaCO3	Na+ mmol/kg	K+ mmol/kg	Mg++ mmol/kg	Ca++ mmol/kg	Cl- mmol/kg	SO4-- mmol/kg	ΣPO4 mmol/kg	SiO2(aq) mmol/kg	CO3-- (DIC) mmol/kg
195	8.85	1.501	422	51.9	6.91	39.4	501	38.4	1.00E-12	0.525	2.6
196	7.6	1.168	238	10.4	7.7	18.5	304	4.25	1.00E-12	1.35	2.4
197	7.75	2.687	1570	70.1	65	136	2040	22.5	1.00E-12	1.08	5.2
199	9.31	29.32	352	10.2	4.4	0.22	166	25.5	0.02	0.013	47.8
200	9.9	31.74	351	10.5	4.94	0.04	161	28.9	1.00E-12	0.033	41.3
201	9.7	29.53	338	14.4	4.44	0.1	159	24.5	1.00E-12	1.00E-09	41.7
202	9.6	31.43	324	11	3.58	0.1	157	17.6	1.00E-12	1.00E-09	46.3
203	9.55	27.85	1.00E-06	13	3.91	0.1	154	1.00E-06	0.0055	1.00E-09	41.9
204	9.7	30.4	330	12	4.28	0.1	163	25.7	0.002	1.00E-09	42.8
205	9.73	29.69	338	10.8	4.4	0.11	160	24.5	0.00347	0.019	41.4
206	9.87	31.03	343	10.9	4.48	0.1	164	25	0.004	0.038	40.9
207	9.88	31.71	347	11.1	4.53	0.09	166	25.4	0.00565	0.121	41.6
208	9.02	2.039	14.3	1.00E-06	5.1	0.3	7	4	0.004	0.004	3.8
209	9.18	0.3384	156.2	5.42	1.4	1.62	63.48	0.7	1.00E-12	1.115	0.6
210	8.05	1.006	293.2	25.32	5.76	4.99	290.6	0.71	1.00E-12	1.132	2
211	8.15	0.6639	330.6	26.34	13.37	34.18	392.1	0.93	1.00E-12	1.481	1.3
212	8.85	1.449	435	26.09	8.64	9.98	409.1	0.58	1.00E-12	0.932	2.6
213	8.18	1.134	587.2	43.48	24.69	29.94	620.7	0.58	1.00E-12	0.932	2.2
214	8.5	2.186	861.2	53.71	26.74	12.97	694	0.61	1.00E-12	0.982	4.1
215	8.28	1.862	900.4	63.94	46.9	33.43	1086	0.77	1.00E-12	1.232	3.5
216	8.8	7.634	1309	327.4	78.17	18.21	1241	0.49	1.00E-12	0.782	13
217	7.46	2.475	3349	164.7	51.43	41.17	3780	0.74	1.00E-12	1.182	4.9
218	7.2	6.009	4480	363.2	143.2	77.35	5473	0.7	1.00E-12	1.115	12
219	7.52	1.914	3001	205.1	53.08	21.51	3075	0.72	1.00E-12	1.148	3.8
220	7.83	3.86	2601	183.9	48.55	25.7	2564	0.37	1.00E-12	0.599	7.5
221	7.68	2.332	2532	168	47.73	20.91	2435	0.47	1.00E-12	0.749	4.6
222	7.64	2.471	2401	157	43.61	17.52	2282	0.44	1.00E-12	0.699	4.9
223	7.7	2.122	2340	150.1	42.38	14.6	2093	0.4	1.00E-12	0.632	4.2
224	7.79	3.307	2462	161.9	43.2	14.3	2113	0.45	1.00E-12	0.716	6.5
225	8.8	1.45	0.25	0.08	3.61	0.66	0.11	0.12	1.00E-12	0.186	2.8
226	8.3	1.504	0.15	0.17	2.48	1.48	0.03	0.03	1.00E-12	0.055	3
227	8.2	1.546	0.09	0.16	1.65	1.97	0.05	0.02	1.00E-12	0.038	3.1
228	8.3	4.476	0.24	0.41	8.6	1.52	0.02	0.02	1.00E-12	0.038	8.9
229	8	13.81	1.32	0.81	29.5	1.84	0.03	0.22	1.00E-12	0.344	27.8
230	8	10.55	0.7	0.17	14.52	0.12	0.06	0.17	0.00758	0.266	21.3
232	8.6	16.03	4.19	0.61	23.66	0.25	0.31	0.35	0.0118	0.566	31
234	8	16.52	2.88	0.49	37.89	1.00E-09	0.04	0.23	1.00E-12	0.37	33.2
235	7.1	28.33	2.11	1.05	52.25	1.36	0.01	0.15	1.00E-12	0.244	63.9

Table G. part 3: *Continued*

Sequence # (sample #)	pH	Carbonate alkalinity mmol/kg as CaCO3	Na+ mmol/kg	K+ mmol/kg	Mg++ mmol/kg	Ca++ mmol/kg	Cl- mmol/kg	SO4-- mmol/kg	ΣPO4 mmol/kg	SiO2(aq) mmol/kg	CO3-- (DIC) mmol/kg
236	7.8	0.1942	0.03	0.03	0.13	0.36	0.01	0.01	1.00E-12	0.023	0.4
237	8.3	3.973	0.87	0.31	8.19	1.74	0.96	0.06	1.00E-12	0.095	7.9
238	8.2	3.198	0.81	0.3	5.84	1.22	0.71	0.07	1.00E-12	0.108	6.4
239	7.9	1.618	0.03	0.4	3.61	0.32	0.05	0.01	1.00E-12	0.021	3.3
240	7.9	0.2446	0.16	0.09	0.18	0.27	1.00E-06	0.03	1.00E-12	0.044	0.5
241	8	1.579	0.17	0.14	2.04	0.83	0.02	0.04	1.05E-04	0.059	3.2
242	8.5	0.4042	0.13	0.03	0.74	0.18	0.01	0.03	2.11E-04	0.048	0.8
243	9.4	0.1114	0.13	0.09	0.37	0.04	0.02	0.03	1.05E-04	0.047	0.2
244	8	1.53	0.16	0.03	2.88	1.2	0.07	0.11	1.00E-12	0.174	3.1
245	8.14	9.75	0.7	0.17	19.5	0.18	0.05	0.26	1.00E-12	0.409	19.5
246	7.98	32.58	3.8	0.37	63.77	0.05	0.21	0.37	1.00E-12	0.595	65.3
247	7.54	20.2	2.82	0.24	32.92	1.7	0.09	0.97	1.00E-12	1.556	42.2
248	8.61	16.23	2.5	0.28	36.49	0.25	3.6	0.22	1.00E-12	1.107	31.2
249	8.56	16.25	3.31	0.32	35.59	0.23	3.1	0.26	1.00E-12	1.203	31.4
250	10.1	214	317.4	2.47	1.39	0.08	3.6	0.22	1.00E-12	0.057	252
251	10.4	146.2	286.1	2.21	1.56	0.1	3.1	0.26	1.00E-12	0.142	162.8
252	10.1	216.1	346.5	1.48	0.26	0.11	8.5	0.48	0.31	0.053	254.3
253	10.4	146.3	286	2.26	1.57	0.09	3.1	0.21	0.1	0.128	162.9
254	10.1	309.5	502.3	9.2	1.9	0.09	34.8	13.8	0.4	0.05	355.5
255	10.7	114.2	219.8	4.27	1.21	0.12	16.1	7.01	0.2	0.036	121.3
256	10.1	390.7	762.9	7.09	0.62	0.12	23	27.72	4.1	0.189	443.9
257	10.3	324.7	858.4	6.88	1.04	0.21	22.8	31.31	4.41	0.584	357.3
258	7.4	2.041	0.96	0.38	1.32	0.45	0.03	0.22	1.00E-12	0.35	4.4
259	8.4	9.465	2.91	0.31	8.64	0.12	0.14	0.22	1.00E-12	0.35	18.7
260	7.9	9.938	6.22	0.08	9.13	0.5	0.17	0.18	1.00E-12	0.283	20.2
261	9	52.16	180.1	9.85	2.26	0.02	7.76	0.34	1.00E-12	0.549	95.2
262	8.6	14.77	35.02	2.05	0.41	0.05	0.87	0.18	1.00E-12	0.283	28.8
263	8.3	11.52	16.53	1.07	3.66	0.05	0.34	0.08	1.00E-12	0.133	22.9
264	8.8	25.36	80.47	5.75	3.33	0.02	3.1	0.34	1.00E-12	0.549	48.2
265	9.5	54.95	145.7	9.85	1.73	1.00E-09	5.5	0.15	1.00E-12	0.233	87.4
266	9.4	24.96	67.42	4.09	0.41	0.01	1.75	0.15	1.00E-12	0.233	42.2
267	9.4	33.41	73.95	5.24	3.21	0.05	1.13	0.15	1.00E-12	0.233	56
268	8.7	23.75	77.64	6.39	1.69	0.01	2.2	0.22	1.00E-12	0.35	45.7
269	9.1	179.3	429.8	29.67	0.62	1.00E-09	12.7	0.44	1.00E-12	0.699	308.5
271	9.8	73.54	1.00E-06	1.00E-06	1.00E-09	1.00E-09	198.6	1.00E-06	1.00E-12	1.00E-09	96.3
272	9.7	143.5	704.6	13.71	1.00E-09	1.00E-09	397.8	1.63	0.579	2.613	189
274	9.7	195.5	952.6	18.31	1.00E-09	1.00E-09	541.7	1.79	0.821	2.863	250.7
275	9.6	191.1	956.9	19.23	0.02	0.03	544.5	1.5	0.779	2.397	254.8

Table G. part 3: *Continued*

Sequence # (sample #)	pH	Carbonate alkalinity mmol/kg as CaCO3	Na+ mmol/kg	K+ mmol/kg	Mg++ mmol/kg	Ca++ mmol/kg	Cl- mmol/kg	SO4-- mmol/kg	ΣPO4 mmol/kg	SiO2(aq) mmol/kg	CO3-- (DIC) mmol/kg
278	9.7	175.5	848.2	16.73	1.00E-09	1.00E-09	471.1	1.42	0.737	2.264	227.7
283	9.9	73.8	348.9	6.45	1.00E-09	1.00E-09	218.9	0.99	1.00E-12	1.581	94.2
284	9.8	66.92	364.1	7.55	1.00E-09	1.00E-09	209.9	1.46	0.347	2.33	89.2
285	9.8	64.77	334.5	7.57	0.07	0.02	191.3	1.4	1.00E-12	2.23	86.7
287	9.6	33.43	123.1	2.94	0.01	0.06	45.14	1.15	1.00E-12	1.831	51.3
288	9.5	13.84	50.46	1.00E-06	0.01	0.05	17.77	0.9	1.00E-12	1.431	22.8
289	9.6	30.27	105.7	2.92	0.02	0.05	38.09	1.43	1.00E-12	2.28	46.7
290	9	6.16	15.57	0.79	0.21	0.45	1.00E-06	0.6	1.00E-12	0.965	11.6
291	9.1	7.465	19.57	0.92	0.16	0.32	4.29	0.6	1.00E-12	0.965	13.8
292	8.9	4.56	11.48	0.69	0.14	0.35	2.34	0.94	1.00E-12	1.498	8.7
293	9.2	7.718	20.4	1.13	0.2	0.3	4.57	0.71	1.00E-12	1.132	14
294	8.8	5.087	12.7	0.82	0.19	0.32	2.76	0.67	1.00E-12	1.065	9.8
295	8.9	4.665	11.48	0.69	0.14	0.35	2.37	0.9	1.00E-12	1.431	8.9
296	8.5	6.043	5.96	0.72	1.81	1.47	0.59	0.23	1.00E-12	0.366	11.9
297	9.7	5.314	10.18	0.82	0.74	0.4	1.13	0.2	1.00E-12	0.316	8.5
298	9.8	95.02	574.2	12.48	1.00E-09	1.00E-09	330.1	0.76	0.337	1.215	123.4
299	8.4	2.166	2.35	0.16	0.58	0.85	0.56	0.41	0.0105	0.649	4.3
300	8.8	4.776	8.35	0.41	1.23	1.3	1.75	0.36	1.00E-12	0.583	9.2
301	7.1	0.4298	0.31	0.07	0.16	0.2	0.03	0.32	1.00E-12	0.516	1
302	7.9	1.028	0.52	0.09	0.33	0.47	0.06	0.23	1.00E-12	0.366	2.1
303	8.7	8.19	780.8	26.01	459.2	12.82	657.2	0.21	1.00E-12	0.333	13
304	8.8	4.669	196.2	1.00E-06	101.5	2.92	59.16	0.17	1.00E-12	0.266	8.5
306	9.4	19.93	35.93	1.00E-06	134.9	1.92	43.78	0.54	1.00E-12	0.865	29.6
307	8.7	5.041	67.29	2.81	65.42	1.78	4.15	0.04	1.00E-12	0.067	9.5
308	8.9	78.22	102.6	1.00E-06	49.04	0.47	7.11	0.1	1.00E-12	0.166	142.1
309	8.9	6.401	101.3	1.00E-06	46.57	0.55	9.17	0.23	1.00E-12	0.366	11.8
310	8.7	4.517	62.98	1.00E-06	53.82	32.64	12.07	0.09	1.00E-12	0.15	8.4
311	8.9	2.978	17.88	4.6	41.88	3.02	1.83	0.18	1.00E-12	0.283	5.5
313	8.9	3.593	25.1	1.00E-06	28.1	1.14	4.32	0.22	1.00E-12	0.35	6.7
314	8.3	2.319	12.14	1.00E-06	15.18	2.1	1.46	0.14	1.00E-12	0.228	4.6
315	8.3	1.713	10.92	1.00E-06	11.85	4.84	1.58	0.04	1.00E-12	0.07	3.4
316	8.5	3.31	22.92	0.42	6.87	1.1	5.02	0.15	1.00E-12	0.233	6.5
317	7.8	1.61	9.26	1.00E-06	6.83	2.16	0.19	0.11	1.00E-12	0.168	3.3
319	8.7	3.46	3.63	1.00E-06	8.68	0.87	0.53	0.09	1.00E-12	0.15	6.7
320	8.6	1.996	2.11	1.00E-06	7.53	1.17	0.08	0.06	1.00E-12	0.103	3.9
321	8.7	2.472	10.96	0.57	2.91	1.49	2.96	0.1	1.00E-12	0.166	4.8
322	8.7	3.659	6.96	3.61	5.8	0.05	0.38	0.08	1.00E-12	0.13	7.1
323	8.6	2.61	1.63	1.00E-06	7.57	1.04	0.51	0.11	1.00E-12	0.175	5.1

Table G. part 3: *Continued*

Sequence # (sample #)	pH	Carbonate alkalinity mmol/kg as CaCO3	Na+ mmol/kg	K+ mmol/kg	Mg++ mmol/kg	Ca++ mmol/kg	Cl- mmol/kg	SO4-- mmol/kg	ΣPO4 mmol/kg	SiO2(aq) mmol/kg	CO3-- (DIC) mmol/kg
325	8.8	4.726	9.7	1.00E-06	3.22	0.52	0.28	0.04	1.00E-12	0.07	9.1
329	8.9	3.104	0.71	1.00E-06	7.2	1.2	0.18	0.2	1.00E-12	0.326	5.9
330	8.9	1.94	2.13	1.00E-06	4.57	1.26	0.09	0.08	1.00E-12	0.133	3.7
331	8.4	2.018	7.35	1.00E-06	2.2	1.31	1.65	0.19	1.00E-12	0.3	4
332	8.7	2.008	1.68	1.00E-06	5.23	1.03	0.21	0.41	1.00E-12	0.656	3.9
333	8.8	4.627	3.65	1.00E-06	5.6	0.22	0.58	0.12	1.00E-12	0.186	8.9
334	8.7	2.108	3.9	1.00E-06	3.4	0.9	0.25	0.07	1.00E-12	0.113	4.1
335	8.8	4.362	1.93	1.00E-06	4.53	0.22	0.05	0.32	1.00E-12	0.511	8.4
336	8.7	3.497	1.42	1.00E-06	3.92	0.38	0.04	0.04	1.00E-12	0.057	6.8
337	8.7	3.342	1.57	1.00E-06	3.66	0.47	0.06	0.07	1.00E-12	0.11	6.5
338	7.9	1.863	1.23	1.00E-06	1.84	1.59	0.05	0.12	1.00E-12	0.191	3.8
340	8.6	2.703	1.18	1.00E-06	2.81	0.58	0.25	0.09	1.00E-12	0.15	5.3
341	8.4	1.461	1.52	1.00E-06	1.46	1.2	0.61	0.18	1.00E-12	0.293	2.9
342	8.7	3.546	1.22	1.00E-06	3.31	0.28	0.05	0.14	1.00E-12	0.228	6.9
343	8.2	1.197	0.21	1.00E-06	1.86	1.24	0.06	0.19	1.00E-12	0.296	2.4
345	8.7	2.979	1.26	1.00E-06	2.48	0.59	0.05	0.06	1.00E-12	0.1	5.8
346	8.5	2.228	0.61	1.00E-06	1.39	1.06	0.01	0.06	1.00E-12	0.093	4.4
347	8.6	2.237	1.00E-06	1.00E-06	1.00E-09	1.00E-09	0.06	0.37	1.00E-12	0.588	4.4
348	8	1.924	0.84	1.00E-06	1.37	0.78	0.03	0.07	1.00E-12	0.12	3.9
349	8.5	1.619	0.71	1.00E-06	1.29	0.57	1.00E-06	0.03	1.00E-12	0.045	3.2
352	8.1	1.438	0.29	1.00E-06	0.73	0.84	0.01	0.16	1.00E-12	0.25	2.9
353	8.1	1.388	0.28	1.00E-06	0.6	0.89	0.04	0.09	1.00E-12	0.138	2.8
356	10	56.24	147.5	18.7	0.99	0.2	25.53	0.21	1.00E-12	0.333	73.1
357	9.6	22.89	57.85	7.29	0.36	0.16	10.3	0.01	1.00E-12	0.015	36.2
358	9.7	44.65	267.1	7.55	1.03	0.1	162.5	0.04	0.0695	0.072	63.2
359	9.7	208.9	943.9	29.41	1.52	0.11	409.1	0.15	1.00E-12	0.233	272.4
361	6.1	0.01853	0.03	0.01	1.00E-09	0.06	0.01	0.02	1.00E-12	0.03	0.1
368	8	3.46	19.57	0.17	0.19	0.35	9.14	0.76	1.00E-12	1.215	7
370	7.8	2.58	2.7	0.25	0.58	0.95	0.22	0.48	0.0116	0.766	5.3
371	8.3	3.912	4.96	0.41	0.74	1.02	0.42	0.64	1.00E-12	1.015	7.8
372	7.5	1.46	1.3	0.13	0.29	0.7	0.1	0.35	0.00632	0.566	3.1
373	9.6	29.46	374.5	1	8.02	0.2	213.6	0.03	0.126	0.055	43.2
374	8.9	10.28	70.03	2.53	4.53	0.18	54.17	0.01	6.32E-04	0.022	19.2
375	7.5	0.7996	0.87	1.00E-06	0.08	0.4	0.16	0.24	1.00E-12	0.383	1.7
376	7.5	0.9422	1.87	0.09	0.53	0.82	1.44	0.29	1.00E-12	0.466	2
377	9.2	16.65	101.3	2.43	4.32	0.18	45.99	0.06	0.0147	0.093	29.3
378	9.3	17.1	101.3	2.46	4.32	0.17	46.27	0.04	0.0158	0.057	29.3
381	7.5	0.6584	0.43	0.06	0.19	0.4	0.17	0.2	0.00421	0.316	1.4

Table G. part 3: *Continued*

Sequence # (sample #)	pH	Carbonate alkalinity mmol/kg as CaCO3	Na+ mmol/kg	K+ mmol/kg	Mg++ mmol/kg	Ca++ mmol/kg	Cl- mmol/kg	SO4-- mmol/kg	ΣPO4 mmol/kg	SiO2(aq) mmol/kg	CO3-- (DIC) mmol/kg
382	7.6	3.1	839.5	13.04	30.9	11.55	710.9	0.09	0.00737	0.151	6.3
383	9.8	66.92	364.1	7.55	0.06	0.03	209.9	1.46	0.347	2.33	89.2
384	9.8	34.38	165.3	4.5	0.49	0.1	99.31	0.72	0.126	1.148	47.8
385	6.9	0.3976	0.61	0.06	0.29	0.24	0.48	0.37	0.00337	0.599	1
386	7.4	2.075	3636	104.1	296.2	6.01	3950	0.06	0.00526	0.103	4.1
387	6.7	2.144	548.1	14.6	12.22	23.6	609.4	0.5	1.00E-12	0.799	5.3
388	7.3	1.457	305.8	23.12	2.88	28.44	375.2	0.4	1.00E-12	0.632	3.1
389	7.6	1.54	44.8	1.23	3	3.17	53.88	0.37	1.05E-04	0.599	3.2
390	7.1	1.69	109.6	7.29	3.79	13.37	123.3	0.36	1.00E-12	0.583	3.8
392	7.4	2.693	1.00E-06	1.00E-06	1.03	1.77	2.4	1.00E-06	1.00E-12	1.00E-09	5.8
393	7.4	3.258	1.00E-06	1.00E-06	3.54	0.32	8.52	1.00E-06	1.00E-12	1.00E-09	7
394	6.9	2.377	1.00E-06	1.00E-06	2.72	4.19	7.59	1.00E-06	1.00E-12	1.00E-09	5.9
395	8.5	1.924	0.65	0.05	0.58	1.55	0.51	0.12	1.00E-12	0.2	3.8
396	7.1	0.3461	4184	74.94	55.96	44.16	4401	0.08	1.00E-12	0.123	0.7
397	8.7	2.107	1.44	0.51	2.43	1.56	0.29	1.00E-06	1.00E-12	1.00E-09	4.1
398	9.1	8.213	70.03	1.43	8.52	0.68	23.37	1.00E-06	1.00E-12	1.00E-09	14.9
399	9.2	10.88	67.86	5.45	9.26	0.42	7.72	1.00E-06	1.00E-12	1.00E-09	19.4
400	9	8.923	107	5.01	50.2	1.64	9.67	1.00E-06	1.00E-12	1.00E-09	16.1
401	9	19.33	561.1	27.88	493.7	3.83	198.9	1.00E-06	1.00E-12	1.00E-09	28.6
402	8.9	6.206	126.6	5.4	102	3.39	21.68	1.00E-06	1.00E-12	1.00E-09	11.1
403	9.2	9.929	106.6	13.17	132.1	1.31	19.82	1.00E-06	1.00E-12	1.00E-09	16.1
404	8.8	11.67	2553	25.83	740.6	13.75	299.9	1.00E-06	1.00E-12	1.00E-09	18.5
405	8.8	2.262	20.66	1.92	16.54	3.44	4.5	1.00E-06	1.00E-12	1.00E-09	4.3
406	8.9	5.461	277.5	10.31	159.2	5.04	81.53	1.00E-06	1.00E-12	1.00E-09	9.5
408	8.6	6.132	13.66	3.35	18.1	0.67	2.7	1.00E-06	1.00E-12	1.00E-09	11.9
409	8.3	2.663	9.79	0.56	4.69	2.27	1.37	1.00E-06	1.00E-12	1.00E-09	5.3
410	9	4.577	212.3	6.01	58.84	3.22	158.7	1.00E-06	1.00E-12	1.00E-09	8
411	8.8	4.441	23.97	1.94	5.72	1.92	6.95	1.00E-06	1.00E-12	1.00E-09	8.5
412	9	7.674	413.2	18.75	107.8	3.77	133.4	1.00E-06	1.00E-12	1.00E-09	13.3
413	8.7	2.257	27.45	0.03	35.75	4.07	1.31	1.00E-06	1.00E-12	1.00E-09	4.3
414	8.8	6.145	101.3	5.86	19.05	2.32	29.17	1.00E-06	1.00E-12	1.00E-09	11.6
415	9.2	9.828	16.14	1.15	2.88	0.17	1.99	1.00E-06	1.00E-12	1.00E-09	17.8
416	8.6	5.859	839.5	25.32	191.7	9.56	233.8	1.00E-06	1.00E-12	1.00E-09	10.8
417	8.9	11.37	34.62	1.56	4.98	0.37	0.8	1.00E-06	1.00E-12	1.00E-09	21.5
418	8.3	2.674	14.09	1.64	17.49	2.52	1.6	1.00E-06	1.00E-12	1.00E-09	5.3
419	9.2	16.26	115.3	3.86	4.07	0.23	24.51	1.00E-06	1.00E-12	1.00E-09	28.8
420	9.2	16.21	245.3	11.94	29.29	0.45	34.5	1.00E-06	1.00E-12	1.00E-09	28.2
421	8.9	3.704	188.8	19.18	181.9	9.48	21.08	1.00E-06	1.00E-12	1.00E-09	6.4

Table G. part 3: *Continued*

Sequence # (sample #)	pH	Carbonate alkalinity mmol/kg as CaCO3	Na+ mmol/kg	K+ mmol/kg	Mg++ mmol/kg	Ca++ mmol/kg	Cl- mmol/kg	SO4-- mmol/kg	ΣPO4 mmol/kg	SiO2(aq) mmol/kg	CO3-- (DIC) mmol/kg
422	8.8	1.918	1.7	0.41	2.39	2.24	0.21	1.00E-06	1.00E-12	1.00E-09	3.7
423	9.2	12.44	82.64	3.86	1.28	0.43	18.43	1.00E-06	1.00E-12	1.00E-09	22.2
424	8.4	2.484	7.26	1.56	13	2.72	2.23	1.00E-06	1.00E-12	1.00E-09	4.9
425	9.3	10.89	22.01	1.66	6.54	0.12	1.22	1.00E-06	1.00E-12	1.00E-09	19.2
426	8.3	2.359	1.87	0.41	4.57	1.02	0.4	1.00E-06	1.00E-12	1.00E-09	4.7
427	8.6	5.127	13.57	1.71	6.17	1.9	2.76	1.00E-06	1.00E-12	1.00E-09	10
428	8.3	1.807	2.44	0.36	2.72	2.48	1.27	1.00E-06	1.00E-12	1.00E-09	3.6
429	9.7	41.1	351.5	5.47	15.26	0.31	54.45	1.00E-06	1.00E-12	1.00E-09	60.2
430	8.9	2.435	134.8	13.07	236.6	7.93	15.03	1.00E-06	1.00E-12	1.00E-09	4.1
431	8.8	7.373	258.8	11.87	50.61	2.67	66.55	1.00E-06	1.00E-12	1.00E-09	13.7
432	9.2	8.877	57.42	6.19	11.27	0.3	13.33	1.00E-06	1.00E-12	1.00E-09	15.8
433	8.8	5.04	1875	16.04	674.8	12.55	144.8	1.00E-06	1.00E-12	1.00E-09	8.1
434	9.9	3.871	27.97	3.27	34.85	2.41	4.93	1.00E-06	1.00E-12	1.00E-09	5.3
435	8.4	2.371	1.57	0.38	2.55	2.35	0.26	1.00E-06	1.00E-12	1.00E-09	4.7
436	8.3	1.856	0.87	0.41	2.51	1.62	0.22	1.00E-06	1.00E-12	1.00E-09	3.7
437	8.5	5.412	70.47	1.18	7.98	1.39	6.5	1.00E-06	1.00E-12	1.00E-09	10.6
439	8.3	2.409	2.44	0.61	3.29	1.49	0.66	1.00E-06	1.00E-12	1.00E-09	4.8
440	9.6	0.5116	40.76	2.07	12.47	6.07	20.89	1.00E-06	1.00E-12	1.00E-09	0.8
441	8.6	4.571	41.19	2.28	38.43	1.52	2.96	1.00E-06	1.00E-12	1.00E-09	8.8
442	8.9	5.815	91.34	4.3	106.6	1.97	6	1.00E-06	1.00E-12	1.00E-09	10.4
443	9.2	12.24	117.9	1.56	2.14	0.23	94.68	1.00E-06	1.00E-12	1.00E-09	21.3
444	9	5.242	30.32	1.59	10.78	2.99	14.61	1.00E-06	1.00E-12	1.00E-09	9.7
445	8.6	2.147	7.48	0.77	4.03	1.45	1	1.00E-06	1.00E-12	1.00E-09	4.2
446	9	13.4	28.58	1.2	3.41	0.15	1.74	1.00E-06	1.00E-12	1.00E-09	25
447	8.8	3.975	3.52	1.56	12.22	1.32	0.72	1.00E-06	1.00E-12	1.00E-09	7.6
448	8.6	3.098	54.81	3.66	124.3	3.61	5.92	1.00E-06	1.00E-12	1.00E-09	5.8
449	9.1	3.297	465.4	3.66	63.77	10.11	10.38	1.00E-06	1.00E-12	1.00E-09	5.8
450	9.1	12.98	30.97	2.38	1.28	0.24	8.18	1.00E-06	1.00E-12	1.00E-09	23.8
451	8.7	5.665	43.37	3.02	11.97	0.8	11.48	1.00E-06	1.00E-12	1.00E-09	10.9
452	9	3.687	14.75	1.28	6.79	0.68	3.87	1.00E-06	1.00E-12	1.00E-09	6.9
453	9.4	6.518	268.8	15.73	64.6	1.33	79.84	1.00E-06	1.00E-12	1.00E-09	10.3
454	8.5	5.558	210.5	4.6	22.96	4.22	38.06	1.00E-06	1.00E-12	1.00E-09	10.8
455	9	8.504	139.2	3.35	9.55	0.93	15.25	1.00E-06	1.00E-12	1.00E-09	15.7
456	8.8	4.948	11.48	1.28	5.14	0.85	2.49	1.00E-06	1.00E-12	1.00E-09	9.5
457	8.3	1.209	12.18	0.59	12.3	4.14	1.66	1.00E-06	1.00E-12	1.00E-09	2.4
458	8.7	2.935	131.4	5.83	97.51	6.74	96.09	1.00E-06	1.00E-12	1.00E-09	5.4
459	8.6	4.677	38.32	8.77	72	1.97	7.7	1.00E-06	1.00E-12	1.00E-09	8.9
460	8.6	8.467	2049	28.9	715.9	11.13	487.5	1.00E-06	1.00E-12	1.00E-09	14

Table G. part 3: *Continued*

Sequence # (sample #)	pH	Carbonate alkalinity mmol/kg as CaCO3	Na+ mmol/kg	K+ mmol/kg	Mg++ mmol/kg	Ca++ mmol/kg	Cl- mmol/kg	SO4-- mmol/kg	ΣPO4 mmol/kg	SiO2(aq) mmol/kg	CO3-- (DIC) mmol/kg
461	9.8	80.04	796	6.14	2.1	0.28	127.8	1.00E-06	1.00E-12	1.00E-09	110.4
462	9.3	2.945	117.9	3.76	24.65	2.15	34.36	1.00E-06	1.00E-12	1.00E-09	5
473	8.5	2.951	117.4	2.46	7.78	12.62	115.7	1.00E-06	1.00E-12	1.00E-09	5.7
474	8.5	2.643	126.1	2.56	6.97	14.97	121.3	1.00E-06	1.00E-12	1.00E-09	5.1
475	8.3	2.248	147.9	2.92	10.01	21.19	148.1	1.00E-06	1.00E-12	1.00E-09	4.4
476	8.4	3.338	124	2.66	7.91	14.55	122.7	1.00E-06	1.00E-12	1.00E-09	6.5
477	8.4	3.09	178.3	4.22	16.46	8.73	169.3	1.00E-06	1.00E-12	1.00E-09	6
478	8.6	3.053	182.7	3.96	17.26	9.16	174.9	1.00E-06	1.00E-12	1.00E-09	5.8
479	8.6	2.37	187	4.09	17.53	9.23	180.6	1.00E-06	1.00E-12	1.00E-09	4.5
480	8.6	3.057	193.6	4.22	17.98	9.78	184.8	1.00E-06	1.00E-12	1.00E-09	5.8
481	8.6	2.688	195.7	3.96	17.88	9.55	186.2	1.00E-06	1.00E-12	1.00E-09	5.1
482	8.6	2.369	189.2	4.22	17.07	8.5	180.6	1.00E-06	1.00E-12	1.00E-09	4.5
483	8.5	2.239	182.7	4.22	19.26	8.3	179.2	1.00E-06	1.00E-12	1.00E-09	4.3
484	8.6	2.524	169.6	3.84	17.7	8.08	165	1.00E-06	1.00E-12	1.00E-09	4.8
485	8.6	2.258	155.7	3.32	16.46	7.24	155.2	1.00E-06	1.00E-12	1.00E-09	4.3
486	8	1.991	86.99	0.84	7.61	10.48	78.99	1.00E-06	1.00E-12	1.00E-09	4
487	8.8	1.723	18.7	0.54	2.5	3	16.36	1.00E-06	1.00E-12	1.00E-09	3.3
488	8.9	1.743	17.4	0.41	2.43	3.02	15.52	1.00E-06	1.00E-12	1.00E-09	3.3
489	7.7	1.642	6.09	0.18	1.03	1.12	4.51	1.00E-06	1.00E-12	1.00E-09	3.4
490	8.9	1.901	17.4	0.41	2.28	2.97	15.8	1.00E-06	1.00E-12	1.00E-09	3.6
522	8.38	4.034	3.33	0.19	2.54	2.3	0.52	0.69	0.161	1.104	8
523	10.61	111.5	236.6	1.24	1.09	1.37	20.84	0.49	0.291	0.783	120.2
524	10.65	57.38	122.4	0.22	0.93	1.97	11.84	0.47	0.355	0.748	62.4
525	10.28	151.7	309.3	7.45	0.74	2.4	34.15	0.65	1.87	1.033	172.6
526	10.44	561.6	1595	22.36	4.9	3.82	74.63	0.71	0.71	1.139	595.9
527	8.3	8.398	8.92	0.45	4.79	1.12	0.38	0.31	1.00E-12	0.498	16.7
528	8.47	8.94	8.96	0.45	5.02	1.02	0.37	0.65	0.194	1.033	17.6
529	9.9	235.2	513.4	7.83	3.48	1.57	39.49	1.02	0.355	1.638	293.6
530	10.1	282.3	672.5	10.67	2	1.62	49.68	1.25	0.323	1.994	327.9
531	7.45	15.31	11.05	0.66	6.87	1.37	0.94	0.45	0.0323	0.712	32.5
532	7.71	15.48	10.7	0.51	6.85	1.22	0.68	0.4	1.00E-12	0.641	31.9
533	7.77	14.68	11	0.67	7.27	0.55	0.6	0.42	0.0645	0.676	30.1
534	7.99	17.38	14.35	0.91	7.36	0.6	0.59	0.24	1.00E-12	0.392	35.1
535	8.07	42.62	66.03	2.83	3.61	0.37	0.47	0.29	0.226	0.463	85.4
536	10.16	479.8	881.3	15.29	1.15	0.3	101.9	0.37	0.888	0.588	532
537	9.96	564.1	1021	19.33	0.37	0.4	105.7	0.45	1.19	0.712	649.3
538	10.33	608.2	1129	22.28	1.11	0.45	1.37	0.51	0.581	0.819	652.2
539	10.43	431.9	810	15.44	1.07	0.37	96.75	0.33	0.226	0.534	459.9

Table G. part 3: *Continued*

Sequence # (sample #)	pH	Carbonate alkalinity mmol/kg as CaCO3	Na+ mmol/kg	K+ mmol/kg	Mg++ mmol/kg	Ca++ mmol/kg	Cl- mmol/kg	SO4-- mmol/kg	ΣPO4 mmol/kg	SiO2(aq) mmol/kg	CO3-- (DIC) mmol/kg
540	8.31	13.2	10.53	0.58	5.38	0.7	0.58	0.69	1.00E-12	1.104	26.2
541	8.24	14.63	10.53	1.04	12.25	1.12	0.7	0.42	1.00E-12	0.676	29.1
542	8.38	12.66	23.1	0.46	8.59	0.6	1.26	0.2	1.00E-12	0.32	25
543	9.8	277.6	555.6	11.15	0.93	2.15	48.96	2.36	3.58	3.774	353.8
544	9.8	217.3	399.6	6.83	0.47	1.75	14.62	1.36	1.58	2.172	282.9
545	10.1	301.6	662.5	10.95	2.36	1.47	50.79	1.25	0.743	1.994	348.7
546	10.13	359.2	925.7	13.58	0.56	1.4	69.35	1.58	1.39	2.528	409.2
547	10.22	1028	1961	37.55	5.23	3.67	133.9	1.71	1.55	2.742	1095
548	9.82	306.4	605	12.33	0.67	1.55	61.33	1.38	1.36	2.207	384.9
549	9.48	147.8	308.1	5.47	2.05	0.82	20.82	0.71	0.839	1.139	224.2
550	10.01	458.7	870	16.6	0.8	1.8	60.67	1.76	0.839	2.813	529.4
551	10.01	700.7	1551	22.43	0.81	2.27	78.66	1.78	1.36	2.848	791.2
552	10.26	659	1220	22.87	3.82	1.67	90.55	1.02	0.194	1.638	709.5
553	10.22	650	1246	20.85	2.25	2.17	97.44	1.02	0.387	1.638	704.7
554	10.28	655.7	1281	22.15	3.32	3.82	100.8	1.96	0.775	3.133	703.9
555	10.44	478.9	922.4	4.94	0.34	1.12	49.52	0.49	2.1	0.783	508.7
556	10.27	585.7	1241	6.64	0.49	2.3	82.88	0.58	2.55	0.925	633.1
557	9.9	619.9	1310	8.93	0.78	2.02	106.6	0.87	4.13	1.389	722.3
558	10.5	280.4	615.4	2.03	0.26	1.97	38.41	0.91	1.52	1.46	300.2
559	10.15	695.7	1400	11.74	0.87	1.35	80.49	1.2	3.42	1.923	761.9
560	8.84	5.47	7.92	0.23	1.98	0.37	0.63	0.11	1.00E-12	0.178	10.5
561	10.12	1178	2306	20.17	0.26	0.67	194.6	0.8	3.07	1.282	1266
562	10.24	600.6	1312	10.18	0.24	1.7	93.02	2.23	4.1	3.56	651.6
563	9.58	1766	3738	55.91	1.78	2.47	219.1	2.18	15.7	3.489	2088
564	9.84	1.6182	4351	47.16	1.24	1.22	20093.7	2.65	13.6	4.237	2641
565	10.27	485.1	991.4	6.37	0.23	1.52	6416	1.54	2.29	2.457	487.7
566	8.63	5.273	9.92	0.21	1.9	0.5	1.02	0.22	1.00E-12	0.356	10.3
567	9.78	1750	3540	38.75	2.85	2.27	334.4	2.41	9.3	3.845	1962
568	9.89	1943	4019	48.26	0.91	2.79	250.9	2.65	12.7	4.237	2132
569	10.15	393.8	1059	11.3	0.7	1.52	118.7	1.18	3.26	1.887	443.1
570	9.68	2094	4286	96.25	3.46	5.21	442.4	5.5	38.3	8.794	2386
571	9.69	1614	3455	48.24	1.37	1.87	400.2	1.63	13.5	2.599	1854
572	8.17	3.836	4.65	0.03	1.5	0.5	0.08	0.18	1.00E-12	0.285	7.7
573	8.53	5.393	2.7	0.12	2.97	1.25	0.86	0.36	1.00E-12	0.57	10.6
574	10.18	337.2	558	18.89	0.36	0.31	27.6	0.27	0.307	0.427	379.9
575	9.59	50.6	80.01	4.25	2.04	0.17	3.57	0.09	0.0645	0.142	78.2
576	8.95	11.59	29.53	0.83	0.67	0.32	6.19	0.24	0.194	0.392	21.8
577	8.15	4.085	2.31	0.09	3.81	1.12	1.19	0.22	1.00E-12	0.356	8.2

Table G. part 3: *Continued*

Sequence # (sample #)	pH	Carbonate alkalinity mmol/kg as CaCO3	Na+ mmol/kg	K+ mmol/kg	Mg++ mmol/kg	Ca++ mmol/kg	Cl- mmol/kg	SO4-- mmol/kg	ΣPO4 mmol/kg	SiO2(aq) mmol/kg	CO3-- (DIC) mmol/kg
578	8.8	6.018	56.67	0.3076	0.04124	0.175	46.64	0.1043	0.01044	0.4996	11.45
579	10.4	195.8	1218	3.211	1.00E-09	1.00E-09	817.2	2.011	0.07043	4.126	207.9
580	10.2	253.9	1460	4.414	1.00E-09	1.00E-09	946.6	2.995	0.07992	6.486	275.4
581	9.8	409.5	2012	5.554	1.00E-09	1.00E-09	1225	0.05897	0.3148	8.066	473
582	9.5	524.6	2582	6.88	1.00E-09	1.00E-09	1570	0.004828	0.4059	6.604	647.4
583	9.4	624.4	2786	7.779	1.00E-09	1.00E-09	1690	0.005757	0.5954	7.218	785.8
584	9.3	743.3	3249	8.621	1.00E-09	1.00E-09	1850	0.00569	0.8258	12.32	959.4
585	9.2	1050	3992	11.39	1.00E-09	1.00E-09	2136	0.007421	1.207	72.97	1377
586	10.45	1662	5263	45.01	1.00E-09	1.00E-09	1800	29	0.9273	12.2	1714
587	10.45	1653	4915	49.87	1.00E-09	1.00E-09	1816	13	0.9169	14.9	1701
588	10.55	1526	5437	50.9	1.00E-09	1.00E-09	2395	38	0.7293	15.96	1565
589	10.55	1770	5524	45.27	1.00E-09	1.00E-09	2031	18	0.5522	13.02	1816
590	10.55	1577	5698	47.32	1.00E-09	1.00E-09	2194	50	0.9585	18.31	1620
591	10.55	1571	5589	50.9	1.00E-09	1.00E-09	2378	22	0.9377	16.31	1613
592	10.25	1501	5742	58.31	1.00E-09	1.00E-09	2381	23	0.896	17.56	1583
593	10.5	1570	5524	51.15	1.00E-09	1.00E-09	2304	20	0.7293	15.81	1616
594	9.5	1227	4785	39.13	1.00E-09	1.00E-09	1430	11	0.6876	8.954	1510
595	10.1	1616	4698	38.88	1.00E-09	1.00E-09	1450	11	0.9273	9.487	1717
596	9.25	808.8	2784	26.86	1.00E-09	1.00E-09	767.2	6	0.5105	5.742	1123
597	10.52	1576	4828	37.6	1.00E-09	1.00E-09	1644	16	0.5314	13.35	1616
598	10.4	1518	5568	1.00E-09	1.00E-09	1.00E-09	2403	27	0.9169	19.14	1573
599	10.45	1679	5394	38.62	1.00E-09	1.00E-09	1808	19	0.5835	16.81	1733
600	9.9	1362	3984	39.64	1.00E-09	1.00E-09	1354	10	0.5939	8.305	1490
601	9.97	1055	2727	27.62	1.00E-09	1.00E-09	516.2	46	1.354	2.58	1160
602	9.85	67.49	192.3	7.34	1.00E-09	1.00E-09	32.72	9.755	0.1146	2.114	91.32
603	9.4	673.1	2131	22.79	1.00E-09	1.00E-09	674.1	7.089	0.2501	4.843	893.2
604	9.33	742.6	2353	23.76	1.00E-09	1.00E-09	795.4	6.225	0.2396	5.526	996.5
605	10.55	1190	4828	53.46	1.00E-09	1.00E-09	2474	22.49	1.00E-12	18.31	1218
606	10.45	1647	5046	42.71	1.00E-09	1.00E-09	1819	17.7	0.6772	14.91	1696
607	10.45	1501	5394	45.78	1.00E-09	1.00E-09	2090	19.68	1.00E-12	17.31	1550
608	10.3	1504	4611	33.76	1.00E-09	1.00E-09	1591	15.41	1.00E-12	12.8	1565
609	10.3	1496	4480	33.76	1.00E-09	1.00E-09	1585	16.03	0.6043	13.2	1555
610	10.15	1470	4202	29.16	1.00E-09	1.00E-09	1371	14.57	1.011	11.42	1551
611	9.8	1193	3415	25.83	1.00E-09	1.00E-09	1066	9.182	0.5835	8.355	1338
612	10.5	1146	5089	56.52	1.00E-09	1.00E-09	2702	25.51	0.9064	20.64	1178
613	9.9	1395	5263	50.13	1.00E-09	1.00E-09	2465	27.17	0.5835	14.98	1536
614	9.5	1293	3832	26.09	1.00E-09	1.00E-09	1041	7.589	0.5522	4.344	1570
615	10.9	296.8	1270	48.53	1.00E-09	1.00E-09	540.3	164.8	0.5797	1.00E-09	302.2

Table G. part 3: *Continued*

Sequence # (sample #)	pH	Carbonate alkalinity mmol/kg as CaCO3	Na+ mmol/kg	K+ mmol/kg	Mg++ mmol/kg	Ca++ mmol/kg	Cl- mmol/kg	SO4-- mmol/kg	ΣPO4 mmol/kg	SiO2(aq) mmol/kg	CO3-- (DIC) mmol/kg
616	11	317	2848	21.31	1.00E-09	1.00E-09	2008	245.8	2.319	1.00E-09	319.6
617	11	800.3	4446	41.75	1.00E-09	1.00E-09	3138	169.2	4.916	1.00E-09	806.2
618	10.9	79.7	4360	25.61	1.00E-09	1.00E-09	3585	365.8	0.09731	1.00E-09	80.48
619	11	120.7	2047	13.07	1.00E-09	1.00E-09	1630	163.9	0.1011	1.00E-09	122
620	11.2	593.6	4286	46.54	1.00E-09	1.00E-09	3200	240	2.163	1.00E-09	596.3
621	10.5	61.32	144.1	6.006	0.03503	1.00E-09	29.03	0.5005	0.04589	3.457	68.29
622	9.4	53.8	165	7	1.00E-09	1.00E-09	56	1.5	0.03126	1.922	87.15
623	10.2	42.17	115.1	12.01	1.00E-09	0.05505	28.03	8.007	0.1053	0.9262	51.22
624	9.2	39.23	109.2	1.00E-06	0.04006	0.03506	33.05	2.504	0.06783	0.3067	68.4

Table G. part 4: Aqueous chemistry database of alkaline lake waters compiled from published literature, as well as corresponding results from calculations described in chapters 2 and 3, and investigated in detail in chapter 4.

Sequence # (sample #)	Dissolved solids mg/kg	Ionic strength molal	Activity of H2O	ALK/(Ca+Mg)	Charge imbalance eq/kg	Charge imbalance error percentage	Water type	Fluid density g/cm³
1	7755	0.1478	0.9962	0.74663643	-0.007194	-0.02873	Na-Cl	1.001
2	8220	0.1512	0.9959	1.40448113	0.003353	0.01271	Na-Cl	1.002
3	10402	0.1869	0.995	10.245283	-0.0006543	-0.001999	Na-Cl	1.003
4	14408.6	0.2998	0.9933	0.32804533	0.0003207	0.0006774	Na-Cl	1.006
5	116923	2.871	0.9442	89.9389002	0.02692	0.00679	Na-CO3	1.079
6	105129	2.401	0.9501	50.5812221	-0.006331	-0.00183	Na-Cl	1.071
7	142994	3.538	0.928	74.8690293	-0.1695	-0.03531	Na-Cl	1.099
8	192606	5.215	0.8951	170.263852	0.4465	0.06785	Na-CO3	1.139
9	17531.6	0.3323	0.9917	1.84214876	-0.009259	-0.0166	Na-Cl	1.008
10	23975	0.4864	0.9893	0.48944099	-0.007498	-0.009804	Na-Cl	1.012
11	6297	0.1293	0.9975	0.70011947	-1.016E-05	-0.000053	Na-Cl	1
12	11496.3	0.234	0.9949	0.47552083	0.002707	0.007368	Na-Cl	1.004
13	14602.4	0.2502	0.993	50.475	-0.002743	-0.006107	Na-Cl	1.006
14	47293.5	1.006	0.9787	0.31963257	-0.01553	-0.01021	Na-Cl	1.029
15	25629.5	0.5021	0.9893	24.5555556	-0.06941	-0.08841	Na-Cl	1.013
16	19620.5	0.3319	0.9902	6.67850467	-0.01591	-0.026	Na-Cl	1.009
17	50608.9	0.9598	0.9713	0.4223578	-0.05988	-0.03506	Na-Cl	1.031
18	2459	0.04747	0.9989	0.79070681	-0.000928	-0.0122	Na-Cl	0.9977
19	7369	0.157	0.9963	0.23932247	0.01805	0.07043	Na-Cl	1.001
20	100170	2.321	0.9561	217.666667	-0.1554	-0.04782	Na-CO3	1.067
21	83428.5	1.84	0.9677	160.57971	-0.1579	-0.06199	Na-Cl	1.055
22	24455.1	0.4801	0.9896	7.89052288	-0.02382	-0.03158	Na-Cl	1.013
23	4926	0.08678	0.9976	1.54116059	-0.01407	-0.09276	Na-Cl	0.9993
24	9858	0.1821	0.9959	4.06643952	-0.008311	-0.02844	Na-Cl	1.003
25	2795	0.04438	0.9987	20.7958524	0.01038	0.127	Na-HCO3	0.9979
26	1237	0.02044	0.9995	60.3028576	0.001854	0.05494	Na-HCO3	0.9968
27	613.5	0.009432	0.9997	21.6888577	0.0001842	0.01152	Na-HCO3	0.9964
28	647.4	0.01214	0.9997	27.0833333	-0.0000204	-0.001086	Na-CO3	0.9964
29	488	0.008564	0.9998	24.9530663	0.0004682	0.0347	Na-CO3	0.9963
30	2651	0.04283	0.999	157.737723	-0.03118	-0.4513	Na-HCO3	0.9978
31	1457	0.02844	0.9994	26.1586914	-0.008125	-0.1939	Na-CO3	0.997
32	1107	0.01551	0.9996	28.8078892	-0.0006788	-0.02471	Na-HCO3	0.9968
33	996.9	0.01332	0.9996	26.4654088	0.001775	0.07199	Na-HCO3	0.9967
34	3060	0.05244	0.9987	112.271051	-0.001692	-0.01927	Na-HCO3	0.9981
35	2124	0.03909	0.9988	4.60882353	0.04682	0.6375	Na-Cl	0.9974
36	268.9	0.004732	0.9999	7.11522288	0.0004738	0.06399	Na-CO3	0.9962

Table G. part 4: *Continued*

Sequence # (sample #)	Dissolved solids mg/kg	Ionic strength molal	Activity of H2O	ALK/(Ca+Mg)	Charge imbalance eq/kg	Charge imbalance percentage	Charge imbalance error	Water type	Fluid density g/cm³
37	1405	0.0216	0.9994	55.6626987	0.0004897		0.01339	Na-HCO3	0.997
38	5085	0.09503	0.9976	213.690352	0.003432		0.02124	Na-Cl	0.9994
39	848.7	0.01432	0.9996	38.8950686	0.001743		0.0734	Na-HCO3	0.9966
40	270.9	0.005102	0.9999	11.9306765	0.0019		0.2302	Na-CO3	0.9962
41	1030	0.01419	0.9996	20.0960267	0.001571		0.06063	Na-HCO3	0.9967
42	13812.7	0.2406	0.993	43.1861199	-0.01082		-0.02458	Na-Cl	1.005
43	16005.9	0.2755	0.992	52.147752	-0.05294		-0.1049	Na-Cl	1.007
44	15650.8	0.3239	0.9927	75.5666252	-0.05359		-0.1031	Na-Cl	1.007
45	17497.1	0.3564	0.9918	72.2402779	-0.05549		-0.09592	Na-Cl	1.008
46	16223.6	0.3246	0.9924	74.595066	-0.04922		-0.09241	Na-Cl	1.007
47	16087.6	0.3297	0.9925	80.6381897	-0.05433		-0.1024	Na-Cl	1.007
48	14261.8	0.2957	0.9935	79.8984127	-0.05347		-0.1142	Na-Cl	1.006
49	5618	0.1005	0.9974	4.6603117	-0.009847		-0.05803	Na-Cl	0.9998
50	5245	0.09761	0.9976	5.27499023	-0.01303		-0.0812	Na-Cl	0.9995
51	9487	0.1821	0.9962	2.3804193	-0.02011		-0.07247	Na-Cl	1.002
52	7394	0.1377	0.9971	2.09410591	-0.01929		-0.09149	Na-Cl	1.001
53	7856	0.1489	0.9971	2.04097443	-0.01552		-0.07032	Na-SO4	1.001
54	24798.4	0.4788	0.9892	2.30763514	-0.007077		-0.009223	Na-Cl	1.013
55	5238	0.09867	0.998	1.91444692	-0.009096		-0.06164	Na-SO4	0.9995
56	3974	0.08952	0.9986	0.51113294	-0.004053		-0.03448	Mg-SO4	0.9987
57	14879.4	0.2512	0.994	9.73182781	-0.01747		-0.04216	Na-HCO3	1.006
58	70662.9	1.417	0.9688	3.31168176	-0.0353		-0.01629	Na-Cl	1.045
59	5865	0.1135	0.9979	3.36614563	-0.02022		-0.1235	Na-CO3	1
60	93882.2	2.108	0.969	4.82367323	-0.03057		-0.01124	Na-SO4	1.062
61	23113.4	0.4568	0.9906	2.22204532	-0.03352		-0.04817	Na-Cl	1.012
62	17229	0.3447	0.9926	0.56759419	-0.01058		-0.01976	Na-Cl	1.008
63	6236	0.1053	0.9971	4.49743171	-0.004399		-0.0236	Na-Cl	1
64	28146.1	0.517	0.9886	3.01673971	-0.04224		-0.05188	Na-Cl	1.015
65	126008	2.608	0.938	3.5579388	-0.1755		-0.04563	Na-Cl	1.086
66	146.6	0.002556	0.9999	0.75454545	0.0008451		0.2314	Na-HCO3	0.9961
67	238.8	0.004591	0.9999	0.43942029	0.0006129		0.09367	Na-SO4	0.9962
68	304.6	0.005486	0.9999	0.55333333	0.0008945		0.12	Na-SO4	0.9962
69	538.4	0.009249	0.9998	1.54388889	0.001879		0.1307	Na-SO4	0.9964
70	2127	0.04278	0.9992	4.85111111	0.006732		0.1102	Na-SO4	0.9974
71	379.1	0.007904	0.9999	0.38012658	0.001406		0.1358	Na-SO4	0.9963
72	596	0.01339	0.9998	0.28933333	0.001335		0.0767	Na-SO4	0.9964
73	888.9	0.01874	0.9997	0.39830508	0.002634		0.1079	Na-SO4	0.9966
74	960	0.0205	0.9996	0.31527586	0.001067		0.03768	Na-SO4	0.9967

Table G. part 4: *Continued*

Sequence # (sample #)	Dissolved solids mg/kg	Ionic strength molal	Activity of H2O	ALK/(Ca+Mg)	Charge imbalance eq/kg	Charge imbalance error percentage	Water type	Fluid density g/cm³
75	7314	0.1399	0.997	13.2754098	0.02924	0.1344	Na-SO4	1.001
76	44144.7	0.9007	0.9816	268.347826	0.1714	0.125	Na-SO4	1.026
77	70321.4	1.52	0.9715	406.375	0.2367	0.1083	Na-SO4	1.045
78	173202	4.163	0.9098	1.57E+11	0.7098	0.1262	Na-Cl	1.123
79	188538	4.636	0.9007	1.6945E+11	0.7593	0.1244	Na-Cl	1.135
80	3679	0.07328	0.9982	19.3333333	0.03748	0.3056	Na-CO3	0.9985
81	9200	0.1459	0.9959	26	0.01305	0.04996	Na-Cl	1.002
82	153794	3.705	0.9194	3334.61538	0.5617	0.1094	Na-Cl	1.108
83	222504	6.081	0.8937	2213.04348	1.085	0.1516	Na-SO4	1.163
84	242448	6.58	0.8801	706.5	1.592	0.2071	Na-SO4	1.18
85	382768	12.21	0.71	1908.33333	1.175	0.09843	Na-SO4	1.306
86	262.3	0.003571	0.9999	2.022	0.001353	0.2175	Na-HCO3	0.9962
87	2074	0.03335	0.999	27.52	0.0161	0.2663	Na-HCO3	0.9974
88	941.6	0.01415	0.9996	22.3333333	0.006197	0.2424	Na-HCO3	0.9966
89	443.9	0.006858	0.9998	1.04538462	0.004035	0.3654	Na-HCO3	0.9963
90	594.4	0.007589	0.9997	1.87375	0.003896	0.2977	Na-HCO3	0.9964
91	7487	0.1367	0.9967	6.97954545	0.04742	0.2128	Na-CO3	1.001
92	5829	0.1109	0.9971	116.5	0.06232	0.3264	Na-Cl	0.9999
93	273.9	0.004543	0.9999	1.19	0.002059	0.2915	Na-HCO3	0.9962
94	434.1	0.004983	0.9999	3.66875	-0.003524	-0.4262	Ca-HCO3	0.9963
95	599.2	0.01121	0.9998	0.713125	0.005634	0.3485	Na-HCO3	0.9964
96	242	0.003699	0.9999	0.95355556	0.0009753	0.1805	Na-HCO3	0.9962
97	568.7	0.008487	0.9998	1.40470588	0.002106	0.1571	Na-HCO3	0.9964
98	244.4	0.003158	0.9999	1.08033333	-0.0003519	-0.08129	Ca-HCO3	0.9962
99	848.3	0.01862	0.9996	0.4738	0.01582	0.5805	Na-HCO3	0.9966
100	693.6	0.01209	0.9998	0.83564103	0.002864	0.1732	Mg-HCO3	0.9965
101	290.3	0.004379	0.9999	1.18957143	-0.001182	-0.2052	Ca-HCO3	0.9962
102	312.2	0.005121	0.9999	1.09416667	0.002319	0.2964	Na-HCO3	0.9962
103	303.6	0.004661	0.9999	1.05909091	0.002245	0.3152	Na-HCO3	0.9962
104	294.9	0.004926	0.9999	0.89538462	0.002127	0.2939	Na-HCO3	0.9962
105	2015	0.03649	0.999	8.71166667	0.02597	0.4051	Na-HCO3	0.9974
106	185.3	0.0033	0.9999	0.554	0.001366	0.3243	Ca-HCO3	0.9961
107	210.9	0.003808	0.9999	0.44521429	0.00215	0.445	Ca-HCO3	0.9962
108	2058	0.02995	0.9991	9.78285714	0.0131	0.2444	Na-HCO3	0.9974
109	178.5	0.00287	0.9999	0.81266667	0.0008345	0.2113	Ca-HCO3	0.9961
110	1696	0.0311	0.9991	10.6225	0.02366	0.4331	Na-HCO3	0.9972
111	774.1	0.01257	0.9997	1.481	0.007025	0.338	Na-HCO3	0.9965
115	2220	0.03754	0.9988	2007000000	0.01856	0.2577	Na-Cl	0.9975

Table G. part 4: *Continued*

Sequence # (sample #)	Dissolved solids mg/kg	Ionic strength molal	Activity of H2O	ALK/(Ca+Mg)	Charge imbalance eq/kg	Charge imbalance error percentage	Water type	Fluid density g/cm³
116	6509	0.1193	0.9964	9.86125	0.05279	0.2359	Na-Cl	1
117	2945	0.04666	0.9985	8.52619048	0.01944	0.2154	Na-Cl	0.998
118	17159.6	0.303	0.9911	25.0875	-0.005156	-0.009279	Na-Cl	1.008
119	16051.1	0.295	0.9912	26.7	0.1141	0.2082	Na-Cl	1.007
120	6093	0.1112	0.9966	13.376	0.039	0.187	Na-Cl	1
121	5749	0.1038	0.9969	13.876	0.03312	0.1703	Na-Cl	0.9999
125	1003	0.01672	0.9995	1.41625	0.006185	0.2171	Na-HCO3	0.9967
126	4127	0.07127	0.9977	3.76823529	0.04239	0.3082	Na-Cl	0.9988
127	2732	0.04694	0.9985	4.08526316	0.04352	0.4889	Na-HCO3	0.9978
128	2704	0.05131	0.9986	1.19811321	0.03513	0.3837	Na-Cl	0.9978
129	778.6	0.02196	0.9996	0.27101449	0.01443	0.4915	Mg-HCO3	0.9965
130	781.9	0.02299	0.9996	0.23441558	0.01605	0.5312	Mg-HCO3	0.9965
131	896.7	0.02765	0.9996	0.26444444	0.01826	0.544	Mg-HCO3	0.9966
132	634.7	0.02075	0.9997	0.16337662	0.0147	0.5808	Mg-HCO3	0.9964
133	625.7	0.01611	0.9997	0.28212766	0.01013	0.4521	Mg-Cl	0.9964
134	532.9	0.008527	0.9998	1.41	0.003111	0.2212	Na-HCO3	0.9964
135	3358	0.07396	0.9988	0.425625	0.009227	0.09143	Na-SO4	0.9983
136	1568	0.02502	0.9993	3.95642857	0.007508	0.1663	Na-HCO3	0.9971
137	559.5	0.01039	0.9997	0.665	0.005001	0.3085	Na-HCO3	0.9964
138	2351	0.0379	0.9988	4.43357143	0.01988	0.2745	Na-Cl	0.9976
139	44967.4	0.8967	0.9771	0.02078467	0.002896	0.001951	Na-Cl	1.027
140	27452.7	0.5488	0.9864	0.01397899	-0.005942	-0.00654	Na-Cl	1.015
141	14288.4	0.2787	0.993	0.09236453	0.003094	0.006597	Na-Cl	1.006
142	66363.2	1.359	0.9696	0.05624685	-0.05162	-0.02473	Na-Cl	1.042
143	30354.6	0.5766	0.9848	0.07851772	0.005106	0.005153	Na-Cl	1.017
144	32145.5	0.6083	0.9842	0.07427948	-0.02579	-0.02493	Na-Cl	1.018
145	21135.2	0.389	0.9894	0.09055814	-0.006428	-0.009372	Na-Cl	1.01
146	68694.5	1.368	0.9615	0.02386052	-0.05453	-0.02369	Na-Cl	1.044
147	11331.5	0.2272	0.9956	0.11543046	-0.002572	-0.007623	Na-SO4	1.004
148	116943	2.48	0.9426	0.08267635	0.01826	0.005027	Na-Cl	1.079
149	10921.5	0.211	0.996	0.30167364	0.009763	0.03142	Na-SO4	1.003
150	117783	2.347	0.9265	0.16936813	-0.001435	-0.000365	Na-Cl	1.08
151	58324	1.103	0.9686	0.15632184	-0.006002	-0.003132	Na-Cl	1.036
152	27795.4	0.5794	0.9875	13.2873563	0.1721	0.19	Na-CO3	1.015
153	1421	0.0243	0.9992	0.21528302	0.0007226	0.01612	Na-Cl	0.997
154	28212.7	0.5143	0.9844	0.04533702	-0.01279	-0.01346	Na-Cl	1.015
155	13764.9	0.2481	0.9925	0.07225528	-0.0041	-0.008849	Na-Cl	1.005
156	102106	1.946	0.9366	0.07062324	-0.1161	-0.0341	Na-Cl	1.068

Table G. part 4: *Continued*

Sequence # (sample #)	Dissolved solids mg/kg	Ionic strength molal	Activity of H2O	ALK/(Ca+Mg)	Charge imbalance eq/kg	Charge imbalance error percentage	Water type	Fluid density g/cm³
157	320947	8.298	0.6675	0.02728552	-0.2504	-0.02319	Na-Cl	1.248
158	12534.2	0.2225	0.9932	0.13049482	-0.006933	-0.01664	Na-Cl	1.004
159	546.6	0.01032	0.9998	0.35152381	0.001898	0.133	Na-Cl	0.9964
160	11942.2	0.2159	0.9936	0.11142035	0.002318	0.005802	Na-Cl	1.004
161	1401	0.02656	0.9993	0.31609677	0.001047	0.0237	Na-Cl	0.997
162	14192.8	0.254	0.9923	0.08372361	-0.01056	-0.0223	Na-Cl	1.006
163	142748	2.927	0.9041	0.02708525	-0.1841	-0.03848	Na-Cl	1.099
164	178.8	0.002886	0.9999	0.10589286	0.00007292	0.01489	Na-Cl	0.9961
165	223762	5.02	0.8169	0.02676757	-0.1453	-0.01927	Na-Cl	1.164
166	354.4	0.005782	0.9998	0.42112903	0.0002921	0.02865	Na-Cl	0.9962
167	252720	5.947	0.7788	0.01243309	-0.302	-0.03555	Na-Cl	1.189
168	395578	10.5	0.6303	0.02230561	3.293	0.267	Na-Cl	1.318
169	661	0.01134	0.9997	0.42311475	0.00109	0.05607	Na-Cl	0.9965
170	1331	0.02362	0.9993	0.34971154	0.001629	0.03909	Na-Cl	0.9969
171	3369	0.06159	0.9983	0.20904918	0.00324	0.02971	Na-Cl	0.9983
172	7686	0.1388	0.996	0.19709497	0.001633	0.006502	Na-Cl	1.001
173	23952.2	0.4379	0.9877	0.29278467	-0.005186	-0.006628	Na-Cl	1.012
174	58324.2	1.103	0.9686	0.15686918	-0.00603	-0.003147	Na-Cl	1.036
175	118369	2.363	0.9264	0.16792196	-0.01265	-0.003208	Na-Cl	1.081
176	467.3	0.01466	0.9998	0.1316129	0.009612	0.5332	Mg-Cl	0.9963
177	116943	2.48	0.9426	0.08267635	0.01826	0.005027	Na-Cl	1.079
178	320592	8.286	0.6681	0.02728552	-0.2404	-0.02228	Na-Cl	1.248
179	260608	6.924	0.8378	2181.11111	1.371	0.1622	Na-Cl	1.195
180	8503	0.148	0.9954	2.38021201	0.01223	0.04374	Na-Cl	1.002
181	28673.5	0.5252	0.9843	0.08788274	-0.02418	-0.0252	Na-Cl	1.016
182	118369	2.363	0.9264	0.16799818	-0.01269	-0.003218	Na-Cl	1.081
183	403.9	0.007536	0.9999	0.06075238	0.0003068	0.03166	Na-SO4	0.9963
184	22551.4	0.4287	0.9885	0.04678095	-0.01718	-0.02302	Na-Cl	1.011
185	134225	2.879	0.9265	710	0.1084	0.02495	Na-Cl	1.093
186	32145.5	0.6083	0.9842	0.07427948	-0.02579	-0.02493	Na-Cl	1.018
187	64591	1.315	0.9667	0.06461194	-0.04728	-0.02228	Na-Cl	1.041
188	34199.4	0.7834	0.9824	433.870968	0.3066	0.246	Na-CO3	1.019
189	28439.8	0.6068	0.9858	126.61194	0.1955	0.198	Na-Cl	1.015
190	343.4	0.005191	0.9999	0.65361702	0.001298	0.1575	Na-H3SiO4	0.9962
191	9626	0.1673	0.995	1.49382022	-0.001147	-0.003676	Na-Cl	1.003
192	72218.2	1.412	0.9616	0.15268226	-0.02182	-0.009252	Na-Cl	1.046
193	18077.8	0.3483	0.9923	0.3020979	0.0008256	0.001491	Na-Cl	1.008
194	337616	9.093	0.681	0.08705572	-0.3846	-0.03548	Na-Cl	1.264

Table G. part 4: *Continued*

Sequence # (sample #)	Dissolved solids mg/kg	Ionic strength molal	Activity of H2O	ALK/(Ca+Mg)	Charge imbalance eq/kg	Charge imbalance error percentage	Water type	Fluid density g/cm³
195	35121.3	0.6812	0.9825	0.03241201	-0.01471	-0.01284	Na-Cl	1.02
196	18219.5	0.3443	0.9903	0.04458015	-0.01408	-0.02287	Na-Cl	1.008
197	120733	2.599	0.9219	0.01336816	-0.04853	-0.01176	Na-Cl	1.082
199	19849.4	0.3685	0.9902	6.34632035	0.09481	0.1474	Na-Cl	1.009
200	19587.2	0.3843	0.9904	6.37349398	0.08815	0.1362	Na-Cl	1.009
201	18963.1	0.3627	0.9906	6.50440529	0.09342	0.1499	Na-Cl	1.009
202	18035	0.3387	0.9909	8.54076087	0.0864	0.1457	Na-Cl	1.008
203	8610	0.1279	0.9966	6.94513716	-0.1902	-0.8504	K-Cl	1.002
204	19005.3	0.3632	0.9907	6.94063927	0.07459	0.1202	Na-Cl	1.009
205	18840.3	0.362	0.9907	6.58314856	0.08843	0.1424	Na-Cl	1.009
206	19119.2	0.3718	0.9906	6.77510917	0.086	0.1358	Na-Cl	1.009
207	19378.3	0.3772	0.9904	6.86363636	0.08606	0.1342	Na-Cl	1.009
208	1329	0.03108	0.9994	0.37759259	0.005742	0.1325	Na-SO4	0.9969
209	6333	0.1212	0.9962	0.11205298	0.1018	0.4361	Na-Cl	1
210	18632.1	0.3347	0.9896	0.0935814	0.04594	0.07246	Na-Cl	1.009
211	24485.6	0.4837	0.9867	0.01396215	0.05664	0.06687	Na-Cl	1.013
212	26409.7	0.4876	0.985	0.07781955	0.08484	0.09314	Na-Cl	1.014
213	39252.3	0.7669	0.9777	0.02075783	0.1157	0.08484	Na-Cl	1.023
214	48043.1	0.9316	0.9715	0.05504911	0.2945	0.1739	Na-Cl	1.029
215	64545.1	1.27	0.962	0.02317939	0.03343	0.01509	Na-Cl	1.041
216	90409.7	1.799	0.9455	0.0792073	0.5701	0.1851	Na-Cl	1.06
217	220785	4.918	0.8176	0.02672786	-0.0877	-0.01172	Na-Cl	1.162
218	318676	8.2	0.669	0.02724552	-0.2028	-0.01887	Na-Cl	1.246
219	188551	4.057	0.855	0.02566028	0.2749	0.04273	Na-Cl	1.135
220	160626	3.366	0.8837	0.05198653	0.3607	0.06554	Na-Cl	1.113
221	153475	3.198	0.8901	0.03397436	0.3966	0.07515	Na-Cl	1.108
222	144385	2.974	0.8986	0.04042205	0.3924	0.07899	Na-Cl	1.1
223	135815	2.786	0.9058	0.03724114	0.5059	0.1076	Na-Cl	1.094
224	139948	2.892	0.9019	0.05751304	0.6183	0.1273	Na-Cl	1.097
225	320.9	0.01013	0.9999	0.33957845	0.005435	0.4674	Mg-HCO3	0.9962
226	319.5	0.00948	0.9999	0.37979798	0.005073	0.4575	Mg-HCO3	0.9962
227	321.9	0.008791	0.9999	0.42707182	0.004251	0.4076	Ca-HCO3	0.9962
228	837.8	0.02431	0.9997	0.44229249	0.01156	0.4012	Mg-HCO3	0.9966
229	2583	0.07585	0.9991	0.44065093	0.03578	0.3984	Mg-HCO3	0.9977
230	1709	0.03979	0.9994	0.72062842	0.008185	0.1626	Mg-HCO3	0.9972
232	2672	0.06126	0.9991	0.67043078	0.01678	0.2174	Mg-HCO3	0.9978
234	3068	0.09225	0.9989	0.43599894	0.04445	0.4069	Mg-HCO3	0.9981
235	5218	0.137	0.9982	0.52844619	0.05304	0.3196	Mg-HCO3	0.9995

Table G. part 4: *Continued*

Sequence # (sample #)	Dissolved solids mg/kg	Ionic strength molal	Activity of H2O	ALK/(Ca+Mg)	Charge imbalance eq/kg	Charge imbalance error percentage	Water type	Fluid density g/cm³
236	46.36	0.001227	1	0.39632653	0.00062	0.4261	Ca-HCO3	0.996
237	827.1	0.02431	0.9997	0.4001007	0.01173	0.4033	Mg-HCO3	0.9966
238	648.8	0.018	0.9998	0.4529745	0.007834	0.3568	Mg-HCO3	0.9964
239	320.9	0.009684	0.9999	0.41170483	0.004957	0.4306	Mg-HCO3	0.9962
240	58.24	0.001328	1	0.54355556	0.0005985	0.3529	Ca-HCO3	0.996
241	294.6	0.007484	0.9999	0.55017422	0.002764	0.3006	Mg-HCO3	0.9962
242	84.35	0.002384	1	0.43934783	0.001108	0.3875	Mg-HCO3	0.9961
243	36.64	0.001136	1	0.27170732	0.0006907	0.5069	Mg-HCO3	0.996
244	334.7	0.009931	0.9999	0.375	0.004962	0.4294	Mg-HCO3	0.9962
245	1741	0.04874	0.9994	0.49542683	0.01949	0.3342	Mg-HCO3	0.9972
246	5696	0.1582	0.9981	0.51049828	0.063	0.3318	Mg-HCO3	0.9998
247	3674	0.09175	0.9988	0.58347776	0.02933	0.2601	Mg-HCO3	0.9985
248	3081	0.0855	0.9989	0.44175286	0.03611	0.3556	Mg-HCO3	0.9981
249	3082	0.08474	0.9989	0.45365717	0.03584	0.3537	Mg-HCO3	0.9981
250	22786.2	0.5648	0.9918	145.578231	-0.1098	-0.1461	Na-CO3	1.012
251	16662.8	0.4287	0.9933	88.0722892	-0.005211	-0.008924	Na-CO3	1.007
252	23756.9	0.5879	0.9913	584.054054	-0.09398	-0.1189	Na-CO3	1.012
253	16671.8	0.429	0.9933	88.1325301	-0.005558	-0.009513	Na-CO3	1.007
254	35988.6	0.9071	0.9873	155.527638	-0.1673	-0.1402	Na-CO3	1.021
255	13827.6	0.3603	0.9946	85.8646617	-0.03308	-0.06851	Na-CO3	1.005
256	48472.6	1.25	0.9824	527.972973	-0.09763	-0.05957	Na-CO3	1.029
257	45840.9	1.188	0.9816	259.76	0.1224	0.07604	Na-CO3	1.028
258	393.3	0.006676	0.9999	1.15310734	0.0003187	0.03393	Mg-HCO3	0.9963
259	1479	0.02795	0.9995	1.08047945	0.0006045	0.01574	Mg-HCO3	0.997
260	1653	0.03228	0.9994	1.03198339	0.004905	0.1086	Mg-HCO3	0.9971
261	10722.5	0.1652	0.9952	22.877193	0.08089	0.2653	Na-HCO3	1.003
262	2717	0.03582	0.9989	32.1086957	0.007124	0.1039	Na-HCO3	0.9978
263	1934	0.02781	0.9992	3.10512129	0.00122	0.02554	Na-HCO3	0.9973
264	5270	0.07854	0.9977	7.57014925	0.03764	0.2592	Na-HCO3	0.9996
265	9313	0.1605	0.996	31.7630058	0.04245	0.1563	Na-HCO3	1.002
266	4381	0.07027	0.9981	59.4285714	0.02011	0.1625	Na-HCO3	0.999
267	5461	0.08711	0.9977	10.2484663	0.016	0.1075	Na-HCO3	0.9997
268	4981	0.07222	0.9978	13.9705882	0.03694	0.2703	Na-HCO3	0.9994
269	30365.8	0.4818	0.9876	289.193548	0.08805	0.1058	Na-HCO3	1.017
271	12867.2	0.2266	0.9957	3.677E+10	-0.3458	-1	Na-Cl	1.005
272	42696.8	0.8408	0.9788	7.175E+10	0.02743	0.01947	Na-Cl	1.025
274	57462.7	1.165	0.9711	9.775E+10	0.03113	0.0163	Na-Cl	1.036
275	57886.3	1.151	0.9707	3822	0.04358	0.02283	Na-Cl	1.036

Table G. part 4: *Continued*

Sequence # (sample #)	Dissolved solids mg/kg	Ionic strength molal	Activity of H2O	ALK/(Ca+Mg)	Charge imbalance eq/kg	Charge imbalance error percentage	Water type	Fluid density g/cm³
278	51018.3	1.024	0.9745	8.775E+10	0.03703	0.02187	Na-Cl	1.031
283	21957.6	0.4263	0.9892	3.69E+10	-0.01432	-0.01976	Na-Cl	1.011
284	21871.1	0.4159	0.9891	3.346E+10	0.02273	0.03154	Na-Cl	1.011
285	20336.2	0.3857	0.9899	719.666667	0.01711	0.02564	Na-Cl	1.01
287	7914	0.1385	0.9963	477.571429	0.01094	0.04534	Na-Cl	1.001
288	3371	0.05517	0.9984	230.666667	0.002708	0.02754	Na-HCO3	0.9983
289	7045	0.1218	0.9968	432.428571	0.006131	0.02903	Na-Cl	1.001
290	1239	0.01727	0.9995	9.33333333	0.003866	0.1253	Na-HCO3	0.9968
291	1617	0.02292	0.9993	15.5520833	0.0007131	0.01713	Na-HCO3	0.9971
292	1108	0.015	0.9996	9.30612245	-0.0004558	-0.01725	Na-HCO3	0.9968
293	1690	0.02437	0.9993	15.436	0.0006917	0.01582	Na-HCO3	0.9971
294	1169	0.01585	0.9995	9.9745098	0.0000855	0.002981	Na-HCO3	0.9968
295	1113	0.01504	0.9995	9.52040816	-0.000609	-0.02292	Na-HCO3	0.9968
296	1058	0.0161	0.9996	1.84237805	-0.000185	-0.007289	Na-HCO3	0.9967
297	900.7	0.01492	0.9996	4.66140351	0.0005583	0.02319	Na-HCO3	0.9966
298	33061.3	0.644	0.983	4.751E+10	0.06345	0.05717	Na-Cl	1.019
299	470.4	0.007298	0.9998	1.51468531	-0.0004406	-0.04034	Na-HCO3	0.9963
300	984.1	0.01531	0.9996	1.88774704	0.001432	0.05767	Na-HCO3	0.9967
301	143.2	0.001993	1	1.19388889	-0.0004311	-0.1641	Ca-HCO3	0.9961
302	216	0.003408	0.9999	1.285	-0.0003775	-0.07928	Ca-HCO3	0.9962
303	54771.6	1.774	0.9683	0.01735096	1.074	0.4452	Mg-Cl	1.034
304	9742	0.3409	0.9948	0.04471366	0.3345	0.7143	Mg-Cl	1.003
306	7638	0.3022	0.997	0.14566584	0.2147	0.6226	Mg-Cl	1.001
307	4051	0.1736	0.998	0.07501488	0.1886	0.8825	Mg-HCO3	0.9987
308	12478.6	0.2017	0.9956	1.57988285	0.02175	0.07021	Na-HCO3	1.004
309	4571	0.1522	0.9975	0.13584465	0.171	0.8099	Na-Cl	0.9991
310	5021	0.2108	0.9978	0.05224381	0.2129	0.8504	Mg-Cl	0.9994
311	2165	0.1025	0.999	0.06632517	0.1029	0.8837	Mg-HCO3	0.9975
313	1910	0.07458	0.999	0.12287962	0.07041	0.7678	Mg-HCO3	0.9973
314	1091	0.04345	0.9995	0.13420139	0.04009	0.766	Mg-HCO3	0.9967
315	1004	0.04093	0.9995	0.10263631	0.03903	0.8013	Mg-HCO3	0.9967
316	1357	0.03324	0.9993	0.4153074	0.02708	0.5371	Na-HCO3	0.9969
317	692.7	0.0244	0.9996	0.17908788	0.02357	0.768	Mg-HCO3	0.9965
319	774.1	0.02374	0.9997	0.36230366	0.01459	0.5068	Mg-HCO3	0.9965
320	530.9	0.02007	0.9998	0.22942529	0.01507	0.6571	Mg-HCO3	0.9964
321	822.1	0.01828	0.9996	0.56181818	0.012	0.4327	Na-HCO3	0.9966
322	905.9	0.02041	0.9996	0.62547009	0.01407	0.483	Mg-HCO3	0.9966
323	613.2	0.02045	0.9997	0.30313589	0.01258	0.5279	Mg-HCO3	0.9964

Table G. part 4: *Continued*

Sequence # (sample #)	Dissolved solids mg/kg	Ionic strength molal	Activity of H2O	ALK/(Ca+Mg)	Charge imbalance eq/kg	Charge imbalance error percentage	Water type	Fluid density g/cm³
325	894.6	0.01666	0.9996	1.26363636	0.00699	0.2708	Na-HCO3	0.9966
329	645.2	0.01941	0.9998	0.36952381	0.01007	0.4505	Mg-HCO3	0.9964
330	455.3	0.01418	0.9998	0.33276158	0.00932	0.5517	Mg-HCO3	0.9963
331	613.7	0.01372	0.9997	0.57492877	0.008205	0.4076	Na-HCO3	0.9964
332	532.7	0.01581	0.9998	0.32076677	0.008865	0.478	Mg-HCO3	0.9964
333	814.7	0.01765	0.9997	0.79501718	0.004677	0.1969	Mg-HCO3	0.9966
334	480.8	0.01254	0.9998	0.49023256	0.007696	0.4662	Mg-HCO3	0.9963
335	739.9	0.01474	0.9997	0.91831579	0.001537	0.07859	Mg-HCO3	0.9965
336	566.1	0.01237	0.9998	0.81325581	0.002615	0.161	Mg-HCO3	0.9964
337	555.5	0.01205	0.9998	0.80920097	0.002668	0.1681	Mg-HCO3	0.9964
338	391.9	0.009471	0.9999	0.54314869	0.004039	0.3382	Mg-HCO3	0.9963
340	468.3	0.01007	0.9998	0.79734513	0.001951	0.1468	Mg-HCO3	0.9963
341	352	0.008071	0.9999	0.54924812	0.002878	0.2733	Mg-HCO3	0.9962
342	569.5	0.01122	0.9998	0.98774373	0.00071	0.04711	Mg-HCO3	0.9964
343	284.1	0.007814	0.9999	0.38612903	0.003532	0.3878	Mg-HCO3	0.9962
345	480	0.009531	0.9998	0.97035831	0.001064	0.0825	Mg-HCO3	0.9963
346	370.1	0.007338	0.9999	0.90938776	0.0008192	0.08404	Mg-HCO3	0.9963
347	342.3	0.003123	0.9999	1118500000	-0.005314	-1	H-HCO3	0.9962
348	335.6	0.006719	0.9999	0.89488372	0.001094	0.121	Mg-HCO3	0.9962
349	271.1	0.005654	0.9999	0.87043011	0.001072	0.1421	Mg-HCO3	0.9962
352	265.2	0.004987	0.9999	0.91592357	0.0001982	0.03028	Ca-HCO3	0.9962
353	245.2	0.004646	0.9999	0.93154362	0.0002408	0.03905	Ca-HCO3	0.9962
356	9530	0.1937	0.9958	47.2605042	0.02941	0.09656	Na-CO3	1.002
357	4197	0.07072	0.9982	44.0192308	0.009806	0.0808	Na-HCO3	0.9988
358	16072.8	0.2948	0.9918	39.5132743	0.02443	0.04635	Na-Cl	1.007
359	53903.6	1.106	0.9732	128.159509	0.1488	0.08263	Na-Cl	1.033
361	12.6	0.0002039	1	0.30883333	0.00007372	0.2974	Ca-SO4	0.996
368	1371	0.02054	0.9993	6.40740741	0.003207	0.08358	Na-Cl	0.9969
370	546	0.008113	0.9998	1.68627451	-0.000378	-0.03085	Na-HCO3	0.9964
371	802	0.01145	0.9997	2.22272727	-0.0007453	-0.04111	Na-HCO3	0.9965
372	328	0.004879	0.9999	1.47474747	-0.0003288	-0.04632	Ca-HCO3	0.9962
373	19062.9	0.3546	0.9895	3.58394161	0.1172	0.1789	Na-Cl	1.009
374	4918	0.08323	0.9975	2.18259023	0.006616	0.04274	Na-Cl	0.9993
375	191.8	0.002746	0.9999	1.66583333	-0.000413	-0.1018	Na-HCO3	0.9961
376	319.3	0.005898	0.9999	0.69792593	0.0007491	0.08777	Na-HCO3	0.9962
377	5963	0.102	0.997	3.7	0.03218	0.1709	Na-Cl	1
378	5969	0.1029	0.997	3.80846325	0.03096	0.1639	Na-Cl	1
381	161.5	0.002565	0.9999	1.1159322	-0.0002276	-0.06407	Ca-HCO3	0.9961

Table G. part 4: *Continued*

Sequence # (sample #)	Dissolved solids mg/kg	Ionic strength molal	Activity of H2O	ALK/(Ca+Mg)	Charge imbalance eq/kg	Charge imbalance error percentage	Water type	Fluid density g/cm³
382	46627.4	0.912	0.9722	0.07302709	0.2201	0.133	Na-Cl	1.028
383	21873.7	0.4159	0.9891	743.555556	0.02288	0.03175	Na-Cl	1.011
384	10583.7	0.1942	0.9948	58.2711864	0.0002529	0.0007429	Na-Cl	1.003
385	179.5	0.002773	0.9999	0.75018868	-0.0002912	-0.07773	Na-HCO3	0.9961
386	235402	5.82	0.7864	0.00686609	0.3897	0.04698	Na-Cl	1.174
387	36422.3	0.6853	0.9793	0.05985483	0.01961	0.01571	Na-Cl	1.021
388	22708.6	0.4261	0.9877	0.0465198	0.01261	0.01638	Na-Cl	1.011
389	3453	0.06469	0.9982	0.24959481	0.0006502	0.005608	Na-Cl	0.9983
390	8099	0.1578	0.9957	0.09848485	0.02378	0.08546	Na-Cl	1.001
392	527.9	0.00934	0.9998	0.96178571	-0.002204	-0.1668	Ca-HCO3	0.9964
393	819.6	0.0152	0.9997	0.84404145	-0.007332	-0.3232	Mg-Cl	0.9966
394	844	0.01975	0.9997	0.34399421	0.001443	0.05568	Ca-Cl	0.9966
395	366.5	0.006812	0.9999	0.90328638	0.0002646	0.02866	Ca-HCO3	0.9963
396	258336	6.108	0.7611	0.00345685	0.05731	0.006468	Na-Cl	1.193
397	434.6	0.01076	0.9998	0.52807018	0.005227	0.38	Mg-HCO3	0.9963
398	3635	0.07212	0.9981	0.89271739	0.04881	0.3894	Na-Cl	0.9985
399	3468	0.06781	0.9982	1.12396694	0.06137	0.5304	Na-HCO3	0.9983
400	5262	0.1662	0.9973	0.17212577	0.1849	0.7977	Na-HCO3	0.9996
401	34924	1.438	0.9833	0.03885193	1.34	0.7496	Mg-Cl	1.02
402	7179	0.2894	0.9964	0.05888604	0.3061	0.8324	Mg-Cl	1.001
403	7907	0.3343	0.9964	0.07442471	0.3419	0.8436	Mg-Cl	1.001
404	90007.6	3.241	0.9463	0.01547027	3.761	0.8558	Na-Cl	1.059
405	1511	0.05442	0.9992	0.11321321	0.05294	0.7602	Mg-Cl	0.997
406	14321.4	0.5204	0.9925	0.03325012	0.5216	0.7446	Mg-Cl	1.006
408	1732	0.05145	0.9992	0.32669153	0.03862	0.5811	Mg-HCO3	0.9972
409	822.9	0.02203	0.9996	0.38261494	0.01742	0.5733	Na-HCO3	0.9966
410	12787.2	0.3174	0.9929	0.07375121	0.173	0.3429	Na-Cl	1.005
411	1607	0.03496	0.9992	0.58128272	0.02479	0.4499	Na-HCO3	0.9971
412	18540.4	0.5163	0.9896	0.06878193	0.5036	0.6345	Na-Cl	1.009
413	1972	0.09484	0.999	0.05668006	0.1006	0.9085	Mg-HCO3	0.9973
414	4854	0.1152	0.9973	0.28755264	0.1074	0.5719	Na-Cl	0.9993
415	1647	0.02506	0.9993	3.22229508	0.0009118	0.0216	Na-HCO3	0.9971
416	34277.9	0.9884	0.9802	0.0291116	1.02	0.6767	Na-Cl	1.019
417	2330	0.03933	0.999	2.12523364	0.0224	0.3326	Na-HCO3	0.9976
418	1293	0.05072	0.9994	0.13363318	0.04853	0.7857	Mg-HCO3	0.9969
419	5531	0.09791	0.9971	3.78139535	0.06972	0.3847	Na-Cl	0.9997
420	9772	0.2158	0.9945	0.54505716	0.246	0.6655	Na-Cl	1.003
421	11027.5	0.5022	0.9949	0.01935416	0.5606	0.9144	Mg-Cl	1.003

Table G. part 4: *Continued*

Sequence # (sample #)	Dissolved solids mg/kg	Ionic strength molal	Activity of H2O	ALK/(Ca+Mg)	Charge imbalance eq/kg	Charge imbalance error percentage	Water type	Fluid density g/cm³
422	435.8	0.01173	0.9998	0.41425486	0.007067	0.486	Mg-HCO3	0.9963
423	4104	0.07003	0.9979	7.2748538	0.04618	0.3505	Na-HCO3	0.9988
424	1030	0.03875	0.9995	0.15801527	0.03278	0.7052	Mg-HCO3	0.9967
425	1945	0.03369	0.9992	1.63513514	0.01216	0.2273	Na-HCO3	0.9973
426	511.1	0.01461	0.9998	0.42200358	0.008226	0.4524	Mg-HCO3	0.9964
427	1312	0.02913	0.9994	0.63531599	0.0179	0.4192	Na-HCO3	0.9969
428	499.7	0.01395	0.9998	0.3475	0.008219	0.4647	Mg-HCO3	0.9963
429	14256.6	0.2838	0.9923	2.63969171	0.2472	0.4919	Na-Cl	1.006
430	10460.7	0.5759	0.9957	0.00995788	0.6159	0.9439	Mg-Cl	1.003
431	10943.5	0.2819	0.9938	0.13838213	0.2943	0.6498	Na-Cl	1.003
432	3281	0.06711	0.9983	0.76724287	0.05383	0.4833	Na-Cl	0.9982
433	66262.1	2.563	0.9639	0.00733251	3.109	0.9108	Na-Cl	1.042
434	2213	0.08876	0.9989	0.10389157	0.09111	0.8486	Mg-Cl	0.9975
435	502.4	0.01285	0.9998	0.48387755	0.006599	0.408	Mg-HCO3	0.9963
436	394.9	0.01064	0.9998	0.44939467	0.005526	0.4201	Mg-HCO3	0.9963
437	2792	0.06268	0.9984	0.57758805	0.07272	0.6825	Na-HCO3	0.9979
439	535	0.01353	0.9998	0.5039749	0.007022	0.3973	Mg-HCO3	0.9964
440	2355	0.0688	0.9987	0.02759439	0.05767	0.5726	Na-Cl	0.9976
441	2671	0.1056	0.9986	0.11441802	0.1102	0.8339	Mg-HCO3	0.9978
442	5782	0.2689	0.9973	0.05355992	0.2926	0.9101	Mg-HCO3	0.9999
443	7486	0.1268	0.996	5.16455696	0.004587	0.01898	Na-Cl	1.001
444	2249	0.05313	0.9989	0.38068264	0.03307	0.4129	Na-Cl	0.9975
445	649.4	0.01731	0.9997	0.39178832	0.01373	0.575	Mg-HCO3	0.9964
446	2377	0.03582	0.999	3.76404494	0.007511	0.1199	Na-HCO3	0.9976
447	979.8	0.03206	0.9996	0.29357459	0.02266	0.5943	Mg-HCO3	0.9967
448	5131	0.2901	0.9978	0.02422015	0.3011	0.9323	Mg-Cl	0.9995
449	13518.3	0.3932	0.9918	0.04462642	0.5987	0.9509	Na-Cl	1.005
450	2585	0.03784	0.9989	8.53947368	0.001827	0.02644	Na-HCO3	0.9977
451	2509	0.0588	0.9987	0.44361785	0.0484	0.5236	Na-Cl	0.9977
452	1139	0.02726	0.9994	0.4935743	0.01907	0.4759	Na-HCO3	0.9968
453	11873.3	0.3166	0.9933	0.09886243	0.3208	0.6448	Na-Cl	1.004
454	7753	0.1867	0.9954	0.20448859	0.2197	0.6938	Na-Cl	1.001
455	5097	0.1073	0.997	0.81145038	0.1302	0.6772	Na-Cl	0.9994
456	1140	0.02349	0.9995	0.82604341	0.01181	0.334	Na-HCO3	0.9968
457	972.8	0.04099	0.9995	0.07354015	0.04145	0.8411	Mg-HCO3	0.9967
458	9624	0.3288	0.995	0.02815348	0.2428	0.5464	Mg-Cl	1.003
459	3867	0.1775	0.9982	0.06322834	0.1766	0.8502	Mg-Cl	0.9986
460	84214.6	2.991	0.9487	0.01164601	3.025	0.7514	Na-Cl	1.055

Table G. part 4: *Continued*

Sequence # (sample #)	Dissolved solids mg/kg	Ionic strength molal	Activity of H2O	ALK/(Ca+Mg)	Charge imbalance eq/kg	Charge imbalance error percentage	Water type	Fluid density g/cm³
461	29820	0.6142	0.9832	33.6302521	0.5183	0.4751	Na-Cl	1.016
462	5065	0.1325	0.997	0.10988806	0.1339	0.6335	Na-Cl	0.9994
473	7939	0.1616	0.9957	0.14465686	0.0387	0.1379	Na-Cl	1.001
474	8379	0.1718	0.9955	0.1204649	0.04561	0.1533	Na-Cl	1.002
475	10125.2	0.2152	0.9945	0.07205128	0.06038	0.1656	Na-Cl	1.003
476	8476	0.1731	0.9954	0.14861977	0.04184	0.1398	Na-Cl	1.002
477	11381.4	0.2312	0.9937	0.12266773	0.05713	0.1403	Na-Cl	1.004
478	11695.4	0.2384	0.9935	0.1155564	0.05807	0.1386	Na-Cl	1.004
479	11931.7	0.2438	0.9934	0.08856502	0.05894	0.1375	Na-Cl	1.004
480	12349.5	0.2519	0.9932	0.11012248	0.062	0.1401	Na-Cl	1.004
481	12383	0.2526	0.9931	0.0979949	0.06257	0.1407	Na-Cl	1.004
482	11947	0.2426	0.9933	0.09264763	0.0589	0.1374	Na-Cl	1.004
483	11780.9	0.2426	0.9935	0.08124093	0.0581	0.1368	Na-Cl	1.004
484	10945.2	0.2249	0.9939	0.09790535	0.0546	0.1387	Na-Cl	1.003
485	10163.6	0.2081	0.9944	0.09527426	0.0464	0.1271	Na-Cl	1.003
486	5681	0.1218	0.9969	0.11006081	0.04095	0.1984	Na-Cl	0.9998
487	1413	0.03006	0.9993	0.31327273	0.01022	0.2073	Na-Cl	0.997
488	1347	0.02875	0.9993	0.31981651	0.009443	0.2017	Na-Cl	0.9969
489	582.2	0.01127	0.9997	0.76372093	0.002764	0.1512	Na-Cl	0.9964
490	1370	0.02862	0.9993	0.36209524	0.008432	0.1796	Na-Cl	0.9969
522	892.8	0.01651	0.9997	0.83347107	0.00262	0.1172	Mg-HCO3	0.9966
523	13696	0.3487	0.9943	45.3252033	-0.004434	-0.009188	Na-CO3	1.005
524	7257	0.1778	0.9969	19.7862069	-0.001749	-0.007011	Na-CO3	1.001
525	19465	0.4702	0.9922	48.3121019	-0.02193	-0.03333	Na-CO3	1.009
526	76537.4	2.101	0.9667	64.4036697	0.4319	0.1531	Na-CO3	1.05
527	1474	0.02496	0.9995	1.42098139	0.003034	0.08028	Mg-HCO3	0.997
528	1616	0.02622	0.9994	1.48013245	0.0009832	0.02494	Mg-HCO3	0.9971
529	31664.9	0.7174	0.9872	46.5742574	0.01605	0.01553	Na-CO3	1.018
530	37851.5	0.9233	0.9843	77.9834254	0.07054	0.05422	Na-CO3	1.022
531	2574	0.0385	0.9991	1.85800971	-0.004471	-0.0746	Mg-HCO3	0.9977
532	2511	0.03773	0.9991	1.91821561	-0.005305	-0.09017	Mg-HCO3	0.9977
533	2408	0.03686	0.9992	1.87723785	-0.003829	-0.06677	Mg-HCO3	0.9976
534	2767	0.04097	0.999	2.18341709	-0.00505	-0.07687	Na-HCO3	0.9979
535	7016	0.08654	0.9974	10.7085427	-0.0103	-0.06358	Na-HCO3	1.001
536	56718.8	1.495	0.9787	330.896552	-0.1656	-0.08441	Na-CO3	1.035
537	67358.3	1.737	0.9749	732.597403	-0.1963	-0.08616	Na-CO3	1.043
538	66332.4	1.876	0.9756	389.871795	-0.06682	-0.02816	Na-CO3	1.042
539	50461.1	1.367	0.9808	299.930556	-0.1344	-0.07517	Na-CO3	1.031

Table G. part 4: *Continued*

Sequence # (sample #)	Dissolved solids mg/kg	Ionic strength molal	Activity of H2O	ALK/(Ca+Mg)	Charge imbalance eq/kg	Charge imbalance error percentage	Water type	Fluid density g/cm³
540	2172	0.0317	0.9992	2.17105263	-0.005612	-0.1122	Na-HCO3	0.9975
541	2501	0.04647	0.9991	1.09424084	0.006629	0.1	Mg-HCO3	0.9977
542	2387	0.04255	0.999	1.37758433	0.01425	0.2137	Na-HCO3	0.9976
543	37324	0.8298	0.9856	90.1298701	-0.04706	-0.03976	Na-CO3	1.022
544	27625.3	0.6016	0.9895	97.8828829	-0.04665	-0.05414	Na-CO3	1.015
545	38966.2	0.9596	0.9843	78.7467363	0.02049	0.01538	Na-CO3	1.023
546	49510.9	1.241	0.9791	183.265306	0.1466	0.08449	Na-CO3	1.03
547	117985	3.478	0.9551	115.505618	-0.1831	-0.04359	Na-CO3	1.08
548	40348.7	0.9162	0.9843	138.018018	-0.06025	-0.04644	Na-CO3	1.024
549	21959.2	0.3986	0.9913	51.4982578	-0.002026	-0.0032	Na-HCO3	1.011
550	55303.1	1.404	0.9791	176.423077	-0.09435	-0.05042	Na-CO3	1.034
551	87651.3	2.351	0.9652	227.5	0.09021	0.02946	Na-CO3	1.058
552	75260.6	2.097	0.972	120.03643	-0.1593	-0.05996	Na-CO3	1.049
553	75743.3	2.09	0.9714	147.058824	-0.1268	-0.0475	Na-CO3	1.049
554	77014.3	2.137	0.9708	91.8347339	-0.104	-0.03818	Na-CO3	1.05
555	54122.3	1.504	0.9795	328.013699	-0.08417	-0.04337	Na-CO3	1.033
556	70308.6	1.932	0.9725	209.928315	-0.009362	-0.003731	Na-CO3	1.045
557	78497.5	2.02	0.9693	221.392857	-0.03422	-0.01279	Na-CO3	1.051
558	34104.7	0.9044	0.9862	125.73991	0.01511	0.01236	Na-CO3	1.019
559	82047.9	2.269	0.9687	313.378378	-0.06775	-0.0234	Na-CO3	1.054
560	937.9	0.01445	0.9996	2.32765957	0.0007376	0.03113	Na-HCO3	0.9966
561	137373	4.105	0.9461	1266.66667	-0.2337	-0.04781	Na-CO3	1.095
562	74072	2.023	0.9708	309.587629	0.01459	0.005541	Na-CO3	1.048
563	223985	6.781	0.8984	415.529412	0.00975	0.001285	Na-CO3	1.164
564							Na-Cl	1.193
565	280446	6.512	0.8421	277.2	-6.398	-0.7622	Na-Cl	1.213
566	1009	0.01583	0.9996	2.19708333	0.002694	0.1024	Na-HCO3	0.9967
567	214537	6.72	0.9038	341.796875	-0.2747	-0.0369	Na-CO3	1.157
568	233478	7.699	0.8911	525.135135	-0.1015	-0.01231	Na-CO3	1.172
569	56361.6	1.423	0.9759	177.387387	0.1569	0.07896	Na-CO3	1.035
570	266986	8.788	0.8664	241.522491	-0.3431	-0.0376	Na-CO3	1.201
571	209024	6.298	0.9047	498.148148	-0.1553	-0.02167	Na-CO3	1.152
572	670.1	0.01047	0.9997	1.918	0.0005029	0.03032	Na-HCO3	0.9965
573	934.9	0.01573	0.9997	1.27796209	-0.00145	-0.06424	Mg-HCO3	0.9966
574	37547.7	0.9719	0.9863	503.283582	-0.1258	-0.09822	Na-CO3	1.022
575	6962	0.119	0.9973	22.8959276	-0.0175	-0.0925	Na-HCO3	1.001
576	2355	0.03344	0.999	11.7070707	0.001798	0.02912	Na-HCO3	0.9976
577	777.5	0.01586	0.9997	0.82860041	0.002325	0.1077	Mg-HCO3	0.9965

Table G. part 4: *Continued*

Sequence # (sample #)	Dissolved solids mg/kg	Ionic strength molal	Activity of H2O	ALK/(Ca+Mg)	Charge imbalance eq/kg	Charge imbalance error percentage	Water type	Fluid density g/cm³
578	3717	0.05927	0.998	27.8301887	-0.001584	-0.01362	Na-Cl	0.9985
579	70183.9	1.511	0.9624	9.79E+10	0.004153	0.001703	Na-Cl	1.045
580	84750.5	1.858	0.9544	1.2695E+11	-0.001913	-0.0006528	Na-Cl	1.056
581	119139	2.703	0.9345	2.0475E+11	-0.03317	-0.008152	Na-Cl	1.081
582	154954	3.561	0.9096	2.623E+11	-0.03503	-0.00672	Na-Cl	1.109
583	172370	4.027	0.8987	3.122E+11	-0.1501	-0.02617	Na-Cl	1.122
584	199643	4.785	0.8776	3.7165E+11	-0.08647	-0.0131	Na-Cl	1.144
585	256759	6.541	0.8322	5.25E+11	-0.2649	-0.03203	Na-Cl	1.192
586	293538	9.759	0.787	8.31E+11	0.1115	0.01062	Na-CO3	1.224
587	284221	9.339	0.8014	8.265E+11	-0.1993	-0.01968	Na-CO3	1.216
588	311095	10.22	0.7499	7.63E+11	-0.05149	-0.004669	Na-CO3	1.24
589	312836	10.68	0.7569	8.85E+11	-0.05223	-0.004667	Na-CO3	1.241
590	314531	10.49	0.7467	7.885E+11	0.278	0.02479	Na-CO3	1.243
591	315388	10.46	0.7422	7.855E+11	0.05796	0.005165	Na-CO3	1.243
592	317752	10.36	0.7374	7.505E+11	0.3529	0.03138	Na-CO3	1.246
593	311206	10.28	0.75	7.85E+11	0.07483	0.006756	Na-CO3	1.24
594	255262	7.152	0.8339	6.135E+11	0.9103	0.1042	Na-CO3	1.191
595	266176	8.521	0.8291	8.08E+11	0.0227	0.002402	Na-CO3	1.2
596	161332	3.704	0.9173	4.044E+11	0.4106	0.07879	Na-CO3	1.114
597	270639	8.785	0.8174	7.88E+11	0.02312	0.002381	Na-CO3	1.204
598	312151	10.22	0.7463	7.59E+11	0.05485	0.00495	Na-CO3	1.241
599	297160	9.923	0.7807	8.395E+11	0.2103	0.01974	Na-CO3	1.227
600	232565	6.921	0.8636	6.81E+11	-0.08343	-0.01026	Na-CO3	1.172
601	156675	4.433	0.9291	5.275E+11	0.03039	0.005548	Na-CO3	1.11
602	12519.6	0.2509	0.9948	3.3745E+10	0.01076	0.02769	Na-CO3	1.004
603	128907	2.934	0.9378	3.3655E+11	0.1164	0.02776	Na-CO3	1.089
604	144578	3.311	0.9285	3.713E+11	0.0805	0.01723	Na-CO3	1.101
605	277810	8.423	0.7889	5.95E+11	-0.03481	-0.003553	Na-Cl	1.21
606	287190	9.46	0.7962	8.235E+11	-0.07527	-0.007342	Na-CO3	1.218
607	296501	9.617	0.7724	7.505E+11	0.2919	0.02757	Na-CO3	1.227
608	260428	8.25	0.8302	7.52E+11	0.00309	0.0003327	Na-CO3	1.195
609	256754	8.102	0.8354	7.48E+11	-0.1083	-0.01186	Na-CO3	1.192
610	242121	7.52	0.8548	7.35E+11	-0.1227	-0.01429	Na-CO3	1.18
611	199559	5.646	0.8936	5.965E+11	-0.03831	-0.005536	Na-CO3	1.144
612	290205	8.804	0.767	5.73E+11	0.07805	0.007642	Na-Cl	1.221
613	306773	9.522	0.7589	6.975E+11	-0.009776	-0.0009192	Na-CO3	1.236
614	221930	6.14	0.8773	6.465E+11	0.2114	0.02817	Na-CO3	1.163
615	84303.6	2.02	0.9645	1.484E+11	-0.1479	-0.0531	Na-CO3	1.055

Table G. part 4: *Continued*

Sequence # (sample #)	Dissolved solids mg/kg	Ionic strength molal	Activity of H2O	ALK/(Ca+Mg)	Charge imbalance eq/kg	Charge imbalance error percentage	Water type	Fluid density g/cm³
616	180537	4.36	0.8927	1.585E+11	-0.2725	-0.04533	Na-Cl	1.129
617	280224	8.014	0.782	4.0015E+11	-0.6049	-0.06314	Na-Cl	1.212
618	268328	6.665	0.7828	3.985E+10	-0.09152	-0.01033	Na-Cl	1.202
619	128463	2.77	0.9266	6.035E+10	-0.141	-0.0331	Na-Cl	1.088
620	272879	7.483	0.7903	2.968E+11	-0.5427	-0.05894	Na-Cl	1.206
621	9065	0.21	0.9961	1750.49952	-0.006109	-0.01994	Na-CO3	1.002
622	11636.6	0.194	0.9948	2.69E+10	0.0046	0.01355	Na-HCO3	1.004
623	8068	0.1709	0.9966	766.030867	-0.002348	-0.009149	Na-CO3	1.001
624	8116	0.1267	0.9965	522.231097	-0.007429	-0.03288	Na-HCO3	1.001

Table G. part 5: Aqueous chemistry database of alkaline lake waters compiled from published literature, as well as corresponding results from calculations described in chapters 2 and 3, and investigated in detail in chapter 4.

Sequence # (sample #)	CO2(aq) activity	CO3-- activity	Ca++ activity	CaCO3 activity	CaH2PO4+ activity	CaHCO3+ activity	CaHPO4 activity	CaOH+ activity	CaPO4- activity	Cl- activity	H+ activity
1	0.00000654	0.0008654	0.00004953	0.00006073	3.555E-22	4.153E-06	2.576E-18	1.751E-08	3.855E-17	0.07377	3.981E-10
2	0.00001166	0.0009729	0.00003673	0.00005063	4.492E-22	4.358E-06	2.586E-18	1.031E-08	3.073E-17	0.07036	5.012E-10
3	0.00001208	0.00401	8.382E-06	0.00004762	6.655E-23	2.054E-06	7.645E-19	4.69E-09	1.813E-17	0.0681	2.512E-10
4	0.00001026	0.0006186	0.0000549	0.00004811	3.433E-22	4.866E-06	1.682E-18	1.308E-08	1.702E-17	0.1243	5.888E-10
5	1.224E-06	0.02024	5.002E-06	0.0001434	3.382E-25	8.54E-07	2.815E-20	1.924E-08	4.835E-18	0.5089	3.467E-11
6	8.181E-06	0.01636	9.251E-06	0.0002145	3.499E-24	3.683E-06	1.01E-19	1.241E-08	6.013E-18	0.5064	1E-10
7	7.853E-07	0.01845	5.332E-06	0.0001393	1.166E-25	6.902E-07	1.167E-20	2.423E-08	2.41E-18	0.7653	2.884E-11
8	6.468E-07	0.02322	4.226E-06	0.000139	5.532E-26	5.471E-07	6.968E-21	2.333E-08	1.812E-18	0.9496	2.291E-11
9	4.331E-06	0.002271	0.00001242	0.00003997	3.819E-23	0.00000137	5.523E-19	8.721E-09	1.649E-17	0.1325	1.995E-10
10	0.00002599	0.0005936	0.0001834	0.0001542	1.96E-21	0.0000253	5.922E-18	2.684E-08	3.694E-17	0.1656	9.55E-10
11	0.00002306	0.0006382	0.0001613	0.0001459	2.688E-21	0.00002182	8.904E-18	2.61E-08	6.09E-17	0.03313	8.71E-10
12	0.00001562	0.0004517	0.0002334	0.0001493	3.132E-21	0.00002183	1.062E-17	3.853E-08	7.431E-17	0.08039	8.511E-10
13	0.00004053	0.003076	0.00002432	0.000106	4.021E-22	9.556E-06	2.211E-18	6.501E-09	2.509E-17	0.09321	5.248E-10
14	1.222E-06	0.001003	0.00002743	0.00003896	1.516E-23	0.00000106	2.76E-19	2.393E-08	1.037E-17	0.3199	1.585E-10
15	0.00001975	0.01033	4.795E-06	0.00007021	1.817E-23	2.406E-06	2.627E-19	3.358E-09	7.843E-18	0.103	1.995E-10
16	0.000076	0.001584	0.00002279	0.00005116	5.314E-22	8.786E-06	1.533E-18	3.188E-09	9.133E-18	0.1632	1E-09
17	0.00001746	0.0007122	0.0001436	0.0001449	5.508E-22	0.00001762	2.245E-18	2.783E-08	1.889E-17	0.5903	7.079E-10
18	0.00001257	0.000419	0.0002182	0.0001296	4.531E-21	0.00001767	1.646E-17	3.876E-08	1.234E-16	0.01997	7.943E-10
19	8.908E-06	0.0002961	0.00008219	0.00003448	9.378E-22	4.704E-06	3.407E-18	1.456E-08	2.555E-17	0.07757	7.943E-10
20	0.00002129	0.01706	2.825E-06	0.00006829	2.075E-24	1.859E-06	3.778E-20	2.408E-09	1.42E-18	0.3778	1.585E-10
21	0.00000519	0.01271	2.786E-06	0.00005017	1.512E-24	7.859E-07	4.785E-20	4.175E-09	3.125E-18	0.2664	9.12E-11
22	8.832E-06	0.004622	9.394E-06	0.00006152	3.362E-23	2.108E-06	4.862E-19	6.582E-09	1.451E-17	0.1179	1.995E-10
23	9.209E-06	0.001165	0.00004771	0.00007878	5.083E-22	5.512E-06	3.6E-18	1.65E-08	5.264E-17	0.04657	4.074E-10
24	0.0000143	0.002382	0.0000353	0.0001191	3.408E-22	7.259E-06	2.771E-18	1.399E-08	4.652E-17	0.0458	3.548E-10
25	0.0000106	0.001406	0.00009747	0.0001941	3.076E-12	0.00001327	2.23E-08	3.454E-08	3.336E-07	0.01193	3.981E-10
26	2.314E-06	0.001939	0.00002288	0.00006285	1.32E-13	1.711E-06	2.403E-09	2.038E-08	9.032E-08	0.0009131	1.585E-10
27	2.409E-06	0.0008036	0.00005703	0.00006493	1.008E-21	2.801E-06	1.158E-17	3.206E-08	2.747E-16	0.0002606	2.512E-10
28	5.023E-07	0.001676	0.00003666	0.00008704	6.63E-13	1.187E-06	2.408E-08	6.518E-08	1.806E-06	0.0005436	7.943E-11
29	5.548E-07	0.001168	0.0000299	0.00004948	1.932E-22	8.498E-07	5.575E-18	4.223E-08	3.321E-16	0.0000666	1E-10
30	6.664E-06	0.003521	0.00001438	0.00007171	1.758E-22	2.458E-06	2.542E-18	1.017E-08	7.588E-17	0.01207	1.995E-10
31	1.089E-06	0.003631	0.00004916	0.0002529	8.585E-12	0.00000345	3.118E-07	8.737E-08	0.00002338	0.002186	7.943E-11
32	9.357E-06	0.0007839	0.00006866	0.00007626	1.236E-10	6.564E-06	7.118E-07	1.934E-08	0.00000846	0.0008408	5.012E-10
33	0.00001371	0.0004571	0.00007897	0.00005115	7.53E-11	6.978E-06	2.735E-07	1.404E-08	2.051E-06	0.0006905	7.943E-10
34	6.651E-06	0.003512	0.00001806	0.00008985	6.162E-13	3.079E-06	8.911E-09	1.277E-08	2.66E-07	0.007099	1.995E-10
35	4.272E-06	0.0003576	0.00007987	0.00004047	8.888E-10	3.483E-06	5.117E-06	2.248E-08	0.00006081	0.004119	5.012E-10
36	3.066E-07	0.0006455	0.00005913	0.00005408	1.494E-13	9.288E-07	4.312E-09	8.352E-08	2.568E-07	0.00007351	1E-10

Table G. part 5: *Continued*

Sequence # (sample #)	CO2(aq) activity	CO3-- activity	Ca++ activity	CaCO3 activity	CaH2PO4+ activity	CaHCO3+ activity	CaHPO4 activity	CaOH+ activity	CaPO4- activity	Cl- activity	H+ activity
37	4.974E-06	0.001659	0.00002853	0.00006705	3.193E-11	2.893E-06	3.668E-07	1.603E-08	8.697E-06	0.0007719	2.512E-10
38	2.238E-06	0.0047	7.442E-06	0.00004956	3.143E-12	8.512E-07	9.07E-08	1.049E-08	5.402E-06	0.02905	1E-10
39	1.718E-06	0.001439	0.00003273	0.00006674	1.15E-12	1.817E-06	2.094E-08	2.916E-08	7.868E-07	0.0004401	1.585E-10
40	1.248E-07	0.0006597	0.00004397	0.00004109	1.259E-22	4.453E-07	5.758E-18	9.842E-08	5.435E-16	0.0001991	6.31E-11
41	0.00001143	0.0006042	0.0000965	0.0000826	1.241E-11	8.952E-06	5.674E-08	2.159E-08	5.356E-07	0.0005501	6.31E-10
42	0.00001894	0.002498	0.00001352	0.00004784	1.707E-22	3.271E-06	1.237E-18	4.762E-09	1.851E-17	0.1147	3.981E-10
43	0.00002044	0.002694	0.0000192	0.00007328	2.143E-22	5.011E-06	1.553E-18	6.759E-09	2.324E-17	0.1461	3.981E-10
44	1.168E-06	0.009714	7.954E-06	0.0001095	8.7E-24	9.423E-07	5.009E-19	2.225E-08	5.953E-17	0.1017	5.012E-11
45	1.816E-06	0.009527	0.00001068	0.0001441	1.409E-23	1.561E-06	6.446E-19	2.37E-08	6.085E-17	0.1159	6.31E-11
46	2.684E-06	0.008887	8.539E-06	0.0001075	1.6E-23	1.467E-06	5.812E-19	1.507E-08	4.358E-17	0.1082	7.943E-11
47	1.853E-06	0.009724	9.258E-06	0.0001275	1.308E-23	1.382E-06	5.982E-19	2.057E-08	5.648E-17	0.1023	6.31E-11
48	1.926E-06	0.01012	9.056E-06	0.0001299	1.37E-23	1.407E-06	6.264E-19	2.014E-08	5.914E-17	0.08369	6.31E-11
49	4.609E-06	0.002431	0.00004548	0.0001566	2.784E-22	5.368E-06	4.026E-18	3.211E-08	1.202E-16	0.03739	1.995E-10
50	0.0000016	0.003361	0.00007602	0.000362	1.639E-22	6.217E-06	4.73E-18	1.071E-07	2.817E-16	0.0346	1E-10
51	4.274E-06	0.003569	0.0001011	0.0005113	2.451E-22	0.00001392	4.463E-18	8.978E-08	1.677E-16	0.04333	1.585E-10
52	4.259E-06	0.003559	0.000256	0.001291	4.725E-22	0.00003514	8.601E-18	2.275E-07	3.233E-16	0.03541	1.585E-10
53	0.00000834	0.002774	0.0001368	0.0005378	6.084E-22	0.0000232	6.988E-18	7.671E-08	1.657E-16	0.02645	2.512E-10
54	0.00002631	0.0008685	0.00005449	0.00006705	7.874E-22	9.147E-06	2.86E-18	9.585E-09	2.145E-17	0.1399	7.943E-10
55	5.762E-06	0.001919	0.0003066	0.0008335	1.251E-21	0.00003596	1.437E-17	1.721E-07	3.407E-16	0.01928	2.512E-10
56	0.00002195	0.0004615	0.00005603	0.00003663	1.107E-21	6.291E-06	3.195E-18	7.903E-09	1.903E-17	0.01442	1E-09
57	0.00009185	0.003046	0.0002316	0.0009997	4.437E-21	0.0001364	1.612E-17	4.094E-08	1.209E-16	0.04376	7.943E-10
58	0.00001195	0.002438	0.00002643	0.00009128	6.05E-23	4.958E-06	5.521E-19	1.144E-08	1.04E-17	0.3917	3.162E-10
59	3.556E-06	0.004714	0.00003384	0.000226	9.303E-23	4.886E-06	2.132E-18	3.788E-08	1.009E-16	0.01459	1.259E-10
60	0.00002176	0.001767	0.00002617	0.00006549	8.591E-23	5.638E-06	4.946E-19	7.145E-09	5.878E-18	0.1453	5.012E-10
61	4.727E-06	0.003925	0.0004213	0.002343	4.346E-22	0.00006377	7.912E-18	3.72E-07	2.973E-16	0.1112	1.585E-10
62	6.944E-06	0.0009156	0.001518	0.001969	3.476E-21	0.0001346	2.519E-17	5.347E-07	3.769E-16	0.1113	3.981E-10
63	0.00003058	0.001017	0.00006508	0.00009381	1.898E-21	0.0000128	6.894E-18	1.154E-08	5.17E-17	0.04185	7.943E-10
64	0.0000801	0.004187	0.0002044	0.001213	1.626E-21	0.0001314	7.437E-18	4.524E-08	7.021E-17	0.1175	6.31E-10
65	0.0003032	0.005988	0.0002997	0.002543	9.647E-22	0.0004367	2.784E-18	3.971E-08	1.658E-17	0.7812	1E-09
66	0.0001362	2.867E-07	0.0001399	5.684E-08	7.042E-19	9.763E-07	2.032E-17	1.977E-10	1.21E-18	0.0001514	0.0000001
67	0.0001936	1.622E-07	0.0002995	6.883E-08	1.729E-18	1.874E-06	3.147E-17	2.669E-10	1.183E-18	0.001023	1.585E-07
68	0.000137	4.57E-07	0.0004086	2.645E-07	1.69E-18	3.609E-06	6.138E-17	7.266E-10	4.603E-18	0.0004251	7.943E-08
69	0.0000406	5.392E-06	0.0002121	1.621E-06	2.163E-19	3.504E-06	4.957E-17	2.38E-09	2.345E-17	0.001411	1.259E-08
70	8.329E-07	0.0004401	0.00005626	0.00003508	5.356E-22	1.202E-06	7.745E-18	3.98E-08	2.312E-16	0.0008171	1.995E-10
71	0.0002982	3.961E-07	0.0005781	3.244E-07	2.695E-18	7.014E-06	6.177E-17	6.485E-10	2.923E-18	0.0008952	1.259E-07
72	0.0001986	6.625E-07	0.0004461	4.187E-07	1.451E-18	5.713E-06	5.269E-17	7.931E-10	3.951E-18	0.001677	7.943E-08
73	0.0003517	1.173E-06	0.0003508	5.831E-07	1.046E-18	7.955E-06	3.8E-17	6.237E-10	2.85E-18	0.00121	7.943E-08
74	0.0002719	9.07E-07	0.0008238	1.059E-06	2.506E-18	0.00001444	9.102E-17	1.464E-09	6.825E-18	0.0043	7.943E-08

Table G. part 5: *Continued*

Sequence # (sample #)	CO2(aq) activity	CO3-- activity	Ca++ activity	CaCO3 activity	CaH2PO4+ activity	CaHCO3+ activity	CaHPO4 activity	CaOH+ activity	CaPO4- activity	Cl- activity	H+ activity
75	8.739E-06	0.0007302	0.00009005	0.00009316	1.734E-21	0.00000802	9.981E-18	2.53E-08	1.186E-16	0.01729	5.012E-10
76	9.775E-06	0.005074	7.165E-06	0.0000515	2.274E-23	1.765E-06	3.288E-19	4.979E-09	9.817E-18	0.1298	1.995E-10
77	5.329E-06	0.006877	5.512E-06	0.0000537	6.804E-24	1.161E-06	1.559E-19	6.008E-09	7.378E-18	0.1797	1.259E-10
78	0.00002579	0.01241	3.599E-14	6.328E-13	2.154E-32	2.169E-14	3.115E-28	2.318E-17	9.3E-27	0.8519	1.995E-10
79	0.00002689	0.01281	3.571E-14	6.479E-13	1.873E-32	2.22E-14	2.709E-28	2.277E-17	8.086E-27	0.9352	1.995E-10
80	4.849E-07	0.004056	0.00001948	0.000112	3.466E-23	9.638E-07	1.995E-18	5.481E-08	2.371E-16	0.009661	5.012E-11
81	0.000683	0.00009036	0.0001331	0.00001704	6.779E-20	0.00003684	1.554E-17	1.487E-09	7.351E-18	0.04722	1.259E-08
82	0.00002308	0.01779	0.00000192	0.00004838	9.484E-25	1.317E-06	1.727E-20	1.573E-09	6.489E-19	0.7449	1.585E-10
83	0.00001037	0.01951	3.286E-06	0.00009082	7.577E-25	0.00000156	2.186E-20	4.148E-09	1.302E-18	0.5673	1E-10
84	0.00002351	0.01094	9.268E-06	0.0001437	5.352E-24	4.925E-06	7.739E-20	5.775E-09	2.31E-18	0.7012	1.995E-10
85	0.0000348	0.02071	6.925E-06	0.0002032	7.243E-25	5.531E-06	1.319E-20	4.382E-09	4.956E-19	4.926	1.585E-10
86	0.00001001	0.00002108	0.00007395	2.209E-06	2.27E-20	0.0000012	2.071E-17	3.303E-09	3.901E-17	0.000657	3.162E-09
87	5.709E-06	0.0007576	0.0000303	0.00003252	8.232E-22	2.224E-06	5.967E-18	1.074E-08	8.927E-17	0.006677	3.981E-10
88	3.056E-06	0.0004058	0.0000432	0.00002483	1.358E-21	1.698E-06	9.84E-18	1.532E-08	1.472E-16	0.002396	3.981E-10
89	0.00002069	0.00002748	0.0003336	0.00001298	9.106E-20	8.878E-06	6.6E-17	1.183E-08	9.875E-17	0.0006443	3.981E-09
90	8.579E-06	0.00007188	0.0004364	0.00004444	4.282E-20	0.0000121	7.796E-17	3.889E-08	2.93E-16	0.0009153	1.585E-09
91	0.00000428	0.005667	0.00002507	0.0002012	9.204E-23	4.351E-06	2.109E-18	2.803E-08	9.981E-17	0.01354	1.259E-10
92	3.741E-06	0.003127	0.00001234	0.00005468	9.558E-23	1.489E-06	1.74E-18	1.097E-08	6.54E-17	0.01513	1.585E-10
93	0.00003736	0.00001247	0.000578	0.00001021	3.515E-19	0.00001393	1.277E-16	1.028E-08	9.574E-17	0.00009328	7.943E-09
94	0.00003562	0.00007499	0.0004013	0.00004263	9.551E-20	0.00002315	8.715E-17	1.792E-08	1.642E-16	0.00003711	3.162E-09
95	0.00002617	0.00005508	0.001073	0.00008371	1.408E-19	0.00004547	1.285E-16	4.791E-08	2.42E-16	0.0007235	3.162E-09
96	0.0000871	2.906E-06	0.0003001	1.236E-06	5.474E-19	0.00000533	6.287E-17	1.687E-09	1.491E-17	0.0002815	2.512E-08
97	0.0002347	7.828E-06	0.0004565	5.063E-06	6.799E-19	0.00002184	7.81E-17	2.566E-09	1.852E-17	0.0006388	2.512E-08
98	0.0001574	2.091E-06	0.0003836	1.136E-06	1.012E-18	7.769E-06	7.332E-17	1.361E-09	1.097E-17	0.0001884	3.981E-08
99	0.0001776	9.387E-06	0.0002743	3.648E-06	2.139E-19	0.0000125	3.093E-17	1.941E-09	9.235E-18	0.0008878	1.995E-08
100	0.0001233	0.00002594	0.0009626	0.00003538	4.291E-19	0.00006077	1.238E-16	1.359E-08	7.375E-17	0.0003607	0.00000001
101	0.00004183	5.556E-06	0.0002823	2.223E-06	2.953E-19	4.806E-06	6.768E-17	3.168E-09	3.202E-17	0.0001862	1.259E-08
102	0.00008278	6.937E-06	0.0004998	4.911E-06	5.641E-19	0.00001337	1.027E-16	4.454E-09	3.859E-17	0.00009296	1.585E-08
103	0.0004692	9.877E-07	0.0005104	7.143E-07	2.289E-18	0.00001227	6.606E-17	7.209E-10	3.935E-18	0.00009324	0.0000001
104	0.0003714	1.239E-06	0.0005791	1.017E-06	2.22E-18	0.00001387	8.064E-17	1.03E-09	6.047E-18	0.0001862	7.943E-08
105	0.00000207	0.001094	0.0001027	0.0001591	8.312E-22	5.452E-06	1.202E-17	7.261E-08	3.589E-16	0.003954	1.995E-10
106	0.0001706	9.02E-07	0.0005381	6.877E-07	1.845E-18	7.452E-06	8.436E-17	1.205E-09	7.964E-18	0.00009421	6.31E-08
107	0.0002527	5.319E-07	0.000604	4.552E-07	2.622E-18	7.818E-06	7.566E-17	8.53E-10	4.507E-18	0.00009387	0.0000001
108	0.00001257	0.0006642	0.00009645	0.00009077	3.624E-21	9.837E-06	1.657E-17	2.157E-08	1.564E-16	0.002727	6.31E-10
109	0.0002374	7.922E-07	0.0003905	4.383E-07	1.619E-18	5.979E-06	5.88E-17	6.944E-10	4.409E-18	0.00009452	7.943E-08
110	1.741E-06	0.00092	0.00005651	0.00007366	5.913E-22	2.524E-06	8.551E-18	3.997E-08	2.553E-16	0.002889	1.995E-10
111	0.0001124	0.00002366	0.0005293	0.00001774	3.153E-19	0.00003048	9.098E-17	7.473E-09	5.419E-17	0.0005391	0.00000001
115	0.00001248	0.0002624	3.825E-13	1.422E-13	2.894E-29	2.442E-14	8.349E-26	5.396E-17	4.973E-25	0.01414	1E-09

Table G. part 5: *Continued*

Sequence # (sample #)	CO2(aq) activity	CO3-- activity	Ca++ activity	CaCO3 activity	CaH2PO4+ activity	CaHCO3+ activity	CaHPO4 activity	CaOH+ activity	CaPO4- activity	Cl- activity	H+ activity
116	4.825E-06	0.001012	0.00002081	0.00002983	2.881E-22	0.00000162	2.629E-18	9.261E-09	4.952E-17	0.04952	3.162E-10
117	0.0006322	0.00002106	0.00001662	4.959E-07	2.222E-20	2.139E-06	2.552E-18	9.331E-11	6.052E-19	0.01674	2.512E-08
118	6.563E-06	0.00217	0.0001093	0.000336	5.913E-22	0.0000145	6.793E-18	6.091E-08	1.611E-16	0.1563	2.512E-10
119	0.00001292	0.001701	1.382E-13	3.331E-13	1.803E-30	2.278E-14	1.307E-26	4.862E-17	1.956E-25	0.1188	3.981E-10
120	2.986E-06	0.0009929	0.00002159	0.00003037	2.406E-22	0.00000131	2.764E-18	1.21E-08	6.554E-17	0.05101	2.512E-10
121	4.352E-06	0.0009133	0.00002256	0.0000292	3.301E-22	1.586E-06	3.012E-18	1.005E-08	5.673E-17	0.04764	3.162E-10
125	0.0005127	6.807E-06	0.0005657	5.456E-06	1.076E-18	0.00003731	7.797E-17	2.006E-09	1.167E-17	0.003722	3.981E-08
126	0.0005447	0.00001813	0.0002159	5.547E-06	2.487E-19	0.00002393	2.857E-17	1.211E-09	6.776E-18	0.02749	2.512E-08
127	0.0001686	0.00008902	0.0001533	0.00001933	5.353E-20	0.00002095	2.448E-17	3.426E-09	2.311E-17	0.005627	6.31E-09
128	0.0001072	0.00008972	0.0002311	0.00002938	4.545E-20	0.00002529	2.617E-17	6.505E-09	3.11E-17	0.01297	5.012E-09
129	0.00002629	0.00003491	5.167E-13	2.556E-14	7.015E-29	1.748E-14	5.084E-26	1.833E-17	7.607E-26	0.002645	3.981E-09
130	0.0001057	8.855E-06	0.0002615	3.281E-06	1.302E-19	8.931E-06	2.37E-17	2.33E-09	8.907E-18	0.002731	1.585E-08
131	0.0002087	0.00001103	0.000347	5.424E-06	1.773E-19	0.00001859	2.565E-17	2.456E-09	7.656E-18	0.001576	1.995E-08
132	0.0001883	0.0000025	0.000323	1.144E-06	3.728E-19	7.823E-06	2.702E-17	1.146E-09	4.043E-18	0.001771	3.981E-08
133	0.00006279	8.338E-06	0.0001721	2.033E-06	8.86E-20	4.396E-06	2.031E-17	1.93E-09	9.608E-18	0.002767	1.259E-08
134	0.0004195	2.218E-06	0.0002601	8.173E-07	8.377E-19	8.857E-06	3.831E-17	5.822E-10	3.617E-18	0.001368	6.31E-08
135	0.00004288	0.00005689	0.0007041	0.00005676	8.84E-20	0.00003881	6.407E-17	2.495E-08	9.587E-17	0.006879	3.981E-09
136	0.0002017	0.00004243	0.000289	0.00001737	1.775E-19	0.00002984	5.12E-17	4.08E-09	3.05E-17	0.005012	0.00000001
137	0.0001794	3.776E-06	0.0006971	0.00000373	1.166E-18	0.00002026	1.064E-16	3.113E-09	2.004E-17	0.002266	3.162E-08
138	0.0003501	0.00002931	0.000264	0.00001096	2.345E-19	0.00002984	4.27E-17	2.35E-09	1.605E-17	0.01142	1.585E-08
139	0.00001705	8.036E-06	0.005351	0.00006093	2.398E-19	0.00006914	1.047E-16	1.118E-07	9.442E-17	0.4298	6.607E-09
140	0.00001154	4.783E-06	0.006805	0.00004612	4.06E-19	0.00005607	1.655E-16	1.339E-07	1.392E-16	0.2775	7.079E-09
141	6.832E-06	0.00003934	0.001222	0.0000681	3.424E-20	0.00002229	5.184E-17	8.995E-08	1.621E-16	0.1315	1.905E-09
142	0.00001328	0.0000271	0.001938	0.00007442	3.748E-20	0.00004042	3.42E-17	8.395E-08	6.442E-17	0.4501	3.162E-09
143	4.002E-06	0.00004159	0.001885	0.000111	2.418E-20	0.00002694	4.94E-17	1.856E-07	2.083E-16	0.2739	1.413E-09
144	0.00001144	0.00002598	0.002233	0.0000822	6.85E-20	0.00004264	6.545E-17	1.028E-07	1.291E-16	0.2925	3.02E-09
145	0.00001324	0.00001001	0.001082	0.00001535	1.008E-19	0.00001383	5.542E-17	2.881E-08	6.29E-17	0.2027	5.248E-09
146	0.00003721	9.482E-06	0.00689	0.00009255	2.612E-19	0.0001417	8.455E-17	1.05E-07	5.651E-17	0.7787	8.913E-09
147	4.674E-07	0.00002244	0.0002978	9.469E-06	4.596E-21	1.074E-06	2.007E-17	6.339E-08	1.81E-16	0.04434	6.607E-10
148	0.00001598	0.0001263	0.002827	0.0005057	1.115E-20	0.0001377	2.029E-17	2.375E-07	7.627E-17	0.882	1.585E-09
149	6.454E-08	0.00034	0.0008791	0.0004234	1.353E-22	4.588E-06	6.188E-18	0.00000196	5.842E-16	0.03943	6.31E-11
150	0.00005606	0.00006899	0.001638	0.0001601	1.979E-20	0.0001095	1.434E-17	5.385E-08	2.146E-17	1.393	3.981E-09
151	0.00001878	0.00003829	0.000489	0.00002653	1.315E-20	0.00001441	1.2E-17	2.116E-08	2.261E-17	0.5631	3.162E-09
152	9.51E-07	0.01138	2.426E-06	0.00003911	1.475E-24	0.00000028	1.021E-19	8.118E-09	1.459E-17	0.08391	4.169E-11
153	2.713E-07	0.0000286	0.0003155	0.00001279	4.851E-21	9.809E-07	3.134E-17	9.971E-08	4.179E-16	0.017	4.467E-10
154	6.321E-06	0.00001436	0.002083	0.00004239	6.829E-20	0.00002199	6.524E-17	9.59E-08	1.287E-16	0.3312	3.02E-09
155	0.00001922	5.056E-06	0.00137	9.812E-06	2.547E-19	0.00001502	8.247E-17	2.155E-08	5.512E-17	0.1666	8.913E-09
156	0.0002089	2.599E-06	0.007815	0.00002878	1.253E-18	0.0001968	9.081E-17	2.597E-08	1.359E-17	1.262	3.981E-08

Table G. part 5: *Continued*

Sequence # (sample #)	CO2(aq) activity	CO3-- activity	Ca++ activity	CaCO3 activity	CaH2PO4+ activity	CaHCO3+ activity	CaHPO4 activity	CaOH+ activity	CaPO4- activity	Cl- activity	H+ activity
157	0.0002246	7.927E-07	0.2786	0.0003129	2.383E-18	0.003391	1.09E-16	4.163E-07	1.029E-17	10.56	6.31E-08
158	0.00001186	0.00001716	0.001406	0.0000342	1.09E-19	0.00002233	8.273E-17	5.19E-08	1.296E-16	0.1505	3.802E-09
159	0.0003228	5.397E-07	0.0007839	5.993E-07	3.241E-18	0.00001155	8.335E-17	9.867E-10	4.425E-18	0.002297	1.122E-07
160	0.00002371	9.894E-06	0.001327	0.0000186	2.029E-19	0.00002261	8.27E-17	2.63E-08	6.959E-17	0.1411	7.079E-09
161	0.00005041	5.316E-06	0.0004146	3.123E-06	2.779E-19	7.576E-06	5.677E-17	4.144E-09	2.394E-17	0.01455	1.413E-08
162	0.00001066	0.00001116	0.001364	0.00002157	1.167E-19	0.00001655	7.541E-17	4.28E-08	1.006E-16	0.1711	4.467E-09
163	0.00005655	7.112E-06	0.01391	0.0001402	2.857E-19	0.0002962	6.702E-17	1.444E-07	3.245E-17	1.981	1.23E-08
164	1.926E-08	7.046E-06	0.0001157	1.156E-06	1.523E-21	4.761E-08	1.832E-17	6.815E-08	4.55E-16	0.001679	2.399E-10
165	0.0001489	2.129E-06	0.03574	0.0001078	8.662E-19	0.0006422	7.208E-17	1.189E-07	1.238E-17	4.172	3.467E-08
166	1.125E-06	0.00001638	0.0002182	5.064E-06	1.844E-20	1.046E-06	4.425E-17	2.563E-08	2.192E-16	0.003908	1.202E-09
167	0.0003019	3.932E-07	0.07989	0.00004451	3.35E-18	0.0008577	8.615E-17	7.834E-08	4.573E-18	5.528	1.122E-07
168	0.0001988	2.638E-06	0.03533	0.000132	1.361E-18	0.0007172	1.242E-16	9.946E-08	2.34E-17	13.32	3.162E-08
169	1.604E-06	0.00001118	0.0002051	3.248E-06	2.572E-20	9.693E-07	4.27E-17	1.666E-08	1.464E-16	0.005912	1.738E-09
170	2.034E-06	0.00001554	0.0002435	5.361E-06	2.35E-20	1.528E-06	4.085E-17	2.072E-08	1.466E-16	0.01364	1.66E-09
171	2.461E-06	0.00002976	0.0005822	0.00002454	2.478E-20	5.557E-06	5.424E-17	6.227E-08	2.451E-16	0.03561	1.318E-09
172	2.191E-06	0.00003178	0.0004718	0.00002124	1.528E-20	4.386E-06	3.667E-17	5.521E-08	1.817E-16	0.08038	1.202E-09
173	3.728E-06	0.0001229	0.000617	0.0001074	6.341E-21	0.00001465	2.303E-17	1.084E-07	1.727E-16	0.2323	7.943E-10
174	0.00001785	0.00003991	0.0004888	0.00002764	1.252E-20	0.00001434	1.196E-17	2.215E-08	2.359E-17	0.5631	3.02E-09
175	0.00005588	0.00006877	0.001638	0.0001596	1.959E-20	0.0001092	1.42E-17	5.386E-08	2.124E-17	1.39	3.981E-09
176	0.00001173	0.0000103	0.0003061	4.464E-06	5.934E-20	3.755E-06	3.496E-17	8.825E-09	4.252E-17	0.001372	4.898E-09
177	0.00001598	0.0001263	0.002827	0.0005057	1.115E-20	0.0001377	2.029E-17	2.375E-07	7.627E-17	0.882	1.585E-09
178	0.0002265	8.001E-07	0.2754	0.0003122	2.382E-18	0.003383	1.089E-16	4.12E-07	1.028E-17	10.53	6.31E-08
179	0.00001294	0.02874	3.435E-06	0.0001399	3.897E-25	2.141E-06	1.262E-20	4.561E-09	8.432E-19	1.817	8.913E-11
180	5.135E-06	0.000679	0.00002116	0.00002035	2.735E-22	1.392E-06	1.982E-18	7.472E-09	2.966E-17	0.088	3.981E-10
181	0.00001456	0.00004782	0.004637	0.0003141	8.485E-20	0.0001355	9.747E-17	2.567E-07	2.311E-16	0.3455	2.512E-09
182	0.00005589	0.00006877	0.001633	0.0001592	1.953E-20	0.0001088	1.416E-17	5.369E-08	2.118E-17	1.39	3.981E-09
183	1.94E-08	0.00001625	0.0005851	0.00001347	1.135E-21	3.668E-07	2.067E-17	5.214E-07	7.767E-16	0.0005567	1.585E-10
184	0.00001121	0.00001117	0.002375	0.00003757	1.382E-19	0.0000295	8.725E-17	7.254E-08	1.137E-16	0.2319	4.571E-09
185	0.00002052	0.004002	8.646E-06	0.00004903	9.053E-24	2.663E-06	8.261E-20	3.578E-09	1.556E-18	1.022	3.162E-10
186	0.00001144	0.00002598	0.002233	0.0000822	6.85E-20	0.00004264	6.545E-17	1.028E-07	1.291E-16	0.2925	3.02E-09
187	0.00002688	0.0000499	0.003379	0.0002389	5.169E-20	0.0001359	4.504E-17	1.394E-07	8.102E-17	0.6016	3.311E-09
188	2.158E-07	0.01861	4.825E-06	0.0001272	9.567E-25	3.384E-07	1.782E-19	4.324E-08	6.854E-17	0.1225	1.549E-11
189	3.854E-07	0.01268	0.0000156	0.0002802	5.308E-24	1.209E-06	6.097E-19	8.648E-08	1.446E-16	0.1251	2.512E-11
190	1.614E-08	0.0001353	0.0002716	0.00005205	1.225E-22	4.481E-07	7.051E-18	7.654E-07	8.38E-16	0.0004814	5.012E-11
191	4.903E-06	0.0001628	0.0003874	0.00008933	7.952E-21	0.00001219	2.888E-17	6.854E-08	2.166E-16	0.1014	7.943E-10
192	0.0000348	0.00002805	0.002768	0.00011	8.963E-20	0.00009468	5.16E-17	7.503E-08	6.133E-17	0.6518	5.012E-09
193	4.504E-06	0.0001491	0.001197	0.0002528	1.096E-20	0.00003449	3.981E-17	2.111E-07	2.985E-16	0.1107	7.943E-10
194	0.0005495	0.00003136	0.005097	0.0002265	6.869E-21	0.0006165	1.25E-18	3.094E-08	4.7E-19	9.694	1.585E-08

Table G. part 5: *Continued*

Sequence # (sample #)	CO2(aq) activity	CO3-- activity	Ca++ activity	CaCO3 activity	CaH2PO4+ activity	CaHCO3+ activity	CaHPO4 activity	CaOH+ activity	CaPO4- activity	Cl- activity	H+ activity
195	3.472E-06	0.00003599	0.00759	0.0003871	4.022E-20	0.0000939	8.216E-17	7.457E-07	3.465E-16	0.3485	1.413E-09
196	0.00008281	2.736E-06	0.004624	0.00001793	1.618E-18	0.00007734	1.858E-16	2.575E-08	4.406E-17	0.2207	2.512E-08
197	0.00008054	4.943E-06	0.03638	0.0002547	1.006E-18	0.0007781	1.632E-16	2.664E-07	5.465E-17	1.718	1.778E-08
199	0.00002449	0.002128	0.00002573	0.00007756	6.138E-12	6.525E-06	3.616E-08	7.347E-09	4.398E-07	0.1173	4.898E-10
200	3.133E-06	0.004121	3.423E-06	0.00001999	8.942E-24	4.321E-07	2.05E-19	3.804E-09	9.697E-18	0.1116	1.259E-10
201	0.00000646	0.003384	9.622E-06	0.00004613	4.414E-23	1.581E-06	6.384E-19	6.748E-09	1.906E-17	0.1115	1.995E-10
202	0.00001017	0.003361	9.947E-06	0.00004737	6.31E-23	2.044E-06	7.248E-19	5.543E-09	1.719E-17	0.1111	2.512E-10
203	0.0000119	0.003144	0.00001446	0.00006443	6.049E-13	3.119E-06	6.193E-09	7.225E-09	1.309E-07	0.1119	2.818E-10
204	6.583E-06	0.003449	9.596E-06	0.00004689	8.731E-14	1.607E-06	1.263E-09	6.73E-09	3.769E-08	0.1137	1.995E-10
205	5.795E-06	0.003485	0.00001045	0.00005159	1.529E-13	0.00000165	2.37E-09	7.852E-09	7.58E-08	0.1121	1.862E-10
206	3.501E-06	0.004012	8.796E-06	0.00005	1.006E-13	1.158E-06	2.151E-09	9.124E-09	9.499E-08	0.1142	1.349E-10
207	0.00000342	0.004104	7.797E-06	0.00004533	1.221E-13	1.026E-06	2.672E-09	8.274E-09	1.207E-07	0.1154	1.318E-10
208	5.693E-06	0.0001313	0.0001239	0.00002306	1.623E-11	3.783E-06	4.903E-08	1.832E-08	3.058E-07	0.005984	9.55E-10
209	5.359E-07	0.00002575	0.0004651	0.00001697	7.765E-21	1.925E-06	3.391E-17	9.906E-08	3.057E-16	0.05025	6.607E-10
210	0.00002484	6.515E-06	0.001208	0.00001115	2.112E-19	0.00001706	6.836E-17	1.894E-08	4.569E-17	0.2112	8.913E-09
211	0.00001183	4.904E-06	0.0073	0.00005071	4.433E-19	0.00006166	1.807E-16	1.437E-07	1.52E-16	0.2879	7.079E-09
212	4.183E-06	0.00004348	0.002114	0.0001302	2.784E-20	0.00003159	5.687E-17	2.082E-07	2.398E-16	0.2949	1.413E-09
213	0.00001777	8.381E-06	0.005739	0.00006815	2.745E-19	0.00007733	1.199E-16	0.00000012	1.081E-16	0.4536	6.607E-09
214	0.00001515	0.00003098	0.00216	0.00009478	5.517E-20	0.00005148	5.034E-17	9.372E-08	9.482E-17	0.5164	3.162E-09
215	0.0000201	0.00001478	0.006968	0.0001459	1.495E-19	0.0001315	8.221E-17	1.804E-07	9.331E-17	0.7983	5.248E-09
216	0.00001888	0.0001496	0.002713	0.0005749	1.492E-20	0.0001565	2.716E-17	2.286E-07	1.021E-16	1.011	1.585E-09
217	0.0001498	2.145E-06	0.03557	0.0001081	8.817E-19	0.0006438	7.337E-17	1.185E-07	1.26E-17	4.202	3.467E-08
218	0.0002265	8.014E-07	0.2752	0.0003125	2.406E-18	0.003386	1.1E-16	4.122E-07	1.039E-17	10.55	6.31E-08
219	0.0001312	0.00000259	0.01034	0.00003794	4.059E-19	0.0001968	3.878E-17	4.135E-08	7.648E-18	3.121	3.02E-08
220	0.0001257	0.00001069	0.008577	0.0001299	2.335E-19	0.0003301	4.555E-17	7.239E-08	1.834E-17	2.394	1.479E-08
221	0.0001133	4.864E-06	0.006492	0.00004474	2.857E-19	0.0001606	3.946E-17	3.907E-08	1.125E-17	2.234	2.089E-08
222	0.0001345	4.848E-06	0.005018	0.00003447	2.799E-19	0.0001356	3.525E-17	2.78E-08	9.166E-18	2.03	2.291E-08
223	0.0001017	4.873E-06	0.003634	0.00002509	2.097E-19	0.00008598	3.033E-17	2.33E-08	9.055E-18	1.847	1.995E-08
224	0.0001281	9.245E-06	0.003431	0.00004493	1.601E-19	0.0001252	2.848E-17	2.695E-08	1.046E-17	1.916	1.622E-08
225	7.845E-06	0.00006575	0.0003987	0.00003714	2.278E-20	0.00001011	4.148E-17	3.553E-08	1.559E-16	0.0001001	1.585E-09
226	0.0000282	0.00002363	0.0009413	0.00003152	1.963E-19	0.00002713	1.13E-16	2.653E-08	1.343E-16	0.00002737	5.012E-09
227	0.00003689	0.00001951	0.001276	0.00003526	3.531E-19	0.00003821	1.615E-16	2.856E-08	1.524E-16	0.00004572	6.31E-09
228	0.00007858	0.00006584	0.0007502	0.00006998	9.754E-20	0.00006024	5.615E-17	2.114E-08	6.674E-17	0.00001758	5.012E-09
229	0.0004558	0.00009586	0.0006094	0.00008277	8.774E-20	0.0001422	2.532E-17	8.6E-09	1.508E-17	0.00002528	0.00000001
230	0.0003694	0.00007773	0.00005059	5.571E-06	8.483E-11	9.569E-06	2.448E-08	7.142E-10	1.458E-08	0.00005146	0.00000001
232	0.0001196	0.0003986	0.00007788	0.00004399	3.917E-11	0.00001898	4.499E-08	4.376E-09	1.067E-07	0.0002608	2.512E-09
234	0.0005369	0.0001129	3.038E-13	4.86E-14	3.975E-29	8.347E-14	1.147E-26	4.287E-18	6.832E-27	0.00003357	0.00000001
235	0.007474	0.00002489	0.0003606	0.00001272	2.782E-19	0.0001735	1.011E-17	6.401E-10	7.579E-19	8.318E-06	7.943E-08

Table G. part 5: *Continued*

Sequence # (sample #)	CO2(aq) activity	CO3-- activity	Ca++ activity	CaCO3 activity	CaH2PO4+ activity	CaHCO3+ activity	CaHPO4 activity	CaOH+ activity	CaPO4- activity	Cl- activity	H+ activity
236	0.00001275	1.068E-06	0.0003057	4.626E-07	4.487E-19	1.259E-06	8.169E-17	2.724E-09	3.07E-17	9.626E-06	1.585E-08
237	0.00006972	0.00005842	0.000865	0.00007159	1.128E-19	0.00006163	6.495E-17	2.437E-08	7.72E-17	0.0008437	5.012E-09
238	0.00007339	0.0000388	0.0006649	0.00003655	1.351E-19	0.00003961	6.18E-17	1.488E-08	5.835E-17	0.0006314	6.31E-09
239	0.00007868	0.00001045	0.0002052	3.038E-06	1.143E-19	6.569E-06	2.619E-17	2.302E-09	1.239E-17	0.00004558	1.259E-08
240	0.00001271	1.689E-06	0.0002271	5.434E-07	2.739E-19	1.175E-06	6.278E-17	2.549E-09	2.97E-17	9.61E-10	1.259E-08
241	0.00006131	0.00001291	0.0005561	0.00001017	3.022E-11	0.00001746	8.718E-09	7.855E-09	5.193E-09	0.00001838	0.00000001
242	5.041E-06	0.00001061	0.000142	2.134E-06	7.725E-12	1.159E-06	7.048E-09	6.342E-09	1.328E-08	9.497E-06	3.162E-09
243	1.431E-07	0.00001901	0.00003337	8.984E-07	1.228E-13	6.143E-08	8.899E-10	1.184E-08	1.332E-08	0.00001927	3.981E-10
244	0.00005852	0.00001232	0.0007624	0.0000133	3.319E-19	0.00002285	9.577E-17	1.077E-08	5.705E-17	0.00006375	0.00000001
245	0.0002391	0.00009586	0.00007025	9.541E-06	9.518E-21	0.00001187	3.791E-18	1.369E-09	3.117E-18	0.0000427	7.244E-09
246	0.001055	0.0002022	0.00001163	3.332E-06	1.214E-21	5.992E-06	3.346E-19	1.566E-10	1.904E-19	0.0001746	1.047E-08
247	0.001961	0.00004956	0.0005324	0.00003738	2.059E-19	0.0001852	2.06E-17	2.604E-09	4.255E-18	0.00007503	2.884E-08
248	0.000111	0.0003875	0.00007035	0.00003862	2.24E-21	0.00001628	2.633E-18	4.044E-09	6.389E-18	0.003014	2.455E-09
249	0.0001278	0.0003542	0.00006573	0.00003299	2.402E-21	0.0000156	2.517E-18	3.367E-09	5.443E-18	0.002596	2.754E-09
250	7.032E-06	0.02327	1.905E-06	0.0000628	2.725E-24	8.568E-07	9.898E-20	3.359E-09	7.422E-18	0.002129	7.943E-11
251	1.629E-06	0.02149	0.00000259	0.00007884	2.116E-24	5.391E-07	1.534E-19	9.127E-09	2.295E-17	0.001936	3.981E-11
252	7.048E-06	0.02331	2.463E-06	0.00008133	1.095E-12	0.00000111	3.976E-08	4.341E-09	2.982E-06	0.005027	7.943E-11
253	1.629E-06	0.02149	2.238E-06	0.00006813	1.837E-13	4.658E-07	1.332E-08	7.886E-09	1.992E-06	0.001935	3.981E-11
254	7.702E-06	0.02537	1.776E-06	0.00006382	6.939E-13	8.707E-07	2.521E-08	3.117E-09	0.00000189	0.01926	7.943E-11
255	3.631E-07	0.0191	3.012E-06	0.00008149	2.248E-13	2.793E-07	3.251E-08	2.121E-08	9.705E-06	0.01018	1.995E-11
256	8.314E-06	0.02725	0.00000157	0.00006062	5.114E-12	8.271E-07	1.858E-07	2.743E-09	0.00001393	0.01244	7.943E-11
257	0.0000033	0.02715	2.217E-06	0.00008526	5.346E-12	7.339E-07	3.078E-07	6.132E-09	0.00003658	0.01293	5.012E-11
258	0.0003222	0.00000428	0.0003066	1.859E-06	6.568E-19	0.00001271	4.76E-17	1.088E-09	7.123E-18	0.00002763	3.981E-08
259	0.00013	0.0001725	0.00005276	0.0000129	6.329E-21	8.819E-06	4.587E-18	1.871E-09	6.864E-18	0.0001214	3.981E-09
260	0.0004484	0.00005953	0.0002264	0.0000191	8.032E-20	0.00004129	1.841E-17	2.539E-09	8.71E-18	0.0001467	1.259E-08
261	0.0001318	0.002762	2.477E-06	9.693E-06	1.045E-22	1.665E-06	3.014E-19	3.482E-10	1.795E-18	0.005941	1E-09
262	0.0001257	0.0004188	0.00001755	0.00001041	3.056E-21	4.491E-06	3.511E-18	9.856E-10	8.326E-18	0.0007347	2.512E-09
263	0.0002045	0.0001712	0.00002177	5.282E-06	5.12E-21	4.547E-06	2.947E-18	6.132E-10	3.503E-18	0.000293	5.012E-09
264	0.0001196	0.001	4.514E-06	6.395E-06	3.324E-22	1.741E-06	6.051E-19	4.013E-10	2.274E-18	0.002503	1.585E-09
265	0.00003098	0.006496	7.517E-14	6.918E-13	9.924E-31	3.757E-14	9.055E-27	3.344E-17	1.706E-25	0.004098	3.162E-10
266	0.00002302	0.003052	0.00000139	6.008E-06	3.286E-23	4.108E-07	2.381E-19	4.922E-10	3.563E-18	0.0014	3.981E-10
267	0.00002875	0.00381	5.875E-06	0.00003171	1.047E-22	2.168E-06	7.592E-19	2.08E-09	1.136E-17	0.0008881	3.981E-10
268	0.0001468	0.0007746	2.486E-06	2.728E-06	2.65E-22	9.348E-07	3.832E-19	1.756E-10	1.144E-18	0.001785	1.995E-09
269	0.000271	0.00893	5.177E-14	6.55E-13	1.083E-30	8.936E-14	3.936E-27	9.092E-18	2.951E-26	0.00888	7.943E-10
271	0.00001039	0.008671	6.579E-14	8.082E-13	2.576E-31	2.2E-14	4.69E-27	5.838E-17	1.763E-25	0.1301	1.585E-10
272	0.00002202	0.0114	4.071E-14	6.574E-13	6.912E-20	2.253E-14	9.996E-16	2.821E-17	2.984E-14	0.258	1.995E-10
274	0.00002551	0.0131	3.586E-14	6.655E-13	6.298E-20	2.281E-14	9.107E-16	2.465E-17	2.719E-14	0.3468	1.995E-10
275	0.00003743	0.01212	1.157E-06	0.00001987	2.512E-12	8.572E-07	2.885E-08	6.316E-10	6.841E-07	0.3528	2.512E-10

Table G. part 5: *Continued*

Sequence # (sample #)	CO2(aq) activity	CO3-- activity	Ca++ activity	CaCO3 activity	CaH2PO4+ activity	CaHCO3+ activity	CaHPO4 activity	CaOH+ activity	CaPO4- activity	Cl- activity	H+ activity
278	0.00002453	0.01264	3.699E-14	6.623E-13	6.696E-20	2.27E-14	9.683E-16	2.552E-17	2.891E-14	0.3029	1.995E-10
283	6.853E-06	0.009004	5.536E-14	7.063E-13	1.633E-31	1.527E-14	3.743E-27	6.145E-17	1.771E-25	0.1469	1.259E-10
284	9.513E-06	0.007885	5.518E-14	6.165E-13	7.544E-20	1.678E-14	1.373E-15	4.865E-17	5.162E-14	0.143	1.585E-10
285	9.452E-06	0.007842	1.227E-06	0.00001363	5.02E-24	3.711E-07	9.139E-20	1.083E-09	3.435E-18	0.1309	1.585E-10
287	0.00001399	0.004651	5.901E-06	0.00003889	6.627E-23	1.678E-06	7.612E-19	3.306E-09	1.805E-17	0.03388	2.512E-10
288	9.765E-06	0.002053	9.195E-06	0.00002674	1.825E-22	1.452E-06	1.666E-18	4.101E-09	3.137E-17	0.01442	3.162E-10
289	0.00001306	0.004342	5.231E-06	0.00003218	6.197E-23	1.388E-06	7.118E-19	2.932E-09	1.688E-17	0.02887	2.512E-10
290	0.00002026	0.0004263	0.0001842	0.0001112	1.175E-20	0.0000191	3.389E-17	2.6E-08	2.019E-16	8.791E-10	1E-09
291	0.00001847	0.0006158	0.0001132	0.0000988	5.843E-21	0.00001348	2.122E-17	2.012E-08	1.592E-16	0.003706	7.943E-10
292	0.00001962	0.0002605	0.0001631	0.00006019	1.455E-20	0.00001302	3.335E-17	1.829E-08	1.578E-16	0.002069	1.259E-09
293	0.00001447	0.0007645	0.00009761	0.0001057	3.877E-21	0.00001146	1.773E-17	2.184E-08	1.674E-16	0.003931	6.31E-10
294	0.00002807	0.0002351	0.0001511	0.00005033	1.747E-20	0.0000137	3.18E-17	1.346E-08	1.195E-16	0.002435	1.585E-09
295	0.00002007	0.0002665	0.0001625	0.00006137	1.45E-20	0.00001327	3.323E-17	1.823E-08	1.572E-16	0.002095	1.259E-09
296	0.00006813	0.0001434	0.0007482	0.000152	1.037E-19	0.00008255	9.459E-17	3.341E-08	1.782E-16	0.0005231	3.162E-09
297	2.286E-06	0.001208	0.0001162	0.0001989	9.119E-22	6.818E-06	1.319E-17	8.224E-08	3.937E-16	0.0009975	1.995E-10
298	0.00001142	0.009405	4.781E-14	6.371E-13	4.729E-20	1.734E-14	8.609E-16	4.189E-17	3.236E-14	0.2199	1.585E-10
299	0.00003275	0.00004349	0.0005436	0.0000335	1.456E-09	0.0000229	1.055E-06	1.929E-08	1.579E-06	0.0005132	3.981E-09
300	0.00002571	0.0002154	0.0006348	0.0001937	4.197E-20	0.00005273	7.64E-17	5.655E-08	2.871E-16	0.001554	1.585E-09
301	0.0001408	4.698E-07	0.0001593	1.061E-07	7.365E-19	1.447E-06	2.675E-17	2.834E-10	2.006E-18	0.00002855	7.943E-08
302	0.00005211	6.921E-06	0.0003523	3.454E-06	3.624E-19	7.469E-06	8.306E-17	3.952E-09	3.93E-17	0.00005638	1.259E-08
303	0.00002292	0.0001173	0.00096	0.0001596	4.838E-21	0.00005469	6.996E-18	6.581E-08	2.089E-17	0.7302	1.995E-09
304	0.00001518	0.0001265	0.0004493	0.00008056	5.377E-21	0.00002193	9.789E-18	3.984E-08	3.679E-17	0.0508	1.585E-09
306	6.209E-06	0.0008222	0.0002777	0.0003235	4.377E-22	0.00002212	3.172E-18	9.822E-08	4.746E-17	0.0376	3.981E-10
307	0.00002438	0.0001287	0.0003841	0.00007001	7.218E-21	0.00002399	1.044E-17	2.714E-08	3.116E-17	0.003541	1.995E-09
308	0.0002178	0.00288	0.00005548	0.0002264	9.747E-22	0.00004895	2.234E-18	6.197E-09	1.057E-17	0.005502	1.259E-09
309	0.00001821	0.0002413	0.0001226	0.00004191	1.791E-21	9.062E-06	4.104E-18	1.372E-08	1.942E-17	0.007695	1.259E-09
310	0.00001978	0.0001044	0.006446	0.0009531	6.884E-20	0.0003266	9.955E-17	4.554E-07	2.972E-16	0.01034	1.995E-09
311	8.362E-06	0.000111	0.000859	0.000135	1.005E-20	0.0000292	2.303E-17	9.628E-08	1.09E-16	0.001557	1.259E-09
313	0.0000111	0.0001473	0.0003681	0.00007681	5.953E-21	0.00001661	1.364E-17	4.127E-08	6.456E-17	0.003668	1.259E-09
314	0.00003874	0.00003245	0.0008814	0.00004053	8.591E-20	0.00003488	4.946E-17	2.483E-08	5.878E-17	0.001261	5.012E-09
315	0.00002853	0.0000239	0.002088	0.00007071	1.952E-19	0.00006086	1.124E-16	5.883E-08	1.335E-16	0.001367	5.012E-09
316	0.00003514	0.00007393	0.0004903	0.00005135	4.686E-20	0.00002789	4.276E-17	2.188E-08	8.054E-17	0.004336	3.162E-09
317	0.00009358	0.00000784	0.001103	0.00001225	5.12E-19	0.00003336	9.321E-17	9.829E-09	3.503E-17	0.0001675	1.585E-08
319	0.00002228	0.0001178	0.0004166	0.00006951	2.088E-20	0.00002382	3.02E-17	2.949E-08	9.016E-17	0.0004665	1.995E-09
320	0.00001685	0.0000562	0.0006122	0.00004874	4.011E-20	0.00002103	4.607E-17	3.442E-08	1.092E-16	0.00007105	2.512E-09
321	0.0000167	0.00008826	0.0007757	0.000097	5.305E-20	0.00003324	7.671E-17	5.489E-08	2.29E-16	0.002622	1.995E-09
322	0.00002456	0.0001298	0.00002447	0.0000045	1.804E-21	1.542E-06	2.609E-18	1.731E-09	7.789E-18	0.0003355	1.995E-09
323	0.00002204	0.00007352	0.0005348	0.0000557	3.58E-20	0.00002403	4.112E-17	3.006E-08	9.751E-17	0.000452	2.512E-09

Table G. part 5: *Continued*

Sequence # (sample #)	CO2(aq) activity	CO3-- activity	Ca++ activity	CaCO3 activity	CaH2PO4+ activity	CaHCO3+ activity	CaHPO4 activity	CaOH+ activity	CaPO4- activity	Cl- activity	H+ activity
325	0.00002519	0.0002111	0.0002515	0.0000752	1.681E-20	0.00002047	3.06E-17	2.24E-08	1.15E-16	0.0002486	1.585E-09
329	0.00001187	0.0001576	0.0005874	0.0001312	1.717E-20	0.00002836	3.935E-17	6.589E-08	1.862E-16	0.0001597	1.259E-09
330	7.743E-06	0.0001028	0.0006895	0.0001005	2.309E-20	0.00002172	5.291E-17	7.735E-08	2.504E-16	0.00008088	1.259E-09
331	0.0000293	0.0000389	0.0007549	0.00004161	1.318E-19	0.00002845	9.552E-17	2.678E-08	1.429E-16	0.00148	3.981E-09
332	0.0000135	0.00007138	0.0005599	0.00005661	3.377E-20	0.0000194	4.884E-17	3.963E-08	1.458E-16	0.0001878	1.995E-09
333	0.00002412	0.0002021	0.0001064	0.00003047	5.955E-21	8.295E-06	1.084E-17	9.483E-09	4.075E-17	0.0005145	1.585E-09
334	0.00001458	0.00007711	0.0005145	0.0000562	3.787E-20	0.00001926	5.477E-17	3.641E-08	1.635E-16	0.0002255	1.995E-09
335	0.00002319	0.0001943	0.0001105	0.00003043	6.878E-21	8.283E-06	1.252E-17	9.848E-09	4.706E-17	0.00004465	1.585E-09
336	0.0000243	0.0001285	0.0002092	0.00003809	1.689E-20	0.00001305	2.442E-17	1.481E-08	7.291E-17	0.00003603	1.995E-09
337	0.00002328	0.0001231	0.000261	0.0000455	2.117E-20	0.00001559	3.061E-17	1.847E-08	9.138E-17	0.0000541	1.995E-09
338	0.00009026	0.00001199	0.001017	0.00001727	6.108E-19	0.00003734	1.4E-16	1.141E-08	6.624E-17	0.00004557	1.259E-08
340	0.00002452	0.00008179	0.000345	0.00003997	3.881E-20	0.00001725	4.458E-17	1.94E-08	1.057E-16	0.000227	2.512E-09
341	0.00002182	0.00002899	0.0007781	0.00003195	1.523E-19	0.00002185	1.104E-16	2.76E-08	1.652E-16	0.0005587	3.981E-09
342	0.00002494	0.0001319	0.0001562	0.00002918	1.404E-20	9.998E-06	2.031E-17	1.105E-08	6.062E-17	0.00004517	1.995E-09
343	0.00002886	0.00001526	0.0008196	0.00001772	2.511E-19	0.0000192	1.148E-16	1.835E-08	1.084E-16	0.00005508	6.31E-09
345	0.00002116	0.0001119	0.0003455	0.00005475	3.132E-20	0.00001876	4.529E-17	2.445E-08	1.352E-16	0.00004547	1.995E-09
346	0.00002627	0.0000553	0.0006829	0.0000535	1.073E-19	0.00002906	9.793E-17	3.05E-08	1.845E-16	9.184E-06	3.162E-09
347	0.00002194	0.00007321	6.989E-13	7.249E-14	2.068E-28	3.127E-14	2.376E-25	3.93E-17	5.634E-25	0.00005631	2.512E-09
348	0.00007512	0.00001581	0.000529	0.00001185	3.107E-19	0.00002035	8.966E-17	7.471E-09	5.341E-17	0.00002764	0.00000001
349	0.00001944	0.00004092	0.0003888	0.00002254	7.25E-20	0.00001224	6.615E-17	1.736E-08	1.246E-16	9.268E-10	3.162E-09
352	0.00004493	0.00001499	0.0005958	0.00001265	3.141E-19	0.00001726	1.141E-16	1.059E-08	8.556E-17	0.0000093	7.943E-09
353	0.00004347	0.0000145	0.0006402	0.00001315	3.434E-19	0.00001795	1.247E-16	1.138E-08	9.354E-17	0.00003729	7.943E-09
356	4.895E-06	0.01026	0.00001049	0.0001526	3.537E-23	2.621E-06	1.021E-18	1.476E-08	6.08E-17	0.01825	1E-10
357	0.00001114	0.00371	0.00001984	0.0001043	2.632E-22	4.498E-06	3.023E-18	1.113E-08	7.169E-17	0.008181	2.512E-10
358	0.00001045	0.00548	7.952E-06	0.00006174	3.145E-12	2.116E-06	4.549E-08	5.583E-09	1.358E-06	0.115	1.995E-10
359	0.00002923	0.01504	3.662E-06	0.00007805	8.95E-24	2.675E-06	1.294E-19	2.523E-09	3.864E-18	0.2653	1.995E-10
361	0.00006293	2.1E-09	0.00005603	1.667E-10	5.073E-19	2.274E-08	1.843E-18	9.964E-12	1.382E-20	9.837E-06	7.943E-07
368	0.0001278	0.00002689	0.0001828	6.963E-06	1.318E-19	0.00001196	3.803E-17	2.58E-09	2.265E-17	0.007966	0.00000001
370	0.0001594	0.00001336	0.0006109	0.00001156	7.315E-09	0.00003147	1.332E-06	5.443E-09	5.005E-07	0.0002008	1.585E-08
371	0.00007339	0.00006149	0.0005861	0.00005106	1.768E-19	0.00004395	1.018E-16	1.651E-08	1.21E-16	0.0003777	5.012E-09
372	0.0001847	3.889E-06	0.0004972	0.00000274	6.748E-09	0.00001488	6.157E-07	2.221E-09	1.16E-07	0.00009294	3.162E-08
373	9.161E-06	0.003024	0.00002101	0.00009002	1.344E-11	3.884E-06	1.544E-07	1.169E-08	3.661E-06	0.1548	2.512E-10
374	0.00003635	0.0004817	0.00005276	0.00003601	1.518E-12	7.785E-06	3.478E-09	5.905E-09	1.646E-08	0.04324	1.259E-09
375	0.0001031	2.171E-06	0.0003088	9.498E-07	7.674E-19	5.158E-06	7.002E-17	1.379E-09	1.319E-17	0.0001511	3.162E-08
376	0.0001184	2.493E-06	0.0005729	2.023E-06	1.132E-18	0.00001099	1.033E-16	2.559E-09	1.945E-17	0.001331	3.162E-08
377	0.00002507	0.001322	0.00003609	0.00006757	1.215E-11	7.323E-06	5.555E-08	8.054E-09	5.244E-07	0.03624	6.31E-10
378	0.00001907	0.001594	0.00003154	0.00007121	8.913E-12	6.129E-06	5.131E-08	8.862E-09	6.098E-07	0.03637	5.012E-10
381	0.00008509	1.791E-06	0.0003122	7.924E-07	3.183E-09	4.304E-06	2.904E-07	1.395E-09	5.47E-08	0.0001609	3.162E-08

Table G. part 5: *Continued*

Sequence # (sample #)	CO2(aq) activity	CO3-- activity	Ca++ activity	CaCO3 activity	CaH2PO4+ activity	CaHCO3+ activity	CaHPO4 activity	CaOH+ activity	CaPO4- activity	Cl- activity	H+ activity
382	0.0002012	6.525E-06	0.002058	0.00001902	3.385E-09	0.00008206	3.889E-07	1.125E-08	9.222E-08	0.5254	2.512E-08
383	9.507E-06	0.007881	1.657E-06	0.00001851	2.244E-12	5.038E-07	4.085E-08	1.461E-09	1.535E-06	0.1431	1.585E-10
384	6.326E-06	0.005275	8.276E-06	0.00006185	5.768E-12	1.683E-06	1.05E-07	7.338E-09	3.946E-06	0.07211	1.585E-10
385	0.0002049	2.721E-07	0.0001846	7.117E-08	3.407E-09	1.539E-06	7.809E-08	2.071E-10	3.695E-09	0.0004532	1.259E-07
386	0.0001915	2.001E-06	0.004758	0.00001349	3.653E-10	0.00009221	2.647E-08	1.328E-08	3.961E-09	5.842	3.981E-08
387	0.001149	5.951E-07	0.005119	4.316E-06	7.859E-18	0.0001479	1.136E-16	3.549E-09	3.393E-18	0.434	1.995E-07
388	0.0002034	1.684E-06	0.00667	0.00001591	4.153E-18	0.000137	2.391E-16	1.857E-08	2.842E-17	0.2715	5.012E-08
389	0.0001318	4.389E-06	0.001302	8.096E-06	1.125E-10	0.00003493	1.292E-08	7.307E-09	3.065E-09	0.04389	2.512E-08
390	0.000424	1.409E-06	0.004039	8.059E-06	5.875E-18	0.0001099	2.134E-16	7.151E-09	1.6E-17	0.0953	7.943E-08
392	0.0004174	5.543E-06	0.001154	9.061E-06	2.166E-18	0.00006196	1.57E-16	4.093E-09	2.349E-17	0.002182	3.981E-08
393	0.0004948	0.00000657	0.0001916	1.783E-06	2.946E-19	0.00001219	2.135E-17	6.794E-10	3.195E-18	0.007573	3.981E-08
394	0.001126	1.496E-06	0.002353	4.986E-06	7.244E-18	0.0001078	1.66E-16	2.639E-09	7.855E-18	0.006695	1.259E-07
395	0.00002271	0.0000478	0.001018	0.00006892	1.579E-19	0.00003743	1.441E-16	4.545E-08	2.714E-16	0.0004693	3.162E-09
396	0.0000399	1.013E-07	0.06561	9.419E-06	2.483E-18	0.0001285	9.021E-17	8.88E-08	6.764E-18	6.129	7.943E-08
397	0.00001463	0.00007734	0.000923	0.0001011	6.294E-20	0.00003466	9.102E-17	6.533E-08	2.717E-16	0.000263	1.995E-09
398	0.0000165	0.0005494	0.0001907	0.0001484	3.882E-21	0.00002025	1.41E-17	3.385E-08	1.057E-16	0.01918	7.943E-10
399	0.00001655	0.0008734	0.0001033	0.0001278	1.745E-21	0.00001385	7.98E-18	2.308E-08	7.534E-17	0.006382	6.31E-10
400	0.00001822	0.0003825	0.0003356	0.0001819	3.436E-21	0.00003123	9.914E-18	4.727E-08	5.906E-17	0.008102	1E-09
401	0.00002108	0.0004364	0.000212	0.000131	6.896E-22	0.00002251	1.99E-18	2.944E-08	1.185E-17	0.2381	1E-09
402	0.00001473	0.0001949	0.0005438	0.0001502	4.785E-21	0.00003247	1.097E-17	6.08E-08	5.189E-17	0.01883	1.259E-09
403	7.526E-06	0.0003966	0.000184	0.0001034	6.203E-22	0.0000112	2.836E-18	4.104E-08	2.678E-17	0.01751	6.31E-10
404	0.00003501	0.0002777	0.0004159	0.0001636	2.438E-21	0.00004454	4.439E-18	3.508E-08	1.668E-17	0.6029	1.585E-09
405	9.855E-06	0.00008253	0.001297	0.0001517	2.897E-20	0.00004129	5.275E-17	1.155E-07	1.983E-16	0.003847	1.585E-09
406	0.00001173	0.0001546	0.000584	0.0001279	4.255E-21	0.00002766	9.753E-18	6.504E-08	4.615E-17	0.07373	1.259E-09
408	0.0000471	0.000157	0.0002481	0.00005519	1.169E-20	0.00002381	1.343E-17	1.394E-08	3.185E-17	0.002304	2.512E-09
409	0.00004733	0.00003965	0.001168	0.00006563	1.845E-19	0.0000565	1.062E-16	3.291E-08	1.263E-16	0.001208	5.012E-09
410	0.0000081	0.0001693	0.0006111	0.0001466	4.822E-21	0.00002518	1.391E-17	8.571E-08	8.288E-17	0.1259	1E-09
411	0.00002168	0.0001816	0.0007934	0.0002041	3.21E-20	0.00005556	5.844E-17	7.065E-08	2.196E-16	0.005969	1.585E-09
412	0.00001294	0.0002696	0.0004557	0.0001741	3.242E-21	0.0000299	9.354E-18	6.369E-08	5.572E-17	0.1143	1E-09
413	0.00001178	0.00006224	0.001221	0.0001076	2.609E-20	0.00003689	3.773E-17	8.633E-08	1.126E-16	0.001116	1.995E-09
414	0.00002578	0.0002155	0.000616	0.0001881	1.664E-20	0.00005119	3.029E-17	5.475E-08	1.138E-16	0.02385	1.585E-09
415	0.00001764	0.0009322	0.0000516	0.00006815	1.55E-21	7.385E-06	7.087E-18	1.154E-08	6.69E-17	0.001716	6.31E-10
416	0.00003246	0.0001062	0.0007708	0.0001159	1.276E-20	0.00005002	1.465E-17	4.249E-08	3.475E-17	0.2252	2.512E-09
417	0.0000436	0.0005785	0.0001184	0.00009702	5.746E-21	0.00002098	1.317E-17	1.327E-08	6.231E-17	0.0006783	1.259E-09
418	0.00004399	0.00003684	0.0009974	0.00005206	8.975E-20	0.00004482	5.167E-17	2.809E-08	6.141E-17	0.001375	5.012E-09
419	0.00002506	0.001322	0.00004501	0.00008428	1.098E-21	9.133E-06	5.022E-18	1.005E-08	4.741E-17	0.01957	6.31E-10
420	0.00001986	0.001044	0.00006929	0.0001025	7.152E-22	0.00001111	3.271E-18	1.543E-08	3.088E-17	0.02776	6.31E-10
421	7.784E-06	0.0001029	0.001049	0.0001529	6.824E-21	0.00003306	1.564E-17	1.171E-07	7.4E-17	0.01983	1.259E-09

Table G. part 5: *Continued*

Sequence # (sample #)	CO2(aq) activity	CO3-- activity	Ca++ activity	CaCO3 activity	CaH2PO4+ activity	CaHCO3+ activity	CaHPO4 activity	CaOH+ activity	CaPO4- activity	Cl- activity	H+ activity
422	0.00001012	0.00008478	0.001295	0.0001556	5.501E-20	0.00004235	1.001E-16	1.154E-07	3.764E-16	0.0001899	1.585E-09
423	0.00002049	0.001081	0.00009892	0.0001515	2.853E-21	0.00001642	1.304E-17	2.21E-08	1.232E-16	0.01497	6.31E-10
424	0.00003253	0.00004319	0.001186	0.00007258	9.18E-20	0.00004962	6.653E-17	4.206E-08	9.955E-17	0.001931	3.981E-09
425	0.00001348	0.001129	0.00003187	0.00005095	5.327E-22	4.386E-06	3.067E-18	8.975E-09	3.645E-17	0.00104	5.012E-10
426	0.00004322	0.00003622	0.0005856	0.00003005	1.061E-19	0.00002587	6.106E-17	1.65E-08	7.256E-17	0.0003589	5.012E-09
427	0.00004245	0.0001415	0.0008448	0.0001694	5.817E-20	0.00007309	6.682E-17	4.748E-08	1.585E-16	0.002396	2.512E-09
428	0.00003298	0.00002763	0.001453	0.00005688	2.557E-19	0.00004896	1.472E-16	4.094E-08	1.75E-16	0.001141	5.012E-09
429	0.0000099	0.005195	0.00002364	0.000174	9.577E-23	5.961E-06	1.385E-18	1.66E-08	4.135E-17	0.04124	1.995E-10
430	4.732E-06	0.00006258	0.0007952	0.0000705	4.575E-21	0.00001524	1.048E-17	8.884E-08	4.961E-17	0.01475	1.259E-09
431	0.00002695	0.0002244	0.0004514	0.0001435	8.423E-21	0.00003907	1.533E-17	3.998E-08	5.763E-17	0.05456	1.585E-09
432	0.00001311	0.0006923	0.00008017	0.00007864	1.202E-21	8.522E-06	5.498E-18	1.792E-08	5.191E-17	0.01104	6.31E-10
433	0.00001494	0.0001207	0.0004018	0.00006872	2.62E-21	0.00001871	4.77E-18	3.452E-08	1.793E-17	0.2523	1.585E-09
434	2.506E-07	0.0003325	0.0006686	0.0003149	2.659E-22	0.00000681	6.094E-18	7.493E-07	2.883E-16	0.004179	1.259E-10
435	0.00003411	0.00004531	0.001376	0.00008835	1.908E-19	0.00006041	1.383E-16	4.883E-08	2.069E-16	0.0002343	3.981E-09
436	0.00003457	0.00002897	0.001002	0.00004113	2.042E-19	0.0000354	1.176E-16	2.824E-08	1.398E-16	0.0001997	5.012E-09
437	0.00005476	0.0001151	0.0004756	0.00007755	4.483E-20	0.00004212	4.09E-17	2.121E-08	7.704E-17	0.005451	3.162E-09
439	0.00004431	0.00003713	0.0008689	0.00004571	1.673E-19	0.00003934	9.631E-17	2.448E-08	1.145E-16	0.0005934	5.012E-09
440	1.464E-07	0.00004878	0.002183	0.0001509	2.08E-21	6.511E-06	2.39E-17	1.226E-06	5.667E-16	0.01752	2.512E-10
441	0.00003175	0.0001058	0.0004265	0.00006392	1.331E-20	0.00002758	1.528E-17	2.395E-08	3.624E-17	0.002505	2.512E-09
442	0.00001373	0.0001819	0.0003251	0.00008379	2.841E-21	0.00001812	6.512E-18	3.638E-08	3.081E-17	0.005257	1.259E-09
443	0.00001786	0.000941	0.00005193	0.00006923	1.183E-21	7.503E-06	5.41E-18	1.158E-08	5.107E-17	0.07272	6.31E-10
444	0.00001348	0.0002834	0.001045	0.0004197	1.617E-20	0.00007208	4.664E-17	1.475E-07	2.778E-16	0.01231	1E-09
445	0.0000186	0.00006204	0.0007808	0.00006863	6.412E-20	0.00002961	7.365E-17	4.389E-08	1.747E-16	0.0008907	2.512E-09
446	0.00004026	0.0008466	0.00004385	0.0000526	2.055E-21	9.033E-06	5.929E-18	6.188E-09	3.531E-17	0.001473	1E-09
447	0.00001869	0.0001566	0.0005685	0.0001261	1.744E-20	0.00003432	3.175E-17	5.065E-08	1.193E-16	0.0006268	1.585E-09
448	0.00001809	0.00006022	0.0005866	0.00005005	9.99E-21	0.00002159	1.148E-17	3.291E-08	2.721E-17	0.005267	2.512E-09
449	4.799E-06	0.0001588	0.001207	0.0002716	7.724E-21	0.00003706	2.806E-17	2.129E-07	2.104E-16	0.009064	7.943E-10
450	0.00003016	0.001005	0.00006573	0.00009362	2.871E-21	0.00001277	1.043E-17	1.168E-08	7.82E-17	0.006862	7.943E-10
451	0.00003401	0.0001796	0.0002799	0.00007123	1.331E-20	0.00002441	1.925E-17	1.979E-08	5.748E-17	0.009646	1.995E-09
452	0.0000107	0.0002251	0.0002932	0.00009349	7.847E-21	0.00001606	2.264E-17	4.139E-08	1.349E-16	0.00337	1E-09
453	3.033E-06	0.0004002	0.0002039	0.0001156	5.841E-22	7.905E-06	4.234E-18	7.187E-08	6.334E-17	0.0658	3.981E-10
454	0.00004963	0.000104	0.0008921	0.0001315	5.062E-20	0.0000714	4.619E-17	3.967E-08	8.7E-17	0.03095	3.162E-09
455	0.00002212	0.0004642	0.0002219	0.000146	5.893E-21	0.00002507	1.7E-17	3.126E-08	1.013E-16	0.01243	1E-09
456	0.00002525	0.0002115	0.0003826	0.0001146	1.95E-20	0.00003121	3.551E-17	3.408E-08	1.335E-16	0.002179	1.585E-09
457	0.00002019	0.00001691	0.001792	0.00004295	1.715E-19	0.00003697	9.874E-17	5.048E-08	1.173E-16	0.001437	5.012E-09
458	0.00001247	0.00006563	0.001161	0.0001079	1.557E-20	0.00003698	2.252E-17	8.176E-08	6.722E-17	0.08082	1.995E-09
459	0.00002962	0.00009866	0.0004294	0.00006002	9.569E-21	0.00002589	1.099E-17	2.41E-08	2.606E-17	0.006581	2.512E-09
460	0.00004451	0.0001409	0.000423	0.00008443	3.424E-21	0.00003643	3.933E-18	2.257E-08	9.328E-18	0.8593	2.512E-09

Table G. part 5: *Continued*

Sequence # (sample #)	CO2(aq) activity	CO3-- activity	Ca++ activity	CaCO3 activity	CaH2PO4+ activity	CaHCO3+ activity	CaHPO4 activity	CaOH+ activity	CaPO4- activity	Cl- activity	H+ activity
461	0.00001242	0.01023	0.00001185	0.0001718	4.755E-23	4.678E-06	8.656E-19	1.039E-08	3.253E-17	0.09413	1.585E-10
462	0.00000252	0.0002106	0.0005354	0.0001597	2.782E-21	0.00001375	1.602E-17	1.505E-07	1.903E-16	0.02813	5.012E-10
473	0.00002552	0.0000535	0.003613	0.0002739	1.52E-19	0.0001488	1.387E-16	1.607E-07	2.612E-16	0.08997	3.162E-09
474	0.00002258	0.00004731	0.004182	0.0002803	1.637E-19	0.0001522	1.493E-16	1.859E-07	2.813E-16	0.09415	3.162E-09
475	0.00003095	0.0000258	0.005455	0.0001994	3.175E-19	0.0001716	1.828E-16	1.529E-07	2.172E-16	0.1143	5.012E-09
476	0.00003694	0.00004884	0.004064	0.0002812	2.173E-19	0.0001923	1.575E-16	1.435E-07	2.357E-16	0.09515	3.981E-09
477	0.00003337	0.00004404	0.00221	0.0001379	1.224E-19	0.00009428	8.87E-17	7.791E-08	1.327E-16	0.1291	3.981E-09
478	0.00001934	0.00006411	0.002279	0.000207	6.844E-20	0.00008931	7.862E-17	1.273E-07	1.864E-16	0.1333	2.512E-09
479	0.00001496	0.00004957	0.002296	0.0001612	6.81E-20	0.00006955	7.822E-17	1.282E-07	1.855E-16	0.1374	2.512E-09
480	0.00001917	0.00006353	0.002385	0.0002147	6.908E-20	0.00009263	7.935E-17	1.332E-07	1.882E-16	0.1405	2.512E-09
481	0.00001687	0.0000559	0.002335	0.0001849	6.82E-20	0.00007977	7.834E-17	1.304E-07	1.858E-16	0.1415	2.512E-09
482	0.00001502	0.00004977	0.002119	0.0001494	6.527E-20	0.00006446	7.497E-17	1.184E-07	1.778E-16	0.1373	2.512E-09
483	0.00001847	0.00003864	0.002076	0.0001136	8.306E-20	0.00006172	7.579E-17	9.212E-08	1.428E-16	0.1366	3.162E-09
484	0.00001614	0.00005353	0.002061	0.0001563	6.411E-20	0.00006745	7.365E-17	1.152E-07	1.746E-16	0.1262	2.512E-09
485	0.00001464	0.00004856	0.001915	0.0001317	6.281E-20	0.00005682	7.215E-17	1.071E-07	1.711E-16	0.1189	2.512E-09
486	0.00006218	0.00001305	0.003317	0.00006133	6.439E-19	0.0001053	1.858E-16	4.671E-08	1.107E-16	0.06282	0.00000001
487	8.505E-06	0.00007123	0.001433	0.0001446	5.388E-20	0.00003937	9.81E-17	1.276E-07	3.687E-16	0.01408	1.585E-09
488	6.595E-06	0.00008754	0.001444	0.0001791	3.865E-20	0.00003873	8.859E-17	1.619E-07	4.192E-16	0.01339	1.259E-09
489	0.0001261	6.664E-06	0.000703	6.637E-06	7.841E-19	0.00002275	1.134E-16	4.975E-09	3.385E-17	0.004069	1.995E-08
490	7.215E-06	0.00009577	0.001415	0.000192	3.869E-20	0.00004152	8.866E-17	1.587E-07	4.195E-16	0.01363	1.259E-09
522	0.0000603	0.00007303	0.001193	0.0001234	2.96E-08	0.00008837	0.00002049	4.041E-08	0.00002928	0.0004619	4.169E-09
523	5.463E-07	0.01898	0.00003622	0.0009738	2.949E-12	4.106E-06	3.467E-07	2.072E-07	0.00008412	0.01341	2.455E-11
524	3.181E-07	0.01332	0.00007307	0.001379	4.972E-12	5.302E-06	6.408E-07	4.596E-07	0.0001705	0.008318	2.239E-11
525	0.00000268	0.02032	0.00004636	0.001335	6.076E-11	0.00001203	0.00000334	1.238E-07	0.0003791	0.02122	5.248E-11
526	2.268E-06	0.03501	0.00004385	0.002175	5.19E-12	0.00001356	4.125E-07	1.649E-07	0.00006767	0.04316	3.631E-11
527	0.0001489	0.0001247	0.0005192	0.00009175	9.476E-20	0.00007898	5.455E-17	1.462E-08	6.484E-17	0.0003307	5.012E-09
528	0.0001044	0.0001914	0.0004334	0.0001175	1.022E-08	0.00006837	8.702E-06	1.805E-08	0.0000153	0.0003206	3.388E-09
529	0.00001676	0.02198	0.00003696	0.001151	2.38E-11	0.00002489	5.455E-07	4.094E-08	0.00002581	0.02404	1.259E-10
530	7.812E-06	0.02566	0.00003157	0.001148	9.407E-12	0.00001566	3.417E-07	5.526E-08	0.00002562	0.02928	7.943E-11
531	0.001947	0.00003252	0.0005919	0.00002728	1.957E-08	0.0001662	1.591E-06	2.354E-09	2.671E-07	0.0007982	3.548E-08
532	0.001076	0.0000595	0.0005225	0.00004405	3.126E-19	0.0001475	4.625E-17	3.782E-09	1.413E-17	0.0005778	1.95E-08
533	0.0008893	0.00006486	0.0002356	0.00002165	8.096E-09	0.00006316	1.376E-06	1.958E-09	4.825E-07	0.0005107	1.698E-08
534	0.0006223	0.000125	0.000241	0.00004267	7.851E-20	0.00007499	2.214E-17	3.323E-09	1.289E-17	0.0004986	1.023E-08
535	0.00118	0.0003419	0.0001019	0.00004936	7.777E-09	0.00007216	2.636E-06	1.687E-09	1.845E-06	0.0003748	8.511E-09
536	6.847E-06	0.02947	4.622E-06	0.000193	2.161E-12	2.293E-06	9.013E-08	9.236E-09	7.761E-06	0.05397	6.918E-11
537	0.00001728	0.02949	6.185E-06	0.0002584	5.684E-12	4.867E-06	1.496E-07	7.767E-09	8.126E-06	0.05595	1.096E-10
538	3.622E-06	0.034	5.505E-06	0.0002652	9.043E-13	2.131E-06	5.579E-08	1.622E-08	7.104E-06	0.0007063	4.677E-11
539	1.999E-06	0.0299	0.00000582	0.0002466	3.522E-13	1.573E-06	2.735E-08	2.17E-08	4.385E-06	0.05125	3.715E-11

Table G. part 5: *Continued*

Sequence # (sample #)	CO2(aq) activity	CO3-- activity	Ca++ activity	CaCO3 activity	CaH2PO4+ activity	CaHCO3+ activity	CaHPO4 activity	CaOH+ activity	CaPO4- activity	Cl- activity	H+ activity
540	0.0002247	0.000197	0.0002892	0.00008072	5.194E-20	0.0000679	3.06E-17	8.333E-09	3.721E-17	0.0004962	4.898E-09
541	0.0002833	0.0001799	0.0004212	0.0001074	5.816E-20	0.0001061	2.916E-17	1.033E-08	3.019E-17	0.0005922	5.754E-09
542	0.000177	0.0002143	0.0002266	0.00006881	2.853E-20	0.00004926	1.975E-17	7.672E-09	2.821E-17	0.001069	4.169E-09
543	0.00002686	0.02218	0.00004092	0.001286	3.117E-10	0.00003501	5.675E-06	3.595E-08	0.0002133	0.02906	1.585E-10
544	0.00002456	0.02037	0.0000408	0.001177	1.709E-10	0.00003205	3.111E-06	3.598E-08	0.0001169	0.008958	1.585E-10
545	7.946E-06	0.0261	0.00002703	0.0009992	1.791E-11	0.00001363	6.506E-07	4.73E-08	0.00004879	0.02941	7.943E-11
546	7.545E-06	0.0283	0.00002162	0.0008671	2.22E-11	0.00001104	8.642E-07	4.034E-08	0.00006944	0.04016	7.413E-11
547	6.383E-06	0.03535	0.00003745	0.001876	9.019E-12	0.00001941	4.319E-07	8.385E-08	0.00004269	0.07031	6.026E-11
548	0.00002585	0.02338	0.0000321	0.001063	8.364E-11	0.00002764	1.594E-06	2.949E-08	0.00006275	0.03589	1.514E-10
549	0.00006632	0.01262	0.00003171	0.0005671	2.135E-10	0.00003225	0.00000186	1.341E-08	0.00003347	0.01398	3.311E-10
550	0.0000134	0.02892	0.00002925	0.001199	1.977E-11	0.00002012	5.838E-07	4.14E-08	0.00003558	0.03302	9.772E-11
551	0.00001555	0.03309	0.00002858	0.00134	2.038E-11	0.00002249	6.019E-07	3.988E-08	0.00003669	0.04331	9.772E-11
552	0.00000482	0.03266	0.00002205	0.00102	1.108E-12	9.629E-06	5.819E-08	5.508E-08	6.307E-06	0.04662	5.495E-11
553	5.762E-06	0.03246	0.00002879	0.001324	3.246E-12	0.0000137	1.555E-07	6.556E-08	0.00001537	0.05069	6.026E-11
554	4.408E-06	0.03271	0.00004864	0.002254	8.286E-12	0.00002032	4.556E-07	1.271E-07	0.00005171	0.05254	5.248E-11
555	2.017E-06	0.03156	0.00001333	0.000596	6.618E-12	3.716E-06	5.259E-07	5.08E-08	0.00008628	0.02599	3.631E-11
556	4.565E-06	0.0324	0.00002708	0.001243	2.008E-11	0.00001147	1.079E-06	6.927E-08	0.0001197	0.04406	5.37E-11
557	0.0000235	0.03025	0.00002718	0.001165	8.853E-11	0.00002519	2.029E-06	2.956E-08	0.000096	0.0584	1.259E-10
558	1.326E-06	0.02752	0.00002839	0.001107	1.202E-11	6.013E-06	1.097E-06	1.251E-07	0.0002066	0.02186	3.162E-11
559	8.097E-06	0.03295	0.00001525	0.000712	1.866E-11	8.657E-06	7.607E-07	2.948E-08	0.000064	0.04229	7.079E-11
560	0.00002694	0.0002713	0.0001764	0.0000678	1.33E-20	0.00001683	2.656E-17	1.723E-08	1.094E-16	0.0005609	1.445E-09
561	0.00001025	0.03546	6.659E-06	0.0003346	3.619E-12	4.359E-06	1.377E-07	1.173E-08	0.00001081	0.1054	7.586E-11
562	5.239E-06	0.03234	0.00001851	0.0008482	2.413E-11	8.383E-06	0.00000121	4.412E-08	0.0001252	0.04974	5.754E-11
563	0.0001401	0.03829	0.0000276	0.001497	2.26E-10	0.00006763	2.479E-06	1.331E-08	0.00005614	0.1635	2.63E-10
564	2.88E-08	2.2208E-05	0.00129569	4.0766E-05	1.5195E-10	1.012E-06	3.0332E-06	9.6917E-07	0.000125	5.564165	1.4454E-10
565	4.159E-07	0.002556	0.0005578	0.00202	2.205E-17	0.00001863	1.185E-12	1.235E-06	1.314E-10	3.286	5.37E-11
566	0.00004371	0.0001674	0.0002507	0.00005944	3.106E-20	0.00002393	3.823E-17	1.51E-08	9.715E-17	0.0009049	2.344E-09
567	0.00005522	0.03815	0.00002394	0.001294	5.629E-11	0.00003688	9.786E-07	1.842E-08	0.00003512	0.2303	1.66E-10
568	0.00003794	0.04288	0.00002434	0.001479	5.269E-11	0.00003272	0.00000118	2.378E-08	0.00005457	0.1898	1.288E-10
569	6.956E-06	0.02851	0.00002017	0.0008149	4.037E-11	9.908E-06	1.645E-06	3.928E-08	0.0001384	0.06836	7.079E-11
570	0.00009952	0.04158	0.00005421	0.003194	4.945E-10	0.0001146	0.00000683	3.176E-08	0.0001947	0.3705	2.089E-10
571	0.00007949	0.03632	0.00002152	0.001107	1.037E-10	0.00003883	1.466E-06	1.347E-08	0.00004277	0.278	2.042E-10
572	0.00009861	0.0000454	0.0003008	0.00001935	1.222E-19	0.00002247	5.214E-17	6.283E-09	4.593E-17	0.00007235	6.761E-09
573	0.00005634	0.0001361	0.000645	0.0001244	7.512E-20	0.00006305	7.344E-17	3.086E-08	1.482E-16	0.0007643	2.951E-09
574	0.00000584	0.02778	5.583E-06	0.0002197	1.314E-12	2.493E-06	5.737E-08	1.177E-08	5.172E-06	0.01518	6.607E-11
575	0.00002191	0.006964	0.0000125	0.0001234	8.492E-12	5.446E-06	9.533E-08	6.853E-09	2.209E-06	0.002676	2.57E-10
576	0.00004089	0.0006831	0.00009465	0.0000916	1.246E-09	0.00001765	3.203E-06	1.19E-08	0.00001701	0.005235	1.122E-09
577	0.0001068	0.00004487	0.0006226	0.00003958	1.742E-19	0.00004812	7.102E-17	1.242E-08	5.975E-17	0.00106	7.079E-09

Table G. part 5: *Continued*

Sequence # (sample #)	CO2(aq) activity	CO3-- activity	Ca++ activity	CaCO3 activity	CaH2PO4+ activity	CaHCO3+ activity	CaHPO4 activity	CaOH+ activity	CaPO4- activity	Cl- activity	H+ activity
578	0.00002956	0.0002473	0.00006333	0.00002218	6.082E-11	6.039E-06	1.107E-07	5.633E-09	4.162E-07	0.03789	1.585E-09
579	1.082E-06	0.01383	3.63E-14	7.11E-13	4.962E-22	4.862E-15	3.596E-17	1.239E-16	5.381E-15	0.5173	3.981E-11
580	2.966E-06	0.01497	3.409E-14	7.23E-13	7.126E-22	7.835E-15	3.259E-17	7.283E-17	3.076E-15	0.6026	6.31E-11
581	0.00002128	0.01667	3.167E-14	7.477E-13	4.659E-21	2.035E-14	8.481E-17	2.637E-17	3.188E-15	0.8141	1.585E-10
582	0.00008351	0.01599	3.446E-14	7.807E-13	9.35E-21	4.24E-14	8.531E-17	1.4E-17	1.607E-15	1.153	3.162E-10
583	0.0001376	0.01642	3.422E-14	7.961E-13	1.398E-20	5.443E-14	1.013E-16	1.091E-17	1.516E-15	1.277	3.981E-10
584	0.0002353	0.0173	3.334E-14	8.174E-13	1.968E-20	7.036E-14	1.133E-16	8.246E-18	1.346E-15	1.541	5.012E-10
585	0.0004555	0.02004	3.101E-14	8.806E-13	2.032E-20	9.543E-14	9.291E-17	5.777E-18	8.772E-16	2.125	6.31E-10
586	3.469E-06	0.04565	1.578E-14	1.021E-12	6.996E-23	6.22E-15	5.69E-18	4.944E-17	9.552E-16	2.258	3.548E-11
587	3.137E-06	0.04204	1.662E-14	9.898E-13	6.189E-23	6.032E-15	5.033E-18	5.301E-17	8.449E-16	2.027	3.548E-11
588	2.198E-06	0.04368	1.92E-14	1.188E-12	2.292E-23	5.752E-15	2.347E-18	7.216E-17	4.959E-16	3.401	2.818E-11
589	2.464E-06	0.04942	1.608E-14	1.126E-12	1.814E-23	5.449E-15	1.857E-18	6.099E-17	3.924E-16	2.868	2.818E-11
590	2.443E-06	0.04835	1.707E-14	1.17E-12	3.849E-23	5.661E-15	3.941E-18	6.389E-17	8.329E-16	3.358	2.818E-11
591	2.361E-06	0.04645	1.826E-14	1.201E-12	3.008E-23	5.815E-15	3.079E-18	6.791E-17	6.508E-16	3.554	2.818E-11
592	9.487E-06	0.04657	1.841E-14	1.215E-12	1.352E-22	1.173E-14	6.939E-18	3.41E-17	7.35E-16	3.785	5.623E-11
593	0.0000029	0.0458	1.814E-14	1.177E-12	3.153E-23	6.391E-15	2.877E-18	6.076E-17	5.419E-16	3.337	3.162E-11
594	0.0001901	0.03338	1.935E-14	9.151E-13	6.451E-21	4.97E-14	5.886E-17	7.208E-18	1.109E-15	1.625	3.162E-10
595	0.00001462	0.04044	1.55E-14	8.882E-13	4.522E-22	1.212E-14	1.643E-17	2.286E-17	1.232E-15	1.477	7.943E-11
596	0.0003669	0.02241	2.303E-14	7.311E-13	2.532E-20	7.061E-14	1.299E-16	5.307E-18	1.376E-15	0.5866	5.623E-10
597	2.199E-06	0.04149	1.565E-14	9.199E-13	3.663E-23	4.771E-15	3.5E-18	5.983E-17	6.903E-16	1.752	3.02E-11
598	4.396E-06	0.04358	1.934E-14	1.194E-12	6.138E-23	8.167E-15	4.449E-18	5.123E-17	6.657E-16	3.537	3.981E-11
599	3.623E-06	0.04731	1.548E-14	1.038E-12	4.465E-23	6.323E-15	3.631E-18	4.811E-17	6.096E-16	2.371	3.548E-11
600	0.00002911	0.0334	1.745E-14	8.255E-13	9.345E-22	1.785E-14	2.142E-17	1.691E-17	1.013E-15	1.146	1.259E-10
601	0.00001888	0.03216	1.328E-14	6.054E-13	4.267E-21	1.114E-14	1.149E-16	1.627E-17	6.387E-15	0.3219	1.072E-10
602	9.492E-06	0.009962	4.987E-14	7.039E-13	2.775E-20	1.708E-14	5.669E-16	4.961E-17	2.391E-14	0.02266	1.413E-10
603	0.0001762	0.02195	2.324E-14	7.227E-13	1.036E-20	4.941E-14	7.511E-17	7.733E-18	1.124E-15	0.451	3.981E-10
604	0.0002399	0.02143	2.411E-14	7.321E-13	1.021E-20	5.881E-14	6.297E-17	6.76E-18	8.019E-16	0.5508	4.677E-10
605	0.00000159	0.03325	2.361E-14	1.112E-12	4.371E-35	5.383E-15	4.475E-30	9.336E-17	9.458E-28	2.89	2.818E-11
606	3.239E-06	0.04313	1.641E-14	1.003E-12	4.815E-23	6.111E-15	3.916E-18	5.202E-17	6.573E-16	2.121	3.548E-11
607	0.00000342	0.04417	1.759E-14	1.101E-12	7.746E-35	6.709E-15	6.299E-30	5.41E-17	1.057E-27	2.822	3.548E-11
608	5.573E-06	0.03878	1.635E-14	8.982E-13	2.087E-34	7.732E-15	1.202E-29	3.826E-17	1.428E-27	1.591	5.012E-11
609	5.375E-06	0.03764	1.657E-14	8.834E-13	1.227E-22	7.604E-15	7.065E-18	3.901E-17	8.397E-16	1.521	5.012E-11
610	0.00001009	0.03624	1.588E-14	8.152E-13	4.832E-22	9.912E-15	1.97E-17	2.708E-17	1.657E-15	1.2	7.079E-11
611	0.0000411	0.03078	1.715E-14	7.48E-13	2.06E-21	2.036E-14	3.751E-17	1.366E-17	1.41E-15	0.79	1.585E-10
612	2.083E-06	0.03363	2.468E-14	1.176E-12	4.49E-23	6.388E-15	4.097E-18	8.457E-17	7.718E-16	3.512	3.162E-11
613	0.00003666	0.03696	2.235E-14	1.171E-12	3.644E-22	2.531E-14	8.351E-18	1.903E-17	3.951E-16	3.378	1.259E-10
614	0.0001668	0.03081	1.846E-14	8.06E-13	5.374E-21	4.378E-14	4.903E-17	7.236E-18	9.236E-16	0.8831	3.162E-10
615	1.328E-07	0.01701	2.435E-14	5.869E-13	3.692E-22	1.269E-15	8.463E-17	2.635E-16	4.004E-14	0.3047	1.259E-11

Table G. part 5: *Continued*

Sequence # (sample #)	CO2(aq) activity	CO3-- activity	Ca++ activity	CaCO3 activity	CaH2PO4+ activity	CaHCO3+ activity	CaHPO4 activity	CaOH+ activity	CaPO4- activity	Cl- activity	H+ activity
616	5.616E-08	0.01055	5.268E-14	7.877E-13	9.199E-23	1.353E-15	2.654E-17	6.642E-16	1.581E-14	1.509	1E-11
617	1.254E-07	0.02065	4.058E-14	1.187E-12	1.607E-23	2.039E-15	4.638E-18	4.483E-16	2.762E-15	3.494	1E-11
618	2.443E-08	0.00254	2.522E-13	9.077E-13	3.689E-24	1.963E-15	8.454E-19	2.215E-15	4E-16	4.415	1.259E-11
619	2.868E-08	0.005596	8.027E-14	6.363E-13	2.187E-23	1.093E-15	6.309E-18	1.051E-15	3.758E-15	1.132	1E-11
620	3.799E-08	0.01588	5.205E-14	1.171E-12	3.714E-24	1.269E-15	1.698E-18	9.209E-16	1.603E-15	3.509	6.31E-12
621	6.303E-07	0.01322	4.021E-14	7.53E-13	2.005E-21	4.09E-15	1.83E-16	1.789E-16	3.446E-14	0.02009	3.162E-11
622	0.00003972	0.005248	8.611E-14	6.403E-13	4.199E-20	4.378E-14	3.043E-16	3.039E-17	4.553E-15	0.04086	3.981E-10
623	1.694E-06	0.008928	2.953E-06	0.00003735	7.52E-13	4.047E-07	3.439E-08	6.588E-09	3.247E-06	0.01999	6.31E-11
624	0.00005814	0.003064	0.00000442	0.00001918	8.81E-12	2.079E-06	4.029E-08	9.86E-10	3.803E-07	0.02507	6.31E-10

Table G. part 6: Aqueous chemistry database of alkaline lake waters compiled from published literature, as well as corresponding results from calculations described in chapters 2 and 3, and investigated in detail in chapter 4.

Sequence # (sample #)	H2PO4- activity	H3PO4 activity	H3SiO4- activity	HCO3- activity	HPO4-- activity	HSO4- activity	K+ activity	Mg++ activity	MgCO3 activity	MgH2PO4+ activity	MgHPO4 activity	MgOH+ activity
1	7.176E-19	4.026E-26	2.509E-13	0.007529	1.138E-16	7.363E-11	7.367E-10	0.00324	0.002376	3.136E-20	2.55E-16	0.00001264
2	1.223E-18	8.638E-26	2.148E-13	0.01066	1.54E-16	9.702E-11	7.355E-10	0.001974	0.001627	3.256E-20	2.103E-16	6.117E-06
3	7.94E-19	2.811E-26	3.23E-13	0.02201	1.995E-16	2.277E-11	7.29E-10	0.0004316	0.001467	4.623E-21	5.958E-17	2.666E-06
4	6.254E-19	5.189E-26	1.859E-13	0.00796	6.704E-17	2.472E-10	0.00264	0.007265	0.003808	6.128E-20	3.369E-16	0.00001911
5	6.763E-21	3.305E-29	3.368E-13	0.01533	1.231E-17	1.645E-11	0.05996	0.000157	0.002693	1.432E-23	1.337E-18	6.668E-06
6	3.782E-20	5.33E-28	3.105E-13	0.03576	2.388E-17	5.087E-11	0.07696	0.000269	0.00373	1.372E-22	4.443E-18	3.986E-06
7	2.188E-21	8.892E-30	3.303E-13	0.01163	4.789E-18	1.379E-11	0.07538	0.0002572	0.00402	7.591E-24	8.521E-19	0.00001291
8	1.309E-21	4.226E-30	3.067E-13	0.01163	3.607E-18	1.668E-11	0.07421	0.0001187	0.002335	2.096E-24	2.961E-19	7.232E-06
9	3.074E-19	8.645E-27	3.432E-13	0.009903	9.727E-17	9.164E-11	0.004938	0.001858	0.003576	7.705E-21	1.25E-16	0.0000144
10	1.069E-18	1.438E-25	1.268E-13	0.01239	7.064E-17	7.746E-10	6.469E-10	0.005475	0.002754	7.893E-20	2.676E-16	8.845E-06
11	1.666E-18	2.045E-25	1.428E-13	0.01215	1.207E-16	3.663E-10	7.435E-10	0.004008	0.002168	9.008E-20	3.348E-16	7.159E-06
12	1.342E-18	1.61E-25	1.428E-13	0.008401	9.955E-17	4.846E-10	7.005E-10	0.003952	0.001513	7.155E-20	2.722E-16	7.204E-06
13	1.653E-18	1.223E-25	2.032E-13	0.03528	1.988E-16	8.229E-11	0.001619	0.00008761	0.0002284	1.953E-21	1.205E-17	2.585E-07
14	5.527E-20	1.234E-27	3.255E-13	0.003472	2.201E-17	1.805E-10	5.989E-10	0.009303	0.007903	6.935E-21	1.417E-16	0.00008959
15	3.788E-19	1.065E-26	3.259E-13	0.04506	1.199E-16	6.508E-11	0.00958	0.0002936	0.002571	1.5E-21	2.434E-17	0.00000227
16	2.331E-18	3.286E-25	1.243E-13	0.03462	1.472E-16	1.182E-10	0.006812	0.0009568	0.001285	3.009E-20	9.742E-17	1.478E-06
17	3.835E-19	3.827E-26	1.525E-13	0.01102	3.42E-17	2.752E-11	0.009143	0.01061	0.006403	5.489E-20	2.51E-16	0.0000227
18	2.077E-18	2.325E-25	1.573E-13	0.007274	1.65E-16	5.347E-11	0.0003734	0.002661	0.0009451	7.455E-20	3.039E-16	5.219E-06
19	1.141E-18	1.277E-25	1.528E-13	0.00514	9.068E-17	9.091E-11	0.001296	0.006364	0.001597	9.796E-20	3.993E-16	0.00001245
20	7.345E-20	1.641E-27	2.78E-13	0.05908	2.926E-17	9.333E-11	0.02931	0.0000667	0.0009642	6.609E-23	1.35E-18	6.275E-07
21	5.43E-20	6.979E-28	3.293E-13	0.02534	3.758E-17	1.007E-10	0.1228	0.00006288	0.0006774	4.605E-23	1.635E-18	0.00000104
22	3.579E-19	1.006E-26	3.277E-13	0.02015	1.132E-16	1.596E-10	0.005278	0.0006175	0.002419	2.981E-21	4.836E-17	4.776E-06
23	1.065E-18	6.117E-26	2.531E-13	0.01037	1.651E-16	2.134E-11	7.772E-10	0.001965	0.00194	2.824E-20	2.244E-16	7.503E-06
24	9.655E-19	4.828E-26	2.658E-13	0.01847	1.718E-16	1.744E-10	0.003059	0.0009249	0.001867	1.205E-20	1.099E-16	4.049E-06
25	3.156E-09	1.771E-16	2.63E-13	0.01223	5.005E-07	2.509E-13	0.005011	0.00002724	0.00003245	1.16E-12	9.433E-09	1.066E-07
26	5.768E-10	1.288E-17	4.569E-13	0.006714	2.298E-07	4.011E-13	0.005021	4.835E-06	7.943E-06	3.762E-14	7.685E-10	4.755E-08
27	1.768E-18	6.259E-26	3.661E-13	0.004411	4.444E-16	1.811E-12	0.001485	7.599E-06	5.175E-06	1.813E-22	2.336E-18	4.717E-08
28	1.808E-09	2.024E-17	6.086E-13	0.002909	1.437E-06	9.546E-14	0.002023	0.0000039	5.538E-06	9.514E-14	3.877E-09	7.656E-08
29	6.461E-19	9.106E-27	5.701E-13	0.002552	4.079E-16	1.113E-13	0.002217	0.00001295	0.00001282	1.129E-22	3.654E-18	2.019E-07
30	1.223E-18	3.438E-26	3.96E-13	0.01535	3.868E-16	1.686E-13	0.001673	1.602E-06	4.778E-06	2.641E-23	4.286E-19	1.251E-08
31	1.746E-08	1.955E-16	5.836E-13	0.006302	0.00001388	6.579E-13	0.001849	8.478E-06	0.00002608	1.997E-12	8.14E-08	1.664E-07
32	1.801E-07	1.272E-14	2.288E-13	0.008585	0.00002268	7.993E-12	0.002576	4.114E-06	2.733E-06	9.994E-12	6.456E-08	1.28E-08
33	9.535E-08	1.067E-14	1.601E-13	0.007935	7.577E-06	3.967E-12	0.003186	5.436E-06	2.106E-06	6.991E-12	2.849E-08	1.067E-08
34	3.413E-09	9.596E-17	3.922E-13	0.01531	0.00000108	5.276E-13	0.003499	4.557E-06	0.00001356	2.098E-13	3.404E-09	3.557E-08
35	1.113E-06	7.86E-14	2.246E-13	0.003917	0.0001402	1.847E-11	0.006073	0.0001306	0.00003959	1.961E-09	0.00001267	4.06E-07
36	2.527E-10	3.561E-18	5.795E-13	0.001411	1.595E-07	2.772E-14	0.001264	0.00005281	0.00002889	1.8E-13	5.829E-09	8.235E-07

Table G. part 6: *Continued*

Sequence # (sample #)	H2PO4- activity	H3PO4 activity	H3SiO4- activity	HCO3- activity	HPO4-- activity	HSO4- activity	K+ activity	Mg++ activity	MgCO3 activity	MgH2PO4+ activity	MgHPO4 activity	MgOH+ activity
37	1.119E-07	3.962E-15	3.586E-13	0.009105	0.00002812	2.213E-12	0.004666	5.458E-06	7.672E-06	8.239E-12	1.062E-07	3.387E-08
38	4.224E-08	5.952E-16	5.008E-13	0.01027	0.00002666	2.022E-13	0.008406	2.324E-06	9.258E-06	1.324E-12	4.287E-08	3.616E-08
39	3.514E-09	7.848E-17	4.626E-13	0.004985	0.0000014	1.354E-13	0.002207	3.816E-06	4.655E-06	1.809E-13	3.695E-09	3.754E-08
40	2.863E-19	2.546E-27	6.706E-13	0.0009095	2.865E-16	1.741E-14	0.001452	8.584E-06	4.799E-06	3.316E-23	1.701E-18	2.122E-07
41	1.286E-08	1.143E-15	1.923E-13	0.008331	1.286E-06	1.541E-12	0.002313	0.00001752	8.972E-06	3.039E-12	1.559E-08	4.329E-08
42	1.263E-18	7.085E-26	0.00005093	0.02174	2.002E-16	4.636E-11	0.0004514	0.00008926	0.000189	1.521E-21	1.236E-17	3.472E-07
43	1.116E-18	6.262E-26	0.00004406	0.02343	1.77E-16	3.58E-11	0.0004126	0.00007453	0.0001701	1.122E-21	9.125E-18	2.896E-07
44	1.094E-19	7.726E-28	0.0001657	0.01064	1.378E-16	5.89E-12	0.00135	0.00004973	0.0004094	7.338E-23	4.74E-18	1.536E-06
45	1.32E-19	1.174E-27	0.0002156	0.01314	1.321E-16	7.334E-12	0.001533	0.000053	0.0004278	9.439E-23	4.843E-18	1.299E-06
46	1.874E-19	2.097E-27	0.0002315	0.01543	1.489E-16	7.484E-12	0.001505	0.00005305	0.0003995	1.341E-22	5.465E-18	1.034E-06
47	1.413E-19	1.256E-27	0.0002463	0.01341	1.414E-16	6.914E-12	0.001547	0.00004649	0.0003831	8.862E-23	4.547E-18	1.141E-06
48	1.513E-19	1.345E-27	0.0002403	0.01396	1.513E-16	6.277E-12	0.001511	0.00004573	0.0003922	9.33E-23	4.787E-18	1.123E-06
49	6.122E-19	1.721E-26	0.0004649	0.0106	1.937E-16	3.486E-11	0.0009298	0.0005894	0.001214	4.867E-21	7.898E-17	4.595E-06
50	2.156E-19	3.039E-27	0.0006515	0.007344	1.361E-16	1.622E-11	0.0008374	0.0004195	0.001195	1.22E-21	3.95E-17	6.526E-06
51	2.424E-19	5.415E-27	0.000189	0.01236	9.655E-17	7.727E-11	0.004608	0.001441	0.004358	4.712E-21	9.626E-17	0.00001413
52	1.846E-19	4.122E-27	0.0001928	0.01233	7.351E-17	5.142E-11	0.003871	0.001487	0.004484	3.702E-21	7.561E-17	0.00001459
53	4.447E-19	1.574E-26	0.000147	0.01523	1.117E-16	1.291E-10	0.003976	0.001698	0.003993	1.019E-20	1.313E-16	0.00001051
54	1.445E-18	1.618E-25	4.793E-06	0.01508	1.148E-16	7.853E-10	0.00144	0.001251	0.000921	2.439E-20	9.941E-17	0.00000243
55	4.079E-19	1.444E-26	0.00007164	0.01053	1.025E-16	1.046E-10	0.002689	0.001171	0.001904	6.444E-21	8.305E-17	7.256E-06
56	1.976E-18	2.785E-25	1.288E-13	0.01008	1.248E-16	3.989E-10	0.0009858	0.005056	0.001977	1.348E-19	4.363E-16	7.874E-06
57	1.916E-18	2.144E-25	0.00002985	0.05288	1.522E-16	3.686E-10	0.0003206	0.0004962	0.001281	1.282E-20	5.226E-17	9.684E-07
58	2.289E-19	1.02E-26	0.00001612	0.01684	4.569E-17	3.976E-10	0.06445	0.001753	0.003621	5.413E-21	5.542E-17	8.376E-06
59	2.749E-19	4.878E-27	4.54E-13	0.01297	1.379E-16	4.365E-11	0.003373	0.001032	0.004124	3.829E-21	9.847E-17	0.00001276
60	3.283E-19	2.319E-26	0.00002062	0.01935	4.135E-17	1.236E-09	0.02074	0.0009607	0.001438	4.255E-21	2.749E-17	2.897E-06
61	1.031E-19	2.304E-27	3.612E-13	0.01359	4.108E-17	1.381E-10	0.01058	0.001548	0.005148	2.154E-21	4.399E-17	0.00001509
62	2.289E-19	1.285E-26	0.00009164	0.007965	3.63E-17	3.006E-10	0.001065	0.002607	0.002023	8.051E-21	6.547E-17	0.00001014
63	2.916E-18	3.264E-25	0.00003367	0.01766	2.317E-16	1.338E-10	0.0009557	0.0008035	0.0006927	3.161E-20	1.288E-16	1.573E-06
64	7.955E-19	7.074E-26	1.719E-13	0.05774	7.959E-17	4.072E-10	0.00506	0.002729	0.009683	2.928E-20	1.503E-16	6.668E-06
65	3.219E-19	4.536E-26	1.125E-13	0.1308	2.032E-17	7.473E-10	0.0141	0.007482	0.03797	3.249E-20	1.052E-16	0.00001095
66	5.032E-16	7.091E-21	4.807E-07	0.0006265	3.176E-16	2.152E-09	0.0001699	0.0002041	4.958E-08	1.385E-18	4.485E-17	3.183E-09
67	5.772E-16	1.289E-20	2.643E-07	0.0005618	2.299E-16	6.816E-09	0.0002041	0.0001955	2.687E-08	1.522E-18	3.109E-17	1.923E-09
68	4.135E-16	4.629E-21	0.00000121	0.0007932	3.286E-16	5.167E-09	0.0005441	0.0001253	4.853E-08	6.992E-19	2.85E-17	2.46E-09
69	1.019E-16	1.809E-22	8.885E-06	0.001483	5.112E-16	1.177E-09	0.0005509	0.0001188	5.43E-07	1.634E-19	4.202E-17	1.472E-08
70	9.519E-19	2.677E-26	0.000154	0.001919	3.012E-16	9.325E-11	0.001997	0.00008154	0.00003041	1.047E-21	1.699E-17	6.369E-07
71	4.663E-16	8.272E-21	5.545E-07	0.00109	2.338E-16	8.822E-09	0.0002814	0.0004474	1.502E-07	2.814E-18	7.236E-17	5.541E-09
72	3.252E-16	3.64E-21	7.805E-07	0.00115	2.584E-16	1.062E-08	0.0002304	0.0008404	4.718E-07	3.686E-18	1.502E-16	1.65E-08
73	2.982E-16	3.338E-21	2.107E-06	0.002036	2.37E-16	1.449E-08	0.0007653	0.001185	1.178E-06	4.766E-18	1.942E-16	2.325E-08
74	3.042E-16	3.405E-21	6.244E-07	0.001574	2.417E-16	1.347E-08	0.0005715	0.0006532	5.021E-07	2.68E-18	1.092E-16	1.282E-08

Table G. part 6: *Continued*

Sequence # (sample #)	H2PO4- activity	H3PO4 activity	H3SiO4- activity	HCO3- activity	HPO4-- activity	HSO4- activity	K+ activity	Mg++ activity	MgCO3 activity	MgH2PO4+ activity	MgHPO4 activity	MgOH+ activity
75	1.925E-18	1.36E-25	0.0002276	0.007997	2.425E-16	3.78E-10	0.005506	0.00002314	0.00001432	6.011E-22	3.882E-18	7.18E-08
76	3.174E-19	8.924E-27	0.0009002	0.02212	1.004E-16	2.673E-10	0.03583	8.422E-06	0.00003621	3.605E-23	5.85E-19	6.461E-08
77	1.234E-19	2.19E-27	0.001777	0.01892	6.189E-17	2.047E-10	0.04735	7.284E-06	0.00004245	1.213E-23	3.119E-19	8.767E-08
78	5.985E-20	1.683E-27	0.002297	0.05411	1.894E-17	2.453E-10	0.1009	5.328E-14	5.603E-13	4.302E-32	6.98E-28	3.789E-16
79	5.246E-20	1.475E-27	0.002174	0.05584	1.66E-17	2.624E-10	0.1101	5.4E-14	5.861E-13	3.821E-32	6.2E-28	3.802E-16
80	1.779E-19	1.257E-27	0.001247	0.004443	2.241E-16	2.299E-12	0.005525	0.00008089	0.0002781	1.941E-22	1.254E-17	2.512E-06
81	5.093E-17	9.036E-23	0.00003859	0.02486	2.554E-16	4.341E-09	0.009852	0.00004378	3.352E-06	3.008E-20	7.735E-18	5.402E-09
82	4.94E-20	1.103E-27	0.001429	0.0616	1.968E-17	1.115E-10	0.07736	2.345E-06	0.00003535	1.563E-24	3.193E-20	2.122E-08
83	2.306E-20	3.25E-28	0.005625	0.04263	1.456E-17	1.751E-10	0.1275	2.703E-06	0.00004468	8.407E-25	2.722E-20	3.767E-08
84	5.774E-20	1.624E-27	0.004407	0.04772	1.827E-17	4.961E-10	0.09952	5.274E-06	0.00004891	4.108E-24	6.665E-20	3.628E-08
85	1.046E-20	2.336E-28	0.004034	0.07173	4.166E-18	4.415E-10	0.3418	0.00000467	0.00008195	6.589E-25	1.346E-20	3.262E-08
86	3.069E-17	1.368E-23	0.00003733	0.001457	6.127E-16	9.052E-12	0.000374	0.0002254	4.026E-06	9.331E-20	9.553E-17	1.111E-07
87	2.717E-18	1.525E-25	0.0004241	0.006591	4.309E-16	2.611E-11	0.00452	0.00003544	0.00002276	1.299E-21	1.056E-17	1.387E-07
88	3.143E-18	1.763E-25	0.0003783	0.00353	4.984E-16	1.384E-11	0.002033	9.724E-06	3.344E-06	4.123E-22	3.353E-18	3.808E-08
89	2.73E-17	1.532E-23	0.00005238	0.00239	4.329E-16	7.533E-12	0.0006378	0.0005442	0.00001267	2.004E-19	1.63E-16	2.131E-07
90	9.813E-18	2.192E-24	0.00023	0.002489	3.908E-16	2.001E-11	0.0003636	0.0000647	3.941E-06	8.565E-21	1.75E-17	6.365E-08
91	3.672E-19	6.514E-27	0.002195	0.01559	1.841E-16	1.522E-11	0.01586	0.0004694	0.002254	2.325E-21	5.979E-17	5.796E-06
92	7.743E-19	1.729E-26	0.000375	0.01083	3.084E-16	2.917E-11	0.007186	6.397E-06	0.00001695	6.681E-23	1.365E-18	6.276E-08
93	6.081E-17	6.807E-23	0.00000766	0.002164	4.832E-16	1.063E-11	0.00009257	0.0001466	1.548E-06	1.202E-19	4.9E-17	2.877E-08
94	2.38E-17	1.061E-23	0.00001866	0.005182	4.751E-16	4.186E-12	0.0001847	0.0001405	8.929E-06	4.512E-20	4.619E-17	6.929E-08
95	1.313E-17	5.85E-24	0.00005121	0.003806	2.62E-16	1.71E-12	0.0006212	0.0008605	0.00004016	1.524E-19	1.56E-16	4.243E-07
96	1.824E-16	6.456E-22	4.914E-06	0.001595	4.583E-16	1.74E-10	0.0002797	0.000379	9.332E-07	9.324E-19	1.202E-16	2.353E-08
97	1.489E-16	5.272E-22	6.142E-06	0.004297	3.743E-16	1.499E-10	0.001082	0.000665	4.411E-06	1.336E-18	1.722E-16	4.128E-08
98	2.637E-16	1.48E-21	4.274E-06	0.001819	4.182E-16	2.793E-10	0.00009369	0.0003103	5.498E-07	1.104E-18	8.977E-17	1.215E-08
99	7.799E-17	2.193E-22	0.00001234	0.004093	2.467E-16	9.697E-16	0.00129	0.002502	0.0000199	2.632E-18	4.271E-16	1.955E-07
100	4.457E-17	6.282E-23	0.00002595	0.00567	2.814E-16	5.201E-12	0.000353	0.001422	0.00003126	8.549E-19	2.768E-16	2.217E-07
101	1.046E-16	1.856E-22	0.00001096	0.001529	5.244E-16	6.903E-10	0.0002788	0.000217	1.022E-06	3.061E-19	7.872E-17	2.688E-08
102	1.129E-16	2.521E-22	5.818E-06	0.002402	4.495E-16	2.075E-11	0.0002764	0.0003615	2.125E-06	5.504E-19	1.124E-16	3.557E-08
103	4.485E-16	6.321E-21	9.304E-07	0.002158	2.831E-16	6.65E-11	0.0002774	0.0002944	2.464E-07	1.781E-18	5.767E-17	4.591E-09
104	3.834E-16	4.292E-21	9.756E-07	0.002151	3.047E-16	1.038E-10	0.0002767	0.0003654	3.837E-07	1.89E-18	7.702E-17	7.174E-09
105	8.097E-19	2.277E-26	0.0004391	0.004769	2.562E-16	1.656E-11	0.002742	0.0000619	0.00005738	6.761E-22	1.097E-17	4.834E-07
106	3.428E-16	3.048E-21	1.719E-06	0.001244	3.43E-16	4.34E-15	0.00009344	0.0003866	2.955E-07	1.788E-18	9.174E-17	9.556E-09
107	4.342E-16	6.119E-21	1.396E-06	0.001162	2.741E-16	6.709E-15	0.000186	0.0004553	2.053E-07	2.667E-18	8.634E-17	7.101E-09
108	3.757E-18	3.341E-25	0.0007795	0.009158	3.759E-16	3.93E-11	0.001095	0.0001496	0.00008418	7.579E-21	3.889E-17	3.693E-07
109	4.145E-16	4.64E-21	9.756E-07	0.001375	3.294E-16	5.639E-15	0.0000939	0.0003145	2.111E-07	1.758E-18	7.166E-17	6.173E-09
110	1.046E-18	2.943E-26	0.0002411	0.004011	3.311E-16	1.641E-11	0.003026	0.00006724	0.00005242	9.491E-22	1.54E-17	5.251E-07
111	5.958E-17	8.396E-23	0.00001527	0.005171	3.761E-16	1.114E-10	0.0008845	0.0006639	0.00001331	5.336E-19	1.727E-16	1.035E-07
115	7.565E-18	1.066E-24	0.00007834	0.005734	4.775E-16	4.082E-11	8.289E-10	4.126E-13	9.175E-14	4.211E-29	1.363E-25	6.427E-16

Table G. part 6: *Continued*

Sequence # (sample #)	H2PO4- activity	H3PO4 activity	H3SiO4- activity	HCO3- activity	HPO4-- activity	HSO4- activity	K+ activity	Mg++ activity	MgCO3 activity	MgH2PO4+ activity	MgHPO4 activity	MgOH+ activity
116	1.385E-18	6.171E-26	0.00005848	0.006994	2.764E-16	2.861E-11	0.00001498	0.0001683	0.0001443	3.144E-21	3.219E-17	8.271E-07
117	1.337E-16	4.733E-22	4.295E-06	0.01156	3.36E-16	5.236E-10	8.123E-10	0.0003421	6.105E-06	6.169E-19	7.951E-17	2.12E-08
118	5.411E-19	1.916E-26	0.001308	0.01191	1.36E-16	3.974E-11	0.001617	1.695E-13	3.117E-13	1.237E-30	1.594E-26	1.043E-15
119	1.304E-18	7.318E-26	0.0001446	0.0148	2.068E-16	6.647E-11	0.00006789	0.0001145	0.000165	2.014E-21	1.638E-17	4.444E-07
120	1.114E-18	3.945E-26	0.00006692	0.00545	2.801E-16	2.236E-11	7.566E-10	0.0001001	0.0000842	1.504E-21	1.939E-17	6.192E-07
121	1.463E-18	6.519E-26	0.0000589	0.006311	2.92E-16	2.882E-11	7.618E-10	0.0001042	0.00008062	2.055E-21	2.104E-17	5.121E-07
125	1.901E-16	1.067E-21	2.719E-06	0.005922	3.015E-16	2.063E-10	0.00008706	0.0008084	4.663E-06	2.074E-18	1.686E-16	3.166E-08
126	1.152E-16	4.078E-22	3.679E-06	0.009954	2.895E-16	4.577E-10	0.00001563	0.0004043	6.214E-06	6.284E-19	8.099E-17	2.505E-08
127	3.492E-17	3.105E-23	0.00001194	0.01227	3.494E-16	8.035E-11	0.0000242	0.0005965	0.000045	2.81E-19	1.442E-16	1.472E-07
128	1.966E-17	1.389E-23	8.948E-06	0.009826	2.477E-16	1.951E-11	7.999E-06	0.001876	0.0001426	4.976E-19	3.214E-16	5.829E-07
129	1.358E-17	7.616E-24	0.00002985	0.003037	2.153E-16	7.234E-11	0.000017	0.003646	0.0001079	6.676E-19	5.429E-16	1.428E-06
130	4.978E-17	1.112E-22	0.00000872	0.003067	1.982E-16	1.393E-10	8.454E-10	0.003814	0.00002862	2.561E-18	5.231E-16	3.752E-07
131	5.111E-17	1.437E-22	0.00001157	0.00481	1.617E-16	7.954E-11	0.00003321	0.005082	0.00004751	3.504E-18	5.685E-16	3.971E-07
132	1.154E-16	6.475E-22	3.884E-06	0.002175	1.83E-16	7.109E-10	0.00002553	0.003866	8.189E-06	6.018E-18	4.894E-16	1.514E-07
133	5.148E-17	9.134E-23	0.00001095	0.002294	2.581E-16	1.259E-10	0.00001737	0.002555	0.00001805	1.774E-18	4.563E-16	3.164E-07
134	3.221E-16	2.864E-21	1.964E-06	0.003058	3.222E-16	1.158E-09	9.034E-10	0.0005289	9.94E-07	2.298E-18	1.179E-16	1.307E-08
135	1.255E-17	7.044E-24	0.00002229	0.00495	1.991E-16	2.058E-09	7.867E-06	0.001808	0.00008715	3.061E-19	2.489E-16	7.072E-07
136	6.14E-17	8.653E-23	1.525E-14	0.009272	3.876E-16	4.882E-10	0.00001702	0.0004019	0.00001445	3.329E-19	1.078E-16	6.264E-08
137	1.672E-16	7.452E-22	4.885E-06	0.00261	3.338E-16	1.795E-10	0.00003572	0.0007055	2.258E-06	1.591E-18	1.629E-16	3.478E-08
138	8.883E-17	1.984E-22	6.778E-06	0.01015	3.538E-16	1.397E-10	0.00001649	0.0003621	8.994E-06	4.339E-19	8.863E-17	3.559E-08
139	4.481E-18	4.172E-24	0.00002022	0.00116	4.281E-17	3.578E-09	0.02631	0.005023	0.00003421	3.036E-19	1.488E-16	1.159E-06
140	5.966E-18	5.952E-24	0.00003127	0.00074	5.319E-17	2.727E-09	0.01669	0.002906	0.00001178	2.338E-19	1.069E-16	6.314E-07
141	2.802E-18	7.524E-25	0.00007372	0.001638	9.282E-17	8.405E-10	0.00543	0.002619	0.0000873	9.898E-20	1.682E-16	2.128E-06
142	1.934E-18	8.618E-25	0.00004385	0.001873	3.86E-17	4.016E-09	0.03172	0.004806	0.0001104	1.254E-19	1.284E-16	2.298E-06
143	1.283E-18	2.554E-25	0.00008567	0.001284	5.734E-17	7.775E-10	0.01671	0.001807	0.00006368	3.128E-20	7.169E-17	1.965E-06
144	3.068E-18	1.306E-24	0.0000346	0.001715	6.412E-17	1.695E-09	0.02812	0.002416	0.00005321	9.999E-20	1.072E-16	1.228E-06
145	9.318E-18	6.891E-24	0.00003187	0.001148	1.121E-16	2.18E-09	0.01695	0.001352	0.00001147	1.699E-19	1.048E-16	3.974E-07
146	3.791E-18	4.761E-24	0.00002052	0.001847	2.685E-17	2.506E-09	0.03745	0.01125	0.00009042	5.754E-19	2.09E-16	1.893E-06
147	1.543E-18	1.437E-25	0.0001933	0.000324	1.474E-16	7.405E-10	0.003851	0.0002935	5.582E-06	6.11E-21	2.994E-17	6.898E-07
148	3.943E-19	8.806E-26	0.00006206	0.004373	1.57E-17	1.987E-09	0.1852	0.01561	0.00167	8.3E-20	1.695E-16	0.00001448
149	1.539E-20	1.369E-28	0.0003457	0.0004687	1.54E-17	6.253E-11	0.03295	0.0004409	0.000127	9.154E-23	4.697E-18	0.00001085
150	1.208E-18	6.778E-25	0.00005681	0.006002	1.916E-17	1.089E-09	0.06397	0.01211	0.0007082	1.974E-19	1.605E-16	4.396E-06
151	2.69E-18	1.199E-24	0.0000516	0.002646	5.37E-17	1.556E-09	0.03275	0.003447	0.0001118	1.251E-19	1.28E-16	1.646E-06
152	6.08E-20	3.572E-28	0.002708	0.01036	9.207E-17	2.167E-11	0.04765	0.0003323	0.003204	2.726E-22	2.117E-17	0.00001228
153	1.537E-18	9.679E-26	0.000338	0.0002792	2.173E-16	1.634E-11	0.000943	0.0002373	0.00000575	4.921E-21	3.566E-17	8.277E-07
154	3.279E-18	1.395E-24	0.00005321	0.000948	6.853E-17	1.852E-10	0.01691	0.002707	0.00003295	1.197E-19	1.284E-16	1.376E-06
155	1.86E-17	2.336E-23	0.00001046	0.0009848	1.317E-16	4.425E-10	0.008948	0.00155	6.643E-06	3.89E-19	1.413E-16	2.693E-07
156	1.603E-17	8.996E-23	0.00000277	0.002261	2.542E-17	2.549E-09	0.06072	0.001581	3.481E-06	3.419E-19	2.78E-17	5.799E-08

Table G. part 6: *Continued*

Sequence # (sample #)	H2PO4- activity	H3PO4 activity	H3SiO4- activity	HCO3- activity	HPO4-- activity	HSO4- activity	K+ activity	Mg++ activity	MgCO3 activity	MgH2PO4+ activity	MgHPO4 activity	MgOH+ activity
157	8.555E-19	7.607E-24	1.801E-06	0.001093	8.559E-19	3.631E-09	0.2593	1.105	0.0007423	1.275E-17	6.543E-16	0.00001823
158	7.75E-18	4.153E-24	0.00004999	0.001426	1.287E-16	2.115E-10	0.009631	0.001085	0.00001578	1.134E-19	9.659E-17	4.42E-07
159	4.135E-16	6.538E-21	1.838E-06	0.001323	2.326E-16	6.975E-09	0.0003764	0.0005238	2.395E-07	2.922E-18	8.43E-17	7.279E-09
160	1.529E-17	1.526E-23	0.00004456	0.001531	1.364E-16	4.584E-10	0.007221	0.001651	0.00001384	3.407E-19	1.558E-16	3.614E-07
161	6.703E-17	1.334E-22	0.00001172	0.001641	2.995E-16	8.747E-10	0.001045	0.001179	0.00000531	1.066E-18	2.443E-16	1.301E-07
162	8.56E-18	5.389E-24	0.00003792	0.00109	1.21E-16	2.668E-10	0.01034	0.001548	0.00001465	1.788E-19	1.296E-16	5.364E-07
163	2.054E-18	3.562E-24	0.00001427	0.001912	1.054E-17	1.345E-09	0.07645	0.02438	0.0001469	6.755E-19	1.778E-16	2.794E-06
164	1.316E-18	4.449E-26	0.0002175	0.00003694	3.463E-16	2.645E-12	0.0001036	0.0001006	6.005E-07	1.786E-21	2.41E-17	6.538E-07
165	2.423E-18	1.184E-23	4.499E-06	0.001613	4.412E-18	3.118E-09	0.1054	0.07023	0.0001267	2.296E-18	2.144E-16	0.00000258
166	8.451E-18	1.432E-24	0.00009061	0.0004304	4.437E-16	3.965E-12	0.0002944	0.0002202	3.057E-06	2.51E-20	6.759E-17	2.856E-07
167	4.193E-18	6.63E-23	6.722E-07	0.0009641	2.359E-18	8.911E-09	0.1653	0.2384	0.00007945	1.349E-17	3.891E-16	2.581E-06
168	3.854E-18	1.718E-23	3.588E-06	0.001823	7.693E-18	3.234E-09	2.397	0.07471	0.000167	3.884E-18	3.976E-16	2.322E-06
169	1.254E-17	3.071E-24	0.00008203	0.0004245	4.555E-16	1.017E-10	0.000519	0.0001663	1.575E-06	2.814E-20	5.242E-17	1.492E-07
170	9.647E-18	2.256E-24	0.00008287	0.0005634	3.67E-16	1.397E-10	0.001022	0.0002919	3.844E-06	3.799E-20	7.411E-17	2.742E-07
171	4.257E-18	7.909E-25	0.0001392	0.0008573	2.038E-16	1.8E-10	0.001856	0.0006089	0.00001535	3.496E-20	8.587E-17	7.191E-07
172	3.238E-18	5.487E-25	0.0001136	0.000835	1.7E-16	2.704E-10	0.004668	0.0006144	0.00001655	2.684E-20	7.227E-17	7.938E-07
173	1.028E-18	1.151E-25	0.0001863	0.002133	8.168E-17	3.065E-10	0.01418	0.001331	0.0001385	1.845E-20	7.519E-17	0.00000258
174	2.56E-18	1.09E-24	0.0000538	0.002634	5.352E-17	1.486E-09	0.03275	0.003446	0.0001165	1.19E-19	1.276E-16	1.724E-06
175	1.196E-18	6.708E-25	0.00005682	0.005983	1.896E-17	1.187E-09	0.064	0.01228	0.0007156	1.981E-19	1.611E-16	4.457E-06
176	1.939E-17	1.338E-23	0.00001913	0.001102	2.499E-16	1.708E-10	0.0005068	0.0026	0.00002268	6.799E-19	4.494E-16	8.276E-07
177	3.943E-19	8.806E-26	0.00006206	0.004373	1.57E-17	1.987E-09	0.1852	0.01561	0.00167	8.3E-20	1.695E-16	0.00001448
178	8.647E-19	7.689E-24	1.804E-06	0.001103	8.651E-19	3.637E-09	0.2589	1.09	0.0007393	1.272E-17	6.526E-16	0.00001801
179	1.135E-20	1.425E-28	0.001973	0.05597	8.036E-18	8.149E-11	0.5945	4.265E-06	0.0001039	6.528E-25	2.371E-20	6.253E-08
180	1.293E-18	7.253E-26	0.0002836	0.005907	2.05E-16	2.231E-11	0.005288	0.0007244	0.0004168	1.263E-20	1.027E-16	2.825E-06
181	1.83E-18	6.478E-25	0.00006794	0.002625	4.598E-17	3.047E-17	0.024	0.002662	0.0001079	6.572E-20	8.47E-17	1.627E-06
182	1.196E-18	6.71E-25	0.00005682	0.005983	1.896E-17	1.187E-09	0.064	0.01228	0.0007157	1.981E-19	1.611E-16	4.457E-06
183	1.94E-19	4.334E-27	0.0005843	0.00005629	7.728E-17	1.616E-11	0.0007748	0.00007048	9.708E-07	1.845E-22	3.768E-18	6.934E-07
184	5.821E-18	3.749E-24	0.00004465	0.001115	8.038E-17	1.617E-09	0.006414	0.002382	0.00002255	1.871E-19	1.325E-16	8.035E-07
185	1.047E-19	4.666E-27	0.0005139	0.02766	2.09E-17	2.979E-10	0.03905	6.394E-06	0.00002169	9.031E-24	9.246E-20	2.922E-08
186	3.068E-18	1.306E-24	0.0000346	0.001715	6.412E-17	1.695E-09	0.02812	0.002416	0.00005321	9.999E-20	1.072E-16	1.228E-06
187	1.53E-18	7.138E-25	0.00004012	0.003611	2.916E-17	2.36E-09	0.02056	0.009885	0.000418	2.04E-19	1.994E-16	4.501E-06
188	1.983E-20	4.327E-29	0.001195	0.006298	8.08E-17	8.838E-13	0.02064	0.00000481	0.00007584	1.286E-24	2.689E-19	4.758E-07
189	3.403E-20	1.205E-28	0.001558	0.006959	8.551E-17	5.749E-12	0.02805	0.00001362	0.0001464	6.253E-24	8.06E-19	8.338E-07
190	4.509E-20	3.185E-28	0.001166	0.0001481	5.679E-17	1.6E-12	9.243E-06	0.00001927	2.208E-06	1.172E-23	7.57E-19	5.994E-07
191	2.053E-18	2.298E-25	0.0002377	0.002825	1.631E-16	1.437E-10	0.005902	0.0001014	0.00001399	2.807E-21	1.144E-17	1.981E-07
192	3.238E-18	2.287E-24	0.00003097	0.003072	4.078E-17	3.59E-09	0.01512	0.001472	0.00003499	6.431E-20	4.154E-17	4.406E-07
193	9.16E-19	1.025E-25	0.000097	0.002589	7.279E-17	7.239E-10	0.0196	0.000648	0.00008189	8.007E-21	3.263E-17	1.262E-06
194	1.348E-19	3.01E-25	7.076E-07	0.01086	5.367E-19	1.003E-08	0.6578	1.803	0.04793	3.278E-18	6.696E-16	0.0001209

Table G. part 6: *Continued*

Sequence # (sample #)	H2PO4- activity	H3PO4 activity	H3SiO4- activity	HCO3- activity	HPO4-- activity	HSO4- activity	K+ activity	Mg++ activity	MgCO3 activity	MgH2PO4+ activity	MgHPO4 activity	MgOH+ activity
195	5.299E-19	1.055E-25	0.00004798	0.001111	2.368E-17	5.715E-10	0.03242	0.001472	0.00004489	1.052E-20	2.411E-17	1.596E-06
196	3.498E-17	1.238E-22	8.255E-06	0.001502	8.791E-17	1.641E-09	0.006969	0.002025	4.695E-06	9.555E-19	1.231E-16	1.245E-07
197	2.764E-18	6.928E-24	8.936E-06	0.001921	9.813E-18	1.669E-09	0.03915	0.02202	0.00009225	8.213E-19	1.495E-16	1.781E-06
199	2.386E-08	1.647E-15	2.703E-06	0.02278	3.075E-06	2.175E-10	0.006783	0.0006231	0.001124	2.006E-10	1.326E-06	1.965E-06
200	2.613E-19	4.635E-27	0.00001324	0.01134	1.31E-16	6.137E-11	0.007036	0.0005445	0.001902	1.919E-21	4.934E-17	0.00000668
201	4.588E-19	1.29E-26	3.398E-13	0.01476	1.451E-16	8.563E-11	0.009663	0.0005394	0.001547	3.339E-21	5.417E-17	4.177E-06
202	6.343E-19	2.246E-26	3.076E-13	0.01845	1.594E-16	8.025E-11	0.007434	0.0004498	0.001281	3.849E-21	4.961E-17	2.768E-06
203	4.182E-09	1.661E-16	3.122E-13	0.01936	9.367E-07	6.432E-18	0.01026	0.0007865	0.002096	4.437E-11	5.097E-07	4.337E-06
204	9.098E-10	2.558E-17	3.396E-13	0.01504	2.878E-07	8.861E-11	0.00808	0.0005217	0.001525	6.403E-12	1.039E-07	0.00000404
205	1.464E-09	3.841E-17	6.649E-06	0.01418	4.962E-07	7.977E-11	0.007258	0.0005304	0.001567	1.047E-11	1.821E-07	4.401E-06
206	1.143E-09	2.174E-17	0.00001497	0.01183	5.35E-07	5.791E-11	0.007329	0.0005075	0.001725	7.827E-12	1.878E-07	5.811E-06
207	1.566E-09	2.909E-17	0.00004796	0.01182	7.498E-07	5.7E-11	0.007455	0.0005066	0.001762	1.07E-11	2.628E-07	5.936E-06
208	1.309E-08	1.762E-15	5.444E-07	0.002741	8.655E-07	1.674E-10	8.396E-10	0.002268	0.0002525	4.006E-10	1.358E-06	3.702E-06
209	1.669E-18	1.554E-25	0.0001977	0.0003717	1.595E-16	1.426E-11	0.004005	0.0004084	8.911E-06	9.198E-21	4.507E-17	9.604E-07
210	1.748E-17	2.196E-23	0.00001915	0.001269	1.238E-16	1.077E-10	0.01704	0.001454	8.026E-06	3.429E-19	1.245E-16	2.517E-07
211	6.073E-18	6.059E-24	0.00003125	0.0007586	5.415E-17	8.597E-11	0.01668	0.003011	0.00001251	2.466E-19	1.128E-16	6.544E-07
212	1.317E-18	2.622E-25	0.00008594	0.001342	5.886E-17	1.144E-11	0.01675	0.00194	0.00007149	3.448E-20	7.902E-17	0.00000211
213	4.782E-18	4.453E-24	0.00002088	0.00121	4.569E-17	4.001E-11	0.0262	0.005109	0.00003629	3.296E-19	1.615E-16	1.179E-06
214	2.554E-18	1.138E-24	0.00004368	0.002141	5.099E-17	1.977E-11	0.03145	0.004842	0.0001271	1.668E-19	1.708E-16	0.00000232
215	2.146E-18	1.587E-24	0.00003399	0.001695	2.581E-17	2.884E-11	0.03724	0.0111	0.000139	3.212E-19	1.982E-16	3.172E-06
216	5.5E-19	1.228E-25	0.00006208	0.00518	2.191E-17	5.338E-12	0.179	0.0133	0.001686	9.87E-20	2.016E-16	0.00001238
217	2.479E-18	1.211E-23	4.498E-06	0.001625	4.513E-18	6.71E-11	0.1047	0.06836	0.0001243	2.286E-18	2.134E-16	2.514E-06
218	8.745E-19	7.776E-24	1.795E-06	0.001105	8.749E-19	1.001E-10	0.2583	1.067	0.0007249	1.259E-17	6.46E-16	0.00001765
219	3.925E-18	1.67E-23	5.258E-06	0.001709	8.204E-18	6.968E-11	0.1223	0.03551	0.00007793	1.88E-18	2.015E-16	1.568E-06
220	2.722E-18	5.675E-24	5.715E-06	0.003456	1.162E-17	2.054E-11	0.1061	0.0215	0.0001949	7.897E-19	1.729E-16	2.004E-06
221	4.401E-18	1.296E-23	5.125E-06	0.002221	1.33E-17	3.876E-11	0.09617	0.0192	0.00007916	1.14E-18	1.767E-16	1.276E-06
222	5.577E-18	1.801E-23	4.404E-06	0.002427	1.537E-17	4.201E-11	0.08956	0.01594	0.00006549	1.199E-18	1.695E-16	9.751E-07
223	5.771E-18	1.623E-23	0.00000459	0.002125	1.826E-17	3.633E-11	0.08431	0.01314	0.00005428	1.023E-18	1.66E-16	9.306E-07
224	4.666E-18	1.066E-23	6.347E-06	0.003276	1.816E-17	3.335E-11	0.09014	0.01298	0.0001017	8.169E-19	1.631E-16	1.126E-06
225	5.714E-18	1.276E-24	0.00001643	0.002277	2.276E-16	1.027E-11	0.00007117	0.00225	0.0001254	1.735E-19	3.544E-16	2.214E-06
226	2.086E-17	1.473E-23	1.648E-06	0.002588	2.627E-16	8.131E-12	0.0001517	0.001606	0.00003215	4.517E-19	2.918E-16	4.996E-07
227	2.767E-17	2.461E-23	9.106E-07	0.00269	2.769E-16	6.906E-12	0.0001434	0.001087	0.00001797	4.057E-19	2.082E-16	2.686E-07
228	1.3E-17	9.183E-24	1.136E-06	0.007211	1.638E-16	4.077E-12	0.0003436	0.004399	0.0002454	7.715E-19	4.983E-16	1.368E-06
229	1.44E-17	2.029E-23	5.241E-06	0.02095	9.089E-17	5.847E-11	0.0006049	0.0102	0.0008287	1.981E-18	6.414E-16	0.00000159
230	1.677E-07	2.363E-13	4.056E-06	0.01698	1.058E-06	5.925E-11	0.0001367	0.006448	0.0004247	1.458E-08	4.721E-06	1.005E-06
232	5.029E-08	1.78E-14	0.00003246	0.02188	1.264E-06	2.63E-11	0.0004706	0.008167	0.002759	5.54E-09	7.141E-06	5.066E-06
234	1.308E-17	1.844E-23	5.635E-06	0.02467	8.259E-17	5.73E-11	0.0003568	0.01203	0.001151	2.123E-18	6.872E-16	1.874E-06
235	7.716E-17	8.638E-22	4.766E-07	0.04321	6.132E-17	2.53E-10	0.0007236	0.01438	0.0003034	1.497E-17	6.102E-16	2.819E-07

Table G. part 6: *Continued*

Sequence # (sample #)	H2PO4- activity	H3PO4 activity	H3SiO4- activity	HCO3- activity	HPO4-- activity	HSO4- activity	K+ activity	Mg++ activity	MgCO3 activity	MgH2PO4+ activity	MgHPO4 activity	MgOH+ activity
236	1.468E-16	3.279E-22	2.231E-07	0.00037	5.847E-16	1.242E-11	0.00002877	0.0001107	1.002E-07	2.192E-19	4.477E-17	1.089E-08
237	1.304E-17	9.213E-24	2.841E-06	0.006398	1.643E-16	1.225E-11	0.00026	0.004206	0.0002082	7.4E-19	4.78E-16	1.308E-06
238	2.033E-17	1.807E-23	2.585E-06	0.005349	2.033E-16	2.009E-11	0.0002575	0.003272	0.0001076	8.97E-19	4.602E-16	8.084E-07
239	5.569E-17	9.881E-23	2.556E-07	0.002875	2.792E-16	6.901E-12	0.0003565	0.002347	0.00002078	1.763E-18	4.534E-16	2.907E-07
240	1.206E-16	2.14E-22	5.359E-07	0.0004646	6.047E-16	2.956E-11	0.00008619	0.000152	2.175E-07	2.473E-19	6.359E-17	1.883E-08
241	5.433E-09	7.657E-15	9.01E-07	0.00282	3.43E-08	2.331E-11	0.0001265	0.001389	0.00001519	1.018E-10	3.295E-08	2.166E-07
242	5.441E-09	2.425E-15	2.241E-06	0.0007333	1.086E-07	6.917E-12	0.00002831	0.0005887	5.294E-06	4.321E-11	4.423E-08	2.903E-07
243	3.68E-10	2.065E-17	0.00001305	0.0001653	5.835E-08	9.543E-13	0.00008647	0.0003111	5.011E-06	1.545E-12	1.256E-08	1.219E-06
244	4.354E-17	6.136E-23	2.657E-06	0.002692	2.748E-16	5.91E-11	0.00002671	0.001858	0.00001939	1.091E-18	3.532E-16	2.897E-07
245	1.355E-17	1.383E-23	8.544E-06	0.01518	1.181E-16	6.012E-11	0.0001337	0.007978	0.0006481	1.458E-18	6.516E-16	1.716E-06
246	1.044E-17	1.541E-23	8.659E-06	0.04627	6.295E-17	7.86E-11	0.0002497	0.01569	0.002688	2.21E-18	6.832E-16	2.332E-06
247	3.868E-17	1.572E-22	0.00000833	0.03124	8.465E-17	6.989E-10	0.0001757	0.0108	0.0004535	5.633E-18	6.323E-16	5.831E-07
248	3.184E-18	1.102E-24	0.00006469	0.02078	8.188E-17	1.389E-11	0.0002068	0.01117	0.003669	4.8E-19	6.33E-16	7.092E-06
249	3.655E-18	1.419E-24	0.00006319	0.02132	8.377E-17	1.853E-11	0.0002366	0.01103	0.00331	5.437E-19	6.39E-16	6.237E-06
250	1.431E-19	1.601E-27	0.00002366	0.0404	1.137E-16	2.06E-13	0.001789	0.00004667	0.0009204	9.007E-23	3.671E-18	9.088E-07
251	8.171E-20	4.584E-28	0.00006942	0.01869	1.296E-16	1.527E-13	0.001594	0.00005794	0.001055	6.386E-23	5.193E-18	2.255E-06
252	4.445E-08	4.976E-16	0.00002186	0.04046	0.00003533	4.415E-13	0.001064	8.577E-06	0.0001694	5.143E-12	2.096E-07	1.669E-07
253	8.21E-09	4.606E-17	0.00006257	0.0187	0.00001302	1.232E-13	0.00163	0.00005803	0.001057	6.427E-12	5.227E-07	2.258E-06
254	3.908E-08	4.375E-16	0.00001894	0.04404	0.00003106	9.187E-12	0.006565	0.00005326	0.001145	2.808E-11	1.144E-06	1.032E-06
255	7.464E-09	2.099E-17	0.0000194	0.008327	0.00002361	2.249E-12	0.003131	0.00005028	0.0008137	5.062E-12	8.214E-07	3.909E-06
256	3.257E-07	3.646E-15	0.00006673	0.0473	0.0002588	1.492E-11	0.004928	0.00001407	0.000325	6.183E-11	0.00000252	2.715E-07
257	2.412E-07	1.704E-15	0.0002234	0.02974	0.0003038	1.191E-11	0.004591	0.00002273	0.0005231	7.396E-11	4.778E-06	6.944E-07
258	2.142E-16	1.202E-21	0.00000136	0.003723	3.397E-16	5.416E-10	0.0003462	0.0009169	3.326E-06	2.65E-18	2.155E-16	3.592E-08
259	1.2E-17	6.73E-24	0.00001305	0.01501	1.902E-16	3.593E-11	0.0002585	0.004108	0.0006007	6.647E-19	5.406E-16	1.608E-06
260	3.548E-17	6.294E-23	3.442E-06	0.01638	1.779E-16	8.862E-11	0.00006585	0.004351	0.0002195	2.082E-18	5.355E-16	5.387E-07
261	4.218E-18	5.944E-25	0.00006975	0.06036	2.662E-16	9.106E-12	0.007024	0.0003483	0.0008152	1.982E-20	6.415E-17	5.406E-07
262	1.742E-17	6.166E-24	0.00001628	0.02299	4.377E-16	2.033E-11	0.001697	0.0001628	0.00005778	3.826E-20	4.931E-17	1.01E-07
263	2.351E-17	1.661E-23	3.977E-06	0.01876	2.962E-16	1.811E-11	0.0008987	0.001731	0.0002513	5.492E-19	3.548E-16	5.384E-07
264	7.363E-18	1.645E-24	0.00004771	0.03464	2.933E-16	1.88E-11	0.004428	0.0008819	0.0007474	8.76E-20	1.789E-16	8.658E-07
265	1.32E-18	5.884E-26	0.00006688	0.04489	2.635E-16	1.244E-12	0.007219	0.000179	0.0009853	3.188E-21	3.264E-17	8.792E-07
266	2.364E-18	1.326E-25	0.00006032	0.02655	3.749E-16	2.185E-12	0.003227	0.00007583	0.0001961	2.418E-21	1.967E-17	2.965E-07
267	1.783E-18	1E-25	0.00005982	0.03314	2.827E-16	1.979E-12	0.004058	0.0005102	0.001647	1.227E-20	9.978E-17	1.994E-06
268	1.066E-17	2.998E-24	0.00002476	0.03377	3.373E-16	1.596E-11	0.00496	0.0004836	0.0003175	6.955E-20	1.128E-16	3.772E-07
269	2.093E-18	2.343E-25	0.0001026	0.155	1.663E-16	5.271E-12	0.01907	0.00004242	0.000321	1.198E-21	4.881E-18	8.225E-08
271	3.916E-19	8.746E-27	3.932E-13	0.03003	1.56E-16	2.636E-18	7.944E-10	9.899E-14	7.274E-13	5.229E-31	1.068E-26	9.699E-16
272	1.698E-07	4.775E-15	0.000803	0.0497	0.00005372	3.173E-12	0.008878	5.959E-14	5.756E-13	1.365E-19	2.215E-15	4.559E-16
274	1.756E-07	4.938E-15	0.0008402	0.05711	0.00005555	2.746E-12	0.01169	5.272E-14	5.852E-13	1.249E-19	2.026E-15	4.002E-16
275	2.171E-07	7.684E-15	0.0006437	0.06654	0.00005455	2.949E-12	0.01218	1.122E-06	0.00001152	3.284E-12	4.233E-08	6.759E-09

Table G. part 6: *Continued*

Sequence # (sample #)	H2PO4- activity	H3PO4 activity	H3SiO4- activity	HCO3- activity	HPO4-- activity	HSO4- activity	K+ activity	Mg++ activity	MgCO3 activity	MgH2PO4+ activity	MgHPO4 activity	MgOH+ activity
278	1.81E-07	5.091E-15	0.0006767	0.05511	0.00005728	2.406E-12	0.01073	5.43E-14	5.816E-13	1.326E-19	2.152E-15	4.136E-16
283	2.95E-19	5.233E-27	0.000626	0.02477	1.479E-16	1.843E-12	0.004441	7.731E-14	5.899E-13	3.076E-31	7.91E-27	9.474E-16
284	1.367E-07	3.053E-15	0.000856	0.02731	0.00005445	3.558E-12	0.005145	8.229E-14	5.499E-13	1.518E-19	3.1E-15	8.009E-16
285	4.09E-19	9.136E-27	0.0008264	0.02716	1.629E-16	3.555E-12	0.0052	5.919E-06	0.00003933	3.266E-23	6.671E-19	5.766E-08
287	1.123E-18	3.975E-26	0.0006034	0.02553	2.822E-16	7.879E-12	0.002203	1.336E-06	5.264E-06	2.023E-23	2.607E-19	8.261E-09
288	1.985E-18	8.847E-26	0.0004332	0.01418	3.963E-16	1.115E-11	8.094E-10	2.373E-06	4.128E-06	6.356E-23	6.507E-19	1.169E-08
289	1.185E-18	4.194E-26	0.0007574	0.02384	2.977E-16	1.033E-11	0.002215	2.839E-06	0.00001045	4.537E-23	5.847E-19	1.757E-08
290	6.378E-18	8.989E-25	0.0001272	0.009316	4.026E-16	3.264E-11	0.0006892	0.00009781	0.00003533	8.415E-21	2.724E-17	1.525E-07
291	5.16E-18	5.776E-25	0.0001535	0.01069	4.101E-16	2.416E-11	0.0007901	0.00006618	0.00003454	4.606E-21	1.877E-17	1.298E-07
292	8.922E-18	1.583E-24	0.000162	0.007168	4.474E-16	6.622E-11	0.0006077	0.00007204	0.0000159	8.67E-21	2.23E-17	8.92E-08
293	3.972E-18	3.532E-25	0.000216	0.01054	3.974E-16	2.236E-11	0.0009672	0.00007749	0.0000502	4.152E-21	2.131E-17	1.914E-07
294	1.156E-17	2.583E-24	0.00009385	0.008143	4.605E-16	5.863E-11	0.0007195	0.00009839	0.0000196	1.535E-20	3.135E-17	9.677E-08
295	8.921E-18	1.583E-24	0.0001548	0.007331	4.473E-16	6.334E-11	0.0006076	0.00007189	0.00001624	8.652E-21	2.225E-17	8.902E-08
296	1.386E-17	6.175E-24	0.00001702	0.009908	2.766E-16	3.69E-11	0.0006274	0.0009894	0.0001202	1.849E-19	1.893E-16	4.877E-07
297	7.848E-19	2.207E-26	0.0001302	0.005269	2.483E-16	2.232E-12	0.0007239	0.0002708	0.0002773	2.867E-21	4.651E-17	2.116E-06
298	9.891E-08	2.209E-15	0.0004223	0.03257	0.00003939	1.436E-12	0.008162	6.952E-14	5.541E-13	9.275E-20	1.895E-15	6.725E-16
299	2.678E-07	1.502E-13	0.00002428	0.003784	4.246E-06	1.005E-10	0.0001455	0.0003851	0.00001419	1.391E-09	1.131E-06	1.508E-07
300	6.611E-18	1.477E-24	0.00005139	0.00746	2.633E-16	3.005E-11	0.0003592	0.0006538	0.0001193	5.83E-20	1.191E-16	6.431E-07
301	4.622E-16	5.174E-21	1.007E-06	0.0008155	3.673E-16	1.934E-09	0.00006653	0.000129	5.135E-08	8.042E-19	3.278E-17	2.532E-09
302	1.029E-16	1.825E-22	4.457E-06	0.001904	5.158E-16	2.028E-10	0.00008418	0.0002513	1.474E-06	3.488E-19	8.969E-17	3.113E-08
303	5.039E-19	1.417E-25	0.00002189	0.005116	1.594E-17	4.734E-12	0.01149	0.037	0.003679	2.515E-19	4.081E-16	0.000028
304	1.197E-18	2.673E-25	0.00002251	0.004383	4.766E-17	5.241E-12	6.025E-10	0.01588	0.001703	2.563E-19	5.235E-16	0.00001554
306	1.576E-19	8.844E-27	0.0002088	0.007153	2.499E-17	3.747E-12	6.087E-10	0.02099	0.01462	4.462E-20	3.629E-16	0.00008196
307	1.879E-18	5.285E-25	4.689E-06	0.00561	5.946E-17	1.796E-12	0.001868	0.01433	0.001563	3.634E-19	5.896E-16	0.00001118
308	1.757E-18	3.117E-25	0.00001737	0.07924	8.81E-17	2.639E-12	6.879E-10	0.007331	0.01789	1.738E-19	4.468E-16	9.041E-06
309	1.461E-18	2.591E-25	0.00003843	0.006638	7.324E-17	7.274E-12	6.873E-10	0.01072	0.002192	2.112E-19	5.431E-16	0.00001325
310	1.068E-18	3.003E-25	0.00001047	0.00455	3.378E-17	3.459E-12	6.434E-10	0.01078	0.0009534	1.553E-19	2.52E-16	8.408E-06
311	1.17E-18	2.076E-25	0.00002993	0.003053	5.866E-17	5.617E-12	0.003294	0.01215	0.001142	1.917E-19	4.93E-16	0.00001503
313	1.617E-18	2.869E-25	0.00003721	0.004052	8.109E-17	7.975E-12	7.511E-10	0.009369	0.001169	2.044E-19	5.256E-16	0.0000116
314	9.747E-18	6.885E-24	6.805E-06	0.003554	1.228E-16	2.39E-11	7.959E-10	0.006464	0.0001778	8.499E-19	5.49E-16	0.00000201
315	9.345E-18	6.601E-24	0.00000209	0.002617	1.177E-16	6.78E-12	8.001E-10	0.005168	0.0001047	6.515E-19	4.209E-16	1.607E-06
316	9.558E-18	4.26E-24	0.0000108	0.005109	1.908E-16	1.961E-11	0.0003463	0.003155	0.0001977	4.068E-19	4.165E-16	1.555E-06
317	4.641E-17	1.037E-22	1.628E-06	0.002715	1.848E-16	7.337E-11	8.394E-10	0.003522	0.0000234	2.205E-18	4.504E-16	3.465E-07
319	5.012E-18	1.409E-24	0.0000107	0.005135	1.586E-16	7.558E-12	8.41E-10	0.004347	0.0004339	2.94E-19	4.77E-16	3.397E-06
320	6.551E-18	2.319E-24	5.942E-06	0.003085	1.646E-16	6.577E-12	8.502E-10	0.00404	0.0001924	3.57E-19	4.601E-16	2.507E-06
321	6.839E-18	1.923E-24	0.00001186	0.003848	2.164E-16	9.765E-12	0.0004919	0.001573	0.0001176	1.451E-19	2.354E-16	1.229E-06
322	7.374E-18	2.073E-24	9.281E-06	0.005661	2.333E-16	7.538E-12	0.003085	0.002985	0.0003284	2.969E-19	4.817E-16	2.332E-06
323	6.694E-18	2.37E-24	0.0000101	0.004035	1.682E-16	1.204E-11	8.498E-10	0.004022	0.0002506	3.632E-19	4.681E-16	2.497E-06

Table G. part 6: *Continued*

Sequence # (sample #)	H2PO4- activity	H3PO4 activity	H3SiO4- activity	HCO3- activity	HPO4-- activity	HSO4- activity	K+ activity	Mg++ activity	MgCO3 activity	MgH2PO4+ activity	MgHPO4 activity	MgOH+ activity
325	6.684E-18	1.493E-24	6.167E-06	0.00731	2.662E-16	3.236E-12	8.685E-10	0.001683	0.0003011	1.518E-19	3.101E-16	1.656E-06
329	2.923E-18	5.187E-25	0.00003519	0.004337	1.466E-16	1.116E-11	8.538E-10	0.003732	0.0004985	1.472E-19	3.784E-16	4.621E-06
330	3.348E-18	5.94E-25	0.00001439	0.002829	1.679E-16	4.958E-12	8.723E-10	0.002605	0.000227	1.177E-19	3.026E-16	3.227E-06
331	1.746E-17	9.795E-24	0.00001121	0.003385	2.768E-16	3.964E-11	8.782E-10	0.0013	0.00004287	3.062E-19	2.49E-16	5.093E-07
332	6.033E-18	1.696E-24	0.00004689	0.003112	1.909E-16	3.924E-11	8.672E-10	0.002946	0.0001782	2.397E-19	3.89E-16	2.302E-06
333	5.595E-18	1.25E-24	0.00001638	0.006999	2.229E-16	9.122E-12	8.627E-10	0.002922	0.0005004	2.206E-19	4.505E-16	2.875E-06
334	7.362E-18	2.07E-24	8.086E-06	0.003362	2.329E-16	7.311E-12	8.804E-10	0.002015	0.0001317	2.001E-19	3.246E-16	1.574E-06
335	6.223E-18	1.39E-24	0.00004506	0.006731	2.479E-16	2.568E-11	8.736E-10	0.002462	0.0004054	2.067E-19	4.221E-16	2.422E-06
336	8.072E-18	2.27E-24	4.079E-06	0.005602	2.554E-16	4.184E-12	8.812E-10	0.002287	0.000249	2.49E-19	4.04E-16	1.787E-06
337	8.109E-18	2.28E-24	7.873E-06	0.005366	2.566E-16	7.382E-12	8.827E-10	0.00215	0.0002242	2.352E-19	3.816E-16	0.00000168
338	6.008E-17	1.066E-22	2.325E-06	0.003298	3.012E-16	8.29E-11	8.938E-10	0.001197	0.00001216	9.704E-19	2.495E-16	1.483E-07
340	1.125E-17	3.983E-24	8.677E-06	0.00449	2.827E-16	1.25E-11	8.917E-10	0.001746	0.000121	2.65E-19	3.415E-16	1.084E-06
341	1.958E-17	1.098E-23	0.00001096	0.002522	3.104E-16	4.155E-11	9.023E-10	0.0009683	0.00002378	2.557E-19	2.079E-16	3.793E-07
342	8.992E-18	2.528E-24	0.00001632	0.00575	2.845E-16	1.517E-11	8.871E-10	0.001964	0.0002195	2.382E-19	3.865E-16	1.535E-06
343	3.063E-17	2.724E-23	7.094E-06	0.002104	3.065E-16	6.871E-11	9.022E-10	0.00125	0.00001616	5.165E-19	2.65E-16	3.089E-07
345	9.065E-18	2.549E-24	7.165E-06	0.004877	2.868E-16	6.745E-12	8.947E-10	0.001533	0.0001453	1.875E-19	3.042E-16	1.198E-06
346	1.572E-17	7.004E-24	4.334E-06	0.003821	3.137E-16	1.122E-11	9.059E-10	0.0009273	0.00004345	1.966E-19	2.013E-16	4.573E-07
347	2.959E-17	1.048E-23	0.00003411	0.004018	7.437E-16	6.801E-11	9.406E-10	7.372E-13	4.573E-14	2.943E-28	3.793E-25	4.577E-16
348	5.874E-17	8.279E-23	1.833E-06	0.003455	3.708E-16	4.244E-11	9.096E-10	0.0009481	0.0000127	7.513E-19	2.432E-16	1.478E-07
349	1.865E-17	8.312E-24	2.098E-06	0.002827	3.723E-16	5.981E-12	9.164E-10	0.000904	0.00003135	2.274E-19	2.328E-16	4.458E-07
352	5.272E-17	5.901E-23	4.787E-06	0.002602	4.189E-16	8.181E-11	9.216E-10	0.000528	6.706E-06	3.755E-19	1.53E-16	1.037E-07
353	5.365E-17	6.005E-23	2.643E-06	0.002518	4.263E-16	4.649E-11	9.238E-10	0.0004394	0.0000054	3.179E-19	1.296E-16	8.626E-08
356	3.371E-19	4.75E-27	0.0001547	0.02243	2.128E-16	4.943E-13	0.01379	0.00007424	0.0006456	3.375E-22	1.093E-17	1.153E-06
357	1.327E-18	4.697E-26	5.135E-06	0.02037	3.334E-16	9.046E-14	0.005787	0.00006082	0.0001912	1.089E-21	1.403E-17	3.769E-07
358	3.956E-08	1.112E-15	0.00002503	0.0239	0.00001251	1.494E-13	0.005271	0.0001124	0.0005221	5.999E-11	9.733E-07	8.715E-07
359	2.444E-19	6.873E-27	0.00006872	0.0656	7.733E-17	2.518E-13	0.01856	0.00006941	0.0008849	2.289E-22	3.713E-18	5.28E-07
361	9.054E-16	1.014E-19	5.865E-09	0.00003645	7.195E-17	1.408E-09	9.832E-06	9.346E-13	1.663E-18	1.141E-26	4.652E-26	1.835E-18
368	7.211E-17	1.016E-22	0.00001854	0.005876	4.552E-16	3.947E-10	0.0001469	0.0001025	2.335E-06	9.967E-20	3.227E-17	1.597E-08
370	1.197E-06	2.675E-12	7.427E-06	0.004626	4.769E-06	4.58E-10	0.0002263	0.0003838	4.344E-06	6.2E-09	1.266E-06	3.776E-08
371	3.017E-17	2.131E-23	0.0000304	0.006735	3.799E-16	1.811E-10	0.0003651	0.0004468	0.00002328	1.818E-19	1.174E-16	1.39E-07
372	1.357E-06	6.047E-12	2.765E-06	0.002687	2.709E-06	7.335E-10	0.0001202	0.0002099	6.918E-07	3.842E-09	3.934E-07	1.035E-08
373	6.397E-08	2.264E-15	0.00001691	0.0166	0.00001608	1.352E-13	0.0006676	0.001079	0.002764	9.307E-10	0.000012	6.626E-06
374	2.876E-09	5.103E-16	2.334E-06	0.01325	1.442E-07	4.053E-13	0.00196	0.001473	0.0006015	5.717E-11	1.47E-07	1.821E-06
375	2.485E-16	1.108E-21	1.871E-06	0.0015	4.961E-16	5.531E-10	9.422E-10	0.00006257	1.151E-07	2.097E-19	2.147E-17	3.085E-09
376	1.976E-16	8.805E-22	2.277E-06	0.001722	3.944E-16	5.834E-10	0.00008256	0.0003753	7.926E-07	1E-18	1.024E-16	1.85E-08
377	3.366E-08	2.993E-15	0.00001717	0.01822	3.368E-06	1.173E-12	0.001843	0.001038	0.001162	4.712E-10	2.418E-06	2.557E-06
378	2.826E-08	1.996E-15	0.00001244	0.01745	3.559E-06	6.193E-13	0.001867	0.0009798	0.001323	3.735E-10	2.413E-06	0.00000304
381	1.019E-06	4.543E-12	1.544E-06	0.001238	2.035E-06	4.619E-10	0.00005661	0.0001499	2.276E-07	2.061E-09	2.11E-07	7.393E-09

Table G. part 6: *Continued*

Sequence # (sample #)	H2PO4- activity	H3PO4 activity	H3SiO4- activity	HCO3- activity	HPO4-- activity	HSO4- activity	K+ activity	Mg++ activity	MgCO3 activity	MgH2PO4+ activity	MgHPO4 activity	MgOH+ activity
382	1.645E-07	5.825E-13	9.147E-07	0.003582	4.135E-07	2.272E-11	0.007685	0.006013	0.00003325	1.335E-08	0.00000172	3.629E-07
383	1.354E-07	3.024E-15	0.000856	0.0273	0.00005392	3.558E-12	0.005145	4.939E-06	0.00003299	9.02E-12	1.843E-07	4.807E-08
384	6.969E-08	1.557E-15	0.0004572	0.01827	0.00002776	2.612E-12	0.00329	0.00005836	0.0002609	5.487E-11	1.121E-06	5.713E-07
385	1.846E-06	3.275E-11	7.38E-07	0.0007486	9.254E-07	3.4E-09	0.00005653	0.0002257	5.205E-08	5.619E-09	1.445E-07	2.796E-09
386	7.677E-09	4.307E-14	3.223E-07	0.00174	1.217E-08	7.395E-12	0.05964	0.3755	0.0006367	3.889E-08	3.163E-06	0.00001157
387	1.535E-16	4.317E-21	6.181E-07	0.002595	4.857E-17	1.066E-09	0.009078	0.002871	1.448E-06	5.947E-18	9.649E-17	2.198E-08
388	6.227E-17	4.398E-22	1.945E-06	0.001844	7.843E-17	2.76E-10	0.01507	0.0007118	1.016E-06	5.978E-19	3.862E-17	2.187E-08
389	8.642E-09	3.059E-14	3.674E-06	0.002409	2.172E-08	3.11E-10	0.0009745	0.001252	4.657E-06	1.459E-10	1.881E-08	7.759E-08
390	1.455E-16	1.628E-21	1.136E-06	0.002445	1.156E-16	6.486E-10	0.005261	0.001171	1.397E-06	2.297E-18	9.363E-17	2.289E-08
392	1.877E-16	1.053E-21	3.885E-15	0.004822	2.976E-16	2.195E-15	8.961E-10	0.0006848	3.217E-06	1.734E-18	1.41E-16	2.682E-08
393	1.538E-16	8.63E-22	3.885E-15	0.005716	2.439E-16	1.981E-15	8.742E-10	0.002166	0.00001206	4.493E-18	3.654E-16	8.481E-08
394	3.079E-16	5.462E-21	1.232E-15	0.004115	1.544E-16	5.376E-15	8.557E-10	0.001548	1.963E-06	6.43E-18	1.654E-16	1.917E-08
395	1.552E-17	6.915E-24	9.322E-06	0.003303	3.098E-16	2.273E-11	0.00004549	0.0003932	0.00001593	8.23E-20	8.426E-17	1.939E-07
396	3.785E-18	4.237E-23	1.871E-07	0.0001759	3.008E-18	1.572E-11	0.04895	0.133	0.00001142	6.792E-18	2.768E-16	1.988E-06
397	6.819E-18	1.918E-24	7.161E-14	0.003372	2.157E-16	1.064E-16	0.0004527	0.001491	0.00009775	1.372E-19	2.226E-16	1.166E-06
398	2.035E-18	2.279E-25	1.559E-13	0.009536	1.618E-16	2.743E-17	0.001109	0.002645	0.001231	7.262E-20	2.96E-16	5.183E-06
399	1.69E-18	1.502E-25	1.869E-13	0.01204	1.69E-16	2.272E-17	0.004238	0.002613	0.001934	5.955E-20	3.056E-16	6.447E-06
400	1.024E-18	1.443E-25	1.27E-13	0.008359	6.464E-17	2.443E-17	0.003402	0.01074	0.003483	1.484E-19	4.804E-16	0.00001671
401	3.253E-19	4.585E-26	1.17E-13	0.009536	2.054E-17	1.666E-17	0.01205	0.02804	0.01037	1.231E-19	3.984E-16	0.000043
402	8.799E-19	1.561E-25	1.035E-13	0.005362	4.412E-17	2.527E-17	0.003305	0.01665	0.00275	1.976E-19	5.081E-16	0.00002055
403	3.371E-19	2.998E-26	1.767E-13	0.005468	3.373E-17	1.205E-17	0.007814	0.01911	0.006423	8.691E-20	4.459E-16	0.00004707
404	5.862E-19	1.309E-25	7.831E-14	0.009618	2.335E-17	3.309E-17	0.00923	0.02293	0.005395	1.813E-19	3.704E-16	0.00002135
405	2.233E-18	4.989E-25	8.723E-14	0.002858	8.896E-17	5.089E-17	0.001497	0.006373	0.0004457	1.92E-19	3.922E-16	6.267E-06
406	7.286E-19	1.293E-25	1.017E-13	0.004253	3.654E-17	2.264E-17	0.005699	0.01874	0.002455	1.842E-19	4.737E-16	0.00002304
408	4.714E-18	1.669E-24	5.74E-14	0.00862	1.185E-16	8.289E-17	0.00263	0.00701	0.0009329	4.458E-19	5.745E-16	4.349E-06
409	1.579E-17	1.116E-23	2.991E-14	0.004343	1.989E-16	2.224E-16	0.000475	0.002468	0.00008292	5.258E-19	3.396E-16	7.676E-07
410	7.891E-19	1.112E-25	1.244E-13	0.0037	4.981E-17	1.818E-17	0.003833	0.01161	0.001666	1.236E-19	4.001E-16	0.00001798
411	4.046E-18	9.037E-25	8.761E-14	0.006289	1.611E-16	6.486E-17	0.001596	0.002497	0.0003843	1.363E-19	2.784E-16	2.455E-06
412	7.115E-19	1.003E-25	1.223E-13	0.005892	4.491E-17	1.815E-17	0.01073	0.01342	0.003067	1.288E-19	4.17E-16	0.00002071
413	2.138E-18	6.011E-25	7.05E-14	0.002714	6.763E-17	5.141E-17	0.00002173	0.01085	0.0005723	3.129E-19	5.076E-16	8.472E-06
414	2.701E-18	6.033E-25	8.638E-14	0.007464	1.076E-16	4.538E-17	0.004265	0.005259	0.0009605	1.916E-19	3.915E-16	5.161E-06
415	3.003E-18	2.671E-25	1.908E-13	0.01285	3.005E-16	3.012E-17	0.0009789	0.001063	0.0008396	4.306E-20	2.209E-16	2.625E-06
416	1.655E-18	5.858E-25	5.493E-14	0.005828	4.159E-17	4.129E-17	0.01267	0.01585	0.001426	3.538E-19	4.56E-16	9.646E-06
417	4.854E-18	8.613E-25	1.072E-13	0.01592	2.434E-16	5.283E-17	0.001276	0.001818	0.0008911	1.19E-19	3.061E-16	2.249E-06
418	8.998E-18	6.356E-24	2.983E-14	0.004035	1.133E-16	1.618E-16	0.001284	0.007019	0.0002191	8.52E-19	5.503E-16	2.183E-06
419	2.439E-18	2.169E-25	1.849E-13	0.01822	2.441E-16	2.08E-17	0.002917	0.0009407	0.001054	3.096E-20	1.588E-16	2.319E-06
420	1.032E-18	9.178E-26	1.8E-13	0.0144	1.033E-16	1.61E-17	0.008017	0.004945	0.004377	6.886E-20	3.533E-16	0.00001216
421	6.503E-19	1.154E-25	1.019E-13	0.00283	3.261E-17	2.348E-17	0.01042	0.02021	0.001762	1.773E-19	4.56E-16	0.00002491

Table G. part 6: *Continued*

Sequence # (sample #)	H2PO4- activity	H3PO4 activity	H3SiO4- activity	HCO3- activity	HPO4-- activity	HSO4- activity	K+ activity	Mg++ activity	MgCO3 activity	MgH2PO4+ activity	MgHPO4 activity	MgOH+ activity
422	4.247E-18	9.487E-25	8.828E-14	0.002936	1.692E-16	8.148E-17	0.0003619	0.001434	0.000103	8.215E-20	1.678E-16	1.411E-06
423	2.884E-18	2.564E-25	1.866E-13	0.01491	2.885E-16	2.345E-17	0.003023	0.0003465	0.0003174	1.348E-20	6.915E-17	8.545E-07
424	7.74E-18	4.343E-24	3.724E-14	0.003758	1.227E-16	1.389E-16	0.001255	0.005768	0.0002111	6.022E-19	4.897E-16	2.258E-06
425	1.672E-18	1.181E-25	2.255E-13	0.01236	2.106E-16	2.158E-17	0.001378	0.002124	0.002032	4.791E-20	3.095E-16	6.605E-06
426	1.811E-17	1.279E-23	2.994E-14	0.003967	2.281E-16	2.454E-16	0.0003569	0.002686	0.00008243	6.561E-19	4.238E-16	8.355E-07
427	6.886E-18	2.437E-24	5.759E-14	0.007769	1.73E-16	1.048E-16	0.001423	0.00289	0.0003466	2.684E-19	3.46E-16	1.793E-06
428	1.76E-17	1.243E-23	2.994E-14	0.003026	2.217E-16	2.45E-16	0.0003146	0.001623	0.00003801	3.854E-19	2.489E-16	5.05E-07
429	4.052E-19	1.139E-26	3.496E-13	0.02265	1.282E-16	4.552E-18	0.003655	0.001485	0.006538	8.118E-21	1.317E-16	0.00001152
430	5.753E-19	1.021E-25	1.015E-13	0.001722	2.885E-17	2.264E-17	0.006793	0.02374	0.001259	1.842E-19	4.737E-16	0.00002928
431	1.866E-18	4.168E-25	8.495E-14	0.007773	7.432E-17	3.495E-17	0.007577	0.008782	0.00167	2.211E-19	4.516E-16	8.588E-06
432	1.5E-18	1.334E-25	1.869E-13	0.009546	1.5E-16	2.21E-17	0.004815	0.003392	0.00199	6.861E-20	3.521E-16	8.369E-06
433	6.521E-19	1.456E-25	7.963E-14	0.00418	2.597E-17	3.55E-17	0.005958	0.02174	0.002224	1.912E-19	3.906E-16	0.00002062
434	3.977E-20	7.056E-28	4.679E-13	0.0009147	1.994E-17	3.405E-18	0.002403	0.01017	0.002865	5.454E-21	1.403E-16	0.0001258
435	1.386E-17	7.778E-24	3.737E-14	0.003941	2.198E-16	1.99E-16	0.0003336	0.001535	0.00005892	2.87E-19	2.334E-16	6.011E-07
436	2.038E-17	1.44E-23	2.995E-14	0.003173	2.567E-16	2.65E-16	0.0003638	0.001585	0.00003891	4.357E-19	2.815E-16	4.931E-07
437	9.425E-18	4.2E-24	4.62E-14	0.007953	1.881E-16	1.162E-16	0.0009191	0.002814	0.0002744	3.577E-19	3.662E-16	1.385E-06
439	1.925E-17	1.36E-23	2.994E-14	0.004066	2.425E-16	2.521E-16	0.0005342	0.001966	0.00006186	5.107E-19	3.299E-16	6.117E-07
440	9.528E-20	3.373E-27	3.44E-13	0.0002678	2.394E-17	7.732E-18	0.00159	0.004536	0.0001875	5.83E-21	7.514E-17	0.00002812
441	3.12E-18	1.104E-24	5.706E-14	0.005807	7.841E-17	6.535E-17	0.001635	0.01099	0.0009856	4.627E-19	5.963E-16	6.816E-06
442	8.739E-19	1.55E-25	1.037E-13	0.005004	4.382E-17	2.536E-17	0.002642	0.01785	0.002752	2.104E-19	5.412E-16	0.00002205
443	2.278E-18	2.025E-25	1.834E-13	0.01297	2.279E-16	1.738E-17	0.001169	0.0005602	0.0004467	1.721E-20	8.831E-17	1.379E-06
444	1.547E-18	2.18E-25	1.3E-13	0.006194	9.763E-17	3.451E-17	0.001259	0.004031	0.0009682	8.41E-20	2.723E-16	0.00000628
445	8.212E-18	2.907E-24	5.773E-14	0.003405	2.064E-16	1.21E-16	0.0006646	0.002231	0.0001173	2.472E-19	3.186E-16	1.385E-06
446	4.686E-18	6.604E-25	1.307E-13	0.0185	2.958E-16	4.341E-17	0.000993	0.001189	0.0008532	7.517E-20	2.434E-16	1.853E-06
447	3.068E-18	6.853E-25	8.768E-14	0.005422	1.222E-16	5.955E-17	0.001278	0.005527	0.0007332	2.287E-19	4.672E-16	5.436E-06
448	1.703E-18	6.028E-25	5.641E-14	0.003306	4.28E-17	4.758E-17	0.002196	0.02027	0.001034	4.656E-19	6.001E-16	0.00001256
449	6.399E-19	7.163E-26	1.481E-13	0.002757	5.085E-17	1.896E-17	0.002166	0.007677	0.001033	6.627E-20	2.701E-16	0.00001495
450	4.368E-18	4.889E-25	1.579E-13	0.01745	3.471E-16	3.45E-17	0.001971	0.0004251	0.0003622	2.505E-20	1.021E-16	8.337E-07
451	4.756E-18	1.337E-24	7.084E-14	0.007831	1.505E-16	6.979E-17	0.002365	0.004386	0.0006676	2.814E-19	4.566E-16	3.424E-06
452	2.676E-18	3.772E-25	1.312E-13	0.004918	1.689E-16	4.349E-17	0.001072	0.003128	0.0005966	1.129E-19	3.656E-16	4.875E-06
453	2.865E-19	1.607E-26	2.41E-13	0.003482	4.542E-17	8.365E-18	0.009849	0.01033	0.003502	3.99E-20	3.245E-16	0.00004018
454	5.674E-18	2.529E-24	4.577E-14	0.007187	1.133E-16	8.275E-17	0.003135	0.00493	0.0004345	3.773E-19	3.863E-16	0.00000242
455	2.655E-18	3.742E-25	1.282E-13	0.01014	1.676E-16	3.266E-17	0.00247	0.002438	0.0009589	8.731E-20	2.827E-16	0.00000379
456	5.098E-18	1.139E-24	8.79E-14	0.007326	2.031E-16	7.214E-17	0.001085	0.002485	0.0004454	1.709E-19	3.49E-16	2.444E-06
457	9.57E-18	6.759E-24	2.985E-14	0.001853	1.205E-16	1.714E-16	0.0004721	0.005363	0.00007688	6.924E-19	4.472E-16	1.668E-06
458	1.342E-18	3.772E-25	6.919E-14	0.002862	4.244E-17	3.542E-17	0.003555	0.01709	0.0009507	3.093E-19	5.019E-16	0.00001329
459	2.229E-18	7.889E-25	5.676E-14	0.005415	5.6E-17	5.362E-17	0.005787	0.01588	0.001328	4.775E-19	6.154E-16	9.844E-06
460	8.096E-19	2.866E-25	5.301E-14	0.007734	2.034E-17	4.355E-17	0.01073	0.02842	0.003393	3.104E-19	4E-16	0.00001674

Table G. part 6: *Continued*

Sequence # (sample #)	H2PO4- activity	H3PO4 activity	H3SiO4- activity	HCO3- activity	HPO4-- activity	HSO4- activity	K+ activity	Mg++ activity	MgCO3 activity	MgH2PO4+ activity	MgHPO4 activity	MgOH+ activity
461	4.012E-19	8.961E-27	3.508E-13	0.03544	1.598E-16	2.6E-18	0.003731	0.000115	0.0009976	6.226E-22	1.272E-17	1.113E-06
462	5.196E-19	3.67E-26	2.164E-13	0.002306	6.544E-17	1.371E-17	0.002682	0.006352	0.001134	4.452E-20	2.876E-16	0.00001971
473	4.206E-18	1.875E-24	4.585E-14	0.003697	8.396E-17	7.164E-17	0.00176	0.002293	0.000104	1.301E-19	1.332E-16	1.126E-06
474	3.914E-18	1.744E-24	4.583E-14	0.003269	7.813E-17	6.967E-17	0.001817	0.002003	0.00008029	1.057E-19	1.083E-16	9.832E-07
475	5.819E-18	4.11E-24	2.959E-14	0.002825	7.329E-17	9.833E-17	0.002009	0.002649	0.00005791	2.08E-19	1.343E-16	8.198E-07
476	5.348E-18	3E-24	3.69E-14	0.004249	8.479E-17	8.707E-17	0.001887	0.002275	0.00009418	1.641E-19	1.335E-16	8.873E-07
477	5.539E-18	3.107E-24	3.68E-14	0.003831	8.782E-17	7.929E-17	0.002898	0.004305	0.0001607	3.217E-19	2.616E-16	1.676E-06
478	3.003E-18	1.063E-24	5.645E-14	0.003519	7.547E-17	4.924E-17	0.00271	0.004451	0.0002418	1.803E-19	2.324E-16	2.746E-06
479	2.966E-18	1.05E-24	5.643E-14	0.002721	7.455E-17	4.872E-17	0.002792	0.004512	0.0001895	1.805E-19	2.327E-16	2.783E-06
480	2.896E-18	1.025E-24	5.641E-14	0.003487	7.278E-17	4.804E-17	0.002868	0.00455	0.000245	1.777E-19	2.291E-16	2.805E-06
481	2.921E-18	1.034E-24	5.64E-14	0.003068	7.341E-17	4.805E-17	0.002691	0.00453	0.0002146	1.785E-19	2.301E-16	2.793E-06
482	3.08E-18	1.09E-24	5.644E-14	0.002732	7.74E-17	4.905E-17	0.002885	0.004404	0.0001857	1.83E-19	2.358E-16	2.716E-06
483	4.001E-18	1.783E-24	4.564E-14	0.00267	7.988E-17	6.139E-17	0.00288	0.004976	0.0001629	2.686E-19	2.75E-16	2.438E-06
484	3.11E-18	1.101E-24	5.65E-14	0.002938	7.816E-17	5.048E-17	0.002645	0.004668	0.0002117	1.958E-19	2.524E-16	0.00000288
485	3.281E-18	1.161E-24	5.656E-14	0.002665	8.245E-17	5.212E-17	0.00231	0.004492	0.0001848	1.988E-19	2.562E-16	2.773E-06
486	1.941E-17	2.735E-23	1.52E-14	0.002852	1.225E-16	2.539E-16	0.0006174	0.002451	0.00002711	6.418E-19	2.078E-16	3.811E-07
487	3.759E-18	8.397E-25	8.771E-14	0.002467	1.497E-16	6.683E-17	0.0004519	0.001227	0.00007408	6.224E-20	1.271E-16	1.207E-06
488	2.676E-18	4.748E-25	1.076E-13	0.002408	1.342E-16	5.366E-17	0.0003442	0.001199	0.00008896	4.329E-20	1.113E-16	1.485E-06
489	1.115E-16	3.136E-22	7.717E-15	0.002906	3.529E-16	1.112E-15	0.0001602	0.0006547	3.697E-06	9.851E-19	1.598E-16	5.116E-08
490	2.733E-18	4.85E-25	1.076E-13	0.002635	1.371E-16	5.389E-17	0.0003445	0.001124	0.00009124	4.145E-20	1.066E-16	1.392E-06
522	2.482E-06	1.458E-12	0.00003946	0.006653	0.00003758	1.395E-10	0.0001651	0.001394	0.0000863	4.668E-08	0.00003625	5.215E-07
523	8.143E-09	2.817E-17	0.0004192	0.01018	0.00002094	2.008E-13	0.0009044	0.00004607	0.0007409	5.06E-12	6.674E-07	0.00000291
524	6.805E-09	2.147E-17	0.000453	0.006516	0.00001919	2.526E-13	0.0001672	0.00005718	0.0006454	5.248E-12	7.59E-07	3.971E-06
525	1.311E-07	9.693E-16	0.0004801	0.02331	0.0001576	4.712E-13	0.005327	0.00002741	0.0004721	4.846E-11	2.989E-06	8.082E-07
526	1.184E-08	6.056E-17	0.0003914	0.02778	0.00002058	1.316E-13	0.01466	0.0000733	0.002175	1.17E-11	1.044E-06	3.044E-06
527	1.825E-17	1.289E-23	0.00001489	0.01366	2.299E-16	6.862E-11	0.0003798	0.002374	0.000251	5.845E-19	3.776E-16	7.384E-07
528	2.358E-06	1.126E-12	0.00004493	0.01417	0.00004393	9.665E-11	0.0003791	0.002345	0.0003803	7.461E-08	0.00007129	1.079E-06
529	6.439E-08	1.142E-15	0.0005884	0.06047	0.00003229	1.384E-12	0.005344	0.0001156	0.002152	1.004E-10	2.581E-06	1.413E-06
530	2.98E-08	3.336E-16	0.000758	0.04454	0.00002368	9.064E-13	0.007226	0.00005426	0.00118	2.181E-11	8.889E-07	1.049E-06
531	3.306E-06	1.653E-11	3.102E-06	0.02522	5.881E-06	6.051E-10	0.0005378	0.003155	0.00008696	1.407E-07	0.00001284	1.386E-07
532	5.982E-17	1.644E-22	5.061E-06	0.02535	1.937E-16	2.979E-10	0.0004163	0.00314	0.0001583	2.534E-18	4.208E-16	2.51E-07
533	3.436E-06	8.222E-12	6.119E-06	0.02407	0.00001277	2.769E-10	0.0005481	0.003328	0.000183	1.543E-07	0.00002941	3.054E-07
534	3.258E-17	4.699E-23	5.846E-06	0.02795	2.01E-16	9.276E-11	0.000738	0.00321	0.00034	1.411E-18	4.463E-16	4.887E-07
535	7.632E-06	9.154E-12	8.264E-06	0.0636	0.0000566	7.765E-11	0.002152	0.001131	0.0003276	1.164E-07	0.00004428	2.066E-07
536	4.676E-08	4.559E-16	0.0002044	0.04456	0.00004266	1.476E-13	0.01089	0.00002445	0.0006106	1.542E-11	7.216E-07	5.394E-07
537	9.191E-08	1.42E-15	0.0002214	0.07067	0.00005291	2.519E-13	0.01373	7.582E-06	0.0001895	9.4E-12	2.775E-07	1.051E-07
538	1.643E-08	1.083E-16	0.000279	0.03476	0.00002217	1.164E-13	0.01591	0.00001755	0.0005057	3.889E-12	2.692E-07	5.709E-07
539	6.052E-09	3.169E-17	0.0002031	0.02428	0.00001028	7.604E-14	0.01103	0.00002291	0.0005805	1.87E-12	1.63E-07	9.432E-07

Table G. part 6: *Continued*

Sequence # (sample #)	H2PO4- activity	H3PO4 activity	H3SiO4- activity	HCO3- activity	HPO4-- activity	HSO4- activity	K+ activity	Mg++ activity	MgCO3 activity	MgH2PO4+ activity	MgHPO4 activity	MgOH+ activity
540	1.796E-17	1.24E-23	0.00003375	0.02109	2.315E-16	1.405E-10	0.0004819	0.002443	0.0004078	5.918E-19	3.912E-16	7.772E-07
541	1.381E-17	1.12E-23	0.00001767	0.02263	1.515E-16	8.372E-11	0.0008298	0.004985	0.0007601	9.285E-19	5.224E-16	0.00000135
542	1.259E-17	7.395E-24	0.0000114	0.01952	1.906E-16	3.171E-11	0.0003715	0.003513	0.0006379	5.965E-19	4.633E-16	1.313E-06
543	7.617E-07	1.701E-14	0.001235	0.07683	0.0003034	3.545E-12	0.007618	0.00002919	0.0005488	3E-10	6.127E-06	2.831E-07
544	4.189E-07	9.357E-15	0.0007461	0.07055	0.0001669	2.539E-12	0.004744	0.00001706	0.0002945	9.64E-11	1.969E-06	1.661E-07
545	6.627E-08	7.419E-16	0.0007508	0.0453	0.00005267	8.618E-13	0.007496	0.00006247	0.001382	5.584E-11	2.276E-06	1.207E-06
546	1.027E-07	1.073E-15	0.0009131	0.04585	0.00008743	8.717E-13	0.009044	0.00001266	0.0003035	1.753E-11	7.656E-07	2.607E-07
547	2.408E-08	2.045E-16	0.0007862	0.04654	0.00002523	2.969E-13	0.0288	0.00006455	0.001934	2.097E-11	1.127E-06	1.596E-06
548	2.606E-07	5.558E-15	0.0007204	0.07734	0.0001087	1.832E-12	0.008439	0.00002019	0.0004001	7.097E-11	1.518E-06	2.048E-07
549	6.733E-07	3.142E-14	0.0002978	0.09134	0.0001284	3.701E-12	0.003751	0.0001168	0.001249	1.061E-09	0.00001037	5.454E-07
550	6.759E-08	9.309E-16	0.0009366	0.06177	0.00004366	1.07E-12	0.01157	0.00001753	0.0004296	1.598E-11	5.294E-07	2.738E-07
551	7.131E-08	9.822E-16	0.0008458	0.07067	0.00004607	7.415E-13	0.01547	0.00001278	0.0003584	1.229E-11	4.073E-07	1.968E-07
552	5.027E-09	3.893E-17	0.0005376	0.03922	5.774E-06	2.46E-13	0.01654	0.00006336	0.001754	4.296E-12	2.531E-07	1.748E-06
553	1.128E-08	9.576E-17	0.0005333	0.04274	0.00001181	2.726E-13	0.01496	0.0000378	0.00104	5.75E-12	3.089E-07	9.503E-07
554	1.704E-08	1.26E-16	0.00103	0.03751	0.00002049	4.505E-13	0.01587	0.00005445	0.001509	1.251E-11	7.719E-07	1.571E-06
555	4.965E-08	2.54E-16	0.0002897	0.02504	0.00008632	1.036E-13	0.003511	6.349E-06	0.0001698	4.252E-12	3.792E-07	2.671E-07
556	7.417E-08	5.613E-16	0.000311	0.03803	0.00008718	1.516E-13	0.004654	8.272E-06	0.0002272	8.276E-12	4.989E-07	2.336E-07
557	3.258E-07	5.78E-15	0.000407	0.08323	0.0001633	5.186E-13	0.006164	0.00001454	0.0003728	6.39E-11	1.643E-06	1.746E-07
558	4.234E-08	1.887E-16	0.0006229	0.01902	0.00008451	2.578E-13	0.001415	6.429E-06	0.0001499	3.672E-12	3.759E-07	3.127E-07
559	1.224E-07	1.221E-15	0.0006011	0.05097	0.0001091	3.568E-13	0.008362	0.0000136	0.0003798	2.246E-11	1.027E-06	2.903E-07
560	7.542E-18	1.536E-24	0.00001705	0.00857	3.294E-16	8.571E-12	0.000202	0.001043	0.0002397	1.061E-19	2.376E-16	1.124E-06
561	5.435E-08	5.811E-16	0.0003457	0.05878	0.00004523	1.517E-13	0.01605	3.128E-06	0.00009401	2.294E-12	9.789E-08	6.085E-08
562	1.303E-07	1.057E-15	0.001176	0.04066	0.000143	6.049E-13	0.007102	0.00000397	0.0001088	6.98E-12	3.927E-07	1.044E-07
563	8.189E-07	3.035E-14	0.0006869	0.2201	0.0001965	1.071E-12	0.04924	0.00002347	0.0007614	2.592E-10	0.00000319	1.25E-07
564	1.1727E-08	2.3889E-16	0.0011285	7.0146E-05	5.1215E-06	9.1264E-13	0.03222552	0.00263633	4.9625E-05	4.1716E-10	9.3433E-06	2.1772E-05
565	3.954E-15	2.992E-23	0.0008562	0.003	4.647E-12	7.163E-14	0.01121	0.0001427	0.0003091	7.61E-18	4.588E-13	3.489E-06
566	1.239E-17	4.094E-24	0.00002193	0.008575	3.337E-16	2.723E-11	0.0001834	0.001025	0.0001454	1.714E-19	2.367E-16	6.817E-07
567	2.351E-07	5.498E-15	0.0008448	0.1383	0.00008942	7.178E-13	0.03617	0.00003524	0.001139	1.118E-10	0.00000218	2.993E-07
568	2.165E-07	3.93E-15	0.0009488	0.1207	0.0001061	5.724E-13	0.04825	9.321E-06	0.0003387	2.722E-11	6.84E-07	1.006E-07
569	2.001E-07	1.997E-15	0.0006672	0.04411	0.0001784	5.578E-13	0.007506	0.00001507	0.000364	4.067E-11	0.00000186	3.239E-07
570	9.122E-07	2.686E-14	0.001772	0.1899	0.0002756	1.78E-12	0.1049	0.00004686	0.001651	5.766E-10	8.935E-06	3.03E-07
571	4.821E-07	1.387E-14	0.0005538	0.162	0.0001491	6.362E-13	0.04238	0.00001926	0.0005928	1.253E-10	1.986E-06	1.331E-07
572	4.061E-17	3.869E-23	6.384E-06	0.006708	3.792E-16	6.963E-11	0.00002678	0.000939	0.00003613	5.144E-19	2.463E-16	2.166E-07
573	1.165E-17	4.844E-24	0.0000283	0.008779	2.491E-16	5.289E-11	0.0001046	0.001642	0.0001894	2.579E-19	2.829E-16	8.673E-07
574	2.353E-08	2.191E-16	0.0001643	0.0401	0.00002248	1.438E-13	0.01348	9.056E-06	0.0002132	2.875E-12	1.409E-07	2.108E-07
575	6.792E-08	2.46E-15	0.00004657	0.03912	0.00001668	6.576E-13	0.003255	0.0002171	0.001281	1.989E-10	2.505E-06	1.314E-06
576	1.316E-06	2.081E-13	0.0000465	0.01675	0.00007404	1.221E-11	0.0006933	0.0002449	0.0001418	4.348E-09	0.00001254	3.401E-07
577	2.799E-17	2.792E-23	0.00000762	0.006941	2.496E-16	7.595E-11	0.00007819	0.002198	0.00008356	8.297E-19	3.794E-16	4.84E-07

Table G. part 6: *Continued*

Sequence # (sample #)	H2PO4- activity	H3PO4 activity	H3SiO4- activity	HCO3- activity	HPO4-- activity	HSO4- activity	K+ activity	Mg++ activity	MgCO3 activity	MgH2PO4+ activity	MgHPO4 activity	MgOH+ activity
578	9.604E-08	2.145E-14	0.00004353	0.008563	3.825E-06	6.194E-12	0.000247	0.00001607	3.367E-06	2.082E-11	4.253E-08	1.578E-08
579	1.367E-09	7.67E-18	0.001634	0.01203	2.168E-06	4.932E-13	0.002067	5.211E-14	6.106E-13	9.61E-22	7.815E-17	1.965E-15
580	2.091E-09	1.859E-17	0.002325	0.02064	2.091E-06	9.862E-13	0.002848	4.896E-14	6.211E-13	1.381E-21	7.084E-17	1.155E-15
581	1.471E-08	3.286E-16	0.002231	0.05772	0.00000586	3.591E-14	0.003659	4.627E-14	6.535E-13	9.182E-21	1.876E-16	4.255E-16
582	2.713E-08	1.209E-15	0.001384	0.1105	5.417E-06	4.778E-15	0.004608	5.297E-14	7.179E-13	1.939E-20	1.985E-16	2.376E-16
583	4.087E-08	2.293E-15	0.001343	0.1429	0.00000648	6.413E-15	0.005385	5.431E-14	7.558E-13	2.994E-20	2.435E-16	1.912E-16
584	5.902E-08	4.169E-15	0.001999	0.1895	7.433E-06	7.221E-15	0.006102	5.556E-14	8.147E-13	4.423E-20	2.857E-16	1.517E-16
585	6.552E-08	5.826E-15	0.01005	0.2763	6.555E-06	9.697E-15	0.00904	5.724E-14	9.722E-13	5.059E-20	2.596E-16	1.177E-16
586	4.433E-10	2.217E-18	0.003289	0.03539	7.887E-07	1.807E-12	0.05078	2.373E-14	9.181E-13	1.419E-22	1.295E-17	8.21E-16
587	3.725E-10	1.862E-18	0.004022	0.0326	6.626E-07	7.82E-13	0.0568	2.479E-14	8.834E-13	1.246E-22	1.137E-17	8.733E-16
588	1.194E-10	4.741E-19	0.004497	0.0269	2.674E-07	1.922E-12	0.05935	3.061E-14	1.133E-12	4.929E-23	5.662E-18	1.27E-15
589	1.128E-10	4.481E-19	0.003554	0.03044	2.527E-07	8.757E-13	0.05686	2.479E-14	1.038E-12	3.772E-23	4.333E-18	1.038E-15
590	2.255E-10	8.955E-19	0.005109	0.02978	5.05E-07	2.608E-12	0.05435	2.698E-14	1.105E-12	8.205E-23	9.425E-18	1.115E-15
591	1.648E-10	6.544E-19	0.004581	0.02861	3.69E-07	1.125E-12	0.06037	2.905E-14	1.143E-12	6.456E-23	7.416E-18	1.193E-15
592	7.347E-10	5.822E-18	0.004709	0.05723	8.247E-07	2.469E-12	0.06464	2.957E-14	1.167E-12	2.93E-22	1.687E-17	6.047E-16
593	1.738E-10	7.747E-19	0.004401	0.03165	3.47E-07	1.145E-12	0.0597	2.867E-14	1.113E-12	6.723E-23	6.883E-18	1.061E-15
594	3.333E-08	1.486E-15	0.001694	0.2306	6.654E-06	7.929E-12	0.02957	2.912E-14	8.236E-13	1.309E-20	1.341E-16	1.198E-16
595	2.917E-09	3.265E-17	0.00238	0.0702	2.318E-06	1.54E-12	0.03992	2.195E-14	7.522E-13	8.636E-22	3.52E-17	3.573E-16
596	1.099E-07	8.711E-15	0.0009041	0.2753	0.00001234	1.142E-11	0.01693	3.22E-14	6.113E-13	4.774E-20	2.748E-16	8.19E-17
597	2.341E-10	9.963E-19	0.003644	0.02738	4.893E-07	8.499E-13	0.03983	2.283E-14	8.028E-13	7.21E-23	7.729E-18	9.639E-16
598	3.173E-10	1.78E-18	0.005282	0.03791	5.031E-07	1.977E-12	1.146E-12	3.094E-14	1.143E-12	1.325E-22	1.077E-17	9.047E-16
599	2.884E-10	1.442E-18	0.004533	0.03668	5.132E-07	1.199E-12	0.04382	2.326E-14	9.326E-13	9.051E-23	8.259E-18	7.983E-16
600	5.356E-09	9.502E-17	0.002005	0.09188	2.686E-06	2.403E-12	0.03568	2.43E-14	6.877E-13	1.755E-21	4.514E-17	2.599E-16
601	3.212E-08	4.85E-16	0.0006708	0.07531	0.00001892	1.242E-11	0.02078	1.671E-14	4.555E-13	7.24E-21	2.188E-16	2.26E-16
602	5.564E-08	1.108E-15	0.0008506	0.03075	0.00002487	2.813E-11	0.005284	7.265E-14	6.133E-13	5.453E-20	1.25E-15	7.979E-16
603	4.459E-08	2.502E-15	0.0009308	0.1909	0.00000707	1.066E-11	0.01475	3.136E-14	5.832E-13	1.886E-20	1.534E-16	1.152E-16
604	4.234E-08	2.791E-15	0.0009692	0.2191	5.714E-06	9.928E-12	0.01557	3.34E-14	6.068E-13	1.908E-20	1.321E-16	1.034E-16
605	1.851E-22	7.354E-31	0.005355	0.02048	4.147E-19	1.193E-12	0.05275	3.741E-14	1.054E-12	9.342E-35	1.073E-29	1.633E-15
606	2.934E-10	1.467E-18	0.004028	0.03344	5.22E-07	1.082E-12	0.04826	2.456E-14	8.976E-13	9.72E-23	8.869E-18	8.595E-16
607	4.403E-22	2.202E-30	0.004787	0.03425	7.833E-19	1.297E-12	0.0492	2.72E-14	1.018E-12	1.615E-34	1.474E-29	9.233E-16
608	1.276E-21	9.016E-30	0.003407	0.04247	1.608E-18	1.385E-12	0.034	2.358E-14	7.749E-13	4.061E-34	2.623E-29	6.092E-16
609	7.407E-10	5.232E-18	0.003516	0.04122	9.329E-07	1.427E-12	0.03405	2.391E-14	7.625E-13	2.389E-22	1.543E-17	6.215E-16
610	3.043E-09	3.036E-17	0.002946	0.05606	2.714E-06	1.867E-12	0.0281	2.219E-14	6.813E-13	9.109E-22	4.165E-17	4.178E-16
611	1.201E-08	2.683E-16	0.001976	0.1066	4.784E-06	3.134E-12	0.02096	2.291E-14	5.977E-13	3.713E-21	7.584E-17	2.015E-16
612	1.819E-10	8.107E-19	0.006054	0.02324	3.631E-07	1.554E-12	0.0559	3.992E-14	1.138E-12	9.795E-23	1.003E-17	1.51E-15
613	1.63E-09	2.892E-17	0.003592	0.1017	8.173E-07	6.342E-12	0.05231	3.674E-14	1.151E-12	8.079E-22	2.078E-17	3.454E-16
614	2.91E-08	1.297E-15	0.0008328	0.2129	0.00000581	5.191E-12	0.02051	2.52E-14	6.581E-13	9.895E-21	1.013E-16	1.09E-16
615	1.516E-09	2.69E-18	3.798E-13	0.00468	7.603E-06	9.631E-12	0.03177	3.747E-14	5.402E-13	7.664E-22	1.971E-16	4.477E-15

Table G. part 6: *Continued*

Sequence # (sample #)	H2PO4- activity	H3PO4 activity	H3SiO4- activity	HCO3- activity	HPO4-- activity	HSO4- activity	K+ activity	Mg++ activity	MgCO3 activity	MgH2PO4+ activity	MgHPO4 activity	MgOH+ activity
616	1.746E-10	2.461E-19	3.455E-13	0.002306	1.102E-06	6.366E-12	0.01439	8.467E-14	7.573E-13	1.995E-22	6.458E-17	1.179E-14
617	3.961E-11	5.582E-20	3.191E-13	0.004512	0.00000025	3.11E-12	0.03877	6.665E-14	1.166E-12	3.561E-23	1.153E-17	8.129E-15
618	1.462E-12	2.595E-21	3.525E-13	0.0006988	7.333E-09	1.048E-11	0.01715	4.069E-13	8.758E-13	8.026E-24	2.064E-18	3.945E-14
619	2.724E-11	3.839E-20	3.846E-13	0.001223	1.72E-07	6.106E-12	0.008108	1.174E-13	5.567E-13	4.314E-23	1.397E-17	1.697E-14
620	7.135E-12	6.344E-21	3.308E-13	0.002189	7.138E-08	2.909E-12	0.03938	8.418E-14	1.132E-12	8.102E-24	4.157E-18	1.644E-14
621	4.987E-09	2.222E-17	0.001979	0.009134	9.955E-06	3.487E-13	0.004495	2.154E-06	0.00002413	1.449E-13	1.484E-08	1.058E-07
622	4.876E-08	2.736E-15	0.0004749	0.04566	7.732E-06	1.381E-11	0.005065	1.173E-13	5.218E-13	7.717E-20	6.276E-16	4.572E-16
623	2.547E-08	2.265E-16	0.0004896	0.01231	0.00002548	1.236E-11	0.009018	8.309E-14	6.286E-13	2.855E-20	1.465E-15	2.047E-15
624	1.993E-07	1.772E-14	0.00005624	0.04224	0.00001994	4.409E-11	7.5E-10	6.706E-06	0.00001741	1.803E-11	9.252E-08	1.652E-08

Table G. part 7: Aqueous chemistry database of alkaline lake waters compiled from published literature, as well as corresponding results from calculations described in chapters 2 and 3, and investigated in detail in chapter 4.

Sequence # (sample #)	MgPO4- activity	Na+ activity	OH- activity	PO4--- activity	SO4-- activity	SiO2(aq) activity	CO2(g) bar	CO2(g) fugacity	Amrph^silica log Q/K	Anhydrite log Q/K	Aragonite log Q/K	Brucite log Q/K
1	1.785E-16	0.07504	0.00002514	1.292E-19	0.001942	6.48E-13	0.0001921	0.0001921	-9.475	-2.655	0.8516	-0.8048
2	1.169E-16	0.08987	0.00001996	1.389E-19	0.002032	6.989E-13	0.0003423	0.0003423	-9.442	-2.765	0.7726	-1.22
3	6.608E-17	0.1183	0.00003979	3.59E-19	0.0009518	5.277E-13	0.0003548	0.0003548	-9.564	-3.736	0.746	-1.281
4	1.594E-16	0.1191	0.00001695	5.145E-20	0.004407	7.144E-13	0.0003013	0.0003013	-9.432	-2.255	0.7505	-0.7966
5	1.075E-17	1.291	0.0002736	1.605E-19	0.004981	8.433E-14	0.00003595	0.00003595	-10.36	-3.242	1.225	-0.04592
6	1.238E-17	1.082	0.00009544	1.079E-19	0.00534	2.215E-13	0.0002403	0.0002403	-9.941	-2.945	1.4	-0.7268
7	8.231E-18	1.608	0.0003233	7.504E-20	0.005021	7.122E-14	0.00002306	0.00002306	-10.43	-3.211	1.212	0.3134
8	3.602E-18	2.474	0.0003925	7.116E-20	0.007643	5.646E-14	0.00001899	0.00001899	-10.53	-3.129	1.211	0.1461
9	1.746E-16	0.1773	0.00004993	2.203E-19	0.004821	4.483E-13	0.0001272	0.0001272	-9.635	-2.861	0.6699	-0.4502
10	7.806E-17	0.2178	0.00001041	3.343E-20	0.008514	7.968E-13	0.0007634	0.0007634	-9.385	-1.445	1.256	-1.343
11	1.071E-16	0.05058	0.00001151	6.266E-20	0.004415	8.052E-13	0.0006771	0.0006771	-9.381	-1.786	1.232	-1.391
12	8.909E-17	0.108	0.00001174	5.286E-20	0.005977	7.904E-13	0.0004588	0.0004588	-9.389	-1.494	1.242	-1.38
13	6.398E-18	0.1583	0.00001901	1.712E-19	0.001646	6.964E-13	0.00119	0.00119	-9.444	-3.036	1.094	-2.616
14	2.49E-16	0.4188	0.00006204	6.277E-20	0.01195	3.468E-13	0.0000359	0.0000359	-9.746	-2.123	0.6588	0.4379
15	3.399E-17	0.2365	0.00004981	2.715E-19	0.003424	4.278E-13	0.0005801	0.0005801	-9.655	-3.423	0.9146	-1.254
16	2.714E-17	0.1976	9.948E-06	6.652E-20	0.001241	8.16E-13	0.002232	0.002232	-9.375	-3.187	0.7771	-2.14
17	9.879E-17	0.4878	0.00001378	2.183E-20	0.0004081	7.37E-13	0.0005127	0.0005127	-9.419	-2.87	1.229	-0.8116
18	1.066E-16	0.0196	0.00001263	9.39E-20	0.0007066	8.062E-13	0.0003693	0.0003693	-9.38	-2.45	1.181	-1.488
19	1.4E-16	0.06754	0.0000126	5.16E-20	0.001201	7.872E-13	0.0002616	0.0002616	-9.39	-2.644	0.6058	-1.112
20	2.373E-18	1.008	0.0000606	8.343E-20	0.006182	3.103E-13	0.0006253	0.0006253	-9.795	-3.396	0.9025	-1.727
21	4.994E-18	0.6615	0.0001066	1.862E-19	0.01159	2.065E-13	0.0001524	0.0001524	-9.971	-3.129	0.7687	-1.262
22	6.753E-17	0.2422	0.00004983	2.565E-19	0.008397	4.299E-13	0.0002594	0.0002594	-9.653	-2.741	0.8572	-0.9305
23	1.535E-16	0.04556	0.0000246	1.832E-19	0.0005498	6.671E-13	0.0002705	0.0002705	-9.462	-3.219	0.9646	-1.041
24	8.631E-17	0.09632	0.0000282	2.188E-19	0.005161	6.122E-13	0.0004201	0.0004201	-9.5	-2.378	1.144	-1.25
25	6.602E-09	0.03244	0.0000252	5.682E-10	6.616E-06	6.76E-13	0.0003112	0.0003112	-9.456	-4.829	1.356	-2.878
26	1.351E-09	0.01036	0.00006335	6.552E-10	0.00002657	4.668E-13	0.00006797	0.00006797	-9.617	-4.854	0.8665	-2.828
27	2.591E-18	0.005644	0.00003998	7.995E-19	0.00007569	5.924E-13	0.00007075	0.00007075	-9.514	-4.003	0.8806	-3.031
28	1.36E-08	0.006253	0.0001264	8.176E-09	0.00001262	3.114E-13	0.00001475	0.00001475	-9.793	-4.973	1.008	-2.321
29	1.018E-17	0.004007	0.0001004	1.843E-18	0.00001169	3.672E-13	0.0000163	0.0000163	-9.722	-5.095	0.7626	-2
30	5.984E-19	0.01414	0.0000503	8.761E-19	8.871E-06	5.098E-13	0.0001957	0.0001957	-9.579	-5.533	0.9238	-3.508
31	2.855E-07	0.01242	0.0001264	7.896E-08	0.00008694	2.988E-13	0.00003198	0.00003198	-9.811	-4.007	1.471	-1.984
32	3.589E-08	0.009004	0.00002004	2.045E-08	0.0001674	7.389E-13	0.0002748	0.0002748	-9.418	-3.578	0.9505	-3.898
33	9.995E-09	0.008289	0.00001264	4.311E-09	0.00005242	8.194E-13	0.0004026	0.0004026	-9.373	-4.021	0.777	-4.177
34	4.753E-09	0.03161	0.00005028	2.446E-09	0.00002776	5.052E-13	0.0001953	0.0001953	-9.583	-4.938	1.022	-3.054
35	7.041E-06	0.04264	0.00002002	1.264E-07	0.0003869	7.266E-13	0.0001255	0.0001255	-9.425	-3.148	0.6753	-2.397
36	1.624E-08	0.002109	0.0001005	7.21E-10	0.00000291	3.732E-13	9.006E-06	9.006E-06	-9.714	-5.403	0.8012	-1.389

Table G. part 7: *Continued*

Sequence # (sample #)	MgPO4- activity	Na+ activity	OH- activity	PO4--- activity	SO4-- activity	SiO2(aq) activity	CO2(g) bar	CO2(g) fugacity	Amrph^silica log Q/K	Anhydrite log Q/K	Aragonite log Q/K	Brucite log Q/K
37	1.178E-07	0.01126	0.00003997	5.06E-08	0.00009247	5.806E-13	0.0001461	0.0001461	-9.523	-4.217	0.8946	-3.175
38	1.194E-07	0.05621	0.0001002	1.205E-07	0.00002123	3.24E-13	0.00006573	0.00006573	-9.776	-5.44	0.7633	-2.748
39	6.495E-09	0.008976	0.00006336	3.991E-09	8.969E-06	4.724E-13	0.00005046	0.00005046	-9.612	-5.171	0.8926	-2.931
40	7.513E-18	0.003115	0.0001592	2.052E-18	2.897E-06	2.725E-13	3.664E-06	3.664E-06	-9.851	-5.533	0.682	-1.778
41	6.886E-09	0.009495	0.00001592	9.214E-10	0.00002564	7.82E-13	0.0003357	0.0003357	-9.393	-4.245	0.9852	-3.469
42	8.653E-18	0.155	0.00002506	2.273E-19	0.001223	0.0001324	0.0005563	0.0005563	-1.165	-3.42	0.748	-2.367
43	6.386E-18	0.1633	0.00002503	2.009E-19	0.000944	0.0001148	0.0006004	0.0006004	-1.227	-3.38	0.9332	-2.447
44	2.635E-17	0.1675	0.000199	1.242E-18	0.001234	0.00005425	0.00003429	0.00003429	-1.552	-3.646	1.107	-0.8217
45	2.139E-17	0.1865	0.0001579	9.462E-19	0.00122	0.00008903	0.00005335	0.00005335	-1.337	-3.523	1.227	-0.9949
46	1.917E-17	0.173	0.0001255	8.472E-19	0.0009891	0.0001202	0.00007883	0.00007883	-1.206	-3.712	1.1	-1.194
47	2.008E-17	0.1706	0.000158	1.013E-18	0.00115	0.0001016	0.00005441	0.00005441	-1.28	-3.611	1.174	-1.051
48	2.114E-17	0.1496	0.0001582	1.084E-18	0.001044	0.00009891	0.00005658	0.00005658	-1.291	-3.662	1.182	-1.057
49	1.103E-16	0.05841	0.00005022	4.387E-19	0.001834	0.0006003	0.0001354	0.0001354	-0.508	-2.717	1.263	-0.9438
50	1.1E-16	0.05463	0.0001002	6.152E-19	0.001703	0.0004215	0.000047	0.000047	-0.6616	-2.526	1.627	-0.4914
51	1.692E-16	0.0818	0.00006315	2.753E-19	0.005118	0.0001943	0.0001255	0.0001255	-0.9979	-1.924	1.777	-0.3566
52	1.329E-16	0.05949	0.0000632	2.096E-19	0.003406	0.0001979	0.0001251	0.0001251	-0.9899	-1.698	2.179	-0.3423
53	1.456E-16	0.06267	0.00003988	2.011E-19	0.005395	0.0002391	0.0002449	0.0002449	-0.9079	-1.77	1.799	-0.6845
54	3.487E-17	0.2502	0.00001251	6.534E-20	0.01038	0.00002505	0.0007728	0.0007728	-1.888	-1.886	0.8946	-1.824
55	9.211E-17	0.0437	0.00003991	1.844E-19	0.004371	0.0001163	0.0001692	0.0001692	-1.221	-1.511	1.989	-0.8452
56	1.216E-16	0.01888	0.00001003	5.638E-20	0.004188	8.317E-13	0.0006447	0.0006447	-9.366	-2.268	0.632	-1.409
57	1.833E-17	0.1367	0.00001257	8.662E-20	0.004871	0.0001545	0.002698	0.002698	-1.097	-1.586	2.068	-2.222
58	4.883E-17	0.6202	0.00003078	6.531E-20	0.0132	0.00003498	0.000351	0.000351	-1.743	-2.096	1.029	-0.8957
59	2.179E-16	0.04643	0.00007963	4.949E-19	0.00364	3.696E-13	0.0001044	0.0001044	-9.719	-2.548	1.422	-0.3
60	1.528E-17	0.7974	0.00001942	3.729E-20	0.0259	0.00007087	0.0006389	0.0006389	-1.436	-1.807	0.8844	-1.557
61	7.733E-17	0.2031	0.00006279	1.172E-19	0.009145	3.756E-13	0.0001388	0.0001388	-9.712	-1.052	2.438	-0.3305
62	4.582E-17	0.1546	0.00002505	4.121E-20	0.007926	0.0002384	0.0002039	0.0002039	-0.9091	-0.558	2.363	-0.9023
63	4.518E-17	0.06523	0.00001261	1.319E-19	0.001768	0.0001732	0.0008981	0.0008981	-1.048	-2.577	1.04	-2.01
64	6.635E-17	0.2334	0.00001574	5.701E-20	0.006775	7.147E-13	0.002353	0.002353	-9.432	-1.497	2.152	-1.286
65	2.93E-17	1.194	9.423E-06	9.183E-21	0.007845	8.231E-13	0.008905	0.008905	-9.371	-1.267	2.473	-1.294
66	1.25E-19	0.001124	1.005E-07	1.436E-21	0.0002259	0.0003095	0.004	0.004	-0.7957	-3.138	-2.177	-6.802
67	5.465E-20	0.001838	6.338E-08	6.556E-22	0.0004514	0.0002698	0.005685	0.005685	-0.8554	-2.507	-2.094	-7.221
68	9.995E-20	0.001874	1.265E-07	1.87E-21	0.0006829	0.0006189	0.004023	0.004023	-0.4948	-2.193	-1.509	-6.814
69	9.3E-19	0.005833	7.978E-07	1.835E-20	0.0009815	0.0007205	0.001193	0.001193	-0.4288	-2.32	-0.7221	-5.237
70	2.372E-17	0.02549	0.00005031	6.822E-19	0.004906	0.0001982	0.00002446	0.00002446	-0.9894	-2.197	0.6133	-1.801
71	1.601E-19	0.002199	7.979E-08	8.393E-22	0.0007357	0.0004496	0.008759	0.008759	-0.6336	-2.01	-1.421	-6.661
72	5.27E-19	0.004103	1.264E-07	1.47E-21	0.001403	0.0003994	0.005833	0.005833	-0.685	-1.842	-1.31	-5.988
73	6.813E-19	0.005887	1.264E-07	1.348E-21	0.001915	0.001079	0.01033	0.01033	-0.2536	-1.811	-1.166	-5.839
74	3.832E-19	0.007166	1.264E-07	1.375E-21	0.00178	0.0003196	0.007987	0.007987	-0.7818	-1.472	-0.9071	-6.097

Table G. part 7: *Continued*

Sequence # (sample #)	MgPO4- activity	Na+ activity	OH- activity	PO4--- activity	SO4-- activity	SiO2(aq) activity	CO2(g) bar	CO2(g) fugacity	Amrph^silica log Q/K	Anhydrite log Q/K	Aragonite log Q/K	Brucite log Q/K
75	2.158E-18	0.08653	0.00001998	2.187E-19	0.007917	0.0007389	0.0002567	0.0002567	-0.4178	-1.785	1.037	-3.15
76	8.169E-19	0.4561	0.00004942	2.274E-19	0.01407	0.0012	0.0002871	0.0002871	-0.2071	-2.635	0.78	-2.803
77	6.903E-19	0.702	0.00007753	2.222E-19	0.01707	0.001526	0.0001565	0.0001565	-0.1029	-2.665	0.7982	-2.475
78	9.747E-28	1.994	0.00004581	4.289E-20	0.01291	0.003565	0.0007575	0.0007575	0.2657	-10.97	-7.131	-11.07
79	8.658E-28	2.198	0.00004535	3.759E-20	0.0138	0.003443	0.0007897	0.0007897	0.2505	-10.95	-7.12	-11.07
80	6.971E-17	0.05746	0.0002001	2.021E-18	0.0004815	0.0004038	0.00001424	0.00001424	-0.6803	-3.666	1.117	-0.6057
81	1.712E-19	0.09163	7.947E-07	9.168E-21	0.00362	0.003154	0.02006	0.02006	0.2125	-1.955	0.2996	-5.674
82	5.613E-20	1.814	0.00005828	5.611E-20	0.007388	0.001725	0.000678	0.000678	-0.04952	-3.487	0.7528	-3.215
83	7.583E-20	2.493	0.00008978	6.579E-20	0.01838	0.004535	0.0003046	0.0003046	0.3701	-2.857	1.026	-2.778
84	9.307E-20	2.788	0.00004431	4.138E-20	0.0261	0.007309	0.0006906	0.0006906	0.5774	-2.255	1.226	-3.101
85	2.366E-20	6.86	0.000045	1.188E-20	0.02924	0.008167	0.001022	0.001022	0.6257	-2.332	1.376	-3.14
86	8.416E-18	0.002432	3.177E-06	8.757E-20	0.00003005	0.0007603	0.0002941	0.0002941	-0.4054	-4.291	-0.5877	-3.759
87	7.394E-18	0.02736	0.00002521	4.891E-19	0.0006886	0.001089	0.0001677	0.0001677	-0.2492	-3.319	0.5803	-2.763
88	2.346E-18	0.01186	0.00002522	5.658E-19	0.0003648	0.0009705	0.00008976	0.00008976	-0.2994	-3.441	0.4632	-3.325
89	1.141E-17	0.00392	2.523E-06	4.914E-20	0.00001986	0.001343	0.0006076	0.0006076	-0.1582	-3.817	0.1816	-3.576
90	3.075E-18	0.006003	6.337E-06	1.115E-19	0.0001326	0.002348	0.000252	0.000252	0.08436	-2.876	0.716	-3.701
91	1.323E-16	0.0825	0.00007954	6.61E-19	0.001269	0.001791	0.0001257	0.0001257	-0.03333	-3.136	1.372	-0.6433
92	2.399E-18	0.08902	0.0000632	8.794E-19	0.001932	0.0003849	0.0001099	0.0001099	-0.7011	-3.261	0.8061	-2.709
93	1.719E-18	0.002315	1.265E-06	2.75E-20	0.00001404	0.0003919	0.001097	0.001097	-0.6933	-3.729	0.07712	-4.746
94	4.069E-18	0.0006469	3.176E-06	6.79E-20	0.00001389	0.00038	0.001046	0.001046	-0.7066	-3.892	0.6979	-3.964
95	1.375E-17	0.003642	3.176E-06	3.745E-20	5.675E-06	0.001043	0.0007685	0.0007685	-0.268	-3.854	0.991	-3.177
96	1.333E-18	0.001026	3.999E-07	8.247E-21	0.00007272	0.0007949	0.002558	0.002558	-0.3861	-3.299	-0.84	-5.333
97	1.91E-18	0.002889	3.999E-07	6.734E-21	0.00006264	0.0009938	0.006892	0.006892	-0.2891	-3.182	-0.2274	-5.089
98	6.283E-19	0.00009372	2.523E-07	4.748E-21	0.00007364	0.001096	0.004623	0.004623	-0.2467	-3.187	-0.8763	-5.82
99	5.964E-18	0.008695	5.033E-07	5.589E-21	5.102E-10	0.001587	0.005215	0.005215	-0.0858	-8.492	-0.3698	-4.314
100	7.711E-18	0.001502	1.004E-06	1.272E-20	0.00000546	0.001672	0.00362	0.00362	-0.06318	-3.918	0.617	-3.959
101	1.742E-18	0.0005581	7.979E-07	1.883E-20	0.0005756	0.0008884	0.001229	0.001229	-0.3378	-2.427	-0.5849	-4.976
102	1.977E-18	0.002212	6.338E-07	1.282E-20	0.00001374	0.0005939	0.002431	0.002431	-0.5127	-3.801	-0.2406	-4.954
103	1.607E-19	0.002035	1.004E-07	1.28E-21	6.981E-06	0.0005992	0.01378	0.01378	-0.5088	-4.086	-1.078	-6.643
104	2.702E-19	0.001661	1.265E-07	1.733E-21	0.00001372	0.0004991	0.01091	0.01091	-0.5882	-3.738	-0.9246	-6.349
105	1.532E-17	0.03412	0.0000503	5.802E-19	0.0008713	0.0005653	0.00006081	0.00006081	-0.5341	-2.687	1.27	-1.921
106	4.051E-19	0.0002804	1.592E-07	2.457E-21	7.221E-10	0.0006983	0.00501	0.00501	-0.4424	-8.049	-1.094	-6.125
107	2.406E-19	0.000465	1.005E-07	1.239E-21	7.043E-10	0.0008987	0.007422	0.007422	-0.3328	-8.01	-1.274	-6.454
108	1.717E-17	0.02617	0.00001591	2.692E-19	0.0006538	0.003173	0.0003693	0.0003693	0.215	-2.839	1.026	-2.538
109	2.514E-19	0.0004697	1.265E-07	1.874E-21	7.453E-10	0.0004991	0.006974	0.006974	-0.5883	-8.174	-1.29	-6.415
110	2.15E-17	0.02948	0.00005031	7.499E-19	0.0008635	0.0003103	0.00005114	0.00005114	-0.7947	-2.95	0.9354	-1.885
111	4.813E-18	0.007969	1.004E-06	1.7E-20	0.0001169	0.0009835	0.003302	0.003302	-0.2936	-2.847	0.3172	-4.29
115	3.798E-26	0.03771	0.00001003	2.158E-19	0.0004285	0.0005056	0.0003665	0.0003665	-0.5826	-11.42	-7.779	-11.5

Table G. part 7: *Continued*

Sequence # (sample #)	MgPO4- activity	Na+ activity	OH- activity	PO4--- activity	SO4-- activity	SiO2(aq) activity	CO2(g) bar	CO2(g) fugacity	Amrph^silica log Q/K	Anhydrite log Q/K	Aragonite log Q/K	Brucite log Q/K
116	2.836E-17	0.1039	0.00003165	3.951E-19	0.0009498	0.0001199	0.0001417	0.0001417	-1.207	-3.342	0.5429	-1.889
117	8.819E-19	0.04346	3.993E-07	6.045E-21	0.0002188	0.0006967	0.01857	0.01857	-0.4433	-4.078	-1.236	-5.379
118	1.768E-26	0.1949	0.00003964	2.447E-19	0.001661	0.002154	0.0001928	0.0001928	0.04684	-2.379	1.595	-10.69
119	1.146E-17	0.2305	0.00002501	2.348E-19	0.001753	0.0003771	0.0003794	0.0003794	-0.7099	-11.25	-7.409	-2.261
120	2.151E-17	0.0942	0.00003986	5.039E-19	0.0009343	0.000109	0.00008769	0.00008769	-1.249	-3.334	0.5507	-1.915
121	1.854E-17	0.08709	0.00003167	4.173E-19	0.0009568	0.0001207	0.0001278	0.0001278	-1.205	-3.304	0.5336	-2.097
125	1.18E-18	0.0109	2.522E-07	3.423E-21	0.00005441	0.0006976	0.01506	0.01506	-0.4428	-3.15	-0.1949	-5.405
126	8.984E-19	0.0682	3.99E-07	5.209E-21	0.0001913	0.0005977	0.016	0.016	-0.5099	-3.022	-0.1877	-5.307
127	6.367E-18	0.0507	0.00000159	2.503E-20	0.0001337	0.0004865	0.004951	0.004951	-0.5993	-3.327	0.3544	-3.938
128	1.787E-17	0.04269	2.002E-06	2.233E-20	0.00004087	0.0002896	0.003148	0.003148	-0.8246	-3.663	0.5362	-3.24
129	3.8E-17	0.007068	2.523E-06	2.444E-20	0.0001907	0.0007657	0.0007722	0.0007722	-0.4023	-11.64	-8.524	-2.751
130	9.196E-18	0.006608	6.336E-07	5.653E-21	0.00009226	0.0008905	0.003104	0.003104	-0.3368	-3.256	-0.4158	-3.931
131	7.938E-18	0.003661	5.033E-07	3.663E-21	0.00004185	0.001488	0.00613	0.00613	-0.1139	-3.476	-0.1975	-4.006
132	3.425E-18	0.003922	2.523E-07	2.077E-21	0.0001874	0.0009961	0.005529	0.005529	-0.2881	-2.856	-0.8733	-4.725
133	1.01E-17	0.006003	7.977E-07	9.268E-21	0.000105	0.000888	0.001844	0.001844	-0.338	-3.382	-0.6237	-3.905
134	5.206E-19	0.005607	1.592E-07	2.308E-21	0.0001927	0.0007983	0.01232	0.01232	-0.3843	-2.938	-1.019	-5.989
135	1.742E-17	0.0313	0.00000252	2.26E-20	0.005426	0.0005728	0.00126	0.00126	-0.5284	-1.056	0.8222	-3.056
136	3.003E-18	0.02014	1.004E-06	1.752E-20	0.0005125	9.836E-13	0.005923	0.005923	-9.294	-2.468	0.3081	-4.508
137	1.435E-18	0.005543	3.176E-07	4.771E-21	0.00005959	0.0009951	0.00527	0.00527	-0.2885	-3.02	-0.3601	-5.264
138	1.558E-18	0.03594	6.331E-07	1.009E-20	0.00009251	0.0006934	0.01028	0.01028	-0.4454	-3.25	0.1082	-4.954
139	6.274E-18	0.3914	1.486E-06	2.929E-21	0.005685	0.0009008	0.0005008	0.0005008	-0.3318	-0.1551	0.853	-3.071
140	4.208E-18	0.2223	0.0000014	3.396E-21	0.004043	0.001465	0.0003391	0.0003391	-0.1206	-0.1987	0.7321	-3.361
141	2.459E-17	0.1398	5.236E-06	2.202E-20	0.004631	0.0009172	0.0002006	0.0002006	-0.3239	-0.8856	0.9014	-2.26
142	1.131E-17	0.5866	0.00000308	5.517E-21	0.01333	0.0009497	0.0003899	0.0003899	-0.3088	-0.226	0.9399	-2.457
143	1.414E-17	0.2967	7.004E-06	1.835E-20	0.005778	0.0008034	0.0001175	0.0001175	-0.3815	-0.6012	1.114	-2.168
144	9.889E-18	0.2833	3.274E-06	9.597E-21	0.005894	0.0006945	0.0003359	0.0003359	-0.4447	-0.5191	0.9831	-2.703
145	5.564E-18	0.2056	1.894E-06	9.652E-21	0.00436	0.0011	0.0003889	0.0003889	-0.2449	-0.9647	0.2542	-3.43
146	6.534E-18	0.6069	1.084E-06	1.362E-21	0.002952	0.001274	0.001093	0.001093	-0.1813	-0.33	1.035	-2.995
147	1.263E-17	0.114	0.00001514	1.009E-19	0.01177	0.0008296	0.00001373	0.00001373	-0.3675	-1.094	0.04449	-2.288
148	2.98E-17	0.886	5.975E-06	4.478E-21	0.01316	0.0007127	0.0004693	0.0004693	-0.4335	-0.06752	1.772	-1.37
149	2.074E-17	0.07399	0.0001586	1.103E-19	0.0104	0.0001416	1.896E-06	1.896E-06	-1.135	-0.6771	1.695	-0.07112
150	1.123E-17	1.308	2.338E-06	2.175E-21	0.002873	0.001696	0.001647	0.001647	-0.05688	-0.9656	1.273	-2.295
151	1.128E-17	0.5871	3.077E-06	7.674E-21	0.005167	0.00112	0.0005515	0.0005515	-0.2372	-1.236	0.4919	-2.602
152	1.415E-16	0.3046	0.000238	9.982E-19	0.005457	0.0007453	0.00002793	0.00002793	-0.4141	-3.516	0.6604	0.1586
153	2.224E-17	0.01687	0.00002247	2.198E-19	0.0003841	0.0009735	7.967E-06	7.967E-06	-0.2981	-2.555	0.1749	-2.037
154	1.184E-17	0.2778	3.275E-06	1.026E-20	0.0006439	0.001068	0.0001857	0.0001857	-0.258	-1.511	0.6954	-2.653
155	4.417E-18	0.1416	1.119E-06	6.68E-21	0.0005213	0.0006094	0.0005646	0.0005646	-0.5015	-1.785	0.05995	-3.828
156	1.946E-19	1.092	2.364E-07	2.886E-22	0.0006721	0.0008094	0.006135	0.006135	-0.3782	-0.918	0.5272	-5.17

Table G. part 7: *Continued*

Sequence # (sample #)	MgPO4- activity	Na+ activity	OH- activity	PO4--- activity	SO4-- activity	SiO2(aq) activity	CO2(g) bar	CO2(g) fugacity	Amrph^silica log Q/K	Anhydrite log Q/K	Aragonite log Q/K	Brucite log Q/K
157	2.889E-18	8.231	1.063E-07	6.131E-24	0.0006041	0.001643	0.006596	0.006596	-0.07087	0.5878	1.564	-3.02
158	7.078E-18	0.1269	2.625E-06	1.53E-20	0.000584	0.00124	0.0003484	0.0003484	-0.1929	-1.724	0.6022	-3.242
159	2.093E-19	0.003123	8.952E-08	9.371E-22	0.0006526	0.001329	0.00948	0.00948	-0.163	-1.929	-1.154	-6.493
160	6.131E-18	0.1238	0.00000141	8.706E-21	0.0006797	0.002058	0.0006963	0.0006963	0.02701	-1.683	0.3377	-3.6
161	4.818E-18	0.01297	7.107E-07	9.584E-21	0.0006501	0.001068	0.001481	0.001481	-0.258	-2.208	-0.4373	-4.341
162	8.082E-18	0.1416	2.232E-06	1.224E-20	0.0006269	0.001107	0.0003131	0.0003131	-0.2421	-1.706	0.402	-3.229
163	4.026E-18	1.615	7.383E-07	3.872E-22	0.001148	0.001383	0.001661	0.001661	-0.1456	-0.4351	1.215	-2.993
164	2.799E-17	0.001715	0.00004188	6.525E-19	0.0001158	0.000336	5.657E-07	5.657E-07	-0.7601	-3.511	-0.869	-1.87
165	1.722E-18	3.637	2.367E-07	5.75E-23	0.000944	0.001505	0.004372	0.004372	-0.1088	-0.1101	1.101	-3.521
166	1.566E-17	0.003407	8.355E-06	1.668E-19	0.00003462	0.0007017	0.00003304	0.00003304	-0.4403	-3.76	-0.2273	-2.929
167	9.663E-19	4.401	6.973E-08	9.502E-24	0.0008338	0.0008006	0.008867	0.008867	-0.383	0.1853	0.7166	-4.052
168	3.503E-18	5.443	2.002E-07	1.1E-22	0.001074	0.001839	0.00584	0.00584	-0.02191	-0.05937	1.189	-3.64
169	8.403E-18	0.007602	5.779E-06	1.185E-19	0.0006143	0.0009185	0.00004711	0.00004711	-0.3233	-2.538	-0.4202	-3.371
170	1.244E-17	0.01586	6.049E-06	9.993E-20	0.0008835	0.0008867	0.00005974	0.00005974	-0.3386	-2.305	-0.2026	-3.087
171	1.815E-17	0.03859	7.608E-06	6.989E-20	0.001434	0.001186	0.00007227	0.00007227	-0.2123	-1.717	0.4582	-2.569
172	1.675E-17	0.08576	8.323E-06	6.392E-20	0.002361	0.0008865	0.00006434	0.00006434	-0.3387	-1.592	0.3954	-2.487
173	2.637E-17	0.2441	0.00001249	4.647E-20	0.004051	0.0009767	0.0001095	0.0001095	-0.2966	-1.24	1.099	-1.799
174	1.177E-17	0.5871	3.222E-06	8.01E-21	0.005166	0.001115	0.0005242	0.0005242	-0.2391	-1.236	0.5097	-2.562
175	1.127E-17	1.31	2.338E-06	2.152E-21	0.003131	0.001697	0.001641	0.001641	-0.05669	-0.9282	1.271	-2.289
176	2.557E-17	0.002957	2.051E-06	2.306E-20	0.0003661	0.0006035	0.0003446	0.0003446	-0.5057	-2.589	-0.2821	-3.077
177	2.98E-17	0.886	5.975E-06	4.478E-21	0.01316	0.0007127	0.0004693	0.0004693	-0.4335	-0.06752	1.772	-1.37
178	2.882E-18	8.202	1.064E-07	6.197E-24	0.0006052	0.001642	0.006651	0.006651	-0.0711	0.5836	1.563	-3.025
179	7.412E-20	3.097	0.00009443	4.075E-20	0.009599	0.001613	0.0003801	0.0003801	-0.07866	-3.12	1.214	-2.536
180	7.19E-17	0.1008	0.00002512	2.327E-19	0.0005882	0.0007336	0.0001508	0.0001508	-0.4209	-3.543	0.3768	-1.456
181	9.394E-18	0.2534	3.937E-06	8.274E-21	1.274E-10	0.001134	0.0004276	0.0004276	-0.2317	-7.867	1.565	-2.5
182	1.127E-17	1.31	2.338E-06	2.153E-21	0.003131	0.001697	0.001641	0.001641	-0.0567	-0.9296	1.27	-2.289
183	6.624E-18	0.001898	0.00006338	2.204E-19	0.001071	0.0005965	5.697E-07	5.697E-07	-0.5108	-1.841	0.1977	-1.664
184	8.075E-18	0.2174	2.173E-06	7.948E-21	0.003713	0.001345	0.0003293	0.0003293	-0.1577	-0.693	0.6431	-3.065
185	8.146E-20	1.54	0.00002943	2.987E-20	0.009889	0.001219	0.0006026	0.0006026	-0.2004	-2.706	0.7586	-3.373
186	9.889E-18	0.2833	3.274E-06	9.597E-21	0.005894	0.0006945	0.0003359	0.0003359	-0.4447	-0.5191	0.9831	-2.703
187	1.678E-17	0.5798	2.933E-06	3.98E-21	0.007483	0.0009152	0.0007895	0.0007895	-0.3249	-0.2354	1.446	-2.186
188	4.837E-18	0.4794	0.0006372	2.358E-18	0.000599	0.0001235	6.338E-06	6.338E-06	-1.195	-4.177	1.173	-0.8253
189	8.94E-18	0.3633	0.0003943	1.539E-18	0.002403	0.0002593	0.00001132	0.00001132	-0.8726	-3.065	1.516	-0.7901
190	4.208E-18	0.003634	0.0002004	5.122E-19	0.0003351	0.0003762	4.741E-07	4.741E-07	-0.711	-2.679	0.7846	-1.227
191	4.013E-18	0.1079	0.00001258	9.281E-20	0.0019	0.001228	0.000144	0.000144	-0.1972	-1.771	1.019	-2.91
192	2.309E-18	0.7495	1.928E-06	3.678E-21	0.007519	0.001081	0.001022	0.001022	-0.2526	-0.32	1.11	-3.378
193	1.145E-17	0.1614	0.00001255	4.142E-20	0.009567	0.0005038	0.0001323	0.0001323	-0.5841	-0.5796	1.471	-2.107
194	1.177E-17	6.14	4.317E-07	1.531E-23	0.006644	0.0001557	0.01614	0.01614	-1.094	-0.1086	1.423	-1.59

Table G. part 7: *Continued*

Sequence # (sample #)	MgPO4- activity	Na+ activity	OH- activity	PO4--- activity	SO4-- activity	SiO2(aq) activity	CO2(g) bar	CO2(g) fugacity	Amrph^silica log Q/K	Anhydrite log Q/K	Aragonite log Q/K	Brucite log Q/K
195	4.756E-18	0.2832	6.987E-06	7.577E-21	0.004248	0.0004521	0.000102	0.000102	-0.6311	-0.1299	1.656	-2.26
196	1.366E-18	0.1665	3.961E-07	1.582E-21	0.0006859	0.001361	0.002432	0.002432	-0.1524	-1.137	0.3217	-4.614
197	2.343E-18	1.14	5.208E-07	2.494E-22	0.0009852	0.001204	0.002365	0.002365	-0.2058	-0.08397	1.474	-3.34
199	7.541E-07	0.2419	0.00002031	2.838E-09	0.004661	8.694E-06	0.0007192	0.0007192	-2.347	-2.559	0.9579	-1.706
200	1.092E-16	0.2422	0.00007904	4.703E-19	0.005118	0.00001094	0.00009201	0.00009201	-2.247	-3.395	0.3689	-0.5844
201	7.564E-17	0.2335	0.00004988	3.288E-19	0.004505	4.448E-13	0.0001897	0.0001897	-9.638	-3.001	0.7322	-0.9882
202	5.503E-17	0.225	0.00003963	2.868E-19	0.003354	5.066E-13	0.0002986	0.0002986	-9.582	-3.115	0.7437	-1.267
203	5.039E-07	8.03E-10	0.00003552	1.502E-09	2.396E-10	5.704E-13	0.0003496	0.0003496	-9.53	-10.1	0.8773	-1.119
204	1.451E-07	0.2289	0.00004988	6.52E-10	0.004662	4.446E-13	0.0001933	0.0001933	-9.638	-2.988	0.7393	-1.003
205	2.724E-07	0.2339	0.00005345	1.204E-09	0.004497	8.123E-06	0.0001702	0.0001702	-2.377	-2.966	0.7808	-0.9355
206	3.88E-07	0.2373	0.00007377	1.793E-09	0.004506	0.00001325	0.0001028	0.0001028	-2.164	-3.04	0.7672	-0.6748
207	5.554E-07	0.2399	0.00007548	2.571E-09	0.004539	0.0000415	0.0001005	0.0001005	-1.668	-3.089	0.7246	-0.6557
208	3.962E-07	0.01206	0.00001051	4.096E-10	0.00184	3.351E-06	0.0001672	0.0001672	-2.761	-2.28	0.4311	-1.717
209	1.901E-17	0.1169	0.00001515	1.091E-19	0.0002265	0.0008477	0.00001574	0.00001574	-0.3582	-2.616	0.2978	-2.144
210	3.894E-18	0.2055	1.115E-06	6.28E-21	0.0001268	0.001122	0.0007295	0.0007295	-0.2363	-2.453	0.1154	-3.859
211	4.439E-18	0.221	0.0000014	3.457E-21	0.0001275	0.001463	0.0003475	0.0003475	-0.1211	-1.67	0.7733	-3.345
212	1.559E-17	0.2953	7.005E-06	1.883E-20	0.000085	0.0008056	0.0001229	0.0001229	-0.3803	-2.384	1.183	-2.137
213	6.811E-18	0.384	1.487E-06	3.126E-21	0.00006357	0.0009293	0.000522	0.000522	-0.3183	-2.076	0.9017	-3.063
214	1.505E-17	0.5538	3.086E-06	7.288E-21	0.00006565	0.0009422	0.0004448	0.0004448	-0.3123	-2.487	1.045	-2.452
215	1.052E-17	0.6004	1.841E-06	2.223E-21	0.00005769	0.001241	0.0005904	0.0005904	-0.1925	-2.034	1.232	-2.54
216	3.544E-17	0.8364	5.993E-06	6.247E-21	0.00003536	0.0007086	0.0005544	0.0005544	-0.436	-2.656	1.828	-1.437
217	1.715E-18	3.605	2.369E-07	5.882E-23	0.00002032	0.001502	0.004401	0.004401	-0.1097	-1.779	1.102	-3.532
218	2.853E-18	8.144	1.065E-07	6.267E-24	0.00001665	0.00163	0.006653	0.006653	-0.07426	-0.9772	1.563	-3.033
219	1.859E-18	2.705	2.844E-07	1.228E-22	0.00002422	0.001399	0.003854	0.003854	-0.1407	-2.24	0.6473	-3.658
220	3.256E-18	2.098	6.002E-07	3.55E-22	0.00001458	0.0006969	0.003693	0.003693	-0.4432	-2.541	1.182	-3.227
221	2.356E-18	1.991	4.28E-07	2.876E-22	0.00001947	0.00087	0.003328	0.003328	-0.3469	-2.536	0.7189	-3.57
222	2.061E-18	1.839	3.941E-07	3.032E-22	0.00001925	0.0008045	0.00395	0.00395	-0.3809	-2.653	0.6056	-3.722
223	2.319E-18	1.725	4.561E-07	4.136E-22	0.00001911	0.0007186	0.002988	0.002988	-0.4299	-2.797	0.4677	-3.679
224	2.801E-18	1.811	5.587E-07	5.061E-22	0.00002158	0.0008148	0.003761	0.003761	-0.3754	-2.769	0.7208	-3.508
225	6.229E-17	0.0002226	6.338E-06	6.49E-20	0.00006804	0.0001677	0.0002304	0.0002304	-1.062	-3.205	0.638	-2.16
226	1.622E-17	0.0001339	2.004E-06	2.369E-20	0.00001703	0.00005318	0.0008282	0.0008282	-1.561	-3.433	0.5667	-3.306
227	9.192E-18	0.00008069	1.592E-06	1.983E-20	0.00001149	0.000037	0.001084	0.001084	-1.718	-3.472	0.6155	-3.676
228	2.77E-17	0.0002015	2.004E-06	1.477E-20	0.00000854	0.00003669	0.002308	0.002308	-1.722	-3.832	0.9132	-2.869
229	1.787E-17	0.0009918	1.004E-06	4.108E-21	0.00006138	0.000338	0.01339	0.01339	-0.7574	-3.065	0.9861	-3.104
230	1.315E-07	0.0005652	1.004E-06	4.784E-11	0.0000622	0.0002615	0.01085	0.01085	-0.869	-4.14	-0.1858	-3.303
232	7.92E-07	0.003249	3.996E-06	2.274E-10	0.0001099	0.000526	0.003512	0.003512	-0.5654	-3.706	0.7115	-2.001
234	1.915E-17	0.002113	1.004E-06	3.733E-21	0.00006015	0.0003636	0.01577	0.01577	-0.7258	-12.38	-8.245	-3.033
235	2.14E-18	0.001471	1.263E-07	3.489E-22	0.00003343	0.0002446	0.2195	0.2195	-0.8979	-3.557	0.1726	-4.756

Table G. part 7: *Continued*

Sequence # (sample #)	MgPO4- activity	Na+ activity	OH- activity	PO4--- activity	SO4-- activity	SiO2(aq) activity	CO2(g) bar	CO2(g) fugacity	Amrph^silica log Q/K	Anhydrite log Q/K	Aragonite log Q/K	Brucite log Q/K
236	7.869E-19	0.00002877	6.339E-07	1.667E-20	8.226E-06	0.00002277	0.0003744	0.0003744	-1.929	-4.238	-1.267	-5.468
237	2.657E-17	0.0007311	2.004E-06	1.481E-20	0.00002567	0.00009173	0.002048	0.002048	-1.324	-3.292	0.9231	-2.888
238	2.032E-17	0.0006963	1.592E-06	1.457E-20	0.00003342	0.0001051	0.002155	0.002155	-1.265	-3.292	0.6311	-3.197
239	1.003E-17	0.00002676	7.979E-07	1.002E-20	5.755E-06	0.00002072	0.002311	0.002311	-1.97	-4.566	-0.4492	-3.942
240	1.407E-18	0.0001533	7.98E-07	2.171E-20	0.00002465	0.00004344	0.0003734	0.0003734	-1.648	-3.89	-1.197	-5.13
241	9.181E-10	0.0001537	1.005E-06	1.55E-12	0.00002447	0.00005803	0.001801	0.001801	-1.523	-3.504	0.07545	-3.969
242	3.897E-09	0.0001227	3.177E-06	1.552E-11	0.00002296	0.00004564	0.000148	0.000148	-1.627	-4.125	-0.6025	-3.342
243	8.79E-09	0.0001249	0.00002523	6.624E-11	0.00002516	0.00003344	4.202E-06	4.202E-06	-1.762	-4.714	-0.9783	-1.819
244	9.841E-18	0.0001426	1.004E-06	1.242E-20	0.00006204	0.0001711	0.001719	0.001719	-1.053	-2.963	0.1922	-3.843
245	2.506E-17	0.0005529	1.386E-06	7.366E-21	0.00008712	0.000399	0.007023	0.007023	-0.6854	-3.852	0.04778	-2.931
246	1.818E-17	0.002596	9.576E-07	2.717E-21	0.0000788	0.000586	0.03099	0.03099	-0.5185	-4.676	-0.4091	-2.958
247	6.108E-18	0.002081	3.479E-07	1.327E-21	0.0002544	0.001551	0.05758	0.05758	-0.0959	-2.507	0.6409	-4
248	7.185E-17	0.001859	4.088E-06	1.508E-20	0.00005938	0.001025	0.003261	0.003261	-0.2759	-4.017	0.655	-1.845
249	6.464E-17	0.002464	3.644E-06	1.375E-20	0.00007063	0.001123	0.003753	0.003753	-0.236	-3.972	0.5865	-1.95
250	1.288E-17	0.2223	0.0001254	6.469E-19	0.00002723	0.0000123	0.0002065	0.0002065	-2.196	-5.924	0.8662	-1.25
251	3.634E-17	0.2014	0.0002507	1.471E-18	0.00004026	0.00001803	0.00004783	0.00004783	-2.03	-5.62	0.9649	-0.5549
252	7.353E-07	0.2412	0.0001254	2.01E-07	0.00005835	0.00001138	0.000207	0.000207	-2.23	-5.481	0.9785	-1.986
253	3.658E-06	0.2013	0.0002507	1.478E-07	0.0000325	0.00001625	0.00004783	0.00004783	-2.075	-5.777	0.9015	-0.5541
254	4.014E-06	0.3427	0.0001249	1.767E-07	0.001214	0.00000994	0.0002262	0.0002262	-2.289	-4.305	0.8732	-1.197
255	0.00001147	0.1583	0.0005008	5.349E-07	0.001183	2.519E-06	0.00001066	0.00001066	-2.885	-4.086	0.9793	-0.01534
256	8.839E-06	0.5011	0.0001243	1.473E-06	0.001971	0.00003536	0.0002442	0.0002442	-1.738	-4.148	0.8508	-1.779
257	0.00002656	0.5484	0.0001968	2.739E-06	0.002495	0.0000748	0.00009692	0.00009692	-1.412	-3.896	0.9989	-1.171
258	1.508E-18	0.0008753	2.523E-07	3.857E-21	0.0001428	0.0003486	0.009464	0.009464	-0.744	-2.997	-0.6625	-5.35
259	3.783E-17	0.002433	2.522E-06	2.159E-20	0.00009474	0.000335	0.003817	0.003817	-0.7614	-3.939	0.1787	-2.699
260	1.185E-17	0.005136	7.975E-07	6.386E-21	0.00007389	0.0002793	0.01317	0.01317	-0.8403	-3.415	0.3491	-3.674
261	1.787E-17	0.1295	9.998E-06	1.203E-19	0.00009559	0.0004534	0.003872	0.003872	-0.6299	-5.264	0.05464	-2.574
262	5.469E-18	0.02908	3.995E-06	7.876E-20	0.00008498	0.000264	0.00369	0.00369	-0.8648	-4.465	0.08568	-3.701
263	1.972E-17	0.01392	2.003E-06	2.671E-20	0.00003794	0.0001285	0.006005	0.006005	-1.177	-4.721	-0.209	-3.274
264	3.146E-17	0.06229	6.324E-06	8.363E-20	0.0001245	0.0004891	0.003513	0.003513	-0.597	-4.889	-0.126	-2.569
265	2.875E-17	0.107	0.00003164	3.767E-19	0.00004131	0.0001373	0.0009098	0.0009098	-1.149	-13.15	-7.092	-1.863
266	1.376E-17	0.05331	0.00002519	4.256E-19	0.00005762	0.0001552	0.000676	0.000676	-1.096	-5.735	-0.153	-2.434
267	6.983E-17	0.0574	0.00002518	3.209E-19	0.00005218	0.000154	0.0008443	0.0008443	-1.099	-5.152	0.5694	-1.606
268	1.576E-17	0.06057	5.024E-06	7.64E-20	0.00008395	0.0003195	0.004312	0.004312	-0.7819	-5.319	-0.496	-3.029
269	1.712E-18	0.2791	0.00001249	9.464E-20	0.00006967	0.0005381	0.007959	0.007959	-0.5555	-13.08	-7.116	-3.295
271	1.878E-26	8.042E-10	0.00006311	4.447E-19	1.746E-10	4.048E-13	0.0003052	0.0003052	-9.679	-18.58	-7.024	-10.52
272	3.093E-15	0.4726	0.00004928	1.217E-07	0.000167	0.001077	0.0006468	0.0006468	-0.2542	-12.81	-7.114	-10.96
274	2.829E-15	0.6353	0.00004889	1.258E-07	0.0001445	0.001145	0.0007492	0.0007492	-0.2277	-12.92	-7.109	-11.02
275	4.695E-08	0.6357	0.00003882	9.815E-08	0.0001233	0.001105	0.001099	0.001099	-0.2431	-5.484	0.3664	-3.888

Table G. part 7: *Continued*

Sequence # (sample #)	MgPO4- activity	Na+ activity	OH- activity	PO4--- activity	SO4-- activity	SiO2(aq) activity	CO2(g) bar	CO2(g) fugacity	Amrph^silica log Q/K	Anhydrite log Q/K	Aragonite log Q/K	Brucite log Q/K
278	3.004E-15	0.5653	0.00004906	1.297E-07	0.0001266	0.0009154	0.0007204	0.0007204	-0.3248	-12.97	-7.111	-11
283	1.751E-26	0.2452	0.00007894	5.31E-19	0.0001536	0.0005186	0.0002013	0.0002013	-0.5716	-12.71	-7.083	-10.43
284	5.449E-15	0.2537	0.00006269	1.553E-07	0.0002357	0.0008929	0.0002794	0.0002794	-0.3356	-12.52	-7.142	-10.61
285	1.173E-18	0.2345	0.00006275	4.646E-19	0.0002355	0.0008606	0.0002776	0.0002776	-0.3516	-5.177	0.2028	-2.749
287	2.892E-19	0.09288	0.00003985	5.078E-19	0.0003293	0.000983	0.0004109	0.0004109	-0.2938	-4.35	0.658	-3.79
288	5.733E-19	0.04101	0.00003172	5.663E-19	0.0003702	0.0008847	0.0002868	0.0002868	-0.3396	-4.106	0.4954	-3.738
289	6.485E-19	0.08068	0.00003987	5.357E-19	0.0004319	0.001233	0.0003835	0.0003835	-0.1955	-4.284	0.5758	-3.462
290	7.59E-18	0.0136	0.00001004	1.82E-19	0.0003426	0.0008196	0.000595	0.000595	-0.3728	-2.838	1.114	-3.122
291	6.585E-18	0.01684	0.00001264	2.333E-19	0.0003192	0.0007861	0.0005424	0.0005424	-0.3909	-3.08	1.063	-3.092
292	4.934E-18	0.01013	7.976E-06	1.606E-19	0.0005522	0.001315	0.0005763	0.0005763	-0.1676	-2.684	0.8478	-3.455
293	9.408E-18	0.0175	0.00001591	2.847E-19	0.0003721	0.0008787	0.0004249	0.0004249	-0.3425	-3.078	1.092	-2.823
294	5.511E-18	0.01116	6.336E-06	1.313E-19	0.0003883	0.0009587	0.0008243	0.0008243	-0.3047	-2.87	0.77	-3.519
295	4.924E-18	0.01013	7.976E-06	1.606E-19	0.0005282	0.001256	0.0005895	0.0005895	-0.1875	-2.705	0.8561	-3.456
296	1.668E-17	0.005202	3.176E-06	3.953E-20	0.0001225	0.0003469	0.002001	0.002001	-0.7462	-2.676	1.25	-3.117
297	6.495E-17	0.008991	0.00005033	5.624E-19	0.0001175	0.0001673	0.00006714	0.00006714	-1.063	-3.503	1.367	-1.28
298	3.331E-15	0.3881	0.00006231	1.123E-07	0.00009511	0.0004459	0.0003353	0.0003353	-0.6371	-12.98	-7.128	-10.68
299	7.916E-08	0.002139	2.523E-06	4.82E-10	0.0002649	0.0006226	0.0009618	0.0009618	-0.4922	-2.48	0.5932	-3.727
300	2.094E-17	0.007326	6.336E-06	7.509E-20	0.000199	0.0005249	0.0007551	0.0007551	-0.5664	-2.537	1.355	-2.697
301	1.15E-19	0.0002947	1.265E-07	2.09E-21	0.0002556	0.000515	0.004135	0.004135	-0.5746	-3.028	-1.906	-6.802
302	1.985E-18	0.0004866	7.979E-07	1.852E-20	0.0001691	0.0003613	0.00153	0.00153	-0.7285	-2.863	-0.3934	-4.912
303	5.698E-17	0.4	4.875E-06	3.611E-21	0.00002491	0.0003	0.0006731	0.0006731	-0.8093	-3.26	1.271	-1.172
304	9.203E-17	0.1213	6.305E-06	1.359E-20	0.00003472	0.0002322	0.0004458	0.0004458	-0.9206	-3.445	0.9743	-1.316
306	2.54E-16	0.02236	0.00002516	2.838E-20	0.0000988	0.0005385	0.0001824	0.0001824	-0.5552	-3.2	1.578	0.007315
307	8.233E-17	0.04525	5.025E-06	1.347E-20	0.00000945	0.00006048	0.000716	0.000716	-1.505	-4.078	0.9134	-1.557
308	9.888E-17	0.07136	7.944E-06	3.163E-20	0.00002201	0.0001421	0.006397	0.006397	-1.134	-4.552	1.423	-1.451
309	1.202E-16	0.07034	0.00000796	2.629E-20	0.00006066	0.000313	0.0005349	0.0005349	-0.7908	-3.767	0.6905	-1.284
310	3.518E-17	0.04105	5.024E-06	7.653E-21	0.0000182	0.0001351	0.0005809	0.0005809	-1.156	-2.569	2.047	-1.681
311	1.091E-16	0.01289	7.972E-06	2.106E-20	0.00004684	0.0002431	0.0002456	0.0002456	-0.9006	-3.034	1.199	-1.228
313	1.163E-16	0.01895	7.972E-06	2.911E-20	0.0000665	0.0003022	0.0003259	0.0003259	-0.8061	-3.249	0.9536	-1.341
314	3.052E-17	0.009693	2.003E-06	1.107E-20	0.00005007	0.0002199	0.001138	0.001138	-0.9443	-2.994	0.6759	-2.702
315	2.34E-17	0.008761	2.003E-06	1.061E-20	0.0000142	0.00006751	0.0008378	0.0008378	-1.457	-3.166	0.9177	-2.799
316	3.67E-17	0.01895	3.175E-06	2.727E-20	0.00006512	0.0002203	0.001032	0.001032	-0.9434	-3.134	0.7787	-2.614
317	7.917E-18	0.007786	6.336E-07	5.271E-21	0.0000486	0.0001662	0.002748	0.002748	-1.066	-2.909	0.1565	-3.965
319	6.66E-17	0.003058	5.033E-06	3.592E-20	0.00003977	0.0001375	0.0006543	0.0006543	-1.148	-3.419	0.9103	-2.074
320	5.104E-17	0.001796	3.999E-06	2.962E-20	0.00002749	0.00009615	0.0004948	0.0004948	-1.303	-3.412	0.7561	-2.306
321	3.287E-17	0.009474	5.033E-06	4.901E-20	0.00005137	0.0001525	0.0004904	0.0004904	-1.103	-3.038	1.055	-2.516
322	6.727E-17	0.005956	5.033E-06	5.284E-20	0.00003966	0.0001193	0.0007213	0.0007213	-1.21	-4.651	-0.2785	-2.237
323	5.192E-17	0.001387	3.998E-06	3.027E-20	0.00005033	0.0001634	0.0006473	0.0006473	-1.073	-3.208	0.814	-2.308

Table G. part 7: *Continued*

Sequence # (sample #)	MgPO4- activity	Na+ activity	OH- activity	PO4--- activity	SO4-- activity	SiO2(aq) activity	CO2(g) bar	CO2(g) fugacity	Amrph^silica log Q/K	Anhydrite log Q/K	Aragonite log Q/K	Brucite log Q/K
325	5.451E-17	0.008436	6.336E-06	7.592E-20	0.00002143	0.00006298	0.0007399	0.0007399	-1.487	-3.907	0.9444	-2.286
329	8.375E-17	0.0006071	7.978E-06	5.262E-20	0.00009308	0.0002854	0.0003486	0.0003486	-0.8309	-2.901	1.186	-1.74
330	6.697E-17	0.00186	7.978E-06	6.027E-20	0.00004134	0.0001167	0.0002274	0.0002274	-1.219	-3.183	1.07	-1.896
331	1.743E-17	0.006463	2.523E-06	3.143E-20	0.0001045	0.0002875	0.0008604	0.0008604	-0.8278	-2.741	0.6874	-3.198
332	5.432E-17	0.001459	5.034E-06	4.323E-20	0.0002064	0.0006027	0.0003965	0.0003965	-0.5063	-2.575	0.8211	-2.243
333	7.92E-17	0.003154	6.337E-06	6.355E-20	0.00006042	0.0001673	0.0007084	0.0007084	-1.063	-3.83	0.5521	-2.047
334	4.533E-17	0.003437	5.034E-06	5.276E-20	0.00003847	0.0001039	0.0004284	0.0004284	-1.27	-3.342	0.818	-2.408
335	7.421E-17	0.001688	6.337E-06	7.068E-20	0.0001701	0.00046	0.0006812	0.0006812	-0.6236	-3.364	0.5515	-2.121
336	5.642E-17	0.001253	5.034E-06	5.785E-20	0.00002201	0.00005243	0.0007138	0.0007138	-1.567	-3.975	0.649	-2.353
337	5.329E-17	0.001387	5.034E-06	5.812E-20	0.00003884	0.0001012	0.0006836	0.0006836	-1.281	-3.632	0.7263	-2.38
338	5.522E-18	0.0011	7.979E-07	1.081E-20	0.00006913	0.0001885	0.002651	0.002651	-1.011	-2.791	0.3054	-4.234
340	3.788E-17	0.001053	3.999E-06	5.087E-20	0.00005225	0.0001404	0.0007201	0.0007201	-1.139	-3.382	0.67	-2.67
341	1.455E-17	0.001373	2.523E-06	3.524E-20	0.0001096	0.000281	0.000641	0.000641	-0.8377	-2.708	0.5727	-3.326
342	5.397E-17	0.001083	5.034E-06	6.444E-20	0.00007981	0.0002098	0.0007325	0.0007325	-0.9646	-3.543	0.5332	-2.419
343	1.17E-17	0.0001896	1.592E-06	2.195E-20	0.0001143	0.0002883	0.0008475	0.0008475	-0.8266	-2.667	0.3166	-3.615
345	4.248E-17	0.001128	5.034E-06	6.496E-20	0.00003549	0.00009207	0.0006213	0.0006213	-1.322	-3.55	0.8066	-2.527
346	1.773E-17	0.000553	3.176E-06	4.484E-20	0.00003724	0.00008827	0.0007715	0.0007715	-1.341	-3.233	0.7965	-3.145
347	4.207E-26	9.412E-10	3.999E-06	1.338E-19	0.0002842	0.0005518	0.0006444	0.0006444	-0.5446	-11.34	-8.072	-12.04
348	6.777E-18	0.0007646	1.004E-06	1.676E-20	0.00004455	0.000118	0.002206	0.002206	-1.214	-3.266	0.1419	-4.135
349	2.051E-17	0.000651	3.177E-06	5.321E-20	0.00001985	0.00004273	0.0005709	0.0005709	-1.656	-3.751	0.4211	-3.156
352	5.367E-18	0.0002674	1.265E-06	2.384E-20	0.0001081	0.0002449	0.001319	0.001319	-0.8974	-2.829	0.1704	-4.189
353	4.545E-18	0.0002588	1.265E-06	2.426E-20	0.00006144	0.0001352	0.001277	0.001277	-1.155	-3.044	0.1873	-4.269
356	3.045E-17	0.1085	0.0001	9.616E-19	0.00005189	0.0001005	0.0001438	0.0001438	-1.284	-4.902	1.252	-1.245
357	1.556E-17	0.04602	0.00003992	5.999E-19	3.781E-06	8.336E-06	0.0003272	0.0003272	-2.365	-5.763	1.086	-2.13
358	1.359E-06	0.1902	0.00004994	2.835E-08	7.862E-06	0.00003269	0.0003069	0.0003069	-1.772	-5.842	0.8588	-1.668
359	5.185E-18	0.6137	0.000049	1.752E-19	0.00001325	0.00009321	0.0008586	0.0008586	-1.317	-5.952	0.9606	-1.894
361	1.632E-29	0.0000295	1.265E-08	4.094E-23	0.00001861	0.00002999	0.001848	0.001848	-1.809	-4.62	-4.71	-16.94
368	8.99E-19	0.01696	1.004E-06	2.057E-20	0.0004144	0.001195	0.003754	0.003754	-0.209	-2.759	-0.08898	-5.102
370	2.226E-08	0.002446	6.337E-07	1.36E-10	0.0003033	0.0007582	0.004681	0.004681	-0.4066	-2.37	0.1311	-4.928
371	6.529E-18	0.004423	2.004E-06	3.426E-20	0.0003794	0.0009817	0.002155	0.002155	-0.2944	-2.291	0.7763	-3.862
372	3.466E-09	0.001202	3.177E-07	3.871E-11	0.0002435	0.0005632	0.005426	0.005426	-0.5357	-2.555	-0.4941	-5.79
373	0.00001331	0.2579	0.00003957	2.892E-08	5.652E-06	0.00002793	0.000269	0.000269	-1.84	-5.564	1.023	-0.8883
374	3.254E-08	0.05481	0.00000796	5.178E-11	3.379E-06	0.00001902	0.001068	0.001068	-2.007	-5.387	0.6246	-2.146
375	1.892E-19	0.00082	3.177E-07	7.09E-21	0.0001836	0.0003811	0.003029	0.003029	-0.7054	-2.885	-0.9542	-6.316
376	9.021E-19	0.001717	3.176E-07	5.637E-21	0.0001937	0.0004637	0.003478	0.003478	-0.6202	-2.593	-0.6258	-5.538
377	1.068E-06	0.07756	0.00001587	2.412E-09	0.00001952	0.0000702	0.0007363	0.0007363	-1.44	-4.79	0.898	-1.699
378	1.341E-06	0.0776	0.00001998	3.21E-09	0.00001297	0.00004039	0.0005602	0.0005602	-1.68	-5.026	0.9207	-1.523
381	1.859E-09	0.0004058	3.177E-07	2.908E-11	0.0001533	0.0003144	0.002499	0.002499	-0.7889	-2.958	-1.033	-5.936

Table G. part 7: *Continued*

Sequence # (sample #)	MgPO4- activity	Na+ activity	OH- activity	PO4--- activity	SO4-- activity	SiO2(aq) activity	CO2(g) bar	CO2(g) fugacity	Amrph^silica log Q/K	Anhydrite log Q/K	Aragonite log Q/K	Brucite log Q/K
382	1.908E-08	0.5449	3.888E-07	7.44E-12	9.495E-06	0.0001565	0.005908	0.005908	-1.092	-3.347	0.3475	-4.157
383	3.239E-07	0.2537	0.00006269	1.538E-07	0.0002357	0.0008929	0.0002792	0.0002792	-0.3356	-5.046	0.3355	-2.828
384	0.00000197	0.1223	0.00006306	7.915E-08	0.000173	0.0004715	0.0001858	0.0001858	-0.6129	-4.482	0.8595	-1.75
385	3.198E-10	0.000575	7.979E-08	3.322E-12	0.0002836	0.0005983	0.006017	0.006017	-0.5095	-2.919	-2.079	-6.959
386	2.213E-08	3.892	1.984E-07	1.382E-13	0.00000195	0.0001336	0.005625	0.005625	-1.161	-3.671	0.1981	-2.946
387	1.347E-19	0.3689	4.931E-08	1.1E-22	0.0000561	0.000828	0.03375	0.03375	-0.3684	-2.18	-0.2967	-6.272
388	2.147E-19	0.2096	1.98E-07	7.072E-22	0.00005782	0.0006433	0.005974	0.005974	-0.478	-2.052	0.2699	-5.67
389	2.086E-10	0.03583	3.992E-07	3.908E-13	0.00013	0.0005963	0.003871	0.003871	-0.5109	-2.41	-0.02355	-4.816
390	3.284E-19	0.08065	1.259E-07	6.577E-22	0.00008572	0.0005861	0.01245	0.01245	-0.5184	-2.099	-0.02551	-5.847
392	9.869E-19	8.971E-10	2.523E-07	3.379E-21	5.788E-10	9.962E-13	0.01226	0.01226	-9.288	-7.814	0.02538	-5.477
393	2.557E-18	8.763E-10	2.523E-07	2.769E-21	5.224E-10	9.964E-13	0.01453	0.01453	-9.288	-8.638	-0.6807	-4.977
394	3.66E-19	8.577E-10	7.977E-08	5.542E-22	4.483E-10	9.994E-13	0.03308	0.03308	-9.287	-7.615	-0.234	-6.122
395	7.424E-18	0.0005918	3.176E-06	4.427E-20	0.00007545	0.0001899	0.000667	0.000667	-1.008	-2.753	0.9065	-3.518
396	9.71E-19	5.38	9.626E-08	1.711E-23	2.078E-06	0.0001652	0.001172	0.001172	-1.068	-2.504	0.04221	-4.025
397	3.109E-17	0.001279	5.034E-06	4.887E-20	5.598E-10	9.203E-13	0.0004296	0.0004296	-9.322	-7.925	1.073	-2.539
398	1.038E-16	0.05464	0.00001262	9.204E-20	3.625E-10	8.007E-13	0.0004845	0.0004845	-9.383	-8.799	1.24	-1.491
399	1.349E-16	0.05299	0.00001589	1.211E-19	3.78E-10	7.619E-13	0.000486	0.000486	-9.404	-9.047	1.175	-1.296
400	1.339E-16	0.07344	0.00001002	2.921E-20	2.565E-10	8.223E-13	0.0005351	0.0005351	-9.371	-8.703	1.328	-1.083
401	1.11E-16	0.2683	9.878E-06	9.282E-21	1.749E-10	7.792E-13	0.0006191	0.0006191	-9.395	-9.069	1.186	-0.6789
402	1.125E-16	0.07903	7.951E-06	1.584E-20	2.107E-10	8.447E-13	0.0004325	0.0004325	-9.36	-8.579	1.245	-1.094
403	1.969E-16	0.06466	0.00001586	2.416E-20	2.004E-10	7.232E-13	0.000221	0.000221	-9.427	-9.072	1.083	-0.4338
404	6.511E-17	1.125	5.998E-06	6.658E-21	2.192E-10	8.923E-13	0.001028	0.001028	-9.336	-8.678	1.282	-1.2
405	6.895E-17	0.01617	6.334E-06	2.537E-20	3.371E-10	8.916E-13	0.0002894	0.0002894	-9.336	-7.998	1.249	-1.708
406	1.048E-16	0.1593	0.00000792	1.312E-20	1.888E-10	8.364E-13	0.0003444	0.0003444	-9.364	-8.596	1.175	-1.046
408	6.373E-17	0.01076	3.996E-06	2.131E-20	3.464E-10	9.297E-13	0.001383	0.001383	-9.318	-8.704	0.8101	-2.067
409	1.888E-17	0.008318	2.004E-06	1.794E-20	4.658E-10	9.659E-13	0.00139	0.00139	-9.301	-7.903	0.8853	-3.12
410	1.115E-16	0.1397	9.975E-06	2.251E-20	1.908E-10	8.123E-13	0.0002379	0.0002379	-9.377	-8.572	1.234	-1.053
411	4.894E-17	0.01978	6.334E-06	4.595E-20	4.296E-10	8.955E-13	0.0006369	0.0006369	-9.334	-8.106	1.378	-2.115
412	1.162E-16	0.2458	9.942E-06	2.03E-20	1.905E-10	8.041E-13	0.0003801	0.0003801	-9.381	-8.7	1.309	-0.9933
413	7.088E-17	0.02	0.00000503	1.532E-20	2.705E-10	9.076E-13	0.000346	0.000346	-9.329	-8.12	1.1	-1.677
414	6.882E-17	0.07441	6.322E-06	3.068E-20	3.006E-10	8.862E-13	0.0007572	0.0007572	-9.339	-8.371	1.343	-1.793
415	9.755E-17	0.01376	0.00001591	2.152E-19	5.012E-10	7.76E-13	0.0005181	0.0005181	-9.397	-9.226	0.9017	-1.686
416	5.058E-17	0.4512	0.00000392	7.483E-21	1.726E-10	9.247E-13	0.0009534	0.0009534	-9.32	-8.514	1.132	-1.729
417	6.774E-17	0.02839	7.972E-06	8.738E-20	4.405E-10	8.71E-13	0.001281	0.001281	-9.346	-8.921	1.055	-2.053
418	3.059E-17	0.01107	2.003E-06	1.022E-20	3.388E-10	9.639E-13	0.001292	0.001292	-9.302	-8.109	0.7847	-2.666
419	7.014E-17	0.08773	0.00001588	1.748E-19	3.461E-10	7.555E-13	0.0007361	0.0007361	-9.408	-9.446	0.9939	-1.741
420	1.56E-16	0.167	0.00001584	7.397E-20	2.679E-10	7.392E-13	0.0005832	0.0005832	-9.418	-9.37	1.079	-1.023
421	1.009E-16	0.106	7.939E-06	1.171E-20	1.958E-10	8.348E-13	0.0002286	0.0002286	-9.365	-8.326	1.253	-1.011

Table G. part 7: *Continued*

Sequence # (sample #)	MgPO4- activity	Na+ activity	OH- activity	PO4--- activity	SO4-- activity	SiO2(aq) activity	CO2(g) bar	CO2(g) fugacity	Amrph^silica log Q/K	Anhydrite log Q/K	Aragonite log Q/K	Brucite log Q/K
422	2.95E-17	0.001502	6.338E-06	4.824E-20	5.397E-10	9.012E-13	0.0002972	0.0002972	-9.332	-7.794	1.26	-2.356
423	3.054E-17	0.06505	0.00001589	2.067E-19	3.901E-10	7.615E-13	0.0006017	0.0006017	-9.405	-9.052	1.249	-2.174
424	3.427E-17	0.005858	2.522E-06	1.393E-20	3.664E-10	9.555E-13	0.0009555	0.0009555	-9.306	-8	0.929	-2.551
425	1.72E-16	0.01831	0.00002003	1.899E-19	4.521E-10	7.289E-13	0.0003958	0.0003958	-9.424	-9.48	0.7754	-1.185
426	2.356E-17	0.00163	2.004E-06	2.057E-20	5.14E-10	9.664E-13	0.00127	0.00127	-9.301	-8.16	0.546	-3.083
427	3.837E-17	0.01132	3.997E-06	3.113E-20	4.379E-10	9.326E-13	0.001247	0.001247	-9.317	-8.07	1.297	-2.452
428	1.384E-17	0.002134	2.004E-06	1.999E-20	5.132E-10	9.665E-13	0.0009685	0.0009685	-9.301	-7.766	0.8231	-3.302
429	1.839E-16	0.2378	0.00004996	2.904E-19	2.395E-10	4.561E-13	0.0002908	0.0002908	-9.627	-9.885	1.309	-0.547
430	1.048E-16	0.0728	7.946E-06	1.036E-20	1.888E-10	8.301E-13	0.000139	0.000139	-9.367	-8.462	0.9164	-0.9403
431	7.938E-17	0.1687	6.299E-06	2.119E-20	2.315E-10	8.778E-13	0.0007915	0.0007915	-9.343	-8.619	1.225	-1.574
432	1.555E-16	0.04488	0.0000159	1.075E-19	3.677E-10	7.62E-13	0.0003852	0.0003852	-9.404	-9.169	0.9639	-1.183
433	6.867E-17	0.82	0.00000611	7.406E-21	2.352E-10	8.746E-13	0.0004388	0.0004388	-9.345	-8.663	0.9053	-1.207
434	3.104E-16	0.02067	0.00007971	7.159E-20	2.839E-10	3.801E-13	0.00000736	0.00000736	-9.706	-8.36	1.566	0.6942
435	1.633E-17	0.00138	2.523E-06	2.496E-20	5.246E-10	9.583E-13	0.001002	0.001002	-9.305	-7.78	1.014	-3.126
436	1.565E-17	0.0007726	2.004E-06	2.315E-20	5.551E-10	9.669E-13	0.001015	0.001015	-9.301	-7.893	0.6823	-3.312
437	3.227E-17	0.05513	3.172E-06	2.689E-20	3.856E-10	9.437E-13	0.001608	0.001608	-9.312	-8.375	0.9578	-2.664
439	1.834E-17	0.002139	2.004E-06	2.187E-20	5.28E-10	9.666E-13	0.001301	0.001301	-9.301	-7.977	0.7282	-3.219
440	8.334E-17	0.0315	0.00003994	4.308E-20	3.231E-10	5.579E-13	0.0000043	0.0000043	-9.54	-7.79	1.247	-0.2565
441	6.614E-17	0.02975	3.994E-06	1.411E-20	2.731E-10	9.253E-13	0.0009326	0.0009326	-9.32	-8.572	0.8739	-1.872
442	1.198E-16	0.05712	7.958E-06	1.573E-20	2.115E-10	8.451E-13	0.0004033	0.0004033	-9.359	-8.801	0.9914	-1.063
443	3.9E-17	0.08972	0.00001586	1.632E-19	2.892E-10	7.509E-13	0.0005247	0.0005247	-9.411	-9.462	0.9085	-1.967
444	7.586E-17	0.02412	0.00001003	4.413E-20	3.623E-10	8.386E-13	0.0003958	0.0003958	-9.363	-8.06	1.691	-1.508
445	3.534E-17	0.006464	3.998E-06	3.713E-20	5.055E-10	9.343E-13	0.0005463	0.0005463	-9.316	-8.042	0.9047	-2.564
446	6.78E-17	0.02371	0.00001004	1.337E-19	4.557E-10	8.434E-13	0.001182	0.001182	-9.36	-9.338	0.7891	-2.038
447	8.213E-17	0.00289	6.336E-06	3.485E-20	3.944E-10	8.955E-13	0.0005489	0.0005489	-9.334	-8.288	1.169	-1.77
448	6.656E-17	0.03353	0.00000399	7.7E-21	1.988E-10	9.165E-13	0.0005313	0.0005313	-9.324	-8.571	0.7676	-1.607
449	9.473E-17	0.2815	0.00001254	2.893E-20	2.506E-10	7.698E-13	0.000141	0.000141	-9.4	-8.158	1.502	-1.034
450	3.581E-17	0.02573	0.00001263	1.975E-19	4.559E-10	8.094E-13	0.0008859	0.0008859	-9.378	-9.162	1.04	-2.284
451	6.376E-17	0.03413	5.028E-06	3.409E-20	3.672E-10	9.125E-13	0.0009989	0.0009989	-9.326	-8.626	0.9209	-2.071
452	1.019E-16	0.01238	0.00001004	7.636E-20	4.566E-10	8.454E-13	0.0003142	0.0003142	-9.359	-8.512	1.039	-1.617
453	2.271E-16	0.1723	0.00002507	5.157E-20	2.206E-10	6.26E-13	0.00008909	0.00008909	-9.49	-8.985	1.131	-0.3039
454	3.403E-17	0.1454	3.162E-06	1.619E-20	2.747E-10	9.406E-13	0.001458	0.001458	-9.313	-8.249	1.187	-2.423
455	7.875E-17	0.1034	0.00001002	7.575E-20	3.428E-10	8.305E-13	0.0006495	0.0006495	-9.367	-8.757	1.232	-1.728
456	6.136E-17	0.00975	6.336E-06	5.791E-20	4.778E-10	8.979E-13	0.0007416	0.0007416	-9.333	-8.376	1.128	-2.117
457	2.486E-17	0.009772	2.003E-06	1.087E-20	3.591E-10	9.643E-13	0.000593	0.000593	-9.302	-7.83	0.7011	-2.783
458	7.009E-17	0.0824	0.00000501	9.614E-21	1.864E-10	8.978E-13	0.0003663	0.0003663	-9.333	-8.303	1.101	-1.484
459	6.826E-17	0.02559	3.992E-06	1.008E-20	2.241E-10	9.212E-13	0.00087	0.00087	-9.322	-8.655	0.8465	-1.713
460	4.437E-17	0.9378	3.794E-06	3.661E-21	1.82E-10	9.525E-13	0.001307	0.001307	-9.308	-8.752	0.9947	-1.504

Table G. part 7: *Continued*

Sequence # (sample #)	MgPO4- activity	Na+ activity	OH- activity	PO4--- activity	SO4-- activity	SiO2(aq) activity	CO2(g) bar	CO2(g) fugacity	Amrph^silica log Q/K	Anhydrite log Q/K	Aragonite log Q/K	Brucite log Q/K
461	2.236E-17	0.4949	0.00006233	4.557E-19	1.722E-10	3.702E-13	0.0003647	0.0003647	-9.718	-10.33	1.303	-1.466
462	1.599E-16	0.085	0.00001999	5.901E-20	2.872E-10	7.024E-13	0.00007401	0.00007401	-9.44	-8.451	1.272	-0.7116
473	1.174E-17	0.08564	3.163E-06	1.2E-20	2.378E-10	9.417E-13	0.0007496	0.0007496	-9.312	-7.704	1.506	-2.755
474	9.538E-18	0.09134	3.162E-06	1.117E-20	2.313E-10	9.416E-13	0.0006631	0.0006631	-9.313	-7.653	1.516	-2.814
475	7.467E-18	0.1043	1.994E-06	6.609E-21	2.06E-10	9.655E-13	0.000909	0.000909	-9.302	-7.588	1.368	-3.094
476	9.341E-18	0.08976	2.512E-06	9.626E-21	2.296E-10	9.546E-13	0.001085	0.001085	-9.307	-7.668	1.517	-2.959
477	1.831E-17	0.1259	2.508E-06	9.97E-21	2.091E-10	9.552E-13	0.00098	0.00098	-9.306	-7.974	1.208	-2.683
478	2.578E-17	0.1286	3.974E-06	1.358E-20	2.058E-10	9.25E-13	0.000568	0.000568	-9.32	-7.967	1.384	-2.269
479	2.581E-17	0.1314	3.973E-06	1.341E-20	2.036E-10	9.249E-13	0.0004392	0.0004392	-9.32	-7.969	1.276	-2.263
480	2.541E-17	0.1355	3.972E-06	1.309E-20	2.008E-10	9.249E-13	0.0005631	0.0005631	-9.32	-7.958	1.4	-2.26
481	2.552E-17	0.137	3.972E-06	1.321E-20	2.008E-10	9.249E-13	0.0004954	0.0004954	-9.32	-7.967	1.335	-2.262
482	2.616E-17	0.1331	3.973E-06	1.393E-20	2.05E-10	9.25E-13	0.000441	0.000441	-9.32	-8	1.243	-2.274
483	2.423E-17	0.1283	3.156E-06	1.142E-20	2.038E-10	9.415E-13	0.0005426	0.0005426	-9.313	-8.012	1.124	-2.421
484	2.8E-17	0.12	3.975E-06	1.406E-20	2.11E-10	9.25E-13	0.0004741	0.0004741	-9.32	-8	1.262	-2.248
485	2.842E-17	0.1111	3.977E-06	1.483E-20	2.178E-10	9.252E-13	0.0004298	0.0004298	-9.32	-8.018	1.188	-2.264
486	5.789E-18	0.06485	1.002E-06	5.538E-21	2.666E-10	9.846E-13	0.001826	0.001826	-9.293	-7.692	0.8559	-3.725
487	2.235E-17	0.0157	6.334E-06	4.27E-20	4.426E-10	8.964E-13	0.0002498	0.0002498	-9.334	-7.836	1.228	-2.424
488	2.464E-17	0.01466	7.974E-06	4.818E-20	4.474E-10	8.731E-13	0.0001937	0.0001937	-9.345	-7.828	1.321	-2.234
489	2.232E-18	0.005427	5.034E-07	7.993E-21	5.848E-10	9.919E-13	0.003702	0.003702	-9.29	-8.024	-0.1098	-4.896
490	2.359E-17	0.01467	7.974E-06	4.92E-20	4.493E-10	8.731E-13	0.0002119	0.0002119	-9.345	-7.835	1.352	-2.262
522	2.423E-06	0.002898	2.409E-06	4.074E-09	0.0003513	0.00106	0.001771	0.001771	-0.2612	-2.016	1.16	-3.208
523	7.575E-06	0.1696	0.0004069	3.856E-07	0.00008588	0.00006701	0.00001605	0.00001605	-1.46	-4.146	2.057	-0.2336
524	9.446E-06	0.09223	0.0004474	3.874E-07	0.0001184	0.0000657	9.342E-06	9.342E-06	-1.469	-3.701	2.208	-0.05746
525	0.00001587	0.2167	0.0001899	1.358E-06	0.00009426	0.00001648	0.00007871	0.00007871	-1.069	-3.998	2.194	-1.121
526	8.008E-06	0.9643	0.0002675	2.562E-07	0.00003806	0.00009791	0.0000666	0.0000666	-1.296	-4.416	2.406	-0.3963
527	2.099E-17	0.007546	2.003E-06	2.073E-20	0.0001437	0.0004812	0.004373	0.004373	-0.6041	-2.765	1.031	-3.137
528	5.862E-06	0.007568	2.963E-06	5.86E-09	0.0002994	0.0009814	0.003067	0.003067	-0.2945	-2.525	1.138	-2.802
529	5.712E-06	0.3424	0.00007878	1.159E-07	0.0001154	0.0004894	0.0004923	0.0004923	-0.5967	-4.008	2.129	-1.26
530	3.118E-06	0.4401	0.0001245	1.347E-07	0.0001198	0.0004001	0.0002294	0.0002294	-0.6842	-4.061	2.128	-1.191
531	1.008E-07	0.009042	2.829E-07	7.491E-11	0.000179	0.00071	0.05718	0.05718	-0.4351	-2.613	0.504	-4.714
532	6.013E-18	0.008769	5.148E-07	4.489E-21	0.0001604	0.0006364	0.03159	0.03159	-0.4826	-2.715	0.7121	-4.196
533	4.824E-07	0.009033	5.911E-07	3.399E-10	0.0001712	0.0006702	0.02612	0.02612	-0.4602	-3.033	0.4038	-4.05
534	1.215E-17	0.01169	9.808E-07	8.877E-21	0.00009517	0.0003859	0.01828	0.01828	-0.6999	-3.278	0.6983	-3.626
535	1.449E-06	0.05061	1.177E-06	3.006E-09	0.00009578	0.0004553	0.03465	0.03465	-0.6281	-3.649	0.7616	-3.921
536	2.906E-06	0.5838	0.0001421	2.787E-07	0.00002239	0.00009508	0.0002011	0.0002011	-1.308	-5.623	1.354	-1.422
537	7.052E-07	0.6698	0.00008932	2.181E-07	0.00002412	0.0001644	0.0005074	0.0005074	-1.07	-5.465	1.481	-2.334
538	1.603E-06	0.7226	0.0002095	2.142E-07	0.00002612	0.00008827	0.0001064	0.0001064	-1.341	-5.481	1.492	-1.229
539	1.222E-06	0.5396	0.0002652	1.251E-07	0.00002148	0.00005051	0.00005871	0.00005871	-1.583	-5.541	1.46	-0.9088

Table G. part 7: *Continued*

Sequence # (sample #)	MgPO4- activity	Na+ activity	OH- activity	PO4--- activity	SO4-- activity	SiO2(aq) activity	CO2(g) bar	CO2(g) fugacity	Amrph^silica log Q/K	Anhydrite log Q/K	Aragonite log Q/K	Brucite log Q/K
540	2.225E-17	0.008778	0.00000205	2.136E-20	0.0003012	0.001066	0.006599	0.006599	-0.2587	-2.698	0.9752	-3.105
541	2.529E-17	0.008438	1.744E-06	1.19E-20	0.0001527	0.0006557	0.00832	0.00832	-0.4697	-2.83	1.099	-2.935
542	3.096E-17	0.01872	2.408E-06	2.066E-20	0.00007984	0.0003067	0.0052	0.0052	-0.7997	-3.381	0.9058	-2.807
543	0.00001077	0.3697	0.00006247	8.652E-07	0.0002348	0.001297	0.0007887	0.0007887	-0.1734	-3.656	2.177	-2.059
544	3.462E-06	0.2716	0.00006272	4.758E-07	0.0001682	0.0007776	0.0007214	0.0007214	-0.3956	-3.802	2.139	-2.289
545	7.983E-06	0.4362	0.0001245	2.997E-07	0.0001139	0.0003963	0.0002334	0.0002334	-0.6883	-4.15	2.068	-1.13
546	2.877E-06	0.5897	0.0001327	5.331E-07	0.0001234	0.0004546	0.0002216	0.0002216	-0.6287	-4.212	2.006	-1.768
547	0.00000521	1.263	0.0001592	1.892E-07	0.00005173	0.0003344	0.0001875	0.0001875	-0.7622	-4.351	2.341	-0.902
548	2.794E-06	0.4015	0.00006534	3.245E-07	0.0001271	0.0007246	0.0007592	0.0007592	-0.4263	-4.028	2.095	-2.181
549	8.727E-06	0.211	0.00003007	1.752E-07	0.0001173	0.0006462	0.001948	0.001948	-0.476	-4.068	1.822	-2.092
550	1.509E-06	0.5683	0.0001007	2.019E-07	0.0001149	0.0006147	0.0003936	0.0003936	-0.4977	-4.112	2.147	-1.867
551	1.161E-06	0.9674	0.00009922	2.13E-07	0.00007965	0.0005713	0.0004568	0.0004568	-0.5296	-4.281	2.195	-2.016
552	1.283E-06	0.7913	0.0001777	4.749E-08	0.00004699	0.0002013	0.0001416	0.0001416	-0.9825	-4.623	2.077	-0.8148
553	1.428E-06	0.8053	0.000162	8.861E-08	0.0000475	0.0002193	0.0001692	0.0001692	-0.9454	-4.502	2.19	-1.12
554	4.098E-06	0.8254	0.0001858	1.765E-07	0.00009011	0.0003693	0.0001295	0.0001295	-0.719	-3.997	2.421	-0.8418
555	2.909E-06	0.6038	0.000271	1.075E-06	0.00002996	0.00007058	0.00005925	0.00005925	-1.438	-5.037	1.843	-1.447
556	2.588E-06	0.793	0.0001819	7.337E-07	0.00002963	0.0001137	0.0001341	0.0001341	-1.231	-4.734	2.163	-1.679
557	3.636E-06	0.834	0.00007735	5.864E-07	0.00004325	0.0003511	0.0006901	0.0006901	-0.7409	-4.568	2.134	-2.177
558	3.312E-06	0.4102	0.0003133	1.208E-06	0.00008559	0.0001304	0.00003893	0.00003893	-1.171	-4.253	2.112	-1.316
559	4.041E-06	0.8927	0.0001375	6.965E-07	0.00005291	0.000292	0.0002378	0.0002378	-0.8211	-4.731	1.921	-1.706
560	4.579E-17	0.006966	6.948E-06	1.03E-19	0.00006225	0.0001588	0.0007911	0.0007911	-1.086	-3.598	0.8995	-2.414
561	3.595E-07	1.51	0.0001253	2.695E-07	0.000021	0.0001887	0.0003009	0.0003009	-1.011	-5.493	1.593	-2.425
562	1.901E-06	0.8343	0.0001695	1.123E-06	0.0001103	0.0004624	0.0001539	0.0001539	-0.6214	-4.328	1.997	-2.059
563	3.379E-06	2.594	0.00003431	3.377E-07	0.00004275	0.001441	0.004114	0.004114	-0.1276	-4.566	2.243	-2.675
564	1.8009E-05	5.76102819	5.3199E-05	1.6014E-08	6.6283E-05	0.00179267	8.458E-07	8.458E-07	-0.0329	-2.7044	0.6785	-0.2432
565	2.38E-12	3.276	0.0001575	3.911E-14	0.000014	0.0004175	0.00001221	0.00001221	-0.6658	-3.746	2.374	-0.5669
566	2.813E-17	0.008678	4.284E-06	6.434E-20	0.000122	0.0003313	0.001284	0.001284	-0.7662	-3.153	0.8423	-2.842
567	0.00000366	2.536	0.00005471	2.435E-07	0.00004541	0.001105	0.001622	0.001622	-0.243	-4.602	2.18	-2.093
568	1.479E-06	2.905	0.00006949	3.722E-07	0.00004665	0.000991	0.001114	0.001114	-0.2903	-4.583	2.238	-2.463
569	7.319E-06	0.6722	0.0001385	1.139E-06	0.00008271	0.0003194	0.0002043	0.0002043	-0.7821	-4.416	1.979	-1.655
570	0.00001191	3.436	0.00004166	5.962E-07	0.00008941	0.003174	0.002923	0.002923	0.2153	-3.953	2.573	-2.206
571	0.00000271	2.449	0.00004452	0.00000033	0.00003271	0.0008894	0.002335	0.002335	-0.3373	-4.791	2.112	-2.534
572	1.015E-17	0.004156	1.486E-06	2.535E-20	0.0001081	0.0002781	0.002896	0.002896	-0.8423	-3.126	0.3549	-3.8
573	2.671E-17	0.002357	3.403E-06	3.815E-20	0.0001881	0.0005382	0.001655	0.001655	-0.5555	-2.554	1.163	-2.837
574	5.94E-07	0.377	0.00015	1.538E-07	0.00002285	0.00007183	0.0001715	0.0001715	-1.43	-5.533	1.41	-1.807
575	2.715E-06	0.06127	0.00003898	2.933E-08	0.00002686	0.00007749	0.0006436	0.0006436	-1.397	-5.112	1.159	-1.598
576	3.115E-06	0.02474	8.945E-06	2.982E-08	0.0001142	0.0003367	0.001201	0.001201	-0.7592	-3.604	1.03	-2.824
577	1.493E-17	0.00201	1.419E-06	1.593E-20	0.0001126	0.0003476	0.003138	0.003138	-0.7454	-2.792	0.6656	-3.47

Table G. part 7: *Continued*

Sequence # (sample #)	MgPO4- activity	Na+ activity	OH- activity	PO4--- activity	SO4-- activity	SiO2(aq) activity	CO2(g) bar	CO2(g) fugacity	Amrph^silica log Q/K	Anhydrite log Q/K	Aragonite log Q/K	Brucite log Q/K
578	7.477E-09	0.04589	6.326E-06	1.091E-09	0.00004103	0.0004459	0.0008681	0.0008681	-0.6371	-4.224	0.4143	-4.308
579	5.469E-16	0.8348	0.0002428	2.461E-08	0.0001301	0.0004524	0.00003177	0.00003177	-0.6309	-12.96	-7.08	-9.628
580	3.128E-16	1.009	0.000152	1.498E-08	0.0001641	0.001037	0.00008712	0.00008712	-0.2706	-12.89	-7.073	-10.06
581	3.297E-16	1.442	0.00005923	1.671E-08	2.379E-06	0.002607	0.000625	0.000625	0.1297	-14.76	-7.058	-10.91
582	1.749E-16	1.961	0.0000289	7.742E-09	1.586E-07	0.003406	0.002453	0.002453	0.2458	-15.9	-7.039	-11.47
583	1.704E-16	2.201	0.00002268	7.356E-09	1.691E-07	0.004262	0.004041	0.004041	0.3432	-15.88	-7.031	-11.67
584	1.588E-16	2.687	0.00001759	6.703E-09	1.512E-07	0.008378	0.00691	0.00691	0.6368	-15.94	-7.019	-11.88
585	1.146E-16	3.819	0.00001325	4.695E-09	1.613E-07	0.05897	0.01338	0.01338	1.484	-15.94	-6.987	-12.11
586	1.017E-16	5.68	0.0002228	1.005E-08	0.0005345	0.001213	0.0001019	0.0001019	-0.2025	-12.71	-6.923	-10.04
587	8.925E-17	5.279	0.0002269	8.441E-09	0.0002314	0.001431	0.00009215	0.00009215	-0.1308	-13.05	-6.936	-10.01
588	5.597E-17	6.957	0.0002673	4.288E-09	0.0007158	0.001451	0.00006455	0.00006455	-0.1247	-12.5	-6.857	-9.776
589	4.284E-17	6.756	0.0002698	4.052E-09	0.0003262	0.001126	0.00007235	0.00007235	-0.235	-12.92	-6.88	-9.86
590	9.317E-17	6.979	0.0002662	8.098E-09	0.0009713	0.001663	0.00007176	0.00007176	-0.0656	-12.42	-6.864	-9.835
591	7.331E-17	7.22	0.0002646	5.917E-09	0.0004191	0.001509	0.00006935	0.00006935	-0.1077	-12.75	-6.852	-9.808
592	8.358E-17	7.224	0.0001317	6.628E-09	0.0004609	0.003136	0.0002786	0.0002786	0.21	-12.71	-6.847	-10.41
593	6.064E-17	6.919	0.0002383	4.96E-09	0.00038	0.001593	0.00008518	0.00008518	-0.08418	-12.8	-6.861	-9.904
594	1.181E-16	3.908	0.00002649	9.51E-09	0.0002632	0.004961	0.005584	0.005584	0.4092	-12.93	-6.97	-11.81
595	1.235E-16	4.399	0.0001049	1.319E-08	0.0002035	0.001771	0.0004294	0.0004294	-0.03826	-13.14	-6.983	-10.73
596	1.362E-16	1.831	0.00001639	9.917E-09	0.0002131	0.00389	0.01078	0.01078	0.3036	-12.95	-7.068	-12.18
597	7.131E-17	4.771	0.0002719	7.323E-09	0.0002954	0.00106	0.00006458	0.00006458	-0.2609	-12.97	-6.968	-9.889
598	7.538E-17	7.106	0.0001883	5.712E-09	0.0005212	0.002431	0.0001291	0.0001291	0.09933	-12.63	-6.855	-10.08
599	6.485E-17	5.867	0.0002211	6.537E-09	0.0003546	0.001699	0.0001064	0.0001064	-0.05624	-12.9	-6.916	-10.06
600	9.991E-17	3.387	0.00006891	9.641E-09	0.0002004	0.002179	0.0008551	0.0008551	0.05195	-13.09	-7.015	-11.05
601	5.688E-16	1.832	0.00008711	7.98E-08	0.001217	0.000536	0.0005545	0.0005545	-0.5572	-12.43	-7.15	-11.01
602	2.465E-15	0.1387	0.00007075	7.956E-08	0.002091	0.0007818	0.0002788	0.0002788	-0.3933	-11.62	-7.084	-10.56
603	1.073E-16	1.402	0.00002366	8.027E-09	0.000281	0.002713	0.005175	0.005175	0.1471	-12.82	-7.073	-11.87
604	7.866E-17	1.585	0.00001994	5.522E-09	0.0002228	0.003386	0.007046	0.007046	0.2432	-12.91	-7.067	-11.99
605	1.061E-28	5.515	0.0002812	6.65E-21	0.0004444	0.001561	0.0000467	0.0000467	-0.0929	-12.62	-6.886	-9.645
606	6.964E-17	5.425	0.0002254	6.649E-09	0.0003202	0.001452	0.00009514	0.00009514	-0.1245	-12.92	-6.931	-10.02
607	1.157E-28	6.071	0.0002187	9.978E-21	0.0003837	0.001833	0.0001004	0.0001004	-0.02326	-12.81	-6.89	-10
608	1.458E-28	4.373	0.0001664	1.45E-20	0.0002901	0.001595	0.0001637	0.0001637	-0.08354	-12.96	-6.978	-10.3
609	8.578E-17	4.237	0.0001675	8.413E-09	0.0002989	0.001626	0.0001579	0.0001579	-0.07537	-12.94	-6.986	-10.29
610	1.639E-16	3.702	0.0001213	1.732E-08	0.0002769	0.001838	0.0002964	0.0002964	-0.02216	-13	-7.021	-10.6
611	1.333E-16	2.608	0.00005664	1.364E-08	0.0002076	0.002525	0.001207	0.001207	0.1158	-13.09	-7.058	-11.25
612	8.835E-17	6.204	0.0002437	5.19E-09	0.0005158	0.002095	0.00006117	0.00006117	0.03481	-12.53	-6.861	-9.741
613	4.598E-17	6.444	0.00006056	2.934E-09	0.0005288	0.005055	0.001077	0.001077	0.4173	-12.57	-6.863	-10.99
614	8.925E-17	2.922	0.00002787	8.303E-09	0.0001723	0.002203	0.0049	0.0049	0.05665	-13.14	-7.025	-11.82
615	4.362E-15	0.8515	0.0007697	2.73E-07	0.008031	3.309E-14	0.0000039	0.0000039	-10.77	-11.35	-7.163	-8.77

Table G. part 7: *Continued*

Sequence # (sample #)	MgPO4- activity	Na+ activity	OH- activity	PO4--- activity	SO4-- activity	SiO2(aq) activity	CO2(g) bar	CO2(g) fugacity	Amrph^silica log Q/K	Anhydrite log Q/K	Aragonite log Q/K	Brucite log Q/K
616	1.799E-15	2.397	0.0008968	4.983E-08	0.006682	2.792E-14	1.649E-06	1.649E-06	-10.84	-11.09	-7.035	-8.283
617	3.212E-16	5.773	0.0007856	1.13E-08	0.003265	3.359E-14	3.683E-06	3.683E-06	-10.76	-11.52	-6.857	-8.502
618	4.568E-17	5.255	0.0006247	2.633E-10	0.008736	4.663E-14	7.175E-07	7.175E-07	-10.62	-10.3	-6.974	-7.915
619	3.891E-16	1.542	0.0009309	7.772E-09	0.00641	2.884E-14	8.424E-07	8.424E-07	-10.83	-10.93	-7.128	-8.109
620	1.836E-16	5.356	0.001258	5.113E-09	0.00484	2.152E-14	1.116E-06	1.116E-06	-10.95	-11.24	-6.863	-7.991
621	1.307E-07	0.1071	0.0003165	1.423E-07	0.0001158	0.0004061	0.00001851	0.00001851	-0.6778	-12.97	-7.055	-1.782
622	4.392E-16	0.1205	0.0000251	8.778E-09	0.0003641	0.00123	0.001166	0.001166	-0.1965	-12.14	-7.125	-11.25
623	6.468E-15	0.08649	0.0001587	1.825E-07	0.002056	0.0002002	0.00004975	0.00004975	-0.9849	-3.855	0.6404	-9.795
624	4.086E-08	0.08262	0.00001587	1.428E-08	0.0007336	0.0002301	0.001707	0.001707	-0.9245	-4.127	0.3511	-3.889

Table G. part 8: Aqueous chemistry database of alkaline lake waters compiled from published literature, as well as corresponding results from calculations described in chapters 2 and 3, and investigated in detail in chapter 4.

Sequence # (sample #)	Calcite log Q/K	Carnallite log Q/K	Dolomite log Q/K	Epsomite log Q/K	Gaylussite log Q/K	Gypsum log Q/K	Halite log Q/K	Hydroxyapatite log Q/K	Magnesite log Q/K	Mirabilite log Q/K	Monohydrocalcite log Q/K	Nahcolite log Q/K
1	1.123	-19.36	4.163	-3.332	-3.267	-2.44	-3.827	-20.24	2.282	-3.764	0.2876	-2.846
2	1.044	-19.64	3.919	-3.528	-3.139	-2.55	-3.769	-20.89	2.117	-3.589	0.2084	-2.616
3	1.017	-20.35	3.848	-4.521	-2.314	-3.522	-3.664	-22.56	2.072	-3.684	0.1814	-2.182
4	1.022	-11.78	4.267	-2.634	-3.119	-2.042	-3.4	-21.38	2.487	-3.02	0.1852	-2.621
5	1.496	-10.39	4.59	-4.4	0.8294	-3.073	-1.753	-23.9	2.336	-1.117	0.6375	-1.301
6	1.671	-10.03	4.907	-4.118	0.772	-2.77	-1.831	-23.53	2.478	-1.213	0.8149	-1.01
7	1.483	-9.586	4.752	-4.235	0.9299	-3.057	-1.48	-24.67	2.51	-0.9976	0.6174	-1.326
8	1.483	-9.741	4.515	-4.498	1.325	-3.007	-1.199	-25.16	2.274	-0.5974	0.6008	-1.139
9	0.9411	-12.02	4.159	-3.192	-2.293	-2.649	-3.199	-22.25	2.459	-2.642	0.1039	-2.353
10	1.528	-18.15	4.632	-2.483	-2.116	-1.235	-3.013	-19.54	2.346	-2.227	0.6893	-2.167
11	1.503	-20.3	4.504	-2.879	-3.359	-1.569	-4.346	-18.95	2.242	-3.745	0.6687	-2.809
12	1.514	-19.19	4.357	-2.761	-2.845	-1.279	-3.631	-18.36	2.086	-2.965	0.6777	-2.64
13	1.365	-14.29	3.388	-4.981	-1.833	-2.823	-3.401	-21.53	1.265	-3.201	0.5281	-1.85
14	0.93	-17.13	4.492	-2.138	-1.941	-1.922	-2.443	-22.07	2.804	-1.558	0.08706	-2.435
15	1.186	-12.87	4.26	-4.15	-1.146	-3.214	-3.184	-24.04	2.316	-2.551	0.3475	-1.57
16	1.048	-11.9	3.821	-4.074	-2.251	-2.976	-3.062	-23.19	2.015	-3.144	0.2104	-1.762
17	1.5	-9.106	4.971	-3.571	-1.403	-2.677	-2.111	-20.5	2.712	-2.926	0.6542	-1.867
18	1.452	-15.43	4.092	-3.848	-4.414	-2.232	-4.977	-17.73	1.881	-5.358	0.6178	-3.444
19	0.877	-12.75	3.744	-3.247	-4.07	-2.428	-3.851	-20.63	2.109	-4.064	0.04173	-3.057
20	1.174	-11.42	3.822	-4.64	0.2457	-3.216	-1.989	-26.64	1.89	-1.183	0.3207	-0.8225
21	1.04	-11.25	3.535	-4.357	-0.3559	-2.939	-2.324	-25.38	1.737	-1.224	0.192	-1.373
22	1.128	-12.63	4.176	-3.436	-1.531	-2.532	-3.114	-22.66	2.289	-2.139	0.2903	-1.909
23	1.236	-20.15	4.188	-4.093	-3.455	-3.003	-4.243	-19.87	2.194	-4.739	0.4012	-2.923
24	1.415	-13.91	4.351	-3.453	-2.319	-2.163	-3.925	-20.24	2.177	-3.124	0.58	-2.347
25	1.627	-16.97	2.803	-7.867	-3.275	-4.611	-4.982	10.17	0.4171	-6.95	0.7932	-2.999
26	1.138	-21.06	1.702	-8.012	-4.615	-4.636	-6.594	7.604	-0.1941	-7.334	0.3039	-3.755
27	1.152	-23.03	1.53	-7.36	-5.51	-3.785	-7.402	-17.35	-0.3802	-7.405	0.3181	-4.201
28	1.279	-22.23	1.687	-8.428	-4.975	-4.755	-7.039	12.22	-0.3507	-8.095	0.4454	-4.338
29	1.034	-24.4	1.806	-7.94	-5.763	-4.876	-8.144	-17.27	0.01367	-8.514	0.2001	-4.588
30	1.195	-18.66	1.538	-8.97	-4.03	-5.315	-5.338	-20.13	-0.4148	-7.542	0.361	-3.261
31	1.742	-20.12	2.823	-7.253	-3.58	-3.789	-6.136	15.81	0.3223	-6.661	0.9084	-3.704
32	1.222	-21.53	1.323	-7.282	-5.046	-3.359	-6.691	13.97	-0.6574	-6.656	0.3879	-3.709
33	1.048	-21.58	1.036	-7.666	-5.525	-3.803	-6.812	12.05	-0.7707	-7.232	0.2145	-3.779
34	1.293	-18.58	2.09	-8.021	-3.234	-4.721	-5.219	8.706	0.0383	-6.349	0.4587	-2.913
35	0.9465	-17.59	2.208	-5.419	-4.313	-2.931	-5.325	16.67	0.5034	-4.945	0.1124	-3.375
36	1.072	-23.91	2.197	-7.933	-6.54	-5.184	-8.38	9.991	0.3666	-9.675	0.2388	-5.124

Table G. part 8: *Continued*

Sequence # (sample #)	Calcite log Q/K	Carnallite log Q/K	Dolomite log Q/K	Epsomite log Q/K	Gaylussite log Q/K	Gypsum log Q/K	Halite log Q/K	Hydroxyapatite log Q/K	Magnesite log Q/K	Mirabilite log Q/K	Monohydrocalcite log Q/K	Nahcolite log Q/K
37	1.166	-21.26	1.715	-7.418	-4.582	-3.999	-6.631	13.55	-0.2092	-6.72	0.3319	-3.587
38	1.035	-16.66	1.665	-8.433	-2.869	-5.223	-4.357	12.16	-0.1276	-5.97	0.1999	-2.836
39	1.164	-22.47	1.496	-8.586	-4.842	-4.952	-6.973	10.74	-0.4262	-7.929	0.33	-3.947
40	0.9532	-23.34	1.298	-8.724	-6.311	-5.315	-7.778	-16.09	-0.413	-9.338	0.1195	-5.145
41	1.256	-21.5	1.873	-7.468	-5.078	-4.027	-6.852	10.57	-0.1412	-7.425	0.4226	-3.699
42	1.019	-14.56	2.96	-5.102	-2.287	-3.207	-3.32	-22.32	1.182	-3.349	0.1826	-2.07
43	1.204	-14.37	3.099	-5.296	-2.026	-3.168	-3.192	-21.72	1.137	-3.42	0.3673	-2.015
44	1.379	-14.5	3.655	-5.353	-1.271	-3.434	-3.339	-20.36	1.518	-3.279	0.5419	-2.347
45	1.498	-14.25	3.794	-5.333	-1.069	-3.312	-3.235	-20.18	1.537	-3.195	0.6609	-2.208
46	1.371	-14.34	3.637	-5.422	-1.291	-3.5	-3.298	-20.9	1.507	-3.349	0.5339	-2.171
47	1.445	-14.46	3.693	-5.414	-1.189	-3.399	-3.328	-20.4	1.489	-3.294	0.6082	-2.238
48	1.453	-14.74	3.711	-5.46	-1.276	-3.449	-3.472	-20.36	1.499	-3.446	0.6165	-2.278
49	1.534	-14.88	4.283	-4.093	-2.622	-2.501	-4.231	-18.53	1.99	-4.001	0.6996	-2.806
50	1.898	-15.17	4.639	-4.272	-2.175	-2.309	-4.293	-16.67	1.983	-4.091	1.063	-2.994
51	2.048	-13.61	5.352	-3.263	-1.652	-1.709	-4.02	-17.3	2.545	-3.268	1.213	-2.593
52	2.45	-13.93	5.766	-3.424	-1.526	-1.482	-4.246	-15.64	2.558	-3.718	1.615	-2.732
53	2.07	-14.24	5.336	-3.166	-1.969	-1.554	-4.35	-17.25	2.507	-3.473	1.235	-2.618
54	1.166	-12.67	3.794	-3.039	-2.192	-1.676	-3.026	-21.22	1.87	-2.021	0.3275	-2.021
55	2.26	-14.98	5.204	-3.416	-2.25	-1.294	-4.644	-15.61	2.186	-3.874	1.426	-2.934
56	0.9032	-15.16	3.863	-2.798	-4.953	-2.05	-5.135	-21.45	2.202	-4.618	0.06905	-3.318
57	2.339	-15.22	5.111	-3.754	-0.9882	-1.372	-3.793	-17.71	2.013	-2.853	1.503	-1.738
58	1.3	-9.581	4.523	-2.851	-0.8666	-1.904	-2.184	-22.4	2.465	-1.218	0.4524	-1.578
59	1.693	-15.3	4.973	-3.551	-2.374	-2.331	-4.739	-18.81	2.521	-3.901	0.8589	-2.818
60	1.156	-11.63	3.978	-2.819	-0.9321	-1.616	-2.506	-23.35	2.064	-0.7068	0.3083	-1.409
61	2.709	-12	6.085	-2.997	-0.1716	-0.8419	-3.216	-15.32	2.618	-2.251	1.871	-2.156
62	2.634	-12.77	5.604	-2.826	-1.112	-0.3456	-3.334	-14.29	2.212	-2.541	1.797	-2.507
63	1.312	-14.59	3.816	-3.976	-3.128	-2.361	-4.134	-19.92	1.746	-3.923	0.4768	-2.536
64	2.423	-12.01	6.073	-2.887	-0.3134	-1.288	-3.132	-18.43	2.892	-2.269	1.585	-1.468
65	2.745	-8.795	6.988	-2.545	1.467	-1.104	-1.6	-20.2	3.485	-1.016	1.883	-0.4036
66	-1.906	-23.25	-3.546	-5.456	-13.42	-2.92	-8.339	-26.24	-2.399	-8.331	-2.74	-5.75
67	-1.823	-20.7	-3.729	-5.174	-13.15	-2.289	-7.296	-25.81	-2.665	-7.603	-2.656	-5.583
68	-1.238	-21.61	-2.888	-5.187	-12.1	-1.974	-7.669	-23.47	-2.408	-7.407	-2.072	-5.425
69	-0.4509	-20.07	-1.052	-5.053	-9.258	-2.101	-6.655	-21.12	-1.359	-6.264	-1.285	-4.66
70	0.8845	-20.38	2.032	-4.519	-4.731	-1.979	-6.251	-17.49	0.3889	-4.286	0.05053	-3.908
71	-1.15	-20.37	-2.309	-4.602	-11.94	-1.791	-7.276	-23.96	-1.918	-7.236	-1.983	-5.218
72	-1.039	-19.37	-1.701	-4.048	-11.06	-1.623	-6.732	-23.59	-1.42	-6.414	-1.872	-4.924
73	-0.8948	-19.12	-1.16	-3.764	-10.36	-1.592	-6.717	-24.23	-1.023	-5.966	-1.729	-4.519
74	-0.6359	-17.86	-1.271	-4.055	-10.04	-1.253	-6.081	-22.35	-1.393	-5.827	-1.47	-4.545

Table G. part 8: *Continued*

Sequence # (sample #)	Calcite log Q/K	Carnallite log Q/K	Dolomite log Q/K	Epsomite log Q/K	Gaylussite log Q/K	Gypsum log Q/K	Halite log Q/K	Hydroxyapatite log Q/K	Magnesite log Q/K	Mirabilite log Q/K	Monohydrocalcite log Q/K	Nahcolite log Q/K
75	1.309	-16.52	2.129	-4.865	-3.03	-1.569	-4.395	-18.35	0.06187	-3.027	0.4737	-2.757
76	1.051	-13.56	2.274	-5.102	-1.035	-2.432	-2.798	-23.4	0.4647	-1.401	0.2095	-1.594
77	1.069	-13.1	2.361	-5.112	-0.533	-2.471	-2.469	-23.81	0.5338	-0.9872	0.2232	-1.474
78	-6.859	-19.05	-13.45	-13.57	-7.441	-10.83	-1.34	-67.1	-7.346	-0.4865	-7.734	-0.5645
79	-6.849	-18.92	-13.42	-13.56	-7.354	-10.82	-1.257	-67.3	-7.326	-0.4168	-7.728	-0.5085
80	1.388	-16.73	3.497	-5.534	-2.558	-3.449	-4.826	-17.78	1.35	-4.593	0.5541	-3.19
81	0.5708	-14.68	0.7604	-4.932	-4.628	-1.74	-3.934	-23.04	-0.5687	-3.322	-0.2646	-2.24
82	1.024	-11.67	2.237	-6.136	0.5392	-3.341	-1.439	-28.02	0.4543	-0.7658	0.1539	-0.5493
83	1.298	-11.82	2.612	-5.765	1.067	-2.736	-1.42	-26.45	0.556	-0.2169	0.4151	-0.5711
84	1.497	-11.41	2.85	-5.369	1.08	-2.147	-1.279	-25.11	0.5953	-0.03377	0.6078	-0.4735
85	1.647	-8.942	3.225	-6.025	1.823	-2.411	-0.04121	-27.36	0.8195	-0.1353	0.6649	0.09448
86	-0.3165	-20.95	-0.04745	-6.289	-9.291	-4.073	-7.367	-20.77	-0.4893	-8.537	-1.15	-5.048
87	0.8515	-17.65	1.873	-5.735	-4.467	-3.101	-5.308	-19.57	0.263	-5.079	0.01751	-3.341
88	0.7344	-19.9	0.9229	-6.57	-5.58	-3.222	-6.116	-18.61	-0.5699	-6.078	-0.09935	-3.976
89	0.4528	-20.36	1.22	-6.086	-7.992	-3.598	-7.168	-18.35	0.008722	-8.303	-0.3809	-4.626
90	0.9872	-21.07	1.247	-6.187	-6.67	-2.657	-6.83	-16.3	-0.4985	-7.108	0.1535	-4.423
91	1.643	-15.07	4.66	-4.354	-1.847	-2.92	-4.522	-19.09	2.259	-3.864	0.8081	-2.488
92	1.077	-17.14	1.971	-6.036	-2.605	-3.044	-4.441	-20.35	0.1351	-3.614	0.2424	-2.613
93	0.3483	-24.29	0.2023	-6.806	-8.897	-3.51	-8.236	-18.21	-0.9043	-8.91	-0.4853	-4.898
94	0.9691	-25.21	1.584	-6.829	-8.604	-3.673	-9.19	-17.43	-0.1433	-10.02	0.1355	-5.072
95	1.262	-20.02	2.53	-6.431	-6.944	-3.635	-7.149	-16.07	0.5097	-8.911	0.4285	-4.456
96	-0.5688	-21.96	-0.9346	-5.679	-11.15	-3.081	-8.109	-21.71	-1.124	-8.903	-1.402	-5.384
97	0.04378	-20.06	0.3526	-5.5	-9.211	-2.963	-7.304	-21.06	-0.4495	-8.069	-0.7899	-4.504
98	-0.6051	-23.04	-1.201	-5.76	-13.41	-2.969	-9.323	-22.09	-1.354	-10.98	-1.439	-6.366
99	-0.0986	-18.98	0.8645	-10.01	-8.318	-8.274	-6.682	-22.31	0.2048	-12.2	-0.9324	-4.046
100	0.8882	-20.96	2.047	-6.23	-8.415	-3.699	-7.836	-18.21	0.4009	-9.697	0.05449	-4.667
101	-0.3137	-22.74	-0.6402	-5.023	-11.15	-2.209	-8.553	-20.46	-1.085	-8.533	-1.147	-5.667
102	0.03061	-23.43	0.02221	-6.423	-9.509	-3.583	-8.257	-19.82	-0.7667	-8.959	-0.803	-4.872
103	-0.8067	-23.51	-1.751	-6.807	-11.26	-3.868	-8.292	-23.58	-1.702	-9.326	-1.64	-4.955
104	-0.6534	-22.52	-1.405	-6.419	-11.19	-3.52	-8.08	-22.81	-1.51	-9.209	-1.487	-5.045
105	1.541	-18.31	2.964	-5.39	-3.426	-2.469	-5.44	-16.39	0.6647	-4.785	0.707	-3.386
106	-0.8232	-23.85	-1.688	-10.67	-13.04	-7.83	-9.148	-22.42	-1.623	-15.03	-1.657	-6.055
107	-1.002	-23.48	-2.026	-10.61	-13.01	-7.791	-8.93	-23.26	-1.782	-14.6	-1.836	-5.865
108	1.297	-18.81	2.887	-5.132	-4.116	-2.621	-5.717	-18.03	0.8311	-5.139	0.4633	-3.218
109	-1.019	-23.93	-2.03	-10.75	-12.85	-7.956	-8.923	-23.57	-1.77	-14.57	-1.852	-5.787
110	1.207	-18.64	2.59	-5.358	-3.962	-2.732	-5.64	-17.36	0.6254	-4.915	0.3726	-3.525
111	0.5884	-20.37	1.377	-5.23	-7.305	-2.628	-6.937	-19.13	0.03021	-6.917	-0.2453	-3.983
115	-7.508	-31.35	-14.88	-13.88	-13.01	-11.21	-4.843	-60.53	-8.131	-5.007	-8.342	-3.263

Table G. part 8: *Continued*

Sequence # (sample #)	Calcite log Q/K	Carnallite log Q/K	Dolomite log Q/K	Epsomite log Q/K	Gaylussite log Q/K	Gypsum log Q/K	Halite log Q/K	Hydroxyapatite log Q/K	Magnesite log Q/K	Mirabilite log Q/K	Monohydrocalcite log Q/K	Nahcolite log Q/K
116	0.8141	-16.85	2.638	-4.926	-3.225	-3.127	-3.859	-20.56	1.065	-3.791	-0.02106	-2.736
117	-0.9652	-22.22	-0.5154	-5.25	-7.439	-3.86	-4.708	-28.4	-0.3084	-5.177	-1.799	-2.896
118	1.866	-22.33	-4.976	-13.7	-1.307	-2.168	-3.086	-17.49	-7.6	-3.025	1.028	-2.232
119	-7.138	-15.24	-5.256	-4.844	-10.27	-11.04	-3.132	-62.23	1.123	-2.856	-7.975	-2.065
120	0.8219	-21.34	2.411	-5.159	-3.31	-3.118	-3.888	-20.07	0.8312	-3.883	-0.01319	-2.887
121	0.8048	-21.4	2.375	-5.13	-3.431	-3.088	-3.952	-20.31	0.8123	-3.939	-0.03022	-2.857
125	0.07628	-18.77	0.4092	-5.477	-8.086	-2.932	-5.962	-21.68	-0.4254	-6.978	-0.7575	-3.788
126	0.08345	-17.22	0.541	-5.238	-6.065	-2.806	-4.297	-23.02	-0.3008	-4.847	-0.7511	-2.766
127	0.6256	-18.92	1.943	-5.222	-5.088	-3.109	-5.115	-21.12	0.5591	-5.257	-0.2086	-2.804
128	0.8074	-17.82	2.626	-5.239	-5.052	-3.445	-4.827	-20.28	1.06	-5.921	-0.02679	-2.975
129	-8.253	-19.27	-6.556	-4.278	-16.08	-11.43	-6.298	-63.31	0.9388	-6.809	-9.087	-4.266
130	-0.1446	-23.51	0.9763	-4.574	-8.628	-3.037	-6.314	-22.3	0.3625	-7.183	-0.9784	-4.291
131	0.07369	-19.51	1.415	-4.793	-8.827	-3.258	-6.809	-22.35	0.5827	-8.039	-0.7601	-4.352
132	-0.6021	-19.59	-0.02467	-4.26	-10.09	-2.638	-6.728	-23.54	-0.1808	-7.328	-1.436	-4.667
133	-0.3525	-19.36	0.5683	-4.692	-8.945	-3.163	-6.35	-22.46	0.1625	-7.21	-1.186	-4.459
134	-0.7482	-25.24	-1.087	-5.112	-9.975	-2.72	-6.685	-24.08	-1.097	-7.005	-1.582	-4.363
135	1.093	-18.67	2.698	-3.131	-5.233	-0.8385	-5.237	-17.74	0.8462	-4.066	0.2593	-3.407
136	0.5793	-19.4	1.403	-4.807	-6.256	-2.249	-5.566	-20.41	0.0658	-5.472	-0.2546	-3.326
137	-0.08892	-19.86	-0.07104	-5.496	-9.095	-2.801	-6.471	-20.69	-0.7404	-7.525	-0.9226	-4.437
138	0.3794	-18.38	0.9975	-5.598	-6.115	-3.033	-4.957	-21.52	-0.1401	-5.714	-0.4548	-3.035
139	1.124	-9.369	2.323	-2.734	-3.905	0.04359	-2.344	-16.23	0.4401	-1.947	0.2806	-2.94
140	1.003	-10.35	1.739	-3.091	-4.723	0.008205	-2.78	-15.54	-0.02302	-2.545	0.1637	-3.381
141	1.173	-11.84	2.778	-3.057	-4.027	-0.6729	-3.306	-16.26	0.8469	-2.86	0.3359	-3.238
142	1.211	-9.267	2.918	-2.406	-2.956	-0.03396	-2.148	-17.29	0.9488	-1.259	0.3641	-2.557
143	1.385	-10.58	2.853	-3.147	-3.155	-0.3957	-2.66	-15.43	0.7099	-2.147	0.5447	-3.017
144	1.254	-10.14	2.644	-3.014	-3.531	-0.3141	-2.652	-16.24	0.6319	-2.181	0.4138	-2.911
145	0.5254	-11.08	1.249	-3.381	-4.941	-0.7552	-2.95	-18.04	-0.03451	-2.567	-0.3128	-3.224
146	1.306	-8.133	2.926	-2.717	-3.306	-0.1453	-1.896	-16.82	0.8621	-1.921	0.4551	-2.548
147	0.3157	-14.35	0.7267	-3.594	-5.299	-0.8787	-3.866	-16.88	-0.3473	-2.621	-0.5198	-4.03
148	2.043	-7.187	4.93	-1.986	-1.159	0.09998	-1.677	-16.46	2.129	-1.029	1.184	-2.009
149	1.966	-13.39	3.734	-3.47	-2.842	-0.4617	-4.105	-13.4	1.01	-3.048	1.131	-4.057
150	1.544	-7.208	4.058	-2.81	-1.619	-0.8131	-1.309	-18.99	1.756	-1.426	0.6771	-1.703
151	0.7631	-9.109	2.476	-2.965	-3.255	-1.045	-2.051	-19.85	0.9545	-1.674	-0.0843	-2.406
152	0.9316	-12.39	4.102	-3.899	-1.142	-3.309	-3.162	-23.15	2.412	-2.137	0.0926	-2.098
153	0.4461	-16.29	0.87	-5.162	-6.715	-2.337	-5.113	-15.57	-0.3344	-5.751	-0.3878	-4.925
154	0.9666	-10.15	2.149	-3.925	-4.092	-1.306	-2.606	-16.3	0.4238	-3.158	0.1262	-3.177
155	0.3312	-11.54	0.8177	-4.234	-5.749	-1.572	-3.197	-18.24	-0.2717	-3.8	-0.5057	-3.453
156	0.7984	-8.216	1.004	-4.292	-3.922	-0.756	-1.431	-19.22	-0.5524	-2.167	-0.06359	-2.205

Table G. part 8: *Continued*

Sequence # (sample #)	Calcite log Q/K	Carnallite log Q/K	Dolomite log Q/K	Epsomite log Q/K	Gaylussite log Q/K	Gypsum log Q/K	Halite log Q/K	Hydroxyapatite log Q/K	Magnesite log Q/K	Mirabilite log Q/K	Monohydrocalcite log Q/K	Nahcolite log Q/K
157	1.835	-2.856	4.37	-2.524	-2.383	0.4554	0.369	-16.83	1.777	-1.93	0.8256	-1.643
158	0.8734	-11.8	1.736	-4.338	-4.769	-1.511	-3.289	-16.73	0.104	-3.842	0.03684	-3.34
159	-0.8829	-18.95	-1.839	-4.586	-11.23	-1.711	-6.714	-23.11	-1.715	-6.984	-1.717	-4.981
160	0.6089	-11.82	1.414	-4.089	-5.294	-1.47	-3.327	-17.86	0.04718	-3.797	-0.2275	-3.32
161	-0.1661	-15.75	0.2232	-4.237	-8.286	-1.989	-5.294	-20.56	-0.369	-5.751	-1	-4.27
162	0.6732	-11.45	1.503	-4.155	-5.063	-1.494	-3.186	-17.16	0.07159	-3.721	-0.1637	-3.409
163	1.486	-6.432	3.317	-2.979	-2.534	-0.3039	-1.065	-17.1	1.073	-1.748	0.6086	-2.108
164	-0.5978	-20.64	-1.155	-6.053	-10.35	-3.292	-7.111	-16.06	-1.316	-8.255	-1.431	-6.796
165	1.372	-5.127	3.139	-2.913	-2.687	-0.06701	-0.3889	-18.02	1.009	-1.569	0.4507	-1.829
166	0.04387	-18.74	0.1933	-6.238	-8.747	-3.542	-6.446	-17.16	-0.6089	-8.183	-0.7898	-5.431
167	0.9878	-4.158	2.552	-2.581	-3.743	0.1869	-0.1838	-19.15	0.806	-1.664	0.04569	-1.97
168	1.46	-2.906	3.347	-3.618	-2.719	-0.2414	0.2903	-17.28	1.129	-2.288	0.4261	-1.601
169	-0.149	-18.08	-0.2874	-5.111	-8.409	-2.319	-5.917	-17.9	-0.8967	-6.238	-0.9828	-5.089
170	0.06864	-16.45	0.3176	-4.71	-7.41	-2.087	-5.235	-17.73	-0.5094	-5.442	-0.7653	-4.646
171	0.7294	-14.63	1.58	-4.183	-5.698	-1.499	-4.432	-16.2	0.09212	-4.465	-0.105	-4.078
172	0.6666	-13.17	1.55	-3.97	-5.043	-1.376	-3.732	-16.74	0.1246	-3.564	-0.1687	-3.743
173	1.37	-10.99	3.176	-3.425	-2.862	-1.032	-2.816	-16.39	1.047	-2.457	0.5314	-2.881
174	0.7809	-9.109	2.512	-2.966	-3.22	-1.045	-2.051	-19.78	0.9723	-1.674	-0.06653	-2.408
175	1.543	-7.205	4.061	-2.767	-1.621	-0.7758	-1.31	-19	1.761	-1.388	0.6757	-1.703
176	-0.01087	-18.8	1.009	-4.141	-9.127	-2.37	-6.962	-19.61	0.2615	-7.282	-0.8446	-5.084
177	2.043	-7.187	4.93	-1.986	-1.159	0.09998	-1.677	-16.46	2.129	-1.029	1.184	-2.009
178	1.834	-2.863	4.367	-2.526	-2.381	0.4521	0.3664	-16.84	1.775	-1.929	0.8251	-1.641
179	1.485	-9.609	3.166	-6.045	1.471	-3.055	-0.8198	-26.96	0.9224	-0.591	0.5746	-0.3585
180	0.648	-12.93	2.932	-4.503	-3.593	-3.329	-3.622	-21.32	1.526	-4.03	-0.1876	-2.823
181	1.837	-9.95	3.534	-10.64	-2.78	-7.662	-2.628	-14.76	0.9388	-9.942	0.9961	-2.775
182	1.541	-7.205	4.06	-2.767	-1.623	-0.7772	-1.31	-19.01	1.761	-1.388	0.6744	-1.703
183	0.4689	-21.36	0.1202	-5.242	-8.834	-1.623	-7.546	-13.78	-1.107	-7.201	-0.3648	-6.569
184	0.9143	-11.08	1.932	-3.208	-4.458	-0.4843	-2.867	-16.53	0.259	-2.592	0.07563	-3.213
185	1.03	-11.1	2.03	-5.55	-0.228	-2.554	-1.373	-25.87	0.2421	-0.7475	0.1631	-0.9681
186	1.254	-10.14	2.644	-3.014	-3.531	-0.3141	-2.652	-16.24	0.6319	-2.181	0.4138	-2.911
187	1.718	-8.772	4.003	-2.353	-2.201	-0.04602	-2.027	-16.53	1.527	-1.533	0.8693	-2.277
188	1.444	-14.11	2.988	-6.713	-0.0333	-3.974	-2.801	-20.1	0.7858	-2.725	0.6026	-2.118
189	1.787	-13.49	3.616	-5.648	-0.09039	-2.858	-2.913	-18.32	1.071	-2.347	0.9471	-2.195
190	1.056	-24.03	1.064	-6.31	-6.762	-2.461	-7.327	-13.84	-0.75	-7.141	0.2222	-5.866
191	1.29	-13.55	2.1	-4.85	-3.513	-1.557	-3.531	-16.5	0.05157	-3.464	0.4546	-3.114
192	1.381	-9.642	2.589	-3.194	-2.576	-0.1351	-1.881	-17.25	0.4499	-1.331	0.5302	-2.235
193	1.742	-12.11	3.32	-3.35	-2.755	-0.3675	-3.318	-15.1	0.8192	-2.424	0.9052	-2.977
194	1.694	-2.297	6.039	-1.209	-1.137	-0.2235	0.2047	-23.72	3.587	-1.056	0.694	-0.7734

Table G. part 8: *Continued*

Sequence # (sample #)	Calcite log Q/K	Carnallite log Q/K	Dolomite log Q/K	Epsomite log Q/K	Gaylussite log Q/K	Gypsum log Q/K	Halite log Q/K	Hydroxyapatite log Q/K	Magnesite log Q/K	Mirabilite log Q/K	Monohydrocalcite log Q/K	Nahcolite log Q/K
195	1.927	-10.07	3.243	-3.377	-2.721	0.07352	-2.576	-13.56	0.558	-2.331	1.086	-3.1
196	0.5929	-11.17	0.9287	-4.006	-5.618	-0.9267	-3.005	-17.92	-0.4225	-3.55	-0.2449	-3.199
197	1.746	-6.901	3.375	-3.03	-2.693	0.06423	-1.278	-15.73	0.8709	-2.032	0.8766	-2.257
199	1.229	-12.52	3.944	-3.686	-1.767	-2.349	-3.117	9.274	1.957	-2.394	0.3912	-1.856
200	0.6401	-12.63	3.583	-3.703	-2.067	-3.184	-3.138	-23.86	2.185	-2.351	-0.1976	-2.159
201	1.003	-12.5	3.857	-3.762	-1.821	-2.791	-3.154	-22.28	2.095	-2.437	0.1657	-2.06
202	1.015	-12.69	3.787	-3.968	-1.843	-2.904	-3.172	-22.48	2.014	-2.596	0.1774	-1.979
203	1.148	-12.29	4.134	-10.85	-18.62	-9.883	-11.62	7.438	2.227	-26.61	0.3134	-10.41
204	1.01	-12.56	3.858	-3.761	-1.823	-2.777	-3.154	5.607	2.089	-2.439	0.1728	-2.061
205	1.052	-12.62	3.911	-3.77	-1.758	-2.756	-3.151	6.621	2.101	-2.436	0.2143	-2.077
206	1.038	-12.61	3.939	-3.789	-1.698	-2.83	-3.137	6.906	2.143	-2.423	0.2007	-2.149
207	0.9958	-12.59	3.906	-3.787	-1.722	-2.879	-3.128	7.123	2.152	-2.411	0.158	-2.145
208	0.7023	-22.72	2.769	-3.5	-6.088	-2.062	-5.712	9.881	1.308	-5.362	-0.1315	-4.078
209	0.569	-14.02	1.183	-5.165	-4.963	-2.4	-3.801	-15.81	-0.1442	-4.313	-0.2663	-3.96
210	0.3866	-10.99	0.9553	-4.885	-5.266	-2.243	-2.932	-18.59	-0.1896	-4.103	-0.4516	-3.181
211	1.045	-10.29	1.806	-4.576	-4.675	-1.462	-2.766	-15.37	0.003165	-4.051	0.2051	-3.373
212	1.454	-10.45	2.972	-4.948	-3.07	-2.178	-2.63	-15.15	0.7602	-3.982	0.6139	-3
213	1.173	-9.292	2.397	-4.676	-3.854	-1.877	-2.329	-15.99	0.4657	-3.912	0.3295	-2.93
214	1.316	-9.084	3.084	-4.705	-2.839	-2.293	-2.114	-16.69	1.01	-3.608	0.47	-2.524
215	1.504	-8.108	3.311	-4.431	-2.924	-1.849	-1.889	-15.92	1.049	-3.637	0.6531	-2.59
216	2.099	-7.085	4.99	-4.617	-1.073	-2.486	-1.643	-16.11	2.133	-3.637	1.241	-1.961
217	1.373	-5.13	3.132	-4.589	-2.688	-1.736	-0.3896	-18.01	1	-3.239	0.4522	-1.83
218	1.834	-2.868	4.359	-4.091	-2.383	-1.108	0.364	-16.83	1.766	-3.489	0.826	-1.643
219	0.9185	-5.618	2.474	-4.661	-3.214	-2.157	-0.6436	-19.65	0.7976	-3.218	0.01688	-1.933
220	1.453	-6.157	3.407	-4.999	-2.212	-2.43	-0.8692	-18.35	1.196	-3.516	0.5659	-1.737
221	0.9901	-6.32	2.553	-4.9	-3.047	-2.419	-0.9219	-19.37	0.8044	-3.404	0.106	-1.952
222	0.8768	-6.531	2.357	-4.957	-3.21	-2.527	-0.9978	-19.9	0.7221	-3.437	-0.003215	-1.948
223	0.7389	-6.744	2.138	-5.02	-3.384	-2.664	-1.067	-20.13	0.6405	-3.461	-0.1377	-2.033
224	0.992	-6.684	2.663	-4.985	-2.82	-2.64	-1.03	-19.91	0.9131	-3.385	0.1136	-1.824
225	0.9092	-23.12	2.672	-4.934	-9.648	-2.986	-9.222	-17.2	1.004	-10.26	0.07554	-5.893
226	0.8379	-24.63	2.009	-5.683	-10.6	-3.215	-10.01	-17.15	0.4131	-11.3	0.004296	-6.058
227	0.8867	-24.16	1.805	-6.023	-11.08	-3.253	-10	-16.82	0.1604	-11.91	0.05305	-6.261
228	1.184	-24.42	3.239	-5.545	-9.459	-3.613	-10.02	-18.26	1.296	-11.25	0.3506	-5.435
229	1.257	-23.33	3.84	-4.325	-7.84	-2.847	-9.171	-20.68	1.824	-9.009	0.4233	-4.28
230	0.08535	-23.25	2.378	-4.518	-9.591	-3.922	-9.106	4.117	1.534	-9.491	-0.7485	-4.615
232	0.9827	-20.5	4.088	-4.169	-6.465	-3.488	-7.642	7.685	2.347	-7.726	0.1487	-3.746
234	-7.974	-23.12	-5.249	-4.263	-16.34	-12.16	-8.719	-67.31	1.967	-8.362	-8.808	-3.88
235	0.4438	-24.56	2.59	-4.442	-8.898	-3.34	-9.482	-25.93	1.388	-8.935	-0.3906	-3.794

Table G. part 8: *Continued*

Sequence # (sample #)	Calcite log Q/K	Carnallite log Q/K	Dolomite log Q/K	Epsomite log Q/K	Gaylussite log Q/K	Gypsum log Q/K	Halite log Q/K	Hydroxyapatite log Q/K	Magnesite log Q/K	Mirabilite log Q/K	Monohydrocalcite log Q/K	Nahcolite log Q/K
236	-0.9953	-27.88	-2.33	-7.16	-15.12	-4.019	-11.13	-20.55	-2.093	-12.95	-1.829	-7.57
237	1.194	-19.51	3.177	-5.087	-8.382	-3.073	-7.78	-17.95	1.224	-9.651	0.3605	-4.927
238	0.9023	-20	2.598	-5.081	-8.894	-3.073	-7.927	-18.64	0.9376	-9.578	0.06858	-5.026
239	-0.178	-23.43	0.8039	-5.989	-13.37	-4.347	-10.48	-21.98	0.2236	-13.17	-1.012	-6.711
240	-0.9254	-39.26	-1.924	-6.546	-13.4	-3.671	-14.4	-20.75	-1.757	-11.02	-1.759	-6.745
241	0.3467	-25.29	1.192	-5.588	-11.24	-3.286	-10.12	4.855	0.0874	-11.02	-0.487	-5.96
242	-0.3313	-27.18	0.05664	-5.988	-12.2	-3.906	-10.5	5.392	-0.3703	-11.25	-1.165	-6.643
243	-0.7071	-26.05	-0.343	-6.225	-12.3	-4.495	-10.19	5.038	-0.3942	-11.19	-1.541	-7.283
244	0.4634	-24.22	1.415	-5.058	-11.21	-2.745	-9.612	-18.75	0.1935	-10.69	-0.3703	-6.013
245	0.319	-23.41	2.795	-4.279	-9.285	-3.633	-9.197	-24.47	1.718	-9.364	-0.5149	-4.674
246	-0.1379	-21.02	2.956	-4.033	-8.077	-4.459	-7.914	-29.83	2.335	-8.069	-0.9724	-3.518
247	0.9121	-22.43	3.233	-3.684	-7.829	-2.289	-8.376	-22.9	1.562	-7.75	0.07794	-3.785
248	0.9262	-17.53	4.155	-4.3	-7.019	-3.8	-6.822	-23.06	2.47	-8.479	0.09214	-4.01
249	0.8577	-17.67	4.042	-4.231	-6.882	-3.754	-6.764	-23.38	2.426	-8.159	0.02365	-3.877
250	1.137	-19.44	3.766	-7.04	-0.8893	-5.712	-4.895	-24.51	1.87	-4.693	0.3002	-1.644
251	1.236	-19.52	3.924	-6.772	-0.9078	-5.407	-4.979	-22.48	1.929	-4.603	0.3996	-2.022
252	1.25	-19.29	3.143	-7.446	-0.7068	-5.27	-4.486	10.52	1.135	-4.294	0.4123	-1.608
253	1.173	-19.51	3.861	-6.864	-0.9714	-5.564	-4.979	10.21	1.93	-4.696	0.3362	-2.022
254	1.144	-15.97	3.867	-5.347	-0.479	-4.097	-3.75	9.641	1.965	-2.688	0.3052	-1.419
255	1.25	-17.12	3.825	-5.361	-1.151	-3.872	-4.363	12.83	1.816	-3.338	0.4145	-2.478
256	1.122	-17.25	3.298	-5.73	-0.1509	-3.944	-3.775	12.13	1.418	-2.169	0.2807	-1.223
257	1.27	-17.03	3.653	-5.422	0.07223	-3.693	-3.719	13.89	1.624	-1.992	0.4285	-1.385
258	-0.3913	-24.5	-0.2053	-5.002	-10.95	-2.778	-9.187	-22.85	-0.5722	-8.748	-1.225	-5.084
259	0.4499	-22.05	2.893	-4.53	-7.612	-3.721	-8.1	-23.43	1.685	-8.04	-0.3839	-4.035
260	0.6203	-22.38	2.626	-4.614	-7.255	-3.197	-7.693	-22.35	1.247	-7.499	-0.2135	-3.673
261	0.3258	-16.63	2.901	-5.611	-3.089	-5.049	-4.684	-27.23	1.817	-4.603	-0.5099	-1.705
262	0.3569	-20.29	1.783	-5.982	-5.166	-4.247	-6.24	-23.93	0.6677	-5.935	-0.4772	-2.772
263	0.06221	-20.74	2.127	-5.304	-6.488	-4.503	-6.959	-25.17	1.306	-6.923	-0.7717	-3.181
264	0.1452	-17.55	2.683	-5.086	-4.341	-4.672	-5.377	-26.6	1.779	-5.113	-0.6894	-2.264
265	-6.821	-17.39	-4.163	-6.262	-10.03	-12.93	-4.928	-62.84	1.899	-5.129	-7.656	-1.916
266	0.1182	-19.51	2.075	-6.485	-4.018	-5.518	-5.697	-26.44	1.198	-5.581	-0.7163	-2.447
267	0.8406	-19.17	3.722	-5.701	-3.135	-4.935	-5.863	-23.68	2.123	-5.561	0.006052	-2.318
268	-0.2248	-18.2	1.941	-5.517	-4.846	-5.102	-5.536	-28.12	1.408	-5.308	-1.059	-2.287
269	-6.844	-16.61	-4.674	-6.686	-9.099	-12.87	-4.176	-65.85	1.412	-4.106	-7.683	-0.9614
271	-6.753	-29.1	-13.23	-20.89	-26.08	-18.36	-11.55	-62.61	-7.232	-26.75	-7.589	-10.21
272	-6.843	-21.43	-13.42	-15.19	-8.553	-12.61	-2.484	-29.45	-7.334	-3.308	-7.686	-1.227
274	-6.837	-21	-13.41	-15.33	-8.248	-12.73	-2.227	-29.68	-7.327	-3.148	-7.684	-1.038
275	0.6376	-13.63	1.363	-8.069	-0.8065	-5.291	-2.219	7.437	-0.03262	-3.218	-0.2089	-0.9711

Table G. part 8: *Continued*

Sequence # (sample #)	Calcite log Q/K	Carnallite log Q/K	Dolomite log Q/K	Epsomite log Q/K	Gaylussite log Q/K	Gypsum log Q/K	Halite log Q/K	Hydroxyapatite log Q/K	Magnesite log Q/K	Mirabilite log Q/K	Monohydrocalcite log Q/K	Nahcolite log Q/K
278	-6.84	-21.19	-13.41	-15.36	-8.359	-12.77	-2.336	-29.57	-7.329	-3.292	-7.684	-1.104
283	-6.812	-22.32	-13.38	-15.08	-9.172	-12.5	-3.014	-62.66	-7.323	-3.868	-7.65	-1.814
284	-6.871	-22.27	-13.47	-14.86	-9.259	-12.31	-3.01	-28.36	-7.354	-3.653	-7.709	-1.757
285	0.474	-14.52	1.733	-7.006	-1.983	-4.967	-3.083	-26.2	0.5007	-3.718	-0.364	-1.794
287	0.9292	-17.28	1.315	-7.487	-2.545	-4.134	-4.072	-22.87	-0.3728	-4.349	0.09401	-2.223
288	0.7666	-24.57	1.047	-7.18	-3.769	-3.889	-4.798	-21.87	-0.4783	-4.999	-0.06772	-2.833
289	0.847	-17.16	1.53	-7.04	-2.778	-4.068	-4.203	-23.06	-0.07514	-4.352	0.01202	-2.313
290	1.386	-38.67	2.598	-5.595	-4.788	-2.62	-12.49	-17.34	0.4541	-5.987	0.5518	-3.495
291	1.334	-18.91	2.537	-5.796	-4.495	-2.862	-5.775	-17.97	0.4442	-5.833	0.5002	-3.342
292	1.119	-19.74	1.985	-5.521	-5.525	-2.465	-6.249	-17.86	0.1074	-6.035	0.2852	-3.737
293	1.364	-18.67	2.729	-5.661	-4.338	-2.86	-5.733	-17.93	0.6066	-5.733	0.5297	-3.332
294	1.041	-19.32	1.998	-5.538	-5.563	-2.651	-6.136	-18.39	0.1982	-6.104	0.2074	-3.639
295	1.127	-19.73	2.002	-5.541	-5.507	-2.486	-6.243	-17.87	0.1164	-6.055	0.2935	-3.727
296	1.521	-20.38	3.265	-5.037	-5.961	-2.458	-7.135	-16.78	0.9858	-7.268	0.6874	-3.885
297	1.638	-20.04	3.745	-5.618	-4.443	-3.285	-6.617	-16.17	1.349	-6.811	0.8044	-3.922
298	-6.856	-21.59	-13.45	-15.35	-8.812	-12.78	-2.639	-29.1	-7.351	-3.705	-7.697	-1.496
299	0.8644	-21.45	1.681	-5.111	-7.907	-2.261	-7.529	12.68	0.05792	-7.704	0.03073	-4.689
300	1.627	-19.39	3.368	-5.006	-5.381	-2.318	-6.514	-16	0.9827	-6.76	0.7928	-3.86
301	-1.635	-26.03	-3.26	-5.601	-14.09	-2.81	-9.645	-25.37	-2.384	-9.44	-2.469	-6.217
302	-0.1222	-24.75	-0.2895	-5.491	-10.98	-2.644	-9.132	-20	-0.9256	-9.184	-0.9559	-5.631
303	1.542	-8.195	4.772	-4.253	-2.324	-3.069	-2.104	-19.17	2.472	-4.326	0.6948	-2.286
304	1.246	-19.25	4.141	-4.394	-3.566	-3.231	-3.78	-18.98	2.137	-5.101	0.4096	-2.872
306	1.849	-19.51	5.678	-3.812	-3.613	-2.984	-4.645	-18.47	3.071	-6.106	1.014	-3.394
307	1.185	-16.26	4.043	-4.993	-4.469	-3.861	-5.365	-19.43	2.1	-6.509	0.3501	-3.193
308	1.694	-22.42	5.611	-4.925	-2.219	-4.337	-4.976	-22.32	3.159	-5.756	0.8588	-1.845
309	0.9617	-21.81	3.967	-4.314	-4.036	-3.55	-4.837	-20.84	2.247	-5.32	0.1271	-2.928
310	2.319	-21.45	4.962	-4.833	-3.511	-2.352	-4.942	-14.05	1.885	-6.309	1.484	-3.326
311	1.47	-17.15	4.192	-4.367	-5.336	-2.816	-6.267	-16.9	1.964	-6.9	0.6358	-4.003
313	1.225	-22.79	3.957	-4.327	-5.123	-3.031	-5.728	-18.32	1.974	-6.412	0.3908	-3.712
314	0.9471	-24.32	2.861	-4.611	-6.64	-2.775	-6.483	-18.28	1.156	-7.116	0.1133	-4.06
315	1.189	-24.31	2.873	-5.255	-6.618	-2.948	-6.492	-16.47	0.9257	-7.751	0.355	-4.237
316	1.05	-17.38	3.01	-4.809	-5.597	-2.916	-5.655	-18.18	1.202	-6.421	0.216	-3.612
317	0.4277	-27.19	1.461	-4.887	-7.966	-2.691	-7.455	-19.26	0.2751	-7.319	-0.4061	-4.272
319	1.181	-25.76	3.483	-4.882	-6.847	-3.201	-7.416	-17.98	1.543	-8.217	0.3477	-4.401
320	1.027	-28.24	2.976	-5.074	-7.784	-3.194	-8.464	-17.49	1.19	-8.84	0.1936	-4.854
321	1.326	-18.19	3.061	-5.213	-5.846	-2.819	-6.175	-16.22	0.9764	-7.124	0.4924	-4.036
322	-0.007343	-19.79	2.173	-5.047	-7.415	-4.433	-7.269	-23.63	1.422	-7.64	-0.8411	-4.07
323	1.085	-25.83	3.148	-4.814	-7.834	-2.99	-7.773	-17.76	1.305	-8.801	0.2515	-4.849

Table G. part 8: *Continued*

Sequence # (sample #)	Calcite log Q/K	Carnallite log Q/K	Dolomite log Q/K	Epsomite log Q/K	Gaylussite log Q/K	Gypsum log Q/K	Halite log Q/K	Hydroxyapatite log Q/K	Magnesite log Q/K	Mirabilite log Q/K	Monohydrocalcite log Q/K	Nahcolite log Q/K
325	1.216	-26.98	3.359	-5.563	-5.678	-3.688	-7.248	-18	1.385	-7.605	0.3818	-3.807
329	1.457	-27.22	3.819	-4.579	-7.849	-2.682	-8.583	-16.53	1.604	-9.252	0.6236	-5.177
330	1.341	-28.25	3.362	-5.087	-7.178	-2.965	-8.393	-16.01	1.262	-8.632	0.5077	-4.876
331	0.9586	-24.76	2.255	-4.987	-6.901	-2.523	-6.589	-17.16	0.5381	-7.148	0.1249	-4.258
332	1.092	-27.1	3.007	-4.336	-7.796	-2.357	-8.132	-17.09	1.157	-8.145	0.2586	-4.94
333	0.8233	-25.8	3.187	-4.873	-6.944	-3.611	-7.36	-20.1	1.605	-8.009	-0.01043	-4.254
334	1.089	-27.02	2.873	-5.23	-7.022	-3.123	-7.681	-17.02	1.025	-8.13	0.2555	-4.535
335	0.8227	-29.05	3.095	-4.498	-7.504	-3.146	-8.693	-19.88	1.514	-8.102	-0.011	-4.542
336	0.9202	-29.36	2.981	-5.418	-7.845	-3.756	-8.915	-18.85	1.302	-9.249	0.08649	-4.751
337	0.9975	-28.85	3.012	-5.198	-7.698	-3.414	-8.695	-18.37	1.257	-8.914	0.1638	-4.726
338	0.5766	-29.32	1.326	-5.202	-9.332	-2.573	-8.87	-18.4	-0.009042	-8.865	-0.257	-5.038
340	0.9412	-27.07	2.688	-5.16	-8.171	-3.164	-8.191	-18.03	0.9887	-9.024	0.1075	-4.923
341	0.8439	-26.15	1.884	-5.094	-8.489	-2.489	-7.685	-16.95	0.2822	-8.472	0.01025	-5.058
342	0.8044	-29.12	2.81	-4.925	-8.076	-3.324	-8.88	-19.35	1.247	-8.816	-0.02925	-4.803
343	0.5878	-29.06	1.46	-4.964	-10.74	-2.448	-9.551	-17.65	0.1143	-10.17	-0.2458	-5.997
345	1.078	-29.22	2.904	-5.384	-7.839	-3.331	-8.86	-17.61	1.068	-9.132	0.2441	-4.857
346	1.068	-31.52	2.37	-5.581	-8.774	-3.014	-9.864	-16.82	0.5439	-9.731	0.2341	-5.273
347	-7.8	-38.24	-15.48	-13.8	-29.06	-11.12	-14.85	-60.24	-8.434	-20.39	-8.634	-11.02
348	0.4131	-30.07	1.181	-5.494	-9.691	-3.047	-9.245	-19.15	0.009867	-9.371	-0.4205	-5.176
349	0.6923	-43.51	1.853	-5.865	-9.139	-3.532	-13.79	-17.82	0.4021	-9.862	-0.1414	-5.333
352	0.4416	-31.74	0.9323	-5.363	-10.6	-2.611	-10.17	-18.33	-0.2676	-9.899	-0.3921	-5.755
353	0.4585	-30.01	0.8551	-5.688	-10.62	-2.825	-9.586	-18.16	-0.3617	-10.17	-0.3752	-5.784
356	1.523	-15.55	3.997	-6.546	-1.474	-4.687	-4.273	-20.39	1.716	-5.019	0.6875	-2.211
357	1.358	-17.05	3.303	-7.763	-2.821	-5.546	-4.994	-20.02	1.187	-6.891	0.5231	-2.626
358	1.13	-13.4	3.512	-7.198	-1.66	-5.631	-3.23	10.11	1.624	-5.368	0.2928	-1.94
359	1.232	-12.02	3.843	-7.238	-0.1437	-5.757	-2.358	-25.21	1.853	-4.206	0.3864	-0.9927
361	-4.439	-36.39	-16.55	-14.88	-21.25	-4.401	-11.11	-33.76	-12.87	-12.58	-5.272	-8.566
368	0.1822	-18.45	0.2147	-5.493	-7	-2.541	-5.439	-21.19	-0.7258	-5.713	-0.6517	-3.599
370	0.4023	-22.48	0.7044	-5.054	-8.765	-2.152	-7.879	10.69	-0.4562	-7.528	-0.4313	-4.544
371	1.047	-21.39	2.079	-4.891	-6.943	-2.073	-7.347	-17.7	0.2729	-6.917	0.2138	-4.123
372	-0.2229	-24.02	-0.7187	-5.411	-10.54	-2.337	-8.522	8.304	-1.254	-8.24	-1.057	-5.088
373	1.294	-12.93	4.4	-6.366	-1.495	-5.354	-2.969	12.15	2.347	-5.257	0.4555	-1.966
374	0.8958	-13.97	3.339	-6.43	-4.019	-5.171	-4.195	5.211	1.685	-6.791	0.06109	-2.736
375	-0.683	-29.02	-1.958	-6.059	-11.59	-2.666	-8.477	-21.94	-2.033	-8.695	-1.517	-5.508
376	-0.3546	-20.47	-0.7913	-5.258	-10.56	-2.374	-7.211	-20.9	-1.195	-8.031	-1.188	-5.127
377	1.169	-14.38	3.899	-5.822	-3.007	-4.574	-4.121	9.691	1.971	-5.73	0.3342	-2.447
378	1.192	-14.39	3.978	-6.024	-2.902	-4.81	-4.119	9.87	2.028	-5.907	0.357	-2.466
381	-0.7617	-23.78	-1.74	-5.758	-12.36	-2.739	-8.755	6.921	-1.737	-9.384	-1.595	-5.896

Table G. part 8: *Continued*

Sequence # (sample #)	Calcite log Q/K	Carnallite log Q/K	Dolomite log Q/K	Epsomite log Q/K	Gaylussite log Q/K	Gypsum log Q/K	Halite log Q/K	Hydroxyapatite log Q/K	Magnesite log Q/K	Mirabilite log Q/K	Monohydrocalcite log Q/K	Nahcolite log Q/K
382	0.6187	-9.577	1.805	-5.448	-4.225	-3.153	-2.113	9.327	0.4277	-4.459	-0.2272	-2.307
383	0.6067	-14.49	1.789	-7.086	-1.782	-4.837	-3.01	9.011	0.4243	-3.653	-0.2316	-1.757
384	1.131	-14.49	3.211	-6.131	-2.053	-4.268	-3.624	11.64	1.322	-4.396	0.2948	-2.248
385	-1.808	-22.26	-3.428	-5.313	-13.92	-2.701	-8.154	2.353	-2.378	-8.815	-2.642	-5.964
386	0.4693	-4.306	2.937	-4.985	-3.641	-3.661	-0.2133	5.662	1.71	-4.36	-0.4687	-1.767
387	-0.02554	-10.06	-0.2006	-4.976	-6.232	-1.98	-2.366	-22.08	-0.9333	-3.994	-0.8682	-2.616
388	0.5411	-11.03	0.212	-5.542	-5.686	-1.844	-2.815	-18.48	-1.087	-4.435	-0.2979	-3.01
389	0.2477	-14.32	0.5799	-4.913	-7.075	-2.193	-4.373	4.506	-0.426	-5.572	-0.5868	-3.661
390	0.2457	-12.61	0.05521	-5.131	-6.871	-1.884	-3.684	-19.86	-0.9488	-5.059	-0.5898	-3.303
392	0.2966	-24.53	0.4682	-10.52	-22.12	-7.595	-13.28	-20.15	-0.5867	-26.12	-0.5371	-10.96
393	-0.4095	-22.42	0.336	-10.07	-22.78	-8.419	-12.75	-24.3	-0.01287	-26.18	-1.243	-10.9
394	0.03716	-22.73	-0.005812	-10.28	-22.99	-7.397	-12.81	-21.45	-0.8013	-26.27	-0.7966	-11.05
395	1.178	-22.06	2.044	-5.647	-8.668	-2.534	-8.126	-15.97	0.108	-9.365	0.3441	-5.306
396	0.3134	-4.865	1.035	-5.508	-4.882	-2.522	-0.0518	-18.68	-0.03632	-4.193	-0.6388	-2.621
397	1.344	-21.24	2.999	-10.2	-7.624	-7.706	-8.043	-15.85	0.896	-13.83	0.5106	-4.963
398	1.511	-15.02	4.266	-10.14	-3.348	-8.581	-4.55	-18.05	1.996	-10.76	0.6765	-2.881
399	1.446	-15.88	4.397	-10.13	-3.238	-8.83	-5.041	-18.92	2.192	-10.77	0.6116	-2.793
400	1.599	-15.05	4.805	-9.687	-3.162	-8.487	-4.795	-18.42	2.448	-10.66	0.7643	-2.809
401	1.457	-9.715	5.137	-9.48	-2.152	-8.865	-2.765	-20.92	2.922	-9.76	0.6159	-2.19
402	1.516	-13.77	4.619	-9.585	-3.476	-8.363	-4.397	-18.27	2.345	-10.68	0.6808	-2.97
403	1.354	-13.44	4.826	-9.547	-3.504	-8.856	-4.516	-19.77	2.714	-10.88	0.5187	-3.049
404	1.553	-8.807	4.95	-9.586	-1.09	-8.508	-1.738	-20.1	2.638	-8.583	0.6957	-1.563
405	1.52	-16.6	3.834	-9.789	-5.217	-7.779	-5.776	-15.86	1.555	-11.84	0.6864	-3.933
406	1.446	-11.72	4.501	-9.593	-3.046	-8.384	-3.5	-18.36	2.296	-10.14	0.6095	-2.767
408	1.081	-16.98	3.715	-9.736	-5.73	-8.486	-6.176	-19.88	1.876	-12.19	0.2474	-3.63
409	1.157	-19.02	2.739	-10.06	-6.476	-7.684	-6.568	-17.04	0.8246	-12.28	0.3228	-4.04
410	1.506	-11.4	4.391	-9.795	-3.061	-8.359	-3.325	-17.46	2.128	-10.25	0.6688	-2.884
411	1.649	-16.4	3.898	-10.09	-4.571	-7.888	-5.498	-16.16	1.491	-11.56	0.8153	-3.503
412	1.58	-11.03	4.731	-9.743	-2.3	-8.49	-3.122	-18.23	2.393	-9.771	0.742	-2.437
413	1.371	-19.82	3.793	-9.655	-5.304	-7.902	-6.221	-16.75	1.664	-11.76	0.5373	-3.863
414	1.614	-13.85	4.26	-9.928	-3.385	-8.154	-4.321	-17.23	1.888	-10.58	0.779	-2.853
415	1.173	-18.61	3.761	-10.39	-4.651	-9.007	-6.197	-19.68	1.83	-11.81	0.339	-3.35
416	1.404	-10.02	4.222	-9.743	-2.375	-8.313	-2.563	-18.79	2.06	-9.328	0.5613	-2.178
417	1.326	-19.47	3.94	-10.22	-4.077	-8.703	-6.285	-19.35	1.856	-11.24	0.4922	-2.943
418	1.056	-17.96	3.061	-9.745	-6.36	-7.891	-6.388	-18.12	1.247	-12.17	0.222	-3.947
419	1.265	-15.02	3.952	-10.62	-2.804	-9.229	-4.335	-20.25	1.929	-10.37	0.4303	-2.394
420	1.35	-13.42	4.656	-10.01	-2.267	-9.156	-3.904	-20.43	2.547	-9.937	0.5143	-2.217
421	1.524	-13.13	4.434	-9.537	-3.494	-8.111	-4.247	-17.23	2.152	-10.47	0.688	-3.12

Table G. part 8: *Continued*

Sequence # (sample #)	Calcite log Q/K	Carnallite log Q/K	Dolomite log Q/K	Epsomite log Q/K	Gaylussite log Q/K	Gypsum log Q/K	Halite log Q/K	Hydroxyapatite log Q/K	Magnesite log Q/K	Mirabilite log Q/K	Monohydrocalcite log Q/K	Nahcolite log Q/K
422	1.531	-21.78	3.208	-10.23	-7.257	-7.575	-8.115	-15.03	0.9188	-13.7	0.6977	-4.953
423	1.52	-15.79	3.686	-10.99	-2.894	-8.835	-4.582	-18.32	1.408	-10.58	0.6853	-2.611
424	1.2	-17.61	3.189	-9.796	-6.7	-7.782	-6.516	-17.24	1.23	-12.69	0.3664	-4.255
425	1.047	-18.81	4.019	-10.14	-4.447	-9.262	-6.29	-20.79	2.214	-11.61	0.2126	-3.243
426	0.8172	-20.68	2.397	-9.98	-8.27	-7.941	-7.803	-18.36	0.822	-13.65	-0.01648	-4.787
427	1.568	-17.58	3.772	-10.02	-5.244	-7.852	-6.137	-16.73	1.446	-12.04	0.7345	-3.653
428	1.094	-19.45	2.338	-10.2	-7.876	-7.547	-7.183	-16.43	0.4858	-13.42	0.2606	-4.787
429	1.58	-13.77	5.059	-10.59	-1.039	-9.673	-3.578	-20.49	2.721	-9.688	0.7429	-1.866
430	1.188	-13.63	3.952	-9.481	-4.371	-8.247	-4.539	-18	2.006	-10.81	0.3521	-3.499
431	1.496	-12.31	4.383	-9.83	-2.782	-8.406	-3.606	-18.39	2.129	-9.995	0.6601	-2.48
432	1.235	-14.99	4.198	-10.03	-3.694	-8.951	-4.875	-19.63	2.205	-10.92	0.4007	-2.966
433	1.176	-10.11	4.188	-9.522	-2.064	-8.476	-2.254	-20.03	2.253	-8.747	0.3269	-2.062
434	1.838	-16.08	4.959	-9.662	-4.082	-8.142	-5.634	-14.85	2.363	-11.71	1.004	-4.321
435	1.286	-21.51	2.72	-10.21	-7.849	-7.561	-8.061	-16.16	0.6762	-13.79	0.4519	-4.862
436	0.9535	-21.67	2.208	-10.18	-8.879	-7.674	-8.382	-17.04	0.4959	-14.27	0.1199	-5.208
437	1.229	-16.71	3.332	-10.09	-4.3	-8.158	-5.092	-18.27	1.344	-10.72	0.3947	-2.956
439	0.9994	-19.99	2.455	-10.1	-7.841	-7.758	-7.466	-17.43	0.6973	-13.4	0.1657	-4.658
440	1.518	-14.74	3.455	-9.957	-4.87	-7.572	-4.828	-13.24	1.179	-11.29	0.6839	-4.671
441	1.145	-16.88	3.803	-9.646	-4.956	-8.354	-5.698	-19.24	1.9	-11.41	0.3109	-3.36
442	1.263	-15.5	4.366	-9.55	-4.04	-8.585	-5.092	-19.39	2.346	-10.96	0.4278	-3.141
443	1.18	-13.94	3.494	-10.92	-3.019	-9.246	-3.755	-20.03	1.556	-10.44	0.3444	-2.532
444	1.962	-15.36	4.612	-9.958	-3.893	-7.842	-5.098	-15.41	1.892	-11.47	1.128	-3.423
445	1.176	-19.31	2.909	-10.07	-6.481	-7.824	-6.81	-16.67	0.9753	-12.46	0.3422	-4.255
446	1.06	-18.76	3.656	-10.39	-4.334	-9.12	-6.027	-20.85	1.837	-11.38	0.2263	-2.955
447	1.44	-19.09	3.97	-9.782	-6.514	-8.069	-7.312	-17.24	1.771	-13.27	0.6063	-4.402
448	1.039	-15.52	3.718	-9.521	-5.205	-8.355	-5.323	-19.34	1.921	-11.45	0.2043	-3.553
449	1.773	-15.26	4.452	-9.86	-2.214	-7.946	-4.163	-15.55	1.92	-9.524	0.9362	-2.708
450	1.311	-16.9	3.534	-10.84	-3.938	-8.944	-5.323	-19.37	1.465	-11.31	0.4767	-2.945
451	1.192	-15.36	3.681	-9.916	-4.56	-8.409	-5.053	-18.91	1.73	-11.16	0.3579	-3.171
452	1.31	-17.22	3.75	-9.966	-5.223	-8.293	-5.95	-17.46	1.682	-11.94	0.4763	-3.813
453	1.402	-11.89	4.611	-9.782	-2.607	-8.772	-3.515	-18.36	2.45	-9.999	0.5659	-2.819
454	1.458	-13.68	3.76	-10	-3.279	-8.034	-3.917	-17.56	1.544	-10.04	0.6226	-2.578
455	1.504	-15.27	4.15	-10.21	-2.877	-8.541	-4.461	-18.07	1.888	-10.24	0.6687	-2.577
456	1.399	-17.89	3.712	-10.05	-5.369	-8.158	-6.243	-17.44	1.555	-12.13	0.565	-3.744
457	0.9723	-18.46	2.522	-9.836	-6.89	-7.611	-6.422	-16.77	0.7917	-12.25	0.1385	-4.34
458	1.373	-11.84	4.015	-9.631	-4.059	-8.089	-3.747	-17.47	1.884	-10.71	0.5367	-3.225
459	1.118	-14.92	3.905	-9.573	-5.146	-8.438	-5.344	-19.67	2.029	-11.63	0.2833	-3.456
460	1.266	-8.181	4.461	-9.565	-1.825	-8.579	-1.664	-21.04	2.437	-8.811	0.4095	-1.737

Table G. part 8: *Continued*

Sequence # (sample #)	Calcite log Q/K	Carnallite log Q/K	Dolomite log Q/K	Epsomite log Q/K	Gaylussite log Q/K	Gypsum log Q/K	Halite log Q/K	Hydroxyapatite log Q/K	Magnesite log Q/K	Mirabilite log Q/K	Monohydrocalcite log Q/K	Nahcolite log Q/K
461	1.575	-13.82	4.238	-11.87	-0.1327	-10.12	-2.902	-21.3	1.905	-9.235	0.7336	-1.353
462	1.543	-13.76	4.261	-9.867	-3.351	-8.235	-4.191	-16.19	1.96	-10.48	0.7079	-3.305
473	1.777	-12.87	3.458	-10.4	-3.708	-7.489	-3.683	-14.92	0.9228	-10.56	0.9415	-3.097
474	1.787	-12.86	3.356	-10.47	-3.696	-7.438	-3.636	-14.69	0.8106	-10.52	0.9515	-3.122
475	1.639	-12.44	3.066	-10.4	-3.995	-7.374	-3.494	-15	0.6687	-10.46	0.8031	-3.128
476	1.788	-12.77	3.427	-10.41	-3.696	-7.454	-3.638	-15.05	0.8799	-10.54	0.9529	-3.016
477	1.479	-11.92	3.349	-10.18	-3.761	-7.76	-3.359	-16.33	1.112	-10.29	0.6426	-2.914
478	1.655	-11.89	3.703	-10.18	-3.403	-7.754	-3.336	-15.66	1.289	-10.28	0.819	-2.942
479	1.547	-11.83	3.489	-10.18	-3.605	-7.756	-3.313	-15.66	1.184	-10.27	0.7103	-3.044
480	1.671	-11.79	3.725	-10.18	-3.346	-7.745	-3.29	-15.61	1.295	-10.25	0.8347	-2.923
481	1.606	-11.81	3.602	-10.18	-3.458	-7.754	-3.283	-15.64	1.238	-10.24	0.7697	-2.974
482	1.514	-11.83	3.447	-10.18	-3.625	-7.787	-3.308	-15.78	1.175	-10.26	0.6773	-3.037
483	1.395	-11.78	3.271	-10.13	-3.886	-7.799	-3.326	-16.19	1.118	-10.29	0.5585	-3.063
484	1.533	-11.95	3.524	-10.14	-3.663	-7.786	-3.39	-15.83	1.232	-10.33	0.6972	-3.05
485	1.459	-12.1	3.39	-10.15	-3.845	-7.804	-3.449	-15.92	1.173	-10.38	0.623	-3.126
486	1.127	-13.76	2.224	-10.31	-5.21	-7.476	-3.96	-16.61	0.339	-10.75	0.2922	-3.33
487	1.5	-16.14	3.034	-10.39	-5.327	-7.618	-5.225	-14.97	0.7756	-11.75	0.6658	-4.009
488	1.593	-16.34	3.206	-10.39	-5.204	-7.61	-5.277	-14.7	0.8551	-11.81	0.7587	-4.05
489	0.1614	-18.48	0.3935	-10.54	-8.616	-7.806	-6.226	-19.8	-0.5262	-12.55	-0.6723	-4.4
490	1.623	-16.34	3.247	-10.42	-5.134	-7.617	-5.269	-14.71	0.8661	-11.8	0.7889	-4.01
522	1.431	-20.98	3.031	-4.43	-6.852	-1.797	-7.443	17.15	0.8419	-7.318	0.5971	-4.312
523	2.328	-17.34	4.862	-6.539	-0.01713	-3.932	-4.213	17.72	1.776	-4.419	1.492	-2.36
524	2.479	-18.6	4.953	-6.298	-0.5432	-3.485	-4.685	19.29	1.716	-4.797	1.644	-2.819
525	2.465	-16.21	4.803	-6.731	0.3579	-3.786	-3.907	19.56	1.58	-4.175	1.628	-1.894
526	2.677	-14.48	5.678	-6.776	2.046	-4.226	-2.951	17.42	2.243	-3.385	1.829	-1.17
527	1.302	-20.82	3.366	-4.588	-5.917	-2.547	-7.173	-18.62	1.306	-6.876	0.4682	-3.584
528	1.409	-20.86	3.654	-4.274	-5.622	-2.307	-7.185	15.52	1.486	-6.555	0.5755	-3.567
529	2.401	-15.43	5.398	-6.033	0.714	-3.801	-3.655	15.48	2.239	-3.711	1.561	-1.281
530	2.399	-15.38	5.135	-6.354	0.9914	-3.856	-3.46	15.54	1.978	-3.49	1.559	-1.305
531	0.7752	-19.4	2.379	-4.37	-6.872	-2.395	-6.712	9.492	0.8452	-6.625	-0.05882	-3.24
532	0.9833	-19.93	2.847	-4.42	-6.428	-2.497	-6.865	-21.19	1.106	-6.699	0.1493	-3.251
533	0.675	-19.95	2.601	-4.366	-6.673	-2.815	-6.906	9.783	1.168	-6.645	-0.159	-3.26
534	0.9695	-19.86	3.165	-4.637	-5.87	-3.06	-6.805	-21.7	1.437	-6.677	0.1355	-3.083
535	1.033	-20.23	3.212	-5.093	-4.1	-3.432	-6.292	11.1	1.421	-5.408	0.1981	-2.09
536	1.625	-14.76	4.075	-7.446	0.5104	-5.423	-3.072	12.37	1.692	-3.998	0.782	-1.182
537	1.752	-15.14	3.694	-7.934	0.7484	-5.268	-2.996	12.48	1.183	-3.863	0.9071	-0.9223
538	1.763	-20.4	4.131	-7.533	0.8889	-5.283	-4.862	12.57	1.61	-3.759	0.9187	-1.198
539	1.731	-14.85	4.159	-7.486	0.5592	-5.339	-3.128	12.1	1.67	-4.075	0.8893	-1.48

Table G. part 8: *Continued*

Sequence # (sample #)	Calcite log Q/K	Carnallite log Q/K	Dolomite log Q/K	Epsomite log Q/K	Gaylussite log Q/K	Gypsum log Q/K	Halite log Q/K	Hydroxyapatite log Q/K	Magnesite log Q/K	Mirabilite log Q/K	Monohydrocalcite log Q/K	Nahcolite log Q/K
540	1.246	-20.17	3.521	-4.255	-5.644	-2.48	-6.931	-19.84	1.516	-6.424	0.4124	-3.33
541	1.37	-19.4	3.915	-4.24	-5.594	-2.612	-6.871	-19.85	1.787	-6.754	0.5364	-3.317
542	1.177	-19.13	3.646	-4.674	-5.019	-3.163	-6.269	-20.34	1.711	-6.344	0.343	-3.035
543	2.449	-15.63	4.852	-6.327	0.8291	-3.449	-3.539	18.22	1.645	-3.343	1.609	-1.144
544	2.41	-17.59	4.544	-6.693	0.4947	-3.592	-4.184	17.44	1.375	-3.738	1.572	-1.315
545	2.339	-15.3	5.144	-6.315	0.931	-3.945	-3.462	16.24	2.046	-3.519	1.499	-1.302
546	2.277	-15.51	4.424	-6.989	1.155	-4.011	-3.196	16.53	1.388	-3.245	1.435	-1.166
547	2.613	-13.64	5.563	-6.735	2.194	-4.172	-2.622	16.46	2.192	-3.07	1.759	-0.8284
548	2.366	-15.47	4.632	-6.758	0.8384	-3.823	-3.411	16.44	1.508	-3.544	1.526	-1.105
549	2.093	-16.27	4.854	-6.009	-0.2458	-3.856	-4.1	15.27	2.003	-4.106	1.256	-1.312
550	2.418	-15.52	4.715	-6.879	1.273	-3.911	-3.297	15.81	1.539	-3.309	1.575	-1.052
551	2.467	-15.22	4.685	-7.219	1.811	-4.093	-2.948	15.82	1.46	-3.068	1.618	-0.7627
552	2.348	-14.38	5.256	-6.732	1.527	-4.429	-3.003	13.55	2.15	-3.441	1.502	-1.106
553	2.461	-14.54	5.142	-6.953	1.652	-4.309	-2.959	14.9	1.923	-3.424	1.615	-1.061
554	2.692	-14.31	5.535	-6.519	1.906	-3.803	-2.933	17	2.085	-3.127	1.846	-1.107
555	2.115	-16.79	4.009	-7.903	1.061	-4.836	-3.374	16.71	1.136	-3.838	1.272	-1.418
556	2.434	-15.88	4.454	-7.814	1.613	-4.539	-3.027	17.58	1.262	-3.637	1.588	-1.118
557	2.406	-15.16	4.641	-7.415	1.591	-4.376	-2.882	16.92	1.477	-3.444	1.559	-0.7561
558	2.384	-17.39	4.224	-7.421	0.9494	-4.046	-3.617	18.56	1.082	-3.688	1.544	-1.705
559	2.192	-15.48	4.436	-7.359	1.472	-4.54	-2.993	16.14	1.485	-3.3	1.344	-0.9395
560	1.171	-20.76	3.215	-5.308	-5.78	-3.379	-6.978	-18.33	1.286	-7.308	0.3369	-3.822
561	1.864	-14.71	3.501	-8.47	1.581	-5.322	-2.368	13.06	0.8791	-3.347	1.006	-0.6494
562	2.268	-15.87	3.969	-7.568	1.486	-4.135	-2.952	17.27	0.9425	-3.03	1.421	-1.067
563	2.515	-12.91	5.06	-7.444	2.623	-4.441	-1.942	15.88	1.787	-2.793	1.634	0.1591
564	2.351	-6.8615	2.3096	-5.6896	-1.8331	-2.7179	-0.0641	20.4579	0.6016	-2.6055	0	-2.991
565	2.645	-9.024	4.799	-7.341	1.64	-3.676	-0.5381	2.263	1.396	-3.356	1.737	-1.605
566	1.114	-20.19	2.94	-5.023	-5.856	-2.935	-6.675	-18.39	1.069	-6.825	0.2797	-3.726
567	2.451	-12.4	5.172	-7.222	2.552	-4.471	-1.803	15.35	1.962	-2.76	1.574	-0.05238
568	2.509	-13.14	4.703	-7.831	2.748	-4.464	-1.829	16.04	1.436	-2.692	1.626	-0.05257
569	2.251	-14.84	4.476	-7.098	1.238	-4.218	-2.908	17.39	1.467	-3.32	1.406	-1.125
570	2.844	-11.31	5.726	-6.933	3.154	-3.859	-1.465	18.17	2.124	-2.386	1.948	0.217
571	2.384	-12.35	4.821	-7.624	2.435	-4.659	-1.737	15.42	1.679	-2.929	1.507	0.001136
572	0.6261	-24.35	1.848	-5.113	-7.55	-2.908	-8.092	-19.67	0.4638	-7.516	-0.2076	-4.152
573	1.434	-20.45	3.376	-4.63	-6.758	-2.336	-7.314	-17.12	1.183	-7.769	0.6005	-4.282
574	1.681	-16.74	3.674	-7.845	0.1778	-5.326	-3.812	12.03	1.235	-4.335	0.8416	-1.418
575	1.431	-18.21	4.202	-6.362	-2.227	-4.896	-5.355	11.03	2.013	-5.794	0.5958	-2.218
576	1.301	-17.95	3.117	-5.675	-4.149	-3.387	-5.458	14.81	1.057	-5.946	0.4672	-2.98
577	0.9368	-20.02	2.523	-4.726	-7.875	-2.574	-7.241	-18.71	0.8279	-8.13	0.1031	-4.453

Table G. part 8: *Continued*

Sequence # (sample #)	Calcite log Q/K	Carnallite log Q/K	Dolomite log Q/K	Epsomite log Q/K	Gaylussite log Q/K	Gypsum log Q/K	Halite log Q/K	Hydroxyapatite log Q/K	Magnesite log Q/K	Mirabilite log Q/K	Monohydrocalcite log Q/K	Nahcolite log Q/K
578	0.6855	-17	0.877	-7.306	-4.672	-4.006	-4.33	9.478	-0.5668	-5.859	-0.149	-3.003
579	-6.809	-21.26	-13.36	-15.4	-7.978	-12.78	-1.935	-31.09	-7.308	-2.996	-7.659	-1.596
580	-6.801	-20.97	-13.34	-15.36	-7.789	-12.71	-1.786	-32.07	-7.301	-2.766	-7.655	-1.279
581	-6.787	-20.55	-13.31	-17.28	-7.464	-14.6	-1.501	-32.5	-7.279	-4.387	-7.65	-0.6773
582	-6.768	-20	-13.25	-18.48	-7.255	-15.76	-1.216	-33.63	-7.238	-5.413	-7.643	-0.2616
583	-6.76	-19.82	-13.22	-18.48	-7.161	-15.75	-1.121	-33.82	-7.216	-5.337	-7.64	-0.09991
584	-6.748	-19.58	-13.17	-18.59	-7.005	-15.83	-0.9527	-34.11	-7.183	-5.315	-7.639	0.1094
585	-6.716	-19.11	-13.06	-18.71	-6.719	-15.88	-0.6608	-34.85	-7.106	-5.213	-7.629	0.4259
586	-6.652	-18.81	-13.02	-15.74	-6.073	-12.7	-0.462	-34.1	-7.131	-1.59	-7.589	-0.2942
587	-6.665	-18.84	-13.05	-16.03	-6.147	-13.03	-0.5405	-34.21	-7.148	-1.939	-7.595	-0.3617
588	-6.586	-18.23	-12.87	-15.65	-5.955	-12.53	-0.1959	-34.7	-7.04	-1.497	-7.544	-0.3253
589	-6.609	-18.53	-12.93	-16.06	-5.93	-12.94	-0.2827	-35.16	-7.078	-1.823	-7.564	-0.2844
590	-6.593	-18.35	-12.88	-15.59	-5.925	-12.45	-0.2002	-34.13	-7.051	-1.38	-7.553	-0.2798
591	-6.581	-18.21	-12.86	-15.94	-5.914	-12.79	-0.1607	-34.4	-7.036	-1.742	-7.544	-0.2825
592	-6.576	-18.11	-12.84	-15.91	-5.922	-12.76	-0.1332	-34.54	-7.027	-1.728	-7.542	0.01888
593	-6.59	-18.28	-12.88	-15.96	-5.943	-12.83	-0.2066	-34.69	-7.048	-1.776	-7.548	-0.2572
594	-6.699	-19.24	-13.12	-15.79	-6.456	-12.87	-0.7673	-34.65	-7.178	-1.971	-7.612	0.3574
595	-6.712	-19.37	-13.17	-16.04	-6.295	-13.08	-0.7573	-34.11	-7.218	-2.005	-7.627	-0.1078
596	-6.797	-20.51	-13.35	-15.55	-7.178	-12.8	-1.539	-34.43	-7.308	-2.307	-7.668	0.105
597	-6.697	-19.17	-13.13	-15.9	-6.229	-12.93	-0.648	-34.44	-7.189	-1.834	-7.618	-0.4815
598	-6.583	-28.9	-12.86	-15.8	-5.946	-12.67	-0.1697	-34.47	-7.036	-1.637	-7.544	-0.1671
599	-6.645	-18.84	-13.01	-15.96	-6.04	-12.89	-0.4265	-34.7	-7.124	-1.775	-7.586	-0.2646
600	-6.744	-19.6	-13.24	-15.88	-6.549	-13	-0.9809	-34.44	-7.257	-2.062	-7.641	-0.1045
601	-6.879	-21.46	-13.56	-15.03	-7.075	-12.27	-1.799	-32.18	-7.436	-1.495	-7.744	-0.4577
602	-6.813	-24.69	-13.36	-13.95	-9.611	-11.41	-4.073	-29.4	-7.306	-3.205	-7.649	-1.967
603	-6.802	-20.87	-13.37	-15.37	-7.376	-12.66	-1.769	-34.53	-7.328	-2.323	-7.663	-0.1698
604	-6.796	-20.58	-13.35	-15.47	-7.296	-12.75	-1.629	-35.01	-7.311	-2.361	-7.662	-0.05697
605	-6.614	-18.27	-12.93	-15.62	-6.194	-12.6	-0.3676	-69.66	-7.071	-1.685	-7.551	-0.5447
606	-6.659	-18.87	-13.04	-15.92	-6.12	-12.9	-0.5091	-34.55	-7.141	-1.802	-7.592	-0.3388
607	-6.619	-18.52	-12.95	-15.89	-6.038	-12.81	-0.3362	-69.88	-7.086	-1.757	-7.565	-0.2796
608	-6.707	-19.31	-13.15	-15.85	-6.311	-12.91	-0.7276	-69.67	-7.205	-1.851	-7.622	-0.3286
609	-6.714	-19.34	-13.17	-15.81	-6.345	-12.88	-0.7608	-34.35	-7.212	-1.838	-7.626	-0.3553
610	-6.749	-19.71	-13.25	-15.81	-6.464	-12.91	-0.9222	-33.64	-7.261	-1.889	-7.651	-0.2804
611	-6.787	-20.25	-13.35	-15.78	-6.78	-12.97	-1.256	-34.11	-7.318	-2.125	-7.669	-0.1535
612	-6.59	-18.04	-12.87	-15.61	-6.124	-12.54	-0.2318	-33.95	-7.038	-1.64	-7.539	-0.4386
613	-6.592	-18.18	-12.87	-15.67	-6.075	-12.59	-0.2322	-35.51	-7.033	-1.643	-7.546	0.2189
614	-6.754	-20.12	-13.27	-15.88	-6.688	-13.03	-1.158	-34.91	-7.276	-2.187	-7.645	0.1964
615	-6.892	-20.9	-13.5	-13.75	-7.949	-11.16	-2.156	-28.32	-7.362	-1.178	-7.741	-1.997

Table G. part 8: *Continued*

Sequence # (sample #)	Calcite log Q/K	Carnallite log Q/K	Dolomite log Q/K	Epsomite log Q/K	Gaylussite log Q/K	Gypsum log Q/K	Halite log Q/K	Hydroxyapatite log Q/K	Magnesite log Q/K	Mirabilite log Q/K	Monohydrocalcite log Q/K	Nahcolite log Q/K
616	-6.764	-19	-13.22	-13.71	-7.298	-10.97	-1.012	-28.79	-7.215	-0.6951	-7.647	-1.855
617	-6.586	-17.93	-12.86	-14.53	-6.352	-11.51	-0.2652	-31.35	-7.027	-0.8176	-7.527	-1.182
618	-6.703	-17.19	-13.1	-13.31	-7.458	-10.29	-0.2045	-32.38	-7.152	-0.4675	-7.643	-2.033
619	-6.857	-19.39	-13.45	-13.47	-7.968	-10.77	-1.328	-30.28	-7.348	-0.9347	-7.724	-2.322
620	-6.592	-17.79	-12.87	-14.22	-6.514	-11.22	-0.2959	-31.64	-7.04	-0.6661	-7.528	-1.528
621	-6.784	-17.45	-5.737	-7.734	-9.681	-12.76	-4.237	-28.46	0.2885	-4.68	-7.619	-2.607
622	-6.854	-23.74	-13.47	-14.5	-10.05	-11.93	-3.878	-31.54	-7.377	-4.086	-7.69	-1.857
623	0.9116	-24.56	-5.626	-13.9	-2.341	-3.639	-4.332	10.89	-7.296	-3.614	0.07657	-2.57
624	0.6223	-23.44	1.527	-6.438	-3.135	-3.912	-4.254	7.448	0.1467	-4.102	-0.2128	-2.055

Table G. part 9: Aqueous chemistry database of alkaline lake waters compiled from published literature, as well as corresponding results from calculations described in chapters 2 and 3, and investigated in detail in chapter 4.

Sequence # (sample #)	Natron log Q/K	Nesquehonite log Q/K	OCP log Q/K	Pirssonite log Q/K	Portlandite log Q/K	Sepiolite log Q/K	Sylvite log Q/K	Thermonatrite log Q/K	Trona log Q/K	Vaterite log Q/K	CO2(aq) act. coef.	CO3-- act. coef.
1	-4.504	-0.3902	-34.45	-3.449	-8.314	-38.91	-11.16	-5.937	-7.519	0.5455	1.025	0.2689
2	-4.297	-0.5549	-34.78	-3.321	-8.645	-40.38	-11.19	-5.729	-7.083	0.4665	1.028	0.2741
3	-3.448	-0.6013	-36.41	-2.495	-8.687	-41.35	-11.2	-4.876	-5.795	0.4399	1.033	0.2533
4	-4.261	-0.1891	-35.3	-3.298	-8.612	-38.63	-4.384	-5.683	-7.041	0.4444	1.051	0.1826
5	-0.8964	-0.4057	-39.26	0.7172	-7.237	-41.26	-2.415	-2.12	-2.181	0.9187	1.586	0.04246
6	-1.115	-0.2561	-38.25	0.6518	-7.884	-41.46	-2.309	-2.363	-2.13	1.093	1.476	0.04946
7	-0.8211	-0.2542	-40.24	0.8403	-7.064	-40.28	-2.139	-1.977	-2.07	0.9062	1.733	0.03375
8	-0.5033	-0.5371	-40.85	1.283	-6.996	-41.61	-2.052	-1.518	-1.44	0.9053	2.489	0.02983
9	-3.358	-0.2186	-36.46	-2.469	-8.319	-38.46	-4.084	-4.773	-5.865	0.3638	1.06	0.1857
10	-3.772	-0.3352	-33.56	-2.289	-8.512	-40.53	-10.87	-5.178	-6.084	0.9502	1.09	0.1428
11	-4.973	-0.4284	-33	-3.543	-8.481	-40.69	-11.51	-6.411	-7.956	0.9261	1.022	0.2898
12	-4.475	-0.5881	-32.59	-3.026	-8.302	-40.69	-11.15	-5.903	-7.28	0.9362	1.042	0.219
13	-3.318	-1.412	-35.2	-2.011	-8.866	-45.97	-4.721	-4.739	-5.327	0.7875	1.046	0.2209
14	-3.023	0.1087	-36.83	-2.1	-7.786	-35.59	-10.62	-4.387	-5.567	0.3527	1.194	0.08528
15	-2.46	-0.3651	-37.85	-1.319	-8.735	-41.8	-3.906	-3.866	-4.176	0.6085	1.078	0.1443
16	-3.426	-0.6652	-36.27	-2.426	-9.457	-43.66	-3.854	-4.836	-5.338	0.471	1.06	0.1859
17	-3.072	0.007363	-34.69	-1.552	-8.374	-38.64	-3.168	-4.406	-5.021	0.9232	1.177	0.08398
18	-5.973	-0.7871	-31.99	-4.599	-8.268	-41.07	-6.027	-7.417	-9.596	0.8745	1.007	0.4237
19	-5.061	-0.5627	-34.47	-4.252	-8.694	-39.63	-4.897	-6.494	-8.288	0.2997	1.027	0.2569
20	-1.131	-0.8354	-40.43	0.1171	-8.794	-44.57	-2.855	-2.403	-1.98	0.5964	1.436	0.04753
21	-1.572	-0.9731	-39.64	-0.5001	-8.31	-43.76	-2.385	-2.892	-3.014	0.4626	1.325	0.06044
22	-2.787	-0.3912	-36.75	-1.704	-8.442	-40.49	-4.106	-4.194	-4.843	0.5511	1.087	0.153
23	-4.802	-0.4763	-34.05	-3.639	-8.349	-39.78	-11.34	-6.24	-7.899	0.6585	1.013	0.3366
24	-3.849	-0.4953	-34.4	-2.5	-8.362	-40.84	-4.753	-5.28	-6.364	0.8381	1.032	0.2549
25	-5.011	-2.252	-4.342	-3.461	-8.018	-47.09	-5.123	-6.453	-8.188	1.05	1.009	0.4541
26	-5.859	-2.862	-7.073	-4.801	-7.847	-47.85	-6.238	-7.305	-9.795	0.5604	1.003	0.5622
27	-6.768	-3.048	-32.03	-5.697	-7.85	-48.05	-7.312	-8.215	-11.15	0.5745	1.001	0.6604
28	-6.36	-3.018	-3.265	-5.161	-7.042	-46.88	-6.859	-7.807	-10.88	0.7018	1.002	0.6306
29	-6.903	-2.654	-32.46	-5.95	-7.33	-45.17	-7.731	-8.35	-11.67	0.4565	1.001	0.6743
30	-5.332	-3.083	-34.4	-4.215	-8.249	-50.35	-5.594	-6.776	-8.773	0.6177	1.003	0.4331
31	-5.429	-2.345	0.1988	-3.766	-6.915	-45.64	-6.293	-6.875	-9.314	1.165	1.003	0.5081
32	-6.374	-3.325	-0.1806	-5.232	-8.37	-50.94	-6.564	-7.82	-10.26	0.6444	1.002	0.5944
33	-6.68	-3.438	-1.766	-5.712	-8.709	-51.78	-6.557	-8.126	-10.64	0.4709	1.002	0.6165
34	-4.635	-2.63	-5.669	-3.42	-8.151	-48.55	-5.505	-6.078	-7.726	0.7156	1.008	0.4245
35	-5.367	-2.165	2.454	-4.498	-8.305	-44.98	-5.502	-6.81	-8.921	0.3692	1.011	0.5033
36	-7.718	-2.301	-5.498	-6.726	-7.034	-42.68	-7.932	-9.165	-13.02	0.4951	1.001	0.7399

Table G. part 9: *Continued*

Sequence # (sample #)	Natron log Q/K	Nesquehonite log Q/K	OCP log Q/K	Pirssonite log Q/K	Portlandite log Q/K	Sepiolite log Q/K	Sylvite log Q/K	Thermonatrite log Q/K	Trona log Q/K	Vaterite log Q/K	CO2(aq) act. coef.	CO3-- act. coef.
37	-5.854	-2.877	-0.8261	-4.768	-8.151	-48.67	-6.343	-7.3	-9.622	0.5885	1.003	0.5524
38	-4.014	-2.798	-2.432	-3.053	-7.936	-48.49	-4.512	-5.452	-7.024	0.4572	1.015	0.3443
39	-6.112	-3.094	-4.097	-5.029	-7.691	-48.23	-6.912	-7.559	-10.24	0.5865	1.002	0.6099
40	-7.369	-3.08	-31.85	-6.497	-6.763	-45.06	-7.439	-8.817	-12.7	0.3759	1.001	0.7348
41	-6.441	-2.809	-3.528	-5.265	-8.422	-49.07	-6.795	-7.887	-10.32	0.6791	1.002	0.6078
42	-3.427	-1.494	-35.97	-2.465	-8.881	4.697	-5.186	-4.847	-5.656	0.4419	1.044	0.2224
43	-3.353	-1.541	-35.52	-2.203	-8.73	4.006	-5.12	-4.77	-5.523	0.6271	1.046	0.1991
44	-2.771	-1.159	-35.58	-1.449	-7.312	8.554	-4.762	-4.191	-5.275	0.8014	1.048	0.1849
45	-2.691	-1.141	-35.33	-1.246	-7.385	9.151	-4.65	-4.106	-5.053	0.9207	1.054	0.1755
46	-2.784	-1.17	-35.76	-1.468	-7.681	9.138	-4.688	-4.201	-5.111	0.7936	1.05	0.1853
47	-2.756	-1.188	-35.48	-1.366	-7.446	9.27	-4.701	-4.174	-5.151	0.8678	1.049	0.1831
48	-2.848	-1.176	-35.43	-1.454	-7.455	9.177	-4.798	-4.27	-5.286	0.8756	1.043	0.1939
49	-4.267	-0.6802	-33.3	-2.806	-7.75	14.34	-5.359	-5.705	-7.247	0.957	1.017	0.3277
50	-4.184	-0.687	-32.27	-2.359	-6.927	15.22	-5.438	-5.622	-7.353	1.321	1.015	0.3312
51	-3.813	-0.1267	-32.62	-1.834	-7.204	13.74	-4.599	-5.246	-6.576	1.471	1.029	0.2502
52	-4.088	-0.1132	-31.36	-1.709	-6.8	13.85	-4.763	-5.524	-6.993	1.873	1.021	0.2825
53	-4.151	-0.1636	-32.31	-2.152	-7.472	12.97	-4.878	-5.587	-6.941	1.493	1.024	0.2753
54	-3.487	-0.811	-34.88	-2.365	-8.879	2.527	-4.596	-4.892	-5.653	0.5885	1.094	0.154
55	-4.62	-0.4841	-31.02	-2.434	-7.121	10.46	-5.185	-6.06	-7.73	1.683	1.016	0.3312
56	-5.965	-0.4669	-34.91	-5.138	-9.059	-40.68	-5.747	-7.407	-9.461	0.3259	1.013	0.3364
57	-3.446	-0.6614	-31.99	-1.167	-8.246	5.684	-5.753	-4.87	-5.346	1.762	1.045	0.2171
58	-2.34	-0.2435	-36.56	-1.012	-8.411	7.083	-2.498	-3.664	-3.992	0.7225	1.285	0.07546
59	-4.177	-0.1486	-33.86	-2.558	-7.478	-38.35	-5.208	-5.617	-7.171	1.116	1.016	0.3094
60	-2.261	-0.6443	-37.1	-1.078	-8.816	6.279	-3.421	-3.586	-3.744	0.5783	1.491	0.05579
61	-3.006	-0.06175	-31.26	-0.3463	-6.59	-38.44	-3.829	-4.417	-5.313	2.132	1.079	0.1537
62	-3.867	-0.4648	-30	-1.289	-6.831	12.09	-4.826	-5.286	-6.532	2.056	1.062	0.1773
63	-4.551	-0.9243	-33.65	-3.311	-8.795	6.834	-5.298	-5.988	-7.26	0.7343	1.019	0.3219
64	-2.867	0.2099	-32.86	-0.4854	-8.105	-40.59	-4.126	-4.27	-4.478	1.846	1.09	0.1397
65	-1.522	0.7349	-34.43	1.364	-8.385	-40.32	-2.858	-2.719	-1.886	2.167	1.557	0.04029
66	-11.62	-5.066	-36.1	-13.6	-12.66	-10.82	-8.489	-13.06	-17.55	-2.483	1	0.7977
67	-11.44	-5.332	-35.6	-13.34	-12.73	-12.85	-7.58	-12.88	-17.2	-2.4	1.001	0.7423
68	-10.97	-5.075	-34	-12.29	-11.99	-9.062	-7.536	-12.42	-16.58	-1.815	1.001	0.7257
69	-8.912	-4.027	-32.96	-9.444	-10.68	-2.359	-7.009	-10.36	-13.75	-1.028	1.002	0.6663
70	-5.722	-2.279	-32.36	-4.916	-7.656	8.02	-6.687	-7.167	-9.81	0.3072	1.009	0.4629
71	-10.89	-4.585	-34.24	-12.12	-12.24	-9.285	-7.499	-12.34	-16.29	-1.727	1.001	0.6833
72	-10.13	-4.088	-34.16	-11.25	-11.96	-6.899	-7.313	-11.58	-15.23	-1.616	1.002	0.6189
73	-9.567	-3.69	-34.69	-10.54	-12.06	-3.714	-6.933	-11.01	-14.27	-1.472	1.003	0.5754
74	-9.509	-4.061	-33.18	-10.22	-11.69	-7.918	-6.509	-10.95	-14.24	-1.213	1.003	0.5605

Table G. part 9: *Continued*

Sequence # (sample #)	Natron log Q/K	Nesquehonite log Q/K	OCP log Q/K	Pirssonite log Q/K	Portlandite log Q/K	Sepiolite log Q/K	Sylvite log Q/K	Thermonatrite log Q/K	Trona log Q/K	Vaterite log Q/K	CO2(aq) act. coef.	CO3-- act. coef.
75	-4.45	-2.609	-32.62	-3.213	-8.254	6.051	-4.921	-5.886	-7.38	0.7314	1.03	0.3041
76	-2.232	-2.227	-37.39	-1.198	-8.567	8.685	-3.232	-3.607	-3.944	0.4739	1.198	0.1194
77	-1.77	-2.171	-38.08	-0.6823	-8.29	10.61	-2.97	-3.105	-3.327	0.4921	1.349	0.08249
78	-0.8921	-10.14	-72.83	-7.505	-16.93	-21.64	-1.966	-1.971	-1.311	-7.437	2.272	0.04069
79	-0.8378	-10.13	-73.03	-7.405	-16.94	-21.75	-1.887	-1.877	-1.166	-7.426	2.492	0.03789
80	-4.056	-1.319	-33.39	-2.743	-6.918	14.66	-5.172	-5.497	-7.423	0.8112	1.016	0.3991
81	-5.313	-3.241	-34.68	-4.809	-10.89	-0.2649	-4.232	-6.745	-7.722	-0.00646	1.029	0.2909
82	-0.7727	-2.322	-41.66	0.4617	-8.996	7.897	-2.139	-1.892	-1.213	0.4467	2.001	0.04156
83	-0.5796	-2.257	-40.75	1.027	-8.387	12.13	-2.041	-1.588	-0.9431	0.7203	3.31	0.03328
84	-0.7997	-2.238	-39.27	1.059	-8.55	12.06	-2.056	-1.748	-1.013	0.9196	4.157	0.03659
85	-0.6736	-2.294	-41.71	2.082	-8.663	11.91	-0.6735	-0.7828	0.4278	1.07	10.83	0.03517
86	-9.08	-3.156	-33.36	-9.478	-9.937	3.693	-7.509	-10.53	-14.31	-0.8938	1.001	0.766
87	-5.426	-2.405	-33.57	-4.652	-8.525	8.613	-5.42	-6.869	-8.946	0.2742	1.007	0.5024
88	-6.421	-3.237	-32.76	-5.766	-8.371	6.067	-6.212	-7.867	-10.58	0.1571	1.003	0.6151
89	-8.55	-2.659	-31.39	-8.179	-9.483	5.907	-7.286	-9.997	-13.36	-0.1245	1.001	0.698
90	-7.763	-3.166	-30.26	-6.856	-8.566	6.863	-7.378	-9.21	-12.37	0.4099	1.002	0.6885
91	-3.603	-0.4124	-34.01	-2.03	-7.61	18.39	-4.568	-5.038	-6.263	1.066	1.026	0.3122
92	-3.793	-2.536	-34.76	-2.788	-8.117	6.118	-4.863	-5.23	-6.58	0.5	1.026	0.3496
93	-9.351	-3.571	-30.89	-9.084	-9.844	-1.981	-8.964	-10.8	-14.43	-0.229	1.001	0.7407
94	-9.679	-2.81	-30.75	-8.791	-9.203	1.065	-9.064	-11.13	-14.93	0.3918	1	0.7208
95	-8.312	-2.158	-29.82	-7.131	-8.776	6.844	-7.247	-9.759	-12.95	0.6849	1.002	0.6332
96	-10.69	-3.791	-33.1	-11.34	-11.13	-2.488	-8.004	-12.14	-16.26	-1.146	1.001	0.7603
97	-9.361	-3.117	-32.64	-9.398	-10.95	-0.9297	-7.06	-10.81	-14.05	-0.5335	1.001	0.668
98	-12.91	-4.021	-33.19	-13.6	-11.42	-3.599	-8.653	-14.36	-19.46	-1.182	1	0.7722
99	-8.326	-2.463	-33.86	-8.505	-10.97	3.391	-6.841	-9.772	-12.55	-0.6759	1.004	0.5721
100	-9.409	-2.266	-30.91	-8.601	-9.823	4.946	-7.795	-10.86	-14.26	0.3109	1.002	0.6161
101	-10.94	-3.752	-32.43	-11.33	-10.56	-0.7666	-8.185	-12.38	-16.79	-0.891	1.001	0.7449
102	-9.645	-3.434	-31.84	-9.695	-10.51	-1.729	-8.49	-11.09	-14.7	-0.5467	1.001	0.7277
103	-10.56	-4.37	-34.01	-11.45	-12.1	-8.463	-8.487	-12.01	-15.7	-1.384	1.001	0.7379
104	-10.64	-4.177	-33.49	-11.38	-11.84	-7.764	-8.188	-12.09	-15.87	-1.231	1.001	0.7311
105	-5.074	-2.004	-31.52	-3.612	-7.395	10.27	-5.865	-6.518	-8.64	0.9637	1.009	0.4974
106	-12.32	-4.291	-33.26	-13.23	-11.68	-5.991	-8.955	-13.77	-18.56	-1.401	1.001	0.7697
107	-12.11	-4.449	-33.76	-13.2	-12.03	-6.649	-8.658	-13.56	-18.16	-1.58	1.001	0.7569
108	-5.521	-1.837	-32.13	-4.302	-8.422	12.3	-6.425	-6.965	-8.919	0.72	1.007	0.5146
109	-11.93	-4.437	-34.07	-13.03	-12.01	-8.025	-8.952	-13.38	-17.9	-1.596	1	0.7827
110	-5.276	-2.043	-32.23	-4.148	-7.655	8.853	-5.958	-6.72	-8.981	0.6293	1.008	0.5203
111	-8	-2.637	-31.57	-7.492	-10.08	2.24	-7.221	-9.446	-12.16	0.01115	1.003	0.625
115	-5.608	-10.8	-65.83	-13.19	-17.22	-28.32	-11.83	-7.051	-9.05	-8.085	1.009	0.4843

Table G. part 9: *Continued*

Sequence # (sample #)	Natron log Q/K	Nesquehonite log Q/K	OCP log Q/K	Pirssonite log Q/K	Portlandite log Q/K	Sepiolite log Q/K	Sylvite log Q/K	Thermonatrite log Q/K	Trona log Q/K	Vaterite log Q/K	CO2(aq) act. coef.	CO3-- act. coef.
116	-4.152	-1.606	-34.6	-3.407	-8.491	6.357	-7.029	-5.586	-7.059	0.2368	1.028	0.3307
117	-6.582	-2.977	-38.53	-7.624	-12.39	-3.016	-11.77	-8.024	-9.656	-1.543	1.011	0.4497
118	-3.297	-10.28	-32.45	-1.482	-7.575	-21.33	-4.497	-4.71	-5.681	1.288	1.057	0.199
119	-3.257	-1.555	-67.89	-10.45	-16.87	7.848	-5.993	-4.671	-5.475	-7.715	1.07	0.2276
120	-4.245	-1.84	-34.32	-3.493	-8.275	6.005	-11.31	-5.679	-7.303	0.2446	1.025	0.3349
121	-4.348	-1.859	-34.39	-3.614	-8.455	5.542	-11.34	-5.784	-7.378	0.2275	1.023	0.3421
125	-8.269	-3.093	-32.95	-8.273	-11.25	-3.114	-7.389	-9.715	-12.24	-0.501	1.003	0.5828
126	-6.259	-2.971	-34.27	-6.249	-11.27	-3.129	-7.267	-7.698	-9.2	-0.4938	1.018	0.3994
127	-5.822	-2.11	-33.42	-5.273	-10.22	1.814	-7.766	-7.264	-8.803	0.04833	1.013	0.4662
128	-5.968	-1.609	-32.96	-5.237	-9.843	3.253	-7.884	-7.41	-9.121	0.2301	1.012	0.4385
129	-7.935	-1.729	-67.54	-16.27	-18.29	7.746	-8.247	-9.381	-12.38	-8.83	1.004	0.5431
130	-8.589	-2.305	-34.03	-8.814	-10.79	3.418	-12.54	-10.04	-13.06	-0.7219	1.004	0.5345
131	-9.007	-2.085	-34.01	-9.013	-10.87	4.453	-8.181	-10.45	-13.54	-0.5036	1.005	0.5007
132	-9.591	-2.848	-34.57	-10.27	-11.5	0.5337	-8.244	-11.04	-14.44	-1.179	1.004	0.5486
133	-8.699	-2.505	-34.22	-9.132	-10.77	3.515	-8.218	-10.15	-13.34	-0.9298	1.003	0.5867
134	-9.333	-3.764	-34.61	-10.16	-11.99	-5.099	-12.81	-10.78	-13.88	-1.326	1.002	0.6717
135	-6.434	-1.822	-31.11	-5.418	-9.159	5.767	-8.166	-7.877	-10.02	0.5161	1.014	0.3815
136	-6.942	-2.602	-32.59	-6.442	-10.35	-52.63	-7.969	-8.387	-10.45	0.002	1.005	0.5321
137	-9.112	-3.408	-32.25	-9.281	-10.96	-1.624	-7.992	-10.56	-13.73	-0.6662	1.002	0.6455
138	-6.602	-2.809	-33.26	-6.3	-10.79	-1.328	-7.625	-8.045	-9.816	-0.1979	1.009	0.4801
139	-5.185	-2.257	-30.05	-4.062	-8.738	6.858	-2.846	-6.543	-8.228	0.5469	1.168	0.09242
140	-5.861	-2.708	-29.4	-4.892	-8.685	6.979	-3.234	-7.255	-9.378	0.426	1.095	0.125
141	-5.32	-1.829	-30.51	-4.205	-8.285	10.17	-4.046	-6.74	-8.716	0.5953	1.051	0.2004
142	-4.339	-1.758	-31.31	-3.103	-8.545	9.442	-2.745	-5.667	-6.972	0.6338	1.274	0.07175
143	-4.678	-1.977	-30.13	-3.322	-7.844	10.18	-3.239	-6.066	-7.824	0.8076	1.11	0.1342
144	-4.925	-2.056	-30.35	-3.697	-8.431	7.663	-2.985	-6.31	-7.964	0.677	1.11	0.1261
145	-5.595	-2.715	-31.36	-5.114	-9.221	5.958	-3.364	-7.001	-8.965	-0.05186	1.071	0.1698
146	-4.802	-1.856	-30.49	-3.442	-8.902	8.045	-2.435	-6.097	-7.397	0.7285	1.257	0.06231
147	-5.729	-3.02	-31.44	-5.48	-7.976	9.799	-4.667	-7.16	-9.927	-0.2616	1.044	0.2336
148	-3.435	-0.6154	-31.26	-1.269	-7.806	13	-1.687	-4.652	-5.423	1.466	1.522	0.04568
149	-4.923	-1.662	-30.46	-3.024	-5.465	14.06	-3.786	-6.355	-9.149	1.389	1.037	0.2471
150	-3.434	-1.01	-32.76	-1.707	-8.858	11.54	-1.95	-4.584	-5.055	0.9666	1.528	0.04615
151	-4.193	-1.754	-33.28	-3.401	-9.144	9.289	-2.634	-5.516	-6.671	0.1858	1.222	0.08715
152	-2.206	-0.2718	-38.01	-1.313	-7.672	19.3	-3.298	-3.605	-4.444	0.3543	1.116	0.1604
153	-7.268	-3.002	-30.49	-6.901	-7.608	11.22	-5.695	-8.713	-12.37	-0.1312	1.004	0.5293
154	-5.198	-2.264	-30.39	-4.259	-8.461	8.982	-3.152	-6.585	-8.504	0.3893	1.093	0.1378
155	-6.202	-2.949	-31.2	-5.926	-9.576	2.831	-3.726	-7.62	-9.812	-0.2461	1.044	0.2108
156	-4.968	-3.305	-31.67	-4.024	-10.17	-1.872	-2.016	-6.16	-7.128	0.2211	1.401	0.05126

Table G. part 9: *Continued*

Sequence # (sample #)	Natron log Q/K	Nesquehonite log Q/K	OCP log Q/K	Pirssonite log Q/K	Portlandite log Q/K	Sepiolite log Q/K	Sylvite log Q/K	Thermonatrite log Q/K	Trona log Q/K	Vaterite log Q/K	CO2(aq) act. coef.	CO3-- act. coef.
157	-5.201	-1.417	-30.61	-2.043	-9.312	8.132	-0.4625	-5.068	-5.622	1.257	4.114	0.01852
158	-5.763	-2.572	-30.44	-4.947	-8.824	7.027	-3.738	-7.184	-9.262	0.2961	1.039	0.2232
159	-10.45	-4.382	-33.62	-11.42	-12.01	-5.788	-6.963	-11.9	-15.62	-1.46	1.002	0.6486
160	-6.022	-2.628	-31	-5.472	-9.389	6.917	-3.892	-7.444	-9.502	0.03159	1.039	0.2271
161	-8.227	-3.037	-32.59	-8.472	-10.49	2.249	-5.718	-9.672	-12.68	-0.7434	1.004	0.5141
162	-5.859	-2.605	-30.71	-5.24	-8.978	6.785	-3.652	-7.276	-9.424	0.09593	1.044	0.2071
163	-4.345	-1.725	-30.83	-2.59	-8.93	8.187	-1.72	-5.398	-6.285	0.9087	1.644	0.03289
164	-9.859	-3.983	-31.08	-10.54	-7.503	9.124	-7.659	-11.31	-16.84	-1.175	1	0.7842
165	-4.604	-1.922	-31.33	-2.611	-9.509	6.162	-1.257	-5.261	-5.913	0.7949	2.43	0.02315
166	-8.897	-3.276	-31.06	-8.934	-8.627	6.803	-6.839	-10.34	-14.51	-0.5334	1.001	0.7127
167	-5.379	-2.187	-31.81	-3.604	-10.22	2.332	-0.939	-5.85	-6.663	0.4105	2.736	0.01886
168	-5.286	-2.14	-30.79	-2.304	-9.659	5.872	0.6043	-4.93	-5.467	0.8828	6.979	0.1693
169	-8.366	-3.564	-31.45	-8.596	-8.974	5.737	-6.413	-9.813	-13.64	-0.7263	1.002	0.6365
170	-7.586	-3.177	-31.39	-7.596	-8.86	6.781	-5.756	-9.031	-12.41	-0.5087	1.004	0.5365
171	-6.536	-2.577	-30.45	-5.882	-8.282	9.611	-5.08	-7.977	-10.79	0.1521	1.011	0.3975
172	-5.823	-2.548	-30.97	-5.225	-8.296	9.177	-4.326	-7.256	-9.735	0.08931	1.026	0.2877
173	-4.364	-1.636	-31.11	-3.032	-7.826	12.17	-3.382	-5.763	-7.385	0.7931	1.082	0.1598
174	-4.175	-1.736	-33.24	-3.365	-9.105	9.437	-2.634	-5.498	-6.655	0.2036	1.222	0.08714
175	-3.435	-1.006	-32.78	-1.709	-8.858	11.57	-1.951	-4.584	-5.056	0.9652	1.531	0.0457
176	-9.221	-2.406	-32.44	-9.313	-9.7	5.819	-7.058	-10.67	-14.49	-0.5882	1.003	0.6017
177	-3.435	-0.6154	-31.26	-1.269	-7.806	13	-1.687	-4.652	-5.423	1.466	1.522	0.04568
178	-5.196	-1.418	-30.62	-2.042	-9.316	8.112	-0.4643	-5.067	-5.618	1.257	4.111	0.01857
179	-0.5033	-1.975	-41.41	1.515	-8.324	10.32	-0.8664	-1.259	-0.4299	0.9078	3.61	0.04075
180	-4.356	-1.147	-35.16	-3.774	-8.685	12.81	-4.232	-5.786	-7.346	0.07069	1.028	0.283
181	-4.756	-1.749	-29.36	-2.947	-7.953	9.75	-2.981	-6.142	-7.659	1.259	1.09	0.1301
182	-3.435	-1.006	-32.78	-1.71	-8.859	11.57	-1.951	-4.584	-5.056	0.9639	1.531	0.0457
183	-9.408	-3.774	-29.86	-9.02	-6.439	11.44	-7.265	-10.86	-16.16	-0.1084	1.001	0.6913
184	-5.503	-2.423	-30.31	-4.63	-8.76	7.941	-3.727	-6.905	-8.858	0.337	1.077	0.1532
185	-1.529	-2.524	-39.56	-0.3156	-8.935	6.371	-2.299	-2.678	-2.415	0.4525	1.724	0.04466
186	-4.925	-2.056	-30.35	-3.697	-8.431	7.663	-2.985	-6.31	-7.964	0.677	1.11	0.1261
187	-4.097	-1.184	-30.76	-2.344	-8.347	10.42	-2.807	-5.413	-6.439	1.14	1.255	0.06754
188	-1.621	-1.904	-36.13	-0.1972	-6.518	10.67	-3.497	-3	-3.86	0.8666	1.169	0.1399
189	-2.014	-1.614	-34.44	-0.2588	-6.425	12.75	-3.355	-3.406	-4.342	1.21	1.126	0.1573
190	-7.924	-3.417	-30.6	-6.949	-5.772	11.99	-9.251	-9.371	-13.97	0.4785	1.001	0.7305
191	-4.92	-2.622	-31.01	-3.693	-8.022	8.331	-4.123	-6.348	-8.199	0.7131	1.031	0.2652
192	-4.147	-2.268	-31.03	-2.713	-8.798	6.084	-2.906	-5.442	-6.43	0.8035	1.298	0.07147
193	-4.619	-1.858	-30.1	-2.932	-7.535	9.219	-3.563	-6.037	-7.752	1.165	1.064	0.1857
194	-3.771	0.419	-36.95	-0.8232	-9.832	7.739	-0.09518	-3.717	-3.392	1.117	4.156	0.01792

Table G. part 9: *Continued*

Sequence # (sample #)	Natron log Q/K	Nesquehonite log Q/K	OCP log Q/K	Pirssonite log Q/K	Portlandite log Q/K	Sepiolite log Q/K	Sylvite log Q/K	Thermonatrite log Q/K	Trona log Q/K	Vaterite log Q/K	CO2(aq) act. coef.	CO3-- act. coef.
195	-4.792	-2.132	-28.87	-2.885	-7.241	8.314	-2.847	-6.17	-8.013	1.35	1.119	0.1108
196	-6.337	-3.102	-30.51	-5.792	-9.949	1.779	-3.713	-7.747	-9.686	0.0156	1.059	0.1667
197	-4.72	-1.902	-29.55	-2.774	-8.816	6.463	-2.072	-5.85	-6.878	1.168	1.537	0.03071
199	-3.123	-0.7233	-4.479	-1.941	-8.784	0.2429	-3.999	-4.532	-5.128	0.6518	1.081	0.1968
200	-2.833	-0.4945	-37.91	-2.242	-8.48	5.328	-4.005	-4.244	-5.142	0.06283	1.081	0.1908
201	-2.95	-0.5838	-36.38	-1.995	-8.431	-40.63	-3.867	-4.361	-5.16	0.4261	1.078	0.1985
202	-2.983	-0.6653	-36.4	-2.019	-8.616	-41.41	-3.983	-4.396	-5.114	0.4376	1.072	0.205
203	-19.88	-0.4442	-6.541	-18.8	-8.549	-40.5	-3.84	-21.32	-30.46	0.5712	1	0.238
204	-2.959	-0.5901	-8.497	-1.998	-8.432	-40.69	-3.936	-4.37	-5.17	0.4332	1.076	0.1949
205	-2.936	-0.5783	-7.58	-1.933	-8.335	3.148	-3.989	-4.347	-5.163	0.4747	1.077	0.1976
206	-2.862	-0.5366	-7.501	-1.873	-8.13	5.467	-3.977	-4.273	-5.161	0.4611	1.078	0.1941
207	-2.844	-0.5277	-7.251	-1.896	-8.162	8.517	-3.965	-4.254	-5.138	0.4185	1.079	0.1925
208	-6.897	-1.36	-3.97	-6.274	-8.673	-2.273	-12.2	-8.342	-11.16	0.125	1.005	0.4996
209	-5.646	-2.816	-30.56	-5.145	-7.782	10.43	-4.596	-7.078	-9.775	-0.008316	1.033	0.347
210	-5.781	-2.87	-31.5	-5.44	-9.633	4.297	-3.344	-7.188	-9.109	-0.1907	1.066	0.1905
211	-5.854	-2.681	-29.25	-4.844	-8.654	7.038	-3.218	-7.249	-9.363	0.4672	1.088	0.1379
212	-4.662	-1.927	-29.9	-3.237	-7.794	10.31	-3.206	-6.051	-7.792	0.8767	1.1	0.1553
213	-5.181	-2.231	-29.84	-4.011	-8.707	6.971	-2.825	-6.541	-8.216	0.5956	1.152	0.1077
214	-4.323	-1.695	-30.76	-2.988	-8.497	9.443	-2.689	-5.658	-6.929	0.7388	1.215	0.1121
215	-4.617	-1.669	-30.06	-3.06	-8.437	9.795	-2.427	-5.913	-7.255	0.9263	1.245	0.06786
216	-3.399	-0.6072	-30.89	-1.187	-7.821	12.73	-1.642	-4.627	-5.348	1.522	1.417	0.07321
217	-4.604	-1.929	-31.3	-2.613	-9.51	6.114	-1.256	-5.265	-5.917	0.7959	2.4	0.02373
218	-5.195	-1.425	-30.6	-2.046	-9.316	8.062	-0.4645	-5.072	-5.625	1.257	4.066	0.01871
219	-4.578	-2.073	-32.51	-3.197	-9.888	5.483	-1.318	-5.413	-6.149	0.3412	2.141	0.03174
220	-4.039	-1.632	-31.73	-2.238	-9.32	5.435	-1.495	-5.004	-5.53	0.8758	1.903	0.03785
221	-4.395	-2.014	-32.33	-3.083	-9.735	4.651	-1.568	-5.388	-6.126	0.4128	1.858	0.04027
222	-4.425	-2.084	-32.66	-3.258	-9.918	3.849	-1.64	-5.454	-6.184	0.2995	1.785	0.04322
223	-4.443	-2.155	-32.86	-3.442	-9.932	3.738	-1.707	-5.504	-6.316	0.1616	1.749	0.04836
224	-4.142	-1.888	-32.8	-2.873	-9.78	4.742	-1.663	-5.186	-5.79	0.4147	1.807	0.04922
225	-10.66	-1.663	-31.12	-9.835	-8.605	6.152	-9.047	-12.11	-16.74	0.3319	1.002	0.6425
226	-11.55	-2.254	-30.44	-10.79	-9.232	-1.427	-9.282	-13	-17.79	0.2606	1.001	0.65
227	-12.07	-2.507	-30.04	-11.27	-9.3	-3.85	-9.083	-13.52	-18.52	0.3094	1.001	0.659
228	-10.75	-1.372	-31.45	-9.645	-9.331	-0.6443	-9.119	-12.2	-16.37	0.6071	1.004	0.5137
229	-9.204	-0.8439	-33.18	-8.026	-10.02	4.2	-8.715	-10.65	-13.66	0.68	1.012	0.3348
230	-9.783	-1.134	-7.304	-9.777	-11.1	2.736	-9.052	-11.23	-14.58	-0.4919	1.005	0.4325
232	-7.555	-0.3215	-5.124	-6.651	-9.715	9.766	-7.811	-8.999	-11.48	0.4054	1.009	0.3687
234	-8.477	-0.7015	-70.51	-16.53	-19.32	4.676	-8.821	-9.921	-12.54	-8.551	1.014	0.3056
235	-9.451	-1.281	-36.4	-9.083	-12.05	-3.25	-9.12	-10.89	-13.42	-0.1335	1.02	0.2445

Table G. part 9: *Continued*

Sequence # (sample #)	Natron log Q/K	Nesquehonite log Q/K	OCP log Q/K	Pirssonite log Q/K	Portlandite log Q/K	Sepiolite log Q/K	Sylvite log Q/K	Thermonatrite log Q/K	Trona log Q/K	Vaterite log Q/K	CO2(aq) act. coef.	CO3-- act. coef.
236	-14.23	-4.76	-32.35	-15.31	-10.72	-12.28	-10.46	-15.68	-21.98	-1.573	1	0.8507
237	-9.682	-1.443	-31.2	-8.568	-9.269	1.665	-7.559	-11.13	-14.79	0.617	1.004	0.5146
238	-9.902	-1.73	-31.58	-9.08	-9.583	0.7834	-7.689	-11.35	-15.11	0.325	1.003	0.5599
239	-13.3	-2.444	-33.81	-13.56	-10.69	-6.424	-8.689	-14.75	-20.2	-0.7553	1.001	0.6469
240	-12.58	-4.424	-32.62	-13.58	-10.65	-9.249	-13.98	-14.02	-19.5	-1.503	1	0.8458
241	-11.69	-2.58	-7.608	-11.43	-10.06	-3.852	-9.533	-13.14	-17.83	-0.2306	1.001	0.6789
242	-11.97	-3.037	-7.478	-12.38	-9.654	-1.969	-10.47	-13.42	-18.8	-0.9086	1	0.8001
243	-11.7	-3.061	-9.003	-12.49	-8.483	3.314	-9.678	-13.15	-19.17	-1.284	1	0.8569
244	-11.78	-2.474	-31.35	-11.39	-9.924	-0.5289	-9.669	-13.22	-17.97	-0.1139	1.002	0.6441
245	-9.711	-0.9503	-36.31	-9.471	-10.68	5.327	-9.143	-11.16	-14.57	-0.2583	1.007	0.4034
246	-8.049	-0.3341	-40.58	-8.262	-11.78	6.217	-8.26	-9.489	-11.74	-0.7152	1.024	0.226
247	-8.849	-1.106	-34.43	-8.014	-11	4.587	-8.78	-10.29	-12.81	0.3348	1.013	0.3046
248	-8.053	-0.1979	-35.85	-7.205	-9.74	12.13	-7.105	-9.496	-12.24	0.3489	1.013	0.3164
249	-7.847	-0.2427	-36.03	-7.067	-9.869	11.94	-7.111	-9.291	-11.9	0.2804	1.013	0.3183
250	-2.15	-0.8078	-38.72	-1.066	-8.333	2.973	-6.319	-3.565	-3.948	0.5601	1.068	0.1296
251	-2.264	-0.7466	-37.41	-1.086	-7.599	6.753	-6.41	-3.685	-4.445	0.6588	1.06	0.1641
252	-2.081	-1.543	-3.793	-0.8824	-8.222	-0.1762	-6.171	-3.494	-3.841	0.6724	1.074	0.128
253	-2.264	-0.7458	-4.658	-1.15	-7.662	6.485	-6.401	-3.686	-4.446	0.5954	1.06	0.164
254	-1.756	-0.7189	-4.533	-0.6493	-8.368	2.625	-4.798	-3.154	-3.314	0.5671	1.114	0.09313
255	-2.519	-0.8577	-2.765	-1.331	-6.932	3.783	-5.396	-3.945	-5.161	0.6732	1.047	0.1773
256	-1.417	-1.272	-1.989	-0.3148	-8.425	3.597	-5.112	-2.795	-2.761	0.5447	1.181	0.07687
257	-1.343	-1.067	-0.7818	-0.09063	-7.876	7.978	-5.126	-2.719	-2.847	0.6928	1.206	0.08881
258	-10.66	-3.239	-33.85	-11.13	-11.52	-4.701	-8.919	-12.11	-15.93	-0.9686	1.001	0.6937
259	-8.168	-0.9831	-35.67	-7.798	-10.28	5.798	-8.403	-9.614	-12.38	-0.1274	1.004	0.4899
260	-7.982	-1.42	-34.22	-7.441	-10.65	1.425	-8.915	-9.427	-11.84	0.04304	1.005	0.4706
261	-3.53	-0.8561	-39.35	-3.269	-10.42	7.08	-5.279	-4.959	-5.401	-0.2515	1.039	0.2979
262	-5.631	-2.001	-36.09	-5.352	-10.36	1.167	-6.804	-7.074	-8.582	-0.2204	1.007	0.4811
263	-6.657	-1.362	-36.83	-6.674	-10.87	1	-7.479	-8.102	-10.02	-0.5151	1.005	0.5039
264	-4.596	-0.8906	-38.58	-4.525	-10.55	7.303	-5.855	-6.035	-7.035	-0.4321	1.018	0.3831
265	-3.321	-0.7728	-68.43	-10.21	-16.93	6.814	-5.429	-4.753	-5.406	-7.398	1.031	0.2889
266	-4.245	-1.471	-39.1	-4.202	-9.865	4.852	-6.245	-5.686	-6.868	-0.4591	1.014	0.3946
267	-4.086	-0.5473	-36.97	-3.319	-9.239	8.142	-6.343	-5.525	-6.579	0.2633	1.016	0.3599
268	-4.731	-1.262	-39.63	-5.03	-11.01	4.35	-5.953	-6.17	-7.193	-0.8021	1.017	0.3971
269	-2.387	-1.271	-70.49	-9.27	-17.9	4.632	-4.671	-3.786	-3.488	-7.422	1.096	0.1721
271	-19.45	-9.905	-68.75	-26.26	-16.39	-79	-10.89	-20.88	-29.83	-7.33	0.998	0.1685
272	-1.862	-10.03	-35.19	-8.712	-16.81	-24.21	-3.54	-3.226	-3.198	-7.42	1.156	0.1114
274	-1.579	-10.03	-35.37	-8.396	-16.88	-24.3	-3.292	-2.912	-2.698	-7.415	1.22	0.08803
275	-1.614	-2.738	-5.559	-0.9548	-9.568	4.113	-3.267	-2.946	-2.665	0.0603	1.221	0.08969

Table G. part 9: *Continued*

Sequence # (sample #)	Natron log Q/K	Nesquehonite log Q/K	OCP log Q/K	Pirssonite log Q/K	Portlandite log Q/K	Sepiolite log Q/K	Sylvite log Q/K	Thermonatrite log Q/K	Trona log Q/K	Vaterite log Q/K	CO2(aq) act. coef.	CO3-- act. coef.
278	-1.681	-10.03	-35.27	-8.512	-16.86	-24.82	-3.388	-3.028	-2.878	-7.417	1.192	0.09729
283	-2.489	-10	-68.92	-9.344	-16.27	-24.01	-4.085	-3.894	-4.448	-7.389	1.072	0.1649
284	-2.517	-10.04	-34.43	-9.431	-16.47	-23.29	-4.033	-3.922	-4.419	-7.448	1.076	0.1727
285	-2.584	-2.18	-39.61	-2.157	-9.126	8.046	-4.067	-3.993	-4.526	-0.1033	1.07	0.1794
287	-3.588	-3.045	-36.56	-2.727	-8.838	4.237	-5.027	-5.021	-5.98	0.3519	1.025	0.2965
288	-4.644	-3.147	-35.55	-3.953	-8.844	4.171	-11.83	-6.085	-7.654	0.1893	1.01	0.4181
289	-3.738	-2.746	-36.7	-2.961	-8.89	6.139	-5.094	-5.173	-6.223	0.2697	1.022	0.3115
290	-6.28	-2.214	-31.32	-4.975	-8.541	6.437	-13.12	-7.726	-9.956	0.8083	1.004	0.5833
291	-5.936	-2.224	-31.94	-4.681	-8.553	6.449	-6.433	-7.381	-9.458	0.7568	1.004	0.5406
292	-6.75	-2.56	-31.59	-5.711	-8.794	6.337	-6.8	-8.196	-10.67	0.5417	1.003	0.598
293	-5.809	-2.061	-32.04	-4.524	-8.417	7.813	-6.32	-7.254	-9.321	0.7863	1.004	0.5324
294	-6.71	-2.469	-31.89	-5.749	-9.027	5.256	-6.656	-8.156	-10.53	0.4639	1.003	0.5903
295	-6.74	-2.551	-31.6	-5.693	-8.795	6.214	-6.795	-8.186	-10.65	0.55	1.003	0.5974
296	-7.588	-1.682	-30.37	-6.147	-8.932	4.217	-7.384	-9.034	-11.65	0.9439	1.002	0.5791
297	-6.187	-1.319	-31.35	-4.629	-7.341	9.667	-7.041	-7.633	-10.29	1.061	1.002	0.6007
298	-2.098	-10.04	-35.11	-8.977	-16.54	-25.42	-3.646	-3.479	-3.717	-7.434	1.124	0.1365
299	-8.877	-2.609	-0.5691	-8.094	-9.271	3.303	-8.027	-10.32	-13.75	0.2871	1.001	0.685
300	-7.114	-1.685	-30.12	-5.568	-8.404	6.976	-7.153	-8.56	-11.16	1.049	1.003	0.5912
301	-12.56	-5.051	-35.49	-14.28	-12.4	-9.491	-9.621	-14.01	-18.96	-2.212	1	0.816
302	-10.96	-3.593	-32.07	-11.16	-10.46	-2.856	-9.223	-12.41	-16.77	-0.6995	1	0.7668
303	-4.041	-0.2374	-33.29	-2.469	-8.452	11.58	-2.976	-5.363	-6.399	0.9651	1.408	0.0459
304	-4.928	-0.5368	-32.95	-3.746	-8.558	10.37	-11.41	-6.355	-7.965	0.6682	1.08	0.186
306	-5.574	0.4	-33.43	-3.796	-7.565	17.86	-11.54	-7.01	-9.14	1.272	1.053	0.1596
307	-5.763	-0.5698	-33.14	-4.653	-8.823	5.902	-6.079	-7.203	-9.132	0.6073	1.039	0.2541
308	-4.028	0.4858	-35.59	-2.4	-9.266	8.551	-12.32	-5.458	-6.041	1.117	1.033	0.2235
309	-5.109	-0.4235	-34.45	-4.22	-8.92	11.28	-12.18	-6.547	-8.211	0.3844	1.037	0.2893
310	-5.939	-0.7847	-28.97	-3.695	-7.599	7.501	-12.08	-7.379	-9.441	1.741	1.044	0.2202
311	-6.914	-0.7046	-31.35	-5.522	-8.073	10.84	-6.19	-8.357	-11.1	0.8926	1.02	0.3114
313	-6.456	-0.6944	-32.4	-5.309	-8.441	10.96	-12.46	-7.9	-10.35	0.6475	1.015	0.3624
314	-7.693	-1.512	-31.55	-6.826	-9.261	4.688	-12.9	-9.139	-11.93	0.3698	1.009	0.4402
315	-7.914	-1.742	-30.1	-6.805	-8.887	1.223	-12.86	-9.36	-12.33	0.6116	1.008	0.4487
316	-6.754	-1.466	-31.59	-5.783	-9.116	5.047	-6.723	-8.199	-10.55	0.4726	1.007	0.4922
317	-8.5	-2.392	-31.62	-8.152	-10.16	-1.094	-13.75	-9.946	-12.95	-0.1496	1.005	0.5304
319	-8.134	-1.124	-31.71	-7.034	-8.787	5.978	-13.31	-9.581	-12.72	0.6042	1.004	0.5235
320	-8.917	-1.477	-31.2	-7.971	-8.819	4.118	-14.12	-10.36	-13.95	0.45	1.004	0.5489
321	-7.278	-1.691	-30.23	-6.032	-8.517	4.48	-6.789	-8.724	-11.5	0.7489	1.004	0.5729
322	-7.513	-1.245	-36.14	-7.601	-10.02	4.954	-6.885	-8.96	-11.76	-0.5846	1.004	0.5563
323	-9.025	-1.362	-31.4	-8.021	-8.878	5.492	-13.32	-10.47	-14.06	0.5079	1.003	0.5441

Table G. part 9: *Continued*

Sequence # (sample #)	Natron log Q/K	Nesquehonite log Q/K	OCP log Q/K	Pirssonite log Q/K	Portlandite log Q/K	Sepiolite log Q/K	Sylvite log Q/K	Thermonatrite log Q/K	Trona log Q/K	Vaterite log Q/K	CO2(aq) act. coef.	CO3-- act. coef.
325	-7	-1.283	-31.72	-5.865	-8.806	3.095	-13.57	-8.446	-10.99	0.6383	1.003	0.582
329	-9.412	-1.064	-30.82	-8.035	-8.237	9.215	-13.77	-10.86	-14.77	0.88	1.003	0.5508
330	-8.625	-1.405	-30.36	-7.364	-8.168	6.261	-14.05	-10.07	-13.68	0.7641	1.002	0.5994
331	-7.965	-2.129	-30.56	-7.087	-9.128	3.403	-12.79	-9.412	-12.4	0.3813	1.003	0.6103
332	-8.994	-1.51	-30.96	-7.983	-8.658	9.153	-13.69	-10.44	-14.12	0.515	1.003	0.5846
333	-7.873	-1.062	-33.44	-7.13	-9.179	6.598	-13.25	-9.32	-12.31	0.246	1.003	0.5651
334	-8.216	-1.642	-30.85	-7.208	-8.695	3.913	-13.6	-9.663	-12.93	0.5119	1.002	0.6184
335	-8.433	-1.154	-33.24	-7.691	-9.163	8.937	-14.31	-9.879	-13.16	0.2454	1.002	0.5895
336	-8.871	-1.365	-32.29	-8.032	-9.086	2.35	-14.4	-10.32	-13.8	0.3429	1.002	0.6127
337	-8.801	-1.411	-31.9	-7.885	-8.99	3.956	-14.22	-10.25	-13.71	0.4202	1.002	0.6169
338	-10.01	-2.676	-30.93	-9.519	-9.999	-1.84	-14.29	-11.46	-15.23	-0.0006747	1.001	0.6513
340	-9.218	-1.679	-31.49	-8.358	-9.068	3.647	-13.59	-10.67	-14.32	0.3639	1.001	0.6408
341	-9.438	-2.385	-30.35	-8.676	-9.115	2.832	-13.2	-10.89	-14.68	0.2666	1.001	0.6726
342	-8.986	-1.42	-32.66	-8.263	-9.213	5.699	-14.3	-10.43	-13.97	0.2271	1.001	0.6255
343	-11.44	-2.553	-30.68	-10.93	-9.492	1.742	-14.2	-12.88	-17.62	0.01051	1.001	0.6758
345	-9.022	-1.599	-31.27	-8.026	-8.868	3.123	-14.29	-10.47	-14.06	0.5005	1.001	0.6475
346	-9.947	-2.123	-30.37	-8.961	-8.972	0.5395	-14.98	-11.39	-15.4	0.4904	1.001	0.6801
347	-21.36	-11.1	-65	-29.25	-17.76	-30.28	-14.18	-22.81	-32.57	-8.378	1	0.7676
348	-10.21	-2.657	-31.59	-9.878	-10.08	-2.665	-14.5	-11.66	-15.57	-0.1642	1.001	0.6916
349	-9.936	-2.265	-31.12	-9.326	-9.216	-1.395	-18.97	-11.38	-15.45	0.115	1.001	0.712
352	-11.15	-2.935	-31.03	-10.79	-9.831	-0.9798	-14.97	-12.59	-17.08	-0.1357	1.001	0.726
353	-11.19	-3.029	-30.88	-10.81	-9.8	-2.847	-14.36	-12.64	-17.15	-0.1188	1.001	0.7331
356	-3.111	-0.9566	-35.13	-1.655	-7.789	8.471	-4.499	-4.542	-5.491	0.9456	1.032	0.2609
357	-4.288	-1.482	-34.24	-3.006	-8.31	-1.551	-5.225	-5.728	-7.09	0.7802	1.012	0.3884
358	-2.913	-1.054	-3.908	-1.837	-8.513	3.847	-4.117	-4.329	-5.008	0.5527	1.055	0.2084
359	-1.54	-0.8496	-38.9	-0.2953	-8.866	5.649	-3.208	-2.881	-2.621	0.6545	1.22	0.09825
361	-16.91	-15.54	-41.43	-21.43	-14.86	-57.46	-10.91	-18.36	-25.66	-5.016	1	0.9357
368	-7.289	-3.394	-33.17	-7.186	-10.54	-0.5002	-6.831	-8.734	-11.07	-0.3951	1.004	0.5569
370	-9.273	-3.123	-1.415	-8.952	-10.42	-0.9895	-8.242	-10.72	-14	-0.175	1.001	0.6724
371	-8.096	-2.394	-30.78	-7.129	-9.438	3.947	-7.76	-9.543	-12.4	0.4702	1.002	0.6292
372	-10.43	-3.921	-3.11	-10.73	-11.11	-5.212	-8.852	-11.87	-15.7	-0.8002	1.001	0.7311
373	-2.917	-0.3333	-2.096	-1.669	-8.293	6.554	-4.885	-4.324	-5.03	0.7164	1.079	0.2018
374	-5.025	-0.9852	-8.03	-4.203	-9.286	0.5325	-4.972	-6.463	-7.936	0.3185	1.015	0.3528
375	-11.01	-4.7	-33.15	-11.78	-11.32	-8.333	-13.75	-12.46	-16.7	-1.26	1	0.7878
376	-10.31	-3.862	-32.37	-10.75	-11.05	-4.71	-7.859	-11.76	-15.62	-0.9319	1.001	0.7107
377	-4.288	-0.6997	-3.986	-3.19	-8.851	5.724	-5.075	-5.724	-6.907	0.5919	1.022	0.34
378	-4.206	-0.6434	-3.948	-3.085	-8.71	4.984	-5.068	-5.642	-6.844	0.6146	1.022	0.3386
381	-11.71	-4.404	-4.291	-12.55	-11.31	-7.316	-8.94	-13.15	-17.78	-1.339	1	0.7936

Table G. part 9: *Continued*

Sequence # (sample #)	Natron log Q/K	Nesquehonite log Q/K	OCP log Q/K	Pirssonite log Q/K	Portlandite log Q/K	Sepiolite log Q/K	Sylvite log Q/K	Thermonatrite log Q/K	Trona log Q/K	Vaterite log Q/K	CO2(aq) act. coef.	CO3-- act. coef.
382	-5.01	-2.276	-2.919	-4.375	-10.32	-2.055	-3.294	-6.348	-7.402	0.04135	1.205	0.1059
383	-2.517	-2.257	-4.532	-1.954	-8.996	7.823	-4.033	-3.922	-4.419	0.02945	1.076	0.1727
384	-3.3	-1.351	-2.598	-2.233	-8.293	10.48	-4.525	-4.728	-5.714	0.5534	1.034	0.2505
385	-12.22	-5.045	-7.43	-14.11	-12.74	-9.728	-8.491	-13.67	-18.37	-2.386	1	0.7882
386	-4.737	-1.27	-6.663	-3.515	-10.54	2.102	-1.358	-5.246	-5.852	-0.108	2.88	0.01896
387	-6.357	-3.628	-32.92	-6.392	-11.71	-6.163	-3.304	-7.723	-9.084	-0.6028	1.13	0.1126
388	-6.36	-3.771	-30.63	-5.857	-10.39	-4.403	-3.288	-7.759	-9.51	-0.03622	1.076	0.15
389	-7.432	-3.095	-7.527	-7.26	-10.49	-1.169	-5.269	-8.873	-11.27	-0.3296	1.011	0.3791
390	-7.232	-3.621	-31.38	-7.053	-11	-5.343	-4.2	-8.663	-10.7	-0.3316	1.028	0.2607
392	-22.53	-3.254	-31.72	-22.31	-10.94	-56.47	-12.61	-23.97	-33.67	-0.2807	1.001	0.6436
393	-22.47	-2.68	-35.1	-22.96	-11.72	-54.47	-12.08	-23.92	-33.55	-0.9868	1.001	0.5722
394	-23.13	-3.469	-32.34	-23.18	-11.63	-59.05	-12.14	-24.58	-34.37	-0.5401	1.002	0.5386
395	-9.952	-2.559	-29.69	-8.855	-8.799	1.045	-8.57	-11.4	-15.44	0.6004	1.001	0.6895
396	-5.893	-3.059	-31.56	-4.713	-10.03	-1.704	-1.423	-6.274	-7.749	-0.2639	3.091	0.02201
397	-9.073	-1.771	-29.93	-7.81	-8.441	-44.93	-7.824	-10.52	-14.22	0.767	1.002	0.635
398	-4.969	-0.6733	-32.25	-3.533	-8.327	-41.1	-5.572	-6.409	-8.026	0.9337	1.017	0.3915
399	-4.793	-0.477	-33.06	-3.423	-8.394	-40.45	-5.468	-6.234	-7.763	0.8687	1.017	0.4108
400	-4.872	-0.2228	-32.66	-3.345	-8.283	-39.4	-5.459	-6.309	-7.855	1.022	1.04	0.2792
401	-3.751	0.2326	-34.97	-2.317	-8.494	-37.94	-3.442	-5.133	-6.065	0.8795	1.353	0.06481
402	-5.105	-0.3265	-32.52	-3.658	-8.274	-39.38	-5.106	-6.539	-8.246	0.9387	1.066	0.1977
403	-4.971	0.04195	-34.15	-3.686	-8.144	-37.14	-4.764	-6.405	-8.191	0.7765	1.072	0.1749
404	-2.868	-0.101	-34.07	-1.205	-8.635	-39.72	-3.154	-4.101	-4.423	0.976	2.368	0.0724
405	-6.844	-1.113	-30.3	-5.403	-8.094	-41.69	-6.139	-8.289	-10.96	0.943	1.011	0.4124
406	-4.614	-0.3807	-32.65	-3.223	-8.246	-39.21	-4.276	-6.033	-7.538	0.8691	1.124	0.1461
408	-6.918	-0.7922	-33.2	-5.916	-9.212	-43.01	-6.117	-8.363	-10.73	0.504	1.01	0.4135
409	-7.738	-1.843	-30.43	-6.662	-9.139	-47.13	-7.141	-9.185	-11.96	0.5792	1.004	0.5441
410	-4.687	-0.5487	-31.96	-3.238	-8.026	-39.32	-4.216	-6.107	-7.729	0.9282	1.066	0.1863
411	-6.327	-1.178	-30.38	-4.757	-8.307	-43.31	-5.921	-7.772	-10.01	1.072	1.008	0.484
412	-4.009	-0.2881	-32.61	-2.474	-8.156	-39.11	-3.811	-5.415	-6.592	1.003	1.133	0.1696
413	-6.783	-1.005	-30.96	-5.49	-8.32	-41.52	-8.515	-8.227	-10.83	0.7941	1.02	0.327
414	-5.11	-0.7821	-31.34	-3.569	-8.419	-42.05	-4.892	-6.547	-8.137	1.036	1.028	0.3337
415	-5.931	-0.8379	-33.51	-4.838	-8.694	-41.96	-6.675	-7.376	-9.461	0.5956	1.004	0.5235
416	-3.927	-0.6331	-32.61	-2.536	-8.736	-41.7	-3.444	-5.297	-6.218	0.8263	1.284	0.1272
417	-5.511	-0.8125	-32.94	-4.263	-8.934	-43.13	-6.963	-6.955	-8.633	0.7489	1.009	0.4716
418	-7.523	-1.421	-31.44	-6.547	-9.208	-45.32	-6.653	-8.968	-11.65	0.4786	1.01	0.4181
419	-4.18	-0.7422	-34.02	-2.987	-8.755	-42.25	-5.143	-5.617	-6.747	0.6878	1.025	0.3655
420	-3.735	-0.1271	-34.39	-2.447	-8.57	-39.44	-4.552	-5.161	-6.115	0.7729	1.062	0.2899
421	-5.134	-0.5217	-31.78	-3.674	-7.99	-39.08	-4.584	-6.562	-8.42	0.9466	1.116	0.1439

Table G. part 9: *Continued*

Sequence # (sample #)	Natron log Q/K	Nesquehonite log Q/K	OCP log Q/K	Pirssonite log Q/K	Portlandite log Q/K	Sepiolite log Q/K	Sylvite log Q/K	Thermonatrite log Q/K	Trona log Q/K	Vaterite log Q/K	CO2(aq) act. coef.	CO3-- act. coef.
422	-8.894	-1.748	-29.46	-7.444	-8.094	-44.25	-8.063	-10.34	-14.03	0.954	1.002	0.6245
423	-4.524	-1.262	-32.43	-3.078	-8.413	-43.97	-5.244	-5.963	-7.31	0.9426	1.017	0.4069
424	-8.006	-1.437	-30.83	-6.886	-8.932	-44.88	-6.515	-9.452	-12.44	0.6229	1.007	0.4537
425	-5.601	-0.4543	-34.61	-4.633	-8.703	-40.12	-6.744	-7.045	-9.024	0.4693	1.006	0.486
426	-9.193	-1.845	-31.45	-8.456	-9.439	-46.98	-7.792	-10.64	-14.16	0.2399	1.002	0.5931
427	-6.919	-1.222	-30.57	-5.43	-8.68	-44.54	-6.367	-8.365	-10.75	0.9911	1.006	0.5026
428	-9.076	-2.182	-29.91	-8.063	-9.044	-47.85	-7.345	-10.52	-14.05	0.517	1.002	0.6006
429	-2.741	0.04423	-34.98	-1.216	-8.039	-38.8	-4.722	-4.158	-4.763	1.003	1.078	0.2615
430	-5.673	-0.6667	-32.42	-4.552	-8.109	-38.81	-4.899	-7.104	-9.341	0.6103	1.126	0.1187
431	-4.397	-0.5464	-32.37	-2.96	-8.557	-41.2	-4.283	-5.82	-7.038	0.9191	1.075	0.239
432	-5.038	-0.4645	-33.65	-3.879	-8.503	-40	-5.174	-6.479	-8.181	0.6578	1.016	0.4036
433	-3.425	-0.462	-33.97	-2.203	-8.634	-39.78	-3.723	-4.729	-5.543	0.5992	1.955	0.07761
434	-6.027	-0.3054	-31.2	-4.267	-6.182	-34.3	-5.898	-7.471	-10.53	1.26	1.018	0.3399
435	-9.24	-1.991	-29.81	-8.036	-8.867	-47.17	-8.007	-10.69	-14.28	0.7083	1.002	0.6103
436	-9.938	-2.171	-30.36	-9.065	-9.205	-47.89	-8.038	-11.39	-15.33	0.3762	1.002	0.6356
437	-5.638	-1.325	-31.66	-4.485	-9.13	-45.37	-6.2	-7.08	-8.771	0.6517	1.018	0.4275
439	-8.946	-1.97	-30.68	-8.027	-9.267	-47.52	-7.399	-10.39	-13.79	0.4221	1.002	0.6046
440	-6.496	-1.49	-29.5	-5.055	-6.268	-37.1	-5.455	-7.938	-11.35	0.9408	1.015	0.3838
441	-6.209	-0.7692	-32.79	-5.141	-8.977	-42.25	-6.287	-7.652	-9.748	0.5678	1.023	0.3188
442	-5.414	-0.3251	-33.42	-4.223	-8.496	-39.25	-5.757	-6.851	-8.728	0.6853	1.059	0.1995
443	-4.313	-1.116	-33.86	-3.201	-8.694	-43.18	-4.97	-5.745	-7.014	0.6024	1.024	0.2998
444	-5.963	-0.7766	-30.15	-4.078	-7.788	-41.05	-5.71	-7.406	-9.565	1.385	1.011	0.4166
445	-7.763	-1.692	-30.48	-6.667	-8.714	-44.99	-7.128	-9.209	-12.2	0.5986	1.003	0.5786
446	-5.502	-0.8314	-34.21	-4.52	-9.165	-43.15	-6.735	-6.946	-8.637	0.483	1.007	0.4769
447	-8.06	-0.8964	-31.31	-6.7	-8.452	-41.92	-6.996	-9.506	-12.64	0.8628	1.006	0.4788
448	-6.354	-0.7493	-33.03	-5.389	-8.84	-41.21	-5.837	-7.793	-10.08	0.4615	1.06	0.1781
449	-4.111	-0.7576	-30.56	-2.39	-7.531	-39.38	-5.607	-5.526	-6.973	1.196	1.129	0.2556
450	-5.357	-1.204	-33.1	-4.124	-8.789	-44.25	-5.769	-6.8	-8.481	0.7335	1.007	0.468
451	-5.86	-0.9383	-32.47	-4.745	-8.96	-43.08	-5.542	-7.303	-9.209	0.6148	1.013	0.4139
452	-6.639	-0.9862	-31.64	-5.409	-8.339	-41.46	-6.342	-8.085	-10.63	0.7329	1.006	0.5158
453	-4.129	-0.2256	-33.19	-2.785	-7.702	-37	-4.088	-5.551	-7.108	0.8251	1.081	0.2214
454	-4.853	-1.129	-31.23	-3.46	-8.86	-44.41	-4.913	-6.282	-7.598	0.8809	1.054	0.3005
455	-4.493	-0.7832	-32.14	-3.06	-8.462	-41.95	-5.413	-5.929	-7.242	0.9263	1.032	0.3737
456	-6.874	-1.113	-31.34	-5.555	-8.624	-43.31	-6.526	-8.32	-10.8	0.8215	1.004	0.5332
457	-7.969	-1.876	-30.34	-7.077	-8.953	-45.78	-7.068	-9.415	-12.49	0.395	1.008	0.4511
458	-5.548	-0.7896	-31.66	-4.24	-8.346	-40.78	-4.441	-6.976	-8.938	0.7952	1.066	0.1691
459	-6.372	-0.6403	-33.22	-5.33	-8.975	-41.62	-5.319	-7.813	-10	0.5404	1.036	0.2394
460	-3.311	-0.2991	-34.61	-1.943	-9.025	-40.77	-2.935	-4.553	-5.048	0.6886	2.085	0.057

Table G. part 9: *Continued*

Sequence # (sample #)	Natron log Q/K	Nesquehonite log Q/K	OCP log Q/K	Pirssonite log Q/K	Portlandite log Q/K	Sepiolite log Q/K	Sylvite log Q/K	Thermonatrite log Q/K	Trona log Q/K	Vaterite log Q/K	CO2(aq) act. coef.	CO3-- act. coef.
461	-1.849	-0.7841	-35.7	-0.2977	-8.147	-43.03	-4.354	-3.231	-3.327	0.9972	1.178	0.2019
462	-5.006	-0.7105	-31.23	-3.534	-7.48	-38.33	-5.022	-6.442	-8.483	0.9655	1.034	0.3177
473	-5.6	-1.75	-29.19	-3.89	-8.252	-45.74	-4.7	-7.031	-8.865	1.2	1.031	0.2592
474	-5.599	-1.862	-29.03	-3.877	-8.189	-45.98	-4.667	-7.029	-8.888	1.21	1.033	0.2527
475	-5.751	-2.005	-29.06	-4.175	-8.474	-47.03	-4.539	-7.177	-9.043	1.062	1.041	0.2225
476	-5.6	-1.793	-29.18	-3.877	-8.401	-46.52	-4.646	-7.03	-8.783	1.211	1.033	0.2501
477	-5.359	-1.563	-30.19	-3.94	-8.667	-45.42	-4.327	-6.782	-8.434	0.9016	1.045	0.2196
478	-5.178	-1.386	-29.94	-3.582	-8.254	-43.84	-4.342	-6.6	-8.28	1.078	1.046	0.2156
479	-5.272	-1.492	-29.94	-3.783	-8.251	-43.82	-4.316	-6.693	-8.476	0.9695	1.047	0.213
480	-5.138	-1.381	-29.9	-3.524	-8.234	-43.81	-4.295	-6.559	-8.22	1.094	1.049	0.2096
481	-5.184	-1.438	-29.93	-3.636	-8.244	-43.82	-4.319	-6.605	-8.317	1.029	1.049	0.2096
482	-5.259	-1.501	-30.03	-3.803	-8.286	-43.86	-4.302	-6.68	-8.455	0.9365	1.047	0.2145
483	-5.4	-1.558	-30.22	-4.064	-8.495	-44.4	-4.305	-6.822	-8.623	0.8176	1.047	0.2125
484	-5.315	-1.443	-30.06	-3.842	-8.297	-43.76	-4.377	-6.739	-8.527	0.9562	1.043	0.2214
485	-5.422	-1.502	-30.12	-4.025	-8.329	-43.82	-4.461	-6.848	-8.711	0.8817	1.04	0.2294
486	-6.449	-2.332	-29.85	-5.393	-9.288	-49.5	-5.311	-7.885	-9.952	0.5498	1.024	0.2969
487	-6.933	-1.892	-29.44	-5.513	-8.05	-44.54	-6.096	-8.378	-11.12	0.9224	1.006	0.4958
488	-6.904	-1.813	-29.37	-5.39	-7.847	-43.85	-6.236	-8.349	-11.13	1.015	1.005	0.5017
489	-8.883	-3.194	-31.76	-8.803	-10.56	-54.16	-7.086	-10.33	-13.46	-0.4159	1.002	0.631
490	-6.864	-1.802	-29.38	-5.32	-7.856	-43.96	-6.228	-8.309	-11.05	1.045	1.005	0.5019
522	-8.389	-1.825	3.597	-7.038	-8.97	6.764	-8.018	-9.835	-12.88	0.8535	1.002	0.5774
523	-2.463	-0.8988	1.219	-0.1967	-6.032	11.46	-5.816	-3.888	-4.986	1.751	1.049	0.1846
524	-3.134	-0.9553	2.407	-0.7262	-5.645	12.12	-6.757	-4.57	-6.125	1.902	1.025	0.261
525	-2.229	-1.097	3.616	0.1811	-6.587	10.25	-4.847	-3.646	-4.279	1.888	1.066	0.154
526	-0.8095	-0.4678	1.161	1.903	-6.313	11.76	-4.098	-2.125	-2.044	2.1	1.418	0.06173
527	-7.326	-1.362	-31.65	-6.104	-9.491	4.99	-7.801	-8.772	-11.09	0.7247	1.004	0.5157
528	-7.138	-1.182	2.221	-5.808	-9.23	8.186	-7.815	-8.583	-10.89	0.8321	1.004	0.5087
529	-1.82	-0.4449	0.3916	0.5438	-7.449	12.52	-4.791	-3.217	-3.239	1.823	1.113	0.1217
530	-1.547	-0.7099	0.1107	0.825	-7.12	12.27	-4.574	-2.933	-2.981	1.822	1.152	0.105
531	-7.754	-1.823	-1.897	-7.058	-11.13	-0.3042	-7.267	-9.198	-11.17	0.1979	1.005	0.4429
532	-7.518	-1.563	-33.04	-6.614	-10.67	1.483	-7.519	-8.963	-10.95	0.406	1.005	0.4453
533	-7.455	-1.5	-1.847	-6.859	-10.89	2.198	-7.453	-8.899	-10.9	0.09766	1.005	0.4506
534	-6.947	-1.231	-33.78	-6.056	-10.44	2.456	-7.334	-8.391	-10.21	0.3922	1.006	0.435
535	-5.244	-1.249	-0.7654	-4.284	-10.66	1.707	-6.993	-6.681	-7.508	0.4555	1.015	0.3414
536	-1.267	-1.003	-2.346	0.3515	-7.84	7.595	-4.131	-2.63	-2.557	1.048	1.207	0.06511
537	-1.164	-1.517	-1.963	0.5945	-8.117	5.37	-4.014	-2.512	-2.181	1.174	1.246	0.05747
538	-1.033	-1.089	-2.558	0.7341	-7.427	8.17	-5.849	-2.384	-2.328	1.186	1.277	0.05634
539	-1.32	-1.023	-3.257	0.3975	-7.198	8.004	-4.148	-2.691	-2.915	1.154	1.187	0.07042

Table G. part 9: *Continued*

Sequence # (sample #)	Natron log Q/K	Nesquehonite log Q/K	OCP log Q/K	Pirssonite log Q/K	Portlandite log Q/K	Sepiolite log Q/K	Sylvite log Q/K	Thermonatrite log Q/K	Trona log Q/K	Vaterite log Q/K	CO2(aq) act. coef.	CO3-- act. coef.
540	-6.997	-1.152	-32.64	-5.83	-9.726	7.19	-7.521	-8.442	-10.51	0.6691	1.004	0.4756
541	-7.071	-0.8814	-32.68	-5.78	-9.702	6.603	-7.208	-8.516	-10.57	0.793	1.007	0.4164
542	-6.303	-0.9576	-33.17	-5.205	-9.691	5.135	-7.301	-7.747	-9.518	0.5997	1.008	0.4434
543	-1.756	-1.041	3.286	0.6611	-7.607	11.87	-4.555	-3.147	-3.033	1.871	1.124	0.1066
544	-2.044	-1.306	2.505	0.3214	-7.605	9.618	-5.271	-3.45	-3.505	1.833	1.087	0.1312
545	-1.548	-0.6413	0.8822	0.7646	-7.188	12.49	-4.557	-2.934	-2.977	1.762	1.149	0.09918
546	-1.274	-1.306	1.21	0.9954	-7.229	10.29	-4.34	-2.639	-2.549	1.7	1.217	0.08721
547	-0.6235	-0.5346	0.7007	2.067	-6.832	12.92	-3.593	-1.892	-1.475	2.035	1.568	0.03256
548	-1.667	-1.18	1.565	0.6719	-7.673	9.862	-4.419	-3.053	-2.901	1.789	1.136	0.0988
549	-2.463	-0.6758	1.087	-0.4214	-8.352	9.927	-5.18	-3.877	-3.928	1.516	1.066	0.1742
550	-1.296	-1.156	0.5903	1.113	-7.338	10.68	-4.318	-2.662	-2.458	1.841	1.204	0.07064
551	-0.8379	-1.253	0.606	1.67	-7.361	9.874	-4.074	-2.147	-1.661	1.889	1.409	0.04958
552	-0.9876	-0.5541	-2.044	1.377	-6.967	11.97	-4.013	-2.324	-2.178	1.771	1.306	0.04982
553	-0.9778	-0.782	-0.7284	1.502	-6.932	10.97	-4.02	-2.312	-2.121	1.884	1.313	0.05054
554	-0.9558	-0.621	1.02	1.758	-6.585	13.44	-3.979	-2.288	-2.142	2.115	1.324	0.04995
555	-1.204	-1.558	0.9734	0.9008	-6.819	6.721	-4.939	-2.571	-2.733	1.537	1.216	0.06656
556	-0.9868	-1.441	1.871	1.462	-6.858	7.029	-4.588	-2.326	-2.191	1.857	1.306	0.05609
557	-0.9873	-1.23	1.952	1.445	-7.599	7.97	-4.344	-2.313	-1.818	1.828	1.329	0.05397
558	-1.57	-1.603	2.386	0.7804	-6.365	8.854	-5.409	-2.963	-3.41	1.806	1.136	0.1024
559	-0.8939	-1.223	0.9219	1.327	-7.35	9.371	-4.351	-2.217	-1.906	1.615	1.358	0.04811
560	-7.057	-1.382	-31.98	-5.967	-8.88	4.991	-7.845	-8.503	-11.06	0.5934	1.002	0.5977
561	-0.5081	-1.86	-1.748	1.467	-7.791	5.327	-3.672	-1.739	-1.148	1.287	1.708	0.02805
562	-0.9512	-1.763	1.793	1.338	-7.084	9.16	-4.352	-2.283	-2.098	1.691	1.329	0.05456
563	-0.2293	-1.019	1.505	2.576	-8.298	9.559	-2.994	-1.258	0.1192	1.937	2.636	0.0206
564	-3.4688	-2.4138	3.803	-1.6717	-6.2458	19.6443	-1.6463		-5.7137	0.3724	1.025	0.2689
565	-1.483	-1.495	-14.83	1.677	-5.669	14.68	-2.334	-2.259	-2.674	2.067	1.206	0.003825
566	-7.076	-1.599	-31.77	-6.043	-9.147	5.198	-7.68	-8.522	-10.98	0.5362	1.003	0.5876
567	-0.2245	-0.8363	0.6382	2.497	-7.955	11.2	-2.979	-1.277	-0.1084	1.874	2.47	0.01951
568	-0.117	-1.381	1.096	2.711	-7.74	9.42	-2.938	-1.114	0.04788	1.932	2.867	0.01876
569	-1.171	-1.232	2.056	1.083	-7.222	9.817	-4.19	-2.523	-2.395	1.673	1.252	0.07831
570	-0.1065	-0.7301	3.283	3.154	-7.836	13.44	-2.31	-0.9939	0.4256	2.266	3.255	0.01694
571	-0.2717	-1.119	0.9395	2.378	-8.18	8.871	-2.829	-1.328	-0.1057	1.806	2.401	0.02092
572	-8.282	-2.204	-32.2	-7.736	-9.988	0.9106	-9.613	-9.729	-12.62	0.04881	1.002	0.6389
573	-8.298	-1.484	-30.71	-6.944	-8.937	6.482	-7.997	-9.744	-12.76	0.8569	1.002	0.5783
574	-1.639	-1.45	-2.805	0.008831	-7.711	5.336	-4.589	-3.032	-3.192	1.104	1.125	0.09085
575	-3.769	-0.657	-2.962	-2.411	-8.531	6.385	-5.96	-5.207	-6.161	0.8533	1.017	0.3059
576	-5.558	-1.611	1.218	-4.335	-8.931	5.311	-6.34	-7.002	-8.718	0.724	1.006	0.4862
577	-8.918	-1.839	-31.53	-8.062	-9.712	2.809	-7.981	-10.36	-13.55	0.3595	1.002	0.578

Table G. part 9: *Continued*

Sequence # (sample #)	Natron log Q/K	Nesquehonite log Q/K	OCP log Q/K	Pirssonite log Q/K	Portlandite log Q/K	Sepiolite log Q/K	Sylvite log Q/K	Thermonatrite log Q/K	Trona log Q/K	Vaterite log Q/K	CO2(aq) act. coef.	CO3-- act. coef.
578	-5.467	-3.236	-3.642	-4.856	-9.406	0.1068	-5.929	-6.907	-8.646	0.1082	1.011	0.4011
579	-1.358	-10.03	-38.18	-8.115	-15.48	-21.19	-3.871	-2.656	-3.003	-7.386	1.289	0.07
580	-1.195	-10.03	-38.75	-7.915	-15.91	-20.77	-3.665	-2.46	-2.494	-7.379	1.363	0.05897
581	-0.9298	-10.03	-38.35	-7.563	-16.76	-21.77	-3.426	-2.113	-1.555	-7.364	1.558	0.04243
582	-0.7976	-10.03	-38.94	-7.318	-17.35	-23.37	-3.175	-1.875	-0.9131	-7.345	1.81	0.03363
583	-0.7383	-10.02	-38.93	-7.208	-17.56	-23.6	-3.062	-1.768	-0.65	-7.337	1.923	0.02935
584	-0.6455	-10.02	-39.02	-7.022	-17.8	-22.71	-2.926	-1.583	-0.2652	-7.325	2.203	0.02627
585	-0.5071	-10.01	-39.56	-6.666	-18.07	-18.63	-2.616	-1.237	0.3742	-7.293	2.849	0.02059
586	-0.0473	-10.11	-41.04	-5.948	-15.92	-20.54	-1.84	-0.5587	0.3078	-7.229	4.388	0.02003
587	-0.06779	-10.1	-41.16	-6.045	-15.88	-19.95	-1.839	-0.6501	0.1568	-7.242	3.891	0.01876
588	-0.09991	-10.08	-41.96	-5.767	-15.67	-19.07	-1.595	-0.4227	0.3918	-7.163	4.768	0.02025
589	-0.03129	-10.11	-42.33	-5.755	-15.74	-20.05	-1.687	-0.3904	0.469	-7.187	4.904	0.01969
590	-0.07142	-10.1	-41.34	-5.731	-15.73	-18.95	-1.639	-0.3777	0.4805	-7.17	5.216	0.02162
591	-0.08575	-10.09	-41.64	-5.713	-15.7	-19.1	-1.568	-0.3682	0.4846	-7.158	5.012	0.0208
592	-0.1124	-10.09	-41.18	-5.712	-16.31	-19.6	-1.511	-0.3695	0.7819	-7.153	5.278	0.02239
593	-0.0833	-10.09	-41.82	-5.756	-15.8	-19.33	-1.6	-0.4069	0.4759	-7.167	4.873	0.02071
594	-0.2567	-10.08	-39.76	-6.406	-17.68	-23.84	-2.218	-0.9944	0.5489	-7.276	3.575	0.0263
595	-0.09558	-10.13	-40.32	-6.238	-16.58	-22.24	-2.129	-0.8107	0.2649	-7.289	3.557	0.0196
596	-0.6742	-10.09	-39.06	-7.253	-18.02	-25.84	-2.903	-1.785	-0.4522	-7.374	1.934	0.03799
597	-0.07535	-10.12	-41.5	-6.154	-15.75	-20.22	-2.056	-0.7353	-0.0395	-7.274	3.709	0.0197
598	-0.1031	-10.08	-41.43	-5.752	-15.97	-18.92	-12.29	-0.4074	0.5632	-7.161	4.912	0.02049
599	-0.03823	-10.11	-41.65	-5.904	-15.93	-19.74	-1.883	-0.5185	0.3742	-7.222	4.572	0.02045
600	-0.2286	-10.11	-40.28	-6.545	-16.89	-22.93	-2.288	-1.103	-0.006566	-7.321	2.797	0.02076
601	-0.461	-10.2	-38	-7.166	-16.81	-26.33	-3.074	-1.622	-0.8465	-7.456	1.924	0.02853
602	-2.915	-9.98	-35.52	-9.792	-16.41	-23.43	-4.822	-4.342	-5.047	-7.39	1.042	0.2253
603	-0.8189	-10.08	-39.44	-7.479	-17.7	-25.52	-3.077	-2.016	-0.9486	-7.379	1.625	0.04221
604	-0.766	-10.07	-39.81	-7.386	-17.83	-25.44	-2.967	-1.924	-0.7484	-7.373	1.725	0.03751
605	-0.1997	-10.05	-76.98	-6.072	-15.54	-18.28	-1.717	-0.7209	-0.1038	-7.192	3.73	0.02066
606	-0.06133	-10.1	-41.5	-6.01	-15.89	-19.96	-1.89	-0.6182	0.2088	-7.237	4.06	0.01924
607	-0.08479	-10.09	-76.88	-5.888	-15.88	-19.32	-1.757	-0.5233	0.3497	-7.196	4.553	0.0214
608	-0.1131	-10.11	-76.3	-6.255	-16.15	-20.79	-2.167	-0.8335	0.02185	-7.285	3.435	0.01987
609	-0.1261	-10.11	-40.98	-6.298	-16.14	-20.68	-2.185	-0.8711	-0.03972	-7.292	3.297	0.01948
610	-0.1602	-10.13	-39.94	-6.446	-16.44	-21.58	-2.372	-0.9949	-0.0786	-7.327	3	0.01976
611	-0.3427	-10.13	-39.73	-6.82	-17.07	-23.29	-2.681	-1.351	-0.2884	-7.364	2.329	0.02349
612	-0.2147	-10.05	-41.2	-5.965	-15.64	-17.94	-1.607	-0.6259	0.08515	-7.167	4.1	0.02142
613	-0.187	-10.06	-41.53	-5.902	-16.9	-20.64	-1.653	-0.5566	0.8073	-7.17	4.472	0.02043
614	-0.3234	-10.11	-39.96	-6.705	-17.65	-25.96	-2.642	-1.26	0.1448	-7.332	2.656	0.02358
615	-1.241	-10.08	-36.24	-8.089	-14.65	-78.56	-2.914	-2.547	-3.295	-7.469	1.366	0.05346

Table G. part 9: *Continued*

Sequence # (sample #)	Natron log Q/K	Nesquehonite log Q/K	OCP log Q/K	Pirssonite log Q/K	Portlandite log Q/K	Sepiolite log Q/K	Sylvite log Q/K	Thermonatrite log Q/K	Trona log Q/K	Vaterite log Q/K	CO2(aq) act. coef.	CO3-- act. coef.
616	-0.8851	-10.03	-37.29	-7.337	-14.18	-77.16	-2.563	-1.889	-2.529	-7.342	2.078	0.02751
617	-0.4052	-10.01	-39.81	-6.219	-14.41	-77.73	-1.768	-0.8919	-0.9156	-7.163	3.467	0.01871
618	-1.392	-10.14	-41.43	-7.326	-13.82	-74.52	-2.021	-1.883	-2.757	-7.28	3.467	0.02355
619	-1.382	-10.11	-38.94	-8.056	-13.97	-76.33	-2.937	-2.532	-3.623	-7.434	1.631	0.04082
620	-0.5387	-10.01	-40.6	-6.395	-13.89	-76.83	-1.759	-1.067	-1.432	-7.169	3.338	0.01954
621	-3.011	-2.384	-35.79	-9.863	-15.21	9.962	-4.944	-4.444	-5.787	-7.361	1.03	0.241
622	-3.315	-10.05	-36.99	-10.23	-17.08	-25.01	-4.584	-4.743	-5.337	-7.432	1.034	0.2532
623	-3.365	-9.967	-3.698	-2.523	-7.939	-23.93	-4.644	-4.8	-6.107	0.3343	1.026	0.2675
624	-3.87	-2.525	-5.316	-3.317	-9.764	0.05659	-11.63	-5.304	-6.095	0.04503	1.022	0.3007

Table G. part 10: Aqueous chemistry database of alkaline lake waters compiled from published literature, as well as corresponding results from calculations described in chapters 2 and 3, and investigated in detail in chapter 4.

Sequence # (sample #)	Ca++ act. coef.	CaCO3 act. coef.	Cl- act. coef.	H+ act. coef.	H2PO4- act. coef.	H3PO4 act. coef.	HCO3- act. coef.	HPO4-- act. coef.	Mg++ act. coef.	MgCO3 act. coef.	Na+ act. coef.	OH- act. coef.	PO4--- act. coef.	SiO2(aq) act. coef.
1	0.3001	1	0.7546	0.7551	0.7068	1	0.7199	0.2619	0.3025	1	0.7446	0.725	0.03765	1
2	0.2948	1	0.7503	0.7525	0.7024	1	0.7141	0.2667	0.2931	1	0.7428	0.7292	0.0404	1
3	0.2777	1	0.7247	0.731	0.6748	1	0.6846	0.2456	0.2596	1	0.7318	0.7163	0.03414	1
4	0.221	1	0.7204	0.7055	0.6328	0.9994	0.6625	0.1735	0.2293	1	0.6904	0.6565	0.01407	1
5	0.05439	1	0.5414	0.6427	0.3049	0.9857	0.3706	0.02573	0.06003	1	0.5998	0.5599	0.0002657	1
6	0.07571	1	0.5527	0.6619	0.3377	0.9814	0.398	0.03142	0.07879	1	0.6051	0.5573	0.00036	1
7	0.06643	1	0.5466	0.7558	0.2913	0.9822	0.3558	0.01773	0.07788	1	0.6264	0.5467	0.0000872	1
8	0.04478	1	0.6389	0.7876	0.2159	0.9811	0.3194	0.01304	0.05644	1	0.5876	0.6557	0.00007564	1
9	0.2085	1	0.6852	0.7076	0.6141	0.999	0.6308	0.1738	0.2155	1	0.6966	0.661	0.01466	1
10	0.178	1	0.6734	0.6771	0.5704	1	0.6033	0.1313	0.1888	1	0.6643	0.6153	0.007554	1
11	0.284	1	0.7656	0.7413	0.7135	1	0.7333	0.2859	0.2879	1	0.7502	0.7301	0.05073	1
12	0.2264	1	0.7224	0.7119	0.6532	1	0.6768	0.2113	0.2368	1	0.7119	0.6816	0.02415	1
13	0.2636	1	0.7065	0.7169	0.6452	0.9997	0.6573	0.2112	0.2367	1	0.7092	0.6975	0.02332	1
14	0.137	1	0.6349	0.6654	0.4819	1	0.5309	0.07081	0.1573	1	0.6234	0.5458	0.001718	1
15	0.1703	1	0.6269	0.6413	0.5463	0.998	0.5655	0.1342	0.1512	1	0.6776	0.6248	0.008761	1
16	0.2605	1	0.6956	0.7273	0.6238	0.9986	0.6374	0.1726	0.2381	1	0.6918	0.6751	0.01305	1
17	0.2139	1	0.6671	0.8148	0.5317	0.9978	0.5599	0.06451	0.2295	1	0.6433	0.5694	0.0008712	1
18	0.4455	1	0.8302	0.816	0.8043	0.9999	0.8146	0.4213	0.4387	1	0.8145	0.8094	0.1231	1
19	0.2925	1	0.77	0.7453	0.7034	0.9997	0.7267	0.25	0.2952	1	0.7287	0.7182	0.03427	1
20	0.07439	1	0.5312	0.6071	0.3366	0.993	0.3906	0.03277	0.0722	1	0.6048	0.5406	0.0004052	1
21	0.07917	1	0.5196	0.5852	0.3583	0.971	0.4106	0.04419	0.08509	1	0.6063	0.5353	0.0008584	1
22	0.1626	1	0.639	0.6573	0.5551	0.9989	0.5765	0.1413	0.1658	1	0.6751	0.6261	0.01012	1
23	0.382	1	0.7854	0.7878	0.7559	1	0.7631	0.3317	0.3716	1	0.7816	0.768	0.06574	1
24	0.2471	1	0.7198	0.7187	0.6705	0.9994	0.6835	0.2485	0.2445	1	0.7336	0.7084	0.03705	1
25	0.4594	1	0.8261	0.8193	0.8042	0.9991	0.8102	0.4508	0.4352	1	0.8209	0.8252	0.1512	1
26	0.5573	1	0.8636	0.8612	0.8531	0.9992	0.8564	0.5603	0.5402	1	0.8681	0.8652	0.2581	1
27	0.6607	1	0.9017	0.9	0.8963	0.9998	0.8981	0.6598	0.6482	1	0.903	0.9013	0.374	1
28	0.6228	1	0.888	0.8885	0.8823	0.9997	0.884	0.6296	0.6148	1	0.8942	0.8885	0.3398	1
29	0.6678	1	0.904	0.9039	0.8993	0.9997	0.9009	0.6734	0.6602	1	0.9079	0.9045	0.3979	1
30	0.492	1	0.8125	0.8221	0.8048	0.9997	0.8055	0.4317	0.4594	1	0.8348	0.8124	0.1256	1
31	0.5082	1	0.8388	0.8419	0.83	0.9997	0.8322	0.5071	0.4946	1	0.8555	0.8396	0.2016	1
32	0.6036	1	0.8801	0.8765	0.8717	0.9996	0.8745	0.5935	0.5818	1	0.88	0.8798	0.2873	1
33	0.6262	1	0.8891	0.8841	0.8805	0.9995	0.8835	0.6154	0.6037	1	0.886	0.8887	0.3143	1
34	0.4348	1	0.8069	0.8029	0.7867	0.9994	0.7916	0.4223	0.4059	1	0.815	0.8078	0.13	1
35	0.4276	1	0.8437	0.8231	0.8124	0.999	0.822	0.4992	0.423	1	0.8222	0.8433	0.2162	1
36	0.7356	1	0.9266	0.9261	0.9236	0.9998	0.9249	0.7394	0.7312	1	0.9283	0.9261	0.4947	1

Table G. part 10: *Continued*

Sequence # (sample #)	Ca++ act. coef.	CaCO3 act. coef.	Cl- act. coef.	H+ act. coef.	H2PO4- act. coef.	H3PO4 act. coef.	HCO3- act. coef.	HPO4-- act. coef.	Mg++ act. coef.	MgCO3 act. coef.	Na+ act. coef.	OH- act. coef.	PO4--- act. coef.	SiO2(aq) act. coef.
37	0.5554	1	0.8615	0.858	0.8505	0.9992	0.8538	0.5508	0.533	1	0.8645	0.8626	0.2449	1
38	0.3423	1	0.7661	0.7694	0.7357	0.9985	0.7423	0.3385	0.329	1	0.7801	0.7677	0.07724	1
39	0.6055	1	0.8823	0.8803	0.8746	0.9997	0.8769	0.6089	0.5916	1	0.8853	0.8828	0.313	1
40	0.7226	1	0.9244	0.9239	0.9209	0.9998	0.9222	0.7341	0.7204	1	0.926	0.9243	0.4903	1
41	0.6194	1	0.886	0.8808	0.8772	0.9996	0.8803	0.607	0.5957	1	0.8832	0.8852	0.3041	1
42	0.2685	1	0.7095	0.7355	0.655	0.9999	0.6635	0.2116	0.2548	1	0.7171	0.6986	0.02228	1
43	0.2746	1	0.6949	0.741	0.6452	0.9999	0.6503	0.1876	0.2602	1	0.7152	0.6813	0.01529	1
44	0.1982	1	0.6597	0.6923	0.607	0.9997	0.6154	0.1752	0.1964	1	0.715	0.6576	0.0154	1
45	0.1944	1	0.6547	0.6902	0.5976	0.9997	0.6067	0.165	0.1913	1	0.7082	0.6513	0.01319	1
46	0.2071	1	0.6642	0.6963	0.6093	0.9997	0.618	0.1752	0.2011	1	0.712	0.6606	0.01514	1
47	0.199	1	0.659	0.6906	0.6051	0.9997	0.6138	0.1734	0.1949	1	0.7131	0.6569	0.015	1
48	0.2055	1	0.6647	0.6909	0.6151	0.9997	0.6233	0.1854	0.1997	1	0.7201	0.6642	0.01788	1
49	0.3314	1	0.7651	0.7705	0.7353	0.9998	0.7418	0.3228	0.327	1	0.7759	0.7577	0.06558	1
50	0.3279	1	0.763	0.7711	0.7362	0.9998	0.7419	0.3265	0.3276	1	0.7808	0.7573	0.06806	1
51	0.2389	1	0.716	0.716	0.669	0.9991	0.683	0.2443	0.2426	1	0.7379	0.7016	0.03563	1
52	0.2783	1	0.7397	0.738	0.7003	0.9993	0.7135	0.2776	0.2777	1	0.756	0.7244	0.04726	1
53	0.2559	1	0.7335	0.7247	0.6893	0.9992	0.7042	0.2709	0.2575	1	0.7484	0.7173	0.04618	1
54	0.1697	1	0.6508	0.6712	0.5619	0.9997	0.5855	0.1414	0.1801	1	0.6708	0.6262	0.0098	1
55	0.2989	1	0.765	0.7588	0.7319	0.9995	0.7446	0.3278	0.3049	1	0.7761	0.7513	0.07197	1
56	0.3189	1	0.7946	0.7617	0.7491	0.9998	0.7686	0.3346	0.3268	1	0.7749	0.756	0.07476	1
57	0.2491	1	0.6986	0.6844	0.6336	0.9999	0.6522	0.2113	0.2129	1	0.7039	0.6869	0.02509	1
58	0.1285	1	0.5829	0.6778	0.4227	0.984	0.4707	0.05578	0.1456	1	0.616	0.5494	0.001124	1
59	0.285	1	0.745	0.7418	0.713	0.9994	0.7225	0.3063	0.2835	1	0.7709	0.7378	0.06228	1
60	0.0781	1	0.5268	0.53	0.3248	0.9943	0.3978	0.04221	0.0964	1	0.5605	0.5014	0.001079	1
61	0.1623	1	0.6451	0.6575	0.562	0.9977	0.5892	0.1427	0.1707	1	0.6785	0.6214	0.01024	1
62	0.1925	1	0.688	0.6883	0.6076	0.9998	0.6445	0.1676	0.2056	1	0.6899	0.6407	0.01394	1
63	0.3425	1	0.7692	0.7692	0.7342	0.9998	0.7423	0.3167	0.3277	1	0.7673	0.7585	0.06148	1
64	0.189	1	0.6521	0.6449	0.551	0.9989	0.5821	0.1299	0.1662	1	0.6593	0.6192	0.00779	1
65	0.1717	1	0.6096	0.7808	0.361	0.9962	0.4291	0.02444	0.1529	1	0.6062	0.5224	0.0001256	1
66	0.7821	1	0.9464	0.9438	0.9439	1	0.9456	0.7976	0.785	1	0.9443	0.9434	0.5922	1
67	0.7164	1	0.93	0.9274	0.9264	1	0.9295	0.742	0.7239	1	0.9283	0.9247	0.4979	1
68	0.6856	1	0.9239	0.921	0.9197	0.9999	0.9238	0.7254	0.6963	1	0.9227	0.9174	0.4753	1
69	0.6155	1	0.9038	0.9018	0.898	0.9999	0.9011	0.6657	0.6269	1	0.9039	0.9	0.3872	1
70	0.3435	1	0.8154	0.8133	0.7977	0.9997	0.8033	0.461	0.3718	1	0.8281	0.814	0.1723	1
71	0.6479	1	0.9131	0.9067	0.9063	1	0.9127	0.683	0.6578	1	0.9085	0.9025	0.412	1
72	0.5621	1	0.8913	0.8841	0.8816	1	0.8885	0.6184	0.5794	1	0.8875	0.8801	0.3268	1
73	0.5078	1	0.8761	0.8662	0.8629	0.9999	0.8707	0.5748	0.5264	1	0.8713	0.8641	0.2773	1
74	0.5042	1	0.8714	0.8638	0.8586	0.9999	0.8693	0.5595	0.5223	1	0.8677	0.8558	0.256	1

Table G. part 10: *Continued*

Sequence # (sample #)	Ca++ act. coef.	CaCO3 act. coef.	Cl- act. coef.	H+ act. coef.	H2PO4- act. coef.	H3PO4 act. coef.	HCO3- act. coef.	HPO4-- act. coef.	Mg++ act. coef.	MgCO3 act. coef.	Na+ act. coef.	OH- act. coef.	PO4--- act. coef.	SiO2(aq) act. coef.
75	0.2256	1	0.7357	0.7261	0.6891	0.999	0.7032	0.2984	0.2401	1	0.747	0.733	0.06441	1
76	0.1017	1	0.6056	0.5924	0.4528	0.9914	0.5022	0.1016	0.1069	1	0.6124	0.6046	0.0068	1
77	0.07586	1	0.572	0.564	0.3738	0.9878	0.4408	0.06357	0.08425	1	0.5776	0.5721	0.002746	1
78	0.07067	1	0.6614	0.7765	0.2449	0.9706	0.3615	0.01908	0.0822	1	0.5514	0.6462	0.000198	1
79	0.06956	1	0.68	0.8138	0.2287	0.9675	0.3508	0.01682	0.08369	1	0.5505	0.6625	0.0001531	1
80	0.3398	1	0.7909	0.7779	0.7559	0.999	0.7653	0.3946	0.3361	1	0.7897	0.7925	0.1227	1
81	0.2923	1	0.7458	0.7429	0.6979	0.9981	0.7105	0.2831	0.2769	1	0.7411	0.7405	0.04959	1
82	0.0632	1	0.6291	0.716	0.2635	0.9791	0.3657	0.02111	0.06606	1	0.5643	0.6365	0.0002271	1
83	0.03399	1	0.7129	0.7055	0.1756	0.9607	0.312	0.01547	0.04653	1	0.497	0.7601	0.0001939	1
84	0.03946	1	0.8312	0.8202	0.1651	0.964	0.3232	0.01611	0.06356	1	0.4757	0.8305	0.0002359	1
85	0.1048	1	1.484	4.395	0.1036	0.8816	0.2344	0.0102	0.3094	1	0.7053	1.152	9.826E-06	1
86	0.7661	1	0.9383	0.935	0.935	0.9999	0.9365	0.7657	0.7615	1	0.935	0.9362	0.5327	1
87	0.4662	1	0.8434	0.8357	0.8239	0.9992	0.8293	0.4995	0.4586	1	0.8376	0.8435	0.1996	1
88	0.5892	1	0.8865	0.8828	0.8773	0.9997	0.88	0.6138	0.5847	1	0.8842	0.8862	0.3195	1
89	0.6986	1	0.92	0.9113	0.9126	0.9999	0.9173	0.6977	0.6911	1	0.9112	0.9128	0.4317	1
90	0.6791	1	0.9148	0.9088	0.9082	0.9999	0.9129	0.6881	0.6736	1	0.909	0.9084	0.4166	1
91	0.2643	1	0.7464	0.7239	0.6919	0.997	0.7085	0.3054	0.2511	1	0.7444	0.7479	0.06903	1
92	0.2815	1	0.7676	0.7464	0.7169	0.9987	0.7307	0.3434	0.2757	1	0.7564	0.769	0.09137	1
93	0.7458	1	0.9326	0.9257	0.9275	1	0.9328	0.7407	0.7384	1	0.9258	0.9237	0.4949	1
94	0.7536	1	0.9274	0.9229	0.9241	1	0.9276	0.721	0.7354	1	0.9237	0.9211	0.446	1
95	0.6439	1	0.9039	0.8877	0.8913	0.9999	0.9031	0.6329	0.6326	1	0.8878	0.8855	0.3436	1
96	0.7634	1	0.938	0.9324	0.934	1	0.9373	0.7602	0.7592	1	0.9326	0.932	0.525	1
97	0.6802	1	0.9121	0.902	0.9037	0.9998	0.9098	0.6676	0.6676	1	0.9023	0.9028	0.3838	1
98	0.7817	1	0.9419	0.9366	0.9386	1	0.9422	0.7723	0.7766	1	0.937	0.9349	0.5408	1
99	0.5688	1	0.8871	0.8608	0.8651	0.9998	0.8759	0.5714	0.558	1	0.8602	0.8698	0.2774	1
100	0.6431	1	0.9011	0.8823	0.8876	0.9999	0.8994	0.6162	0.6263	1	0.8828	0.8813	0.318	1
101	0.7189	1	0.9306	0.9283	0.9275	1	0.9305	0.7448	0.7256	1	0.9299	0.9254	0.4991	1
102	0.7341	1	0.9293	0.9212	0.9234	1	0.9286	0.7276	0.726	1	0.9214	0.9206	0.4748	1
103	0.7438	1	0.9321	0.9245	0.9267	1	0.9318	0.7378	0.7363	1	0.9247	0.9236	0.4909	1
104	0.7384	1	0.9306	0.9223	0.9248	1	0.9305	0.731	0.7312	1	0.9225	0.9208	0.4801	1
105	0.4369	1	0.8396	0.8274	0.8163	0.9995	0.8233	0.4949	0.4346	1	0.8311	0.8384	0.2029	1
106	0.7782	1	0.9419	0.9344	0.9374	1	0.9424	0.7698	0.7736	1	0.9345	0.9325	0.5438	1
107	0.7632	1	0.9385	0.9298	0.9332	1	0.939	0.7568	0.759	1	0.9299	0.9279	0.525	1
108	0.487	1	0.8504	0.8395	0.832	0.9998	0.8375	0.5132	0.473	1	0.8425	0.848	0.2112	1
109	0.7916	1	0.945	0.939	0.9414	1	0.9451	0.7828	0.7864	1	0.9391	0.9379	0.563	1
110	0.4572	1	0.8483	0.8374	0.8275	0.9995	0.8336	0.5178	0.4565	1	0.8408	0.8479	0.2258	1
111	0.6238	1	0.8978	0.8845	0.8856	0.9999	0.8932	0.6246	0.6106	1	0.8848	0.8873	0.3329	1
115	0.4607	1	0.8399	0.8338	0.8193	1	0.8235	0.4815	0.4536	1	0.8306	0.8382	0.1786	1

Table G. part 10: *Continued*

Sequence # (sample #)	Ca++ act. coef.	CaCO3 act. coef.	Cl- act. coef.	H+ act. coef.	H2PO4- act. coef.	H3PO4 act. coef.	HCO3- act. coef.	HPO4-- act. coef.	Mg++ act. coef.	MgCO3 act. coef.	Na+ act. coef.	OH- act. coef.	PO4--- act. coef.	SiO2(aq) act. coef.
116	0.3035	1	0.7712	0.7643	0.7223	1	0.7329	0.323	0.301	1	0.7534	0.7651	0.07071	1
117	0.4497	1	0.8304	0.8194	0.8046	1	0.8105	0.4468	0.4296	1	0.8145	0.8257	0.1469	1
118	0.2404	1	0.695	0.736	0.6327	0.9997	0.6427	0.1854	0.2405	1	0.7043	0.6806	0.01597	1
119	0.2138	1	0.7174	0.715	0.6276	1	0.6479	0.2131	0.2097	1	0.6871	0.7062	0.02719	1
120	0.3155	1	0.7728	0.772	0.73	1	0.7385	0.3274	0.3152	1	0.7612	0.7671	0.07109	1
121	0.326	1	0.7765	0.776	0.7364	1	0.7444	0.3351	0.3244	1	0.7663	0.7709	0.07454	1
125	0.5939	1	0.8854	0.8721	0.8715	1	0.8797	0.5822	0.5788	1	0.8713	0.8732	0.2767	1
126	0.3816	1	0.81	0.7939	0.7709	1	0.7818	0.3945	0.3682	1	0.7843	0.8016	0.1129	1
127	0.4309	1	0.8375	0.8105	0.8022	1	0.8131	0.4638	0.4089	1	0.8077	0.8305	0.174	1
128	0.4278	1	0.8347	0.8065	0.7975	1	0.8107	0.4359	0.4105	1	0.8018	0.8181	0.145	1
129	0.5413	1	0.8808	0.8512	0.8561	1	0.8666	0.5426	0.5365	1	0.8509	0.8598	0.2437	1
130	0.5376	1	0.8802	0.8473	0.8534	1	0.8667	0.534	0.5314	1	0.8465	0.8549	0.2353	1
131	0.5158	1	0.875	0.8318	0.8413	1	0.8589	0.5006	0.5051	1	0.8314	0.8409	0.2024	1
132	0.5475	1	0.8851	0.8523	0.8595	1	0.873	0.5483	0.5448	1	0.8522	0.8591	0.2516	1
133	0.5872	1	0.8919	0.8701	0.8738	1	0.8824	0.5862	0.5828	1	0.8695	0.8755	0.2897	1
134	0.6677	1	0.9113	0.9037	0.9037	1	0.9079	0.6714	0.6616	1	0.9039	0.9047	0.3908	1
135	0.306	1	0.7972	0.7766	0.7616	1	0.7811	0.3796	0.3268	1	0.7917	0.7725	0.1067	1
136	0.5271	1	0.8627	0.852	0.8466	1	0.853	0.5311	0.5109	1	0.8521	0.8557	0.2221	1
137	0.649	1	0.9058	0.8941	0.8955	1	0.9036	0.6451	0.6423	1	0.8936	0.8926	0.3572	1
138	0.4766	1	0.8438	0.8299	0.8197	1	0.8276	0.4779	0.4567	1	0.8261	0.8368	0.1747	1
139	0.172	1	0.662	0.734	0.5174	0.9936	0.5905	0.07448	0.1929	1	0.6324	0.5579	0.001586	1
140	0.1943	1	0.6886	0.7164	0.5746	0.9962	0.6565	0.1104	0.2111	1	0.6552	0.5884	0.004191	1
141	0.2257	1	0.712	0.7247	0.6406	0.9989	0.6694	0.189	0.241	1	0.703	0.6693	0.01737	1
142	0.1409	1	0.6064	0.7053	0.4441	0.992	0.5025	0.05366	0.1687	1	0.6188	0.5286	0.00087	1
143	0.186	1	0.664	0.7213	0.561	0.9962	0.5988	0.1166	0.2043	1	0.6614	0.6134	0.005176	1
144	0.1888	1	0.6584	0.7238	0.5562	0.9937	0.5964	0.1084	0.2079	1	0.6607	0.6032	0.004166	1
145	0.2138	1	0.6841	0.7313	0.6064	0.9964	0.6312	0.1539	0.2302	1	0.6869	0.6497	0.01007	1
146	0.1944	1	0.6653	0.8483	0.49	0.9904	0.5629	0.04317	0.2239	1	0.628	0.5207	0.0003172	1
147	0.183	1	0.6914	0.6961	0.6383	0.9992	0.6563	0.2261	0.2082	1	0.7222	0.6797	0.03226	1
148	0.1433	1	0.6281	0.8376	0.3711	0.9495	0.4651	0.02568	0.1797	1	0.5973	0.5054	0.0001383	1
149	0.1906	1	0.7027	0.6994	0.6444	0.9935	0.6741	0.2369	0.2138	1	0.7245	0.6905	0.03714	1
150	0.2376	1	0.6716	1.129	0.4249	0.9829	0.4802	0.02294	0.2922	1	0.652	0.5316	0.00006583	1
151	0.183	1	0.6382	0.7957	0.4951	0.992	0.5288	0.06427	0.2081	1	0.6391	0.5749	0.001074	1
152	0.1099	1	0.6374	0.612	0.5105	0.9895	0.5508	0.1435	0.1115	1	0.6437	0.6479	0.01475	1
153	0.5287	1	0.8615	0.8635	0.8506	0.9998	0.8549	0.5265	0.5344	1	0.8593	0.8549	0.2097	1
154	0.2274	1	0.6847	0.7667	0.5914	0.9962	0.6219	0.119	0.2421	1	0.6699	0.6272	0.004592	1
155	0.2725	1	0.7239	0.7605	0.6634	0.9982	0.6845	0.1971	0.282	1	0.7125	0.6884	0.01724	1
156	0.2606	1	0.6548	1.106	0.4637	0.9844	0.5143	0.02767	0.3135	1	0.6627	0.5266	0.00008695	1

Table G. part 10: *Continued*

Sequence # (sample #)	Ca++ act. coef.	CaCO3 act. coef.	Cl- act. coef.	H+ act. coef.	H2PO4- act. coef.	H3PO4 act. coef.	HCO3- act. coef.	HPO4-- act. coef.	Mg++ act. coef.	MgCO3 act. coef.	Na+ act. coef.	OH- act. coef.	PO4--- act. coef.	SiO2(aq) act. coef.
157	2.773	1	1.311	8.22	0.2062	0.9279	0.3174	0.00167	5.268	1	1.248	0.4527	7.23E-08	1
158	0.2822	1	0.7287	0.7633	0.6736	0.9981	0.6936	0.2101	0.2908	1	0.7204	0.6972	0.02029	1
159	0.6236	1	0.9039	0.8958	0.8953	0.9999	0.9037	0.6481	0.6309	1	0.897	0.8902	0.3616	1
160	0.2797	1	0.7339	0.7596	0.6759	0.9986	0.6975	0.2148	0.288	1	0.7198	0.6993	0.02185	1
161	0.5125	1	0.8599	0.8542	0.8449	0.9998	0.8524	0.5118	0.5175	1	0.8518	0.8469	0.1984	1
162	0.272	1	0.7209	0.7608	0.6611	0.9979	0.6817	0.1933	0.2819	1	0.7121	0.6856	0.01628	1
163	0.3262	1	0.7016	1.436	0.4239	0.9793	0.4947	0.01353	0.4241	1	0.6921	0.482	0.00001217	1
164	0.7782	1	0.9431	0.9423	0.9412	1	0.9424	0.7838	0.7812	1	0.942	0.9408	0.5594	1
165	0.705	1	0.859	2.866	0.3285	0.9707	0.4258	0.004986	1.063	1	0.8428	0.4834	1.091E-06	1
166	0.718	1	0.9235	0.9216	0.9196	1	0.922	0.7119	0.7178	1	0.9206	0.9191	0.441	1
167	1.045	1	0.9541	3.853	0.3084	0.9541	0.4122	0.003201	1.698	1	0.9344	0.4466	2.81E-07	1
168	0.3532	1	1.809	4.247	0.06565	0.4425	0.2384	0.009003	0.5282	1	0.8225	2.171	1.224E-06	1
169	0.6106	1	0.8965	0.8961	0.8903	0.9999	0.8931	0.6353	0.6196	1	0.8959	0.8923	0.3386	1
170	0.5144	1	0.862	0.8628	0.8509	0.9998	0.8551	0.534	0.5245	1	0.861	0.856	0.2209	1
171	0.3898	1	0.8083	0.8111	0.7841	0.9997	0.794	0.3925	0.4008	1	0.8046	0.7945	0.1036	1
172	0.2977	1	0.7524	0.7697	0.7126	0.9991	0.7239	0.2784	0.3106	1	0.7531	0.7364	0.04404	1
173	0.2105	1	0.6768	0.7355	0.5949	0.9969	0.6156	0.1427	0.2262	1	0.6808	0.6442	0.008244	1
174	0.183	1	0.6381	0.7956	0.4951	0.992	0.5288	0.06427	0.2081	1	0.6391	0.5749	0.001074	1
175	0.2374	1	0.6697	1.128	0.4237	0.9828	0.4789	0.0227	0.2929	1	0.6524	0.5295	0.00006412	1
176	0.5869	1	0.8963	0.8741	0.8786	0.9999	0.8884	0.6013	0.5897	1	0.8745	0.8782	0.3115	1
177	0.1433	1	0.6281	0.8376	0.3711	0.9495	0.4651	0.02568	0.1797	1	0.5973	0.5054	0.0001383	1
178	2.743	1	1.31	8.168	0.2063	0.9279	0.318	0.001681	5.201	1	1.244	0.4538	7.39E-08	1
179	0.06212	1	0.8342	1.172	0.1615	0.8417	0.3079	0.01192	0.07327	1	0.5725	0.9461	0.00006041	1
180	0.3092	1	0.7522	0.7683	0.7078	0.999	0.7159	0.2729	0.3091	1	0.7459	0.7403	0.04175	1
181	0.2315	1	0.6892	0.7661	0.5914	0.9946	0.6404	0.1121	0.2441	1	0.6654	0.6136	0.003818	1
182	0.2375	1	0.6697	1.128	0.4237	0.9828	0.4789	0.0227	0.2929	1	0.6524	0.5295	0.00006413	1
183	0.6319	1	0.9122	0.9095	0.9071	0.9999	0.9129	0.6908	0.6507	1	0.9122	0.9034	0.4245	1
184	0.2146	1	0.687	0.7328	0.6015	0.9986	0.6376	0.1383	0.2311	1	0.679	0.6303	0.007331	1
185	0.1463	1	0.6231	0.9172	0.3427	0.9893	0.4148	0.0228	0.1775	1	0.6174	0.549	0.0001283	1
186	0.1888	1	0.6584	0.7238	0.5562	0.9937	0.5964	0.1084	0.2079	1	0.6607	0.6032	0.004166	1
187	0.1682	1	0.6446	0.7718	0.4746	0.9948	0.5372	0.04945	0.1955	1	0.6234	0.5261	0.0005476	1
188	0.08261	1	0.6295	0.5968	0.4706	0.9953	0.5173	0.1206	0.08295	1	0.6223	0.6459	0.01105	1
189	0.1119	1	0.643	0.6298	0.513	0.9938	0.5502	0.1391	0.1135	1	0.644	0.6512	0.01303	1
190	0.7023	1	0.9255	0.9232	0.9218	1	0.9246	0.7303	0.7095	1	0.9243	0.9215	0.4795	1
191	0.2898	1	0.7384	0.7658	0.6958	0.9989	0.7052	0.2543	0.2989	1	0.7418	0.7254	0.03451	1
192	0.1736	1	0.626	0.8108	0.4619	0.9962	0.5111	0.04959	0.2046	1	0.6322	0.5456	0.000588	1
193	0.182	1	0.6751	0.6898	0.5998	0.9959	0.6319	0.1732	0.2009	1	0.6919	0.6491	0.01594	1
194	1.684	1	1.274	7.611	0.2124	0.8188	0.2754	0.001788	3.643	1	1.124	0.4687	3.214E-08	1

Table G. part 10: *Continued*

Sequence # (sample #)	Ca++ act. coef.	CaCO3 act. coef.	Cl- act. coef.	H+ act. coef.	H2PO4- act. coef.	H3PO4 act. coef.	HCO3- act. coef.	HPO4-- act. coef.	Mg++ act. coef.	MgCO3 act. coef.	Na+ act. coef.	OH- act. coef.	PO4--- act. coef.	SiO2(aq) act. coef.
195	0.1885	1	0.6711	0.7293	0.5504	0.9925	0.6333	0.09362	0.2068	1	0.6475	0.5751	0.002734	1
196	0.2473	1	0.7127	0.7478	0.6325	0.9985	0.6832	0.1529	0.2583	1	0.687	0.6417	0.008829	1
197	0.239	1	0.7406	1.165	0.445	0.9889	0.611	0.01528	0.2983	1	0.6383	0.4281	0.00001668	1
199	0.1902	1	0.6926	0.6874	0.5949	0.9985	0.6203	0.1826	0.1854	1	0.6735	0.6782	0.01935	1
200	0.1705	1	0.6794	0.6787	0.5852	0.9985	0.6096	0.1769	0.1741	1	0.6764	0.6686	0.01853	1
201	0.181	1	0.6882	0.6854	0.594	0.9979	0.6185	0.1843	0.1814	1	0.6777	0.6774	0.0202	1
202	0.1946	1	0.6952	0.6932	0.6047	0.9984	0.6273	0.1913	0.1905	1	0.6821	0.6845	0.02143	1
203	0.4535	1	0.7202	0.8044	0.7321	0.9982	0.7205	0.2309	0.4268	1	0.7961	0.7092	0.01909	1
204	0.1835	1	0.6846	0.6867	0.5946	0.9983	0.6174	0.1812	0.1842	1	0.6803	0.6733	0.01893	1
205	0.1813	1	0.6874	0.6861	0.5947	0.9985	0.6184	0.1837	0.1822	1	0.6788	0.6761	0.0199	1
206	0.1765	1	0.6832	0.6841	0.5908	0.9984	0.6144	0.1802	0.1791	1	0.6787	0.6725	0.01904	1
207	0.1752	1	0.6819	0.6832	0.5889	0.9984	0.6126	0.1785	0.1778	1	0.6779	0.6712	0.01864	1
208	0.4551	1	0.8538	0.8378	0.8327	1	0.8417	0.4985	0.4679	1	0.8419	0.8374	0.196	1
209	0.2888	1	0.7866	0.7627	0.7222	0.9992	0.7426	0.3372	0.292	1	0.7434	0.7744	0.08435	1
210	0.2394	1	0.7133	0.752	0.6302	0.9964	0.6563	0.173	0.248	1	0.6877	0.6779	0.0132	1
211	0.2093	1	0.7164	0.7327	0.5946	0.9962	0.6821	0.122	0.2199	1	0.6521	0.6107	0.005313	1
212	0.21	1	0.7018	0.7501	0.5907	0.9963	0.6304	0.1351	0.2205	1	0.6608	0.6484	0.007217	1
213	0.1855	1	0.7021	0.7587	0.545	0.9937	0.6243	0.08726	0.1991	1	0.6283	0.5913	0.002307	1
214	0.1609	1	0.7084	0.7666	0.5126	0.9921	0.5801	0.0855	0.1732	1	0.6122	0.6218	0.002669	1
215	0.1975	1	0.6876	0.8597	0.5032	0.9905	0.5799	0.04722	0.222	1	0.6238	0.5388	0.0003967	1
216	0.1424	1	0.7407	0.865	0.4268	0.9509	0.5405	0.04199	0.1579	1	0.5812	0.6087	0.0004935	1
217	0.7031	1	0.8662	2.851	0.3325	0.9708	0.431	0.005119	1.038	1	0.8389	0.4896	1.169E-06	1
218	2.747	1	1.313	8.062	0.208	0.9281	0.3209	0.001691	5.097	1	1.239	0.4569	7.562E-08	1
219	0.3999	1	0.8235	1.981	0.3477	0.9652	0.4487	0.008874	0.5435	1	0.7313	0.5443	6.225E-06	1
220	0.2907	1	0.7837	1.545	0.3726	0.9698	0.4745	0.0132	0.3731	1	0.677	0.5535	0.00001846	1
221	0.2684	1	0.7766	1.459	0.3774	0.9726	0.4766	0.01479	0.3411	1	0.6656	0.561	0.00002586	1
222	0.2502	1	0.7612	1.365	0.3865	0.9746	0.4804	0.01697	0.3131	1	0.6554	0.5658	0.00003723	1
223	0.2185	1	0.7625	1.259	0.3878	0.976	0.4849	0.02018	0.2683	1	0.6372	0.584	0.00006553	1
224	0.2114	1	0.7797	1.27	0.3767	0.974	0.4819	0.01992	0.2589	1	0.6326	0.5983	0.00007004	1
225	0.6518	1	0.9097	0.8896	0.896	1	0.9047	0.6425	0.6461	1	0.89	0.8928	0.36	1
226	0.6636	1	0.9119	0.8924	0.899	1	0.9106	0.6501	0.6559	1	0.8927	0.8913	0.369	1
227	0.6741	1	0.914	0.8961	0.9023	1	0.9153	0.6591	0.6658	1	0.8963	0.8917	0.3799	1
228	0.5439	1	0.8783	0.8383	0.8487	0.9999	0.8674	0.5139	0.5262	1	0.8389	0.8442	0.212	1
229	0.388	1	0.8406	0.7479	0.7643	0.9999	0.8047	0.3353	0.3549	1	0.7494	0.7626	0.07756	1
230	0.4928	1	0.8562	0.8042	0.8156	1	0.8348	0.4332	0.4568	1	0.806	0.8158	0.1369	1
232	0.4286	1	0.839	0.7699	0.7818	0.9999	0.8087	0.3692	0.3898	1	0.7733	0.7839	0.0948	1
234	0.362	1	0.8367	0.7298	0.7472	0.9999	0.7894	0.3062	0.3264	1	0.7314	0.7488	0.06271	1
235	0.3276	1	0.8275	0.6906	0.7098	0.9999	0.7683	0.2455	0.2754	1	0.6937	0.7099	0.03619	1

Table G. part 10: *Continued*

Sequence # (sample #)	Ca++ act. coef.	CaCO3 act. coef.	Cl- act. coef.	H+ act. coef.	H2PO4- act. coef.	H3PO4 act. coef.	HCO3- act. coef.	HPO4-- act. coef.	Mg++ act. coef.	MgCO3 act. coef.	Na+ act. coef.	OH- act. coef.	PO4--- act. coef.	SiO2(aq) act. coef.
236	0.8533	1	0.9625	0.9589	0.9607	1	0.9632	0.8507	0.852	1	0.959	0.9575	0.6892	1
237	0.5419	1	0.8781	0.8393	0.849	1	0.8681	0.5147	0.5265	1	0.8396	0.8436	0.2126	1
238	0.5843	1	0.8887	0.8587	0.8668	1	0.8811	0.56	0.5704	1	0.8591	0.8625	0.2581	1
239	0.6626	1	0.9113	0.8915	0.898	0.9999	0.9054	0.647	0.6537	1	0.8917	0.8967	0.3642	1
240	0.8468	1	0.961	0.9577	0.9591	1	0.9612	0.8458	0.8455	1	0.9578	0.9569	0.6791	1
241	0.6946	1	0.9188	0.9038	0.9091	1	0.9168	0.679	0.6858	1	0.9041	0.9045	0.4048	1
242	0.8038	1	0.9496	0.9436	0.9462	1	0.9485	0.8001	0.8016	1	0.9437	0.9448	0.5973	1
243	0.8553	1	0.9637	0.9607	0.962	1	0.9629	0.8569	0.8555	1	0.9608	0.9618	0.7025	1
244	0.6564	1	0.9103	0.8904	0.897	1	0.9078	0.6442	0.6493	1	0.8908	0.8907	0.3609	1
245	0.4514	1	0.8526	0.787	0.8006	1	0.8254	0.4039	0.4225	1	0.7885	0.8007	0.1192	1
246	0.3062	1	0.8266	0.6763	0.6955	0.9999	0.7579	0.227	0.2553	1	0.6794	0.6972	0.03021	1
247	0.3765	1	0.8306	0.7322	0.7479	1	0.7905	0.3054	0.3313	1	0.7353	0.7469	0.06041	1
248	0.3704	1	0.8346	0.7394	0.7538	1	0.7923	0.3168	0.3394	1	0.7414	0.7541	0.06734	1
249	0.3725	1	0.8348	0.7402	0.7546	1	0.7927	0.3187	0.3405	1	0.7422	0.7555	0.06833	1
250	0.1088	1	0.578	0.5644	0.5023	0.9996	0.522	0.1249	0.09327	1	0.6845	0.6015	0.009331	1
251	0.1182	1	0.6141	0.5946	0.5384	0.9997	0.5589	0.1584	0.1098	1	0.6922	0.633	0.01715	1
252	0.1052	1	0.5774	0.562	0.497	0.9998	0.5182	0.1227	0.09036	1	0.6795	0.6015	0.009129	1
253	0.1181	1	0.6139	0.5945	0.5383	0.9997	0.5587	0.1583	0.1098	1	0.6923	0.6328	0.01712	1
254	0.07538	1	0.5336	0.522	0.4362	0.9987	0.4629	0.08646	0.06546	1	0.6577	0.5665	0.004269	1
255	0.1329	1	0.6237	0.6185	0.5634	0.9994	0.5788	0.1719	0.1302	1	0.7101	0.6391	0.01945	1
256	0.05343	1	0.5148	0.4859	0.3847	0.999	0.4238	0.06872	0.04663	1	0.625	0.5592	0.003049	1
257	0.04934	1	0.541	0.4933	0.3885	0.999	0.4364	0.07809	0.04577	1	0.6096	0.5826	0.004772	1
258	0.7058	1	0.9205	0.9107	0.9135	0.9999	0.9183	0.6937	0.6962	1	0.9115	0.9118	0.4196	1
259	0.5458	1	0.866	0.8326	0.8398	1	0.8518	0.4904	0.5103	1	0.8347	0.8413	0.181	1
260	0.5248	1	0.8613	0.8227	0.8305	1	0.8454	0.4711	0.4875	1	0.8243	0.8324	0.1658	1
261	0.3053	1	0.7574	0.7041	0.6791	0.9986	0.7018	0.2927	0.2372	1	0.7113	0.7545	0.06145	1
262	0.5121	1	0.8422	0.8259	0.8208	0.9997	0.8266	0.4803	0.461	1	0.8282	0.8403	0.1729	1
263	0.5529	1	0.8602	0.8387	0.8397	0.9998	0.8472	0.5039	0.507	1	0.8405	0.8492	0.1912	1
264	0.3952	1	0.803	0.767	0.7561	0.9992	0.7702	0.3805	0.3393	1	0.77	0.7963	0.1062	1
265	0.2854	1	0.7381	0.7034	0.6761	0.9986	0.6935	0.2846	0.2356	1	0.7276	0.7399	0.05708	1
266	0.3969	1	0.7964	0.7758	0.762	0.9994	0.7711	0.3925	0.3522	1	0.7872	0.7966	0.114	1
267	0.3748	1	0.7816	0.7565	0.7417	0.9993	0.7531	0.3578	0.3234	1	0.7719	0.7791	0.09125	1
268	0.4071	1	0.8073	0.7741	0.7635	0.9991	0.7762	0.3944	0.3503	1	0.7763	0.8037	0.1155	1
269	0.2347	1	0.678	0.5971	0.542	0.9957	0.5834	0.164	0.1333	1	0.6296	0.6834	0.01712	1
271	0.3831	1	0.6469	0.7629	0.673	1	0.6516	0.1634	0.3478	1	0.7939	0.6401	0.007649	1
272	0.1454	1	0.621	0.6638	0.4939	0.998	0.5229	0.09395	0.1296	1	0.6421	0.6135	0.003724	1
274	0.1263	1	0.6035	0.6674	0.4515	0.9973	0.4874	0.06925	0.1129	1	0.6286	0.5951	0.001838	1
275	0.1351	1	0.6105	0.6718	0.4549	0.9971	0.492	0.07057	0.1174	1	0.6259	0.5996	0.0019	1

Table G. part 10: *Continued*

Sequence # (sample #)	Ca++ act. coef.	CaCO3 act. coef.	Cl- act. coef.	H+ act. coef.	H2PO4- act. coef.	H3PO4 act. coef.	HCO3- act. coef.	HPO4-- act. coef.	Mg++ act. coef.	MgCO3 act. coef.	Na+ act. coef.	OH- act. coef.	PO4--- act. coef.	SiO2(aq) act. coef.
278	0.132	1	0.6102	0.6614	0.4672	0.9975	0.501	0.07901	0.1173	1	0.6325	0.6029	0.002531	1
283	0.1909	1	0.6563	0.6875	0.5797	0.9991	0.594	0.1519	0.1792	1	0.6872	0.6513	0.01097	1
284	0.193	1	0.6666	0.688	0.5825	0.9989	0.5998	0.1591	0.1793	1	0.6816	0.6609	0.01266	1
285	0.1993	1	0.6706	0.6897	0.5909	0.9989	0.6072	0.1665	0.1847	1	0.6866	0.6656	0.01409	1
287	0.3071	1	0.7446	0.7383	0.7003	0.9996	0.7099	0.291	0.2779	1	0.7485	0.7433	0.054	1
288	0.4259	1	0.8088	0.8051	0.7869	1	0.7912	0.4157	0.4029	1	0.8099	0.8073	0.1227	1
289	0.3221	1	0.7526	0.747	0.713	0.9996	0.7215	0.3067	0.2935	1	0.7579	0.7515	0.06081	1
290	0.5804	1	0.878	0.8699	0.8668	0.9999	0.8711	0.583	0.5597	1	0.8725	0.8749	0.2786	1
291	0.55	1	0.8625	0.8569	0.8505	0.9999	0.8541	0.5398	0.527	1	0.8593	0.8602	0.2274	1
292	0.5923	1	0.8831	0.8792	0.8749	0.9999	0.878	0.5975	0.5802	1	0.8813	0.8802	0.2906	1
293	0.5385	1	0.8586	0.8534	0.8462	0.9998	0.8498	0.5315	0.5169	1	0.8564	0.8565	0.2198	1
294	0.594	1	0.8814	0.8765	0.8724	0.9999	0.8756	0.5897	0.577	1	0.878	0.8785	0.2806	1
295	0.5935	1	0.883	0.8791	0.8748	0.9999	0.8779	0.5968	0.5806	1	0.8812	0.8801	0.2895	1
296	0.611	1	0.8857	0.8704	0.8725	0.9999	0.8823	0.5791	0.585	1	0.8718	0.8709	0.2689	1
297	0.6004	1	0.882	0.878	0.8736	0.9999	0.8767	0.6002	0.5874	1	0.8824	0.8793	0.2997	1
298	0.1586	1	0.644	0.6774	0.5296	0.9982	0.5551	0.1189	0.1476	1	0.6536	0.6359	0.006556	1
299	0.6891	1	0.916	0.9088	0.9098	1	0.9155	0.685	0.6819	1	0.9099	0.9064	0.4053	1
300	0.6062	1	0.8869	0.8752	0.8751	0.9999	0.8833	0.591	0.5884	1	0.8765	0.875	0.2845	1
301	0.8032	1	0.9514	0.9499	0.9498	1	0.9514	0.816	0.8063	1	0.9506	0.9484	0.6203	1
302	0.7681	1	0.9394	0.9349	0.9362	1	0.9396	0.7668	0.7649	1	0.9355	0.9332	0.5327	1
303	0.07241	1	1.05	0.6118	0.4411	0.9962	0.7109	0.03576	0.07674	1	0.4843	0.4945	0.0003893	1
304	0.1587	1	0.8504	0.6323	0.6165	1	0.7222	0.1799	0.1576	1	0.6122	0.6646	0.02236	1
306	0.1764	1	0.8522	0.6244	0.6307	1	0.7384	0.1579	0.1732	1	0.6176	0.6331	0.01415	1
307	0.2285	1	0.8499	0.6752	0.6874	0.9996	0.7643	0.252	0.2236	1	0.6697	0.7115	0.04761	1
308	0.3165	1	0.7642	0.6721	0.664	1	0.7038	0.2227	0.2309	1	0.6869	0.7009	0.02818	1
309	0.2465	1	0.8353	0.6978	0.7003	1	0.7582	0.2861	0.2405	1	0.6912	0.7371	0.06432	1
310	0.2057	1	0.852	0.6554	0.6683	1	0.8229	0.2183	0.2029	1	0.6486	0.6598	0.03344	1
311	0.3013	1	0.849	0.7217	0.738	0.9994	0.7972	0.3102	0.2977	1	0.7194	0.7441	0.0727	1
313	0.3529	1	0.8474	0.7558	0.7671	1	0.8059	0.3615	0.3474	1	0.7537	0.7754	0.1007	1
314	0.4368	1	0.8625	0.7986	0.8102	1	0.8401	0.4398	0.4305	1	0.7975	0.8104	0.1556	1
315	0.4446	1	0.8646	0.8027	0.8145	1	0.8524	0.4483	0.4397	1	0.8015	0.8065	0.163	1
316	0.4825	1	0.8627	0.8273	0.8293	0.9999	0.8457	0.491	0.4724	1	0.8256	0.837	0.1955	1
317	0.523	1	0.8808	0.8407	0.8494	1	0.8706	0.5301	0.5171	1	0.8402	0.8465	0.2378	1
319	0.5392	1	0.8795	0.8415	0.8505	1	0.8664	0.5235	0.527	1	0.8419	0.8495	0.2242	1
320	0.558	1	0.8876	0.8508	0.8607	1	0.8771	0.5489	0.5505	1	0.851	0.8574	0.2534	1
321	0.5722	1	0.8851	0.8642	0.8663	0.9999	0.8786	0.5722	0.563	1	0.8637	0.8664	0.2738	1
322	0.5595	1	0.8822	0.8545	0.8589	0.9995	0.869	0.5552	0.5452	1	0.8549	0.8659	0.258	1
323	0.559	1	0.8857	0.8503	0.8596	1	0.8751	0.5442	0.5494	1	0.8507	0.8565	0.2456	1

Table G. part 10: *Continued*

Sequence # (sample #)	Ca++ act. coef.	CaCO3 act. coef.	Cl- act. coef.	H+ act. coef.	H2PO4- act. coef.	H3PO4 act. coef.	HCO3- act. coef.	HPO4-- act. coef.	Mg++ act. coef.	MgCO3 act. coef.	Na+ act. coef.	OH- act. coef.	PO4--- act. coef.	SiO2(aq) act. coef.
325	0.5964	1	0.887	0.868	0.8708	1	0.8786	0.5819	0.5765	1	0.8689	0.8743	0.2803	1
329	0.5668	1	0.8865	0.8536	0.8624	1	0.8773	0.551	0.5569	1	0.8546	0.8585	0.2516	1
330	0.6074	1	0.8983	0.8724	0.8797	1	0.8924	0.5994	0.6001	1	0.8728	0.8755	0.3082	1
331	0.6104	1	0.8966	0.8789	0.8818	1	0.8924	0.61	0.6026	1	0.8788	0.8796	0.3169	1
332	0.5884	1	0.894	0.8671	0.8742	1	0.8868	0.5847	0.5831	1	0.8679	0.8708	0.2899	1
333	0.5911	1	0.8864	0.8622	0.8677	1	0.8765	0.5653	0.5729	1	0.8634	0.8689	0.2604	1
334	0.6256	1	0.9015	0.8806	0.886	1	0.8959	0.6184	0.6165	1	0.8809	0.8841	0.329	1
335	0.6133	1	0.8924	0.8725	0.8773	1	0.8847	0.5898	0.5968	1	0.8742	0.8776	0.286	1
336	0.6393	1	0.9003	0.8807	0.8863	1	0.8938	0.6129	0.6229	1	0.8816	0.8855	0.3147	1
337	0.6412	1	0.9012	0.8823	0.8876	1	0.8952	0.6171	0.6258	1	0.8832	0.8865	0.3202	1
338	0.6638	1	0.911	0.8937	0.8992	1	0.9106	0.6514	0.6549	1	0.8941	0.8914	0.3681	1
340	0.6622	1	0.9076	0.8914	0.8962	1	0.9033	0.641	0.6492	1	0.8921	0.894	0.3498	1
341	0.68	1	0.9156	0.9023	0.9061	1	0.9149	0.6726	0.6741	1	0.9027	0.9001	0.3956	1
342	0.6516	1	0.9029	0.8864	0.891	1	0.8972	0.6258	0.6354	1	0.8876	0.8905	0.3282	1
343	0.6823	1	0.9177	0.9021	0.9074	1	0.917	0.6759	0.6778	1	0.9026	0.9004	0.4034	1
345	0.6715	1	0.9089	0.8942	0.8986	1	0.9052	0.6477	0.6567	1	0.8951	0.8965	0.357	1
346	0.7006	1	0.918	0.9056	0.9097	1	0.9174	0.6803	0.6887	1	0.9062	0.9042	0.4015	1
347	0.7813	1	0.9382	0.9394	0.9379	1	0.9379	0.7679	0.7726	1	0.9408	0.9379	0.5134	1
348	0.7091	1	0.9211	0.9094	0.9134	1	0.9199	0.6918	0.6984	1	0.9099	0.9092	0.4184	1
349	0.7277	1	0.9265	0.9162	0.9198	1	0.925	0.7121	0.7183	1	0.9166	0.9167	0.4491	1
352	0.7367	1	0.9298	0.9212	0.9242	1	0.9301	0.7261	0.7299	1	0.9218	0.9189	0.469	1
353	0.7464	1	0.9319	0.9236	0.9267	1	0.9326	0.7332	0.7389	1	0.924	0.9209	0.4797	1
356	0.2311	1	0.7079	0.6921	0.6506	0.9974	0.6662	0.2543	0.2107	1	0.7288	0.7149	0.0449	1
357	0.3924	1	0.7909	0.7798	0.7611	0.999	0.7689	0.3852	0.3582	1	0.7921	0.7919	0.1072	1
358	0.2321	1	0.6964	0.7114	0.626	0.9989	0.64	0.1963	0.216	1	0.7007	0.6895	0.02033	1
359	0.1127	1	0.6135	0.6291	0.4452	0.9957	0.4902	0.07928	0.09628	1	0.6151	0.6147	0.003073	1
361	0.9342	1	0.9837	0.9832	0.9834	1	0.9838	0.9357	0.9346	1	0.9833	0.9828	0.8591	1
368	0.5545	1	0.8704	0.8668	0.8592	1	0.8628	0.5556	0.5453	1	0.8656	0.8663	0.243	1
370	0.6771	1	0.9123	0.9042	0.9055	1	0.9118	0.6724	0.6679	1	0.9055	0.902	0.3876	1
371	0.6369	1	0.8985	0.8893	0.8898	0.9999	0.8966	0.6291	0.623	1	0.891	0.8882	0.3291	1
372	0.7306	1	0.9291	0.9237	0.9248	1	0.9294	0.7311	0.7263	1	0.9246	0.921	0.475	1
373	0.2077	1	0.711	0.7128	0.6105	0.9999	0.6341	0.186	0.2009	1	0.6755	0.6904	0.01889	1
374	0.3922	1	0.7943	0.7896	0.7599	0.9996	0.7684	0.3474	0.3732	1	0.7788	0.7803	0.07558	1
375	0.7844	1	0.9445	0.9418	0.9422	1	0.9448	0.7878	0.7831	1	0.9423	0.9396	0.5676	1
376	0.7106	1	0.924	0.9174	0.9185	1	0.924	0.7106	0.7089	1	0.9177	0.9141	0.4455	1
377	0.3511	1	0.7833	0.7675	0.7375	0.9997	0.7492	0.3344	0.3267	1	0.7611	0.7724	0.07419	1
378	0.3482	1	0.7813	0.7669	0.7361	0.9997	0.7476	0.333	0.325	1	0.7615	0.7711	0.07355	1
381	0.7918	1	0.9465	0.9432	0.9441	1	0.9468	0.7936	0.7908	1	0.9437	0.9412	0.579	1

Table G. part 10: *Continued*

Sequence # (sample #)	Ca++ act. coef.	CaCO3 act. coef.	Cl- act. coef.	H+ act. coef.	H2PO4- act. coef.	H3PO4 act. coef.	HCO3- act. coef.	HPO4-- act. coef.	Mg++ act. coef.	MgCO3 act. coef.	Na+ act. coef.	OH- act. coef.	PO4--- act. coef.	SiO2(aq) act. coef.
382	0.1725	1	0.7046	0.7761	0.5222	0.9981	0.5817	0.08202	0.1857	1	0.6189	0.6081	0.002173	1
383	0.1929	1	0.6667	0.688	0.5826	0.9989	0.5999	0.1591	0.1793	1	0.6816	0.6609	0.01266	1
384	0.2699	1	0.7185	0.7298	0.6694	0.9994	0.6784	0.2419	0.2542	1	0.7322	0.7147	0.03326	1
385	0.7748	1	0.944	0.9418	0.9417	1	0.9437	0.7881	0.7787	1	0.9424	0.9402	0.5711	1
386	0.6331	1	1.131	3.069	0.3059	0.9811	0.4135	0.003783	0.9711	1	0.8183	0.4842	6.363E-07	1
387	0.2115	1	0.6863	0.7773	0.5639	0.9979	0.6196	0.09305	0.2264	1	0.6486	0.596	0.002435	1
388	0.2312	1	0.7071	0.7482	0.6102	0.9967	0.6788	0.1338	0.2416	1	0.67	0.6254	0.006387	1
389	0.4162	1	0.8118	0.8096	0.7837	0.9998	0.8001	0.3741	0.4165	1	0.797	0.7861	0.08877	1
390	0.3034	1	0.7667	0.7577	0.7053	0.999	0.7538	0.2516	0.3065	1	0.7299	0.7107	0.03398	1
392	0.6817	1	0.9085	0.8966	0.9	1	0.9105	0.6436	0.6666	1	0.8967	0.8899	0.3435	1
393	0.6291	1	0.8882	0.8768	0.8773	1	0.8831	0.5717	0.6133	1	0.8756	0.8737	0.2506	1
394	0.5793	1	0.8814	0.8582	0.8624	1	0.8859	0.5381	0.5692	1	0.857	0.8439	0.2261	1
395	0.7064	1	0.9199	0.9095	0.9128	1	0.9218	0.6896	0.697	1	0.9101	0.9041	0.4135	1
396	1.111	1	1.033	4.203	0.2697	0.986	0.3871	0.003418	1.763	1	0.9537	0.5015	6.134E-07	1
397	0.6498	1	0.9065	0.8876	0.8931	0.9999	0.9047	0.6349	0.6396	1	0.8879	0.8869	0.3476	1
398	0.3758	1	0.8179	0.7828	0.769	0.9998	0.7862	0.3876	0.3617	1	0.7773	0.7957	0.1117	1
399	0.3747	1	0.8238	0.7791	0.771	0.9992	0.7899	0.4073	0.3555	1	0.7781	0.8045	0.1328	1
400	0.2363	1	0.8335	0.6893	0.6902	0.9993	0.754	0.2752	0.2288	1	0.6828	0.7307	0.05952	1
401	0.05605	1	1.155	0.5156	0.449	0.996	0.7733	0.05703	0.05595	1	0.4614	0.5362	0.001881	1
402	0.1694	1	0.8623	0.6312	0.6334	0.9992	0.7419	0.1937	0.1665	1	0.6197	0.671	0.02704	1
403	0.1536	1	0.8763	0.6117	0.6167	0.9981	0.7381	0.1713	0.1509	1	0.6017	0.6522	0.02036	1
404	0.02808	1	1.829	0.5496	0.3166	0.996	0.8917	0.04631	0.02836	1	0.4011	0.7416	0.003729	1
405	0.4004	1	0.8537	0.7839	0.7928	0.9997	0.8294	0.4111	0.3956	1	0.7816	0.7955	0.1346	1
406	0.1184	1	0.8914	0.593	0.5671	0.9985	0.7168	0.1384	0.1179	1	0.5657	0.6309	0.01315	1
408	0.4237	1	0.8519	0.7871	0.7963	0.9995	0.8229	0.4125	0.4077	1	0.7865	0.8036	0.1314	1
409	0.5461	1	0.8812	0.8495	0.8554	0.9999	0.874	0.5436	0.5353	1	0.8489	0.8526	0.2468	1
410	0.1989	1	0.7832	0.6857	0.6295	0.9991	0.6939	0.1763	0.2005	1	0.6495	0.6679	0.01691	1
411	0.4806	1	0.8575	0.8256	0.8253	0.9997	0.843	0.4823	0.4675	1	0.8239	0.8325	0.1852	1
412	0.1261	1	0.8406	0.6231	0.5645	0.9973	0.6808	0.156	0.1257	1	0.5838	0.6639	0.01786	1
413	0.3114	1	0.8501	0.7301	0.7459	1	0.804	0.3261	0.3079	1	0.7273	0.751	0.08198	1
414	0.2973	1	0.8135	0.7408	0.727	0.9992	0.7643	0.3282	0.2894	1	0.731	0.7638	0.08168	1
415	0.5526	1	0.8609	0.8477	0.8449	0.9998	0.8504	0.523	0.5204	1	0.8513	0.854	0.212	1
416	0.07966	1	0.9303	0.589	0.4816	0.9963	0.6718	0.1072	0.08043	1	0.5191	0.6463	0.009647	1
417	0.4772	1	0.8458	0.8164	0.8147	0.9998	0.8261	0.4707	0.4436	1	0.818	0.8328	0.1735	1
418	0.4132	1	0.858	0.7862	0.7981	0.9998	0.8325	0.4174	0.4059	1	0.7848	0.7999	0.139	1
419	0.3343	1	0.7939	0.7604	0.7378	0.9995	0.7539	0.3602	0.3099	1	0.7567	0.7851	0.09767	1
420	0.2069	1	0.7967	0.6876	0.6571	0.9983	0.7072	0.2796	0.1964	1	0.674	0.7467	0.067	1
421	0.112	1	0.9303	0.5717	0.5703	0.9973	0.7501	0.139	0.111	1	0.5552	0.6221	0.01406	1

Table G. part 10: *Continued*

Sequence # (sample #)	Ca++ act. coef.	CaCO3 act. coef.	Cl- act. coef.	H+ act. coef.	H2PO4- act. coef.	H3PO4 act. coef.	HCO3- act. coef.	HPO4-- act. coef.	Mg++ act. coef.	MgCO3 act. coef.	Na+ act. coef.	OH- act. coef.	PO4--- act. coef.	SiO2(aq) act. coef.
422	0.6358	1	0.9041	0.8828	0.889	0.9999	0.9037	0.6245	0.6271	1	0.8831	0.8799	0.337	1
423	0.382	1	0.8089	0.7863	0.768	0.9995	0.7795	0.4026	0.3583	1	0.7839	0.8045	0.1232	1
424	0.4582	1	0.8649	0.8071	0.818	0.9998	0.8479	0.4531	0.4506	1	0.8061	0.815	0.1647	1
425	0.4984	1	0.8505	0.8263	0.8248	0.9998	0.8343	0.4853	0.4707	1	0.8303	0.8374	0.1843	1
426	0.6095	1	0.8968	0.871	0.8782	0.9999	0.8902	0.5931	0.5983	1	0.8711	0.875	0.2977	1
427	0.5136	1	0.867	0.8334	0.8374	0.9998	0.8552	0.5018	0.4958	1	0.833	0.8398	0.2017	1
428	0.6135	1	0.898	0.8745	0.8807	0.9999	0.8975	0.6004	0.605	1	0.8743	0.8708	0.3064	1
429	0.1804	1	0.7465	0.671	0.6176	0.9992	0.657	0.2488	0.1664	1	0.667	0.7311	0.05192	1
430	0.1005	1	0.9711	0.5493	0.557	0.9982	0.7642	0.1158	0.09983	1	0.5344	0.591	0.008836	1
431	0.1811	1	0.8108	0.6679	0.6332	0.9983	0.706	0.2284	0.1775	1	0.6447	0.7119	0.04061	1
432	0.3795	1	0.8255	0.7816	0.7733	0.9991	0.7926	0.3999	0.3644	1	0.779	0.8013	0.1242	1
433	0.03017	1	1.627	0.5084	0.3526	0.9976	0.877	0.05669	0.03018	1	0.4083	0.6754	0.004958	1
434	0.3199	1	0.8457	0.7398	0.7511	0.9995	0.7993	0.3383	0.3188	1	0.7374	0.7611	0.08875	1
435	0.6274	1	0.9006	0.878	0.8846	0.9999	0.9003	0.6103	0.6159	1	0.8782	0.875	0.3172	1
436	0.6509	1	0.9076	0.8875	0.8937	0.9999	0.9061	0.6356	0.6413	1	0.8877	0.8864	0.3491	1
437	0.3769	1	0.8362	0.7845	0.7801	0.9998	0.8033	0.4246	0.3642	1	0.7802	0.8098	0.1496	1
439	0.6206	1	0.8986	0.8761	0.8821	0.9999	0.8948	0.6044	0.6089	1	0.8762	0.8771	0.3098	1
440	0.3686	1	0.8367	0.7778	0.7751	0.9997	0.8172	0.3807	0.3695	1	0.771	0.7785	0.1095	1
441	0.3	1	0.8441	0.7238	0.7357	0.9997	0.7877	0.3172	0.2928	1	0.7204	0.7518	0.0773	1
442	0.1741	1	0.8712	0.6295	0.6414	0.9994	0.7502	0.197	0.1709	1	0.6217	0.6714	0.02811	1
443	0.3417	1	0.7623	0.7733	0.7229	0.9998	0.7298	0.2917	0.328	1	0.7552	0.7513	0.04844	1
444	0.4206	1	0.8404	0.7969	0.795	0.9998	0.8205	0.4144	0.4101	1	0.7936	0.8014	0.129	1
445	0.5792	1	0.8901	0.8639	0.8692	0.9999	0.883	0.5781	0.5702	1	0.8636	0.868	0.2844	1
446	0.5054	1	0.8444	0.8244	0.8209	0.9998	0.8286	0.4763	0.464	1	0.8277	0.8361	0.1714	1
447	0.493	1	0.8697	0.8201	0.8307	0.9998	0.8525	0.4785	0.4809	1	0.8203	0.83	0.1841	1
448	0.1656	1	0.8851	0.6161	0.6342	0.9995	0.7593	0.1766	0.1636	1	0.6087	0.65	0.02115	1
449	0.1218	1	0.8614	0.6208	0.5885	0.9995	0.7095	0.2407	0.1207	1	0.5968	0.7283	0.06629	1
450	0.5003	1	0.8367	0.8261	0.8171	0.9997	0.8226	0.4665	0.462	1	0.8285	0.8327	0.1596	1
451	0.4003	1	0.8381	0.7887	0.7863	0.9996	0.8082	0.4113	0.3872	1	0.785	0.8049	0.1311	1
452	0.5162	1	0.8699	0.8391	0.8419	0.9998	0.8551	0.5148	0.5049	1	0.8385	0.8479	0.216	1
453	0.1675	1	0.8144	0.6588	0.6205	0.9978	0.6987	0.2103	0.167	1	0.6335	0.7002	0.03358	1
454	0.2222	1	0.807	0.7024	0.677	0.9994	0.732	0.2916	0.2172	1	0.6855	0.7468	0.07081	1
455	0.2942	1	0.8108	0.7465	0.7302	0.9995	0.7583	0.3677	0.2823	1	0.7387	0.7874	0.1148	1
456	0.547	1	0.874	0.8482	0.851	0.9998	0.8627	0.5326	0.5289	1	0.8483	0.8551	0.2292	1
457	0.442	1	0.8651	0.803	0.8144	0.9999	0.8503	0.4505	0.4384	1	0.8015	0.8093	0.166	1
458	0.1749	1	0.833	0.6446	0.6237	0.9992	0.7279	0.1633	0.1753	1	0.6211	0.6448	0.01538	1
459	0.2286	1	0.8514	0.6705	0.6848	0.9988	0.7664	0.2374	0.2239	1	0.6653	0.7008	0.04018	1
460	0.03537	1	1.614	0.574	0.3417	0.9956	0.84	0.03762	0.03651	1	0.4191	0.6369	0.001392	1

Table G. part 10: *Continued*

Sequence # (sample #)	Ca++ act. coef.	CaCO3 act. coef.	Cl- act. coef.	H+ act. coef.	H2PO4- act. coef.	H3PO4 act. coef.	HCO3- act. coef.	HPO4-- act. coef.	Mg++ act. coef.	MgCO3 act. coef.	Na+ act. coef.	OH- act. coef.	PO4--- act. coef.	SiO2(aq) act. coef.
461	0.1096	1	0.7146	0.6189	0.5116	0.9991	0.5725	0.1779	0.09874	1	0.6032	0.7165	0.0312	1
462	0.2702	1	0.8147	0.7295	0.7143	0.9995	0.7569	0.3117	0.269	1	0.7173	0.7543	0.07447	1
473	0.2955	1	0.7714	0.7503	0.7025	0.9997	0.7516	0.2508	0.2964	1	0.7237	0.7107	0.03462	1
474	0.2866	1	0.7697	0.7462	0.6965	0.9996	0.7519	0.244	0.2883	1	0.7182	0.7044	0.03262	1
475	0.2605	1	0.7643	0.7311	0.6745	0.9996	0.7479	0.2132	0.2635	1	0.6979	0.6794	0.0235	1
476	0.2881	1	0.7689	0.7457	0.6959	0.9996	0.7502	0.2415	0.2887	1	0.7178	0.7033	0.03156	1
477	0.2586	1	0.7542	0.736	0.6675	0.9994	0.7106	0.2088	0.2611	1	0.6978	0.6906	0.02203	1
478	0.2554	1	0.753	0.7347	0.6645	0.9994	0.7089	0.2046	0.2585	1	0.6955	0.6873	0.02094	1
479	0.2531	1	0.7519	0.7346	0.6625	0.9994	0.7072	0.2018	0.2571	1	0.6942	0.6854	0.02019	1
480	0.25	1	0.7508	0.7326	0.659	0.9994	0.7052	0.1983	0.2534	1	0.6913	0.6827	0.01939	1
481	0.2495	1	0.7505	0.733	0.6587	0.9994	0.7044	0.1982	0.2533	1	0.6913	0.6829	0.01937	1
482	0.2537	1	0.7512	0.7357	0.6629	0.9994	0.7055	0.2032	0.2577	1	0.6951	0.6873	0.02055	1
483	0.2535	1	0.753	0.7341	0.663	0.9994	0.7066	0.2015	0.2575	1	0.694	0.6856	0.0201	1
484	0.2607	1	0.7562	0.7368	0.6704	0.9995	0.7126	0.2108	0.264	1	0.6996	0.6918	0.02253	1
485	0.2698	1	0.7585	0.7414	0.6785	0.9995	0.7174	0.2193	0.2732	1	0.7063	0.6978	0.02463	1
486	0.3211	1	0.7908	0.7605	0.7282	0.9999	0.7747	0.2904	0.3214	1	0.7413	0.7328	0.05101	1
487	0.5097	1	0.8596	0.8428	0.8374	0.9999	0.8547	0.4937	0.5054	1	0.8386	0.8342	0.1855	1
488	0.5162	1	0.8617	0.8452	0.8403	0.9999	0.8574	0.4998	0.5119	1	0.8413	0.8363	0.191	1
489	0.6459	1	0.9016	0.8918	0.8919	1	0.8997	0.6304	0.6376	1	0.8907	0.8887	0.3323	1
490	0.518	1	0.8613	0.8459	0.8406	0.9999	0.8571	0.5	0.5133	1	0.842	0.8367	0.1904	1
522	0.5898	1	0.8874	0.8677	0.8716	1	0.886	0.5775	0.5771	1	0.8695	0.8645	0.273	1
523	0.1383	1	0.6349	0.6245	0.5697	0.9998	0.5867	0.1789	0.1332	1	0.707	0.6487	0.02148	1
524	0.2165	1	0.6975	0.6927	0.6553	1	0.6661	0.2572	0.2113	1	0.748	0.7037	0.04625	1
525	0.12	1	0.6092	0.5965	0.531	0.9989	0.5522	0.1472	0.1102	1	0.687	0.6267	0.0138	1
526	0.02536	1	0.5341	0.454	0.3028	0.9966	0.3767	0.04759	0.02365	1	0.5583	0.6092	0.002219	1
527	0.5547	1	0.869	0.843	0.8471	0.9999	0.8593	0.5159	0.5224	1	0.8447	0.8488	0.2055	1
528	0.5446	1	0.8651	0.8405	0.8437	0.9999	0.8552	0.5089	0.5134	1	0.8432	0.8459	0.1983	1
529	0.1002	1	0.5895	0.5531	0.4733	0.9989	0.5072	0.1133	0.08111	1	0.6458	0.6106	0.008248	1
530	0.07061	1	0.5671	0.5273	0.4327	0.9984	0.473	0.09491	0.06102	1	0.6296	0.5984	0.006264	1
531	0.5195	1	0.8469	0.8134	0.8179	0.9999	0.8335	0.4433	0.4648	1	0.8162	0.8205	0.1381	1
532	0.5238	1	0.8476	0.8147	0.8193	0.9999	0.8342	0.4459	0.4681	1	0.8175	0.8221	0.1397	1
533	0.5235	1	0.8492	0.8165	0.821	0.9999	0.834	0.451	0.4705	1	0.8192	0.8257	0.1444	1
534	0.5171	1	0.8428	0.8093	0.8131	0.9999	0.8265	0.4354	0.456	1	0.8122	0.8196	0.1319	1
535	0.4588	1	0.7919	0.7558	0.7496	0.9996	0.7629	0.3411	0.3467	1	0.7611	0.7804	0.07209	1
536	0.04643	1	0.4996	0.4859	0.3649	0.9977	0.4032	0.05611	0.04081	1	0.6249	0.552	0.001827	1
537	0.04529	1	0.4937	0.4727	0.3438	0.9971	0.3871	0.04856	0.03702	1	0.6118	0.5525	0.001348	1
538	0.02879	1	0.4813	0.4388	0.3195	0.9967	0.3689	0.04739	0.02593	1	0.5975	0.5583	0.001655	1
539	0.04532	1	0.503	0.493	0.3763	0.9977	0.412	0.06123	0.04235	1	0.6325	0.5534	0.002244	1

Table G. part 10: *Continued*

Sequence # (sample #)	Ca++ act. coef.	CaCO3 act. coef.	Cl- act. coef.	H+ act. coef.	H2PO4- act. coef.	H3PO4 act. coef.	HCO3- act. coef.	HPO4-- act. coef.	Mg++ act. coef.	MgCO3 act. coef.	Na+ act. coef.	OH- act. coef.	PO4--- act. coef.	SiO2(aq) act. coef.
540	0.5368	1	0.8537	0.8286	0.8311	0.9999	0.8419	0.476	0.4902	1	0.8318	0.8352	0.1642	1
541	0.4778	1	0.8439	0.7967	0.8039	0.9999	0.824	0.4167	0.4328	1	0.7993	0.8075	0.1235	1
542	0.4809	1	0.8461	0.8072	0.8105	0.9999	0.8259	0.4432	0.4408	1	0.8086	0.8208	0.1459	1
543	0.0977	1	0.5713	0.5398	0.4538	0.9984	0.4879	0.09851	0.07529	1	0.6405	0.5963	0.005788	1
544	0.1229	1	0.5958	0.5642	0.498	0.999	0.5258	0.1251	0.09484	1	0.661	0.6152	0.009528	1
545	0.06888	1	0.5564	0.5225	0.4273	0.9984	0.4656	0.08969	0.0594	1	0.6328	0.5895	0.005354	1
546	0.05239	1	0.5505	0.5018	0.3874	0.998	0.4375	0.07535	0.04563	1	0.6055	0.5931	0.004244	1
547	0.01804	1	0.4631	0.4208	0.2418	0.9941	0.306	0.02343	0.01625	1	0.5679	0.584	0.0003713	1
548	0.08999	1	0.5615	0.5321	0.4397	0.9982	0.4748	0.09037	0.0696	1	0.6369	0.5895	0.004803	1
549	0.2021	1	0.6566	0.6153	0.5639	0.9992	0.5899	0.1687	0.1424	1	0.6699	0.662	0.01706	1
550	0.05129	1	0.5142	0.4835	0.3713	0.9975	0.4138	0.06167	0.0425	1	0.6171	0.5638	0.00237	1
551	0.02926	1	0.5023	0.4426	0.2923	0.9966	0.3569	0.03873	0.02434	1	0.5691	0.5852	0.001146	1
552	0.02969	1	0.4761	0.4494	0.3116	0.9965	0.3604	0.04059	0.02675	1	0.5998	0.5512	0.001054	1
553	0.0305	1	0.4808	0.452	0.3123	0.9968	0.3625	0.04102	0.02723	1	0.5973	0.5548	0.00109	1
554	0.02896	1	0.4811	0.4509	0.3087	0.9966	0.3607	0.04023	0.02629	1	0.5947	0.5559	0.001069	1
555	0.03773	1	0.4965	0.4713	0.3568	0.9993	0.3979	0.05756	0.03506	1	0.6191	0.5547	0.002209	1
556	0.03143	1	0.4943	0.4574	0.3214	0.999	0.3736	0.04589	0.02838	1	0.5941	0.5633	0.001482	1
557	0.03946	1	0.5048	0.462	0.3196	0.9986	0.3755	0.04382	0.03152	1	0.5867	0.5702	0.001257	1
558	0.06162	1	0.5498	0.5235	0.4324	0.9997	0.4666	0.09338	0.05797	1	0.6438	0.5851	0.005991	1
559	0.02808	1	0.4823	0.4425	0.2985	0.9982	0.3537	0.03842	0.02456	1	0.5853	0.5634	0.001024	1
560	0.6226	1	0.8895	0.8773	0.8781	1	0.8833	0.5977	0.5989	1	0.8788	0.8814	0.2912	1
561	0.01717	1	0.4672	0.4258	0.2233	0.9967	0.2899	0.01914	0.0152	1	0.5647	0.6063	0.0002335	1
562	0.0306	1	0.4951	0.4563	0.3149	0.9985	0.3696	0.04402	0.02751	1	0.5888	0.5668	0.001383	1
563	0.02318	1	0.5792	0.439	0.168	0.99	0.2653	0.0125	0.0155	1	0.5386	0.8367	0.00007971	1
564	0.3001	1	0.7546	0.7551	0.7068	1	0.7199	0.2619	0.3025	1	0.7446	0.725	0.03765	1
565	19.91	1	0.3685	11.83	1.116	0.9988	0.4194	0.0006504	47.65	1	2.378	0.1698	1.229E-11	1
566	0.6061	1	0.8863	0.8729	0.8735	1	0.8795	0.5875	0.5839	1	0.874	0.8771	0.281	1
567	0.01834	1	0.541	0.4546	0.1716	0.9931	0.2561	0.01153	0.01427	1	0.5627	0.7686	0.00006232	1
568	0.0137	1	0.5798	0.4419	0.1548	0.9912	0.2447	0.01098	0.01109	1	0.554	0.8706	0.0000561	1
569	0.04773	1	0.5435	0.501	0.3703	0.9983	0.4231	0.06562	0.04222	1	0.5989	0.5886	0.003125	1
570	0.02172	1	0.6139	0.4967	0.1478	0.9818	0.2389	0.009554	0.01562	1	0.5877	0.9347	0.00002668	1
571	0.02305	1	0.5494	0.4735	0.1796	0.9915	0.2676	0.01219	0.01712	1	0.5607	0.7544	0.00007116	1
572	0.66	1	0.9038	0.8922	0.8944	1	0.8998	0.6391	0.6411	1	0.8931	0.8947	0.3421	1
573	0.6119	1	0.8879	0.8705	0.874	1	0.8839	0.5786	0.5901	1	0.8721	0.8707	0.2681	1
574	0.06534	1	0.5293	0.5113	0.4229	0.9973	0.453	0.08344	0.05697	1	0.6502	0.5697	0.004243	1
575	0.3372	1	0.7444	0.7295	0.7075	0.9994	0.7171	0.3041	0.2837	1	0.7605	0.7452	0.06061	1
576	0.5143	1	0.8437	0.8337	0.8261	0.9999	0.8311	0.4852	0.4773	1	0.8359	0.8401	0.1751	1
577	0.6069	1	0.8903	0.8688	0.874	1	0.885	0.5782	0.5893	1	0.8696	0.8704	0.2718	1

Table G. part 10: *Continued*

Sequence # (sample #)	Ca++ act. coef.	CaCO3 act. coef.	Cl- act. coef.	H+ act. coef.	H2PO4- act. coef.	H3PO4 act. coef.	HCO3- act. coef.	HPO4-- act. coef.	Mg++ act. coef.	MgCO3 act. coef.	Na+ act. coef.	OH- act. coef.	PO4--- act. coef.	SiO2(aq) act. coef.
578	0.4364	1	0.8095	0.8171	0.789	1	0.7919	0.3963	0.4234	1	0.8067	0.8046	0.1017	1
579	0.1068	1	0.5886	0.7255	0.4273	0.9995	0.4615	0.04972	0.1131	1	0.6373	0.5705	0.0007655	1
580	0.09964	1	0.5826	0.7403	0.3983	0.9993	0.439	0.03908	0.1044	1	0.6327	0.5639	0.0004432	1
581	0.09826	1	0.5854	0.7926	0.3455	0.9991	0.4005	0.02412	0.09642	1	0.6311	0.5642	0.0001461	1
582	0.1267	1	0.6204	0.9165	0.3109	0.9989	0.3803	0.0161	0.1141	1	0.6418	0.5812	0.00005387	1
583	0.1423	1	0.6253	0.9629	0.2946	0.9987	0.3664	0.01323	0.1204	1	0.6539	0.5843	0.00003205	1
584	0.1657	1	0.6669	1.05	0.2656	0.9985	0.351	0.01062	0.1282	1	0.662	0.6203	0.00002021	1
585	0.2416	1	0.7393	1.262	0.2176	0.9979	0.3143	0.007029	0.1538	1	0.711	0.6901	6.794E-06	1
586	0.04318	1	0.8861	1.104	0.1433	0.9911	0.2411	0.006788	0.04811	1	0.7625	0.9498	8.397E-06	1
587	0.04377	1	0.7991	1.069	0.1523	0.9903	0.2417	0.006421	0.04865	1	0.7688	0.867	7.167E-06	1
588	0.08069	1	0.9784	1.58	0.1395	0.9897	0.2348	0.005576	0.09796	1	0.8815	0.9093	4.242E-06	1
589	0.0526	1	0.9704	1.29	0.1346	0.9908	0.2284	0.006264	0.06015	1	0.8405	0.9897	5.309E-06	1
590	0.06505	1	1.049	1.461	0.1324	0.9904	0.2351	0.006338	0.07754	1	0.8395	1.007	6.141E-06	1
591	0.07842	1	1.023	1.58	0.1348	0.9896	0.2323	0.005751	0.09326	1	0.8844	0.9546	4.533E-06	1
592	0.09157	1	1.084	1.618	0.1323	0.9881	0.2385	0.006109	0.1	1	0.8583	1.008	5.625E-06	1
593	0.07344	1	0.9976	1.501	0.1371	0.9897	0.2351	0.005872	0.08583	1	0.8627	0.9494	4.961E-06	1
594	0.07968	1	0.8461	0.9017	0.174	0.9927	0.304	0.01008	0.05621	1	0.6082	0.935	0.00003613	1
595	0.0367	1	0.7474	0.8657	0.159	0.9926	0.2542	0.007603	0.03607	1	0.6871	0.8672	0.00001376	1
596	0.09373	1	0.6413	0.6224	0.2639	0.9955	0.3676	0.02186	0.0555	1	0.5516	0.6859	0.0002258	1
597	0.03644	1	0.7771	0.965	0.1563	0.9928	0.25	0.007078	0.04048	1	0.7207	0.863	0.0000111	1
598	0.08643	1	1.013	1.604	0.1385	1	0.2368	0.005659	0.1009	1	0.8778	0.9259	4.591E-06	1
599	0.04334	1	0.9219	1.12	0.1405	0.9923	0.2406	0.006899	0.04782	1	0.7645	0.9838	8.648E-06	1
600	0.04268	1	0.6497	0.791	0.1865	0.9928	0.2763	0.008677	0.03957	1	0.6524	0.7435	0.00002076	1
601	0.02552	1	0.526	0.5115	0.2236	0.9954	0.3034	0.01703	0.02298	1	0.5665	0.6366	0.0001614	1
602	0.2049	1	0.6837	0.6691	0.6211	0.999	0.6373	0.2192	0.1849	1	0.7125	0.6885	0.03126	1
603	0.08195	1	0.5828	0.597	0.2993	0.9963	0.3779	0.02705	0.05559	1	0.5732	0.615	0.0003133	1
604	0.09125	1	0.5924	0.6261	0.2867	0.9961	0.3693	0.02269	0.05948	1	0.5761	0.6231	0.0001966	1
605	0.09369	1	0.8435	1.526	0.1683	0.9897	0.2633	0.005582	0.1153	1	0.8249	0.7692	5.075E-06	1
606	0.04401	1	0.831	1.086	0.1493	0.9916	0.2421	0.00654	0.04899	1	0.7664	0.8941	0.00000764	1
607	0.05982	1	0.9499	1.307	0.1434	0.9909	0.2466	0.006459	0.06806	1	0.7918	0.9453	7.674E-06	1
608	0.03851	1	0.7394	0.9247	0.1644	0.9936	0.2576	0.007347	0.04102	1	0.7014	0.8249	0.00001279	1
609	0.03858	1	0.7132	0.9123	0.168	0.9937	0.2578	0.007287	0.04121	1	0.703	0.7981	0.00001228	1
610	0.03451	1	0.6636	0.8012	0.1754	0.9946	0.2636	0.008065	0.03489	1	0.6677	0.7697	0.00001737	1
611	0.04024	1	0.5932	0.6736	0.209	0.9955	0.2953	0.01131	0.03523	1	0.6112	0.6849	0.0000446	1
612	0.1206	1	0.9226	1.782	0.1596	0.9889	0.2594	0.005242	0.1507	1	0.8653	0.7955	4.297E-06	1
613	0.1298	1	0.9499	1.63	0.1494	0.9899	0.2503	0.005535	0.1266	1	0.8488	0.8749	4.228E-06	1
614	0.05712	1	0.66	0.6881	0.1961	0.9953	0.2994	0.01114	0.04024	1	0.5933	0.7691	0.00004419	1
615	0.06251	1	0.5164	0.5894	0.35	0.9926	0.3971	0.03863	0.07059	1	0.614	0.5291	0.0006257	1

Table G. part 10: *Continued*

Sequence # (sample #)	Ca++ act. coef.	CaCO3 act. coef.	Cl- act. coef.	H+ act. coef.	H2PO4- act. coef.	H3PO4 act. coef.	HCO3- act. coef.	HPO4-- act. coef.	Mg++ act. coef.	MgCO3 act. coef.	Na+ act. coef.	OH- act. coef.	PO4--- act. coef.	SiO2(aq) act. coef.
616	0.1417	1	0.6159	1.171	0.2918	0.9964	0.3594	0.01087	0.1963	1	0.6898	0.5233	0.00001826	1
617	0.2237	1	0.8015	2.277	0.1936	0.9919	0.2744	0.004201	0.3469	1	0.9346	0.6043	1.669E-06	1
618	0.5695	1	0.901	3.184	0.2278	0.9951	0.3291	0.00453	1.078	1	0.8819	0.5497	2.004E-06	1
619	0.1624	1	0.605	1.002	0.3695	0.9979	0.419	0.02062	0.2084	1	0.6563	0.5219	0.00007219	1
620	0.2739	1	0.7973	2.398	0.2082	0.9911	0.2909	0.004345	0.4513	1	0.9087	0.5738	1.728E-06	1
621	0.2053	1	0.6858	0.6842	0.6389	0.9992	0.6499	0.2357	0.1986	1	0.7367	0.6938	0.03696	1
622	0.2877	1	0.7211	0.7093	0.6641	0.999	0.6773	0.2469	0.2404	1	0.7219	0.7197	0.0363	1
623	0.2333	1	0.7076	0.706	0.6645	0.9983	0.6753	0.262	0.2273	1	0.7454	0.7129	0.04621	1
624	0.3483	1	0.7523	0.741	0.7109	1	0.7199	0.2971	0.2941	1	0.7505	0.7491	0.05408	1

Table G. part 11: Aqueous chemistry database of alkaline lake waters compiled from published literature, as well as corresponding results from calculations described in chapters 2 and 3, and investigated in detail in chapter 4.

Sequence # (sample #)	H+	CO2(aq)	CO3--	Ca++	Cl-	H2PO4-	H3PO4	H3SiO4-	HCO3-	HPO4--	Mg++	Na+	OH-	PO4---	SiO2(aq)
								free mmol/kg							
1	5.231E-07	0.006331	3.193	0.1638	97	1.007E-15	3.995E-23	3.57E-10	10.38	4.311E-13	10.63	100	0.03441	3.405E-15	6.43E-10
2	6.605E-07	0.01125	3.52	0.1236	93	1.727E-15	8.567E-23	3.068E-10	14.8	5.728E-13	6.679	120	0.02715	3.41E-15	6.932E-10
3	3.401E-07	0.01157	15.67	0.02987	93	1.165E-15	2.782E-23	4.778E-10	31.82	8.041E-13	1.645	160	0.05498	1.041E-14	5.222E-10
4	8.227E-07	0.009621	3.339	0.2448	170	9.74E-16	5.118E-23	2.959E-10	11.84	3.808E-13	31.22	170	0.02544	3.604E-15	7.042E-10
5	4.765E-08	0.0006817	421	0.08121	830	1.959E-17	2.961E-26	9.256E-10	36.54	4.226E-13	2.31	1900	0.4315	5.334E-13	7.447E-11
6	1.352E-07	0.00496	296.1	0.1093	820.1	1.002E-16	4.861E-25	8.019E-10	80.4	6.801E-13	3.056	1600	0.1533	2.683E-13	1.982E-10
7	3.271E-08	0.0003883	468.4	0.06878	1200	6.436E-18	7.759E-27	9.39E-10	28	2.315E-13	2.83	2200	0.5068	7.376E-13	6.104E-11
8	2.348E-08	0.0002098	628.6	0.0762	1200	4.895E-18	3.478E-27	9.545E-10	29.39	2.233E-13	1.698	3400	0.4833	7.597E-13	4.559E-11
9	2.77E-07	0.004014	12.02	0.05852	190	4.919E-16	8.502E-24	5.595E-10	15.42	5.499E-13	8.47	250	0.07422	1.476E-14	4.405E-10
10	1.377E-06	0.02328	4.056	1.006	240	1.829E-15	1.404E-22	2.223E-10	20.04	5.253E-13	28.3	320	0.01651	4.32E-15	7.778E-10
11	1.168E-06	0.02242	2.189	0.5646	43	2.32E-15	2.032E-22	1.999E-10	16.46	4.196E-13	13.84	67	0.01566	1.227E-15	8.001E-10
12	1.182E-06	0.01482	2.039	1.019	110	2.031E-15	1.592E-22	2.187E-10	12.27	4.658E-13	16.5	150	0.01703	2.164E-15	7.813E-10
13	7.214E-07	0.03817	13.73	0.09094	130	2.525E-15	1.205E-22	3.138E-10	52.9	9.276E-13	0.3646	220	0.02686	7.237E-15	6.862E-10
14	2.269E-07	0.000975	11.2	0.1907	480	1.093E-16	1.176E-24	6.696E-10	6.231	2.962E-13	56.35	640	0.1083	3.482E-14	3.304E-10
15	3.032E-07	0.01785	69.78	0.02745	160	6.757E-16	1.04E-23	5.832E-10	77.63	8.704E-13	1.892	340	0.07768	3.02E-14	4.169E-10
16	1.348E-06	0.07027	8.356	0.08578	230	3.664E-15	3.226E-22	2E-10	53.25	8.359E-13	3.939	280	0.01445	4.999E-15	8E-10
17	8.249E-07	0.01409	8.052	0.6374	840	6.848E-16	3.641E-23	3.003E-10	18.68	5.033E-13	43.9	720	0.02298	2.379E-14	6.997E-10
18	9.71E-07	0.01245	0.9866	0.4886	24	2.576E-15	2.319E-22	1.958E-10	8.907	3.907E-13	6.051	24	0.01557	7.607E-16	8.042E-10
19	1.058E-06	0.00861	1.144	0.279	100	1.61E-15	1.268E-22	2.186E-10	7.021	3.601E-13	21.4	92	0.01741	1.495E-15	7.814E-10
20	2.349E-07	0.01334	323	0.03418	640.1	1.964E-16	1.487E-24	7.209E-10	136.1	8.036E-13	0.8314	1500	0.1009	1.853E-13	2.793E-10
21	1.429E-07	0.003591	192.8	0.03225	470	1.389E-16	6.588E-25	8.108E-10	56.56	7.795E-13	0.6774	1000	0.1825	1.989E-13	1.893E-10
22	2.961E-07	0.007925	29.47	0.05637	180	6.289E-16	9.828E-24	5.806E-10	34.1	7.817E-13	3.634	350	0.07764	2.472E-14	4.194E-10
23	5.146E-07	0.009042	3.446	0.1243	59	1.403E-15	6.087E-23	3.362E-10	13.53	4.952E-13	5.261	58	0.03188	2.773E-15	6.639E-10
24	4.888E-07	0.01372	9.254	0.1415	63	1.426E-15	4.783E-23	3.938E-10	26.76	6.843E-13	3.746	130	0.03941	5.847E-15	6.062E-10
25	4.846E-07	0.01048	3.086	0.2116	14.4	3.914E-06	1.768E-13	3.259E-10	15.05	0.001107	0.06243	39.4	0.03046	3.748E-06	6.741E-10
26	1.838E-07	0.002305	3.444	0.04101	1.056	6.753E-07	1.288E-14	5.338E-10	7.831	0.0004095	0.008939	11.92	0.07313	2.535E-06	4.662E-10
27	2.789E-07	0.002404	1.216	0.08627	0.2889	1.972E-15	6.257E-23	4.079E-10	4.908	6.731E-13	0.01172	6.246	0.04433	2.137E-15	5.921E-10
28	8.934E-08	0.0005012	2.656	0.05884	0.6117	2.048E-06	2.024E-14	6.888E-10	3.288	0.002281	0.00634	6.988	0.1422	0.00002405	3.112E-10
29	1.106E-07	0.0005539	1.731	0.04476	0.07364	7.181E-16	9.105E-24	6.33E-10	2.831	6.054E-13	0.01961	4.411	0.111	4.631E-15	3.67E-10
30	2.421E-07	0.006624	8.107	0.02914	14.82	1.515E-15	3.43E-23	4.916E-10	19.01	8.936E-13	0.003478	16.89	0.06175	6.958E-15	5.084E-10
31	9.421E-08	0.001084	7.135	0.09658	2.602	0.00002101	1.953E-13	7.016E-10	7.561	0.02733	0.01711	14.5	0.1503	0.0003911	2.984E-10
32	5.712E-07	0.009324	1.317	0.1136	0.9543	0.0002063	1.271E-11	2.619E-10	9.807	0.03817	0.007064	10.22	0.02275	0.00007112	7.381E-10
33	8.976E-07	0.01366	0.7407	0.126	0.7759	0.0001082	1.067E-11	1.814E-10	8.973	0.0123	0.008995	9.346	0.01421	0.00001371	8.186E-10
34	2.478E-07	0.006577	8.249	0.0414	8.77	4.325E-06	9.573E-14	4.963E-10	19.29	0.002549	0.01119	38.67	0.06206	0.00001875	5.037E-10
35	6.076E-07	0.004215	0.709	0.1864	4.872	0.001367	7.851E-11	2.749E-10	4.755	0.2802	0.3081	51.75	0.02369	0.0005833	7.251E-10
36	1.079E-07	0.0003064	0.8721	0.08036	0.07931	2.735E-07	3.561E-15	6.269E-10	1.525	0.0002157	0.07221	2.271	0.1084	1.457E-06	3.731E-10

Table G. part 11: *Continued*

Sequence # (sample #)	H+	CO2(aq)	CO3--	Ca++	Cl-	H2PO4-	H3PO4	H3SiO4-	HCO3-	HPO4--	Mg++	Na+	OH-	PO4---	SiO2(aq)
								free mmol/kg							
37	2.924E-07	0.004951	2.999	0.0513	0.8948	0.0001314	3.959E-12	4.202E-10	10.65	0.05099	0.01023	13.01	0.04627	0.0002063	5.798E-10
38	1.293E-07	0.002193	13.58	0.02163	37.72	0.00005711	5.931E-13	6.777E-10	13.77	0.07837	0.00703	71.69	0.1299	0.001552	3.224E-10
39	1.799E-07	0.001713	2.358	0.054	0.4984	4.014E-06	7.844E-14	5.28E-10	5.68	0.002296	0.006446	10.13	0.07172	0.00001274	4.721E-10
40	6.828E-08	0.0001246	0.8975	0.06083	0.2153	3.109E-16	2.546E-24	7.276E-10	0.986	3.902E-13	0.01191	3.363	0.1722	4.184E-15	2.724E-10
41	7.156E-07	0.01139	0.993	0.1556	0.6202	0.00001464	1.142E-12	2.188E-10	9.454	0.002117	0.02938	10.74	0.01796	3.027E-06	7.812E-10
42	5.338E-07	0.01789	11.08	0.04965	159.4	1.901E-15	6.988E-23	0.07805	32.31	9.33E-13	0.3454	213.2	0.03538	1.006E-14	0.1306
43	5.287E-07	0.01924	13.31	0.06881	206.9	1.702E-15	6.163E-23	0.06897	35.46	9.285E-13	0.2819	224.7	0.03616	1.293E-14	0.1129
44	7.127E-08	0.001097	51.72	0.03951	151.7	1.774E-16	7.607E-25	0.2724	17.02	7.741E-13	0.2493	230.6	0.2979	7.942E-14	0.0534
45	8.982E-08	0.001693	53.35	0.05396	173.9	2.171E-16	1.154E-24	0.3601	21.27	7.865E-13	0.2722	258.7	0.2382	7.05E-14	0.08748
46	1.122E-07	0.002516	47.18	0.04057	160.3	3.025E-16	2.064E-24	0.3794	24.56	8.359E-13	0.2595	239	0.1869	5.506E-14	0.1183
47	8.99E-08	0.001738	52.25	0.04576	152.7	2.298E-16	1.237E-24	0.406	21.49	8.021E-13	0.2347	235.4	0.2367	6.64E-14	0.09993
48	9.003E-08	0.001821	51.45	0.04345	124.1	2.424E-16	1.326E-24	0.3892	22.07	8.047E-13	0.2257	204.8	0.2348	5.975E-14	0.0975
49	2.575E-07	0.004508	7.377	0.1365	48.59	8.279E-16	1.712E-23	0.6321	14.21	5.967E-13	1.792	74.85	0.06591	6.653E-15	0.597
50	1.29E-07	0.001568	10.1	0.2306	45.11	2.914E-16	3.023E-24	0.8848	9.847	4.147E-13	1.274	69.6	0.1317	8.992E-15	0.4193
51	2.193E-07	0.004114	14.13	0.4192	59.95	3.589E-16	5.368E-24	0.2808	17.93	3.915E-13	5.885	109.8	0.08915	7.656E-15	0.1925
52	2.132E-07	0.004142	12.51	0.9131	47.52	2.616E-16	4.095E-24	0.2743	17.15	2.628E-13	5.315	78.11	0.0866	4.403E-15	0.1965
53	3.439E-07	0.008082	9.999	0.5305	35.78	6.4E-16	1.563E-23	0.2117	21.46	4.093E-13	6.544	83.08	0.05516	4.32E-15	0.2372
54	1.154E-06	0.02347	5.499	0.3132	209.6	2.508E-15	1.578E-22	0.008437	25.11	7.921E-13	6.778	363.7	0.01948	6.502E-15	0.02443
55	3.293E-07	0.005642	5.762	1.02	25.07	5.544E-16	1.437E-23	0.09747	14.07	3.111E-13	3.82	56.02	0.05285	2.549E-15	0.1157
56	1.308E-06	0.02158	1.366	0.175	18.08	2.628E-15	2.775E-22	1.716E-10	13.07	3.713E-13	15.41	24.27	0.01322	7.512E-16	8.284E-10
57	1.144E-06	0.08659	13.83	0.9162	61.71	2.979E-15	2.113E-22	0.0464	79.87	7.099E-13	2.296	191.3	0.01803	3.401E-15	0.1522
58	4.336E-07	0.008642	30.02	0.1912	624.5	5.033E-16	9.636E-24	0.03597	33.26	7.614E-13	11.19	935.7	0.05206	5.401E-14	0.03251
59	1.687E-07	0.003479	15.14	0.118	19.47	3.834E-16	4.852E-24	6.326E-10	17.84	4.474E-13	3.62	59.87	0.1073	7.9E-15	3.674E-10
60	8.569E-07	0.01322	28.69	0.3036	249.9	9.161E-16	2.114E-23	0.05328	44.08	8.878E-13	9.031	1289	0.0351	3.13E-14	0.06422
61	2.355E-07	0.004278	24.95	2.536	168.4	1.793E-16	2.256E-24	6.331E-10	22.54	2.811E-13	8.861	292.5	0.09871	1.118E-14	3.669E-10
62	5.684E-07	0.006428	5.076	7.752	159	3.703E-16	1.263E-23	0.1506	12.15	2.128E-13	12.46	220.2	0.03842	2.906E-15	0.2343
63	1.026E-06	0.02983	3.141	0.1888	54.07	3.947E-15	3.245E-22	0.04585	23.64	7.271E-13	2.437	84.48	0.01652	2.131E-15	0.1722
64	9.51E-07	0.07144	29.13	1.052	175.1	1.403E-15	6.883E-23	3.055E-10	96.4	5.956E-13	15.96	344	0.02471	7.113E-15	6.946E-10
65	0.00000112	0.1702	129.9	1.526	1120	7.795E-16	3.981E-23	2.807E-10	266.6	7.267E-13	42.78	1723	0.01577	6.39E-14	7.196E-10
66	0.0001059	0.1361	0.0003593	0.1789	0.16	5.33E-13	7.091E-18	0.0005092	0.6624	3.982E-13	0.2599	1.19	0.0001065	2.424E-18	0.3095
67	0.0001709	0.1934	0.0002185	0.4179	1.1	6.229E-13	1.289E-17	0.0002853	0.6043	3.097E-13	0.27	1.98	0.00006853	1.316E-18	0.2697
68	0.00008622	0.1368	0.0006295	0.5958	0.46	4.495E-13	4.628E-18	0.001315	0.8583	4.529E-13	0.1799	2.03	0.0001378	3.933E-18	0.6187
69	0.00001395	0.04051	0.008088	0.3445	1.56	1.135E-13	1.808E-19	0.009888	1.645	7.674E-13	0.1894	6.45	0.000886	4.736E-17	0.7201
70	2.448E-07	0.000824	0.9488	0.1635	1	1.191E-15	2.672E-23	0.1923	2.384	6.519E-13	0.2189	30.72	0.06168	3.951E-15	0.1977
71	0.0001388	0.2977	0.0005795	0.8919	0.98	5.142E-13	8.269E-18	0.0006115	1.193	3.422E-13	0.6798	2.42	0.00008837	2.037E-18	0.4494
72	0.00008979	0.1981	0.00107	0.7931	1.88	3.686E-13	3.638E-18	0.0008848	1.294	4.176E-13	1.45	4.62	0.0001436	4.497E-18	0.3991
73	0.00009162	0.3503	0.002037	0.6902	1.38	3.453E-13	3.335E-18	0.002439	2.337	4.119E-13	2.249	6.75	0.0001462	4.858E-18	1.078
74	0.00009187	0.2708	0.001617	1.632	4.93	3.539E-13	3.402E-18	0.0007268	1.809	4.316E-13	1.249	8.25	0.0001476	5.367E-18	0.3193

Table G. part 11: *Continued*

Sequence # (sample #)	H+	CO2(aq)	CO3--	Ca++	Cl-	H2PO4-	H3PO4	H3SiO4-	HCO3-	HPO4--	Mg++	Na+	OH-	PO4---	SiO2(aq)
								free mmol/kg							
75	6.852E-07	0.008425	2.384	0.3962	23.33	2.773E-15	1.351E-22	0.3266	11.29	8.068E-13	0.09569	115	0.02706	3.37E-15	0.7335
76	3.22E-07	0.007801	40.61	0.06735	204.9	6.7E-16	8.605E-24	1.843	42.11	9.448E-13	0.07529	712.1	0.07815	3.197E-14	1.147
77	2.076E-07	0.003673	77.52	0.06757	292.2	3.071E-16	2.061E-24	4.162	39.91	9.053E-13	0.08039	1130	0.126	7.525E-14	1.419
78	2.126E-07	0.009388	252.2	4.213E-10	1065	2.022E-16	1.434E-24	6.575	123.8	8.211E-13	5.362E-10	2991	0.05864	1.792E-13	2.949
79	1.99E-07	0.008759	274.4	4.167E-10	1116	1.862E-16	1.238E-24	6.359	129.2	8.01E-13	5.238E-10	3241	0.05557	1.993E-13	2.795
80	6.419E-08	0.0004757	10.13	0.05713	12.17	2.345E-16	1.253E-24	1.638	5.784	5.658E-13	0.2398	72.5	0.2515	1.64E-14	0.4023
81	0.00001679	0.6579	0.3078	0.4512	62.74	7.231E-14	8.97E-20	0.05489	34.66	8.936E-13	0.1567	122.5	0.001063	1.832E-16	3.125
82	1.874E-07	0.009764	362.3	0.02571	1002	1.587E-16	9.54E-25	4.031	142.6	7.89E-13	0.03005	2721	0.07751	2.092E-13	1.461
83	1.103E-07	0.002438	456.2	0.07523	619.3	1.022E-16	2.633E-25	18.13	106.4	7.323E-13	0.04521	3904	0.09192	2.641E-13	3.529
84	1.844E-07	0.004289	226.8	0.1781	639.5	2.652E-16	1.277E-24	14.03	111.9	8.598E-13	0.06291	4444	0.04045	1.33E-13	5.541
85	2.228E-08	0.001986	363.8	0.04083	2051	6.237E-17	1.637E-25	12.45	189.1	2.523E-13	0.009325	6009	0.02414	7.47E-13	5.046
86	3.381E-06	0.01	0.02751	0.09651	0.7	3.282E-14	1.368E-20	0.03991	1.555	8E-13	0.2959	2.6	0.003392	1.643E-16	0.7601
87	4.754E-07	0.005656	1.505	0.06486	7.9	3.291E-15	1.523E-22	0.513	7.932	8.609E-13	0.07713	32.6	0.02983	2.446E-15	1.087
88	4.505E-07	0.003044	0.6591	0.07325	2.7	3.579E-15	1.762E-22	0.4305	4.008	8.113E-13	0.01662	13.4	0.02844	1.769E-15	0.9696
89	4.367E-06	0.02065	0.03934	0.4773	0.7	2.99E-14	1.531E-20	0.05736	2.605	6.202E-13	0.7871	4.3	0.002763	1.138E-16	1.343
90	1.743E-06	0.008559	0.1043	0.6422	1	1.08E-14	2.191E-21	0.2531	2.725	5.677E-13	0.09599	6.6	0.006972	2.674E-16	2.347
91	1.726E-07	0.004141	18.02	0.09414	18	5.268E-16	6.486E-24	3.123	21.84	5.984E-13	1.855	110	0.1056	9.504E-15	1.778
92	2.111E-07	0.003626	8.891	0.04359	19.6	1.074E-15	1.722E-23	0.5174	14.73	8.928E-13	0.02307	117	0.08171	9.569E-15	0.3827
93	8.579E-06	0.03732	0.01682	0.7747	0.1	6.554E-14	6.805E-20	0.008255	2.319	6.522E-13	0.1984	2.5	0.001369	5.554E-17	0.3917
94	3.425E-06	0.03559	0.104	0.5323	0.04	2.575E-14	1.06E-20	0.02018	5.584	6.587E-13	0.191	0.7	0.003447	1.522E-16	0.3798
95	0.00000356	0.0261	0.08693	1.665	0.8	1.472E-14	5.847E-21	0.05741	4.212	4.138E-13	1.359	4.1	0.003585	1.089E-16	1.043
96	0.00002693	0.08703	0.003821	0.393	0.3	1.952E-13	6.455E-19	0.00526	1.701	6.028E-13	0.499	1.1	0.000429	1.57E-17	0.7947
97	0.00002783	0.2342	0.01171	0.6707	0.7	1.647E-13	5.27E-19	0.00679	4.72	5.603E-13	0.9955	3.2	0.0004427	1.754E-17	0.9932
98	0.00004249	0.1573	0.002707	0.4906	0.2	2.809E-13	1.479E-18	0.004553	1.93	5.414E-13	0.3994	0.1	0.0002698	8.777E-18	1.095
99	0.00002316	0.1767	0.01639	0.4818	1	9.007E-14	2.192E-19	0.01425	4.669	4.314E-13	4.48	10.1	0.0005781	2.013E-17	1.586
100	0.00001133	0.123	0.04208	1.496	0.4	5.018E-14	6.278E-20	0.02922	6.299	4.563E-13	2.269	1.7	0.001139	3.997E-17	1.671
101	0.00001356	0.0418	0.007457	0.3926	0.2	1.127E-13	1.855E-19	0.01181	1.642	7.038E-13	0.299	0.6	0.000862	3.771E-17	0.8882
102	0.0000172	0.08267	0.009529	0.6806	0.1	1.222E-13	2.52E-19	0.006298	2.586	6.176E-13	0.4978	2.4	0.0006882	2.699E-17	0.5937
103	0.0001081	0.4687	0.001338	0.686	0.1	4.838E-13	6.319E-18	0.001003	2.316	3.836E-13	0.3997	2.2	0.0001087	2.606E-18	0.599
104	0.0000861	0.371	0.001695	0.7839	0.2	4.144E-13	4.291E-18	0.001054	2.311	4.167E-13	0.4996	1.8	0.0001373	3.61E-18	0.4989
105	2.407E-07	0.002048	2.194	0.2345	4.7	9.899E-16	2.273E-23	0.5359	5.781	5.166E-13	0.1422	40.97	0.05987	2.854E-15	0.5642
106	0.00006751	0.1705	0.001172	0.6913	0.1	3.656E-13	3.048E-18	0.001833	1.319	4.455E-13	0.4997	0.3	0.0001707	4.517E-18	0.6982
107	0.0001075	0.2525	0.0007027	0.7911	0.1	4.652E-13	6.118E-18	0.001495	1.238	3.621E-13	0.5998	0.5	0.0001082	2.359E-18	0.8985
108	0.00000075	0.01246	1.288	0.1976	3.2	4.506E-15	3.334E-22	0.934	10.91	7.309E-13	0.3156	31	0.01872	1.272E-15	3.166
109	0.00008458	0.2373	0.001012	0.4932	0.1	4.402E-13	4.639E-18	0.001036	1.455	4.208E-13	0.3998	0.5	0.0001348	3.328E-18	0.499
110	2.379E-07	0.001725	1.765	0.1234	3.4	1.262E-15	2.939E-23	0.2903	4.804	6.382E-13	0.147	35	0.05923	3.316E-15	0.3097
111	0.0000113	0.1121	0.03783	0.8478	0.6	6.722E-14	8.391E-20	0.01722	5.785	6.017E-13	1.087	9	0.001131	5.102E-17	0.9828
115	1.197E-06	0.01234	0.5406	8.283E-10	16.8	9.213E-15	1.064E-21	0.09552	6.947	9.896E-13	9.077E-10	45.3	0.01194	1.206E-15	0.5045

Table G. part 11: *Continued*

Sequence # (sample #)	H+	CO2(aq)	CO3--	Ca++	Cl-	H2PO4-	H3PO4	H3SiO4-	HCO3-	HPO4--	Mg++	Na+	OH-	PO4---	SiO2(aq)
								free mmol/kg							
116	4.111E-07	0.004662	3.04	0.06812	63.8	1.905E-15	6.131E-23	0.08084	9.48	8.503E-13	0.5556	137	0.04111	5.551E-15	0.1192
117	0.00003056	0.6235	0.04669	0.03685	20.1	1.657E-13	4.719E-19	0.00533	14.22	7.498E-13	0.7939	53.2	0.0004822	4.102E-17	0.6947
118	3.354E-07	0.006104	10.72	0.4468	221	8.407E-16	1.884E-23	2.083	18.22	7.21E-13	6.925E-10	272	0.05725	1.506E-14	2.117
119	5.479E-07	0.01188	7.355	6.364E-10	163	2.045E-15	7.201E-23	0.2289	22.47	9.552E-13	0.5371	330	0.03486	8.499E-15	0.3711
120	3.234E-07	0.002895	2.947	0.06801	65.6	1.517E-15	3.921E-23	0.09169	7.335	8.502E-13	0.3156	123	0.05165	7.045E-15	0.1083
121	4.052E-07	0.004229	2.654	0.06881	61	1.975E-15	6.481E-23	0.08	8.43	8.663E-13	0.3192	113	0.04084	5.567E-15	0.12
125	0.0000456	0.5105	0.01167	0.9516	4.2	2.18E-13	1.066E-18	0.003118	6.725	5.173E-13	1.395	12.5	0.0002886	1.236E-17	0.6969
126	0.00003151	0.5329	0.04522	0.5635	33.8	1.488E-13	4.062E-19	0.004763	12.68	7.309E-13	1.094	86.6	0.0004958	4.596E-17	0.5952
127	7.763E-06	0.1659	0.1904	0.3547	6.7	4.342E-14	3.097E-20	0.01482	15.05	7.512E-13	1.455	62.6	0.001909	1.435E-16	0.4852
128	6.198E-06	0.1056	0.204	0.5389	15.5	2.459E-14	1.385E-20	0.0112	12.09	5.666E-13	4.557	53.1	0.00244	1.537E-16	0.2888
129	4.673E-06	0.02616	0.06424	9.538E-10	3	1.585E-14	7.611E-21	0.03485	3.502	3.964E-13	6.791	8.3	0.002931	1.002E-16	0.7652
130	0.00001869	0.1051	0.01655	0.4861	3.1	5.828E-14	1.111E-19	0.01021	3.536	3.709E-13	7.171	7.8	0.0007406	2.401E-17	0.8898
131	0.00002397	0.2075	0.02202	0.6722	1.8	6.069E-14	1.436E-19	0.01374	5.595	3.227E-13	10.05	4.4	0.000598	1.808E-17	1.486
132	0.00004668	0.1874	0.004554	0.5896	2	1.342E-13	6.47E-19	0.004517	2.489	3.335E-13	7.092	4.6	0.0002935	8.252E-18	0.9955
133	0.00001446	0.06256	0.0142	0.2929	3.1	5.889E-14	9.129E-20	0.01253	2.598	4.401E-13	4.382	6.9	0.0009106	3.197E-17	0.8875
134	0.00006978	0.4186	0.0033	0.3894	1.5	3.562E-13	2.862E-18	0.002172	3.367	4.796E-13	0.799	6.2	0.0001759	5.903E-18	0.7978
135	5.109E-06	0.04216	0.1486	2.293	8.6	1.643E-14	7.02E-21	0.02916	6.315	5.227E-13	5.512	39.4	0.003252	2.11E-16	0.5708
136	0.00001172	0.2003	0.07962	0.5474	5.8	7.241E-14	8.64E-20	1.799E-11	10.85	7.287E-13	0.7855	23.6	0.001171	7.874E-17	9.82E-10
137	0.00003535	0.179	0.005847	1.074	2.5	1.866E-13	7.448E-19	0.005453	2.886	5.171E-13	1.098	6.2	0.0003556	1.335E-17	0.9945
138	0.00001905	0.3461	0.0609	0.5527	13.5	1.081E-13	1.979E-19	0.008255	12.24	7.386E-13	0.791	43.4	0.0007548	5.761E-17	0.6917
139	8.597E-06	0.01395	0.08304	29.71	620	8.271E-15	4.01E-21	0.03972	1.877	5.49E-13	24.87	591	0.002544	1.763E-15	0.8603
140	0.00000961	0.01025	0.03722	34.05	392	1.01E-14	5.811E-21	0.05544	1.096	4.687E-13	13.39	330	0.002314	7.881E-16	1.425
141	2.592E-06	0.006409	0.1935	5.338	182	4.312E-15	7.425E-22	0.1159	2.412	4.84E-13	10.71	196	0.007711	1.249E-15	0.9041
142	4.186E-06	0.00973	0.3526	12.85	693	4.065E-15	8.111E-22	0.0963	3.48	6.716E-13	26.59	885	0.00544	5.921E-15	0.8867
143	1.899E-06	0.003496	0.3004	9.824	400	2.218E-15	2.486E-22	0.154	2.079	4.77E-13	8.576	435	0.01107	3.437E-15	0.779
144	4.038E-06	0.009974	0.1995	11.44	430	5.339E-15	1.272E-21	0.06283	2.783	5.727E-13	11.25	415	0.005253	2.23E-15	0.6722
145	7.024E-06	0.0121	0.05772	4.952	290	1.504E-14	6.77E-21	0.05304	1.781	7.128E-13	5.748	293	0.002853	9.385E-16	1.077
146	9.785E-06	0.02757	0.1417	33.01	1090	7.205E-15	4.477E-21	0.04372	3.056	5.793E-13	46.81	900	0.001939	3.998E-15	1.186
147	9.384E-07	0.0004426	0.09499	1.609	63.4	2.39E-15	1.422E-22	0.2998	0.4881	6.448E-13	1.394	156	0.02202	3.091E-15	0.8202
148	1.671E-06	0.00927	2.441	17.43	1240	9.382E-16	8.19E-23	0.1536	8.301	5.4E-13	76.71	1310	0.01044	2.86E-14	0.6294
149	8.923E-08	0.00006159	1.361	4.562	55.5	2.362E-17	1.363E-25	0.527	0.6878	6.429E-14	2.04	101	0.2272	2.937E-15	0.14
150	3.112E-06	0.03236	1.319	6.083	1830	2.508E-15	6.084E-22	0.1335	11.03	7.368E-13	36.57	1770	0.00388	2.914E-14	1.497
151	3.743E-06	0.01447	0.4138	2.516	831	5.116E-15	1.138E-21	0.1055	4.712	7.867E-13	15.59	865	0.00504	6.727E-15	1.055
152	6.623E-08	0.0008286	68.97	0.02147	128	1.158E-16	3.51E-25	5.026	18.3	6.239E-13	2.897	460.1	0.3572	6.58E-14	0.7247
153	5.166E-07	0.0002697	0.05396	0.596	19.7	1.805E-15	9.666E-23	0.3979	0.3261	4.121E-13	0.4433	19.6	0.02625	1.047E-15	0.9721
154	3.828E-06	0.005618	0.1013	8.9	470	5.388E-15	1.361E-21	0.09246	1.481	5.598E-13	10.87	403	0.005074	2.171E-15	1.038
155	0.00001156	0.01816	0.02366	4.957	227	2.765E-14	2.308E-20	0.01601	1.419	6.592E-13	5.423	196	0.001603	3.82E-16	0.601
156	0.00003231	0.1338	0.04553	26.93	1730	3.105E-14	8.205E-20	0.006227	3.948	8.249E-13	4.527	1480	0.000403	2.98E-15	0.7268

Table G. part 11: *Continued*

Sequence # (sample #)	H+	CO2(aq)	CO3--	Ca++	Cl-	H2PO4-	H3PO4	H3SiO4-	HCO3-	HPO4--	Mg++	Na+	OH-	PO4---	SiO2(aq)
								free mmol/kg							
157	5.212E-06	0.03707	0.02906	68.21	5470	2.817E-15	5.567E-21	0.004589	2.338	3.481E-13	142.5	4480	0.0001594	5.758E-14	1.115
158	4.918E-06	0.01127	0.07593	4.922	204	1.136E-14	4.108E-21	0.0752	2.03	6.048E-13	3.684	174	0.003717	7.444E-16	1.225
159	0.0001252	0.3221	0.0008316	1.256	2.54	4.616E-13	6.535E-18	0.002053	1.463	3.588E-13	0.8297	3.48	0.0001005	2.59E-18	1.328
160	9.209E-06	0.02255	0.04304	4.688	190	2.236E-14	1.51E-20	0.06675	2.168	6.274E-13	5.666	170	0.001992	3.936E-16	2.033
161	0.00001651	0.05012	0.01032	0.8079	16.9	7.922E-14	1.333E-19	0.01389	1.922	5.844E-13	2.275	15.2	0.0008381	4.824E-17	1.066
162	5.788E-06	0.01006	0.05313	4.943	234	1.276E-14	5.323E-21	0.05826	1.576	6.17E-13	5.415	196	0.003209	7.411E-16	1.092
163	7.345E-06	0.02949	0.1854	36.55	2420	4.154E-15	3.118E-21	0.03458	3.313	6.68E-13	49.27	2000	0.001313	2.727E-14	1.185
164	2.545E-07	0.00001925	0.008984	0.1487	1.78	1.398E-15	4.449E-23	0.2311	0.03919	4.418E-13	0.1287	1.82	0.0445	1.166E-15	0.3359
165	9.391E-06	0.04756	0.0714	39.36	3770	5.726E-15	9.469E-21	0.01151	2.941	6.868E-13	51.3	3350	0.0003801	4.09E-14	1.168
166	1.304E-06	0.001123	0.02298	0.3038	4.23	9.187E-15	1.432E-21	0.09856	0.4666	6.231E-13	0.3066	3.7	0.009087	3.781E-16	0.7014
167	0.00002176	0.08246	0.01558	57.11	4330	1.016E-14	5.193E-20	0.001736	1.748	5.507E-13	104.9	3520	0.0001167	2.527E-14	0.5983
168	4.501E-06	0.01722	0.009419	60.45	4450	3.548E-14	2.346E-20	0.008712	4.622	5.165E-13	85.49	4000	0.00005575	5.431E-14	1.111
169	1.938E-06	0.0016	0.01755	0.3356	6.59	1.408E-14	3.07E-21	0.09215	0.4749	7.166E-13	0.2683	8.48	0.006472	3.497E-16	0.9179
170	1.921E-06	0.002022	0.02892	0.4728	15.8	1.132E-14	2.254E-21	0.09746	0.6581	6.863E-13	0.5559	18.4	0.007057	4.518E-16	0.8855
171	0.00000162	0.002425	0.07461	1.488	43.9	5.411E-15	7.885E-22	0.178	1.076	5.177E-13	1.514	47.8	0.009543	6.725E-16	1.182
172	0.00000155	0.00212	0.1096	1.573	106	4.51E-15	5.45E-22	0.1603	1.145	6.06E-13	1.963	113	0.01121	1.44E-15	0.8797
173	1.054E-06	0.003362	0.7504	2.86	335	1.686E-15	1.126E-22	0.3167	3.382	5.585E-13	5.742	350	0.01893	5.502E-15	0.9533
174	3.574E-06	0.01375	0.4313	2.515	831	4.87E-15	1.034E-21	0.11	4.69	7.842E-13	15.59	865	0.005278	7.022E-15	1.05
175	3.113E-06	0.03218	1.327	6.084	1830	2.488E-15	6.017E-22	0.1338	11.01	7.364E-13	36.96	1770	0.003893	2.959E-14	1.496
176	5.601E-06	0.0117	0.0171	0.5212	1.53	2.206E-14	1.338E-20	0.02176	1.24	4.154E-13	4.406	3.38	0.002334	7.399E-17	0.6032
177	1.671E-06	0.00927	2.441	17.43	1240	9.382E-16	8.19E-23	0.1536	8.301	5.4E-13	76.71	1310	0.01044	2.86E-14	0.6294
178	5.248E-06	0.03743	0.02927	68.23	5460	2.847E-15	5.63E-21	0.004595	2.357	3.497E-13	142.5	4480	0.0001593	5.697E-14	1.115
179	5.627E-08	0.002652	521.8	0.0409	1611	5.198E-17	1.252E-25	6.01	134.5	4.986E-13	0.04306	4002	0.07384	4.99E-13	1.193
180	5.138E-07	0.004951	2.379	0.06784	116	1.811E-15	7.199E-23	0.4026	8.181	7.447E-13	2.324	134	0.03364	5.526E-15	0.7274
181	3.185E-06	0.01297	0.3569	19.46	487	3.005E-15	6.326E-22	0.1184	3.981	3.985E-13	10.59	370	0.006232	2.105E-15	1.102
182	3.113E-06	0.03218	1.327	6.065	1830	2.489E-15	6.019E-22	0.1338	11.02	7.365E-13	36.96	1770	0.003893	2.96E-14	1.496
183	1.742E-07	0.00001937	0.0235	0.9256	0.61	2.138E-16	4.332E-24	0.6438	0.06164	1.118E-13	0.1083	2.08	0.07013	5.189E-16	0.5962
184	6.097E-06	0.01017	0.07125	10.81	330	9.459E-15	3.67E-21	0.07553	1.71	5.682E-13	10.08	313	0.003369	1.06E-15	1.314
185	2.985E-07	0.01031	77.6	0.05116	1420	2.646E-16	4.084E-24	1.315	57.74	7.939E-13	0.03119	2160	0.04643	2.016E-13	1.055
186	4.038E-06	0.009974	0.1995	11.44	430	5.339E-15	1.272E-21	0.06283	2.783	5.727E-13	11.25	415	0.005253	2.23E-15	0.6722
187	4.013E-06	0.02003	0.6911	18.79	873	3.015E-15	6.712E-22	0.08591	6.286	5.516E-13	47.3	870	0.005215	6.798E-15	0.8561
188	2.507E-08	0.0001782	128.5	0.05642	188	4.07E-17	4.2E-26	2.381	11.76	6.472E-13	0.05601	744.1	0.953	2.062E-13	0.1193
189	3.876E-08	0.0003325	78.3	0.1355	189	6.446E-17	1.178E-25	2.908	12.29	5.973E-13	0.1166	548.1	0.5883	1.148E-13	0.2519
190	5.427E-08	0.00001612	0.1851	0.3867	0.52	4.89E-17	3.184E-25	1.264	0.1602	7.775E-14	0.02714	3.93	0.2174	1.068E-15	0.3761
191	1.027E-06	0.004709	0.6078	1.324	136	2.922E-15	2.278E-22	0.3439	3.968	6.353E-13	0.3359	144	0.01718	2.664E-15	1.216
192	5.735E-06	0.02487	0.3641	14.8	966	6.504E-15	2.13E-21	0.06717	5.576	7.629E-13	6.677	1100	0.003278	5.803E-15	1.003
193	1.131E-06	0.004155	0.7887	6.456	161	1.5E-15	1.011E-22	0.1603	4.023	4.126E-13	3.168	229	0.01898	2.551E-15	0.4947
194	1.379E-06	0.08758	1.159	2.005	5040	4.202E-16	2.435E-22	0.001861	26.12	1.988E-13	327.9	3620	0.00061	3.155E-13	0.1031

Table G. part 11: *Continued*

Sequence # (sample #)	H+	CO2(aq)	CO3--	Ca++	Cl-	H2PO4-	H3PO4	H3SiO4-	HCO3-	HPO4--	Mg++	Na+	OH-	PO4---	SiO2(aq)
								free mmol/kg							
195	1.869E-06	0.002993	0.3134	38.85	501	9.289E-16	1.026E-22	0.08876	1.693	2.441E-13	6.865	422	0.01172	2.674E-15	0.4362
196	0.00003298	0.0768	0.01612	18.36	304	5.43E-14	1.218E-19	0.01335	2.158	5.645E-13	7.695	238	0.0006059	1.759E-16	1.337
197	0.00001342	0.04608	0.1415	133.8	2040	5.462E-15	6.16E-21	0.02153	2.764	5.646E-13	64.92	1570	0.00107	1.314E-14	1.058
199	6.984E-07	0.02221	10.6	0.1326	166	0.00003931	1.617E-12	0.004479	35.99	0.0165	3.294	352	0.02935	0.0001438	0.008522
200	1.819E-07	0.002841	21.18	0.01969	161	4.377E-16	4.551E-24	0.02228	18.23	7.26E-13	3.067	351	0.1159	2.488E-14	0.01072
201	2.856E-07	0.005882	16.72	0.05216	159	7.577E-16	1.268E-23	5.636E-10	23.4	7.725E-13	2.917	338	0.07224	1.597E-14	4.364E-10
202	3.558E-07	0.009309	16.1	0.05019	157	1.03E-15	2.209E-23	5.025E-10	28.88	8.184E-13	2.318	324	0.05685	1.314E-14	4.975E-10
203	3.474E-07	0.0118	13.1	0.03162	154	5.664E-06	1.65E-13	4.346E-10	26.65	0.004021	1.827	0.000001	0.04966	0.000078	5.655E-10
204	2.85E-07	0.006003	17.36	0.05131	163	1.501E-06	2.514E-14	5.639E-10	23.89	0.001558	2.779	330	0.07268	0.00003379	4.361E-10
205	2.663E-07	0.005278	17.3	0.05655	160	2.415E-06	3.775E-14	0.01103	22.5	0.00265	2.857	338	0.07757	0.00005939	0.00797
206	1.934E-07	0.003185	20.27	0.04888	164	1.898E-06	2.135E-14	0.025	18.88	0.002913	2.779	343	0.1076	0.00009234	0.013
207	1.892E-07	0.003108	20.9	0.04365	166	2.607E-06	2.857E-14	0.08031	18.92	0.00412	2.793	347	0.1103	0.0001352	0.04069
208	1.138E-06	0.005655	0.2625	0.272	7	0.0000157	1.76E-12	0.0006534	3.252	0.001734	4.842	14.3	0.01254	2.087E-06	0.003347
209	8.608E-07	0.0005154	0.07374	1.6	63.48	2.297E-15	1.546E-22	0.2727	0.4974	4.701E-13	1.39	156.2	0.01944	1.285E-15	0.8423
210	0.00001163	0.02288	0.03356	4.952	290.6	2.723E-14	2.163E-20	0.03076	1.897	7.025E-13	5.752	293.2	0.001615	4.668E-16	1.101
211	9.425E-06	0.01061	0.0347	34.02	392.1	9.963E-15	5.933E-21	0.05372	1.085	4.329E-13	13.36	330.6	0.002236	6.347E-16	1.427
212	1.833E-06	0.003704	0.2726	9.798	409.1	2.171E-15	2.562E-22	0.1477	2.073	4.241E-13	8.568	435	0.01052	2.541E-15	0.7844
213	8.367E-06	0.01483	0.07475	29.73	620.7	8.431E-15	4.305E-21	0.03922	1.862	5.03E-13	24.65	587.2	0.002415	1.302E-15	0.8928
214	3.927E-06	0.01187	0.263	12.78	694	4.744E-15	1.092E-21	0.08508	3.512	5.677E-13	26.62	861.2	0.004725	2.6E-15	0.8969
215	5.711E-06	0.0151	0.2038	33.01	1086	3.989E-15	1.499E-21	0.07078	2.735	5.113E-13	46.77	900.4	0.003197	5.241E-15	1.161
216	1.667E-06	0.01211	1.858	17.33	1241	1.172E-15	1.175E-22	0.1374	8.719	4.746E-13	76.62	1309	0.008955	1.151E-14	0.6446
217	9.478E-06	0.04865	0.07044	39.42	3780	5.81E-15	9.722E-21	0.01143	2.939	6.869E-13	51.33	3349	0.000377	3.922E-14	1.171
218	5.332E-06	0.03796	0.02918	68.26	5473	2.864E-15	5.708E-21	0.004563	2.346	3.526E-13	142.7	4480	0.0001588	5.646E-14	1.11
219	0.00001237	0.04974	0.06622	20.98	3075	9.161E-15	1.404E-20	0.01317	3.091	7.502E-13	53.01	3001	0.000424	1.6E-14	1.135
220	8.036E-06	0.05546	0.2371	24.77	2564	6.133E-15	4.912E-21	0.01403	6.114	7.388E-13	48.38	2601	0.0009102	1.614E-14	0.585
221	0.00001212	0.05164	0.1022	20.48	2435	9.872E-15	1.128E-20	0.0125	3.945	7.611E-13	47.66	2532	0.0006458	9.417E-15	0.7365
222	0.00001436	0.06447	0.09598	17.16	2282	1.235E-14	1.581E-20	0.01063	4.323	7.748E-13	43.55	2401	0.0005959	6.968E-15	0.6884
223	0.0000137	0.05026	0.08707	14.37	2093	1.286E-14	1.437E-20	0.01097	3.786	7.818E-13	42.33	2340	0.0006749	5.454E-15	0.621
224	0.00001099	0.06096	0.1615	13.96	2113	1.065E-14	9.416E-21	0.01525	5.847	7.842E-13	43.11	2462	0.0008032	6.214E-15	0.7008
225	1.781E-06	0.007831	0.1023	0.6115	0.11	6.376E-15	1.276E-21	0.01833	2.516	3.541E-13	3.482	0.25	0.007096	1.802E-16	0.1677
226	5.614E-06	0.02815	0.03635	1.418	0.03	2.319E-14	1.473E-20	0.001832	2.841	4.039E-13	2.447	0.15	0.002248	6.417E-17	0.05317
227	7.039E-06	0.03683	0.02959	1.892	0.05	3.066E-14	2.46E-20	0.001009	2.938	4.199E-13	1.632	0.09	0.001785	5.219E-17	0.03699
228	5.974E-06	0.07823	0.1281	1.378	0.02	1.531E-14	9.176E-21	0.001338	8.307	3.184E-13	8.353	0.24	0.002372	6.961E-17	0.03666
229	0.00001334	0.4494	0.2856	1.567	0.03	1.879E-14	2.024E-20	0.006837	25.97	2.704E-13	28.67	1.32	0.001313	5.283E-17	0.3372
230	0.00001241	0.3668	0.1794	0.1025	0.06	0.0002052	2.359E-10	0.004965	20.31	0.002439	14.09	0.7	0.001229	3.488E-07	0.261
232	3.254E-06	0.1182	1.078	0.1813	0.31	0.00006416	1.776E-11	0.0414	26.98	0.003414	20.89	4.19	0.005084	2.392E-06	0.5246
234	0.00001366	0.5277	0.3683	8.367E-10	0.04	1.746E-14	1.838E-20	0.007517	31.16	2.689E-13	36.74	2.88	0.001336	5.934E-17	0.3625
235	0.0001144	7.287	0.1013	1.095	0.009999	1.081E-13	8.593E-19	0.0006677	55.94	2.485E-13	51.94	2.11	0.0001769	9.589E-18	0.2433

Table G. part 11: *Continued*

Sequence # (sample #)	H+	CO2(aq)	CO3--	Ca++	Cl-	H2PO4-	H3PO4	H3SiO4-	HCO3-	HPO4--	Mg++	Na+	OH-	PO4---	SiO2(aq)
								free mmol/kg							
236	0.00001653	0.01274	0.001256	0.3582	0.01	1.528E-13	3.279E-19	0.0002322	0.3841	6.872E-13	0.1299	0.03	0.000662	2.419E-17	0.02277
237	5.967E-06	0.06941	0.1134	1.595	0.96	1.535E-14	9.206E-21	0.003344	7.364	3.189E-13	7.98	0.87	0.002373	6.961E-17	0.09166
238	7.343E-06	0.07314	0.06925	1.137	0.71	2.343E-14	1.806E-20	0.002981	6.067	3.629E-13	5.732	0.81	0.001844	5.639E-17	0.105
239	0.00001412	0.07854	0.01615	0.3096	0.05	6.2E-14	9.878E-20	0.0002845	3.174	4.315E-13	3.589	0.03	0.0008895	2.752E-17	0.02072
240	0.00001314	0.01271	0.001996	0.2682	0.000001	1.257E-13	2.139E-19	0.0005587	0.4833	7.149E-13	0.1798	0.16	0.0008338	3.196E-17	0.04344
241	0.00001106	0.06122	0.019	0.8005	0.02	5.975E-06	7.655E-12	0.0009908	3.075	0.0000505	2.025	0.17	0.00111	3.828E-09	0.05801
242	3.351E-06	0.005038	0.01326	0.1766	0.01	0.00000575	2.425E-12	0.002368	0.773	0.0001357	0.7344	0.13	0.003362	2.599E-08	0.04563
243	4.144E-07	0.0001431	0.02218	0.03901	0.02	3.825E-07	2.065E-14	0.01356	0.1717	0.00006809	0.3637	0.13	0.02624	9.429E-08	0.03344
244	0.00001123	0.05841	0.01912	1.161	0.07	4.852E-14	6.134E-20	0.002961	2.964	4.265E-13	2.86	0.16	0.001127	3.44E-17	0.171
245	0.00000919	0.237	0.2372	0.1554	0.05	1.69E-14	1.381E-20	0.01065	18.35	2.918E-13	18.85	0.7	0.001728	6.171E-17	0.3984
246	0.0000154	1.025	0.8897	0.03777	0.21	1.493E-14	1.532E-20	0.01238	60.7	2.758E-13	61.1	3.8	0.001366	8.943E-17	0.5827
247	0.00003925	1.928	0.1621	1.409	0.09	5.153E-14	1.566E-19	0.01109	39.37	2.762E-13	32.47	2.82	0.0004641	2.188E-17	1.545
248	0.00000331	0.1093	1.221	0.1893	3.6	4.211E-15	1.098E-21	0.08559	26.15	2.577E-13	32.82	2.5	0.005404	2.232E-16	1.021
249	3.709E-06	0.1258	1.109	0.1759	3.1	4.829E-15	1.414E-21	0.08351	26.81	2.62E-13	32.28	3.31	0.004808	2.005E-16	1.12
250	1.375E-07	0.006437	175.4	0.0171	3.6	2.784E-16	1.566E-24	0.04498	75.63	8.898E-13	0.489	317.4	0.2038	6.775E-14	0.01202
251	6.584E-08	0.00151	128.8	0.02155	3.1	1.492E-16	4.51E-25	0.1243	32.89	8.042E-13	0.5188	286.1	0.3894	8.433E-14	0.01773
252	1.38E-07	0.006408	177.8	0.02285	8.501	0.00008733	4.859E-13	0.0419	76.25	0.2811	0.09268	346.5	0.2035	0.0215	0.01111
253	6.585E-08	0.00151	128.9	0.01863	3.1	0.000015	4.531E-14	0.112	32.9	0.08086	0.5199	286	0.3895	0.008488	0.01598
254	1.467E-07	0.006666	262.6	0.02271	34.8	0.00008638	4.223E-13	0.04042	91.72	0.3463	0.7845	502.4	0.2125	0.03991	0.009583
255	3.181E-08	0.0003419	106.2	0.02234	16.1	0.00001307	2.071E-14	0.03352	14.19	0.1354	0.3807	219.8	0.7727	0.02712	0.002484
256	1.556E-07	0.006697	337.4	0.02797	23	0.0008056	3.473E-12	0.1554	106.2	3.584	0.2872	763	0.2115	0.4597	0.03365
257	9.694E-08	0.002612	291.7	0.04287	22.8	0.0005924	1.627E-12	0.5127	65.02	3.712	0.474	858.5	0.3223	0.5478	0.07138
258	0.0000437	0.3218	0.006167	0.4342	0.03	2.344E-13	1.202E-18	0.001488	4.053	4.895E-13	1.317	0.96	0.0002766	9.187E-18	0.3485
259	4.775E-06	0.1293	0.3517	0.09652	0.14	1.426E-14	6.721E-21	0.01552	17.6	3.873E-13	8.038	2.91	0.002994	1.192E-16	0.3345
260	0.00001528	0.4456	0.1263	0.4307	0.17	4.265E-14	6.284E-20	0.004136	19.34	3.77E-13	8.91	6.22	0.0009566	3.846E-17	0.2789
261	1.405E-06	0.1256	9.174	0.008028	7.761	6.144E-15	5.889E-22	0.1004	85.09	8.999E-13	1.453	180.1	0.01311	1.937E-15	0.4486
262	3.033E-06	0.1244	0.8682	0.03418	0.87	2.116E-14	6.151E-21	0.01975	27.73	9.09E-13	0.3523	35.02	0.004741	4.542E-16	0.2633
263	5.964E-06	0.2031	0.3392	0.03931	0.34	2.795E-14	1.658E-20	0.004722	22.1	5.867E-13	3.409	16.53	0.002354	1.394E-16	0.1283
264	2.056E-06	0.1169	2.597	0.01136	3.1	9.687E-15	1.637E-21	0.06244	44.74	7.667E-13	2.585	80.47	0.0079	7.836E-16	0.4866
265	4.454E-07	0.02976	22.27	2.61E-10	5.5	1.935E-15	5.837E-23	0.09702	64.13	9.175E-13	0.7527	145.7	0.04237	6.538E-15	0.136
266	5.109E-07	0.0226	7.699	0.003487	1.75	3.089E-15	1.321E-22	0.07848	34.28	9.509E-13	0.2144	67.42	0.03148	3.717E-15	0.1545
267	5.234E-07	0.02814	10.53	0.01559	1.13	2.391E-15	9.956E-23	0.07981	43.77	7.858E-13	1.569	73.95	0.03214	3.498E-15	0.1532
268	2.565E-06	0.1437	1.941	0.006075	2.2	1.389E-14	2.985E-21	0.0321	43.3	8.508E-13	1.374	77.64	0.00622	6.582E-16	0.3179
269	0.00000129	0.2398	50.33	2.139E-10	12.7	3.745E-15	2.282E-22	0.1773	257.7	9.835E-13	0.3087	429.9	0.01773	5.36E-15	0.5219
271	2.051E-07	0.01028	50.8	1.695E-10	198.6	5.744E-16	8.634E-24	6.005E-10	45.49	9.421E-13	2.81E-10	0.000001	0.09733	5.74E-14	3.996E-10
272	2.878E-07	0.01824	98	2.68E-10	397.9	0.0003292	4.581E-12	1.582	91.01	0.5475	4.402E-10	704.7	0.07691	0.03128	1.031
274	2.818E-07	0.01971	140.3	2.676E-10	541.8	0.0003667	4.667E-12	1.784	110.5	0.7562	4.4E-10	952.8	0.07746	0.06456	1.079
275	3.523E-07	0.02888	127.3	0.008071	544.6	0.0004497	7.262E-12	1.356	127.4	0.7284	0.009	957.1	0.06101	0.04867	1.041

Table G. part 11: *Continued*

Sequence # (sample #)	H+	CO2(aq)	CO3--	Ca++	Cl-	H2PO4-	H3PO4	H3SiO4-	HCO3-	HPO4--	Mg++	Na+	OH-	PO4---	SiO2(aq)
								free mmol/kg							
278	2.863E-07	0.01953	123.3	2.659E-10	471.2	0.0003678	4.844E-12	1.395	104.4	0.6881	4.394E-10	848.3	0.07724	0.04866	0.8689
283	1.791E-07	0.00625	53.41	2.836E-10	218.9	4.977E-16	5.123E-24	1.074	40.79	9.522E-13	4.219E-10	348.9	0.1186	4.736E-14	0.5072
284	2.253E-07	0.008647	44.66	2.798E-10	209.9	0.0002296	2.99E-12	1.457	44.54	0.3348	4.489E-10	364.1	0.09279	0.012	0.8734
285	2.251E-07	0.008657	42.83	0.006032	191.3	6.782E-16	8.961E-24	1.387	43.82	9.586E-13	0.0314	334.5	0.09236	3.231E-14	0.8432
287	3.376E-07	0.01354	15.56	0.01907	45.14	1.591E-15	3.946E-23	0.8558	35.68	9.621E-13	0.004767	123.1	0.05319	9.329E-15	0.9753
288	3.915E-07	0.009634	4.893	0.02152	17.77	2.514E-15	8.817E-23	0.5493	17.87	9.501E-13	0.005872	50.46	0.03916	4.601E-15	0.8818
289	3.339E-07	0.01269	13.84	0.01613	38.09	1.65E-15	4.166E-23	1.056	32.8	9.639E-13	0.009606	105.7	0.05268	8.748E-15	1.224
290	1.148E-06	0.02016	0.7299	0.3169	0.000001	7.349E-15	8.979E-22	0.1464	10.68	6.898E-13	0.1745	15.57	0.01146	6.524E-16	0.8186
291	9.255E-07	0.01836	1.137	0.2056	4.29	6.058E-15	5.768E-22	0.1802	12.5	7.585E-13	0.1254	19.57	0.01467	1.024E-15	0.7849
292	0.00000143	0.01955	0.4352	0.275	2.34	1.019E-14	1.581E-21	0.185	8.155	7.479E-13	0.124	11.48	0.009052	5.52E-16	1.313
293	7.381E-07	0.01438	1.433	0.181	4.57	4.687E-15	3.527E-22	0.2548	12.38	7.465E-13	0.1497	20.4	0.01854	1.293E-15	0.8773
294	1.806E-06	0.02795	0.3978	0.2541	2.76	1.324E-14	2.58E-21	0.1074	9.289	7.8E-13	0.1703	12.7	0.007204	4.674E-16	0.9576
295	1.431E-06	0.02	0.4456	0.2736	2.37	1.019E-14	1.581E-21	0.1767	8.342	7.487E-13	0.1237	11.48	0.009053	5.541E-16	1.254
296	3.629E-06	0.0679	0.2473	1.223	0.59	1.586E-14	6.169E-21	0.01948	11.22	4.771E-13	1.689	5.96	0.003643	1.469E-16	0.3465
297	2.27E-07	0.002278	2.01	0.1934	1.13	8.975E-16	2.205E-23	0.1488	6.005	4.133E-13	0.4606	10.18	0.05719	1.875E-15	0.1672
298	2.262E-07	0.009822	66.65	2.916E-10	330.1	0.0001806	2.14E-12	0.7839	56.75	0.3203	4.554E-10	574.3	0.09476	0.01657	0.4312
299	4.378E-06	0.0327	0.06346	0.7885	0.56	0.0002942	1.502E-10	0.02667	4.131	0.006195	0.5644	2.35	0.002782	1.189E-06	0.6223
300	1.809E-06	0.02562	0.364	1.046	1.75	7.547E-15	1.475E-21	0.05866	8.437	4.451E-13	1.11	8.35	0.007234	2.636E-16	0.5243
301	0.00008361	0.1408	0.0005756	0.1984	0.03	4.865E-13	5.173E-18	0.00106	0.857	4.501E-13	0.1599	0.31	0.0001333	3.369E-18	0.5149
302	0.00001346	0.05207	0.009024	0.4586	0.06	1.099E-13	1.825E-19	0.004759	2.026	6.725E-13	0.3285	0.52	0.0008549	3.476E-17	0.3612
303	3.083E-06	0.01538	2.416	12.53	657.2	1.08E-15	1.345E-22	0.04942	6.803	4.214E-13	455.7	780.8	0.009319	8.769E-15	0.2836
304	2.482E-06	0.01392	0.6738	2.803	59.16	1.922E-15	2.647E-22	0.0361	6.01	2.624E-13	99.79	196.2	0.009395	6.02E-16	0.2299
306	6.327E-07	0.00585	5.111	1.562	43.78	2.48E-16	8.776E-24	0.3307	9.614	1.571E-13	120.3	35.93	0.03943	1.99E-15	0.5344
307	2.943E-06	0.02338	0.5043	1.674	4.15	2.723E-15	5.265E-22	0.006767	7.31	2.35E-13	63.85	67.29	0.007033	2.817E-16	0.06023
308	0.00000185	0.2083	12.73	0.1731	7.111	2.613E-15	3.079E-22	0.02571	111.2	3.906E-13	31.36	102.6	0.01119	1.108E-15	0.1403
309	1.796E-06	0.01747	0.8302	0.495	9.17	2.076E-15	2.58E-22	0.0544	8.716	2.548E-13	44.37	101.3	0.01075	4.069E-16	0.3116
310	3.029E-06	0.01884	0.4716	31.18	12.07	1.59E-15	2.988E-22	0.01557	5.502	1.54E-13	52.86	62.98	0.007576	2.277E-16	0.1344
311	1.741E-06	0.008178	0.3556	2.844	1.83	1.582E-15	2.072E-22	0.0404	3.821	1.887E-13	40.72	17.88	0.01069	2.891E-16	0.2426
313	1.663E-06	0.01091	0.4056	1.041	4.32	2.104E-15	2.864E-22	0.04839	5.018	2.239E-13	26.92	25.1	0.01026	2.886E-16	0.3016
314	6.269E-06	0.03837	0.07364	2.016	1.46	1.202E-14	6.877E-21	0.008389	4.226	2.788E-13	15	12.14	0.00247	7.109E-17	0.2196
315	6.237E-06	0.02826	0.0532	4.693	1.58	1.146E-14	6.594E-21	0.002563	3.067	2.623E-13	11.74	10.92	0.002482	6.507E-17	0.06744
316	3.817E-06	0.03483	0.15	1.015	5.02	1.151E-14	4.254E-21	0.01301	6.033	3.88E-13	6.671	22.92	0.003788	1.393E-16	0.22
317	0.00001884	0.09304	0.01477	2.108	0.19	5.46E-14	1.036E-19	0.001914	3.117	3.484E-13	6.806	9.26	0.000748	2.214E-17	0.1661
319	2.369E-06	0.02217	0.2248	0.7722	0.53	5.889E-15	1.408E-21	0.01257	5.922	3.027E-13	8.242	3.63	0.005921	1.601E-16	0.1374
320	2.951E-06	0.01678	0.1023	1.097	0.08	7.608E-15	2.318E-21	0.0069	3.515	2.998E-13	7.335	2.11	0.004661	1.168E-16	0.0961
321	2.307E-06	0.01662	0.1539	1.354	2.96	7.887E-15	1.922E-21	0.01368	4.376	3.778E-13	2.791	10.96	0.005804	1.789E-16	0.1523
322	2.333E-06	0.02445	0.2332	0.0437	0.38	8.577E-15	2.073E-21	0.01078	6.508	4.198E-13	5.469	6.96	0.005807	2.046E-16	0.1192
323	2.952E-06	0.02195	0.135	0.956	0.51	7.783E-15	2.368E-21	0.01174	4.609	3.089E-13	7.317	1.63	0.004666	1.232E-16	0.1633

Table G. part 11: *Continued*

Sequence # (sample #)	H+	CO2(aq)	CO3--	Ca++	Cl-	H2PO4-	H3PO4	H3SiO4-	HCO3-	HPO4--	Mg++	Na+	OH-	PO4---	SiO2(aq)
								free mmol/kg							
325	1.824E-06	0.02509	0.3624	0.4213	0.28	7.669E-15	1.492E-21	0.007074	8.313	4.571E-13	2.917	9.7	0.007241	2.706E-16	0.06293
329	1.474E-06	0.01183	0.286	1.036	0.18	3.388E-15	5.183E-22	0.04078	4.94	2.659E-13	6.696	0.71	0.009287	2.091E-16	0.2852
330	1.442E-06	0.00772	0.1715	1.135	0.09	3.805E-15	5.938E-22	0.01635	3.169	2.799E-13	4.339	2.13	0.009109	1.954E-16	0.1166
331	4.527E-06	0.0292	0.06371	1.236	1.65	1.979E-14	9.789E-21	0.0127	3.79	4.535E-13	2.157	7.35	0.002866	9.911E-17	0.2873
332	0.0000023	0.01346	0.122	0.951	0.21	6.897E-15	1.695E-21	0.05361	3.507	3.263E-13	5.049	1.68	0.005778	1.49E-16	0.6024
333	1.837E-06	0.02404	0.3573	0.1799	0.58	6.443E-15	1.249E-21	0.01886	7.979	3.939E-13	5.097	3.65	0.007287	2.438E-16	0.1671
334	2.265E-06	0.01454	0.1246	0.8219	0.25	8.305E-15	2.069E-21	0.009121	3.751	3.765E-13	3.267	3.9	0.005691	1.603E-16	0.1039
335	1.815E-06	0.02313	0.3294	0.1801	0.05	7.088E-15	1.389E-21	0.05132	7.603	4.2E-13	4.122	1.93	0.007216	2.47E-16	0.4597
336	2.264E-06	0.02425	0.2096	0.3271	0.04	9.102E-15	2.268E-21	0.0046	6.264	4.164E-13	3.669	1.42	0.005682	1.837E-16	0.0524
337	0.00000226	0.02322	0.1994	0.4068	0.06	9.131E-15	2.279E-21	0.008865	5.99	4.155E-13	3.434	1.57	0.005676	1.814E-16	0.1011
338	0.00001408	0.09009	0.0184	1.531	0.05	6.679E-14	1.065E-19	0.002584	3.62	4.623E-13	1.828	1.23	0.0008948	2.937E-17	0.1884
340	2.817E-06	0.02447	0.1276	0.5207	0.25	1.255E-14	3.981E-21	0.009678	4.968	4.409E-13	2.688	1.18	0.004471	1.454E-16	0.1403
341	4.411E-06	0.02179	0.04308	1.144	0.61	2.16E-14	1.098E-20	0.01209	2.755	4.613E-13	1.436	1.52	0.002802	8.905E-17	0.2809
342	0.00000225	0.02489	0.2107	0.2395	0.05	1.009E-14	2.527E-21	0.01831	6.405	4.543E-13	3.089	1.22	0.00565	1.962E-16	0.2097
343	6.992E-06	0.02881	0.02257	1.201	0.06	3.375E-14	2.723E-20	0.007816	2.293	4.533E-13	1.844	0.21	0.001768	5.44E-17	0.2882
345	0.00000223	0.02112	0.1727	0.5143	0.05	1.008E-14	2.548E-21	0.007969	5.385	4.425E-13	2.333	1.26	0.005613	1.819E-16	0.09203
346	3.491E-06	0.02623	0.08128	0.9744	0.01	1.727E-14	7.002E-21	0.004762	4.164	4.61E-13	1.346	0.61	0.003512	1.116E-16	0.08824
347	2.673E-06	0.02193	0.09533	8.942E-10	0.06	3.154E-14	1.047E-20	0.03636	4.283	9.682E-13	9.538E-10	0.000001	0.004262	2.606E-16	0.5516
348	0.00001099	0.07502	0.02286	0.7458	0.03	6.429E-14	8.276E-20	0.002006	3.755	5.359E-13	1.357	0.84	0.001104	4.004E-17	0.118
349	3.451E-06	0.01942	0.05745	0.5341	0.000001	2.027E-14	8.309E-21	0.002281	3.056	5.226E-13	1.258	0.71	0.003464	1.184E-16	0.04272
352	0.00000862	0.04488	0.02064	0.8086	0.01	5.702E-14	5.9E-20	0.005178	2.796	5.768E-13	0.7232	0.29	0.001376	5.081E-17	0.2448
353	8.599E-06	0.04344	0.01978	0.8574	0.04	5.788E-14	6.004E-20	0.002851	2.699	5.813E-13	0.5945	0.28	0.001373	5.055E-17	0.1351
356	1.431E-07	0.004698	38.96	0.04498	25.53	5.132E-16	4.718E-24	0.2335	33.34	8.288E-13	0.3489	147.5	0.1386	2.121E-14	0.09951
357	3.208E-07	0.01096	9.513	0.05034	10.3	1.736E-15	4.682E-23	0.006699	26.38	8.619E-13	0.1691	57.85	0.0502	5.575E-15	0.008301
358	2.76E-07	0.009745	25.88	0.03371	162.5	0.00006218	1.096E-12	0.03984	36.74	0.06274	0.5121	267.1	0.07127	0.001372	0.03217
359	3.001E-07	0.02268	144.9	0.03075	409.2	5.195E-16	6.532E-24	0.1448	126.6	9.23E-13	0.6821	944	0.07543	5.395E-14	0.0882
361	0.0008079	0.06293	2.244E-06	0.05998	0.01	9.206E-13	1.014E-16	5.963E-06	0.03705	7.69E-14	1E-09	0.03	0.00001287	4.765E-20	0.02999
368	0.00001152	0.1271	0.04822	0.3291	9.14	8.381E-14	1.015E-19	0.02157	6.802	8.182E-13	0.1877	19.57	0.001157	8.456E-17	1.193
370	0.00001752	0.1591	0.01985	0.9017	0.22	0.001322	2.673E-09	0.008197	5.07	0.007089	0.5743	2.7	0.0007023	3.507E-07	0.7578
371	5.631E-06	0.0732	0.09766	0.9195	0.42	3.388E-14	2.129E-20	0.03413	7.505	6.034E-13	0.7166	4.96	0.002254	1.04E-16	0.9809
372	0.00003422	0.1846	0.005318	0.6804	0.1	0.001467	6.046E-09	0.002989	2.891	0.003704	0.2889	1.3	0.0003448	8.147E-08	0.563
373	3.457E-07	0.008326	14.7	0.09925	213.6	0.0001028	2.222E-12	0.0276	25.68	0.08479	5.267	374.5	0.05623	0.001502	0.0274
374	1.587E-06	0.03563	1.359	0.1339	54.17	3.767E-06	5.08E-13	0.003077	17.16	0.0004132	3.929	70.03	0.01015	6.817E-07	0.01892
375	0.00003357	0.1031	0.002755	0.3936	0.16	2.637E-13	1.107E-18	0.001986	1.588	6.296E-13	0.07988	0.87	0.000338	1.249E-17	0.381
376	0.00003446	0.1183	0.003506	0.806	1.44	2.15E-13	8.802E-19	0.002478	1.863	5.549E-13	0.5292	1.87	0.0003474	1.265E-17	0.4635
377	8.172E-07	0.02439	3.864	0.1022	45.99	0.00004537	2.976E-12	0.02322	24.18	0.01001	3.158	101.3	0.02043	0.00003232	0.06978
378	6.497E-07	0.01856	4.679	0.09004	46.27	0.00003816	1.985E-12	0.01685	23.21	0.01063	2.997	101.3	0.02576	0.00004338	0.04015
381	0.00003352	0.08505	0.002257	0.3943	0.17	0.00108	4.542E-09	0.001635	1.307	0.002564	0.1895	0.43	0.0003375	5.022E-08	0.3144

Table G. part 11: *Continued*

Sequence # (sample #)	H+	CO2(aq)	CO3--	Ca++	Cl-	H2PO4-	H3PO4	H3SiO4-	HCO3-	HPO4--	Mg++	Na+	OH-	PO4---	SiO2(aq)
								free mmol/kg							
382	0.00003086	0.1592	0.05873	11.37	710.9	0.0003004	5.564E-10	0.001777	5.871	0.004807	30.87	839.5	0.0006096	3.265E-06	0.1492
383	2.253E-07	0.008642	44.64	0.008403	209.9	0.0002273	2.961E-12	1.457	44.51	0.3315	0.02694	364.1	0.09279	0.01188	0.8735
384	2.149E-07	0.006056	20.83	0.03034	99.32	0.000103	1.541E-12	0.6815	26.64	0.1135	0.2272	165.3	0.0873	0.002355	0.4665
385	0.0001337	0.2048	0.0003452	0.2382	0.48	0.00196	3.274E-08	0.0007836	0.7931	0.001174	0.2898	0.61	0.00008486	5.816E-09	0.5982
386	0.00000992	0.05085	0.0807	5.746	3950	0.00001919	3.357E-11	0.0008438	3.218	0.00246	295.7	3636	0.0003133	0.0001661	0.1022
387	0.0002473	0.9795	0.005093	23.32	609.4	2.623E-13	4.169E-18	0.001135	4.035	5.03E-13	12.22	548.1	0.00007972	4.354E-17	0.7979
388	0.00006546	0.1848	0.01097	28.19	375.2	9.972E-14	4.312E-19	0.003263	2.655	5.726E-13	2.879	305.8	0.0003094	1.082E-16	0.6287
389	0.00003092	0.1299	0.01154	3.117	53.88	0.00001099	3.049E-11	0.00471	3.001	0.00005785	2.995	44.8	0.0005061	4.387E-09	0.5943
390	0.000104	0.409	0.005359	13.2	123.3	2.046E-13	1.617E-18	0.001624	3.217	4.557E-13	3.789	109.6	0.0001757	1.92E-17	0.5814
392	0.00004438	0.4167	0.008607	1.692	2.4	2.085E-13	1.053E-18	4.317E-12	5.293	4.622E-13	1.027	0.000001	0.0002834	9.832E-18	9.957E-10
393	0.00004537	0.4937	0.01147	0.3042	8.52	1.752E-13	8.623E-19	4.432E-12	6.467	4.263E-13	3.528	0.000001	0.0002885	1.104E-17	9.956E-10
394	0.0001466	1.123	0.002775	4.058	7.59	3.567E-13	5.457E-18	1.43E-12	4.641	2.866E-13	2.718	0.000001	0.00009444	2.449E-18	9.986E-10
395	3.475E-06	0.02268	0.06931	1.44	0.51	1.699E-14	6.913E-21	0.01021	3.582	4.49E-13	0.5639	0.65	0.003512	1.07E-16	0.1898
396	0.00001402	0.009574	0.003414	43.82	4401	1.041E-14	3.187E-20	0.0004794	0.337	6.527E-13	55.95	4184	0.0001423	2.069E-14	0.1225
397	2.247E-06	0.0146	0.1217	1.42	0.29	7.632E-15	1.917E-21	8.013E-11	3.726	3.396E-13	2.331	1.44	0.005674	1.405E-16	9.199E-10
398	1.011E-06	0.01616	1.398	0.5056	23.37	2.637E-15	2.271E-22	2.022E-10	12.08	4.158E-13	7.287	70.03	0.01581	8.21E-16	7.978E-10
399	8.071E-07	0.01621	2.119	0.2747	7.72	2.184E-15	1.498E-22	2.407E-10	15.19	4.135E-13	7.325	67.86	0.01969	9.084E-16	7.593E-10
400	1.443E-06	0.01742	1.363	1.413	9.67	1.476E-15	1.437E-22	1.82E-10	11.03	2.336E-13	46.71	107	0.01364	4.883E-16	8.18E-10
401	1.872E-06	0.01504	6.498	3.65	198.9	6.994E-16	4.443E-23	2.48E-10	11.9	3.475E-13	483.6	561.1	0.01778	4.764E-15	7.52E-10
402	0.00000198	0.01372	0.9789	3.187	21.68	1.379E-15	1.551E-22	1.613E-10	7.175	2.261E-13	99.24	126.6	0.01177	5.815E-16	8.387E-10
403	1.023E-06	0.006966	2.25	1.188	19.82	5.423E-16	2.979E-23	2.825E-10	7.35	1.953E-13	125.7	106.6	0.02413	1.177E-15	7.175E-10
404	2.624E-06	0.01346	3.49	13.48	299.9	1.685E-15	1.196E-22	1.88E-10	9.816	4.588E-13	735.6	2553	0.00736	1.625E-15	8.12E-10
405	2.019E-06	0.009729	0.1998	3.235	4.5	2.813E-15	4.982E-22	1.098E-10	3.441	2.161E-13	16.09	20.66	0.00795	1.883E-16	8.902E-10
406	2.093E-06	0.01029	1.043	4.863	81.53	1.267E-15	1.276E-22	1.755E-10	5.849	2.602E-13	156.7	277.5	0.01237	9.833E-16	8.245E-10
408	3.186E-06	0.04657	0.3792	0.5845	2.7	5.91E-15	1.667E-21	7.188E-11	10.46	2.867E-13	17.16	13.66	0.004965	1.619E-16	9.281E-10
409	5.895E-06	0.04708	0.07282	2.138	1.37	1.845E-14	1.115E-20	3.492E-11	4.965	3.656E-13	4.606	9.79	0.002348	7.264E-17	9.651E-10
410	0.00000144	0.007499	0.8975	3.034	158.7	1.238E-15	1.099E-22	1.981E-10	5.264	2.789E-13	57.17	212.3	0.01474	1.315E-15	8.019E-10
411	1.917E-06	0.02149	0.3746	1.648	6.95	4.894E-15	9.025E-22	1.06E-10	7.449	3.336E-13	5.333	23.97	0.007596	2.477E-16	8.94E-10
412	1.575E-06	0.01121	1.56	3.545	133.4	1.237E-15	9.868E-23	2.108E-10	8.494	2.826E-13	104.8	413.2	0.0147	1.115E-15	7.892E-10
413	2.727E-06	0.01153	0.19	3.911	1.31	2.86E-15	5.999E-22	9.422E-11	3.369	2.069E-13	35.17	27.45	0.006684	1.865E-16	9.058E-10
414	2.129E-06	0.02495	0.6427	2.062	29.17	3.698E-15	6.009E-22	1.181E-10	9.718	3.262E-13	18.09	101.3	0.008237	3.738E-16	8.819E-10
415	7.431E-07	0.01754	1.778	0.09322	1.99	3.549E-15	2.667E-22	2.253E-10	15.09	5.735E-13	2.039	16.14	0.0186	1.014E-15	7.747E-10
416	4.119E-06	0.02442	0.806	9.345	233.8	3.319E-15	5.678E-22	1.07E-10	8.377	3.745E-13	190.3	839.5	0.005857	7.491E-16	8.93E-10
417	1.539E-06	0.04312	1.224	0.2475	0.8	5.945E-15	8.595E-22	1.311E-10	19.22	5.16E-13	4.088	34.62	0.00955	5.024E-16	8.69E-10
418	6.366E-06	0.04348	0.088	2.411	1.6	1.126E-14	6.349E-21	3.73E-11	4.84	2.712E-13	17.27	14.09	0.002501	7.344E-17	9.627E-10
419	8.252E-07	0.02432	3.595	0.1339	24.51	3.288E-15	2.158E-22	2.486E-10	24.04	6.739E-13	3.019	115.3	0.02011	1.78E-15	7.514E-10
420	9.087E-07	0.01852	3.567	0.3317	34.5	1.555E-15	9.104E-23	2.681E-10	20.16	3.658E-13	24.94	245.3	0.021	1.093E-15	7.319E-10
421	2.178E-06	0.006896	0.7069	9.268	21.08	1.128E-15	1.144E-22	1.744E-10	3.731	2.321E-13	180.1	188.8	0.01262	8.234E-16	8.256E-10

Table G. part 11: *Continued*

Sequence # (sample #)	H+	CO2(aq)	CO3--	Ca++	Cl-	H2PO4-	H3PO4	H3SiO4-	HCO3-	HPO4--	Mg++	Na+	OH-	PO4---	SiO2(aq)
								free mmol/kg							
422	1.795E-06	0.01009	0.1357	2.036	0.21	4.776E-15	9.483E-22	9.924E-11	3.248	2.708E-13	2.285	1.7	0.0072	1.431E-16	9.008E-10
423	7.992E-07	0.02006	2.646	0.2579	18.43	3.74E-15	2.555E-22	2.416E-10	19.05	7.137E-13	0.9629	82.64	0.01967	1.671E-15	7.584E-10
424	4.927E-06	0.03227	0.0951	2.586	2.23	9.452E-15	4.339E-21	4.546E-11	4.428	2.706E-13	12.79	7.26	0.003091	8.452E-17	9.545E-10
425	6.054E-07	0.01337	2.317	0.06382	1.22	2.023E-15	1.179E-22	2.725E-10	14.79	4.33E-13	4.504	22.01	0.02387	1.028E-15	7.275E-10
426	5.751E-06	0.0431	0.06103	0.9602	0.4	2.061E-14	1.279E-20	3.407E-11	4.454	3.844E-13	4.487	1.87	0.002289	6.906E-17	9.659E-10
427	0.00000301	0.04215	0.2813	1.643	2.76	8.212E-15	2.435E-21	6.865E-11	9.073	3.444E-13	5.822	13.57	0.004753	1.542E-16	9.314E-10
428	5.729E-06	0.03288	0.04599	2.367	1.27	1.997E-14	1.243E-20	3.398E-11	3.37	3.69E-13	2.681	2.44	0.0023	6.52E-17	9.66E-10
429	2.931E-07	0.009057	19.58	0.1292	54.45	6.468E-16	1.124E-23	5.504E-10	33.98	5.08E-13	8.799	351.5	0.06737	5.514E-15	4.497E-10
430	2.268E-06	0.00416	0.5217	7.831	15.03	1.022E-15	1.012E-22	1.786E-10	2.229	2.466E-13	235.3	134.8	0.0133	1.16E-15	8.214E-10
431	2.347E-06	0.0248	0.9287	2.466	66.55	2.915E-15	4.129E-22	1.318E-10	10.89	3.218E-13	48.95	258.8	0.008751	5.161E-16	8.682E-10
432	8.047E-07	0.01287	1.71	0.2105	13.33	1.933E-15	1.33E-22	2.405E-10	12	3.74E-13	9.276	57.42	0.01977	8.627E-16	7.595E-10
433	2.911E-06	0.007137	1.452	12.44	144.8	1.727E-15	1.363E-22	1.834E-10	4.451	4.278E-13	672.7	1875	0.008447	1.395E-15	8.167E-10
434	1.698E-07	0.0002455	0.9761	2.085	4.93	5.283E-17	7.043E-25	6.207E-10	1.142	5.882E-14	31.82	27.97	0.1045	8.049E-16	3.793E-10
435	4.532E-06	0.03403	0.0742	2.193	0.26	1.566E-14	7.775E-21	4.222E-11	4.376	3.6E-13	2.49	1.57	0.002882	7.863E-17	9.578E-10
436	5.645E-06	0.0345	0.04556	1.539	0.22	2.28E-14	1.439E-20	3.35E-11	3.5	4.037E-13	2.471	0.87	0.00226	6.629E-17	9.665E-10
437	0.00000402	0.05366	0.2685	1.258	6.5	1.205E-14	4.189E-21	5.891E-11	9.873	4.419E-13	7.705	70.47	0.003906	1.792E-16	9.411E-10
439	5.718E-06	0.04419	0.06138	1.399	0.66	2.181E-14	1.359E-20	3.392E-11	4.542	4.01E-13	3.227	2.44	0.002284	7.056E-17	9.661E-10
440	3.222E-07	0.0001439	0.1268	5.909	20.89	1.226E-16	3.366E-24	4.434E-10	0.3269	6.274E-14	12.25	40.76	0.05118	3.925E-16	5.566E-10
441	3.461E-06	0.03096	0.331	1.418	2.96	4.23E-15	1.102E-21	7.717E-11	7.353	2.465E-13	37.44	41.19	0.005299	1.82E-16	9.228E-10
442	1.988E-06	0.01289	0.9064	1.857	6	1.355E-15	1.542E-22	1.598E-10	6.632	2.212E-13	103.8	91.34	0.01178	5.564E-16	8.402E-10
443	8.098E-07	0.01732	3.116	0.1509	94.68	3.127E-15	2.011E-22	2.547E-10	17.64	7.754E-13	1.695	117.9	0.02095	3.344E-15	7.453E-10
444	1.252E-06	0.01331	0.6788	2.479	14.61	1.941E-15	2.175E-22	1.633E-10	7.531	2.35E-13	9.806	30.32	0.01249	3.414E-16	8.367E-10
445	2.906E-06	0.01852	0.1072	1.347	1	9.442E-15	2.905E-21	6.635E-11	3.854	3.567E-13	3.911	7.48	0.004603	1.305E-16	9.337E-10
446	0.00000121	0.03989	1.771	0.08655	1.74	5.695E-15	6.59E-22	1.587E-10	22.27	6.196E-13	2.557	28.58	0.01197	7.782E-16	8.414E-10
447	1.931E-06	0.01857	0.3267	1.152	0.72	3.69E-15	6.848E-22	1.054E-10	6.354	2.551E-13	11.48	3.52	0.007626	1.891E-16	8.946E-10
448	4.056E-06	0.01698	0.3364	3.524	5.92	2.671E-15	6.001E-22	8.82E-11	4.332	2.411E-13	123.3	54.81	0.006108	3.622E-16	9.118E-10
449	1.262E-06	0.004193	0.6129	9.78	10.38	1.073E-15	7.07E-23	2.406E-10	3.833	2.084E-13	62.73	465.4	0.01699	4.306E-16	7.594E-10
450	9.591E-07	0.02988	2.142	0.131	8.18	5.332E-15	4.878E-22	1.927E-10	21.16	7.421E-13	0.9178	30.97	0.01513	1.235E-15	8.074E-10
451	2.524E-06	0.03348	0.4328	0.6976	11.48	6.034E-15	1.335E-21	8.981E-11	9.665	3.649E-13	11.3	43.37	0.006232	2.593E-16	9.102E-10
452	0.00000119	0.01063	0.4358	0.5674	3.87	3.175E-15	3.768E-22	1.556E-10	5.745	3.278E-13	6.188	14.75	0.01183	3.532E-16	8.444E-10
453	5.971E-07	0.002772	1.786	1.203	79.84	4.562E-16	1.592E-23	3.814E-10	4.924	2.135E-13	61.08	268.8	0.03537	1.517E-15	6.186E-10
454	4.467E-06	0.04674	0.3434	3.984	38.06	8.317E-15	2.511E-21	6.666E-11	9.743	3.854E-13	22.53	210.5	0.004202	2.268E-16	9.333E-10
455	1.333E-06	0.02132	1.236	0.7506	15.25	3.618E-15	3.724E-22	1.738E-10	13.31	4.535E-13	8.591	139.2	0.01266	6.565E-16	8.263E-10
456	1.866E-06	0.02511	0.3962	0.6985	2.49	5.984E-15	1.138E-21	1.031E-10	8.482	3.808E-13	4.692	11.48	0.007401	2.524E-16	8.969E-10
457	6.235E-06	0.02	0.03746	4.051	1.66	1.174E-14	6.753E-21	3.661E-11	2.177	2.673E-13	12.22	12.18	0.002473	6.542E-17	9.634E-10
458	3.066E-06	0.01158	0.3845	6.571	96.09	2.13E-15	3.739E-22	1.108E-10	3.893	2.573E-13	96.55	131.4	0.007694	6.191E-16	8.892E-10
459	3.732E-06	0.02849	0.4104	1.871	7.7	3.242E-15	7.868E-22	8.232E-11	7.039	2.35E-13	70.66	38.32	0.005675	2.499E-16	9.177E-10
460	4.008E-06	0.01955	2.264	10.95	487.5	2.17E-15	2.636E-22	1.277E-10	8.432	4.952E-13	712.8	2049	0.005456	2.408E-15	8.723E-10

Table G. part 11: *Continued*

Sequence # (sample #)	H+	CO2(aq)	CO3--	Ca++	Cl-	H2PO4-	H3PO4	H3SiO4-	HCO3-	HPO4--	Mg++	Na+	OH-	PO4---	SiO2(aq)
								free mmol/kg							
461	2.485E-07	0.01023	49.19	0.1049	127.8	7.608E-16	8.702E-24	6.408E-10	60.07	8.717E-13	1.13	796.1	0.0844	1.417E-14	3.592E-10
462	6.836E-07	0.002426	0.6596	1.971	34.36	7.238E-16	3.653E-23	3.011E-10	3.032	2.089E-13	23.5	117.9	0.02636	7.885E-16	6.989E-10
473	4.181E-06	0.02457	0.2048	12.13	115.7	5.94E-15	1.86E-21	6.576E-11	4.88	3.321E-13	7.676	117.4	0.004416	3.439E-16	9.342E-10
474	4.202E-06	0.02167	0.1857	14.47	121.3	5.573E-15	1.73E-21	6.629E-11	4.312	3.175E-13	6.889	126.1	0.004452	3.395E-16	9.337E-10
475	6.786E-06	0.02943	0.1148	20.73	148.1	8.54E-15	4.07E-21	4.428E-11	3.74	3.403E-13	9.952	147.9	0.002905	2.784E-16	9.557E-10
476	5.293E-06	0.03547	0.1937	13.99	122.7	7.62E-15	2.976E-21	5.345E-11	5.616	3.482E-13	7.816	124	0.003542	3.024E-16	9.466E-10
477	5.347E-06	0.03157	0.1983	8.449	169.3	8.203E-15	3.074E-21	5.566E-11	5.33	4.159E-13	16.3	178.3	0.00359	4.474E-16	9.443E-10
478	3.379E-06	0.01827	0.2939	8.817	174.9	4.466E-15	1.051E-21	8.582E-11	4.906	3.645E-13	17.02	182.7	0.005714	6.41E-16	9.142E-10
479	3.378E-06	0.01411	0.2299	8.963	180.6	4.424E-15	1.038E-21	8.61E-11	3.802	3.65E-13	17.34	187	0.005728	6.563E-16	9.139E-10
480	3.387E-06	0.01805	0.2994	9.424	184.8	4.34E-15	1.013E-21	8.651E-11	4.884	3.625E-13	17.73	193.6	0.005746	6.671E-16	9.135E-10
481	3.384E-06	0.01588	0.2634	9.243	186.2	4.38E-15	1.022E-21	8.654E-11	4.302	3.657E-13	17.66	195.7	0.005744	6.735E-16	9.135E-10
482	3.373E-06	0.01417	0.2292	8.253	180.6	4.591E-15	1.078E-21	8.603E-11	3.826	3.763E-13	16.88	189.2	0.005711	6.696E-16	9.14E-10
483	4.257E-06	0.01744	0.1796	8.092	179.2	5.964E-15	1.763E-21	6.958E-11	3.734	3.917E-13	19.1	182.7	0.004549	5.613E-16	9.304E-10
484	3.372E-06	0.0153	0.2392	7.822	165	4.588E-15	1.09E-21	8.512E-11	4.078	3.667E-13	17.49	169.6	0.005683	6.174E-16	9.149E-10
485	3.354E-06	0.01393	0.2095	7.024	155.2	4.786E-15	1.15E-21	8.421E-11	3.677	3.722E-13	16.27	155.7	0.005641	5.963E-16	9.158E-10
486	0.00001307	0.0604	0.04371	10.27	78.99	2.65E-14	2.72E-20	2.097E-11	3.661	4.196E-13	7.583	86.99	0.001359	1.079E-16	9.79E-10
487	1.878E-06	0.008446	0.1435	2.808	16.36	4.483E-15	8.386E-22	1.048E-10	2.882	3.029E-13	2.425	18.7	0.007583	2.298E-16	8.952E-10
488	1.488E-06	0.006552	0.1742	2.794	15.52	3.181E-15	4.742E-22	1.281E-10	2.805	2.682E-13	2.339	17.4	0.009522	2.52E-16	8.719E-10
489	0.00002236	0.1257	0.01056	1.088	4.51	1.25E-13	3.135E-19	8.653E-12	3.228	5.595E-13	1.026	6.09	0.0005661	2.404E-17	9.913E-10
490	1.486E-06	0.007168	0.1905	2.728	15.8	3.247E-15	4.843E-22	1.281E-10	3.07	2.738E-13	2.187	17.4	0.009517	2.581E-16	8.719E-10
522	0.0000048	0.0601	0.1264	2.021	0.52	0.002845	1.457E-09	0.04522	7.502	0.06502	2.414	3.33	0.002784	0.00001491	1.059
523	3.877E-08	0.0005135	101.4	0.2583	20.84	0.0000141	2.779E-14	0.7169	17.12	0.1155	0.341	236.6	0.6187	0.01771	0.0661
524	3.209E-08	0.000308	50.67	0.3351	11.84	0.00001031	2.131E-14	0.6828	9.713	0.07406	0.2687	122.4	0.6311	0.008315	0.06523
525	8.628E-08	0.002465	129.4	0.3788	34.15	0.000242	9.515E-13	0.8715	41.39	1.05	0.244	309.3	0.2972	0.09649	0.1616
526	7.387E-08	0.001477	523.8	1.597	74.64	0.0000361	5.612E-14	1.049	68.11	0.3993	2.863	1595	0.4055	0.1066	0.09043
527	5.937E-06	0.1481	0.2415	0.9346	0.38	2.151E-14	1.287E-20	0.01755	15.87	4.45E-13	4.539	8.92	0.002357	1.007E-16	0.4805
528	4.025E-06	0.1038	0.3755	0.7945	0.37	0.002791	1.124E-09	0.05315	16.54	0.08619	4.561	8.96	0.003497	0.0000295	0.9799
529	2.205E-07	0.01458	174.9	0.3574	39.5	0.0001318	1.108E-12	1.164	115.5	0.2759	1.38	513.5	0.125	0.01361	0.474
530	1.45E-07	0.006528	235.1	0.4302	49.69	0.00006627	3.215E-13	1.609	90.62	0.2401	0.8556	672.6	0.2002	0.0207	0.385
531	0.00004351	1.932	0.07325	1.136	0.94	0.004031	1.649E-08	0.003781	30.18	0.01323	6.77	11.05	0.0003439	5.41E-07	0.7082
532	0.00002387	1.067	0.1333	0.9949	0.68	7.283E-14	1.64E-19	0.006158	30.32	4.333E-13	6.692	10.7	0.0006246	3.205E-17	0.6349
533	0.00002075	0.8827	0.1436	0.449	0.6	0.004175	8.204E-09	0.007431	28.79	0.02824	7.057	11	0.0007141	2.347E-06	0.6686
534	0.00001261	0.617	0.2865	0.4648	0.59	3.996E-14	4.686E-20	0.007163	33.72	4.603E-13	7.021	14.35	0.001193	6.714E-17	0.3848
535	0.00001118	1.154	0.9946	0.2206	0.47	0.01011	9.094E-09	0.0109	82.79	0.1648	3.239	66.03	0.001498	0.0000414	0.4521
536	1.343E-07	0.005354	427	0.09391	101.9	0.0001209	4.31E-13	0.4984	104.3	0.7173	0.5652	881.4	0.2429	0.1439	0.0897
537	2.164E-07	0.01293	478.7	0.1274	105.7	0.0002493	1.329E-12	0.5588	170.3	1.016	0.1911	1021	0.1508	0.1509	0.1534
538	9.955E-08	0.002648	563.6	0.1786	1.37	0.000048	1.014E-13	0.7367	87.97	0.4368	0.6321	1129	0.3505	0.1209	0.08243
539	7.157E-08	0.001599	403.2	0.1219	96.76	0.00001527	3.016E-14	0.4861	55.95	0.1595	0.5138	810.1	0.4551	0.05293	0.04796

Table G. part 11: *Continued*

Sequence # (sample #)	H+	CO2(aq)	CO3--	Ca++	Cl-	H2PO4-	H3PO4	H3SiO4-	HCO3-	HPO4--	Mg++	Na+	OH-	PO4---	SiO2(aq)
								free mmol/kg							
540	5.899E-06	0.2232	0.4134	0.5375	0.58	2.156E-14	1.237E-20	0.0405	24.99	4.853E-13	4.972	10.53	0.002449	1.298E-16	1.064
541	7.205E-06	0.2806	0.431	0.8795	0.7	1.713E-14	1.117E-20	0.02191	27.39	3.626E-13	11.49	10.53	0.002155	9.611E-17	0.6541
542	5.152E-06	0.1753	0.4821	0.4702	1.26	1.549E-14	7.378E-21	0.01402	23.58	4.29E-13	7.952	23.1	0.002926	1.413E-16	0.306
543	2.827E-07	0.02301	200.4	0.4033	48.97	0.001616	1.641E-11	2.526	151.6	2.966	0.3733	555.7	0.1009	0.1439	1.249
544	2.732E-07	0.02198	150.9	0.3229	14.62	0.0008182	9.109E-12	1.416	130.5	1.297	0.1749	399.7	0.09916	0.04857	0.7563
545	1.461E-07	0.006645	252.9	0.3771	50.8	0.0001491	7.142E-13	1.613	93.52	0.5644	1.011	662.6	0.203	0.0538	0.381
546	1.405E-07	0.005896	308.5	0.3924	69.36	0.000252	1.022E-12	2.096	99.63	1.103	0.2637	925.9	0.2127	0.1194	0.4322
547	1.263E-07	0.00359	957.7	1.832	133.9	0.00008786	1.815E-13	2.448	134.2	0.9501	3.504	1961	0.2406	0.4497	0.295
548	2.73E-07	0.02185	227.2	0.3424	61.34	0.0005688	5.345E-12	1.512	156.3	1.154	0.2784	605.1	0.1064	0.06486	0.6955
549	5.264E-07	0.06086	70.88	0.1535	20.82	0.001168	3.076E-11	0.5071	151.5	0.7441	0.8023	308.2	0.04444	0.01005	0.6321
550	1.91E-07	0.01051	386.9	0.5389	60.68	0.000172	8.818E-13	2.233	141.1	0.669	0.3896	870.2	0.1687	0.08051	0.5809
551	2.015E-07	0.01008	609.1	0.8915	78.68	0.0002227	8.994E-13	2.327	180.7	1.085	0.4792	1551	0.1547	0.1697	0.5213
552	1.131E-07	0.003414	606.4	0.6867	90.57	0.00001492	3.613E-14	1.452	100.6	0.1316	2.191	1220	0.2982	0.04165	0.1862
553	1.232E-07	0.004059	593.6	0.8726	97.46	0.00003338	8.88E-14	1.436	109	0.2662	1.283	1246	0.2698	0.07515	0.2027
554	1.075E-07	0.003074	604.5	1.55	100.8	0.00005095	1.167E-13	2.793	96.01	0.4702	1.912	1281	0.3086	0.1524	0.3409
555	7.288E-08	0.00157	448.5	0.3342	49.52	0.0001316	2.405E-13	0.7163	59.52	1.419	0.1713	922.5	0.4622	0.4602	0.06677
556	1.092E-07	0.003249	537.1	0.8011	82.89	0.0002146	5.224E-13	0.8194	94.64	1.766	0.271	1241	0.3003	0.4603	0.1057
557	2.512E-07	0.01629	516.7	0.6348	106.6	0.0009396	5.335E-12	1.066	204.3	3.436	0.4252	1310	0.125	0.43	0.3237
558	5.835E-08	0.001127	259.6	0.4451	38.41	0.00009458	1.823E-13	1.334	39.37	0.8742	0.1071	615.5	0.5173	0.1948	0.126
559	1.469E-07	0.005474	628.7	0.4987	80.51	0.0003764	1.123E-12	1.655	132.3	2.607	0.5087	1400	0.224	0.6243	0.2681
560	1.646E-06	0.02685	0.4535	0.283	0.63	8.581E-15	1.535E-21	0.01939	9.693	5.505E-13	1.739	7.92	0.007875	3.533E-16	0.1586
561	1.537E-07	0.005177	1091	0.3346	194.6	0.00021	5.03E-13	1.12	175	2.039	0.1775	2307	0.1783	0.9956	0.1628
562	1.168E-07	0.003652	548.9	0.5603	93.04	0.0003834	9.805E-13	3.133	101.9	3.008	0.1336	1312	0.277	0.7521	0.4282
563	4.654E-07	0.04126	1444	0.9248	219.3	0.003787	2.382E-11	2.373	644.4	12.21	1.176	3742	0.03185	3.291	1.12
564	5.231E-07														
565	3.266E-09	0.000248	480.9	0.02016	6417	2.55E-12	2.156E-20	2.157	5.147	5.142E-06	0.002155	991.5	0.6676	2.29	0.3004
566	2.683E-06	0.04355	0.2846	0.4132	1.02	1.417E-14	4.09E-21	0.02507	9.74	5.675E-13	1.754	9.92	0.004879	2.288E-16	0.3309
567	2.869E-07	0.01757	1537	1.026	334.6	0.001077	4.352E-12	2.979	424.5	6.095	1.941	3542	0.05595	3.071	0.8686
568	2.236E-07	0.01015	1753	1.363	251.1	0.001072	3.041E-12	3.48	378.4	7.412	0.6445	4022	0.06123	5.088	0.7601
569	1.334E-07	0.005242	343.6	0.3989	118.7	0.00051	1.888E-12	1.586	98.4	2.566	0.3368	1059	0.222	0.344	0.3014
570	3.087E-07	0.02243	1801	1.832	442.9	0.004529	2.008E-11	6.474	583.2	21.17	2.201	4291	0.03271	16.4	2.329
571	3.413E-07	0.0262	1374	0.739	400.5	0.002125	1.107E-11	1.897	479.4	9.679	0.8905	3457	0.04671	3.67	0.704
572	7.573E-06	0.09838	0.07102	0.4555	0.08	4.537E-14	3.867E-20	0.007132	7.45	5.929E-13	1.464	4.65	0.001659	7.404E-17	0.2779
573	3.387E-06	0.05617	0.2352	1.053	0.86	1.331E-14	4.839E-21	0.03235	9.923	4.301E-13	2.78	2.7	0.003905	1.421E-16	0.5377
574	1.244E-07	0.004996	294.3	0.08224	27.6	0.00005355	2.115E-13	0.3579	85.21	0.2593	0.153	558.1	0.2534	0.03489	0.06914
575	3.499E-07	0.0214	22.61	0.03683	3.57	0.00009533	2.445E-12	0.06505	54.18	0.05447	0.7598	80.01	0.05195	0.0004806	0.07696
576	1.343E-06	0.04054	1.401	0.1836	6.19	0.001589	2.076E-10	0.05614	20.1	0.1522	0.5119	29.53	0.01062	0.0001699	0.3359
577	8.142E-06	0.1065	0.07756	1.025	1.19	3.2E-14	2.79E-20	0.008714	7.837	4.313E-13	3.726	2.31	0.001629	5.856E-17	0.3473

Table G. part 11: *Continued*

Sequence # (sample #)	H+	CO2(aq)	CO3--	Ca++	Cl-	H2PO4-	H3PO4	H3SiO4-	HCO3-	HPO4--	Mg++	Na+	OH-	PO4---	SiO2(aq)
								free mmol/kg							
578	1.933E-06	0.02913	0.6142	0.1446	46.64	0.0001213	2.137E-11	0.05532	10.77	0.009617	0.03782	56.67	0.007833	0.00001068	0.4443
579	5.103E-08	0.0007803	183.7	3.159E-10	817.3	2.975E-06	7.136E-15	3.706	24.24	0.04054	4.285E-10	1218	0.3959	0.02989	0.4207
580	7.803E-08	0.001992	232.4	3.132E-10	946.8	4.805E-06	1.703E-14	5.538	43.04	0.04899	4.293E-10	1460	0.2467	0.03095	0.9493
581	1.762E-07	0.01203	346.2	2.84E-10	1225	0.00003752	2.898E-13	5.772	127	0.2141	4.229E-10	2013	0.09251	0.1008	2.297
582	2.917E-07	0.039	402	2.299E-10	1571	0.00007378	1.024E-12	3.728	245.6	0.2845	3.925E-10	2583	0.04204	0.1215	2.879
583	3.424E-07	0.05925	463.3	1.991E-10	1691	0.0001149	1.901E-12	3.693	322.8	0.4056	3.736E-10	2788	0.03214	0.1901	3.529
584	3.825E-07	0.08553	527.6	1.612E-10	1851	0.000178	3.344E-12	5.619	432.4	0.5607	3.473E-10	3252	0.02272	0.2656	6.711
585	3.724E-07	0.1191	725	9.562E-11	2141	0.0002243	4.349E-12	29.21	655	0.6947	2.773E-10	4001	0.0143	0.5148	43.93
586	2.271E-08	0.0005588	1611	2.584E-10	1801	2.187E-06	1.581E-15	11.35	103.8	0.08214	3.488E-10	5267	0.1658	0.8458	0.8576
587	2.378E-08	0.0005777	1606	2.719E-10	1817	1.752E-06	1.347E-15	13.89	96.61	0.07393	3.651E-10	4919	0.1875	0.8437	1.025
588	1.23E-08	0.0003178	1487	1.641E-10	2397	5.902E-07	3.303E-16	14.97	79	0.03306	2.155E-10	5442	0.2027	0.6969	1.001
589	1.502E-08	0.0003455	1726	2.102E-10	2033	5.763E-07	3.11E-16	12.26	91.64	0.02774	2.834E-10	5528	0.1875	0.5249	0.7741
590	1.323E-08	0.0003214	1535	1.801E-10	2196	1.168E-06	6.204E-16	17.19	86.93	0.05467	2.387E-10	5704	0.1813	0.9048	1.141
591	1.222E-08	0.0003228	1530	1.595E-10	2380	8.375E-07	4.531E-16	15.29	84.37	0.04397	2.134E-10	5594	0.1899	0.8946	1.034
592	2.373E-08	0.001227	1421	1.373E-10	2383	3.791E-06	4.024E-15	15.44	163.9	0.0922	2.019E-10	5748	0.08926	0.8047	2.142
593	1.452E-08	0.0004103	1525	1.703E-10	2306	8.741E-07	5.397E-16	14.73	92.79	0.04074	2.303E-10	5529	0.173	0.6892	1.098
594	2.614E-07	0.03964	945.9	1.811E-10	1431	0.0001428	1.116E-12	5.265	565.6	0.4919	3.862E-10	4790	0.02112	0.1962	3.698
595	6.738E-08	0.003018	1515	3.102E-10	1451	0.00001347	2.416E-14	8.193	202.8	0.2239	4.469E-10	4701	0.08879	0.704	1.3
596	7.584E-07	0.1593	495.1	2.062E-10	767.9	0.0003497	7.345E-12	2.481	628.7	0.4737	4.87E-10	2786	0.02005	0.03686	3.266
597	2.284E-08	0.0004326	1537	3.134E-10	1645	1.093E-06	7.324E-16	12.59	79.93	0.05045	4.117E-10	4831	0.23	0.4813	0.774
598	1.709E-08	0.0006162	1464	1.541E-10	2406	1.578E-06	1.226E-15	17.49	110.3	0.06122	2.111E-10	5574	0.1401	0.8566	1.674
599	2.23E-08	0.0005575	1627	2.513E-10	1810	1.445E-06	1.022E-15	15.63	107.3	0.05233	3.422E-10	5399	0.1581	0.5317	1.195
600	1.222E-07	0.007994	1236	3.139E-10	1355	0.00002205	7.35E-14	6.637	255.3	0.2377	4.715E-10	3987	0.07118	0.3566	1.674
601	1.767E-07	0.008277	951	4.392E-10	516.4	0.0001212	4.11E-13	2.129	209.4	0.9373	6.135E-10	2728	0.1154	0.4171	0.4522
602	2.085E-07	0.008994	43.67	2.404E-10	32.72	0.00008848	1.095E-12	1.342	47.65	0.112	3.881E-10	192.3	0.1015	0.002514	0.7721
603	5.812E-07	0.09448	453.3	2.472E-10	674.5	0.0001299	2.189E-12	2.481	440.4	0.2278	4.916E-10	2132	0.03354	0.02233	2.365
604	6.395E-07	0.1191	489.2	2.262E-10	796	0.0001264	2.398E-12	2.632	507.9	0.2156	4.808E-10	2355	0.0274	0.02404	2.898
605	1.335E-08	0.0003081	1163	1.822E-10	2476	7.954E-19	5.371E-28	17.2	56.2	5.37E-14	2.346E-10	4832	0.2643	9.472E-13	1.129
606	2.33E-08	0.0005692	1599	2.66E-10	1820	1.402E-06	1.055E-15	13.89	98.53	0.05694	3.577E-10	5050	0.1799	0.6208	1.036
607	1.912E-08	0.0005288	1454	2.071E-10	2092	2.163E-18	1.564E-27	16.04	97.8	8.539E-14	2.814E-10	5399	0.1629	9.155E-13	1.291
608	4.011E-08	0.001201	1444	3.142E-10	1592	5.748E-18	6.716E-27	11.63	122	1.62E-13	4.255E-10	4614	0.1493	8.387E-13	1.181
609	4.086E-08	0.001213	1437	3.194E-10	1586	0.00000328	3.916E-15	12	118.9	0.09522	4.316E-10	4483	0.1561	0.5095	1.209
610	6.701E-08	0.002552	1391	3.49E-10	1372	0.00001316	2.315E-14	10.03	161.3	0.2552	4.822E-10	4205	0.1195	0.7565	1.394
611	1.885E-07	0.01413	1050	3.414E-10	1067	0.00004603	2.158E-13	6.338	289.2	0.3389	5.209E-10	3417	0.06625	0.245	2.022
612	1.261E-08	0.0003609	1116	1.454E-10	2705	8.097E-07	5.825E-16	19.17	63.65	0.04922	1.881E-10	5094	0.2176	0.8581	1.489
613	5.359E-08	0.005689	1256	1.195E-10	2467	7.572E-06	2.027E-14	11.49	281.9	0.1025	2.013E-10	5268	0.04803	0.4816	3.508
614	3.579E-07	0.04891	1017	2.517E-10	1042	0.0001156	1.015E-12	2.632	553.8	0.4062	4.877E-10	3835	0.02822	0.1463	1.716
615	1.956E-08	0.00008903	291.4	3.567E-10	540.3	3.968E-06	2.482E-15	9.697E-10	10.79	0.1802	4.861E-10	1270	1.332	0.3995	3.03E-11

Table G. part 11: *Continued*

Sequence # (sample #)	H+	CO2(aq)	CO3--	Ca++	Cl-	H2PO4-	H3PO4	H3SiO4-	HCO3-	HPO4--	Mg++	Na+	OH-	PO4---	SiO2(aq)
								free mmol/kg							
616	7E-09	0.00002215	314.4	3.046E-10	2008	4.905E-07	2.024E-16	9.772E-10	5.259	0.08311	3.534E-10	2848	1.404	2.236	2.288E-11
617	3.161E-09	0.00002604	794.4	1.306E-10	3138	1.472E-07	4.051E-17	9.759E-10	11.83	0.04284	1.383E-10	4446	0.9358	4.873	2.418E-11
618	2.893E-09	5.155E-06	78.93	3.241E-10	3585	4.697E-09	1.908E-18	9.659E-10	1.554	0.001184	2.761E-10	4360	0.8315	0.09613	3.412E-11
619	8.696E-09	0.00001533	119.5	4.308E-10	1630	6.425E-08	3.353E-17	9.749E-10	2.544	0.007268	4.909E-10	2047	1.555	0.09384	2.514E-11
620	1.913E-09	8.275E-06	590.9	1.382E-10	3200	2.491E-08	4.655E-18	9.844E-10	5.471	0.01195	1.356E-10	4286	1.595	2.151	1.565E-11
621	4.581E-08	0.0006065	54.35	1.941E-10	29.03	7.736E-06	2.204E-14	3.055	13.93	0.04186	0.01075	144.1	0.452	0.003815	0.4024
622	5.548E-07	0.03795	20.49	2.959E-10	56.01	0.00007258	2.707E-12	0.7064	66.63	0.03095	4.824E-10	165	0.03448	0.000239	1.216
623	8.865E-08	0.001638	33.1	0.01255	28.03	0.00003802	2.25E-13	0.7276	18.08	0.09649	3.626E-10	115.1	0.2208	0.003918	0.1986
624	8.447E-07	0.0564	10.11	0.01259	33.05	0.0002781	1.758E-11	0.07851	58.2	0.06657	0.02262	109.2	0.02101	0.000262	0.2282

H

Appendix H

H.1 Raw and processed X-ray diffraction data from commercial and synthetic $CaCO_3$ samples discussed in Chapter 5.

The table is divided in 4 parts, comprising all the data used to generate the diffractograms shown in Chapter 5. It contains raw and processed XRD from commercial $CaCO_3$ powder, synthetic samples from crystal growth (seeds) experiments and constant composition experiments.

APPENDIX I

Table I. part 1: Raw and processed X-ray diffraction data from commercial $CaCO_3$ powder and synthetic samples from crystal growth (seeds) experiments shown in Chapter 5.

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1	5.0129	20.4542	345.5432	1	5.0129	20.4542	5973	1	5.0129	20.4542	324.2911	1	5.0129	20.4542	6488
2	5.0389	20.3487	324.3629	2	5.0389	20.3487	5926.4663	2	5.0389	20.3487	120.8173	2	5.0389	20.3487	6242.4607
3	5.0649	20.2443	241.4327	3	5.0649	20.2443	5818.1829	3	5.0649	20.2443	147.68	3	5.0649	20.2443	6227.258
4	5.0909	20.141	245.1984	4	5.0909	20.141	5796.5953	4	5.0909	20.141	83.732	4	5.0909	20.141	6121.2446
5	5.1169	20.0387	199.8536	5	5.1169	20.0387	5725.8973	5	5.1169	20.0387	220.5046	5	5.1169	20.0387	6215.9517
6	5.1429	19.9375	266.0275	6	5.1429	19.9375	5766.7179	6	5.1429	19.9375	272.3206	6	5.1429	19.9375	6225.7023
7	5.1689	19.8373	96.165	7	5.1689	19.8373	5571.5021	7	5.1689	19.8373	27.8415	7	5.1689	19.8373	5939.1578
8	5.1949	19.7381	133.2103	8	5.1949	19.7381	5583.1941	8	5.1949	19.7381	179.2337	8	5.1949	19.7381	6048.4845
9	5.2209	19.6398	149.322	9	5.2209	19.6398	5573.9525	9	5.2209	19.6398	173.736	9	5.2209	19.6398	6000.9215
10	5.2469	19.5426	13.4396	10	5.2469	19.5426	5412.7169	10	5.2469	19.5426	172.6306	10	5.2469	19.5426	5957.7506
11	5.2729	19.4463	88.8327	11	5.2729	19.4463	5462.7567	11	5.2729	19.4463	227.1594	11	5.2729	19.4463	5970.214
12	5.2989	19.3509	158.8451	12	5.2989	19.3509	5507.4159	12	5.2989	19.3509	197.0699	12	5.2989	19.3509	5898.0591
13	5.3249	19.2565	244.2812	13	5.3249	19.2565	5567.4987	13	5.3249	19.2565	185.1487	13	5.3249	19.2565	5844.0724
14	5.3509	19.163	344.2036	14	5.3509	19.163	5642.0678	14	5.3509	19.163	120.9756	14	5.3509	19.163	5737.8338
15	5.3769	19.0704	204.6882	15	5.3769	19.0704	5477.1992	15	5.3769	19.0704	211.9277	15	5.3769	19.0704	5786.7205
16	5.4029	18.9787	207.8005	16	5.4029	18.9787	5454.9582	16	5.4029	18.9787	217.4585	16	5.4029	18.9787	5750.1859
17	5.4289	18.8879	42.3921	17	5.4289	18.8879	5264.1965	17	5.4289	18.8879	364.0646	17	5.4289	18.8879	5854.7266
18	5.4549	18.7979	175.3674	18	5.4549	18.7979	5371.8185	18	5.4549	18.7979	216.2479	18	5.4549	18.7979	5664.8445
19	5.4809	18.7088	263.5795	19	5.4809	18.7088	5434.6773	19	5.4809	18.7088	280.3594	19	5.4809	18.7088	5686.8905
20	5.5069	18.6206	255.6816	20	5.5069	18.6206	5401.4262	20	5.5069	18.6206	270.8047	20	5.5069	18.6206	5635.2704
21	5.5329	18.5331	286.0366	21	5.5329	18.5331	5406.428	21	5.5329	18.5331	293.592	21	5.5329	18.5331	5615.9922
22	5.5589	18.4465	185.1343	22	5.5589	18.4465	5280.1724	22	5.5589	18.4465	203.2543	22	5.5589	18.4465	5483.5891
23	5.5849	18.3607	235.7251	23	5.5849	18.3607	5305.4099	23	5.5849	18.3607	241.999	23	5.5849	18.3607	5480.2684
24	5.6109	18.2757	169.6183	24	5.6109	18.2757	5213.9498	24	5.6109	18.2757	268.8706	24	5.6109	18.2757	5465.0746
25	5.6369	18.1915	127.2141	25	5.6369	18.1915	5146.1923	25	5.6369	18.1915	200.2478	25	5.6369	18.1915	5354.3864
26	5.6629	18.108	265.4456	26	5.6629	18.108	5259.0705	26	5.6629	18.108	318.9586	26	5.6629	18.108	5431.0317
27	5.6889	18.0253	291.6592	27	5.6889	18.0253	5259.9309	27	5.6889	18.0253	326.5004	27	5.6889	18.0253	5396.5081
28	5.7149	17.9434	345.5432	28	5.7149	17.9434	5288.4617	28	5.7149	17.9434	324.2911	28	5.7149	17.9434	5352.2334
29	5.7409	17.8622	344.1118	29	5.7409	17.8622	5267.8912	29	5.7409	17.8622	317.5026	29	5.7409	17.8622	5330.5565
30	5.7669	17.7817	256.7666	30	5.7669	17.7817	5161.407	30	5.7669	17.7817	300.481	30	5.7669	17.7817	5298.6466
31	5.7929	17.702	109.972	31	5.7929	17.702	4995.4734	31	5.7929	17.702	371.4441	31	5.7929	17.702	5354.7215

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
32	5.8189	17.623	186.1154	32	5.8189	17.623	5052.4778	32	5.8189	17.623	440.2301	32	5.8189	17.623	5408.6191
33	5.8449	17.5446	282.076	33	5.8449	17.5446	5129.2995	33	5.8449	17.5446	458.9919	33	5.8449	17.5446	5412.4926
34	5.8709	17.467	245.9866	34	5.8709	17.467	5074.071	34	5.8709	17.467	376.2285	34	5.8709	17.467	5314.841
35	5.8969	17.3901	210.1874	35	5.8969	17.3901	5019.1328	35	5.8969	17.3901	365.8177	35	5.8969	17.3901	5289.5419
36	5.9229	17.3138	160.1015	36	5.9229	17.3138	4949.9079	36	5.9229	17.3138	350.6955	36	5.9229	17.3138	5259.5314
37	5.9489	17.2382	251.1802	37	5.9489	17.2382	5021.8476	37	5.9489	17.2382	381.9775	37	5.9489	17.2382	5275.9251
38	5.9749	17.1632	333.1675	38	5.9749	17.1632	5084.6959	38	5.9749	17.1632	314.1492	38	5.9749	17.1632	5193.2085
39	6.0009	17.0889	425.3813	39	6.0009	17.0889	5157.7707	39	6.0009	17.0889	266.9602	39	6.0009	17.0889	5131.1311
40	6.0269	17.0153	343.9135	40	6.0269	17.0153	5057.1639	40	6.0269	17.0153	328.5337	40	6.0269	17.0153	5177.8164
41	6.0529	16.9423	386.8761	41	6.0529	16.9423	5080.9875	41	6.0529	16.9423	341.0378	41	6.0529	16.9423	5175.4322
42	6.0789	16.8699	376.0337	42	6.0789	16.8699	5051.0061	42	6.0789	16.8699	317.8847	42	6.0789	16.8699	5137.3908
43	6.1049	16.7981	243.2595	43	6.1049	16.7981	4899.0929	43	6.1049	16.7981	375.6257	43	6.1049	16.7981	5180.2435
44	6.1309	16.7269	263.7865	44	6.1309	16.7269	4900.4808	44	6.1309	16.7269	295.1086	44	6.1309	16.7269	5084.8381
45	6.1569	16.6564	275.7369	45	6.1569	16.6564	4893.2923	45	6.1569	16.6564	268.191	45	6.1569	16.6564	5043.0322
46	6.1829	16.5864	262.7791	46	6.1829	16.5864	4861.1955	46	6.1829	16.5864	321.4051	46	6.1829	16.5864	5081.358
47	6.2089	16.517	354.5823	47	6.2089	16.517	4933.8597	47	6.2089	16.517	356.4834	47	6.2089	16.517	5101.548
48	6.2349	16.4482	345.0109	48	6.2349	16.4482	4905.1493	48	6.2349	16.4482	333.5883	48	6.2349	16.4482	5063.7646
49	6.2609	16.38	337.6601	49	6.2609	16.38	4878.6594	49	6.2609	16.38	271.5729	49	6.2609	16.38	4986.861
50	6.2869	16.3123	388.3221	50	6.2869	16.3123	4910.1824	50	6.2869	16.3123	270.2798	50	6.2869	16.3123	4970.6795
51	6.3129	16.2452	375.1155	51	6.3129	16.2452	4877.8368	51	6.3129	16.2452	310.6362	51	6.3129	16.2452	4996.1476
52	6.3389	16.1786	387.2486	52	6.3389	16.1786	4870.831	52	6.3389	16.1786	309.7994	52	6.3389	16.1786	4980.4226
53	6.3649	16.1126	424.913	53	6.3649	16.1126	4889.3564	53	6.3649	16.1126	336.7012	53	6.3649	16.1126	4992.436
54	6.3909	16.0471	376.6297	54	6.3909	16.0471	4821.934	54	6.3909	16.0471	356.6381	54	6.3909	16.0471	4997.4846
55	6.4169	15.9821	345.5432	55	6.4169	15.9821	4771.7086	55	6.4169	15.9821	324.2911	55	6.4169	15.9821	4950.2494
56	6.4429	15.9177	412.4701	56	6.4429	15.9177	4827.3509	56	6.4429	15.9177	342.3938	56	6.4429	15.9177	4961.7227
57	6.4689	15.8538	469.844	57	6.4689	15.8538	4873.4402	57	6.4689	15.8538	349.8579	57	6.4689	15.8538	4962.5573
58	6.4949	15.7904	401.5565	58	6.4949	15.7904	4793.8681	58	6.4949	15.7904	347.2333	58	6.4949	15.7904	4953.3033
59	6.5209	15.7275	347.2901	59	6.5209	15.7275	4728.3172	59	6.5209	15.7275	389.5199	59	6.5209	15.7275	4988.9606
60	6.5469	15.6651	423.3345	60	6.5469	15.6651	4793.077	60	6.5469	15.6651	387.049	60	6.5469	15.6651	4979.8602
61	6.5729	15.6032	389.1374	61	6.5729	15.6032	4747.5953	61	6.5729	15.6032	340.9073	61	6.5729	15.6032	4927.0891
62	6.5989	15.5418	405.7477	62	6.5989	15.5418	4752.9211	62	6.5989	15.5418	374.9738	62	6.5989	15.5418	4954.5262
63	6.6249	15.4809	405.331	63	6.6249	15.4809	4741.2198	63	6.6249	15.4809	317.4355	63	6.6249	15.4809	4890.3585
64	6.6509	15.4204	421.2602	64	6.6509	15.4204	4745.8645	64	6.6509	15.4204	247.7056	64	6.6509	15.4204	4813.9992
65	6.6769	15.3605	473.0519	65	6.6769	15.3605	4786.3717	65	6.6769	15.3605	308.2422	65	6.6769	15.3605	4867.9064
66	6.7029	15.3009	452.7759	66	6.7029	15.3009	4754.8111	66	6.7029	15.3009	350.9682	66	6.7029	15.3009	4904.003
67	6.7289	15.2419	448.9134	67	6.7289	15.2419	4739.6641	67	6.7289	15.2419	266.869	67	6.7289	15.2419	4813.2744

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
68	6.7549	15.1833	419.9534	68	6.7549	15.1833	4699.4195	68	6.7549	15.1833	267.5424	68	6.7549	15.1833	4807.3183
69	6.7809	15.1251	458.5657	69	6.7809	15.1251	4726.7472	69	6.7809	15.1251	341.3918	69	6.7809	15.1251	4874.5384
70	6.8069	15.0674	468.7796	70	6.8069	15.0674	4725.6765	70	6.8069	15.0674	430.0494	70	6.8069	15.0674	4956.5665
71	6.8329	15.0102	488.7223	71	6.8329	15.0102	4734.3347	71	6.8329	15.0102	278.6436	71	6.8329	15.0102	4798.5314
72	6.8589	14.9533	494.3318	72	6.8589	14.9533	4728.6597	72	6.8589	14.9533	262.8551	72	6.8589	14.9533	4776.1134
73	6.8849	14.8969	502.2465	73	6.8849	14.8969	4725.2898	73	6.8849	14.8969	270.5126	73	6.8849	14.8969	4777.1415
74	6.9109	14.841	474.355	74	6.9109	14.841	4686.1137	74	6.9109	14.841	268.1845	74	6.9109	14.841	4768.184
75	6.9369	14.7854	486.3884	75	6.9369	14.7854	4686.8626	75	6.9369	14.7854	264.1144	75	6.9369	14.7854	4757.4845
76	6.9629	14.7303	576.3435	76	6.9629	14.7303	4765.5331	76	6.9629	14.7303	358.9102	76	6.9629	14.7303	4845.6509
77	6.9889	14.6755	504.7017	77	6.9889	14.6755	4682.6067	77	6.9889	14.6755	319.9373	77	6.9889	14.6755	4800.0486
78	7.0149	14.6212	515.4774	78	7.0149	14.6212	4682.0979	78	7.0149	14.6212	295.8412	78	7.0149	14.6212	4769.3231
79	7.0409	14.5673	410.9543	79	7.0409	14.5673	4566.2902	79	7.0409	14.5673	484.7092	79	7.0409	14.5673	4951.5617
80	7.0669	14.5138	352.9112	80	7.0669	14.5138	4496.9626	80	7.0669	14.5138	334.9124	80	7.0669	14.5138	4795.1354
81	7.0929	14.4606	432.9391	81	7.0929	14.4606	4565.7059	81	7.0929	14.4606	330.3639	81	7.0929	14.4606	4783.9576
82	7.1189	14.4079	345.5432	82	7.1189	14.4079	4467.0255	82	7.1189	14.4079	324.2911	82	7.1189	14.4079	4771.2554
83	7.1449	14.3555	495.6597	83	7.1449	14.3555	4611.5171	83	7.1449	14.3555	413.0426	83	7.1449	14.3555	4854.7595
84	7.1709	14.3035	398.5909	84	7.1709	14.3035	4508.8236	84	7.1709	14.3035	416.4763	84	7.1709	14.3035	4852.9459
85	7.1969	14.2519	402.2265	85	7.1969	14.2519	4506.8343	85	7.1969	14.2519	253.4288	85	7.1969	14.2519	4684.6511
86	7.2229	14.2007	390.898	86	7.2229	14.2007	4489.881	86	7.2229	14.2007	327.1248	86	7.2229	14.2007	4753.0998
87	7.2489	14.1498	366.4184	87	7.2489	14.1498	4459.7766	87	7.2489	14.1498	206.3399	87	7.2489	14.1498	4627.0676
88	7.2749	14.0993	516.6836	88	7.2749	14.0993	4604.417	88	7.2749	14.0993	253.3227	88	7.2749	14.0993	4668.8031
89	7.3009	14.0492	355.9705	89	7.3009	14.0492	4438.079	89	7.3009	14.0492	226.7817	89	7.3009	14.0492	4637.0147
90	7.3269	13.9994	456.061	90	7.3269	13.9994	4532.5448	90	7.3269	13.9994	255.3825	90	7.3269	13.9994	4660.3682
91	7.3529	13.95	446.3508	91	7.3529	13.95	4517.2098	91	7.3529	13.95	379.3399	91	7.3529	13.95	4779.0783
92	7.3789	13.9009	482.3575	92	7.3789	13.9009	4547.5916	92	7.3789	13.9009	339.3348	92	7.3789	13.9009	4733.8259
93	7.4049	13.8521	514.9416	93	7.4049	13.8521	4574.551	93	7.4049	13.8521	313.3382	93	7.4049	13.8521	4702.582
94	7.4309	13.8037	444.7522	94	7.4309	13.8037	4498.7367	94	7.4309	13.8037	384.0255	94	7.4309	13.8037	4768.022
95	7.4569	13.7557	355.0055	95	7.4569	13.7557	4403.3652	95	7.4569	13.7557	221.174	95	7.4569	13.7557	4599.9231
96	7.4829	13.7079	403.3631	96	7.4829	13.7079	4446.098	96	7.4829	13.7079	207.424	96	7.4829	13.7079	4580.9259
97	7.5089	13.6605	346.4561	97	7.5089	13.6605	4383.5662	97	7.5089	13.6605	144.8912	97	7.5089	13.6605	4513.1457
98	7.5349	13.6135	385.9171	98	7.5349	13.6135	4417.4024	98	7.5349	13.6135	138.3982	98	7.5349	13.6135	4501.4054
99	7.5609	13.5667	454.9897	99	7.5609	13.5667	4480.8502	99	7.5609	13.5667	284.8912	99	7.5609	13.5667	4642.6511
100	7.5869	13.5203	523.4465	100	7.5869	13.5203	4543.6822	100	7.5869	13.5203	381.0812	100	7.5869	13.5203	4733.5937
101	7.6129	13.4742	400.1482	101	7.6129	13.4742	4414.7591	101	7.6129	13.4742	252.9679	101	7.6129	13.4742	4600.2331
102	7.6389	13.4284	375.0806	102	7.6389	13.4284	4384.0667	102	7.6389	13.4284	287.9175	102	7.6389	13.4284	4629.9355
103	7.6649	13.3829	484.371	103	7.6649	13.3829	4487.7322	103	7.6649	13.3829	299.1569	103	7.6649	13.3829	4635.9276

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
104	7.6909	13.3378	241.8726	104	7.6909	13.3378	4239.609	104	7.6909	13.3378	263.4005	104	7.6909	13.3378	4594.9238
105	7.7169	13.2929	522.632	105	7.7169	13.2929	4514.7437	105	7.7169	13.2929	253.2028	105	7.7169	13.2929	4579.4788
106	7.7429	13.2483	363.1282	106	7.7429	13.2483	4349.615	106	7.7429	13.2483	345.1638	106	7.7429	13.2483	4666.1925
107	7.7689	13.204	516.6488	107	7.7689	13.204	4497.5109	107	7.7689	13.204	224.3102	107	7.7689	13.204	4540.0915
108	7.7949	13.1601	424.7332	108	7.7949	13.1601	4399.9704	108	7.7949	13.1601	344.4468	108	7.7949	13.1601	4654.9809
109	7.8209	13.1164	520.8688	109	7.8209	13.1164	4490.4812	109	7.8209	13.1164	324.2911	109	7.8209	13.1164	4629.5779
110	7.8469	13.073	393.4865	110	7.8469	13.073	4357.4741	110	7.8469	13.073	238.2748	110	7.8469	13.073	4536.0715
111	7.8729	13.0299	248.538	111	7.8729	13.0299	4206.9007	111	7.8729	13.0299	214.0712	111	7.8729	13.0299	4504.3778
112	7.8989	12.9871	416.3926	112	7.8989	12.9871	4369.1306	112	7.8989	12.9871	371.0512	112	7.8989	12.9871	4653.8677
113	7.9249	12.9445	416.1144	113	7.9249	12.9445	4363.2276	113	7.9249	12.9445	251.7037	113	7.9249	12.9445	4527.0301
114	7.9509	12.9023	385.9968	114	7.9509	12.9023	4327.4851	114	7.9509	12.9023	306.1935	114	7.9509	12.9023	4574.0298
115	7.9769	12.8603	369.7593	115	7.9769	12.8603	4305.6228	115	7.9769	12.8603	339.1621	115	7.9769	12.8603	4599.5083
116	8.0029	12.8186	316.0715	116	8.0029	12.8186	4246.3102	116	8.0029	12.8186	386.9371	116	8.0029	12.8186	4639.7932
117	8.0289	12.7771	529.7337	117	8.0289	12.7771	4454.3476	117	8.0289	12.7771	192.6255	117	8.0289	12.7771	4437.9916
118	8.0549	12.7359	376.8243	118	8.0549	12.7359	4295.8134	118	8.0549	12.7359	252.0678	118	8.0549	12.7359	4489.9437
119	8.0809	12.695	388.5817	119	8.0809	12.695	4301.946	119	8.0809	12.695	325.5351	119	8.0809	12.695	4555.921
120	8.1069	12.6544	449.1384	120	8.1069	12.6544	4356.8778	120	8.1069	12.6544	384.0666	120	8.1069	12.6544	4606.9624
121	8.1329	12.614	393.6647	121	8.1329	12.614	4295.7794	121	8.1329	12.614	483.1454	121	8.1329	12.614	4698.5511
122	8.1589	12.5739	403.2946	122	8.1589	12.5739	4299.7845	122	8.1589	12.5739	368.5901	122	8.1589	12.5739	4576.5057
123	8.1849	12.534	489.1356	123	8.1849	12.534	4380.0006	123	8.1849	12.534	368.9958	123	8.1849	12.534	4569.4213
124	8.2109	12.4944	300.3813	124	8.2109	12.4944	4185.6215	124	8.2109	12.4944	361.4574	124	8.2109	12.4944	4554.3928
125	8.2369	12.455	400.851	125	8.2369	12.455	4280.4664	125	8.2369	12.455	379.4866	125	8.2369	12.455	4564.932
126	8.2629	12.4159	389.1934	126	8.2629	12.4159	4263.1841	126	8.2629	12.4159	275.0489	126	8.2629	12.4159	4453.0041
127	8.2889	12.377	378.3831	127	8.2889	12.377	4246.749	127	8.2889	12.377	349.006	127	8.2889	12.377	4519.4712
128	8.3149	12.3384	348.2655	128	8.3149	12.3384	4211.0066	128	8.3149	12.3384	298.5413	128	8.3149	12.3384	4461.5164
129	8.3409	12.3	413.1485	129	8.3409	12.3	4270.2647	129	8.3409	12.3	247.2369	129	8.3409	12.3	4402.7219
130	8.3669	12.2618	432.5482	130	8.3669	12.2618	4284.0396	130	8.3669	12.2618	186.6831	130	8.3669	12.2618	4334.678
131	8.3929	12.2239	385.5566	131	8.3929	12.2239	4231.4232	131	8.3929	12.2239	314.2257	131	8.3929	12.2239	4454.7305
132	8.4189	12.1862	398.3651	132	8.4189	12.1862	4238.6068	132	8.4189	12.1862	314.1684	132	8.4189	12.1862	4447.1831
133	8.4449	12.1488	367.065	133	8.4449	12.1488	4201.682	133	8.4449	12.1488	274.1481	133	8.4449	12.1488	4399.6728
134	8.4709	12.1116	336.0405	134	8.4709	12.1116	4165.0326	134	8.4709	12.1116	306.3019	134	8.4709	12.1116	4424.3364
135	8.4969	12.0746	403.6852	135	8.4969	12.0746	4227.0525	135	8.4969	12.0746	297.9461	135	8.4969	12.0746	4408.4906
136	8.5229	12.0378	431.3686	136	8.5229	12.0378	4249.1112	136	8.5229	12.0378	324.2911	136	8.5229	12.0378	4427.3455
137	8.5489	12.0013	315.3694	137	8.5489	12.0013	4125.8977	137	8.5489	12.0013	331.5776	137	8.5489	12.0013	4428.7358
138	8.5749	11.9649	311.5781	138	8.5749	11.9649	4114.8923	138	8.5749	11.9649	173.0611	138	8.5749	11.9649	4264.323
139	8.6009	11.9288	344.1156	139	8.6009	11.9288	4140.2157	139	8.6009	11.9288	282.1127	139	8.6009	11.9288	4367.4785

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
140	8.6269	11.8929	357.1846	140	8.6269	11.8929	4146.0704	140	8.6269	11.8929	282.1989	140	8.6269	11.8929	4361.6685
141	8.6529	11.8573	333.8973	141	8.6529	11.8573	4115.569	141	8.6529	11.8573	378.9204	141	8.6529	11.8573	4452.4938
142	8.6789	11.8218	344.9846	142	8.6789	11.8218	4119.4421	142	8.6789	11.8218	392.7707	142	8.6789	11.8218	4460.4479
143	8.7049	11.7866	369.1656	143	8.7049	11.7866	4136.409	143	8.7049	11.7866	316.8969	143	8.7049	11.7866	4378.6779
144	8.7309	11.7516	441.0554	144	8.7309	11.7516	4201.0846	144	8.7309	11.7516	395.5387	144	8.7309	11.7516	4451.4235
145	8.7569	11.7167	453.4881	145	8.7569	11.7167	4206.3031	145	8.7569	11.7167	375.0481	145	8.7569	11.7167	4425.0368
146	8.7829	11.6821	398.5294	146	8.7829	11.6821	4144.1303	146	8.7829	11.6821	218.3695	146	8.7829	11.6821	4262.462
147	8.8089	11.6477	341.9165	147	8.8089	11.6477	4080.3031	147	8.8089	11.6477	222.684	147	8.8089	11.6477	4260.8803
148	8.8349	11.6135	367.7213	148	8.8349	11.6135	4098.8938	148	8.8349	11.6135	263.2531	148	8.8349	11.6135	4295.5531
149	8.8609	11.5795	400.5021	149	8.8609	11.5795	4124.4605	149	8.8609	11.5795	208.2651	149	8.8609	11.5795	4234.6689
150	8.8869	11.5457	366.1769	150	8.8869	11.5457	4082.9211	150	8.8869	11.5457	252.5133	150	8.8869	11.5457	4273.021
151	8.9129	11.5121	415.9853	151	8.9129	11.5121	4125.5153	151	8.9129	11.5121	271.153	151	8.9129	11.5121	4285.7645
152	8.9389	11.4786	384.8322	152	8.9389	11.4786	4087.148	152	8.9389	11.4786	261.9113	152	8.9389	11.4786	4270.6266
153	8.9649	11.4454	389.2606	153	8.9649	11.4454	4084.3623	153	8.9649	11.4454	338.6077	153	8.9649	11.4454	4341.4268
154	8.9909	11.4124	379.5678	154	8.9909	11.4124	4067.4552	154	8.9909	11.4124	308.7575	154	8.9909	11.4124	4305.6804
155	9.0169	11.3795	305.1075	155	9.0169	11.3795	3985.7808	155	9.0169	11.3795	315.3759	155	9.0169	11.3795	4306.4026
156	9.0429	11.3469	341.8247	156	9.0429	11.3469	4015.2839	156	9.0429	11.3469	305.2956	156	9.0429	11.3469	4290.4261
157	9.0689	11.3144	323.755	157	9.0689	11.3144	3990	157	9.0689	11.3144	233.361	157	9.0689	11.3144	4212.5953
158	9.0949	11.2822	357.5012	158	9.0949	11.2822	4016.532	158	9.0949	11.2822	244.5575	158	9.0949	11.2822	4217.8956
159	9.1209	11.2501	345.8777	159	9.1209	11.2501	3997.6944	159	9.1209	11.2501	207.391	159	9.1209	11.2501	4174.8329
160	9.1469	11.2182	330.8566	160	9.1469	11.2182	3975.4591	160	9.1469	11.2182	259.3298	160	9.1469	11.2182	4220.8755
161	9.1729	11.1864	386.3517	161	9.1729	11.1864	4023.74	161	9.1729	11.1864	269.9434	161	9.1729	11.1864	4225.5929
162	9.1989	11.1549	339.2225	162	9.1989	11.1549	3969.3966	162	9.1989	11.1549	267.6928	162	9.1989	11.1549	4217.4461
163	9.2249	11.1235	345.5432	163	9.2249	11.1235	3968.5032	163	9.2249	11.1235	324.2911	163	9.2249	11.1235	4268.1482
164	9.2509	11.0923	382.9796	164	9.2509	11.0923	3998.7587	164	9.2509	11.0923	323.2924	164	9.2509	11.0923	4259.0613
165	9.2769	11.0613	350.5939	165	9.2769	11.0613	3959.1923	165	9.2769	11.0613	323.6459	165	9.2769	11.0613	4251.3267
166	9.3029	11.0304	396.9722	166	9.3029	11.0304	3998.3897	166	9.3029	11.0304	317.301	166	9.3029	11.0304	4236.8936
167	9.3289	10.9998	345.2973	167	9.3289	10.9998	3939.534	167	9.3289	10.9998	308.5577	167	9.3289	10.9998	4220.0622
168	9.3549	10.9693	367.0025	168	9.3549	10.9693	3954.0583	168	9.3549	10.9693	289.9929	168	9.3549	10.9693	4193.4092
169	9.3809	10.9389	471.1801	169	9.3809	10.9389	4051.0551	169	9.3809	10.9389	369.9873	169	9.3809	10.9389	4265.3155
170	9.4069	10.9088	364.7244	170	9.4069	10.9088	3937.4186	170	9.4069	10.9088	384.8922	170	9.4069	10.9088	4272.1323
171	9.4329	10.8788	405.4753	171	9.4329	10.8788	3970.9886	171	9.4329	10.8788	325.9916	171	9.4329	10.8788	4205.1435
172	9.4589	10.8489	384.38	172	9.4589	10.8489	3942.7126	172	9.4589	10.8489	367.7072	172	9.4589	10.8489	4238.771
173	9.4849	10.8193	348.6213	173	9.4849	10.8193	3899.773	173	9.4849	10.8193	378.2873	173	9.4849	10.8193	4241.2629
174	9.5109	10.7897	344.3443	174	9.5109	10.7897	3888.3152	174	9.5109	10.7897	289.8066	174	9.5109	10.7897	4144.6941
175	9.5369	10.7604	361.9035	175	9.5369	10.7604	3898.6935	175	9.5369	10.7604	283.5441	175	9.5369	10.7604	4130.3434

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
176	9.5629	10.7312	420.6	176	9.5629	10.7312	3950.2092	176	9.5629	10.7312	337.0461	176	9.5629	10.7312	4175.7573
177	9.5889	10.7022	404.5164	177	9.5889	10.7022	3926.9448	177	9.5889	10.7022	329.6822	177	9.5889	10.7022	4160.3052
178	9.6149	10.6733	340.0022	178	9.6149	10.6733	3855.2498	178	9.6149	10.6733	432.9148	178	9.6149	10.6733	4255.4497
179	9.6409	10.6446	287.7042	179	9.6409	10.6446	3795.771	179	9.6409	10.6446	369.4836	179	9.6409	10.6446	4183.9303
180	9.6669	10.616	236.507	180	9.6669	10.616	3737.3929	180	9.6669	10.616	317.835	180	9.6669	10.616	4124.1935
181	9.6929	10.5876	336.2751	181	9.6929	10.5876	3829.9802	181	9.6929	10.5876	329.8486	181	9.6929	10.5876	4128.119
182	9.7189	10.5594	224.4131	182	9.7189	10.5594	3710.9374	182	9.7189	10.5594	392.4511	182	9.7189	10.5594	4182.6333
183	9.7449	10.5313	288.3377	183	9.7449	10.5313	3767.6811	183	9.7449	10.5313	358.1988	183	9.7449	10.5313	4140.2929
184	9.7709	10.5033	268.259	184	9.7709	10.5033	3740.4217	184	9.7709	10.5033	332.8102	184	9.7709	10.5033	4106.8162
185	9.7969	10.4755	322.0093	185	9.7969	10.4755	3786.9911	185	9.7969	10.4755	373.6967	185	9.7969	10.4755	4139.6145
186	9.8229	10.4478	300.3365	186	9.8229	10.4478	3758.1374	186	9.8229	10.4478	380.6915	186	9.8229	10.4478	4138.5212
187	9.8489	10.4203	248.8849	187	9.8489	10.4203	3699.5051	187	9.8489	10.4203	308.9834	187	9.8489	10.4203	4058.7249
188	9.8749	10.393	225.7482	188	9.8749	10.393	3669.1875	188	9.8749	10.393	264.0185	188	9.8749	10.393	4005.6719
189	9.9009	10.3657	329.8184	189	9.9009	10.3657	3766.0769	189	9.9009	10.3657	323.4348	189	9.9009	10.3657	4057
190	9.9269	10.3386	345.5432	190	9.9269	10.3386	3774.6209	190	9.9269	10.3386	324.2911	190	9.9269	10.3386	4049.7682
191	9.9529	10.3117	368.7244	191	9.9529	10.3117	3788.6396	191	9.9529	10.3117	276.6257	191	9.9529	10.3117	3994.5242
192	9.9789	10.2849	382.9404	192	9.9789	10.2849	3793.6931	192	9.9789	10.2849	272.7453	192	9.9789	10.2849	3983.0653
193	10.0049	10.2582	271.7562	193	10.0049	10.2582	3673.3463	193	10.0049	10.2582	461.7866	193	10.0049	10.2582	4164.5281
194	10.0309	10.2317	366.9078	194	10.0309	10.2317	3759.3354	194	10.0309	10.2317	330.1668	194	10.0309	10.2317	4025.3298
195	10.0569	10.2053	252.4978	195	10.0569	10.2053	3635.7628	195	10.0569	10.2053	418.1062	195	10.0569	10.2053	4105.6907
196	10.0829	10.1791	399.091	196	10.0829	10.1791	3773.1935	196	10.0829	10.1791	308.844	196	10.0829	10.1791	3988.85
197	10.1089	10.153	132.0133	197	10.1089	10.153	3496.9532	197	10.1089	10.153	283.2529	197	10.1089	10.153	3955.6803
198	10.1349	10.127	278.7631	198	10.1349	10.127	3634.5405	198	10.1349	10.127	254.8664	198	10.1349	10.127	3919.7153
199	10.1609	10.1012	322.1544	199	10.1609	10.1012	3668.7693	199	10.1609	10.1012	342.8174	199	10.1609	10.1012	4000.0878
200	10.1869	10.0754	377.9943	200	10.1869	10.0754	3715.4467	200	10.1869	10.0754	403.6923	200	10.1869	10.0754	4053.3841
201	10.2129	10.0499	327.3061	201	10.2129	10.0499	3655.5959	201	10.2129	10.0499	275.3733	201	10.2129	10.0499	3917.4866
202	10.2389	10.0244	310.3108	202	10.2389	10.0244	3629.4381	202	10.2389	10.0244	440.1786	202	10.2389	10.0244	4074.7134
203	10.2649	9.9991	220.4655	203	10.2649	9.9991	3530.4303	203	10.2649	9.9991	397.2631	203	10.2649	9.9991	4024.2195
204	10.2909	9.9739	261.7283	204	10.2909	9.9739	3562.5306	204	10.2909	9.9739	337.5895	204	10.2909	9.9739	3956.9673
205	10.3169	9.9488	341.6217	205	10.3169	9.9488	3633.2614	205	10.3169	9.9488	295.4081	205	10.3169	9.9488	3907.2074
206	10.3429	9.9239	310.0219	206	10.3429	9.9239	3592.4991	206	10.3429	9.9239	444.7369	206	10.3429	9.9239	4048.9576
207	10.3689	9.8991	294.7412	207	10.3689	9.8991	3568.0558	207	10.3689	9.8991	353.1529	207	10.3689	9.8991	3949.7952
208	10.3949	9.8744	244.1906	208	10.3949	9.8744	3508.3427	208	10.3949	9.8744	325.6615	208	10.3949	9.8744	3914.7253
209	10.4209	9.8498	367.0308	209	10.4209	9.8498	3622.0204	209	10.4209	9.8498	353.9827	209	10.4209	9.8498	3935.4679
210	10.4469	9.8254	373.9843	210	10.4469	9.8254	3619.8114	210	10.4469	9.8254	392.733	210	10.4469	9.8254	3966.6397
211	10.4729	9.801	276.0425	211	10.4729	9.801	3512.707	211	10.4729	9.801	412.7513	211	10.4729	9.801	3979.0795

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
212	10.4989	9.7768	241.9613	212	10.4989	9.7768	3469.4633	212	10.4989	9.7768	480.1661	212	10.4989	9.7768	4038.9158
213	10.5249	9.7527	325.6538	213	10.5249	9.7527	3543.9932	213	10.5249	9.7527	345.9106	213	10.5249	9.7527	3897.0818
214	10.5509	9.7288	449.3227	214	10.5509	9.7288	3658.4997	214	10.5509	9.7288	408.218	214	10.5509	9.7288	3951.8107
215	10.5769	9.7049	300.1662	215	10.5769	9.7049	3500.1806	215	10.5769	9.7049	409.2065	215	10.5769	9.7049	3945.2207
216	10.6029	9.6812	315.4829	216	10.6029	9.6812	3506.3347	216	10.6029	9.6812	340.8943	216	10.6029	9.6812	3869.3299
217	10.6289	9.6576	398.7102	217	10.6289	9.6576	3580.3996	217	10.6289	9.6576	324.2911	217	10.6289	9.6576	3845.1482
218	10.6549	9.6341	351.7242	218	10.6549	9.6341	3524.251	218	10.6549	9.6341	343.441	218	10.6549	9.6341	3855.7029
219	10.6809	9.6107	246.529	219	10.6809	9.6107	3409.8933	219	10.6809	9.6107	356.8441	219	10.6809	9.6107	3860.5108
220	10.7069	9.5874	344.1376	220	10.7069	9.5874	3498.3393	220	10.7069	9.5874	287.3618	220	10.7069	9.5874	3782.4333
221	10.7329	9.5643	253.3964	221	10.7329	9.5643	3398.4357	221	10.7329	9.5643	277.8895	221	10.7329	9.5643	3764.3658
222	10.7589	9.5412	435.3023	222	10.7589	9.5412	3571.179	222	10.7589	9.5412	239.3029	222	10.7589	9.5412	3717.1839
223	10.7849	9.5183	358.3477	223	10.7849	9.5183	3485.0618	223	10.7849	9.5183	256.6454	223	10.7849	9.5183	3725.9313
224	10.8109	9.4955	267.3128	224	10.8109	9.4955	3384.8644	224	10.8109	9.4955	315.9744	224	10.8109	9.4955	3776.6651
225	10.8369	9.4728	350.3449	225	10.8369	9.4728	3458.734	225	10.8369	9.4728	436.4126	225	10.8369	9.4728	3888.508
226	10.8629	9.4502	353.5391	226	10.8629	9.4502	3452.7657	226	10.8629	9.4502	277.7913	226	10.8629	9.4502	3721.2915
227	10.8889	9.4277	291.5735	227	10.8889	9.4277	3381.6375	227	10.8889	9.4277	358.1532	227	10.8889	9.4277	3793.0582
228	10.9149	9.4053	269.8839	228	10.9149	9.4053	3350.7854	228	10.9149	9.4053	426.6335	228	10.9149	9.4053	3852.9434
229	10.9409	9.383	285.5891	229	10.9409	9.383	3357.328	229	10.9409	9.383	310.7094	229	10.9409	9.383	3728.424
230	10.9669	9.3608	312.9795	230	10.9669	9.3608	3375.5559	230	10.9669	9.3608	296.8978	230	10.9669	9.3608	3706.0172
231	10.9929	9.3387	244.3129	231	10.9929	9.3387	3297.7268	231	10.9929	9.3387	341.0371	231	10.9929	9.3387	3741.5613
232	11.0189	9.3168	253.3143	232	11.0189	9.3168	3297.5657	232	11.0189	9.3168	386.2652	232	11.0189	9.3168	3778.1942
233	11.0449	9.2949	298.2481	233	11.0449	9.2949	3333.3369	233	11.0449	9.2949	359.5964	233	11.0449	9.2949	3742.9301
234	11.0709	9.2731	327.3953	234	11.0709	9.2731	3353.3216	234	11.0709	9.2731	312.4799	234	11.0709	9.2731	3687.2185
235	11.0969	9.2515	350.7308	235	11.0969	9.2515	3367.4946	235	11.0969	9.2515	349.6168	235	11.0969	9.2515	3715.7601
236	11.1229	9.2299	396.4753	236	11.1229	9.2299	3404.0765	236	11.1229	9.2299	312.6257	236	11.1229	9.2299	3670.1739
237	11.1489	9.2085	336.6356	237	11.1489	9.2085	3335.0743	237	11.1489	9.2085	308.4556	237	11.1489	9.2085	3657.4085
238	11.1749	9.1871	331.551	238	11.1749	9.1871	3320.8272	238	11.1749	9.1871	256.3164	238	11.1749	9.1871	3596.6742
239	11.2009	9.1659	351.7784	239	11.2009	9.1659	3331.892	239	11.2009	9.1659	274.1246	239	11.2009	9.1659	3605.8871
240	11.2269	9.1447	346.106	240	11.2269	9.1447	3317.0571	240	11.2269	9.1447	306.0613	240	11.2269	9.1447	3629.2286
241	11.2529	9.1236	318.5162	241	11.2529	9.1236	3280.3048	241	11.2529	9.1236	241.9018	241	11.2529	9.1236	3556.4739
242	11.2789	9.1027	322.7659	242	11.2789	9.1027	3275.392	242	11.2789	9.1027	263.026	242	11.2789	9.1027	3569.0029
243	11.3049	9.0818	326.7639	243	11.3049	9.0818	3270.2275	243	11.3049	9.0818	302.2291	243	11.3049	9.0818	3599.6108
244	11.3309	9.061	345.5432	244	11.3309	9.061	3279.8443	244	11.3309	9.061	324.2911	244	11.3309	9.061	3613.0776
245	11.3569	9.0404	323.4099	245	11.3569	9.0404	3247.2621	245	11.3569	9.0404	294.2354	245	11.3569	9.0404	3575.7883
246	11.3829	9.0198	332.4626	246	11.3829	9.0198	3245.8661	246	11.3829	9.0198	299.2539	246	11.3829	9.0198	3573.5733
247	11.4089	8.9993	326.2298	247	11.4089	8.9993	3229.1845	247	11.4089	8.9993	262.0247	247	11.4089	8.9993	3529.1105

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
248	11.4349	8.9789	318.773	248	11.4349	8.9789	3211.279	248	11.4349	8.9789	291.035	248	11.4349	8.9789	3550.8871
249	11.4609	8.9586	341.482	249	11.4609	8.9586	3223.5393	249	11.4609	8.9586	320.3968	249	11.4609	8.9586	3573.0154
250	11.4869	8.9384	331.7469	250	11.4869	8.9384	3203.3554	250	11.4869	8.9384	311.6715	250	11.4869	8.9384	3557.0566
251	11.5129	8.9183	305.6603	251	11.5129	8.9183	3166.8201	251	11.5129	8.9183	272.9979	251	11.5129	8.9183	3511.1493
252	11.5389	8.8982	297.251	252	11.5389	8.8982	3147.962	252	11.5389	8.8982	286.2797	252	11.5389	8.8982	3517.1976
253	11.5649	8.8783	307.7361	253	11.5649	8.8783	3147.9983	253	11.5649	8.8783	345.3241	253	11.5649	8.8783	3569.0084
254	11.5909	8.8585	290.3172	254	11.5909	8.8585	3120.1307	254	11.5909	8.8585	324.4319	254	11.5909	8.8585	3540.8826
255	11.6169	8.8387	302.2574	255	11.6169	8.8387	3121.6222	255	11.6169	8.8387	295.992	255	11.6169	8.8387	3505.2092
256	11.6429	8.819	384.2597	256	11.6429	8.819	3193.1758	256	11.6429	8.819	264.3446	256	11.6429	8.819	3466.3281
257	11.6689	8.7994	430.014	257	11.6689	8.7994	3228.4813	257	11.6689	8.7994	264.3463	257	11.6689	8.7994	3459.0963
258	11.6949	8.7799	415.5327	258	11.6949	8.7799	3203.5512	258	11.6949	8.7799	322.4315	258	11.6949	8.7799	3509.9479
259	11.7209	8.7605	419.272	259	11.7209	8.7605	3196.8417	259	11.7209	8.7605	317.6715	259	11.7209	8.7605	3497.9544
260	11.7469	8.7412	417.6195	260	11.7469	8.7412	3184.7405	260	11.7469	8.7412	224.6804	260	11.7469	8.7412	3397.7296
261	11.7729	8.722	365.9983	261	11.7729	8.722	3122.6706	261	11.7729	8.722	274.2676	261	11.7729	8.722	3440.0832
262	11.7989	8.7028	388.3429	262	11.7989	8.7028	3134.5665	262	11.7989	8.7028	356.0047	262	11.7989	8.7028	3514.5868
263	11.8249	8.6838	437.4101	263	11.8249	8.6838	3173.1849	263	11.8249	8.6838	328.0824	263	11.8249	8.6838	3479.4309
264	11.8509	8.6648	375.4311	264	11.8509	8.6648	3100.7571	264	11.8509	8.6648	329.8812	264	11.8509	8.6648	3473.9962
265	11.8769	8.6459	349.4131	265	11.8769	8.6459	3064.2904	265	11.8769	8.6459	295.3025	265	11.8769	8.6459	3432.1838
266	11.9029	8.6271	422.4244	266	11.9029	8.6271	3126.853	266	11.9029	8.6271	364.1579	266	11.9029	8.6271	3493.8057
267	11.9289	8.6083	438.9055	267	11.9289	8.6083	3132.8854	267	11.9289	8.6083	321.4209	267	11.9289	8.6083	3443.8351
268	11.9549	8.5897	426.0584	268	11.9549	8.5897	3109.5894	268	11.9549	8.5897	246.8863	268	11.9549	8.5897	3362.067
269	11.9809	8.5711	394.8241	269	11.9809	8.5711	3067.9064	269	11.9809	8.5711	205.5699	269	11.9809	8.5711	3313.517
270	12.0069	8.5526	390.9598	270	12.0069	8.5526	3053.5933	270	12.0069	8.5526	305.2748	270	12.0069	8.5526	3405.9883
271	12.0329	8.5342	345.5432	271	12.0329	8.5342	2997.7281	271	12.0329	8.5342	357.768	271	12.0329	8.5342	3451.2479
272	12.0589	8.5159	397.706	272	12.0589	8.5159	3044.9976	272	12.0589	8.5159	279.0393	272	12.0589	8.5159	3365.2856
273	12.0849	8.4976	414.63	273	12.0849	8.4976	3057.0284	273	12.0849	8.4976	322.0611	273	12.0849	8.4976	3401.0739
274	12.1109	8.4794	349.2855	274	12.1109	8.4794	2986.7907	274	12.1109	8.4794	329.2376	274	12.1109	8.4794	3401.0168
275	12.1369	8.4613	309.5159	275	12.1369	8.4613	2942.1278	275	12.1369	8.4613	348.7317	275	12.1369	8.4613	3413.2773
276	12.1629	8.4433	372.7792	276	12.1629	8.4433	3000.4979	276	12.1629	8.4433	289.8589	276	12.1629	8.4433	3347.171
277	12.1889	8.4254	397.684	277	12.1889	8.4254	3020.5096	277	12.1889	8.4254	269.7177	277	12.1889	8.4254	3319.7962
278	12.2149	8.4075	412.7232	278	12.2149	8.4075	3030.6555	278	12.2149	8.4075	210.8229	278	12.2149	8.4075	3253.6677
279	12.2409	8.3897	454.8212	279	12.2409	8.3897	3067.8604	279	12.2409	8.3897	280.3357	279	12.2409	8.3897	3315.947
280	12.2669	8.372	346.5846	280	12.2669	8.372	2954.7306	280	12.2669	8.372	252.6556	280	12.2669	8.372	3281.0333
281	12.2929	8.3544	387.2954	281	12.2929	8.3544	2990.5481	281	12.2929	8.3544	348.1989	281	12.2929	8.3544	3369.3431
282	12.3189	8.3368	397.0144	282	12.3189	8.3368	2995.3739	282	12.3189	8.3368	339.9368	282	12.3189	8.3368	3353.8473
283	12.3449	8.3193	348.9002	283	12.3449	8.3193	2942.3666	283	12.3449	8.3193	335.3814	283	12.3449	8.3193	3342.0584

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
284	12.3709	8.3019	291.1773	284	12.3709	8.3019	2879.7504	284	12.3709	8.3019	302.1797	284	12.3709	8.3019	3301.6231
285	12.3969	8.2845	421.3822	285	12.3969	8.2845	3005.0621	285	12.3969	8.2845	373.2246	285	12.3969	8.2845	3365.4345
286	12.4229	8.2673	328.0818	286	12.4229	8.2673	2906.8685	286	12.4229	8.2673	317.9502	286	12.4229	8.2673	3302.9265
287	12.4489	8.2501	303.6975	287	12.4489	8.2501	2877.591	287	12.4489	8.2501	341.8529	287	12.4489	8.2501	3319.5956
288	12.4749	8.2329	285.2819	288	12.4749	8.2329	2854.2821	288	12.4749	8.2329	356.2465	288	12.4749	8.2329	3326.7556
289	12.5009	8.2159	428.1877	289	12.5009	8.2159	2992.2948	289	12.5009	8.2159	331.7144	289	12.5009	8.2159	3294.99
290	12.5269	8.1989	412.2826	290	12.5269	8.1989	2971.4964	290	12.5269	8.1989	340.4009	290	12.5269	8.1989	3296.4428
291	12.5529	8.182	378.8568	291	12.5529	8.182	2933.1775	291	12.5529	8.182	247.4015	291	12.5529	8.182	3196.2099
292	12.5789	8.1652	317.1942	292	12.5789	8.1652	2866.6216	292	12.5789	8.1652	303.1774	292	12.5789	8.1652	3244.7522
293	12.6049	8.1484	304.1945	293	12.6049	8.1484	2848.7287	293	12.6049	8.1484	235.9229	293	12.6049	8.1484	3170.2641
294	12.6309	8.1317	389.5335	294	12.6309	8.1317	2929.1746	294	12.6309	8.1317	295.8515	294	12.6309	8.1317	3222.9591
295	12.6569	8.115	426.719	295	12.6569	8.115	2961.4669	295	12.6569	8.115	282.0489	295	12.6569	8.115	3201.923
296	12.6829	8.0985	337.51	296	12.6829	8.0985	2867.3646	296	12.6829	8.0985	272.9112	296	12.6829	8.0985	3185.5517
297	12.7089	8.082	346.7866	297	12.7089	8.082	2871.748	297	12.7089	8.082	233.2953	297	12.7089	8.082	3138.7022
298	12.7349	8.0655	345.5432	298	12.7349	8.0655	2865.6114	298	12.7349	8.0655	377.4487	298	12.7349	8.0655	3275.622
299	12.7609	8.0492	308.8085	299	12.7609	8.0492	2822.5684	299	12.7609	8.0492	254.818	299	12.7609	8.0492	3144.5179
300	12.7869	8.0329	309.6694	300	12.7869	8.0329	2817.1211	300	12.7869	8.0329	273.9427	300	12.7869	8.0329	3155.1691
301	12.8129	8.0166	433.3621	301	12.8129	8.0166	2934.5056	301	12.8129	8.0166	258.0139	301	12.8129	8.0166	3130.7669
302	12.8389	8.0005	336.2895	302	12.8389	8.0005	2831.1248	302	12.8389	8.0005	257.6846	302	12.8389	8.0005	3121.9641
303	12.8649	7.9844	425.2337	303	12.8649	7.9844	2913.7607	303	12.8649	7.9844	337.2148	303	12.8649	7.9844	3193.0208
304	12.8909	7.9683	363.2266	304	12.8909	7.9683	2845.4454	304	12.8909	7.9683	351.6287	304	12.8909	7.9683	3198.9613
305	12.9169	7.9524	347.4498	305	12.9169	7.9524	2823.3603	305	12.9169	7.9524	315.8779	305	12.9169	7.9524	3154.737
306	12.9429	7.9365	432.2675	306	12.9429	7.9365	2901.8698	306	12.9429	7.9365	269.0871	306	12.9429	7.9365	3099.4728
307	12.9689	7.9206	330.8352	307	12.9689	7.9206	2794.1293	307	12.9689	7.9206	309.8201	307	12.9689	7.9206	3131.7322
308	12.9949	7.9048	144.1507	308	12.9949	7.9048	2601.1365	308	12.9949	7.9048	382.5158	308	12.9949	7.9048	3195.9545
309	13.0209	7.8891	272.5293	309	13.0209	7.8891	2723.2068	309	13.0209	7.8891	327.0154	309	13.0209	7.8891	3131.9807
310	13.0469	7.8735	254.8743	310	13.0469	7.8735	2699.2436	310	13.0469	7.8735	455.7317	310	13.0469	7.8735	3252.2235
311	13.0729	7.8579	288.5098	311	13.0729	7.8579	2726.5709	311	13.0729	7.8579	420.3086	311	13.0729	7.8579	3208.3269
312	13.0989	7.8423	344.7839	312	13.0989	7.8423	2776.5367	312	13.0989	7.8423	315.6693	312	13.0989	7.8423	3095.2141
313	13.1249	7.8269	255.1843	313	13.1249	7.8269	2680.6288	313	13.1249	7.8269	310.3116	313	13.1249	7.8269	3081.383
314	13.1509	7.8115	203.4646	314	13.1509	7.8115	2622.6009	314	13.1509	7.8115	321.085	314	13.1509	7.8115	3083.683
315	13.1769	7.7961	385.4739	315	13.1769	7.7961	2798.302	315	13.1769	7.7961	284.7711	315	13.1769	7.7961	3038.8956
316	13.2029	7.7808	363.8859	316	13.2029	7.7808	2770.4058	316	13.2029	7.7808	266.3615	316	13.2029	7.7808	3012.0125
317	13.2289	7.7656	310.0505	317	13.2289	7.7656	2710.2621	317	13.2289	7.7656	317.6439	317	13.2289	7.7656	3054.8214
318	13.2549	7.7504	389.2868	318	13.2549	7.7504	2783.1902	318	13.2549	7.7504	272.6169	318	13.2549	7.7504	3001.321
319	13.2809	7.7353	361.2563	319	13.2809	7.7353	2748.8515	319	13.2809	7.7353	323.1414	319	13.2809	7.7353	3043.3721

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
320	13.3069	7.7203	241.8427	320	13.3069	7.7203	2623.1296	320	13.3069	7.7203	281.9728	320	13.3069	7.7203	2993.73
321	13.3329	7.7053	318.2312	321	13.3329	7.7053	2693.2099	321	13.3329	7.7053	299.3379	321	13.3329	7.7053	3002.6217
322	13.3589	7.6904	328.8456	322	13.3589	7.6904	2697.5161	322	13.3589	7.6904	296.7058	322	13.3589	7.6904	2991.5161
323	13.3849	7.6755	362.2287	323	13.3849	7.6755	2724.5908	323	13.3849	7.6755	263.8272	323	13.3849	7.6755	2950.164
324	13.4109	7.6607	350.5029	324	13.4109	7.6607	2706.5568	324	13.4109	7.6607	266.3171	324	13.4109	7.6607	2944.1804
325	13.4369	7.6459	345.5432	325	13.4369	7.6459	2695.2889	325	13.4369	7.6459	324.2911	325	13.4369	7.6459	2993.681
326	13.4629	7.6312	350.9421	326	13.4629	7.6312	2694.7753	326	13.4629	7.6312	302.1267	326	13.4629	7.6312	2962.8105
327	13.4889	7.6166	289.73	327	13.4889	7.6166	2627.6507	327	13.4889	7.6166	386.8009	327	13.4889	7.6166	3038.7786
328	13.5149	7.602	402.6561	328	13.5149	7.602	2734.6643	328	13.5149	7.602	351.7198	328	13.5149	7.602	2994.9914
329	13.5409	7.5875	346.2815	329	13.5409	7.5875	2672.3772	329	13.5409	7.5875	324.0156	329	13.5409	7.5875	2958.5812
330	13.5669	7.573	371.9842	330	13.5669	7.573	2692.1674	330	13.5669	7.573	345.0585	330	13.5669	7.573	2970.918
331	13.5929	7.5586	336.0496	331	13.5929	7.5586	2650.3203	331	13.5929	7.5586	443.2956	331	13.5929	7.5586	3060.449
332	13.6189	7.5442	309.3374	332	13.6189	7.5442	2617.6956	332	13.6189	7.5442	472.8168	332	13.6189	7.5442	3081.2642
333	13.6449	7.5299	329.1993	333	13.6449	7.5299	2631.645	333	13.6449	7.5299	439.1456	333	13.6449	7.5299	3038.8869
334	13.6709	7.5157	391.874	334	13.6709	7.5157	2688.4072	334	13.6709	7.5157	365.1607	334	13.6709	7.5157	2956.1958
335	13.6969	7.5015	328.1474	335	13.6969	7.5015	2618.7681	335	13.6969	7.5015	396.1174	335	13.6969	7.5015	2978.4466
336	13.7229	7.4873	324.0653	336	13.7229	7.4873	2608.7735	336	13.7229	7.4873	375.6465	336	13.7229	7.4873	2949.2695
337	13.7489	7.4732	332.5482	337	13.7489	7.4732	2611.3439	337	13.7489	7.4732	335.1031	337	13.7489	7.4732	2900.0201
338	13.7749	7.4592	352.4586	338	13.7749	7.4592	2625.3418	338	13.7749	7.4592	404.6259	338	13.7749	7.4592	2960.8368
339	13.8009	7.4452	365.7979	339	13.8009	7.4452	2632.7687	339	13.8009	7.4452	407.5491	339	13.8009	7.4452	2955.054
340	13.8269	7.4313	371.8508	340	13.8269	7.4313	2632.909	340	13.8269	7.4313	390.9286	340	13.8269	7.4313	2929.7273
341	13.8529	7.4174	296.1667	341	13.8529	7.4174	2551.3125	341	13.8529	7.4174	380.1147	341	13.8529	7.4174	2910.2074
342	13.8789	7.4036	269.4122	342	13.8789	7.4036	2518.6455	342	13.8789	7.4036	341.8565	342	13.8789	7.4036	2863.2431
343	13.9049	7.3898	332.9922	343	13.9049	7.3898	2576.3129	343	13.9049	7.3898	337.4181	343	13.9049	7.3898	2850.0986
344	13.9309	7.3761	414.3408	344	13.9309	7.3761	2651.749	344	13.9309	7.3761	383.6482	344	13.9309	7.3761	2887.6226
345	13.9569	7.3624	405.9126	345	13.9569	7.3624	2637.4084	345	13.9569	7.3624	379.7012	345	13.9569	7.3624	2874.9696
346	13.9829	7.3488	405.2195	346	13.9829	7.3488	2630.8028	346	13.9829	7.3488	369.0522	346	13.9829	7.3488	2855.6145
347	14.0089	7.3352	346.5638	347	14.0089	7.3352	2566.2345	347	14.0089	7.3352	382.2775	347	14.0089	7.3352	2860.1338
348	14.0349	7.3217	279.7733	348	14.0349	7.3217	2493.5316	348	14.0349	7.3217	406.8879	348	14.0349	7.3217	2876.038
349	14.0609	7.3082	324.6528	349	14.0609	7.3082	2532.4986	349	14.0609	7.3082	423.7266	349	14.0609	7.3082	2884.1707
350	14.0869	7.2948	352.416	350	14.0869	7.2948	2554.3493	350	14.0869	7.2948	465.249	350	14.0869	7.2948	2916.987
351	14.1129	7.2814	370.8663	351	14.1129	7.2814	2566.8871	351	14.1129	7.2814	434.8508	351	14.1129	7.2814	2877.8827
352	14.1389	7.2681	345.5432	352	14.1389	7.2681	2535.6515	352	14.1389	7.2681	324.2911	352	14.1389	7.2681	2758.617
353	14.1649	7.2548	330.7152	353	14.1649	7.2548	2515.4559	353	14.1649	7.2548	348.731	353	14.1649	7.2548	2778.5515
354	14.1909	7.2416	357.1758	354	14.1909	7.2416	2536.5488	354	14.1909	7.2416	448.0589	354	14.1909	7.2416	2873.3741
355	14.2169	7.2284	344.2194	355	14.2169	7.2284	2518.2248	355	14.2169	7.2284	471.3401	355	14.2169	7.2284	2892.1499

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
356	14.2429	7.2153	341.3174	356	14.2429	7.2153	2509.9552	356	14.2429	7.2153	422.8921	356	14.2429	7.2153	2839.1966
357	14.2689	7.2022	340.7149	357	14.2689	7.2022	2503.985	357	14.2689	7.2022	364.5093	357	14.2689	7.2022	2776.3084
358	14.2949	7.1892	356.4071	358	14.2949	7.1892	2514.3097	358	14.2949	7.1892	350.2134	358	14.2949	7.1892	2757.5071
359	14.3209	7.1762	341.3701	359	14.3209	7.1762	2493.905	359	14.3209	7.1762	354.0333	359	14.3209	7.1762	2756.8217
360	14.3469	7.1633	345.1909	360	14.3469	7.1633	2492.3582	360	14.3469	7.1633	390.6771	360	14.3469	7.1633	2788.9601
361	14.3729	7.1504	356.5678	361	14.3729	7.1504	2498.3675	361	14.3729	7.1504	414.3831	361	14.3729	7.1504	2808.1608
362	14.3989	7.1375	324.1191	362	14.3989	7.1375	2460.5511	362	14.3989	7.1375	382.9153	362	14.3989	7.1375	2772.1876
363	14.4249	7.1247	378.9974	363	14.4249	7.1247	2510.0618	363	14.4249	7.1247	375.1095	363	14.4249	7.1247	2759.8764
364	14.4509	7.112	332.0932	364	14.4509	7.112	2457.79	364	14.4509	7.112	379.0316	364	14.4509	7.112	2759.2932
365	14.4769	7.0993	315.2174	365	14.4769	7.0993	2435.5465	365	14.4769	7.0993	333.2177	365	14.4769	7.0993	2708.974
366	14.5029	7.0866	363.3367	366	14.5029	7.0866	2478.2982	366	14.5029	7.0866	317.5865	366	14.5029	7.0866	2688.8374
367	14.5289	7.074	352.7757	367	14.5289	7.074	2462.3696	367	14.5289	7.074	361.8347	367	14.5289	7.074	2728.5802
368	14.5549	7.0614	404.8123	368	14.5549	7.0614	2509.0385	368	14.5549	7.0614	422.1761	368	14.5549	7.0614	2784.4163
369	14.5809	7.0489	383.5211	369	14.5809	7.0489	2482.3797	369	14.5809	7.0489	439.6241	369	14.5809	7.0489	2797.359
370	14.6069	7.0364	342.0858	370	14.6069	7.0364	2435.5768	370	14.6069	7.0364	411.3517	370	14.6069	7.0364	2764.5812
371	14.6329	7.024	371.5364	371	14.6329	7.024	2459.6597	371	14.6329	7.024	395.0846	371	14.6329	7.024	2743.8087
372	14.6589	7.0116	305.4318	372	14.6589	7.0116	2388.1875	372	14.6589	7.0116	377.8247	372	14.6589	7.0116	2722.0435
373	14.6849	6.9993	371.099	373	14.6849	6.9993	2448.4871	373	14.6849	6.9993	348.4691	373	14.6849	6.9993	2688.1826
374	14.7109	6.987	355.1014	374	14.7109	6.987	2427.1218	374	14.7109	6.987	291.3594	374	14.7109	6.987	2626.5675
375	14.7369	6.9747	275.769	375	14.7369	6.9747	2342.4219	375	14.7369	6.9747	307.0238	375	14.7369	6.9747	2637.7266
376	14.7629	6.9625	305.954	376	14.7629	6.9625	2367.2392	376	14.7629	6.9625	309.7627	376	14.7629	6.9625	2635.96
377	14.7889	6.9503	395.5047	377	14.7889	6.9503	2451.4223	377	14.7889	6.9503	407.9606	377	14.7889	6.9503	2729.6526
378	14.8149	6.9382	415.631	378	14.8149	6.9382	2466.181	378	14.8149	6.9382	439.1773	378	14.8149	6.9382	2756.364
379	14.8409	6.9261	345.5432	379	14.8409	6.9261	2390.7256	379	14.8409	6.9261	324.2911	379	14.8409	6.9261	2636.9724
380	14.8669	6.9141	374.9407	380	14.8669	6.9141	2414.4926	380	14.8669	6.9141	351.854	380	14.8669	6.9141	2658.5063
381	14.8929	6.9021	365.6034	381	14.8929	6.9021	2399.5248	381	14.8929	6.9021	335.837	381	14.8929	6.9021	2636.4603
382	14.9189	6.8901	391.7873	382	14.9189	6.8901	2420.0784	382	14.9189	6.8901	387.5508	382	14.9189	6.8901	2682.1451
383	14.9449	6.8782	413.9192	383	14.9449	6.8782	2436.5798	383	14.9449	6.8782	367.7083	383	14.9449	6.8782	2656.2737
384	14.9709	6.8663	321.5679	384	14.9709	6.8663	2338.5981	384	14.9709	6.8663	326.4494	384	14.9709	6.8663	2608.9857
385	14.9969	6.8545	320.5013	385	14.9969	6.8545	2331.9011	385	14.9969	6.8545	370.4311	385	14.9969	6.8545	2646.9385
386	15.0229	6.8427	299.5572	386	15.0229	6.8427	2305.3265	386	15.0229	6.8427	344.3167	386	15.0229	6.8427	2614.795
387	15.0489	6.8309	413.8718	387	15.0489	6.8309	2414.0107	387	15.0489	6.8309	398.3606	387	15.0489	6.8309	2662.81
388	15.0749	6.8192	310.7776	388	15.0749	6.8192	2305.286	388	15.0749	6.8192	385.1335	388	15.0749	6.8192	2643.5539
389	15.1009	6.8075	372.0078	389	15.1009	6.8075	2360.8859	389	15.1009	6.8075	326.6146	389	15.1009	6.8075	2579.006
390	15.1269	6.7959	304.2029	390	15.1269	6.7959	2287.4505	390	15.1269	6.7959	360.0468	390	15.1269	6.7959	2606.4093
391	15.1529	6.7843	356.1587	391	15.1529	6.7843	2333.7759	391	15.1529	6.7843	325.5362	391	15.1529	6.7843	2565.8697

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
392	15.1789	6.7727	400.3921	392	15.1789	6.7727	2372.3789	392	15.1789	6.7727	321.3056	392	15.1789	6.7727	2555.6101
393	15.2049	6.7612	350.0218	393	15.2049	6.7612	2316.3782	393	15.2049	6.7612	267.5614	393	15.2049	6.7612	2495.8369
394	15.2309	6.7498	298.1951	394	15.2309	6.7498	2258.921	394	15.2309	6.7498	351.0875	394	15.2309	6.7498	2573.334
395	15.2569	6.7383	339.0857	395	15.2569	6.7383	2294.1812	395	15.2569	6.7383	408.6173	395	15.2569	6.7383	2624.8348
396	15.2829	6.7269	353.7167	396	15.2829	6.7269	2303.1818	396	15.2829	6.7269	358.6961	396	15.2829	6.7269	2568.8846
397	15.3089	6.7156	436.8482	397	15.3089	6.7156	2380.6829	397	15.3089	6.7156	314.7973	397	15.3089	6.7156	2518.9568
398	15.3349	6.7043	379.9542	398	15.3349	6.7043	2318.1584	398	15.3349	6.7043	290.9705	398	15.3349	6.7043	2489.1011
399	15.3609	6.693	295.528	399	15.3609	6.693	2228.1019	399	15.3609	6.693	446.4816	399	15.3609	6.693	2638.5831
400	15.3869	6.6817	307.0751	400	15.3869	6.6817	2234.0185	400	15.3869	6.6817	333.5015	400	15.3869	6.6817	2519.5741
401	15.4129	6.6705	405.8478	401	15.4129	6.6705	2327.1608	401	15.4129	6.6705	348.9467	401	15.4129	6.6705	2528.9903
402	15.4389	6.6594	384.8096	402	15.4389	6.6594	2300.4921	402	15.4389	6.6594	232.3766	402	15.4389	6.6594	2406.3912
403	15.4649	6.6482	367.0715	403	15.4649	6.6482	2277.1236	403	15.4649	6.6482	348.2165	403	15.4649	6.6482	2516.2021
404	15.4909	6.6371	383.5625	404	15.4909	6.6371	2287.9842	404	15.4909	6.6371	284.1921	404	15.4909	6.6371	2446.1487
405	15.5169	6.6261	377.312	405	15.5169	6.6261	2276.1033	405	15.5169	6.6261	402.0999	405	15.5169	6.6261	2558.0275
406	15.5429	6.6151	345.5432	406	15.5429	6.6151	2238.7041	406	15.5429	6.6151	403.2125	406	15.5429	6.6151	2553.1112
407	15.5689	6.6041	338.1242	407	15.5689	6.6041	2228.2845	407	15.5689	6.6041	334.3211	407	15.5689	6.6041	2478.1907
408	15.5949	6.5932	377.3821	408	15.5949	6.5932	2264.5418	408	15.5949	6.5932	357.3919	408	15.5949	6.5932	2495.2325
409	15.6209	6.5823	405.6335	409	15.6209	6.5823	2289.7926	409	15.6209	6.5823	352.7679	409	15.6209	6.5823	2484.5795
410	15.6469	6.5714	477.6498	410	15.6469	6.5714	2358.8083	410	15.6469	6.5714	382.7037	410	15.6469	6.5714	2508.4863
411	15.6729	6.5605	363.7002	411	15.6729	6.5605	2241.8582	411	15.6729	6.5605	397.7012	411	15.6729	6.5605	2517.4549
412	15.6989	6.5497	413.1589	412	15.6989	6.5497	2288.3163	412	15.6989	6.5497	343.4274	412	15.6989	6.5497	2457.1521
413	15.7249	6.539	334.2017	413	15.7249	6.539	2206.3585	413	15.7249	6.539	313.2958	413	15.7249	6.539	2420.9915
414	15.7509	6.5283	356.8087	414	15.7509	6.5283	2225.9649	414	15.7509	6.5283	404.7384	414	15.7509	6.5283	2506.4051
415	15.7769	6.5176	279.8725	415	15.7769	6.5176	2146.0281	415	15.7769	6.5176	403.411	415	15.7769	6.5176	2499.0488
416	15.8029	6.5069	265.7869	416	15.8029	6.5069	2128.942	416	15.8029	6.5069	437.3877	416	15.8029	6.5069	2526.9965
417	15.8289	6.4963	300.1216	417	15.8289	6.4963	2160.2761	417	15.8289	6.4963	396.8253	417	15.8289	6.4963	2480.4051
418	15.8549	6.4857	322.507	418	15.8549	6.4857	2179.6609	418	15.8549	6.4857	418.7341	418	15.8549	6.4857	2496.2849
419	15.8809	6.4752	293.7474	419	15.8809	6.4752	2147.9007	419	15.8809	6.4752	317.6556	419	15.8809	6.4752	2389.1774
420	15.9069	6.4646	247.8767	420	15.9069	6.4646	2099.0295	420	15.9069	6.4646	379.495	420	15.9069	6.4646	2444.9878
421	15.9329	6.4542	296.9692	421	15.9329	6.4542	2145.1214	421	15.9329	6.4542	444.4986	421	15.9329	6.4542	2503.9624
422	15.9589	6.4437	349.516	422	15.9589	6.4437	2194.6676	422	15.9589	6.4437	345.2078	422	15.9589	6.4437	2398.6426
423	15.9849	6.4333	307.2047	423	15.9849	6.4333	2149.3557	423	15.9849	6.4333	387.5536	423	15.9849	6.4333	2434.9594
424	16.0109	6.4229	273.7634	424	16.0109	6.4229	2112.9139	424	16.0109	6.4229	422.8777	424	16.0109	6.4229	2464.2545
425	16.0369	6.4126	373.1404	425	16.0369	6.4126	2209.2903	425	16.0369	6.4126	393.7977	425	16.0369	6.4126	2429.1456
426	16.0629	6.4023	280.6987	426	16.0629	6.4023	2113.848	426	16.0629	6.4023	366.9734	426	16.0629	6.4023	2396.2923
427	16.0889	6.392	311.6995	427	16.0889	6.392	2141.8483	427	16.0889	6.392	356.6598	427	16.0889	6.392	2379.9497

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
428	16.1149	6.3817	315.2987	428	16.1149	6.3817	2142.4468	428	16.1149	6.3817	281.8946	428	16.1149	6.3817	2299.1555
429	16.1409	6.3715	297.034	429	16.1409	6.3715	2121.1816	429	16.1409	6.3715	361.6917	429	16.1409	6.3715	2372.9236
430	16.1669	6.3614	337.2232	430	16.1669	6.3614	2158.3702	430	16.1669	6.3614	410.9471	430	16.1669	6.3614	2416.15
431	16.1929	6.3512	372.4555	431	16.1929	6.3512	2190.6019	431	16.1929	6.3512	443.5619	431	16.1929	6.3512	2442.7358
432	16.2189	6.3411	334.8272	432	16.2189	6.3411	2149.973	432	16.2189	6.3411	341.3729	432	16.2189	6.3411	2334.5178
433	16.2449	6.331	345.5432	433	16.2449	6.331	2157.6885	433	16.2449	6.331	324.2911	433	16.2449	6.331	2311.4071
434	16.2709	6.321	294.5893	434	16.2709	6.321	2101.1535	434	16.2709	6.321	414.9565	434	16.2709	6.321	2398.1049
435	16.2969	6.3109	295.6035	435	16.2969	6.3109	2096.5867	435	16.2969	6.3109	453.2067	435	16.2969	6.3109	2432.3875
436	16.3229	6.301	270.5697	436	16.3229	6.301	2065.9718	436	16.3229	6.301	403.7664	436	16.3229	6.301	2378.9796
437	16.3489	6.291	326.5886	437	16.3489	6.291	2116.4097	437	16.3489	6.291	389.4932	437	16.3489	6.291	2360.7388
438	16.3749	6.2811	325.9225	438	16.3749	6.2811	2110.1625	438	16.3749	6.2811	346.2612	438	16.3749	6.2811	2313.5392
439	16.4009	6.2712	441.4942	439	16.4009	6.2712	2220.1531	439	16.4009	6.2712	393.3634	439	16.4009	6.2712	2356.6738
440	16.4269	6.2613	342.0115	440	16.4269	6.2613	2115.0893	440	16.4269	6.2613	389.2134	440	16.4269	6.2613	2348.5562
441	16.4529	6.2515	292.0914	441	16.4529	6.2515	2059.5882	441	16.4529	6.2515	335.0127	441	16.4529	6.2515	2290.3879
442	16.4789	6.2417	292.9921	442	16.4789	6.2417	2054.9079	442	16.4789	6.2417	373.9038	442	16.4789	6.2417	2325.3114
443	16.5049	6.232	293.3379	443	16.5049	6.232	2049.6726	443	16.5049	6.232	379.2283	443	16.5049	6.232	2326.6683
444	16.5309	6.2222	395.7012	444	16.5309	6.2222	2146.4548	444	16.5309	6.2222	373.1984	444	16.5309	6.2222	2316.6708
445	16.5569	6.2125	399.1882	445	16.5569	6.2125	2144.3608	445	16.5569	6.2125	339.5021	445	16.5569	6.2125	2279.0068
446	16.5829	6.2028	313.7192	446	16.5829	6.2028	2053.3107	446	16.5829	6.2028	352.6297	446	16.5829	6.2028	2288.1668
447	16.6089	6.1932	292.6094	447	16.6089	6.1932	2026.6199	447	16.6089	6.1932	311.4489	447	16.6089	6.1932	2243.0185
448	16.6349	6.1836	320.9479	448	16.6349	6.1836	2049.3773	448	16.6349	6.1836	309.4005	448	16.6349	6.1836	2237.0025
449	16.6609	6.174	361.899	449	16.6609	6.174	2084.7473	449	16.6609	6.174	390.8669	449	16.6609	6.174	2314.5013
450	16.6869	6.1645	386.8225	450	16.6869	6.1645	2104.0898	450	16.6869	6.1645	442.5901	450	16.6869	6.1645	2362.2569
451	16.7129	6.1549	360.6807	451	16.7129	6.1549	2072.3669	451	16.7129	6.1549	379.0555	451	16.7129	6.1549	2294.7547
452	16.7389	6.1454	343.1453	452	16.7389	6.1454	2049.2505	452	16.7389	6.1454	322.1942	452	16.7389	6.1454	2233.9258
453	16.7649	6.136	325.144	453	16.7649	6.136	2025.6682	453	16.7649	6.136	317.752	453	16.7649	6.136	2225.516
454	16.7909	6.1265	325.7806	454	16.7909	6.1265	2020.7237	454	16.7909	6.1265	330.9585	454	16.7909	6.1265	2234.7549
455	16.8169	6.1171	367.0011	455	16.8169	6.1171	2056.3631	455	16.8169	6.1171	355.2089	455	16.8169	6.1171	2255.0378
456	16.8429	6.1078	370.2315	456	16.8429	6.1078	2054.0125	456	16.8429	6.1078	343.9756	456	16.8429	6.1078	2239.8368
457	16.8689	6.0984	321.6671	457	16.8689	6.0984	1999.867	457	16.8689	6.0984	374.6166	457	16.8689	6.0984	2266.5102
458	16.8949	6.0891	310.6568	458	16.8949	6.0891	1983.2756	458	16.8949	6.0891	358.2298	458	16.8949	6.0891	2246.1558
459	16.9209	6.0798	341.5954	459	16.9209	6.0798	2008.6332	459	16.9209	6.0798	332.4114	459	16.9209	6.0798	2216.3699
460	16.9469	6.0706	345.5432	460	16.9469	6.0706	2007	460	16.9469	6.0706	370.9651	460	16.9469	6.0706	2250.956
461	16.9729	6.0613	355.5282	461	16.9729	6.0613	2013.1004	461	16.9729	6.0613	351.8943	461	16.9729	6.0613	2225.7711
462	16.9989	6.0521	377.1062	462	16.9989	6.0521	2030.7939	462	16.9989	6.0521	305.6743	462	16.9989	6.0521	2173.4369
463	17.0249	6.0429	429.9643	463	17.0249	6.0429	2079.7675	463	17.0249	6.0429	330.6203	463	17.0249	6.0429	2192.2689

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
464	17.0509	6.0338	444.7014	464	17.0509	6.0338	2090.6201	464	17.0509	6.0338	375.5775	464	17.0509	6.0338	2231.1119
465	17.0769	6.0247	359.2813	465	17.0769	6.0247	2001.3155	465	17.0769	6.0247	287.4416	465	17.0769	6.0247	2136.862
466	17.1029	6.0156	337.2461	466	17.1029	6.0156	1975.3958	466	17.1029	6.0156	367.9802	466	17.1029	6.0156	2211.2865
467	17.1289	6.0065	353.7859	467	17.1289	6.0065	1988.0511	467	17.1289	6.0065	459.1841	467	17.1289	6.0065	2296.3762
468	17.1549	5.9975	349.6551	468	17.1549	5.9975	1980.0357	468	17.1549	5.9975	386.8034	468	17.1549	5.9975	2217.8815
469	17.1809	5.9885	401.5838	469	17.1809	5.9885	2028.08	469	17.1809	5.9885	293.4546	469	17.1809	5.9885	2118.4185
470	17.2069	5.9795	380.7197	470	17.2069	5.9795	2003.3313	470	17.2069	5.9795	381.3544	470	17.2069	5.9795	2200.2042
471	17.2329	5.9706	320.9858	471	17.2329	5.9706	1939.713	471	17.2329	5.9706	350.6615	471	17.2329	5.9706	2163.3972
472	17.2589	5.9616	288.346	472	17.2589	5.9616	1903.1886	472	17.2589	5.9616	286.9004	472	17.2589	5.9616	2093.522
473	17.2849	5.9527	340.9919	473	17.2849	5.9527	1951.95	473	17.2849	5.9527	407.4924	473	17.2849	5.9527	2208
474	17.3109	5.9439	334.6562	474	17.3109	5.9439	1941.7298	474	17.3109	5.9439	384.4647	474	17.3109	5.9439	2178.8582
475	17.3369	5.935	310.2172	475	17.3369	5.935	1913.4063	475	17.3369	5.935	323.8301	475	17.3369	5.935	2112.1095
476	17.3629	5.9262	307.8179	476	17.3629	5.9262	1907.1225	476	17.3629	5.9262	357.6735	476	17.3629	5.9262	2139.8387
477	17.3889	5.9174	312.0444	477	17.3889	5.9174	1907.4645	477	17.3889	5.9174	403.0482	477	17.3889	5.9174	2179.0994
478	17.4149	5.9086	372.5004	478	17.4149	5.9086	1964.036	478	17.4149	5.9086	328.4785	478	17.4149	5.9086	2098.4156
479	17.4409	5.8999	405.5773	479	17.4409	5.8999	1993.2284	479	17.4409	5.8999	361.1198	479	17.4409	5.8999	2124.9428
480	17.4669	5.8912	326.9668	480	17.4669	5.8912	1910.7333	480	17.4669	5.8912	343.7383	480	17.4669	5.8912	2101.4472
481	17.4929	5.8825	409.2878	481	17.4929	5.8825	1989.1698	481	17.4929	5.8825	312.5416	481	17.4929	5.8825	2064.1364
482	17.5189	5.8738	414.1302	482	17.5189	5.8738	1990.1277	482	17.5189	5.8738	370.5193	482	17.5189	5.8738	2116
483	17.5449	5.8652	369.1089	483	17.5449	5.8652	1941.2218	483	17.5449	5.8652	365.9781	483	17.5449	5.8652	2105.3447
484	17.5709	5.8566	418.8476	484	17.5709	5.8566	1987.0761	484	17.5709	5.8566	321.5031	484	17.5709	5.8566	2054.7556
485	17.5969	5.848	403.4768	485	17.5969	5.848	1967.8208	485	17.5969	5.848	296.0776	485	17.5969	5.848	2023.216
486	17.6229	5.8394	455.9039	486	17.6229	5.8394	2016.3633	486	17.6229	5.8394	369.794	486	17.6229	5.8394	2090.8183
487	17.6489	5.8309	396.6259	487	17.6489	5.8309	1953.2009	487	17.6489	5.8309	382.2466	487	17.6489	5.8309	2097.1568
488	17.6749	5.8224	330.5676	488	17.6749	5.8224	1883.258	488	17.6749	5.8224	312.2815	488	17.6749	5.8224	2021.0777
489	17.7009	5.8139	295.2491	489	17.7009	5.8139	1844.055	489	17.7009	5.8139	380.1086	489	17.7009	5.8139	2082.7906
490	17.7269	5.8054	378.8145	490	17.7269	5.8054	1923.736	490	17.7269	5.8054	409.5562	490	17.7269	5.8054	2106.1241
491	17.7529	5.797	413.8292	491	17.7529	5.797	1954.8661	491	17.7529	5.797	347.2073	491	17.7529	5.797	2037.6611
492	17.7789	5.7886	427.8788	492	17.7789	5.7886	1965.0312	492	17.7789	5.7886	383.4059	492	17.7789	5.7886	2067.7457
493	17.8049	5.7802	335.7863	493	17.8049	5.7802	1869.0541	493	17.8049	5.7802	356.7302	493	17.8049	5.7802	2034.9558
494	17.8309	5.7719	333.1582	494	17.8309	5.7719	1862.5415	494	17.8309	5.7719	386.2965	494	17.8309	5.7719	2058.408
495	17.8569	5.7635	344.8463	495	17.8569	5.7635	1870.3452	495	17.8569	5.7635	400.4606	495	17.8569	5.7635	2066.4581
496	17.8829	5.7552	369.566	496	17.8829	5.7552	1891.1804	496	17.8829	5.7552	371.7281	496	17.8829	5.7552	2031.6114
497	17.9089	5.7469	281.3026	497	17.9089	5.7469	1799.0324	497	17.9089	5.7469	356.9223	497	17.9089	5.7469	2010.6915
498	17.9349	5.7387	388.1354	498	17.9349	5.7387	1901.9807	498	17.9349	5.7387	409.3641	498	17.9349	5.7387	2057.0193
499	17.9609	5.7304	349.8652	499	17.9609	5.7304	1859.826	499	17.9609	5.7304	452.0566	499	17.9609	5.7304	2093.5976

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
500	17.9869	5.7222	332.3386	500	17.9869	5.7222	1838.4149	500	17.9869	5.7222	383.0856	500	17.9869	5.7222	2018.5126
501	18.0129	5.714	285.2643	501	18.0129	5.714	1787.456	501	18.0129	5.714	304.6011	501	18.0129	5.714	1933.914
502	18.0389	5.7058	279.0777	502	18.0389	5.7058	1777.385	502	18.0389	5.7058	382.9748	502	18.0389	5.7058	2006.1736
503	18.0649	5.6977	396.4822	503	18.0649	5.6977	1890.905	503	18.0649	5.6977	393.8888	503	18.0649	5.6977	2010.9735
504	18.0909	5.6896	395.3254	504	18.0909	5.6896	1885.8637	504	18.0909	5.6896	347.5474	504	18.0909	5.6896	1958.518
505	18.1169	5.6815	384.3588	505	18.1169	5.6815	1871.0125	505	18.1169	5.6815	410.0959	505	18.1169	5.6815	2014.9524
506	18.1429	5.6734	354.5965	506	18.1429	5.6734	1837.3658	506	18.1429	5.6734	368.774	506	18.1429	5.6734	1967.5164
507	18.1689	5.6654	363.0119	507	18.1689	5.6654	1841.8966	507	18.1689	5.6654	369.4751	507	18.1689	5.6654	1962.1034
508	18.1949	5.6573	330.1627	508	18.1949	5.6573	1805.1629	508	18.1949	5.6573	336.7099	508	18.1949	5.6573	1923.2241
509	18.2209	5.6493	369.3444	509	18.2209	5.6493	1840.4601	509	18.2209	5.6493	426.0337	509	18.2209	5.6493	2006.4338
510	18.2469	5.6413	273.1666	510	18.2469	5.6413	1740.3978	510	18.2469	5.6413	335.0614	510	18.2469	5.6413	1909.3474
511	18.2729	5.6334	339.3067	511	18.2729	5.6334	1802.6534	511	18.2729	5.6334	426.0326	511	18.2729	5.6334	1994.2046
512	18.2989	5.6254	389.3747	512	18.2989	5.6254	1848.8369	512	18.2989	5.6254	418.4183	512	18.2989	5.6254	1980.4761
513	18.3249	5.6175	385.3849	513	18.3249	5.6175	1840.9626	513	18.3249	5.6175	392.7033	513	18.3249	5.6175	1948.6471
514	18.3509	5.6096	345.5432	514	18.3509	5.6096	1797.2364	514	18.3509	5.6096	324.2911	514	18.3509	5.6096	1874.1208
515	18.3769	5.6018	283.0998	515	18.3769	5.6018	1730.904	515	18.3769	5.6018	392.189	515	18.3769	5.6018	1939.8953
516	18.4029	5.5939	356.6264	516	18.4029	5.5939	1800.5417	516	18.4029	5.5939	383.7267	516	18.4029	5.5939	1929.3096
517	18.4289	5.5861	378.7747	517	18.4289	5.5861	1818.801	517	18.4289	5.5861	411.7035	517	18.4289	5.5861	1955.1631
518	18.4549	5.5783	383.8626	518	18.4549	5.5783	1820	518	18.4549	5.5783	402.0006	518	18.4549	5.5783	1943.3369
519	18.4809	5.5705	404.0964	519	18.4809	5.5705	1836.3448	519	18.4809	5.5705	403.5076	519	18.4809	5.5705	1942.7205
520	18.5069	5.5628	370.675	520	18.5069	5.5628	1799.0345	520	18.5069	5.5628	394.8562	520	18.5069	5.5628	1931.9457
521	18.5329	5.555	386.0184	521	18.5329	5.555	1810.489	521	18.5329	5.555	335.3649	521	18.5329	5.555	1870.331
522	18.5589	5.5473	424.1464	522	18.5589	5.5473	1844.728	522	18.5589	5.5473	368.512	522	18.5589	5.5473	1901.3548
523	18.5849	5.5396	381.7913	523	18.5849	5.5396	1798.4839	523	18.5849	5.5396	387.4862	523	18.5849	5.5396	1918.2056
524	18.6109	5.532	382.3027	524	18.6109	5.532	1795.1064	524	18.6109	5.532	393.8358	524	18.6109	5.532	1922.4319
525	18.6369	5.5243	371.2702	525	18.6369	5.5243	1780.1849	525	18.6369	5.5243	355.6906	525	18.6369	5.5243	1882.1633
526	18.6629	5.5167	348.8319	526	18.6629	5.5167	1753.8577	526	18.6629	5.5167	304.9476	526	18.6629	5.5167	1829.297
527	18.6889	5.5091	406.9904	527	18.6889	5.5091	1808.1273	527	18.6889	5.5091	341.8456	527	18.6889	5.5091	1864.0716
528	18.7149	5.5015	359.9083	528	18.7149	5.5015	1757.1562	528	18.7149	5.5015	413.1768	528	18.7149	5.5015	1933.2795
529	18.7409	5.4939	408.3285	529	18.7409	5.4939	1801.6875	529	18.7409	5.4939	444.1972	529	18.7409	5.4939	1962.1765
530	18.7669	5.4864	382.2058	530	18.7669	5.4864	1771.6758	530	18.7669	5.4864	405.8287	530	18.7669	5.4864	1921.6847
531	18.7929	5.4789	357.56	531	18.7929	5.4789	1743.141	531	18.7929	5.4789	406.6087	531	18.7929	5.4789	1920.3413
532	18.8189	5.4713	298.0756	532	18.8189	5.4713	1679.7677	532	18.8189	5.4713	356.3523	532	18.8189	5.4713	1867.9615
533	18.8449	5.4639	329.9693	533	18.8449	5.4639	1707.7725	533	18.8449	5.4639	323.8086	533	18.8449	5.4639	1833.2945
534	18.8709	5.4564	363.757	534	18.8709	5.4564	1737.6713	534	18.8709	5.4564	348.3828	534	18.8709	5.4564	1855.7453
535	18.8969	5.449	327.7805	535	18.8969	5.449	1697.8058	535	18.8969	5.449	322.477	535	18.8969	5.449	1827.7162

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
536	18.9229	5.4415	341.9097	536	18.9229	5.4415	1708.0461	536	18.9229	5.4415	267.7729	536	18.9229	5.4415	1770.8887
537	18.9489	5.4342	369.659	537	18.9489	5.4342	1731.9064	537	18.9489	5.4342	325.6258	537	18.9489	5.4342	1826.6183
538	18.9749	5.4268	365.207	538	18.9749	5.4268	1723.5654	538	18.9749	5.4268	393.0304	538	18.9749	5.4268	1891.8995
539	19.0009	5.4194	353.927	539	19.0009	5.4194	1708.3965	539	19.0009	5.4194	358.6333	539	19.0009	5.4194	1855.3791
540	19.0269	5.4121	355.3751	540	19.0269	5.4121	1705.9557	540	19.0269	5.4121	328.5106	540	19.0269	5.4121	1823.133
541	19.0529	5.4048	345.5432	541	19.0529	5.4048	1692.2349	541	19.0529	5.4048	324.2911	541	19.0529	5.4048	1816.7902
542	19.0789	5.3975	391.1725	542	19.0789	5.3975	1735.8273	542	19.0789	5.3975	304.7127	542	19.0789	5.3975	1794.1427
543	19.1049	5.3902	371.7463	543	19.1049	5.3902	1714.3643	543	19.1049	5.3902	318.6575	543	19.1049	5.3902	1805.0183
544	19.1309	5.3829	395.0676	544	19.1309	5.3829	1735.6488	544	19.1309	5.3829	324.6887	544	19.1309	5.3829	1807.9805
545	19.1569	5.3757	461.7739	545	19.1569	5.3757	1800.3182	545	19.1569	5.3757	336.4364	545	19.1569	5.3757	1816.6591
546	19.1829	5.3685	441.8433	546	19.1829	5.3685	1778.3508	546	19.1829	5.3685	355.1775	546	19.1829	5.3685	1832.3312
547	19.2089	5.3613	422.1009	547	19.2089	5.3613	1756.5716	547	19.2089	5.3613	335.1238	547	19.2089	5.3613	1809.2083
548	19.2349	5.3541	431.2837	548	19.2349	5.3541	1763.7175	548	19.2349	5.3541	390.5478	548	19.2349	5.3541	1861.5632
549	19.2609	5.3469	367.6555	549	19.2609	5.3469	1698.0525	549	19.2609	5.3469	390.2327	549	19.2609	5.3469	1858.179
550	19.2869	5.3398	334.2196	550	19.2869	5.3398	1662.5798	550	19.2869	5.3398	389.467	550	19.2869	5.3398	1854.3443
551	19.3129	5.3327	364.3306	551	19.3129	5.3327	1690.654	551	19.3129	5.3327	446.3586	551	19.3129	5.3327	1908.1668
552	19.3389	5.3256	389.3698	552	19.3389	5.3256	1713.6563	552	19.3389	5.3256	411.3151	552	19.3389	5.3256	1870.0542
553	19.3649	5.3185	436.83	553	19.3649	5.3185	1759.0797	553	19.3649	5.3185	358.0095	553	19.3649	5.3185	1813.6795
554	19.3909	5.3114	413.3083	554	19.3909	5.3114	1733.5212	554	19.3909	5.3114	365.1715	554	19.3909	5.3114	1817.7724
555	19.4169	5.3044	386.9886	555	19.4169	5.3044	1705.1647	555	19.4169	5.3044	331.6845	555	19.4169	5.3044	1781.2164
556	19.4429	5.2974	398.1082	556	19.4429	5.2974	1714.2474	556	19.4429	5.2974	363.4927	556	19.4429	5.2974	1809.9554
557	19.4689	5.2904	427.3189	557	19.4689	5.2904	1741.4213	557	19.4689	5.2904	359.0454	557	19.4689	5.2904	1802.4391
558	19.4949	5.2834	447.6443	558	19.4949	5.2834	1759.7099	558	19.4949	5.2834	277.3548	558	19.4949	5.2834	1717.6794
559	19.5209	5.2764	415.0445	559	19.5209	5.2764	1725.0733	559	19.5209	5.2764	334.0073	559	19.5209	5.2764	1771.2628
560	19.5469	5.2694	401.498	560	19.5469	5.2694	1709.49	560	19.5469	5.2694	342.3888	560	19.5469	5.2694	1776.5752
561	19.5729	5.2625	385.1578	561	19.5729	5.2625	1691.113	561	19.5729	5.2625	330.6778	561	19.5729	5.2625	1761.7951
562	19.5989	5.2556	371.7731	562	19.5989	5.2556	1675.6914	562	19.5989	5.2556	383.8815	562	19.5989	5.2556	1811.9297
563	19.6249	5.2487	356.8132	563	19.6249	5.2487	1658.6947	563	19.6249	5.2487	345.5508	563	19.6249	5.2487	1770.5299
564	19.6509	5.2418	343.7779	564	19.6509	5.2418	1643.6225	564	19.6509	5.2418	336.6037	564	19.6509	5.2418	1758.5137
565	19.6769	5.235	338.5567	565	19.6769	5.235	1636.3646	565	19.6769	5.235	368.583	565	19.6769	5.235	1787.424
566	19.7029	5.2281	367.8046	566	19.7029	5.2281	1663.5756	566	19.7029	5.2281	332.0171	566	19.7029	5.2281	1747.789
567	19.7289	5.2213	399.5286	567	19.7289	5.2213	1693.2628	567	19.7289	5.2213	306.6977	567	19.7289	5.2213	1719.4004
568	19.7549	5.2145	410.141	568	19.7549	5.2145	1701.8383	568	19.7549	5.2145	324.2911	568	19.7549	5.2145	1733.9248
569	19.7809	5.2077	361.3505	569	19.7809	5.2077	1651.011	569	19.7809	5.2077	385.3386	569	19.7809	5.2077	1791.6469
570	19.8069	5.201	399.3377	570	19.8069	5.201	1686.9614	570	19.8069	5.201	389.6196	570	19.8069	5.201	1792.6025
571	19.8329	5.1942	423.1656	571	19.8329	5.1942	1708.7525	571	19.8329	5.1942	365.5224	571	19.8329	5.1942	1765.1799

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
572	19.8589	5.1875	398.4748	572	19.8589	5.1875	1682.0249	572	19.8589	5.1875	355.9898	572	19.8589	5.1875	1752.3219
573	19.8849	5.1808	387.6108	573	19.8849	5.1808	1669.1241	573	19.8849	5.1808	355.8867	573	19.8849	5.1808	1748.8934
574	19.9109	5.1741	344.3063	574	19.9109	5.1741	1623.7827	574	19.9109	5.1741	353.165	574	19.9109	5.1741	1742.8463
575	19.9369	5.1674	385.8709	575	19.9369	5.1674	1663.3105	575	19.9369	5.1674	339.9605	575	19.9369	5.1674	1726.3164
576	19.9629	5.1607	398.4089	576	19.9629	5.1607	1673.8117	576	19.9629	5.1607	373.6121	576	19.9629	5.1607	1756.6425
577	19.9889	5.1541	369.118	577	19.9889	5.1541	1642.4839	577	19.9889	5.1541	362.4674	577	19.9889	5.1541	1742.1725
578	20.0149	5.1474	348.085	578	20.0149	5.1474	1619.4141	578	20.0149	5.1474	360.9351	578	20.0149	5.1474	1737.3147
579	20.0409	5.1408	384.9321	579	20.0409	5.1408	1654.2244	579	20.0409	5.1408	394.5807	579	20.0409	5.1408	1767.6349
580	20.0669	5.1342	351.5495	580	20.0669	5.1342	1618.8049	580	20.0669	5.1342	360.881	580	20.0669	5.1342	1730.6098
581	20.0929	5.1277	359.8208	581	20.0929	5.1277	1625.0394	581	20.0929	5.1277	377.4106	581	20.0929	5.1277	1743.8141
582	20.1189	5.1211	358.4048	582	20.1189	5.1211	1621.5866	582	20.1189	5.1211	370.2165	582	20.1189	5.1211	1733.2946
583	20.1449	5.1146	362.3235	583	20.1449	5.1146	1623.4685	583	20.1449	5.1146	361.3374	583	20.1449	5.1146	1721.0901
584	20.1709	5.108	361.2692	584	20.1709	5.108	1620.3773	584	20.1709	5.108	350.8113	584	20.1709	5.108	1707.2385
585	20.1969	5.1015	412.1583	585	20.1969	5.1015	1669.2296	585	20.1969	5.1015	418.0399	585	20.1969	5.1015	1771.1417
586	20.2229	5.095	317.847	586	20.2229	5.095	1572.8816	586	20.2229	5.095	364.0686	586	20.2229	5.095	1713.845
587	20.2489	5.0886	295.0498	587	20.2489	5.0886	1548.0474	587	20.2489	5.0886	290.5899	587	20.2489	5.0886	1637.0409
588	20.2749	5.0821	393.1656	588	20.2749	5.0821	1644.1265	588	20.2749	5.0821	317.0991	588	20.2749	5.0821	1660.2248
589	20.3009	5.0757	348.9649	589	20.3009	5.0757	1597.8889	589	20.3009	5.0757	388.691	589	20.3009	5.0757	1728.4912
590	20.3269	5.0692	425.8627	590	20.3269	5.0692	1672.7499	590	20.3269	5.0692	380.9886	590	20.3269	5.0692	1717.4634
591	20.3529	5.0628	326.4629	591	20.3529	5.0628	1571.3133	591	20.3529	5.0628	297.5602	591	20.3529	5.0628	1630.7097
592	20.3789	5.0564	386.5653	592	20.3789	5.0564	1629.3788	592	20.3789	5.0564	370.5738	592	20.3789	5.0564	1700.3978
593	20.4049	5.0501	437.387	593	20.4049	5.0501	1678.1638	593	20.4049	5.0501	309.3995	593	20.4049	5.0501	1635.8981
594	20.4309	5.0437	361.3581	594	20.4309	5.0437	1600.098	594	20.4309	5.0437	344.8992	594	20.4309	5.0437	1668.0724
595	20.4569	5.0374	345.5432	595	20.4569	5.0374	1582.2463	595	20.4569	5.0374	426.7763	595	20.4569	5.0374	1746.6241
596	20.4829	5.031	375.0956	596	20.4829	5.031	1609.1463	596	20.4829	5.031	322.7706	596	20.4829	5.031	1639.293
597	20.5089	5.0247	303.0604	597	20.5089	5.0247	1534.4587	597	20.5089	5.0247	373.2999	597	20.5089	5.0247	1686.4969
598	20.5349	5.0184	392.3511	598	20.5349	5.0184	1621.0971	598	20.5349	5.0184	351.1979	598	20.5349	5.0184	1661.0695
599	20.5609	5.0122	363.2962	599	20.5609	5.0122	1589.3899	599	20.5609	5.0122	371.7743	599	20.5609	5.0122	1678.3205
600	20.5869	5.0059	412.0319	600	20.5869	5.0059	1635.4732	600	20.5869	5.0059	426.2228	600	20.5869	5.0059	1729.4436
601	20.6129	4.9997	385.4344	601	20.6129	4.9997	1606.2234	601	20.6129	4.9997	272.669	601	20.6129	4.9997	1572.5643
602	20.6389	4.9934	313.3958	602	20.6389	4.9934	1531.5324	602	20.6389	4.9934	329.1274	602	20.6389	4.9934	1625.6973
603	20.6649	4.9872	382.5693	603	20.6649	4.9872	1598.0536	603	20.6649	4.9872	348.5595	603	20.6649	4.9872	1641.804
604	20.6909	4.981	387.2355	604	20.6909	4.981	1600.0674	604	20.6909	4.981	272.536	604	20.6909	4.981	1562.4552
605	20.7169	4.9748	394.3267	605	20.7169	4.9748	1604.5063	605	20.7169	4.9748	302.9611	605	20.7169	4.9748	1589.5548
606	20.7429	4.9687	469.2547	606	20.7429	4.9687	1676.7819	606	20.7429	4.9687	385.4927	606	20.7429	4.9687	1668.761
607	20.7689	4.9625	386.2482	607	20.7689	4.9625	1591.1231	607	20.7689	4.9625	481.8436	607	20.7689	4.9625	1761.7865

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
608	20.7949	4.9564	339.8962	608	20.7949	4.9564	1542.1187	608	20.7949	4.9564	405.2775	608	20.7949	4.9564	1681.895
609	20.8209	4.9503	381.0869	609	20.8209	4.9503	1580.6571	609	20.8209	4.9503	401.8716	609	20.8209	4.9503	1675.1638
610	20.8469	4.9441	413.8019	610	20.8469	4.9441	1610.7197	610	20.8469	4.9441	384.9295	610	20.8469	4.9441	1654.8962
611	20.8729	4.9381	344.7846	611	20.8729	4.9381	1539.0501	611	20.8729	4.9381	343.7782	611	20.8729	4.9381	1610.4195
612	20.8989	4.932	341.5119	612	20.8989	4.932	1533.125	612	20.8989	4.932	330.6219	612	20.8989	4.932	1593.9378
613	20.9249	4.9259	325.4881	613	20.9249	4.9259	1514.4489	613	20.9249	4.9259	397.9385	613	20.9249	4.9259	1657.929
614	20.9509	4.9199	377.1614	614	20.9509	4.9199	1563.4699	614	20.9509	4.9199	421.017	614	20.9509	4.9199	1677.6822
615	20.9769	4.9138	405.2213	615	20.9769	4.9138	1588.8774	615	20.9769	4.9138	402.9675	615	20.9769	4.9138	1656.3072
616	21.0029	4.9078	432.441	616	21.0029	4.9078	1613.4448	616	21.0029	4.9078	372.563	616	21.0029	4.9078	1622.5773
617	21.0289	4.9018	414.564	617	21.0289	4.9018	1592.9154	617	21.0289	4.9018	431.7982	617	21.0289	4.9018	1678.4871
618	21.0549	4.8958	359.8683	618	21.0549	4.8958	1535.5674	618	21.0549	4.8958	369.767	618	21.0549	4.8958	1613.1305
619	21.0809	4.8899	377.5219	619	21.0809	4.8899	1550.5686	619	21.0809	4.8899	359.4898	619	21.0809	4.8899	1599.5279
620	21.1069	4.8839	363.0112	620	21.1069	4.8839	1533.4056	620	21.1069	4.8839	394.037	620	21.1069	4.8839	1630.7497
621	21.1329	4.878	326.6345	621	21.1329	4.878	1494.3765	621	21.1329	4.878	330.5175	621	21.1329	4.878	1563.9048
622	21.1589	4.8721	345.5432	622	21.1589	4.8721	1510.6329	622	21.1589	4.8721	324.2911	622	21.1589	4.8721	1554.353
623	21.1849	4.8661	428.3841	623	21.1849	4.8661	1591.2067	623	21.1849	4.8661	382.0841	623	21.1849	4.8661	1610.4984
624	21.2109	4.8602	394.8845	624	21.2109	4.8602	1555.4401	624	21.2109	4.8602	366.5888	624	21.2109	4.8602	1593.3556
625	21.2369	4.8544	377.6266	625	21.2369	4.8544	1535.9151	625	21.2369	4.8544	340.0516	625	21.2369	4.8544	1565.1708
626	21.2629	4.8485	391.5542	626	21.2629	4.8485	1547.5756	626	21.2629	4.8485	344.5141	626	21.2629	4.8485	1567.9857
627	21.2889	4.8426	414.5958	627	21.2889	4.8426	1568.3502	627	21.2889	4.8426	403.3811	627	21.2889	4.8426	1625.2051
628	21.3149	4.8368	446.4318	628	21.3149	4.8368	1597.9191	628	21.3149	4.8368	350.5172	628	21.3149	4.8368	1570.6937
629	21.3409	4.831	371.9806	629	21.3409	4.831	1521.2008	629	21.3409	4.831	363.9919	629	21.3409	4.831	1582.5208
630	21.3669	4.8252	401.4094	630	21.3669	4.8252	1548.3626	630	21.3669	4.8252	428.2401	630	21.3669	4.8252	1645.1215
631	21.3929	4.8194	412.8244	631	21.3929	4.8194	1557.5104	631	21.3929	4.8194	386.8498	631	21.3929	4.8194	1602.0835
632	21.4189	4.8136	402.2345	632	21.4189	4.8136	1544.6535	632	21.4189	4.8136	346.9818	632	21.4189	4.8136	1560.568
633	21.4449	4.8078	411.0556	633	21.4449	4.8078	1551.2076	633	21.4449	4.8078	350.5398	633	21.4449	4.8078	1562.4784
634	21.4709	4.8021	394.1011	634	21.4709	4.8021	1531.986	634	21.4709	4.8021	393.826	634	21.4709	4.8021	1604.117
635	21.4969	4.7963	376.0339	635	21.4969	4.7963	1511.6517	635	21.4969	4.7963	367.8005	635	21.4969	4.7963	1576.444
636	21.5229	4.7906	375.7473	636	21.5229	4.7906	1509.098	636	21.5229	4.7906	348.5074	636	21.5229	4.7906	1555.5033
637	21.5489	4.7849	305.8376	637	21.5489	4.7849	1436.9213	637	21.5489	4.7849	338.3103	637	21.5489	4.7849	1543.6587
638	21.5749	4.7792	387.3008	638	21.5749	4.7792	1516.1174	638	21.5749	4.7792	306.0808	638	21.5749	4.7792	1509.7815
639	21.6009	4.7735	366.7882	639	21.6009	4.7735	1493.3378	639	21.6009	4.7735	333.4519	639	21.6009	4.7735	1535.5051
640	21.6269	4.7678	369.3179	640	21.6269	4.7678	1493.6003	640	21.6269	4.7678	328.2082	640	21.6269	4.7678	1528.6138
641	21.6529	4.7622	405.9284	641	21.6529	4.7622	1527.9439	641	21.6529	4.7622	359.774	641	21.6529	4.7622	1558.5321
642	21.6789	4.7565	410.4934	642	21.6789	4.7565	1530.2417	642	21.6789	4.7565	319.6289	642	21.6789	4.7565	1516.7393
643	21.7049	4.7509	376.7645	643	21.7049	4.7509	1494.2458	643	21.7049	4.7509	326.7396	643	21.7049	4.7509	1522.2025

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
644	21.7309	4.7453	412.4829	644	21.7309	4.7453	1527.6971	644	21.7309	4.7453	368.6838	644	21.7309	4.7453	1562.4991
645	21.7569	4.7397	414.1105	645	21.7569	4.7397	1527.0576	645	21.7569	4.7397	336.5191	645	21.7569	4.7397	1528.6869
646	21.7829	4.7341	395.3199	646	21.7829	4.7341	1506	646	21.7829	4.7341	308.0793	646	21.7829	4.7341	1498.5995
647	21.8089	4.7285	381.6516	647	21.8089	4.7285	1490.0646	647	21.8089	4.7285	344.7197	647	21.8089	4.7285	1533.5923
648	21.8349	4.723	353.7049	648	21.8349	4.723	1459.8509	648	21.8349	4.723	404.8507	648	21.8349	4.723	1592.0758
649	21.8609	4.7174	345.5432	649	21.8609	4.7174	1449.4221	649	21.8609	4.7174	406.4676	649	21.8609	4.7174	1592.0451
650	21.8869	4.7119	405.0635	650	21.8869	4.7119	1506.3619	650	21.8869	4.7119	348.5981	650	21.8869	4.7119	1532.528
651	21.9129	4.7064	370.4582	651	21.9129	4.7064	1469.1761	651	21.9129	4.7064	336.435	651	21.9129	4.7064	1518.7173
652	21.9389	4.7008	308.4032	652	21.9389	4.7008	1404.5406	652	21.9389	4.7008	346.8782	652	21.9389	4.7008	1527.5129
653	21.9649	4.6954	338.5071	653	21.9649	4.6954	1432.0639	653	21.9649	4.6954	314.8875	653	21.9649	4.6954	1493.8747
654	21.9909	4.6899	356.6917	654	21.9909	4.6899	1447.6681	654	21.9909	4.6899	316.656	654	21.9909	4.6899	1493.9957
655	22.0169	4.6844	365.9071	655	22.0169	4.6844	1454.303	655	22.0169	4.6844	338.7538	655	22.0169	4.6844	1514.4459
656	22.0429	4.6789	407.2296	656	22.0429	4.6789	1493.0449	656	22.0429	4.6789	324.4313	656	22.0429	4.6789	1498.4757
657	22.0689	4.6735	379.7758	657	22.0689	4.6735	1463.0107	657	22.0689	4.6735	356.7909	657	22.0689	4.6735	1529.1878
658	22.0949	4.6681	341.2204	658	22.0949	4.6681	1421.8748	658	22.0949	4.6681	370.0958	658	22.0949	4.6681	1540.8452
659	22.1209	4.6626	409.9238	659	22.1209	4.6626	1487.9977	659	22.1209	4.6626	329.2447	659	22.1209	4.6626	1498.3464
660	22.1469	4.6572	439.8341	660	22.1469	4.6572	1515.3274	660	22.1469	4.6572	336.076	660	22.1469	4.6572	1503.5302
661	22.1729	4.6519	384.3638	661	22.1729	4.6519	1457.2766	661	22.1729	4.6519	349.3882	661	22.1729	4.6519	1515.1949
662	22.1989	4.6465	344.1922	662	22.1989	4.6465	1414.5245	662	22.1989	4.6465	356.7855	662	22.1989	4.6465	1520.9446
663	22.2249	4.6411	328.3652	663	22.2249	4.6411	1396.117	663	22.2249	4.6411	383.589	663	22.2249	4.6411	1546.1005
664	22.2509	4.6357	316.5552	664	22.2509	4.6357	1381.7266	664	22.2509	4.6357	347.8094	664	22.2509	4.6357	1508.6733
665	22.2769	4.6304	352.5081	665	22.2769	4.6304	1415.0989	665	22.2769	4.6304	294.6563	665	22.2769	4.6304	1453.8727
666	22.3029	4.6251	405.726	666	22.3029	4.6251	1465.7363	666	22.3029	4.6251	328.4229	666	22.3029	4.6251	1485.9916
667	22.3289	4.6198	390.2712	667	22.3289	4.6198	1447.701	667	22.3289	4.6198	310.6252	667	22.3289	4.6198	1466.5464
668	22.3549	4.6145	397.4778	668	22.3549	4.6145	1452.3272	668	22.3549	4.6145	308.4907	668	22.3549	4.6145	1462.7644
669	22.3809	4.6092	379.7391	669	22.3809	4.6092	1432.0079	669	22.3809	4.6092	335.3324	669	22.3809	4.6092	1487.9585
670	22.4069	4.6039	360.7415	670	22.4069	4.6039	1410.4298	670	22.4069	4.6039	323.6414	670	22.4069	4.6039	1474.6199
671	22.4329	4.5986	392.6078	671	22.4329	4.5986	1439.7156	671	22.4329	4.5986	340.4707	671	22.4329	4.5986	1489.8016
672	22.4589	4.5934	410.2599	672	22.4589	4.5934	1454.7872	672	22.4589	4.5934	340.5253	672	22.4589	4.5934	1488.2086
673	22.4849	4.5881	382.352	673	22.4849	4.5881	1424.2988	673	22.4849	4.5881	337.5318	673	22.4849	4.5881	1483.5675
674	22.5109	4.5829	400.1546	674	22.5109	4.5829	1439.5209	674	22.5109	4.5829	371.8611	674	22.5109	4.5829	1516.2493
675	22.5369	4.5777	382.1553	675	22.5369	4.5777	1418.9411	675	22.5369	4.5777	327.2554	675	22.5369	4.5777	1469.996
676	22.5629	4.5725	385.6639	676	22.5629	4.5725	1419.8692	676	22.5629	4.5725	324.2911	676	22.5629	4.5725	1465.3842
677	22.5889	4.5673	410.6325	677	22.5889	4.5673	1442.2573	677	22.5889	4.5673	275.7305	677	22.5889	4.5673	1414.2386
678	22.6149	4.5621	375.5426	678	22.6149	4.5621	1404.5869	678	22.6149	4.5621	319.7508	678	22.6149	4.5621	1455.6739
679	22.6409	4.5569	429.0834	679	22.6409	4.5569	1455.5472	679	22.6409	4.5569	354.8452	679	22.6409	4.5569	1488.1833

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
680	22.6669	4.5518	411.1017	680	22.6669	4.5518	1434.985	680	22.6669	4.5518	331.7725	680	22.6669	4.5518	1462.5255
681	22.6929	4.5466	438.9159	681	22.6929	4.5466	1460.2187	681	22.6929	4.5466	324.9598	681	22.6929	4.5466	1453.1278
682	22.7189	4.5415	426.7189	682	22.7189	4.5415	1445.4412	682	22.7189	4.5415	294.4452	682	22.7189	4.5415	1420.0283
683	22.7449	4.5363	414.2171	683	22.7449	4.5363	1430.3589	683	22.7449	4.5363	291.2059	683	22.7449	4.5363	1414.204
684	22.7709	4.5312	419.7158	684	22.7709	4.5312	1433.2771	684	22.7709	4.5312	295.5175	684	22.7709	4.5312	1415.9306
685	22.7969	4.5261	387.645	685	22.7969	4.5261	1398.6258	685	22.7969	4.5261	339.5823	685	22.7969	4.5261	1457.4104
686	22.8229	4.521	443.6737	686	22.8229	4.521	1452.074	686	22.8229	4.521	361.2602	686	22.8229	4.521	1476.5033
687	22.8489	4.516	411.5074	687	22.8489	4.516	1417.3272	687	22.8489	4.516	376.9702	687	22.8489	4.516	1489.6283
688	22.8749	4.5109	404.2623	688	22.8749	4.5109	1407.5016	688	22.8749	4.5109	322.9755	688	22.8749	4.5109	1433.0486
689	22.9009	4.5059	428.7393	689	22.9009	4.5059	1429.3981	689	22.9009	4.5059	306.8077	689	22.9009	4.5059	1414.2958
690	22.9269	4.5008	419.7394	690	22.9269	4.5008	1417.8177	690	22.9269	4.5008	323.4615	690	22.9269	4.5008	1428.3646
691	22.9529	4.4958	425.2733	691	22.9529	4.4958	1420.7711	691	22.9529	4.4958	318.9108	691	22.9529	4.4958	1421.2289
692	22.9789	4.4908	418.2088	692	22.9789	4.4908	1411.1261	692	22.9789	4.4908	329.8475	692	22.9789	4.4908	1429.5807
693	23.0049	4.4858	402.1917	693	23.0049	4.4858	1392.5285	693	23.0049	4.4858	340.5141	693	23.0049	4.4858	1437.6623
694	23.0309	4.4808	395.2437	694	23.0309	4.4808	1383	694	23.0309	4.4808	327.1296	694	23.0309	4.4808	1421.6928
695	23.0569	4.4758	395.2039	695	23.0569	4.4758	1380.3796	695	23.0569	4.4758	284.4019	695	23.0569	4.4758	1376.38
696	23.0829	4.4708	374.5965	696	23.0829	4.4708	1357.1918	696	23.0829	4.4708	336.7108	696	23.0829	4.4708	1426.104
697	23.1089	4.4658	358.0658	697	23.1089	4.4658	1338.0806	697	23.1089	4.4658	339.6273	697	23.1089	4.4658	1426.4355
698	23.1349	4.4609	406.6201	698	23.1349	4.4609	1384.0543	698	23.1349	4.4609	335.2619	698	23.1349	4.4609	1419.4851
699	23.1609	4.456	381.6006	699	23.1609	4.456	1356.4544	699	23.1609	4.456	321.5103	699	23.1609	4.456	1403.1485
700	23.1869	4.451	433.5523	700	23.1869	4.451	1405.8255	700	23.1869	4.451	329.2913	700	23.1869	4.451	1408.3445
701	23.2129	4.4461	351.5292	701	23.2129	4.4461	1321.2219	701	23.2129	4.4461	379.0631	701	23.2129	4.4461	1455.5313
702	23.2389	4.4412	440.2181	702	23.2389	4.4412	1407.3303	702	23.2389	4.4412	354.5158	702	23.2389	4.4412	1428.399
703	23.2649	4.4363	345.5432	703	23.2649	4.4363	1310.075	703	23.2649	4.4363	324.2911	703	23.2649	4.4363	1395.5893
704	23.2909	4.4314	431.0561	704	23.2909	4.4314	1394.8178	704	23.2909	4.4314	368.9365	704	23.2909	4.4314	1439.803
705	23.3169	4.4265	384.2876	705	23.3169	4.4265	1347.2794	705	23.3169	4.4265	360.9917	705	23.3169	4.4265	1431.4265
706	23.3429	4.4217	336.9265	706	23.3429	4.4217	1299.1483	706	23.3429	4.4217	323.3126	706	23.3429	4.4217	1393.3157
707	23.3689	4.4168	368.3889	707	23.3689	4.4168	1329.8407	707	23.3689	4.4168	389.0895	707	23.3689	4.4168	1458.6609
708	23.3949	4.412	463.8723	708	23.3949	4.412	1424.5542	708	23.3949	4.412	355.3874	708	23.3949	4.412	1424.5271
709	23.4209	4.4072	439.7626	709	23.4209	4.4072	1399.6745	709	23.4209	4.4072	363.0921	709	23.4209	4.4072	1431.8001
710	23.4469	4.4023	352.0345	710	23.4469	4.4023	1311.1764	710	23.4469	4.4023	401.3624	710	23.4469	4.4023	1469.6387
711	23.4729	4.3975	430.8177	711	23.4729	4.3975	1389.1896	711	23.4729	4.3975	313.3692	711	23.4729	4.3975	1381.2138
712	23.4989	4.3927	426.8908	712	23.4989	4.3927	1384.4928	712	23.4989	4.3927	367.2474	712	23.4989	4.3927	1434.6602
713	23.5249	4.388	469.2578	713	23.5249	4.388	1426.0897	713	23.5249	4.388	384.1134	713	23.5249	4.388	1451.0946
714	23.5509	4.3832	447.952	714	23.5509	4.3832	1404.0141	714	23.5509	4.3832	326.2246	714	23.5509	4.3832	1392.7741
715	23.5769	4.3784	375.3003	715	23.5769	4.3784	1330.5923	715	23.5769	4.3784	407.9376	715	23.5769	4.3784	1474.0554

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
716	23.6029	4.3737	445.5451	716	23.6029	4.3737	1400.0671	716	23.6029	4.3737	430.8029	716	23.6029	4.3737	1496.489
717	23.6289	4.3689	473.0563	717	23.6289	4.3689	1426.8084	717	23.6289	4.3689	377.216	717	23.6289	4.3689	1442.4704
718	23.6549	4.3642	387.4463	718	23.6549	4.3642	1340.4284	718	23.6549	4.3642	307.4057	718	23.6549	4.3642	1372.2284
719	23.6809	4.3595	385.5458	719	23.6809	4.3595	1337.7579	719	23.6809	4.3595	359.163	719	23.6809	4.3595	1423.554
720	23.7069	4.3547	311.3611	720	23.7069	4.3547	1262.8033	720	23.7069	4.3547	332.54	720	23.7069	4.3547	1396.4993
721	23.7329	4.35	430.4321	721	23.7329	4.35	1381.1043	721	23.7329	4.35	332.6081	721	23.7329	4.35	1396.1357
722	23.7589	4.3453	422.6408	722	23.7589	4.3453	1372.543	722	23.7589	4.3453	323.7518	722	23.7589	4.3453	1386.8477
723	23.7849	4.3407	413.6873	723	23.7849	4.3407	1362.8195	723	23.7849	4.3407	259.628	723	23.7849	4.3407	1322.2921
724	23.8109	4.336	372.3286	724	23.8109	4.336	1320.6909	724	23.8109	4.336	262.6388	724	23.8109	4.336	1324.8713
725	23.8369	4.3313	380.7329	725	23.8369	4.3313	1328.3252	725	23.8369	4.3313	267.0155	725	23.8369	4.3313	1328.8163
726	23.8629	4.3267	354.5369	726	23.8629	4.3267	1301.3592	726	23.8629	4.3267	324.8809	726	23.8629	4.3267	1386.25
727	23.8889	4.322	396.529	727	23.8889	4.322	1342.5814	727	23.8889	4.322	319.9486	727	23.8889	4.322	1380.886
728	23.9149	4.3174	443.5369	728	23.9149	4.3174	1388.8192	728	23.9149	4.3174	340.6621	728	23.9149	4.3174	1401.1678
729	23.9409	4.3128	475.2316	729	23.9409	4.3128	1419.744	729	23.9409	4.3128	331.618	729	23.9409	4.3128	1391.692
730	23.9669	4.3082	406.3594	730	23.9669	4.3082	1350.1018	730	23.9669	4.3082	324.2911	730	23.9669	4.3082	1383.9334
731	23.9929	4.3036	356.0287	731	23.9929	4.3036	1299.0011	731	23.9929	4.3036	359.1317	731	23.9929	4.3036	1416.296
732	24.0189	4.299	426.212	732	24.0189	4.299	1368.4144	732	24.0189	4.299	394.7178	732	24.0189	4.299	1449.4041
733	24.0449	4.2944	414.5128	733	24.0449	4.2944	1355.9453	733	24.0449	4.2944	392.2647	733	24.0449	4.2944	1444.473
734	24.0709	4.2898	447.136	734	24.0709	4.2898	1387.7985	734	24.0709	4.2898	318.3007	734	24.0709	4.2898	1368.031
735	24.0969	4.2853	390.5356	735	24.0969	4.2853	1330.4281	735	24.0969	4.2853	297.3329	735	24.0969	4.2853	1344.5852
736	24.1229	4.2807	374.6056	736	24.1229	4.2807	1313.7281	736	24.1229	4.2807	294.8616	736	24.1229	4.2807	1339.636
737	24.1489	4.2762	398.0773	737	24.1489	4.2762	1336.4298	737	24.1489	4.2762	339.324	737	24.1489	4.2762	1381.6203
738	24.1749	4.2717	405.0429	738	24.1749	4.2717	1342.6255	738	24.1749	4.2717	352.9344	738	24.1749	4.2717	1392.7528
739	24.2009	4.2671	405.8648	739	24.2009	4.2671	1342.6773	739	24.2009	4.2671	345.5635	739	24.2009	4.2671	1382.9039
740	24.2269	4.2626	380.9278	740	24.2269	4.2626	1316.9704	740	24.2269	4.2626	323.78	740	24.2269	4.2626	1358.6424
741	24.2529	4.2581	360.1798	741	24.2529	4.2581	1295.4525	741	24.2529	4.2581	322.1907	741	24.2529	4.2581	1354.575
742	24.2789	4.2536	414.7797	742	24.2789	4.2536	1349.2823	742	24.2789	4.2536	352.7017	742	24.2789	4.2536	1382.6081
743	24.3049	4.2492	375.8495	743	24.3049	4.2492	1309.5822	743	24.3049	4.2492	390.8897	743	24.3049	4.2492	1418.3181
744	24.3309	4.2447	437.1029	744	24.3309	4.2447	1370.0656	744	24.3309	4.2447	471.3342	744	24.3309	4.2447	1496.2846
745	24.3569	4.2402	405.1351	745	24.3569	4.2402	1337.3278	745	24.3569	4.2402	422.3267	745	24.3569	4.2402	1444.7991
746	24.3829	4.2358	358.3035	746	24.3829	4.2358	1289.7263	746	24.3829	4.2358	371.4372	746	24.3829	4.2358	1391.4316
747	24.4089	4.2313	370.729	747	24.4089	4.2313	1301.3817	747	24.4089	4.2313	379.0714	747	24.4089	4.2313	1396.5878
748	24.4349	4.2269	323.369	748	24.4349	4.2269	1253.2518	748	24.4349	4.2269	415.1281	748	24.4349	4.2269	1430.1665
749	24.4609	4.2225	311.0122	749	24.4609	4.2225	1240.125	749	24.4609	4.2225	341.7365	749	24.4609	4.2225	1354.2968
750	24.4869	4.218	314.4521	750	24.4869	4.218	1242.7949	750	24.4869	4.218	301.3277	750	24.4869	4.218	1311.4101
751	24.5129	4.2136	325.6418	751	24.5129	4.2136	1253.2147	751	24.5129	4.2136	342.144	751	24.5129	4.2136	1349.7484

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
752	24.5389	4.2092	388.1625	752	24.5389	4.2092	1314.9654	752	24.5389	4.2092	321.6819	752	24.5389	4.2092	1326.8084
753	24.5649	4.2049	423.8134	753	24.5649	4.2049	1349.8463	753	24.5649	4.2049	281.4291	753	24.5649	4.2049	1284.0775
754	24.5909	4.2005	363.015	754	24.5909	4.2005	1288.278	754	24.5909	4.2005	310.8826	754	24.5909	4.2005	1311.053
755	24.6169	4.1961	353.5501	755	24.6169	4.1961	1278.0431	755	24.6169	4.1961	322.9338	755	24.6169	4.1961	1320.6262
756	24.6429	4.1918	368.3349	756	24.6429	4.1918	1292.0579	756	24.6429	4.1918	318.0456	756	24.6429	4.1918	1313.2601
757	24.6689	4.1874	345.5432	757	24.6689	4.1874	1268.4962	757	24.6689	4.1874	324.2911	757	24.6689	4.1874	1317.0276
758	24.6949	4.1831	352.4889	758	24.6949	4.1831	1273.9106	758	24.6949	4.1831	327.9908	758	24.6949	4.1831	1318.7094
759	24.7209	4.1787	377.7445	759	24.7209	4.1787	1297.635	759	24.7209	4.1787	294.4512	759	24.7209	4.1787	1283.152
760	24.7469	4.1744	389.3853	760	24.7469	4.1744	1307.7445	760	24.7469	4.1744	289.7461	760	24.7469	4.1744	1276.429
761	24.7729	4.1701	359.3507	761	24.7729	4.1701	1276.1786	761	24.7729	4.1701	321.382	761	24.7729	4.1701	1306.0471
762	24.7989	4.1658	331.5171	762	24.7989	4.1658	1246.8138	762	24.7989	4.1658	299.0475	762	24.7989	4.1658	1281.6948
763	24.8249	4.1615	342.6815	763	24.8249	4.1615	1256.4469	763	24.8249	4.1615	294.2686	763	24.8249	4.1615	1274.8981
764	24.8509	4.1572	375.0638	764	24.8509	4.1572	1287.2979	764	24.8509	4.1572	297.1257	764	24.8509	4.1572	1275.7373
765	24.8769	4.1529	388.8133	765	24.8769	4.1529	1299.5162	765	24.8769	4.1529	333.7616	765	24.8769	4.1529	1310.3554
766	24.9029	4.1487	362.301	766	24.9029	4.1487	1271.4726	766	24.9029	4.1487	339.9989	766	24.9029	4.1487	1314.5749
767	24.9289	4.1444	331.1444	767	24.9289	4.1444	1238.7848	767	24.9289	4.1444	333.8199	767	24.9289	4.1444	1306.3781
768	24.9549	4.1402	348.774	768	24.9549	4.1402	1254.8832	768	24.9549	4.1402	340.8628	768	24.9549	4.1402	1311.4031
769	24.9809	4.1359	338.5879	769	24.9809	4.1359	1243.1658	769	24.9809	4.1359	331.0176	769	24.9809	4.1359	1299.5401
770	25.0069	4.1317	352.2481	770	25.0069	4.1317	1255.2947	770	25.0069	4.1317	400.7061	770	25.0069	4.1317	1367.2108
771	25.0329	4.1275	374.7732	771	25.0329	4.1275	1276.2886	771	25.0329	4.1275	405.015	771	25.0329	4.1275	1369.5018
772	25.0589	4.1233	337.4173	772	25.0589	4.1233	1237.4014	772	25.0589	4.1233	326.38	772	25.0589	4.1233	1288.849
773	25.0849	4.119	341.4668	773	25.0849	4.119	1239.9196	773	25.0849	4.119	309.3696	773	25.0849	4.119	1269.8208
774	25.1109	4.1148	367.4183	774	25.1109	4.1148	1264.3399	774	25.1109	4.1148	263.2072	774	25.1109	4.1148	1221.6405
775	25.1369	4.1107	371.7716	775	25.1369	4.1107	1267.1619	775	25.1369	4.1107	293.635	775	25.1369	4.1107	1250.0505
776	25.1629	4.1065	382.4511	776	25.1629	4.1065	1276.3102	776	25.1629	4.1065	338.0876	776	25.1629	4.1065	1292.4853
777	25.1889	4.1023	388.8764	777	25.1889	4.1023	1281.2042	777	25.1889	4.1023	307.0015	777	25.1889	4.1023	1259.3813
778	25.2149	4.0982	384.8134	778	25.2149	4.0982	1275.6099	778	25.2149	4.0982	281.3184	778	25.2149	4.0982	1231.6804
779	25.2409	4.094	344.2474	779	25.2409	4.094	1233.5127	779	25.2409	4.094	307.633	779	25.2409	4.094	1255.9772
780	25.2669	4.0899	314.7875	780	25.2669	4.0899	1202.5215	780	25.2669	4.0899	299.3744	780	25.2669	4.0899	1245.7007
781	25.2929	4.0857	269.5307	781	25.2929	4.0857	1155.7335	781	25.2929	4.0857	345.1515	781	25.2929	4.0857	1289.46
782	25.3189	4.0816	311.3947	782	25.3189	4.0816	1196.0662	782	25.3189	4.0816	286.4917	782	25.3189	4.0816	1228.7824
783	25.3449	4.0775	376.1921	783	25.3449	4.0775	1259.3324	783	25.3449	4.0775	317.7079	783	25.3449	4.0775	1257.9808
784	25.3709	4.0734	345.5432	784	25.3709	4.0734	1227.1523	784	25.3709	4.0734	324.2911	784	25.3709	4.0734	1262.5462
785	25.3969	4.0693	326.5545	785	25.3969	4.0693	1207.2443	785	25.3969	4.0693	375.5391	785	25.3969	4.0693	1312.2801
786	25.4229	4.0652	316.1283	786	25.4229	4.0652	1195.899	786	25.4229	4.0652	286.3231	786	25.4229	4.0652	1221.55
787	25.4489	4.0611	340.0337	787	25.4489	4.0611	1218.8852	787	25.4489	4.0611	321.4559	787	25.4489	4.0611	1255.1687

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
788	25.4749	4.057	395.2745	788	25.4749	4.057	1273.2068	788	25.4749	4.057	303.0508	788	25.4749	4.057	1235.2496
789	25.5009	4.0529	357.8995	789	25.5009	4.0529	1234.9126	789	25.5009	4.0529	318.6777	789	25.5009	4.0529	1249.3625
790	25.5269	4.0489	350.6511	790	25.5269	4.0489	1226.7451	790	25.5269	4.0489	317.3752	790	25.5269	4.0489	1246.5459
791	25.5529	4.0448	332.7588	791	25.5529	4.0448	1207.9336	791	25.5529	4.0448	298.6345	791	25.5529	4.0448	1226.2911
792	25.5789	4.0408	327.8926	792	25.5789	4.0408	1202.1483	792	25.5789	4.0408	315.3396	792	25.5789	4.0408	1241.4821
793	25.6049	4.0367	367.9705	793	25.6049	4.0367	1241.307	793	25.6049	4.0367	362.1068	793	25.6049	4.0367	1286.7353
794	25.6309	4.0327	270.9279	794	25.6309	4.0327	1143.3452	794	25.6309	4.0327	349.0958	794	25.6309	4.0327	1272.2103
795	25.6569	4.0287	339.1001	795	25.6569	4.0287	1210.5982	795	25.6569	4.0287	349.6591	795	25.6569	4.0287	1271.2595
796	25.6829	4.0247	373.2673	796	25.6829	4.0247	1243.8462	796	25.6829	4.0247	373.9775	796	25.6829	4.0247	1294.0638
797	25.7089	4.0207	324.2664	797	25.7089	4.0207	1193.9261	797	25.7089	4.0207	315.076	797	25.7089	4.0207	1233.6482
798	25.7349	4.0167	379.8241	798	25.7349	4.0167	1248.5647	798	25.7349	4.0167	337.6435	798	25.7349	4.0167	1254.7017
799	25.7609	4.0127	321.5251	799	25.7609	4.0127	1189.3466	799	25.7609	4.0127	321.4585	799	25.7609	4.0127	1237.0026
800	25.7869	4.0087	368.863	800	25.7869	4.0087	1235.7653	800	25.7869	4.0087	379.1862	800	25.7869	4.0087	1293.2163
801	25.8129	4.0048	340.2088	801	25.8129	4.0048	1206.1918	801	25.8129	4.0048	382.8002	801	25.8129	4.0048	1295.3162
802	25.8389	4.0008	326.1149	802	25.8389	4.0008	1191.1788	802	25.8389	4.0008	372.7442	802	25.8389	4.0008	1283.7462
803	25.8649	3.9969	280.6799	803	25.8649	3.9969	1144.8246	803	25.8649	3.9969	350.9196	803	25.8649	3.9969	1260.4075
804	25.8909	3.9929	388.9925	804	25.8909	3.9929	1252.2181	804	25.8909	3.9929	337.6006	804	25.8909	3.9929	1245.5744
805	25.9169	3.989	339.2335	805	25.9169	3.989	1201.5399	805	25.9169	3.989	296.3604	805	25.9169	3.989	1202.8202
806	25.9429	3.985	448.4158	806	25.9429	3.985	1309.803	806	25.9429	3.985	290.1673	806	25.9429	3.985	1195.113
807	25.9689	3.9811	276.5741	807	25.9689	3.9811	1137.0421	807	25.9689	3.9811	300.75	807	25.9689	3.9811	1204.1816
808	25.9949	3.9772	293.3345	808	25.9949	3.9772	1152.8834	808	25.9949	3.9772	370.5794	808	25.9949	3.9772	1272.497
809	26.0209	3.9733	335.6474	809	26.0209	3.9733	1194.2771	809	26.0209	3.9733	335.2506	809	26.0209	3.9733	1235.6541
810	26.0469	3.9694	403.4443	810	26.0469	3.9694	1261.1548	810	26.0469	3.9694	314.7075	810	26.0469	3.9694	1213.597
811	26.0729	3.9655	345.5432	811	26.0729	3.9655	1202.3346	811	26.0729	3.9655	324.2911	811	26.0729	3.9655	1221.6665
812	26.0989	3.9616	336.9555	812	26.0989	3.9616	1192.3758	812	26.0989	3.9616	342.2033	812	26.0989	3.9616	1238.2014
813	26.1249	3.9578	343.6092	813	26.1249	3.9578	1197.6586	813	26.1249	3.9578	284.021	813	26.1249	3.9578	1178.6417
814	26.1509	3.9539	274.4002	814	26.1509	3.9539	1127.0786	814	26.1509	3.9539	292.0215	814	26.1509	3.9539	1185.2649
815	26.1769	3.95	317.7785	815	26.1769	3.95	1169.0859	815	26.1769	3.95	306.1362	815	26.1769	3.95	1198.0023
816	26.2029	3.9462	349.5502	816	26.2029	3.9462	1199.4866	816	26.2029	3.9462	249.1447	816	26.2029	3.9462	1139.6334
817	26.2289	3.9423	350.7243	817	26.2289	3.9423	1199.2898	817	26.2289	3.9423	294.576	817	26.2289	3.9423	1183.6875
818	26.2549	3.9385	351.8055	818	26.2549	3.9385	1199	818	26.2549	3.9385	316.4551	818	26.2549	3.9385	1204.1893
819	26.2809	3.9347	364.6629	819	26.2809	3.9347	1210.4863	819	26.2809	3.9347	293.1362	819	26.2809	3.9347	1179.4931
820	26.3069	3.9309	310.7608	820	26.3069	3.9309	1155.2132	820	26.3069	3.9309	337.3235	820	26.3069	3.9309	1222.303
821	26.3329	3.927	310.8283	821	26.3329	3.927	1153.9098	821	26.3329	3.927	325.5322	821	26.3329	3.927	1209.1344
822	26.3589	3.9232	361.956	822	26.3589	3.9232	1203.6665	822	26.3589	3.9232	359.6346	822	26.3589	3.9232	1241.8595
823	26.3849	3.9194	320.1841	823	26.3849	3.9194	1160.5236	823	26.3849	3.9194	391.6248	823	26.3849	3.9194	1272.4724

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
824	26.4109	3.9156	292.8505	824	26.4109	3.9156	1131.8191	824	26.4109	3.9156	338.3191	824	26.4109	3.9156	1217.7893
825	26.4369	3.9119	328.3079	825	26.4369	3.9119	1165.9054	825	26.4369	3.9119	331.2032	825	26.4369	3.9119	1209.2961
826	26.4629	3.9081	323.1195	826	26.4629	3.9081	1159.346	826	26.4629	3.9081	412.2529	826	26.4629	3.9081	1288.9685
827	26.4889	3.9043	339.6407	827	26.4889	3.9043	1174.4963	827	26.4889	3.9043	365.7184	827	26.4889	3.9043	1241.0567
828	26.5149	3.9006	373.3146	828	26.5149	3.9006	1206.7992	828	26.5149	3.9006	280.3495	828	26.5149	3.9006	1154.3105
829	26.5409	3.8968	393.6515	829	26.5409	3.8968	1225.7651	829	26.5409	3.8968	362.2434	829	26.5409	3.8968	1234.8271
830	26.5669	3.8931	406.776	830	26.5669	3.8931	1237.5186	830	26.5669	3.8931	366.0122	830	26.5669	3.8931	1237.2186
831	26.5929	3.8893	459.5562	831	26.5929	3.8893	1288.9278	831	26.5929	3.8893	313.5366	831	26.5929	3.8893	1183.3657
832	26.6189	3.8856	497.1274	832	26.6189	3.8856	1325.1281	832	26.6189	3.8856	342.8045	832	26.6189	3.8856	1211.2562
833	26.6449	3.8819	547.0708	833	26.6449	3.8819	1373.7005	833	26.6449	3.8819	345.2665	833	26.6449	3.8819	1212.3409
834	26.6709	3.8782	672.9508	834	26.6709	3.8782	1498.2095	834	26.6709	3.8782	344.5071	834	26.6709	3.8782	1210.2042
835	26.6969	3.8744	869.946	835	26.6969	3.8744	1693.8337	835	26.6969	3.8744	327.8352	835	26.6969	3.8744	1192.155
836	26.7229	3.8707	1052.0138	836	26.7229	3.8707	1874.5306	836	26.7229	3.8707	353.5125	836	26.7229	3.8707	1216.455
837	26.7489	3.8671	1295.0142	837	26.7489	3.8671	2116.16	837	26.7489	3.8671	432.9964	837	26.7489	3.8671	1294.5616
838	26.7749	3.8634	1466.8855	838	26.7749	3.8634	2286.6603	838	26.7749	3.8634	423.5849	838	26.7749	3.8634	1283.7727
839	26.8009	3.8597	1369.2022	839	26.8009	3.8597	2187.606	839	26.8009	3.8597	448.6115	839	26.8009	3.8597	1307.422
840	26.8269	3.856	1161.7999	840	26.8269	3.856	1978.8327	840	26.8269	3.856	477.3443	840	26.8269	3.856	1334.7776
841	26.8529	3.8524	915.7099	841	26.8529	3.8524	1731.3718	841	26.8529	3.8524	430.3874	841	26.8529	3.8524	1286.4433
842	26.8789	3.8487	654.6962	842	26.8789	3.8487	1468.9871	842	26.8789	3.8487	403.3554	842	26.8789	3.8487	1258.0339
843	26.9049	3.845	501.1826	843	26.9049	3.845	1314.1025	843	26.9049	3.845	323.6655	843	26.9049	3.845	1176.9667
844	26.9309	3.8414	435.0402	844	26.9309	3.8414	1246.5891	844	26.9309	3.8414	293.1507	844	26.9309	3.8414	1145.0746
845	26.9569	3.8378	440.3432	845	26.9569	3.8378	1250.5211	845	26.9569	3.8378	298.3254	845	26.9569	3.8378	1148.8721
846	26.9829	3.8341	410.8654	846	26.9829	3.8341	1219.6723	846	26.9829	3.8341	348.315	846	26.9829	3.8341	1197.4843
847	27.0089	3.8305	357.3057	847	27.0089	3.8305	1164.7417	847	27.0089	3.8305	301.2503	847	27.0089	3.8305	1149.0423
848	27.0349	3.8269	308.7609	848	27.0349	3.8269	1114.8258	848	27.0349	3.8269	325.6584	848	27.0349	3.8269	1172.0731
849	27.0609	3.8233	362.7148	849	27.0609	3.8233	1167.4088	849	27.0609	3.8233	338.1217	849	27.0609	3.8233	1183.1591
850	27.0869	3.8197	378.6628	850	27.0869	3.8197	1181.9857	850	27.0869	3.8197	313.6438	850	27.0869	3.8197	1157.3039
851	27.1129	3.8161	361.6709	851	27.1129	3.8161	1163.6229	851	27.1129	3.8161	307.0944	851	27.1129	3.8161	1149.3771
852	27.1389	3.8125	344.8371	852	27.1389	3.8125	1145.4181	852	27.1389	3.8125	322.7836	852	27.1389	3.8125	1163.689
853	27.1649	3.8089	322.5127	853	27.1649	3.8089	1121.7228	853	27.1649	3.8089	342.5643	853	27.1649	3.8089	1182.0924
854	27.1909	3.8053	310.9716	854	27.1909	3.8053	1108.8106	854	27.1909	3.8053	358.2563	854	27.1909	3.8053	1196.4071
855	27.2169	3.8018	345.6409	855	27.2169	3.8018	1142.109	855	27.2169	3.8018	360.6993	855	27.2169	3.8018	1197.4728
856	27.2429	3.7982	351.3343	856	27.2429	3.7982	1146.4314	856	27.2429	3.7982	329.8805	856	27.2429	3.7982	1165.2766
857	27.2689	3.7947	300.5067	857	27.2689	3.7947	1094.2328	857	27.2689	3.7947	320.1115	857	27.2689	3.7947	1154.1304
858	27.2949	3.7911	337.7602	858	27.2949	3.7911	1130.1153	858	27.2949	3.7911	297.0934	858	27.2949	3.7911	1129.7349
859	27.3209	3.7876	375.0889	859	27.3209	3.7876	1166.0731	859	27.3209	3.7876	283.6894	859	27.3209	3.7876	1114.9536

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
860	27.3469	3.7841	323.3981	860	27.3469	3.7841	1113.0112	860	27.3469	3.7841	320.4156	860	27.3469	3.7841	1150.3025
861	27.3729	3.7805	305.2295	861	27.3729	3.7805	1093.4717	861	27.3729	3.7805	334.6894	861	27.3729	3.7805	1163.199
862	27.3989	3.777	321.3012	862	27.3989	3.777	1108.1724	862	27.3989	3.777	319.1606	862	27.3989	3.777	1146.2928
863	27.4249	3.7735	356.7055	863	27.4249	3.7735	1142.2057	863	27.4249	3.7735	305.139	863	27.4249	3.7735	1130.894
864	27.4509	3.77	379.2695	864	27.4509	3.77	1163.3987	864	27.4509	3.77	315.0524	864	27.4509	3.77	1139.43
865	27.4769	3.7665	345.5432	865	27.4769	3.7665	1128.3015	865	27.4769	3.7665	324.2911	865	27.4769	3.7665	1147.2914
866	27.5029	3.763	331.0223	866	27.5029	3.763	1110.7351	866	27.5029	3.763	313.8025	866	27.5029	3.763	1135.8212
867	27.5289	3.7595	337.0681	867	27.5289	3.7595	1113.7356	867	27.5289	3.7595	273.8594	867	27.5289	3.7595	1094.8967
868	27.5549	3.756	374.5306	868	27.5549	3.756	1148.1527	868	27.5549	3.756	262.5551	868	27.5549	3.756	1082.6108
869	27.5809	3.7526	348.1284	869	27.5809	3.7526	1118.7052	869	27.5809	3.7526	284.0663	869	27.5809	3.7526	1103.1404
870	27.6069	3.7491	296.9068	870	27.6069	3.7491	1064.4382	870	27.6069	3.7491	287.7928	870	27.6069	3.7491	1105.8854
871	27.6329	3.7456	328.7478	871	27.6329	3.7456	1093.2338	871	27.6329	3.7456	327.5242	871	27.6329	3.7456	1144.6352
872	27.6589	3.7422	348.8364	872	27.6589	3.7422	1110.2771	872	27.6589	3.7422	298.4625	872	27.6589	3.7422	1114.592
873	27.6849	3.7387	332.5629	873	27.6849	3.7387	1090.9582	873	27.6849	3.7387	304.0297	873	27.6849	3.7387	1119.1776
874	27.7109	3.7353	317.2987	874	27.7109	3.7353	1072.6486	874	27.7109	3.7353	266.4822	874	27.7109	3.7353	1080.6486
875	27.7369	3.7319	344.2567	875	27.7369	3.7319	1096.5612	875	27.7369	3.7319	271.0455	875	27.7369	3.7319	1084.2304
876	27.7629	3.7284	382.0252	876	27.7629	3.7284	1131.2844	876	27.7629	3.7284	270.4869	876	27.7629	3.7284	1082.6903
877	27.7889	3.725	356.6494	877	27.7889	3.725	1102.8632	877	27.7889	3.725	254.9495	877	27.7889	3.725	1066.1713
878	27.8149	3.7216	382.7815	878	27.8149	3.7216	1125.95	878	27.8149	3.7216	321.7488	878	27.8149	3.7216	1131.989
879	27.8409	3.7182	378.9825	879	27.8409	3.7182	1119.1055	879	27.8409	3.7182	381.7007	879	27.8409	3.7182	1190.9594
880	27.8669	3.7148	385.4833	880	27.8669	3.7148	1122.561	880	27.8669	3.7148	316.251	880	27.8669	3.7148	1124.5281
881	27.8929	3.7114	347.0743	881	27.8929	3.7114	1081.1066	881	27.8929	3.7114	285.6088	881	27.8929	3.7114	1092.9044
882	27.9189	3.708	419.1023	882	27.9189	3.708	1150.0893	882	27.9189	3.708	299.326	882	27.9189	3.708	1105.64
883	27.9449	3.7046	400.8508	883	27.9449	3.7046	1128.7924	883	27.9449	3.7046	296.1353	883	27.9449	3.7046	1101.4678
884	27.9709	3.7013	366.8324	884	27.9709	3.7013	1091.7286	884	27.9709	3.7013	305.0589	884	27.9709	3.7013	1109.4098
885	27.9969	3.6979	341.9602	885	27.9969	3.6979	1063.8111	885	27.9969	3.6979	278.4019	885	27.9969	3.6979	1081.7713
886	28.0229	3.6945	404.4747	886	28.0229	3.6945	1123.2802	886	28.0229	3.6945	283.8626	886	28.0229	3.6945	1086.2505
887	28.0489	3.6912	371.9549	887	28.0489	3.6912	1087.715	887	28.0489	3.6912	313.4096	887	28.0489	3.6912	1114.8159
888	28.0749	3.6878	389.0648	888	28.0749	3.6878	1101.7796	888	28.0749	3.6878	353.9623	888	28.0749	3.6878	1154.3871
889	28.1009	3.6845	403.1725	889	28.1009	3.6845	1112.8419	889	28.1009	3.6845	368.5258	889	28.1009	3.6845	1167.9691
890	28.1269	3.6811	379.4219	890	28.1269	3.6811	1086.0459	890	28.1269	3.6811	372.5699	890	28.1269	3.6811	1171.0316
891	28.1529	3.6778	340.0681	891	28.1529	3.6778	1043.6467	891	28.1529	3.6778	312.903	891	28.1529	3.6778	1110.3832
892	28.1789	3.6745	345.5432	892	28.1789	3.6745	1046.0765	892	28.1789	3.6745	324.2911	892	28.1789	3.6745	1120.7897
893	28.2049	3.6712	382.9171	893	28.2049	3.6712	1082.6521	893	28.2049	3.6712	292.7517	893	28.2049	3.6712	1086.2082
894	28.2309	3.6679	320.8755	894	28.2309	3.6679	1019.8121	894	28.2309	3.6679	297.2946	894	28.2309	3.6679	1087.709
895	28.2569	3.6645	339.3353	895	28.2569	3.6645	1037.4735	895	28.2569	3.6645	361.8818	895	28.2569	3.6645	1149.254

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
896	28.2829	3.6612	386.8879	896	28.2829	3.6612	1084.2278	896	28.2829	3.6612	293.8654	896	28.2829	3.6612	1078.1955
897	28.3089	3.658	402.798	897	28.3089	3.658	1099.3396	897	28.3089	3.658	305.9313	897	28.3089	3.658	1087.2193
898	28.3349	3.6547	336.4473	898	28.3349	3.6547	1032.1905	898	28.3349	3.6547	308.8598	898	28.3349	3.6547	1087.1056
899	28.3609	3.6514	370.2748	899	28.3609	3.6514	1065.2197	899	28.3609	3.6514	297.6694	899	28.3609	3.6514	1072.873
900	28.3869	3.6481	409.5411	900	28.3869	3.6481	1103.6876	900	28.3869	3.6481	327.3629	900	28.3869	3.6481	1099.5244
901	28.4129	3.6448	358.7635	901	28.4129	3.6448	1052.1117	901	28.4129	3.6448	300.412	901	28.4129	3.6448	1069.5313
902	28.4389	3.6416	334.8702	902	28.4389	3.6416	1027.4201	902	28.4389	3.6416	285.9032	902	28.4389	3.6416	1051.9805
903	28.4649	3.6383	345.254	903	28.4649	3.6383	1037.0055	903	28.4649	3.6383	320.7163	903	28.4649	3.6383	1083.7514
904	28.4909	3.6351	401.199	904	28.4909	3.6351	1092.1522	904	28.4909	3.6351	336.7216	904	28.4909	3.6351	1096.7146
905	28.5169	3.6318	358.2384	905	28.5169	3.6318	1048.3932	905	28.5169	3.6318	308.1115	905	28.5169	3.6318	1065.0623
906	28.5429	3.6286	371.3996	906	28.5429	3.6286	1060.7561	906	28.5429	3.6286	283.0629	906	28.5429	3.6286	1036.9715
907	28.5689	3.6253	360.3586	907	28.5689	3.6253	1048.9168	907	28.5689	3.6253	381.0919	907	28.5689	3.6253	1131.9584
908	28.5949	3.6221	353.2512	908	28.5949	3.6221	1041.0111	908	28.5949	3.6221	380.142	908	28.5949	3.6221	1127.9664
909	28.6209	3.6189	376.8214	909	28.6209	3.6189	1063.7828	909	28.6209	3.6189	313.8787	909	28.6209	3.6189	1058.6609
910	28.6469	3.6157	447.462	910	28.6469	3.6157	1133.6252	910	28.6469	3.6157	338.8145	910	28.6469	3.6157	1080.5546
911	28.6729	3.6125	373.9195	911	28.6729	3.6125	1059.2843	911	28.6729	3.6125	348.1263	911	28.6729	3.6125	1086.8243
912	28.6989	3.6093	325.3548	912	28.6989	3.6093	1009.9212	912	28.6989	3.6093	295.6183	912	28.6989	3.6093	1031.2741
913	28.7249	3.6061	394.5962	913	28.7249	3.6061	1078.3643	913	28.7249	3.6061	342.028	913	28.7249	3.6061	1074.6417
914	28.7509	3.6029	343.5144	914	28.7509	3.6029	1026.4841	914	28.7509	3.6029	331.4323	914	28.7509	3.6029	1061.0039
915	28.7769	3.5997	353.8629	915	28.7769	3.5997	1036.0343	915	28.7769	3.5997	357.6772	915	28.7769	3.5997	1084.2066
916	28.8029	3.5965	353.7847	916	28.8029	3.5965	1035.1578	916	28.8029	3.5965	329.353	916	28.8029	3.5965	1052.8403
917	28.8289	3.5933	389.9613	917	28.8289	3.5933	1070.536	917	28.8289	3.5933	355.0679	917	28.8289	3.5933	1075.513
918	28.8549	3.5902	360.8771	918	28.8549	3.5902	1040.6535	918	28.8549	3.5902	329.9542	918	28.8549	3.5902	1047.3572
919	28.8809	3.587	345.5432	919	28.8809	3.587	1024.5213	919	28.8809	3.587	324.2911	919	28.8809	3.587	1038.652
920	28.9069	3.5838	366.7181	920	28.9069	3.5838	1045.9167	920	28.9069	3.5838	415.1092	920	28.9069	3.5838	1128.7856
921	28.9329	3.5807	373.0668	921	28.9329	3.5807	1052.486	921	28.9329	3.5807	328.6581	921	28.9329	3.5807	1041.65
922	28.9589	3.5775	371.6371	922	28.9589	3.5775	1051.2769	922	28.9589	3.5775	385.3412	922	28.9589	3.5775	1097.6486
923	28.9849	3.5744	394.9857	923	28.9849	3.5744	1074.8461	923	28.9849	3.5744	366.7177	923	28.9849	3.5744	1078.3407
924	29.0109	3.5713	345.0487	924	29.0109	3.5713	1025.1297	924	29.0109	3.5713	356.1694	924	29.0109	3.5713	1067.1079
925	29.0369	3.5681	369.6342	925	29.0369	3.5681	1049.9357	925	29.0369	3.5681	359.0732	925	29.0369	3.5681	1069.3272
926	29.0629	3.565	390.4499	926	29.0629	3.565	1070.9719	926	29.0629	3.565	361.2523	926	29.0629	3.565	1070.8219
927	29.0889	3.5619	394.0693	927	29.0889	3.5619	1074.812	927	29.0889	3.5619	418.1399	927	29.0889	3.5619	1127.025
928	29.1149	3.5588	332.2801	928	29.1149	3.5588	1013.2433	928	29.1149	3.5588	396.5098	928	29.1149	3.5588	1104.7105
929	29.1409	3.5557	369.0956	929	29.1409	3.5557	1050.2794	929	29.1409	3.5557	386.1075	929	29.1409	3.5557	1093.6237
930	29.1669	3.5526	377.1203	930	29.1669	3.5526	1058.5247	930	29.1669	3.5526	347.0588	930	29.1669	3.5526	1053.8905
931	29.1929	3.5495	395.454	931	29.1929	3.5495	1077.079	931	29.1929	3.5495	381.6443	931	29.1929	3.5495	1087.7915

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
932	29.2189	3.5464	374.4724	932	29.2189	3.5464	1056.3179	932	29.2189	3.5464	372.6669	932	29.2189	3.5464	1078.1296
933	29.2449	3.5433	368.1912	933	29.2449	3.5433	1050.2573	933	29.2449	3.5433	360.2023	933	29.2449	3.5433	1064.9806
934	29.2709	3.5402	382.8208	934	29.2709	3.5402	1065.1075	934	29.2709	3.5402	387.1212	934	29.2709	3.5402	1091.215
935	29.2969	3.5372	354.5267	935	29.2969	3.5372	1037.034	935	29.2969	3.5372	365.3572	935	29.2969	3.5372	1068.7665
936	29.3229	3.5341	338.6589	936	29.3229	3.5341	1021.3867	936	29.3229	3.5341	378.8454	936	29.3229	3.5341	1081.5703
937	29.3489	3.531	339.9025	937	29.3489	3.531	1022.8509	937	29.3489	3.531	355.4611	937	29.3489	3.531	1057.5015
938	29.3749	3.528	364.0238	938	29.3749	3.528	1047.1928	938	29.3749	3.528	327.885	938	29.3749	3.528	1029.241
939	29.4009	3.5249	347.9735	939	29.4009	3.5249	1031.3631	939	29.4009	3.5249	311.9352	939	29.4009	3.5249	1012.6067
940	29.4269	3.5219	350.7322	940	29.4269	3.5219	1034.3423	940	29.4269	3.5219	355.1377	940	29.4269	3.5219	1055.1247
941	29.4529	3.5188	376.0146	941	29.4529	3.5188	1059.8453	941	29.4529	3.5188	333.9495	941	29.4529	3.5188	1033.2521
942	29.4789	3.5158	358.4238	942	29.4789	3.5158	1042.4751	942	29.4789	3.5158	329.96	942	29.4789	3.5158	1028.5781
943	29.5049	3.5128	367.5902	943	29.5049	3.5128	1051.862	943	29.5049	3.5128	316.2044	943	29.5049	3.5128	1014.138
944	29.5309	3.5097	380.1509	944	29.5309	3.5097	1064.6433	944	29.5309	3.5097	330.482	944	29.5309	3.5097	1027.7311
945	29.5569	3.5067	384.0871	945	29.5569	3.5067	1068.8001	945	29.5569	3.5067	367.6028	945	29.5569	3.5067	1064.1675
946	29.5829	3.5037	345.5432	946	29.5829	3.5037	1030.4768	946	29.5829	3.5037	359.9231	946	29.5829	3.5037	1055.8033
947	29.6089	3.5007	331.8659	947	29.6089	3.5007	1017.6567	947	29.6089	3.5007	333.6935	947	29.6089	3.5007	1028.8892
948	29.6349	3.4977	351.0273	948	29.6349	3.4977	1037.6754	948	29.6349	3.4977	352.0467	948	29.6349	3.4977	1046.5579
949	29.6609	3.4947	344.8403	949	29.6609	3.4947	1032.3457	949	29.6609	3.4947	349.9885	949	29.6609	3.4947	1043.8153
950	29.6869	3.4917	312.4551	950	29.6869	3.4917	1000.8177	950	29.6869	3.4917	350.8675	950	29.6869	3.4917	1044.0099
951	29.7129	3.4887	338.8168	951	29.7129	3.4887	1028.0367	951	29.7129	3.4887	324.8175	951	29.7129	3.4887	1017.2754
952	29.7389	3.4857	325.3748	952	29.7389	3.4857	1015.4519	952	29.7389	3.4857	332.0606	952	29.7389	3.4857	1023.834
953	29.7649	3.4828	316.6565	953	29.7649	3.4828	1007.5909	953	29.7649	3.4828	335.644	953	29.7649	3.4828	1026.7329
954	29.7909	3.4798	358.4265	954	29.7909	3.4798	1050.2182	954	29.7909	3.4798	318.6837	954	29.7909	3.4798	1009.0881
955	29.8169	3.4768	337.4276	955	29.8169	3.4768	1030.0766	955	29.8169	3.4768	367.8179	955	29.8169	3.4768	1057.5378
956	29.8429	3.4739	336.519	956	29.8429	3.4739	1030.0253	956	29.8429	3.4739	352.8255	956	29.8429	3.4739	1041.861
957	29.8689	3.4709	354.8365	957	29.8689	3.4709	1049.1999	957	29.8689	3.4709	309.8776	957	29.8689	3.4709	998.2286
958	29.8949	3.468	322.0915	958	29.8949	3.468	1017.3123	958	29.8949	3.468	328.4208	958	29.8949	3.468	1016.0873
959	29.9209	3.465	283.1109	959	29.9209	3.465	979.1889	959	29.9209	3.465	304.4068	959	29.9209	3.465	991.3889
960	29.9469	3.4621	284.4456	960	29.9469	3.4621	981.3809	960	29.9469	3.4621	331.7211	960	29.9469	3.4621	1018.0187
961	29.9729	3.4592	295.1901	961	29.9729	3.4592	992.9826	961	29.9729	3.4592	374.6569	961	29.9729	3.4592	1060.27
962	29.9989	3.4562	310.3721	962	29.9989	3.4562	1009.0219	962	29.9989	3.4562	347.6773	962	29.9989	3.4562	1032.606
963	30.0249	3.4533	328.5788	963	30.0249	3.4533	1028.0859	963	30.0249	3.4533	355.8509	963	30.0249	3.4533	1040.0951
964	30.0509	3.4504	314.1908	964	30.0509	3.4504	1014.5552	964	30.0509	3.4504	325.626	964	30.0509	3.4504	1009.1858
965	30.0769	3.4475	310.6038	965	30.0769	3.4475	1011.8255	965	30.0769	3.4475	301.959	965	30.0769	3.4475	984.8342
966	30.1029	3.4446	313.2959	966	30.1029	3.4446	1015.3748	966	30.1029	3.4446	333.2843	966	30.1029	3.4446	1015.4752
967	30.1289	3.4417	329.3652	967	30.1289	3.4417	1032.3013	967	30.1289	3.4417	331.0594	967	30.1289	3.4417	1012.5657

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
968	30.1549	3.4388	330.4832	968	30.1549	3.4388	1034.2766	968	30.1549	3.4388	336.1524	968	30.1549	3.4388	1016.9743
969	30.1809	3.4359	282.546	969	30.1809	3.4359	987.1967	969	30.1809	3.4359	324.3773	969	30.1809	3.4359	1004.5147
970	30.2069	3.433	238.8127	970	30.2069	3.433	944.3207	970	30.2069	3.433	308.6206	970	30.2069	3.433	988.0735
971	30.2329	3.4301	258.6438	971	30.2329	3.4301	965.009	971	30.2329	3.4301	334.0094	971	30.2329	3.4301	1012.7778
972	30.2589	3.4272	303.8411	972	30.2589	3.4272	1011.0636	972	30.2589	3.4272	369.5869	972	30.2589	3.4272	1047.6709
973	30.2849	3.4243	345.5432	973	30.2849	3.4243	1053.623	973	30.2849	3.4243	324.2911	973	30.2849	3.4243	1001.6907
974	30.3109	3.4215	307.5294	974	30.3109	3.4215	1014.3371	974	30.3109	3.4215	302.2866	974	30.3109	3.4215	979.2295
975	30.3369	3.4186	277.1569	975	30.3369	3.4186	982.6926	975	30.3369	3.4186	347.1568	975	30.3369	3.4186	1023.6431
976	30.3629	3.4157	278.5695	976	30.3629	3.4157	982.8332	976	30.3629	3.4157	345.8568	976	30.3629	3.4157	1021.8865
977	30.3889	3.4129	272.9044	977	30.3889	3.4129	975.8961	977	30.3889	3.4129	350.4259	977	30.3889	3.4129	1025.999
978	30.4149	3.41	299.8461	978	30.4149	3.41	1001.5658	978	30.4149	3.41	331.4592	978	30.4149	3.41	1006.5757
979	30.4409	3.4072	304.5685	979	30.4409	3.4072	1005.0161	979	30.4409	3.4072	330.068	979	30.4409	3.4072	1004.7279
980	30.4669	3.4044	262.6751	980	30.4669	3.4044	961.8506	980	30.4669	3.4044	345.6347	980	30.4669	3.4044	1019.838
981	30.4929	3.4015	274.0172	981	30.4929	3.4015	971.9207	981	30.4929	3.4015	317.6425	981	30.4929	3.4015	991.3892
982	30.5189	3.3987	321.7907	982	30.5189	3.3987	1018.4222	982	30.5189	3.3987	354.4241	982	30.5189	3.3987	1027.7142
983	30.5449	3.3959	290.254	983	30.5449	3.3959	985.6136	983	30.5449	3.3959	368.456	983	30.5449	3.3959	1041.2895
984	30.5709	3.3931	297.7673	984	30.5709	3.3931	991.8548	984	30.5709	3.3931	325.4641	984	30.5709	3.3931	997.841
985	30.5969	3.3902	288.2983	985	30.5969	3.3902	981.1138	985	30.5969	3.3902	348.4388	985	30.5969	3.3902	1020.3591
986	30.6229	3.3874	321.8319	986	30.6229	3.3874	1013.3753	986	30.6229	3.3874	331.7535	986	30.6229	3.3874	1003.2172
987	30.6489	3.3846	306.3962	987	30.6489	3.3846	996.6676	987	30.6489	3.3846	380.162	987	30.6489	3.3846	1051.169
988	30.6749	3.3818	294.8944	988	30.6749	3.3818	983.8938	988	30.6749	3.3818	350.7509	988	30.6749	3.3818	1021.3014
989	30.7009	3.379	308.4533	989	30.7009	3.379	996.1806	989	30.7009	3.379	384.1513	989	30.7009	3.379	1054.2452
990	30.7269	3.3762	314.9184	990	30.7269	3.3762	1001.3737	990	30.7269	3.3762	371.6811	990	30.7269	3.3762	1041.3183
991	30.7529	3.3735	317.6397	991	30.7529	3.3735	1002.8231	991	30.7529	3.3735	363.9347	991	30.7529	3.3735	1033.1153
992	30.7789	3.3707	317.0866	992	30.7789	3.3707	1000.998	992	30.7789	3.3707	357.2698	992	30.7789	3.3707	1025.9939
993	30.8049	3.3679	316.3453	993	30.8049	3.3679	998.9846	993	30.8049	3.3679	343.3609	993	30.8049	3.3679	1011.6283
994	30.8309	3.3651	335.5459	994	30.8309	3.3651	1016.9131	994	30.8309	3.3651	335.1218	994	30.8309	3.3651	1002.9326
995	30.8569	3.3624	350.5123	995	30.8569	3.3624	1030.6076	995	30.8569	3.3624	277.174	995	30.8569	3.3624	944.5283
996	30.8829	3.3596	372.5056	996	30.8829	3.3596	1051.3288	996	30.8829	3.3596	359.0147	996	30.8829	3.3596	1025.9123
997	30.9089	3.3568	401.3357	997	30.9089	3.3568	1078.8869	997	30.9089	3.3568	414.337	997	30.9089	3.3568	1080.778
998	30.9349	3.3541	384.4639	998	30.9349	3.3541	1060.743	998	30.9349	3.3541	374.2491	998	30.9349	3.3541	1040.2335
999	30.9609	3.3513	364.5541	999	30.9609	3.3513	1039.5612	999	30.9609	3.3513	426.1795	999	30.9609	3.3513	1091.7073
1000	30.9869	3.3486	345.5432	1000	30.9869	3.3486	1019.2784	1000	30.9869	3.3486	419.0215	1000	30.9869	3.3486	1084.0927
1001	31.0129	3.3459	366.4511	1001	31.0129	3.3459	1039.1923	1001	31.0129	3.3459	363.8007	1001	31.0129	3.3459	1028.4153
1002	31.0389	3.3431	322.3205	1002	31.0389	3.3431	994.0678	1002	31.0389	3.3431	310.1131	1002	31.0389	3.3431	974.2711
1003	31.0649	3.3404	322.6844	1003	31.0649	3.3404	993.4377	1003	31.0649	3.3404	315.0508	1003	31.0649	3.3404	978.7522

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1004	31.0909	3.3377	297.5215	1004	31.0909	3.3377	967.2809	1004	31.0909	3.3377	325.3582	1004	31.0909	3.3377	988.603
1005	31.1169	3.3349	286.1355	1005	31.1169	3.3349	954.9009	1005	31.1169	3.3349	278.7441	1005	31.1169	3.3349	941.5323
1006	31.1429	3.3322	334.1327	1006	31.1429	3.3322	1001.9043	1006	31.1429	3.3322	292.3875	1006	31.1429	3.3322	954.719
1007	31.1689	3.3295	297.2224	1007	31.1689	3.3295	964	1007	31.1689	3.3295	284.3608	1007	31.1689	3.3295	946.2358
1008	31.1949	3.3268	298.2163	1008	31.1949	3.3268	964	1008	31.1949	3.3268	351.07	1008	31.1949	3.3268	1012.4884
1009	31.2209	3.3241	299.2103	1009	31.2209	3.3241	964	1009	31.2209	3.3241	290.1418	1009	31.2209	3.3241	951.1036
1010	31.2469	3.3214	301.1926	1010	31.2469	3.3214	964.9884	1010	31.2469	3.3214	306.3093	1010	31.2469	3.3214	966.8145
1011	31.2729	3.3187	309.0475	1011	31.2729	3.3187	971.8494	1011	31.2729	3.3187	293.2527	1011	31.2729	3.3187	953.3012
1012	31.2989	3.316	308.2549	1012	31.2989	3.316	970.0629	1012	31.2989	3.316	292.4395	1012	31.2989	3.316	952.0314
1013	31.3249	3.3134	262.2126	1013	31.3249	3.3134	923.0266	1013	31.3249	3.3134	356.1349	1013	31.3249	3.3134	1015.2702
1014	31.3509	3.3107	272.5645	1014	31.3509	3.3107	932.3846	1014	31.3509	3.3107	279.629	1014	31.3509	3.3107	938.3077
1015	31.3769	3.308	258.2144	1015	31.3769	3.308	917.0405	1015	31.3769	3.308	305.8193	1015	31.3769	3.308	964.0415
1016	31.4029	3.3053	244.2347	1016	31.4029	3.3053	902.0669	1016	31.4029	3.3053	350.0337	1016	31.4029	3.3053	1007.7993
1017	31.4289	3.3027	260.7029	1017	31.4289	3.3027	917.5411	1017	31.4289	3.3027	324.2846	1017	31.4289	3.3027	981.5936
1018	31.4549	3.3	327.6967	1018	31.4549	3.3	983.541	1018	31.4549	3.3	359.4178	1018	31.4549	3.3	1016.2702
1019	31.4809	3.2973	288.3961	1019	31.4809	3.2973	943.2465	1019	31.4809	3.2973	339.3284	1019	31.4809	3.2973	995.7241
1020	31.5069	3.2947	293.9246	1020	31.5069	3.2947	947.781	1020	31.5069	3.2947	245.4749	1020	31.5069	3.2947	901.4141
1021	31.5329	3.292	227.5551	1021	31.5329	3.292	880.4176	1021	31.5329	3.292	296.0658	1021	31.5329	3.292	951.5483
1022	31.5589	3.2894	273.0304	1022	31.5589	3.2894	924.899	1022	31.5589	3.2894	300.6274	1022	31.5589	3.2894	955.6533
1023	31.5849	3.2868	334.5498	1023	31.5849	3.2868	985.4244	1023	31.5849	3.2868	370.9029	1023	31.5849	3.2868	1025.4722
1024	31.6109	3.2841	293.1496	1024	31.6109	3.2841	943.0303	1024	31.6109	3.2841	283.4964	1024	31.6109	3.2841	937.6091
1025	31.6369	3.2815	281.7549	1025	31.6369	3.2815	930.6417	1025	31.6369	3.2815	267.1835	1025	31.6369	3.2815	920.8396
1026	31.6629	3.2789	339.353	1026	31.6629	3.2789	987.2459	1026	31.6629	3.2789	299.3272	1026	31.6629	3.2789	952.5267
1027	31.6889	3.2763	345.5432	1027	31.6889	3.2763	992.4422	1027	31.6889	3.2763	324.2911	1027	31.6889	3.2763	977.034
1028	31.7149	3.2736	279.0478	1028	31.7149	3.2736	922.9763	1028	31.7149	3.2736	365.3978	1028	31.7149	3.2736	1016.6314
1029	31.7409	3.271	334.8319	1029	31.7409	3.271	975.79	1029	31.7409	3.271	304.0861	1029	31.7409	3.271	953.8104
1030	31.7669	3.2684	276.8062	1030	31.7669	3.2684	914.7939	1030	31.7669	3.2684	311.4838	1030	31.7669	3.2684	959.6988
1031	31.7929	3.2658	285.5041	1031	31.7929	3.2658	920.5213	1031	31.7929	3.2658	269.3718	1031	31.7929	3.2658	916.0775
1032	31.8189	3.2632	248.2059	1032	31.8189	3.2632	880.2528	1032	31.8189	3.2632	306.091	1032	31.8189	3.2632	951.2874
1033	31.8449	3.2606	276.4537	1033	31.8449	3.2606	905.5301	1033	31.8449	3.2606	279.742	1033	31.8449	3.2606	923.4291
1034	31.8709	3.258	306.8994	1034	31.8709	3.258	933.0054	1034	31.8709	3.258	263.3205	1034	31.8709	3.258	905.4984
1035	31.8969	3.2554	325.9697	1035	31.8969	3.2554	949.1052	1035	31.8969	3.2554	275.9173	1035	31.8969	3.2554	916.5859
1036	31.9229	3.2529	329.1827	1036	31.9229	3.2529	949.3479	1036	31.9229	3.2529	277.4581	1036	31.9229	3.2529	916.6174
1037	31.9489	3.2503	272.4444	1037	31.9489	3.2503	889.6391	1037	31.9489	3.2503	275.1885	1037	31.9489	3.2503	912.8385
1038	31.9749	3.2477	274.0932	1038	31.9749	3.2477	888.3175	1038	31.9749	3.2477	321.3365	1038	31.9749	3.2477	957.4773
1039	32.0009	3.2451	285.0454	1039	32.0009	3.2451	896.2993	1039	32.0009	3.2451	329.4573	1039	32.0009	3.2451	964.0888

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1040	32.0269	3.2426	316.7275	1040	32.0269	3.2426	925.011	1040	32.0269	3.2426	276.1447	1040	32.0269	3.2426	909.2669
1041	32.0529	3.24	294.5613	1041	32.0529	3.24	899.8743	1041	32.0529	3.24	278.5348	1041	32.0529	3.24	910.1477
1042	32.0789	3.2374	270.9357	1042	32.0789	3.2374	873.2784	1042	32.0789	3.2374	297.6053	1042	32.0789	3.2374	927.7089
1043	32.1049	3.2349	332.42	1043	32.1049	3.2349	931.7923	1043	32.1049	3.2349	362.5541	1043	32.1049	3.2349	991.1484
1044	32.1309	3.2323	316.8164	1044	32.1309	3.2323	913.2182	1044	32.1309	3.2323	318.0912	1044	32.1309	3.2323	945.1762
1045	32.1569	3.2298	287.4396	1045	32.1569	3.2298	880.871	1045	32.1569	3.2298	266.884	1045	32.1569	3.2298	892.4597
1046	32.1829	3.2273	313.4184	1046	32.1829	3.2273	903.8794	1046	32.1829	3.2273	291.6001	1046	32.1829	3.2273	915.6666
1047	32.2089	3.2247	292.3687	1047	32.2089	3.2247	879.8592	1047	32.2089	3.2247	269.4382	1047	32.2089	3.2247	891.9954
1048	32.2349	3.2222	308.1614	1048	32.2349	3.2222	892.6816	1048	32.2349	3.2222	263.6815	1048	32.2349	3.2222	884.7294
1049	32.2609	3.2197	313.4	1049	32.2609	3.2197	894.9497	1049	32.2609	3.2197	274.6571	1049	32.2609	3.2197	894.1957
1050	32.2869	3.2171	320.7577	1050	32.2869	3.2171	899.337	1050	32.2869	3.2171	321.1089	1050	32.2869	3.2171	939.1382
1051	32.3129	3.2146	329.9936	1051	32.3129	3.2146	905.6025	1051	32.3129	3.2146	343.4297	1051	32.3129	3.2146	959.9497
1052	32.3389	3.2121	326.6465	1052	32.3389	3.2121	899.285	1052	32.3389	3.2121	319.8391	1052	32.3389	3.2121	934.8499
1053	32.3649	3.2096	337.8817	1053	32.3649	3.2096	907.5497	1053	32.3649	3.2096	293.8931	1053	32.3649	3.2096	907.3945
1054	32.3909	3.2071	345.5432	1054	32.3909	3.2071	912.2409	1054	32.3909	3.2071	324.2911	1054	32.3909	3.2071	936.2833
1055	32.4169	3.2046	337.783	1055	32.4169	3.2046	904.581	1055	32.4169	3.2046	316.8354	1055	32.4169	3.2046	926.7315
1056	32.4429	3.2021	356.5089	1056	32.4429	3.2021	923.4072	1056	32.4429	3.2021	285.8598	1056	32.4429	3.2021	893.6599
1057	32.4689	3.1996	346.722	1057	32.4689	3.1996	913.7206	1057	32.4689	3.1996	294.4723	1057	32.4689	3.1996	900.1765
1058	32.4949	3.1971	341.4351	1058	32.4949	3.1971	908.534	1058	32.4949	3.1971	302.4404	1058	32.4949	3.1971	906.0485
1059	32.5209	3.1946	350.7476	1059	32.5209	3.1946	917.9469	1059	32.5209	3.1946	311.51	1059	32.5209	3.1946	913.0221
1060	32.5469	3.1921	319.0087	1060	32.5469	3.1921	886.3083	1060	32.5469	3.1921	306.2766	1060	32.5469	3.1921	905.6927
1061	32.5729	3.1896	316.4477	1061	32.5729	3.1896	883.8477	1061	32.5729	3.1896	313.0452	1061	32.5729	3.1896	910.3653
1062	32.5989	3.1872	323.2161	1062	32.5989	3.1872	890.7164	1062	32.5989	3.1872	331.4137	1062	32.5989	3.1872	926.6378
1063	32.6249	3.1847	349.6391	1063	32.6249	3.1847	917.2397	1063	32.6249	3.1847	339.6599	1063	32.6249	3.1847	932.788
1064	32.6509	3.1822	360.996	1064	32.6509	3.1822	928.697	1064	32.6509	3.1822	352.8731	1064	32.6509	3.1822	943.9052
1065	32.6769	3.1798	327.0523	1065	32.6769	3.1798	894.8536	1065	32.6769	3.1798	347.653	1065	32.6769	3.1798	936.5891
1066	32.7029	3.1773	329.4432	1066	32.7029	3.1773	897.3448	1066	32.7029	3.1773	336.9962	1066	32.7029	3.1773	923.8362
1067	32.7289	3.1749	321.8036	1067	32.7289	3.1749	889.8055	1067	32.7289	3.1749	346.8269	1067	32.7289	3.1749	931.5709
1068	32.7549	3.1724	343.8272	1068	32.7549	3.1724	911.9295	1068	32.7549	3.1724	351.3775	1068	32.7549	3.1724	934.0255
1069	32.7809	3.17	351.2747	1069	32.7809	3.17	919.4773	1069	32.7809	3.17	309.4476	1069	32.7809	3.17	889.9996
1070	32.8069	3.1675	323.9456	1070	32.8069	3.1675	892.2485	1070	32.8069	3.1675	297.0935	1070	32.8069	3.1675	875.5495
1071	32.8329	3.1651	319.9799	1071	32.8329	3.1651	888.3831	1071	32.8329	3.1651	356.2648	1071	32.8329	3.1651	932.6248
1072	32.8589	3.1626	312.2854	1072	32.8589	3.1626	880.7891	1072	32.8589	3.1626	347.9207	1072	32.8589	3.1626	922.1846
1073	32.8849	3.1602	287.497	1073	32.8849	3.1602	856.1009	1073	32.8849	3.1602	310.2632	1073	32.8849	3.1602	882.4312
1074	32.9109	3.1578	279.9573	1074	32.9109	3.1578	848.6615	1074	32.9109	3.1578	351.6273	1074	32.9109	3.1578	921.6993
1075	32.9369	3.1554	310.1253	1075	32.9369	3.1554	878.9299	1075	32.9369	3.1554	336.468	1075	32.9369	3.1554	904.4439

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1076	32.9629	3.1529	331.0975	1076	32.9629	3.1529	900.0024	1076	32.9629	3.1529	324.4536	1076	32.9629	3.1529	890.3335
1077	32.9889	3.1505	334.4641	1077	32.9889	3.1505	903.4694	1077	32.9889	3.1505	324.6272	1077	32.9889	3.1505	888.4111
1078	33.0149	3.1481	333.364	1078	33.0149	3.1481	902.4697	1078	33.0149	3.1481	320.0573	1078	33.0149	3.1481	881.7452
1079	33.0409	3.1457	334.783	1079	33.0409	3.1457	903.989	1079	33.0409	3.1457	330.04	1079	33.0409	3.1457	889.6319
1080	33.0669	3.1433	308.0353	1080	33.0669	3.1433	877.3415	1080	33.0669	3.1433	345.3379	1080	33.0669	3.1433	902.8338
1081	33.0929	3.1409	345.5432	1081	33.0929	3.1409	914.9499	1081	33.0929	3.1409	324.2911	1081	33.0929	3.1409	879.691
1082	33.1189	3.1385	355.3094	1082	33.1189	3.1385	924.5879	1082	33.1189	3.1385	337.6273	1082	33.1189	3.1385	894.206
1083	33.1449	3.1361	320.9836	1083	33.1449	3.1361	890.1339	1083	33.1449	3.1361	349.1861	1083	33.1449	3.1361	906.9437
1084	33.1709	3.1337	311.3816	1084	33.1709	3.1337	880.4038	1084	33.1709	3.1337	344.047	1084	33.1709	3.1337	902.9834
1085	33.1969	3.1313	334.2212	1085	33.1969	3.1313	903.1153	1085	33.1969	3.1313	328.8942	1085	33.1969	3.1313	889.0094
1086	33.2229	3.129	317.8282	1086	33.2229	3.129	886.5941	1086	33.2229	3.129	319.0117	1086	33.2229	3.129	880.3058
1087	33.2489	3.1266	327.7232	1087	33.2489	3.1266	896.361	1087	33.2489	3.1266	392.8979	1087	33.2489	3.1266	955.3707
1088	33.2749	3.1242	370.1985	1088	33.2749	3.1242	938.7081	1088	33.2749	3.1242	368.5653	1088	33.2749	3.1242	932.217
1089	33.3009	3.1218	348.3231	1089	33.3009	3.1218	916.7046	1089	33.3009	3.1218	377.124	1089	33.3009	3.1218	941.9545
1090	33.3269	3.1195	352.1499	1090	33.3269	3.1195	920.4032	1090	33.3269	3.1195	362.5412	1090	33.3269	3.1195	928.5505
1091	33.3529	3.1171	304.9886	1091	33.3529	3.1171	873.1138	1091	33.3529	3.1171	339.7353	1091	33.3529	3.1171	906.9235
1092	33.3789	3.1147	361.6047	1092	33.3789	3.1147	929.6018	1092	33.3789	3.1147	351.0224	1092	33.3789	3.1147	919.3894
1093	33.4049	3.1124	354.1419	1093	33.4049	3.1124	922.0109	1093	33.4049	3.1124	380.2222	1093	33.4049	3.1124	949.768
1094	33.4309	3.11	343.2168	1094	33.4309	3.11	910.9576	1094	33.4309	3.11	327.7823	1094	33.4309	3.11	898.5069
1095	33.4569	3.1077	316.6229	1095	33.4569	3.1077	884.2355	1095	33.4569	3.1077	312.2474	1095	33.4569	3.1077	884.1508
1096	33.4829	3.1053	354.5962	1096	33.4829	3.1053	922.0807	1096	33.4829	3.1053	366.4598	1096	33.4829	3.1053	939.542
1097	33.5089	3.103	358.89	1097	33.5089	3.103	926.2463	1097	33.5089	3.103	335.2369	1097	33.5089	3.103	909.498
1098	33.5349	3.1007	341.5005	1098	33.5349	3.1007	908.7287	1098	33.5349	3.1007	327.3631	1098	33.5349	3.1007	902.8031
1099	33.5609	3.0983	359.2182	1099	33.5609	3.0983	926.3182	1099	33.5609	3.0983	349.3778	1099	33.5609	3.0983	925.9966
1100	33.5869	3.096	388.396	1100	33.5869	3.096	955.368	1100	33.5869	3.096	299.969	1100	33.5869	3.096	877.7666
1101	33.6129	3.0937	320.0027	1101	33.6129	3.0937	886.8465	1101	33.6129	3.0937	325.8784	1101	33.6129	3.0937	904.8548
1102	33.6389	3.0914	361.7377	1102	33.6389	3.0914	928.4533	1102	33.6389	3.0914	332.4847	1102	33.6389	3.0914	912.64
1103	33.6649	3.089	367.8063	1103	33.6649	3.089	934.3938	1103	33.6649	3.089	317.882	1103	33.6649	3.089	899.216
1104	33.6909	3.0867	376.6047	1104	33.6909	3.0867	943.0641	1104	33.6909	3.0867	358.7544	1104	33.6909	3.0867	941.2673
1105	33.7169	3.0844	426.3793	1105	33.7169	3.0844	992.7105	1105	33.7169	3.0844	294.9035	1105	33.7169	3.0844	878.5953
1106	33.7429	3.0821	378.4741	1106	33.7429	3.0821	944.6772	1106	33.7429	3.0821	307.1337	1106	33.7429	3.0821	892.0043
1107	33.7689	3.0798	369.2505	1107	33.7689	3.0798	935.3254	1107	33.7689	3.0798	332.769	1107	33.7689	3.0798	918.8184
1108	33.7949	3.0775	345.5432	1108	33.7949	3.0775	911.4901	1108	33.7949	3.0775	324.2911	1108	33.7949	3.0775	911.5193
1109	33.8209	3.0752	436.7406	1109	33.8209	3.0752	1002.7011	1109	33.8209	3.0752	295.0041	1109	33.8209	3.0752	882.427
1110	33.8469	3.0729	388.213	1110	33.8469	3.0729	954.1873	1110	33.8469	3.0729	364.1148	1110	33.8469	3.0729	951.7324
1111	33.8729	3.0706	487.6238	1111	33.8729	3.0706	1053.6118	1111	33.8729	3.0706	352.3526	1111	33.8729	3.0706	940.1649

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1112	33.8989	3.0683	543.6729	1112	33.8989	3.0683	1109.6746	1112	33.8989	3.0683	353.9456	1112	33.8989	3.0683	941.9527
1113	33.9249	3.066	571.0776	1113	33.9249	3.066	1137.0931	1113	33.9249	3.066	404.0516	1113	33.9249	3.066	992.2534
1114	33.9509	3.0638	671.4456	1114	33.9509	3.0638	1237.4748	1114	33.9509	3.0638	407.5165	1114	33.9509	3.0638	995.913
1115	33.9769	3.0615	772.5068	1115	33.9769	3.0615	1338.5497	1115	33.9769	3.0615	513.4242	1115	33.9769	3.0615	1102.0154
1116	34.0029	3.0592	817.2823	1116	34.0029	3.0592	1383.339	1116	34.0029	3.0592	520.1507	1116	34.0029	3.0592	1108.9366
1117	34.0289	3.057	1046.0496	1117	34.0289	3.057	1612.12	1117	34.0289	3.057	533.9201	1117	34.0289	3.057	1122.9008
1118	34.0549	3.0547	1329.7876	1118	34.0549	3.0547	1895.8718	1118	34.0549	3.0547	633.8389	1118	34.0549	3.0547	1223.0143
1119	34.0809	3.0524	1758.3692	1119	34.0809	3.0524	2324.4671	1119	34.0809	3.0524	667.1156	1119	34.0809	3.0524	1256.4857
1120	34.1069	3.0502	2320.122	1120	34.1069	3.0502	2886.2337	1120	34.1069	3.0502	795.0088	1120	34.1069	3.0502	1384.5736
1121	34.1329	3.0479	3594.2219	1121	34.1329	3.0479	4160.3473	1121	34.1329	3.0479	1183.5681	1121	34.1329	3.0479	1773.3276
1122	34.1589	3.0457	5774.1079	1122	34.1589	3.0457	6340.2471	1122	34.1589	3.0457	2007.2881	1122	34.1589	3.0457	2597.2424
1123	34.1849	3.0434	9210.0746	1123	34.1849	3.0434	9776.2275	1123	34.1849	3.0434	3710.6093	1123	34.1849	3.0434	4300.7583
1124	34.2109	3.0412	12025.4527	1124	34.2109	3.0412	12591.6193	1124	34.2109	3.0412	4910.5073	1124	34.2109	3.0412	5500.851
1125	34.2369	3.0389	11369.8929	1125	34.2369	3.0389	11936.0732	1125	34.2369	3.0389	6692.1237	1125	34.2369	3.0389	7282.6622
1126	34.2629	3.0367	9455.0441	1126	34.2629	3.0367	10021.2382	1126	34.2629	3.0367	9581.109	1126	34.2629	3.0367	10171.8421
1127	34.2889	3.0345	8016.7366	1127	34.2889	3.0345	8582.9444	1127	34.2889	3.0345	10367.2492	1127	34.2889	3.0345	10958.177
1128	34.3149	3.0322	5892.4542	1128	34.3149	3.0322	6458.6757	1128	34.3149	3.0322	8565.8914	1128	34.3149	3.0322	9157.0139
1129	34.3409	3.03	3634.7748	1129	34.3409	3.03	4201.0101	1129	34.3409	3.03	6461.0706	1129	34.3409	3.03	7052.3878
1130	34.3669	3.0278	2183.834	1130	34.3669	3.0278	2750.083	1130	34.3669	3.0278	4896.9906	1130	34.3669	3.0278	5488.5026
1131	34.3929	3.0256	1420.1758	1131	34.3929	3.0256	1986.4385	1131	34.3929	3.0256	3119.636	1131	34.3929	3.0256	3711.3427
1132	34.4189	3.0233	1014.5745	1132	34.4189	3.0233	1580.8511	1132	34.4189	3.0233	1557.9352	1132	34.4189	3.0233	2149.8366
1133	34.4449	3.0211	844.018	1133	34.4449	3.0211	1410.3083	1133	34.4449	3.0211	847.2972	1133	34.4449	3.0211	1439.3933
1134	34.4709	3.0189	693.6511	1134	34.4709	3.0189	1259.9552	1134	34.4709	3.0189	640.2279	1134	34.4709	3.0189	1232.5188
1135	34.4969	3.0167	582.1146	1135	34.4969	3.0167	1148.4323	1135	34.4969	3.0167	475.8528	1135	34.4969	3.0167	1068.3384
1136	34.5229	3.0145	514.3122	1136	34.5229	3.0145	1078.9699	1136	34.5229	3.0145	500.6557	1136	34.5229	3.0145	1091.6524
1137	34.5489	3.0123	475.241	1137	34.5489	3.0123	1038.2386	1137	34.5489	3.0123	411.4247	1137	34.5489	3.0123	1000.9324
1138	34.5749	3.0101	443.2384	1138	34.5749	3.0101	1004.576	1138	34.5749	3.0101	357.7691	1138	34.5749	3.0101	945.788
1139	34.6009	3.0079	417.6116	1139	34.6009	3.0079	977.2892	1139	34.6009	3.0079	381.3904	1139	34.6009	3.0079	967.9204
1140	34.6269	3.0057	388.9317	1140	34.6269	3.0057	946.9492	1140	34.6269	3.0057	397.4515	1140	34.6269	3.0057	982.4925
1141	34.6529	3.0036	357.9192	1141	34.6529	3.0036	914.2766	1141	34.6529	3.0036	361.1984	1141	34.6529	3.0036	944.7506
1142	34.6789	3.0014	377.8064	1142	34.6789	3.0014	932.5039	1142	34.6789	3.0014	355.7954	1142	34.6789	3.0014	937.8586
1143	34.7049	2.9992	344.8132	1143	34.7049	2.9992	897.8506	1143	34.7049	2.9992	324.9761	1143	34.7049	2.9992	905.5505
1144	34.7309	2.997	360.1753	1144	34.7309	2.997	911.5527	1144	34.7309	2.997	292.7617	1144	34.7309	2.997	871.8471
1145	34.7569	2.9948	370.9003	1145	34.7569	2.9948	920.6176	1145	34.7569	2.9948	332.4751	1145	34.7569	2.9948	910.0717
1146	34.7829	2.9927	347.7735	1146	34.7829	2.9927	895.8307	1146	34.7829	2.9927	353.7805	1146	34.7829	2.9927	929.8882
1147	34.8089	2.9905	351.1838	1147	34.8089	2.9905	897.5811	1147	34.8089	2.9905	317.1543	1147	34.8089	2.9905	891.773

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1148	34.8349	2.9883	342.9271	1148	34.8349	2.9883	887.6643	1148	34.8349	2.9883	294.7745	1148	34.8349	2.9883	867.9043
1149	34.8609	2.9862	363.1648	1149	34.8609	2.9862	906.242	1149	34.8609	2.9862	322.9918	1149	34.8609	2.9862	894.6328
1150	34.8869	2.984	403.9586	1150	34.8869	2.984	945.3757	1150	34.8869	2.984	331.4615	1150	34.8869	2.984	901.6136
1151	34.9129	2.9819	363.2534	1151	34.9129	2.9819	903.0105	1151	34.9129	2.9819	328.873	1151	34.9129	2.9819	897.5362
1152	34.9389	2.9797	341.5479	1152	34.9389	2.9797	879.6449	1152	34.9389	2.9797	332.2463	1152	34.9389	2.9797	899.4206
1153	34.9649	2.9776	345.4507	1153	34.9649	2.9776	881.8877	1153	34.9649	2.9776	325.9109	1153	34.9649	2.9776	891.5963
1154	34.9909	2.9754	306.6472	1154	34.9909	2.9754	841.4242	1154	34.9909	2.9754	313.4096	1154	34.9909	2.9754	877.606
1155	35.0169	2.9733	315.9629	1155	35.0169	2.9733	849.0798	1155	35.0169	2.9733	291.8022	1155	35.0169	2.9733	854.5098
1156	35.0429	2.9712	337.9866	1156	35.0429	2.9712	869.4435	1156	35.0429	2.9712	290.0367	1156	35.0429	2.9712	851.2553
1157	35.0689	2.969	334.2628	1157	35.0689	2.969	864.0597	1157	35.0689	2.969	290.2035	1157	35.0689	2.969	849.9332
1158	35.0949	2.9669	346.2215	1158	35.0949	2.9669	874.3583	1158	35.0949	2.9669	335.7897	1158	35.0949	2.9669	894.0306
1159	35.1209	2.9648	348.8735	1159	35.1209	2.9648	875.3502	1159	35.1209	2.9648	369.9286	1159	35.1209	2.9648	926.6805
1160	35.1469	2.9626	366.1862	1160	35.1469	2.9626	891.0029	1160	35.1469	2.9626	315.2319	1160	35.1469	2.9626	870.4949
1161	35.1729	2.9605	398.6856	1161	35.1729	2.9605	921.8423	1161	35.1729	2.9605	327.6907	1161	35.1729	2.9605	881.4648
1162	35.1989	2.9584	390.7353	1162	35.1989	2.9584	912.2319	1162	35.1989	2.9584	369.7489	1162	35.1989	2.9584	922.0341
1163	35.2249	2.9563	379.2773	1163	35.2249	2.9563	899.1138	1163	35.2249	2.9563	357.2037	1163	35.2249	2.9563	908
1164	35.2509	2.9542	353.7558	1164	35.2509	2.9542	871.9323	1164	35.2509	2.9542	338.4362	1164	35.2509	2.9542	887.7436
1165	35.2769	2.9521	345.6637	1165	35.2769	2.9521	862.1802	1165	35.2769	2.9521	323.8392	1165	35.2769	2.9521	871.6577
1166	35.3029	2.95	373.5708	1166	35.3029	2.95	888.4273	1166	35.3029	2.95	363.7453	1166	35.3029	2.95	910.0749
1167	35.3289	2.9479	358.3587	1167	35.3289	2.9479	871.5551	1167	35.3289	2.9479	384.0738	1167	35.3289	2.9479	928.9145
1168	35.3549	2.9458	342.8431	1168	35.3549	2.9458	854.3795	1168	35.3549	2.9458	337.6692	1168	35.3549	2.9458	881.021
1169	35.3809	2.9437	348.8941	1169	35.3809	2.9437	858.7704	1169	35.3809	2.9437	329.5506	1169	35.3809	2.9437	871.4135
1170	35.4069	2.9416	377.7753	1170	35.4069	2.9416	885.9916	1170	35.4069	2.9416	366.2294	1170	35.4069	2.9416	906.6034
1171	35.4329	2.9395	394.1624	1171	35.4329	2.9395	900.7186	1171	35.4329	2.9395	356.8237	1171	35.4329	2.9395	895.7088
1172	35.4589	2.9374	395.7192	1172	35.4589	2.9374	900.6154	1172	35.4589	2.9374	317.0301	1172	35.4589	2.9374	854.4262
1173	35.4849	2.9353	346.6192	1173	35.4849	2.9353	849.8554	1173	35.4849	2.9353	282.1241	1173	35.4849	2.9353	818.0314
1174	35.5109	2.9332	362.6195	1174	35.5109	2.9332	864.1957	1174	35.5109	2.9332	287.2493	1174	35.5109	2.9332	821.6676
1175	35.5369	2.9312	393.2159	1175	35.5369	2.9312	893.1319	1175	35.5369	2.9312	326.5492	1175	35.5369	2.9312	859.4786
1176	35.5629	2.9291	391.9482	1176	35.5629	2.9291	890.2042	1176	35.5629	2.9291	356.2485	1176	35.5629	2.9291	887.6891
1177	35.5889	2.927	377.9381	1177	35.5889	2.927	874.5341	1177	35.5889	2.927	329.7287	1177	35.5889	2.927	859.6803
1178	35.6149	2.9249	412.8485	1178	35.6149	2.9249	907.7845	1178	35.6149	2.9249	314.3217	1178	35.6149	2.9249	842.7845
1179	35.6409	2.9229	389.0356	1179	35.6409	2.9229	882.3115	1179	35.6409	2.9229	320.8686	1179	35.6409	2.9229	847.8424
1180	35.6669	2.9208	388.6696	1180	35.6669	2.9208	880.2854	1180	35.6669	2.9208	372.1164	1180	35.6669	2.9208	897.6014
1181	35.6929	2.9188	367.1259	1181	35.6929	2.9188	857.0817	1181	35.6929	2.9188	329.2538	1181	35.6929	2.9188	853.2498
1182	35.7189	2.9167	326.8589	1182	35.7189	2.9167	815.1547	1182	35.7189	2.9167	327.9017	1182	35.7189	2.9167	850.4089
1183	35.7449	2.9147	325.8205	1183	35.7449	2.9147	812.4563	1183	35.7449	2.9147	332.9818	1183	35.7449	2.9147	854

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1184	35.7709	2.9126	350.6455	1184	35.7709	2.9126	835.6212	1184	35.7709	2.9126	345.2097	1184	35.7709	2.9126	864.739
1185	35.7969	2.9106	404.5479	1185	35.7969	2.9106	887.8636	1185	35.7969	2.9106	356.7991	1185	35.7969	2.9106	874.8396
1186	35.8229	2.9085	364.0594	1186	35.8229	2.9085	845.715	1186	35.8229	2.9085	311.7631	1186	35.8229	2.9085	828.3146
1187	35.8489	2.9065	400.2014	1187	35.8489	2.9065	880.197	1187	35.8489	2.9065	351.2228	1187	35.8489	2.9065	866.2854
1188	35.8749	2.9044	405.8852	1188	35.8749	2.9044	884.2208	1188	35.8749	2.9044	333.5369	1188	35.8749	2.9044	847.1106
1189	35.9009	2.9024	345.5432	1189	35.9009	2.9024	822.2188	1189	35.9009	2.9024	324.2911	1189	35.9009	2.9024	836.3759
1190	35.9269	2.9004	370.1457	1190	35.9269	2.9004	846.3689	1190	35.9269	2.9004	356.6655	1190	35.9269	2.9004	869.8085
1191	35.9529	2.8983	379.6687	1191	35.9529	2.8983	855.4397	1191	35.9529	2.8983	298.5355	1191	35.9529	2.8983	812.7365
1192	35.9789	2.8963	458.7606	1192	35.9789	2.8963	934.0792	1192	35.9789	2.8963	325.5583	1192	35.9789	2.8963	840.8175
1193	36.0049	2.8943	437.5023	1193	36.0049	2.8943	912.3686	1193	36.0049	2.8943	329.5521	1193	36.0049	2.8943	845.8693
1194	36.0309	2.8923	395.1216	1194	36.0309	2.8923	869.5357	1194	36.0309	2.8923	345.398	1194	36.0309	2.8923	862.7734
1195	36.0569	2.8903	381.6214	1195	36.0569	2.8903	855.5831	1195	36.0569	2.8903	286.5665	1195	36.0569	2.8903	805
1196	36.0829	2.8882	345.2048	1196	36.0829	2.8882	818.7143	1196	36.0829	2.8882	292.5086	1196	36.0829	2.8882	812.0002
1197	36.1089	2.8862	340.3358	1197	36.1089	2.8862	813.3929	1197	36.1089	2.8862	334.7797	1197	36.1089	2.8862	855.3294
1198	36.1349	2.8842	355.5341	1198	36.1349	2.8842	828.1389	1198	36.1349	2.8842	337.8406	1198	36.1349	2.8842	859.4484
1199	36.1609	2.8822	350.7522	1199	36.1609	2.8822	822.9047	1199	36.1609	2.8822	299.4711	1199	36.1609	2.8822	822.137
1200	36.1869	2.8802	358.8156	1200	36.1869	2.8802	830.5159	1200	36.1869	2.8802	268.9423	1200	36.1869	2.8802	792.6664
1201	36.2129	2.8782	363.5656	1201	36.2129	2.8782	834.8135	1201	36.2129	2.8782	332.1212	1201	36.2129	2.8782	856.9034
1202	36.2389	2.8762	360.5378	1202	36.2389	2.8762	831.3335	1202	36.2389	2.8762	226.2428	1202	36.2389	2.8762	752.0831
1203	36.2649	2.8742	346.9141	1203	36.2649	2.8742	817.2575	1203	36.2649	2.8742	266.2953	1203	36.2649	2.8742	793.1936
1204	36.2909	2.8722	396.7922	1204	36.2909	2.8722	866.6832	1204	36.2909	2.8722	353.4407	1204	36.2909	2.8722	881.3972
1205	36.3169	2.8703	334.0433	1205	36.3169	2.8703	803.482	1205	36.3169	2.8703	311.4145	1205	36.3169	2.8703	840.4291
1206	36.3429	2.8683	345.1082	1206	36.3429	2.8683	814.0946	1206	36.3429	2.8683	266.7164	1206	36.3429	2.8683	796.7891
1207	36.3689	2.8663	392.3424	1207	36.3689	2.8663	860.8766	1207	36.3689	2.8663	303.3183	1207	36.3689	2.8663	834.4491
1208	36.3949	2.8643	418.2988	1208	36.3949	2.8643	886.3807	1208	36.3949	2.8643	259.2624	1208	36.3949	2.8643	791.4514
1209	36.4209	2.8623	434.1485	1209	36.4209	2.8623	901.7781	1209	36.4209	2.8623	317.0733	1209	36.4209	2.8623	850.3203
1210	36.4469	2.8604	418.5543	1210	36.4469	2.8604	885.7315	1210	36.4469	2.8604	267.7264	1210	36.4469	2.8604	802.0316
1211	36.4729	2.8584	351.6813	1211	36.4729	2.8584	818.4062	1211	36.4729	2.8584	274.5889	1211	36.4729	2.8584	809.9522
1212	36.4989	2.8564	407.8213	1212	36.4989	2.8564	874.0939	1212	36.4989	2.8564	278.4991	1212	36.4989	2.8564	814.9205
1213	36.5249	2.8545	498.8043	1213	36.5249	2.8545	964.6247	1213	36.5249	2.8545	334.023	1213	36.5249	2.8545	871.5025
1214	36.5509	2.8525	510.3103	1214	36.5509	2.8525	975.6783	1214	36.5509	2.8525	239.965	1214	36.5509	2.8525	778.5026
1215	36.5769	2.8505	553.0751	1215	36.5769	2.8505	1017.9908	1215	36.5769	2.8505	336.564	1215	36.5769	2.8505	876.1597
1216	36.6029	2.8486	550.8145	1216	36.6029	2.8486	1015.2779	1216	36.6029	2.8486	324.2911	1216	36.6029	2.8486	864.945
1217	36.6289	2.8466	520.1506	1217	36.6289	2.8466	984.1618	1217	36.6289	2.8466	266.4666	1217	36.6289	2.8466	806.0615
1218	36.6549	2.8447	539.7062	1218	36.6549	2.8447	1003.2651	1218	36.6549	2.8447	329.1085	1218	36.6549	2.8447	867.6445
1219	36.6809	2.8427	487.0146	1219	36.6809	2.8427	950.1211	1219	36.6809	2.8427	357.4744	1219	36.6809	2.8427	894.9515

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1220	36.7069	2.8408	537.534	1220	36.7069	2.8408	1000.1882	1220	36.7069	2.8408	338.8684	1220	36.7069	2.8408	875.2866
1221	36.7329	2.8389	481.1618	1221	36.7329	2.8389	943.3638	1221	36.7329	2.8389	343.9043	1221	36.7329	2.8389	879.2636
1222	36.7589	2.8369	406.1145	1222	36.7589	2.8369	867.8642	1222	36.7589	2.8369	335.081	1222	36.7589	2.8369	869.3814
1223	36.7849	2.835	358.3295	1223	36.7849	2.835	819.6269	1223	36.7849	2.835	348.7579	1223	36.7849	2.835	881.9993
1224	36.8109	2.833	358.3451	1224	36.8109	2.833	819.1902	1224	36.8109	2.833	335.3817	1224	36.8109	2.833	867.5643
1225	36.8369	2.8311	318.5617	1225	36.8369	2.8311	778.9545	1225	36.8369	2.8311	250.9303	1225	36.8369	2.8311	782.054
1226	36.8629	2.8292	371.2229	1226	36.8629	2.8292	831.1634	1226	36.8629	2.8292	245.542	1226	36.8629	2.8292	775.6067
1227	36.8889	2.8273	418.4284	1227	36.8889	2.8273	877.9166	1227	36.8889	2.8273	344.0501	1227	36.8889	2.8273	873.056
1228	36.9149	2.8253	371.4912	1228	36.9149	2.8253	830.5271	1228	36.9149	2.8253	314.5322	1228	36.9149	2.8253	842.4792
1229	36.9409	2.8234	355.5239	1229	36.9409	2.8234	814.1075	1229	36.9409	2.8234	296.9577	1229	36.9409	2.8234	823.8458
1230	36.9669	2.8215	375.0063	1230	36.9669	2.8215	833.1376	1230	36.9669	2.8215	257.5068	1230	36.9669	2.8215	783.3359
1231	36.9929	2.8196	365.205	1231	36.9929	2.8196	822.884	1231	36.9929	2.8196	311.285	1231	36.9929	2.8196	836.0553
1232	37.0189	2.8177	377.4865	1232	37.0189	2.8177	834.7132	1232	37.0189	2.8177	296.8624	1232	37.0189	2.8177	820.5737
1233	37.0449	2.8158	398.516	1233	37.0449	2.8158	855.2904	1233	37.0449	2.8158	304.0866	1233	37.0449	2.8158	826.739
1234	37.0709	2.8139	385.2984	1234	37.0709	2.8139	841.6205	1234	37.0709	2.8139	292.5586	1234	37.0709	2.8139	814.1521
1235	37.0969	2.812	405.8305	1235	37.0969	2.812	861.7003	1235	37.0969	2.812	247.6473	1235	37.0969	2.812	768.1819
1236	37.1229	2.8101	365.3486	1236	37.1229	2.8101	820.7661	1236	37.1229	2.8101	291.472	1236	37.1229	2.8101	810.9477
1237	37.1489	2.8082	385.8371	1237	37.1489	2.8082	840.8023	1237	37.1489	2.8082	304.9588	1237	37.1489	2.8082	823.3756
1238	37.1749	2.8063	353.7413	1238	37.1749	2.8063	808.2542	1238	37.1749	2.8063	313.0817	1238	37.1749	2.8063	830.4396
1239	37.2009	2.8044	356.2768	1239	37.2009	2.8044	810.3374	1239	37.2009	2.8044	303.377	1239	37.2009	2.8044	819.676
1240	37.2269	2.8025	349.5598	1240	37.2269	2.8025	803.1681	1240	37.2269	2.8025	305.8227	1240	37.2269	2.8025	821.0628
1241	37.2529	2.8006	371.0019	1241	37.2529	2.8006	824.1579	1241	37.2529	2.8006	332.7986	1241	37.2529	2.8006	846.9798
1242	37.2789	2.7987	351.0338	1242	37.2789	2.7987	803.7376	1242	37.2789	2.7987	312.9882	1242	37.2789	2.7987	826.1104
1243	37.3049	2.7968	345.5432	1243	37.3049	2.7968	797.7947	1243	37.3049	2.7968	324.2911	1243	37.3049	2.7968	836.3545
1244	37.3309	2.795	384.3254	1244	37.3309	2.795	835.3295	1244	37.3309	2.795	291.3506	1244	37.3309	2.795	801.3387
1245	37.3569	2.7931	368.0964	1245	37.3569	2.7931	817.8533	1245	37.3569	2.7931	340.3507	1245	37.3569	2.7931	848.2635
1246	37.3829	2.7912	342.4359	1246	37.3829	2.7912	790.9456	1246	37.3829	2.7912	337.7707	1246	37.3829	2.7912	843.6083
1247	37.4089	2.7893	383.3153	1247	37.4089	2.7893	830.5776	1247	37.4089	2.7893	315.3272	1247	37.4089	2.7893	819.0895
1248	37.4349	2.7875	388.6703	1248	37.4349	2.7875	834.6854	1248	37.4349	2.7875	305.6556	1248	37.4349	2.7875	807.3427
1249	37.4609	2.7856	420.4207	1249	37.4609	2.7856	865.1885	1249	37.4609	2.7856	291.5166	1249	37.4609	2.7856	791.1283
1250	37.4869	2.7837	384.1314	1250	37.4869	2.7837	827.652	1250	37.4869	2.7837	266.2165	1250	37.4869	2.7837	763.753
1251	37.5129	2.7819	349.698	1251	37.5129	2.7819	791.9713	1251	37.5129	2.7819	277.827	1251	37.5129	2.7819	773.2882
1252	37.5389	2.78	369.6542	1252	37.5389	2.78	810.6803	1252	37.5389	2.78	302.6605	1252	37.5389	2.78	796.0465
1253	37.5649	2.7782	397.9626	1253	37.5649	2.7782	837.7414	1253	37.5649	2.7782	290.6387	1253	37.5649	2.7782	781.9494
1254	37.5909	2.7763	385.3696	1254	37.5909	2.7763	823.9011	1254	37.5909	2.7763	333.7991	1254	37.5909	2.7763	823.0346
1255	37.6169	2.7745	381.2093	1255	37.6169	2.7745	818.4936	1255	37.6169	2.7745	307.0442	1255	37.6169	2.7745	794.2045

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1256	37.6429	2.7726	403.8184	1256	37.6429	2.7726	839.8554	1256	37.6429	2.7726	285.7664	1256	37.6429	2.7726	770.8514
1257	37.6689	2.7708	414.2854	1257	37.6689	2.7708	849.0752	1257	37.6689	2.7708	306.3887	1257	37.6689	2.7708	789.3984
1258	37.6949	2.7689	411.1807	1258	37.6949	2.7689	844.7232	1258	37.6949	2.7689	313.2021	1258	37.6949	2.7689	794.1366
1259	37.7209	2.7671	405.6337	1259	37.7209	2.7671	837.929	1259	37.7209	2.7671	294.0399	1259	37.7209	2.7671	772.8991
1260	37.7469	2.7653	388.7014	1260	37.7469	2.7653	819.7493	1260	37.7469	2.7653	283.9902	1260	37.7469	2.7653	760.7742
1261	37.7729	2.7634	381.1701	1261	37.7729	2.7634	810.9708	1261	37.7729	2.7634	308.2704	1261	37.7729	2.7634	782.9791
1262	37.7989	2.7616	391.8865	1262	37.7989	2.7616	820.4399	1262	37.7989	2.7616	323.6624	1262	37.7989	2.7616	796.2958
1263	37.8249	2.7598	403.3429	1263	37.8249	2.7598	830.6491	1263	37.8249	2.7598	349.2619	1263	37.8249	2.7598	819.8201
1264	37.8509	2.7579	433.5394	1264	37.8509	2.7579	859.5984	1264	37.8509	2.7579	360.4949	1264	37.8509	2.7579	828.9778
1265	37.8769	2.7561	438.0266	1265	37.8769	2.7561	862.8382	1265	37.8769	2.7561	355.0506	1265	37.8769	2.7561	821.4582
1266	37.9029	2.7543	400.6417	1266	37.9029	2.7543	824.2061	1266	37.9029	2.7543	351.8397	1266	37.9029	2.7543	816.1721
1267	37.9289	2.7525	403.8482	1267	37.9289	2.7525	826.1654	1267	37.9289	2.7525	355.9488	1267	37.9289	2.7525	818.2059
1268	37.9549	2.7507	442.9269	1268	37.9549	2.7507	863.9967	1268	37.9549	2.7507	362.5344	1268	37.9549	2.7507	822.7163
1269	37.9809	2.7488	405.3496	1269	37.9809	2.7488	825.1722	1269	37.9809	2.7488	342.7559	1269	37.9809	2.7488	800.8625
1270	38.0069	2.747	345.5432	1270	38.0069	2.747	764.1186	1270	38.0069	2.747	324.2911	1270	38.0069	2.747	780.3225
1271	38.0329	2.7452	363.8521	1271	38.0329	2.7452	782.0131	1271	38.0329	2.7452	330.0888	1271	38.0329	2.7452	786.562
1272	38.0589	2.7434	384.6894	1272	38.0589	2.7434	802.4361	1272	38.0589	2.7434	344.3636	1272	38.0589	2.7434	801.2786
1273	38.0849	2.7416	430.8349	1273	38.0849	2.7416	848.1673	1273	38.0849	2.7416	330.5509	1273	38.0849	2.7416	787.9077
1274	38.1109	2.7398	417.4223	1274	38.1109	2.7398	834.3404	1274	38.1109	2.7398	323.6866	1274	38.1109	2.7398	781.4852
1275	38.1369	2.738	366.7003	1275	38.1369	2.738	783.204	1275	38.1369	2.738	360.0175	1275	38.1369	2.738	818.258
1276	38.1629	2.7362	361.6005	1276	38.1629	2.7362	777.69	1276	38.1629	2.7362	373.8351	1276	38.1629	2.7362	832.5174
1277	38.1889	2.7344	407.0381	1277	38.1889	2.7344	822.7132	1277	38.1889	2.7344	317.3971	1277	38.1889	2.7344	776.5211
1278	38.2149	2.7326	390.3514	1278	38.2149	2.7326	805.6122	1278	38.2149	2.7326	306.0311	1278	38.2149	2.7326	765.597
1279	38.2409	2.7309	352.1783	1279	38.2409	2.7309	767.0248	1279	38.2409	2.7309	329.1261	1279	38.2409	2.7309	789.1338
1280	38.2669	2.7291	358.2862	1280	38.2669	2.7291	772.7184	1280	38.2669	2.7291	354.8599	1280	38.2669	2.7291	815.3094
1281	38.2929	2.7273	361.6399	1281	38.2929	2.7273	775.6578	1281	38.2929	2.7273	369.4831	1281	38.2929	2.7273	830.3743
1282	38.3189	2.7255	411.316	1282	38.3189	2.7255	824.9196	1282	38.3189	2.7255	380.3721	1282	38.3189	2.7255	841.7052
1283	38.3449	2.7237	405.479	1283	38.3449	2.7237	818.6682	1283	38.3449	2.7237	328.0213	1283	38.3449	2.7237	789.7962
1284	38.3709	2.7219	406.6492	1284	38.3709	2.7219	819.4241	1284	38.3709	2.7219	336.4015	1284	38.3709	2.7219	798.6182
1285	38.3969	2.7202	362.4075	1285	38.3969	2.7202	774.7681	1285	38.3969	2.7202	330.47	1285	38.3969	2.7202	793.1285
1286	38.4229	2.7184	404.5522	1286	38.4229	2.7184	816.4985	1286	38.4229	2.7184	305.3976	1286	38.4229	2.7184	768.498
1287	38.4489	2.7166	404.3103	1287	38.4489	2.7166	815.8423	1287	38.4489	2.7166	330.8135	1287	38.4489	2.7166	794.3556
1288	38.4749	2.7149	372.212	1288	38.4749	2.7149	783.3297	1288	38.4749	2.7149	366.5956	1288	38.4749	2.7149	830.5795
1289	38.5009	2.7131	359.1001	1289	38.5009	2.7131	769.8035	1289	38.5009	2.7131	331.8371	1289	38.5009	2.7131	796.2629
1290	38.5269	2.7113	399.1175	1290	38.5269	2.7113	809.4066	1290	38.5269	2.7113	346.8344	1290	38.5269	2.7113	811.7019
1291	38.5529	2.7096	428.9226	1291	38.5529	2.7096	838.7973	1291	38.5529	2.7096	312.6967	1291	38.5529	2.7096	778.0061

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1292	38.5789	2.7078	401.1269	1292	38.5789	2.7078	810.5873	1292	38.5789	2.7078	335.6746	1292	38.5789	2.7078	801.4258
1293	38.6049	2.7061	329.417	1293	38.6049	2.7061	738.4631	1293	38.6049	2.7061	341.8695	1293	38.6049	2.7061	808.0625
1294	38.6309	2.7043	371.0606	1294	38.6309	2.7043	779.6924	1294	38.6309	2.7043	315.0823	1294	38.6309	2.7043	781.7171
1295	38.6569	2.7026	340.4614	1295	38.6569	2.7026	748.6789	1295	38.6569	2.7026	352.9324	1295	38.6569	2.7026	820.009
1296	38.6829	2.7008	352.0005	1296	38.6829	2.7008	759.8036	1296	38.6829	2.7008	308.0423	1296	38.6829	2.7008	775.5607
1297	38.7089	2.6991	417.0129	1297	38.7089	2.6991	824.4017	1297	38.7089	2.6991	324.2911	1297	38.7089	2.6991	792.2513
1298	38.7349	2.6973	382.7962	1298	38.7349	2.6973	789.7708	1298	38.7349	2.6973	334.2617	1298	38.7349	2.6973	800.3762
1299	38.7609	2.6956	455.5174	1299	38.7609	2.6956	862.0777	1299	38.7609	2.6956	303.4449	1299	38.7609	2.6956	767.7137
1300	38.7869	2.6939	409.6368	1300	38.7869	2.6939	815.7827	1300	38.7869	2.6939	335.0283	1300	38.7869	2.6939	797.4514
1301	38.8129	2.6921	382.349	1301	38.8129	2.6921	788.0806	1301	38.8129	2.6921	299.3115	1301	38.8129	2.6921	759.8888
1302	38.8389	2.6904	367.6869	1302	38.8389	2.6904	773.0041	1302	38.8389	2.6904	295.0945	1302	38.8389	2.6904	753.8261
1303	38.8649	2.6887	389.0711	1303	38.8649	2.6887	793.9741	1303	38.8649	2.6887	338.8482	1303	38.8649	2.6887	795.7341
1304	38.8909	2.6869	401.3664	1304	38.8909	2.6869	805.855	1304	38.8909	2.6869	378.6847	1304	38.8909	2.6869	833.7248
1305	38.9169	2.6852	408.6325	1305	38.9169	2.6852	812.7069	1305	38.9169	2.6852	322.2297	1305	38.9169	2.6852	775.4241
1306	38.9429	2.6835	342.3632	1306	38.9429	2.6835	746.0232	1306	38.9429	2.6835	288.0957	1306	38.9429	2.6835	739.4444
1307	38.9689	2.6818	325.9989	1307	38.9689	2.6818	729.2446	1307	38.9689	2.6818	352.3769	1307	38.9689	2.6818	801.8799
1308	38.9949	2.68	357.5674	1308	38.9949	2.68	760.3988	1308	38.9949	2.68	328.1219	1308	38.9949	2.68	775.7791
1309	39.0209	2.6783	430.8255	1309	39.0209	2.6783	833.2426	1309	39.0209	2.6783	325.093	1309	39.0209	2.6783	770.9044
1310	39.0469	2.6766	396.716	1310	39.0469	2.6766	798.7187	1310	39.0469	2.6766	412.2256	1310	39.0469	2.6766	856.1914
1311	39.0729	2.6749	373.399	1311	39.0729	2.6749	774.9874	1311	39.0729	2.6749	345.853	1311	39.0729	2.6749	787.973
1312	39.0989	2.6732	366.8827	1312	39.0989	2.6732	768.0569	1312	39.0989	2.6732	332.8476	1312	39.0989	2.6732	773.1219
1313	39.1249	2.6715	337.7816	1313	39.1249	2.6715	738.5414	1313	39.1249	2.6715	365.012	1313	39.1249	2.6715	803.4405
1314	39.1509	2.6698	381.3958	1314	39.1509	2.6698	781.7413	1314	39.1509	2.6698	390.7459	1314	39.1509	2.6698	827.3287
1315	39.1769	2.6681	362.8645	1315	39.1769	2.6681	762.7957	1315	39.1769	2.6681	372.0965	1315	39.1769	2.6681	806.8336
1316	39.2029	2.6664	392.953	1316	39.2029	2.6664	792.4699	1316	39.2029	2.6664	350.2562	1316	39.2029	2.6664	783.1476
1317	39.2289	2.6647	403.3778	1317	39.2289	2.6647	802.4804	1317	39.2289	2.6647	357.5502	1317	39.2289	2.6647	788.5958
1318	39.2549	2.663	401.5147	1318	39.2549	2.663	800.203	1318	39.2549	2.663	342.0856	1318	39.2549	2.663	771.2855
1319	39.2809	2.6613	323.3205	1319	39.2809	2.6613	721.5944	1319	39.2809	2.6613	363.8614	1319	39.2809	2.6613	791.2156
1320	39.3069	2.6596	413.865	1320	39.3069	2.6596	811.7246	1320	39.3069	2.6596	381.179	1320	39.3069	2.6596	806.6874
1321	39.3329	2.6579	355.8617	1321	39.3329	2.6579	753.307	1321	39.3329	2.6579	328.3777	1321	39.3329	2.6579	752.0404
1322	39.3589	2.6562	309.6923	1322	39.3589	2.6562	706.7233	1322	39.3589	2.6562	334.0022	1322	39.3589	2.6562	755.8192
1323	39.3849	2.6545	338.927	1323	39.3849	2.6545	735.5437	1323	39.3849	2.6545	338.7942	1323	39.3849	2.6545	758.7655
1324	39.4109	2.6529	345.5432	1324	39.4109	2.6529	741.7456	1324	39.4109	2.6529	324.2911	1324	39.4109	2.6529	742.4167
1325	39.4369	2.6512	371.895	1325	39.4369	2.6512	767.8865	1325	39.4369	2.6512	372.2848	1325	39.4369	2.6512	791.7731
1326	39.4629	2.6495	389.0138	1326	39.4629	2.6495	784.7944	1326	39.4629	2.6495	367.2076	1326	39.4629	2.6495	788.0585
1327	39.4889	2.6478	375.4125	1327	39.4889	2.6478	770.9822	1327	39.4889	2.6478	375.5889	1327	39.4889	2.6478	797.8026

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1328	39.5149	2.6462	367.6424	1328	39.5149	2.6462	763.0013	1328	39.5149	2.6462	353.9294	1328	39.5149	2.6462	777.5058
1329	39.5409	2.6445	337.2169	1329	39.5409	2.6445	732.365	1329	39.5409	2.6445	300.3156	1329	39.5409	2.6445	725.2547
1330	39.5669	2.6428	309.1044	1330	39.5669	2.6428	704.0416	1330	39.5669	2.6428	344.0008	1330	39.5669	2.6428	770.3026
1331	39.5929	2.6412	374.9686	1331	39.5929	2.6412	769.6949	1331	39.5929	2.6412	375.4193	1331	39.5929	2.6412	803.0838
1332	39.6189	2.6395	374.2357	1332	39.6189	2.6395	768.7511	1332	39.6189	2.6395	333.7474	1332	39.6189	2.6395	762.7746
1333	39.6449	2.6378	360.2933	1333	39.6449	2.6378	754.5979	1333	39.6449	2.6378	329.2286	1333	39.6449	2.6378	759.6186
1334	39.6709	2.6362	387.3025	1334	39.6709	2.6362	781.3962	1334	39.6709	2.6362	322.5115	1334	39.6709	2.6362	754.2642
1335	39.6969	2.6345	392.2988	1335	39.6969	2.6345	786.1817	1335	39.6969	2.6345	311.248	1335	39.6969	2.6345	744.3634
1336	39.7229	2.6329	361.9321	1336	39.7229	2.6329	755.6042	1336	39.7229	2.6329	322.5967	1336	39.7229	2.6329	757.0748
1337	39.7489	2.6312	371.1343	1337	39.7489	2.6312	764.5954	1337	39.7489	2.6312	318.7211	1337	39.7489	2.6312	754.5618
1338	39.7749	2.6296	380.6853	1338	39.7749	2.6296	773.9356	1338	39.7749	2.6296	350.0235	1338	39.7749	2.6296	787.227
1339	39.8009	2.6279	337.0743	1339	39.8009	2.6279	730.1137	1339	39.8009	2.6279	353.4701	1339	39.8009	2.6279	792.0363
1340	39.8269	2.6263	347.3053	1340	39.8269	2.6263	740.1339	1340	39.8269	2.6263	307.6562	1340	39.8269	2.6263	747.5851
1341	39.8529	2.6246	374.5772	1341	39.8529	2.6246	767.1949	1341	39.8529	2.6246	329.8437	1341	39.8529	2.6246	771.1353
1342	39.8789	2.623	414.2208	1342	39.8789	2.623	806.6277	1342	39.8789	2.623	335.6268	1342	39.8789	2.623	778.2811
1343	39.9049	2.6213	363.1128	1343	39.9049	2.6213	755.3088	1343	39.9049	2.6213	290.9788	1343	39.9049	2.6213	734.9958
1344	39.9309	2.6197	388.9869	1344	39.9309	2.6197	780.972	1344	39.9309	2.6197	279.7126	1344	39.9309	2.6197	725.0923
1345	39.9569	2.6181	389.6482	1345	39.9569	2.6181	781.4224	1345	39.9569	2.6181	320.1306	1345	39.9569	2.6181	766.873
1346	39.9829	2.6164	380.3637	1346	39.9829	2.6164	771.9271	1346	39.9829	2.6164	329.3861	1346	39.9829	2.6164	777.4913
1347	40.0089	2.6148	338.1705	1347	40.0089	2.6148	729.523	1347	40.0089	2.6148	337.7132	1347	40.0089	2.6148	787.1811
1348	40.0349	2.6132	365.9014	1348	40.0349	2.6132	757.0431	1348	40.0349	2.6132	269.2782	1348	40.0349	2.6132	720.1087
1349	40.0609	2.6115	392.9455	1349	40.0609	2.6115	783.8763	1349	40.0609	2.6115	278.5352	1349	40.0609	2.6115	730.7285
1350	40.0869	2.6099	368.5315	1350	40.0869	2.6099	759.2514	1350	40.0869	2.6099	318.6664	1350	40.0869	2.6099	772.2224
1351	40.1129	2.6083	399.8588	1351	40.1129	2.6083	790.3679	1351	40.1129	2.6083	324.2911	1351	40.1129	2.6083	779.2098
1352	40.1389	2.6067	371.9885	1352	40.1389	2.6067	762.2867	1352	40.1389	2.6067	314.4273	1352	40.1389	2.6067	768.6953
1353	40.1649	2.6051	370.9416	1353	40.1649	2.6051	761.0289	1353	40.1649	2.6051	278.7147	1353	40.1649	2.6051	732.332
1354	40.1909	2.6034	377.4185	1354	40.1909	2.6034	767.295	1354	40.1909	2.6034	283.1892	1354	40.1909	2.6034	736.1558
1355	40.2169	2.6018	354.4214	1355	40.2169	2.6018	744.087	1355	40.2169	2.6018	271.1624	1355	40.2169	2.6018	723.4783
1356	40.2429	2.6002	385.7499	1356	40.2429	2.6002	775.2047	1356	40.2429	2.6002	274.9889	1356	40.2429	2.6002	726.6541
1357	40.2689	2.5986	392.3051	1357	40.2689	2.5986	781.549	1357	40.2689	2.5986	283.8966	1357	40.2689	2.5986	734.9111
1358	40.2949	2.597	361.1871	1358	40.2949	2.597	750.2201	1358	40.2949	2.597	289.1642	1358	40.2949	2.597	739.528
1359	40.3209	2.5954	348.0247	1359	40.3209	2.5954	736.8468	1359	40.3209	2.5954	285.419	1359	40.3209	2.5954	735.1321
1360	40.3469	2.5938	371.6845	1360	40.3469	2.5938	760.2958	1360	40.3469	2.5938	288.4994	1360	40.3469	2.5938	737.5618
1361	40.3729	2.5922	397.6109	1361	40.3729	2.5922	786.0114	1361	40.3729	2.5922	304.5656	1361	40.3729	2.5922	752.9773
1362	40.3989	2.5906	415.1705	1362	40.3989	2.5906	803.3601	1362	40.3989	2.5906	304.2305	1362	40.3989	2.5906	751.9915
1363	40.4249	2.589	403.8427	1363	40.4249	2.589	791.8214	1363	40.4249	2.589	288.3995	1363	40.4249	2.589	735.5098

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1364	40.4509	2.5874	378.5154	1364	40.4509	2.5874	766.2832	1364	40.4509	2.5874	277.2032	1364	40.4509	2.5874	723.6628
1365	40.4769	2.5858	389.0349	1365	40.4769	2.5858	776.5919	1365	40.4769	2.5858	324.8005	1365	40.4769	2.5858	770.6094
1366	40.5029	2.5842	373.7625	1366	40.5029	2.5842	761.1086	1366	40.5029	2.5842	331.1636	1366	40.5029	2.5842	776.3219
1367	40.5289	2.5826	362.1415	1367	40.5289	2.5826	749.2767	1367	40.5289	2.5826	289.4001	1367	40.5289	2.5826	733.9076
1368	40.5549	2.581	369.6062	1368	40.5549	2.581	756.5306	1368	40.5549	2.581	299.1968	1368	40.5549	2.581	743.0536
1369	40.5809	2.5795	386.554	1369	40.5809	2.5795	773.2676	1369	40.5809	2.5795	305.4991	1369	40.5809	2.5795	748.7052
1370	40.6069	2.5779	407.511	1370	40.6069	2.5779	794.0137	1370	40.6069	2.5779	305.9463	1370	40.6069	2.5779	748.5017
1371	40.6329	2.5763	380.1146	1371	40.6329	2.5763	766.4065	1371	40.6329	2.5763	324.6376	1371	40.6329	2.5763	766.5423
1372	40.6589	2.5747	407.487	1372	40.6589	2.5747	793.568	1372	40.6589	2.5747	340.0914	1372	40.6589	2.5747	781.3455
1373	40.6849	2.5731	409.4684	1373	40.6849	2.5731	795.3385	1373	40.6849	2.5731	316.5565	1373	40.6849	2.5731	757.1598
1374	40.7109	2.5716	355.1212	1374	40.7109	2.5716	740.7805	1374	40.7109	2.5716	326.5812	1374	40.7109	2.5716	766.5338
1375	40.7369	2.57	360.6833	1375	40.7369	2.57	746.1317	1375	40.7369	2.57	331.6291	1375	40.7369	2.57	770.9311
1376	40.7629	2.5684	354.6878	1376	40.7629	2.5684	739.9253	1376	40.7629	2.5684	325.1289	1376	40.7629	2.5684	763.7801
1377	40.7889	2.5669	355.3818	1377	40.7889	2.5669	740.4084	1377	40.7889	2.5669	333.8363	1377	40.7889	2.5669	771.8369
1378	40.8149	2.5653	345.5432	1378	40.8149	2.5653	730.359	1378	40.8149	2.5653	324.2911	1378	40.8149	2.5653	761.641
1379	40.8409	2.5637	346.6682	1379	40.8409	2.5637	731.7292	1379	40.8409	2.5637	308.983	1379	40.8409	2.5637	745.2251
1380	40.8669	2.5622	356.8204	1380	40.8669	2.5622	742.1266	1380	40.8669	2.5622	274.7651	1380	40.8669	2.5622	709.8995
1381	40.8929	2.5606	392.5269	1381	40.8929	2.5606	778.0783	1381	40.8929	2.5606	269.7931	1381	40.8929	2.5606	703.8197
1382	40.9189	2.5591	385.4464	1382	40.9189	2.5591	771.243	1382	40.9189	2.5591	311.9731	1382	40.9189	2.5591	744.8919
1383	40.9449	2.5575	365.3365	1383	40.9449	2.5575	751.3782	1383	40.9449	2.5575	306.5672	1383	40.9449	2.5575	738.3782
1384	40.9709	2.5559	338.4412	1384	40.9709	2.5559	724.7281	1384	40.9709	2.5559	301.0026	1384	40.9709	2.5559	731.7059
1385	40.9969	2.5544	343.4637	1385	40.9969	2.5544	729.9958	1385	40.9969	2.5544	330.5052	1385	40.9969	2.5544	760.1008
1386	41.0229	2.5528	381.0533	1386	41.0229	2.5528	767.8306	1386	41.0229	2.5528	310.4376	1386	41.0229	2.5528	738.9254
1387	41.0489	2.5513	327.8401	1387	41.0489	2.5513	714.8626	1387	41.0489	2.5513	327.8769	1387	41.0489	2.5513	755.2569
1388	41.0749	2.5498	299.0546	1388	41.0749	2.5498	686.3223	1388	41.0749	2.5498	322.6855	1388	41.0749	2.5498	748.9577
1389	41.1009	2.5482	341.8929	1389	41.1009	2.5482	729.4058	1389	41.1009	2.5482	314.7091	1389	41.1009	2.5482	739.8736
1390	41.1269	2.5467	403.1262	1390	41.1269	2.5467	790.8843	1390	41.1269	2.5467	321.7514	1390	41.1269	2.5467	745.8081
1391	41.1529	2.5451	404.6515	1391	41.1529	2.5451	792.6548	1391	41.1529	2.5451	298.0911	1391	41.1529	2.5451	721.0401
1392	41.1789	2.5436	334.7134	1392	41.1789	2.5436	722.9618	1392	41.1789	2.5436	318.6099	1392	41.1789	2.5436	740.4511
1393	41.2049	2.5421	357.4686	1393	41.2049	2.5421	745.9622	1393	41.2049	2.5421	369.2829	1393	41.2049	2.5421	790.0164
1394	41.2309	2.5405	378.7053	1394	41.2309	2.5405	767.4442	1394	41.2309	2.5405	313.8396	1394	41.2309	2.5405	733.4653
1395	41.2569	2.539	342.8874	1395	41.2569	2.539	731.8715	1395	41.2569	2.539	318.3734	1395	41.2569	2.539	736.8913
1396	41.2829	2.5375	360.0284	1396	41.2829	2.5375	749.2576	1396	41.2829	2.5375	344.1546	1396	41.2829	2.5375	761.5647
1397	41.3089	2.5359	352.3073	1397	41.3089	2.5359	741.7818	1397	41.3089	2.5359	315.313	1397	41.3089	2.5359	731.6154
1398	41.3349	2.5344	359.0936	1398	41.3349	2.5344	748.8132	1398	41.3349	2.5344	293.1068	1398	41.3349	2.5344	708.3015
1399	41.3609	2.5329	340.3216	1399	41.3609	2.5329	730.2864	1399	41.3609	2.5329	371.1245	1399	41.3609	2.5329	785.2114

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1400	41.3869	2.5314	353.0637	1400	41.3869	2.5314	743.2737	1400	41.3869	2.5314	328.5098	1400	41.3869	2.5314	741.4889
1401	41.4129	2.5298	377.5822	1401	41.4129	2.5298	768.0374	1401	41.4129	2.5298	297.4341	1401	41.4129	2.5298	709.3055
1402	41.4389	2.5283	322.6725	1402	41.4389	2.5283	713.3728	1402	41.4389	2.5283	310.3239	1402	41.4389	2.5283	721.0875
1403	41.4649	2.5268	344.6771	1403	41.4649	2.5268	735.6226	1403	41.4649	2.5268	324.9909	1403	41.4649	2.5268	734.6468
1404	41.4909	2.5253	353.18	1404	41.4909	2.5253	744.3707	1404	41.4909	2.5253	359.9749	1404	41.4909	2.5253	768.523
1405	41.5169	2.5238	384.2955	1405	41.5169	2.5238	775.7315	1405	41.5169	2.5238	324.2911	1405	41.5169	2.5238	731.7315
1406	41.5429	2.5223	431.2416	1406	41.5429	2.5223	822.9227	1406	41.5429	2.5223	372.65	1406	41.5429	2.5223	779.9287
1407	41.5689	2.5208	384.5858	1407	41.5689	2.5208	776.5121	1407	41.5689	2.5208	338.7993	1407	41.5689	2.5208	745.9164
1408	41.5949	2.5193	429.7604	1408	41.5949	2.5193	821.9319	1408	41.5949	2.5193	317.8479	1408	41.5949	2.5193	724.8033
1409	41.6209	2.5178	353.2597	1409	41.6209	2.5178	745.6765	1409	41.6209	2.5178	311.471	1409	41.6209	2.5178	718.2647
1410	41.6469	2.5163	310.2931	1410	41.6469	2.5163	702.955	1410	41.6469	2.5163	254.9916	1410	41.6469	2.5163	661.6237
1411	41.6729	2.5148	358.1599	1411	41.6729	2.5148	751.067	1411	41.6729	2.5148	286.9123	1411	41.6729	2.5148	693.3827
1412	41.6989	2.5133	364.8452	1412	41.6989	2.5133	757.9975	1412	41.6989	2.5133	326.677	1412	41.6989	2.5133	732.9858
1413	41.7249	2.5118	402.212	1413	41.7249	2.5118	795.6095	1413	41.7249	2.5118	328.8323	1413	41.7249	2.5118	734.9794
1414	41.7509	2.5103	345.5289	1414	41.7509	2.5103	739.1716	1414	41.7509	2.5103	320.1963	1414	41.7509	2.5103	726.1818
1415	41.7769	2.5088	428.4916	1415	41.7769	2.5088	822.3794	1415	41.7769	2.5088	288.1702	1415	41.7769	2.5088	693.994
1416	41.8029	2.5073	461.5855	1416	41.8029	2.5073	855.7186	1416	41.8029	2.5073	343.0153	1416	41.8029	2.5073	748.6774
1417	41.8289	2.5058	486.3726	1417	41.8289	2.5058	880.7508	1417	41.8289	2.5058	329.3489	1417	41.8289	2.5058	734.8494
1418	41.8549	2.5043	620.8724	1418	41.8549	2.5043	1015.4958	1418	41.8549	2.5043	315.4996	1418	41.8549	2.5043	720.8384
1419	41.8809	2.5028	786.3333	1419	41.8809	2.5028	1181.202	1419	41.8809	2.5028	319.4738	1419	41.8809	2.5028	724.6509
1420	41.9069	2.5013	1164.1524	1420	41.9069	2.5013	1559.2662	1420	41.9069	2.5013	341.1506	1420	41.9069	2.5013	746.1661
1421	41.9329	2.4999	1697.2409	1421	41.9329	2.4999	2092.5999	1421	41.9329	2.4999	385.9323	1421	41.9329	2.4999	790.7862
1422	41.9589	2.4984	2138.0795	1422	41.9589	2.4984	2533.6837	1422	41.9589	2.4984	538.8775	1422	41.9589	2.4984	943.5697
1423	41.9849	2.4969	2039.5611	1423	41.9849	2.4969	2435.4105	1423	41.9849	2.4969	699.7304	1423	41.9849	2.4969	1104.261
1424	42.0109	2.4954	1674.0772	1424	42.0109	2.4954	2070.1718	1424	42.0109	2.4954	664.7964	1424	42.0109	2.4954	1069.1653
1425	42.0369	2.494	1654.5212	1425	42.0369	2.494	2050.861	1425	42.0369	2.494	539.3836	1425	42.0369	2.494	943.5909
1426	42.0629	2.4925	1470.7752	1426	42.0629	2.4925	1867.3602	1426	42.0629	2.4925	604.5848	1426	42.0629	2.4925	1008.6304
1427	42.0889	2.491	1181.5234	1427	42.0889	2.491	1578.3535	1427	42.0889	2.491	642.7896	1427	42.0889	2.491	1046.6735
1428	42.1149	2.4895	838.2501	1428	42.1149	2.4895	1235.3255	1428	42.1149	2.4895	476.5773	1428	42.1149	2.4895	880.2996
1429	42.1409	2.4881	621.303	1429	42.1409	2.4881	1018.6235	1429	42.1409	2.4881	363.8356	1429	42.1409	2.4881	767.3963
1430	42.1669	2.4866	575.2976	1430	42.1669	2.4866	972.8633	1430	42.1669	2.4866	394.4005	1430	42.1669	2.4866	797.7995
1431	42.1929	2.4852	484.5879	1431	42.1929	2.4852	882.3989	1431	42.1929	2.4852	436.3964	1431	42.1929	2.4852	839.6337
1432	42.2189	2.4837	435.9019	1432	42.2189	2.4837	833.958	1432	42.2189	2.4837	383.8344	1432	42.2189	2.4837	786.91
1433	42.2449	2.4822	403.2306	1433	42.2449	2.4822	800.0966	1433	42.2449	2.4822	340.6	1433	42.2449	2.4822	743.514
1434	42.2709	2.4808	382.4783	1434	42.2709	2.4808	778.1543	1434	42.2709	2.4808	354.3442	1434	42.2709	2.4808	757.0966
1435	42.2969	2.4793	355.5997	1435	42.2969	2.4793	750.0856	1435	42.2969	2.4793	323.3805	1435	42.2969	2.4793	725.9712

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1436	42.3229	2.4779	360.3653	1436	42.3229	2.4779	753.6611	1436	42.3229	2.4779	336.9393	1436	42.3229	2.4779	739.3683
1437	42.3489	2.4764	340.0919	1437	42.3489	2.4764	732.1976	1437	42.3489	2.4764	304.1468	1437	42.3489	2.4764	706.4143
1438	42.3749	2.475	345.6927	1438	42.3749	2.475	736.6083	1438	42.3749	2.475	313.1442	1438	42.3749	2.475	715.25
1439	42.4009	2.4735	321.273	1439	42.4009	2.4735	710.9985	1439	42.4009	2.4735	286.664	1439	42.4009	2.4735	688.6081
1440	42.4269	2.4721	302.0808	1440	42.4269	2.4721	690.6163	1440	42.4269	2.4721	318.9704	1440	42.4269	2.4721	720.7529
1441	42.4529	2.4706	268.3311	1441	42.4529	2.4706	655.6765	1441	42.4529	2.4706	333.5316	1441	42.4529	2.4706	735.1524
1442	42.4789	2.4692	287.7316	1442	42.4789	2.4692	673.887	1442	42.4789	2.4692	293.2302	1442	42.4789	2.4692	694.6893
1443	42.5049	2.4677	336.6375	1443	42.5049	2.4677	721.6027	1443	42.5049	2.4677	315.4575	1443	42.5049	2.4677	716.755
1444	42.5309	2.4663	329.3502	1444	42.5309	2.4663	713.1254	1444	42.5309	2.4663	336.2748	1444	42.5309	2.4663	737.4107
1445	42.5569	2.4649	320.7593	1445	42.5569	2.4649	703.3444	1445	42.5569	2.4649	311.1374	1445	42.5569	2.4649	712.1116
1446	42.5829	2.4634	349.0965	1446	42.5829	2.4634	730.4915	1446	42.5829	2.4634	306.1349	1446	42.5829	2.4634	706.9474
1447	42.6089	2.462	363.1427	1447	42.6089	2.462	743.3476	1447	42.6089	2.462	308.392	1447	42.6089	2.462	709.0429
1448	42.6349	2.4606	332.5055	1448	42.6349	2.4606	711.5203	1448	42.6349	2.4606	296.5893	1448	42.6349	2.4606	697.0785
1449	42.6609	2.4591	337.6809	1449	42.6609	2.4591	715.5057	1449	42.6609	2.4591	315.3407	1449	42.6609	2.4591	715.6683
1450	42.6869	2.4577	340.1585	1450	42.6869	2.4577	716.7932	1450	42.6869	2.4577	359.7188	1450	42.6869	2.4577	759.8847
1451	42.7129	2.4563	357.2244	1451	42.7129	2.4563	732.669	1451	42.7129	2.4563	327.7563	1451	42.7129	2.4563	727.7606
1452	42.7389	2.4549	357.0739	1452	42.7389	2.4549	731.3284	1452	42.7389	2.4549	262.4032	1452	42.7389	2.4549	662.2458
1453	42.7649	2.4534	351.4925	1453	42.7649	2.4534	724.557	1453	42.7649	2.4534	285.3742	1453	42.7649	2.4534	685.0552
1454	42.7909	2.452	342.8845	1454	42.7909	2.452	714.7589	1454	42.7909	2.452	324.6414	1454	42.7909	2.452	724.1607
1455	42.8169	2.4506	321.564	1455	42.8169	2.4506	692.2483	1455	42.8169	2.4506	329.4964	1455	42.8169	2.4506	728.854
1456	42.8429	2.4492	307.4382	1456	42.8429	2.4492	676.9324	1456	42.8429	2.4492	332.7455	1456	42.8429	2.4492	731.9415
1457	42.8689	2.4478	328.481	1457	42.8689	2.4478	696.7851	1457	42.8689	2.4478	343.1565	1457	42.8689	2.4478	742.1908
1458	42.8949	2.4464	351.0588	1458	42.8949	2.4464	718.1729	1458	42.8949	2.4464	352.9299	1458	42.8949	2.4464	751.8025
1459	42.9209	2.4449	345.5432	1459	42.9209	2.4449	711.4672	1459	42.9209	2.4449	324.2911	1459	42.9209	2.4449	723.0022
1460	42.9469	2.4435	337.5841	1460	42.9469	2.4435	702.4299	1460	42.9469	2.4435	301.1832	1460	42.9469	2.4435	699.7104
1461	42.9729	2.4421	346.4746	1461	42.9729	2.4421	710.2422	1461	42.9729	2.4421	306.1701	1461	42.9729	2.4421	704.5135
1462	42.9989	2.4407	367.8919	1462	42.9989	2.4407	730.5812	1462	42.9989	2.4407	291.7346	1462	42.9989	2.4407	689.8941
1463	43.0249	2.4393	363.6063	1463	43.0249	2.4393	725.2173	1463	43.0249	2.4393	290.8454	1463	43.0249	2.4393	688.821
1464	43.0509	2.4379	335.8587	1464	43.0509	2.4379	696.3915	1464	43.0509	2.4379	318.2678	1464	43.0509	2.4379	716.0595
1465	43.0769	2.4365	347.2861	1465	43.0769	2.4365	706.7407	1465	43.0769	2.4365	308.2301	1465	43.0769	2.4365	705.8381
1466	43.1029	2.4351	367.5937	1466	43.1029	2.4351	725.9701	1466	43.1029	2.4351	280.1844	1466	43.1029	2.4351	677.6085
1467	43.1289	2.4337	368.9646	1467	43.1289	2.4337	726.2627	1467	43.1289	2.4337	298.2783	1467	43.1289	2.4337	695.5185
1468	43.1549	2.4323	358.8003	1468	43.1549	2.4323	715.0201	1468	43.1549	2.4323	307.7357	1468	43.1549	2.4323	704.7921
1469	43.1809	2.4309	380.8703	1469	43.1809	2.4309	736.0119	1469	43.1809	2.4309	277.9734	1469	43.1809	2.4309	674.8459
1470	43.2069	2.4295	425.3947	1470	43.2069	2.4295	779.4581	1470	43.2069	2.4295	287.7605	1470	43.2069	2.4295	684.4491
1471	43.2329	2.4281	384.1318	1471	43.2329	2.4281	737.117	1471	43.2329	2.4281	320.0098	1471	43.2329	2.4281	716.5146

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1472	43.2589	2.4267	356.2845	1472	43.2589	2.4267	708.1914	1472	43.2589	2.4267	308.5929	1472	43.2589	2.4267	704.9138
1473	43.2849	2.4254	358.932	1473	43.2849	2.4254	709.7607	1473	43.2849	2.4254	309.0889	1473	43.2849	2.4254	705.2259
1474	43.3109	2.424	378.0902	1474	43.3109	2.424	727.8407	1474	43.3109	2.424	341.1185	1474	43.3109	2.424	737.0717
1475	43.3369	2.4226	394.5861	1475	43.3369	2.4226	743.2583	1475	43.3369	2.4226	341.2563	1475	43.3369	2.4226	737.0257
1476	43.3629	2.4212	375.2906	1476	43.3629	2.4212	722.8845	1476	43.3629	2.4212	298.0282	1476	43.3629	2.4212	693.6138
1477	43.3889	2.4198	358.7108	1477	43.3889	2.4198	705.2265	1477	43.3889	2.4198	275.0856	1477	43.3889	2.4198	670.4873
1478	43.4149	2.4184	368.9744	1478	43.4149	2.4184	714.4119	1478	43.4149	2.4184	279.0895	1478	43.4149	2.4184	674.3073
1479	43.4409	2.4171	387.9483	1479	43.4409	2.4171	732.3075	1479	43.4409	2.4171	319.6494	1479	43.4409	2.4171	714.6834
1480	43.4669	2.4157	371.5454	1480	43.4669	2.4157	714.8263	1480	43.4669	2.4157	320.0014	1480	43.4669	2.4157	714.8516
1481	43.4929	2.4143	363.2623	1481	43.4929	2.4143	705.4651	1481	43.4929	2.4143	316.989	1481	43.4929	2.4143	711.6553
1482	43.5189	2.4129	354.4857	1482	43.5189	2.4129	695.6102	1482	43.5189	2.4129	329.3989	1482	43.5189	2.4129	723.8814
1483	43.5449	2.4116	325.3989	1483	43.5449	2.4116	665.4452	1483	43.5449	2.4116	291.732	1483	43.5449	2.4116	686.0306
1484	43.5709	2.4102	357.0187	1484	43.5709	2.4102	695.9867	1484	43.5709	2.4102	299.1274	1484	43.5709	2.4102	693.2421
1485	43.5969	2.4088	362.4171	1485	43.5969	2.4088	700.3069	1485	43.5969	2.4088	355.9836	1485	43.5969	2.4088	749.9145
1486	43.6229	2.4075	345.5432	1486	43.6229	2.4075	682.3548	1486	43.6229	2.4075	324.2911	1486	43.6229	2.4075	718.0381
1487	43.6489	2.4061	409.5731	1487	43.6489	2.4061	743.6788	1487	43.6489	2.4061	297.8791	1487	43.6489	2.4061	691.9124
1488	43.6749	2.4047	399.1623	1488	43.6749	2.4047	730.5623	1488	43.6749	2.4047	297.7123	1488	43.6749	2.4047	692.032
1489	43.7009	2.4034	387.3001	1489	43.7009	2.4034	715.9943	1489	43.7009	2.4034	318.3712	1489	43.7009	2.4034	712.9773
1490	43.7269	2.402	372.9489	1490	43.7269	2.402	698.9373	1490	43.7269	2.402	264.9791	1490	43.7269	2.402	659.8715
1491	43.7529	2.4007	363.2279	1491	43.7529	2.4007	686.5105	1491	43.7529	2.4007	269.6684	1491	43.7529	2.4007	664.8471
1492	43.7789	2.3993	381.0987	1492	43.7789	2.3993	701.6755	1492	43.7789	2.3993	304.8287	1492	43.7789	2.3993	700.2938
1493	43.8049	2.398	416.2305	1493	43.8049	2.398	734.1015	1493	43.8049	2.398	312.9379	1493	43.8049	2.398	708.6893
1494	43.8309	2.3966	390.278	1494	43.8309	2.3966	705.4432	1494	43.8309	2.3966	291.986	1494	43.8309	2.3966	688.0237
1495	43.8569	2.3953	362.5844	1495	43.8569	2.3953	675.0438	1495	43.8569	2.3953	275.6823	1495	43.8569	2.3953	672.0064
1496	43.8829	2.3939	388.7746	1496	43.8829	2.3939	698.5282	1496	43.8829	2.3939	269.0335	1496	43.8829	2.3939	665.6439
1497	43.9089	2.3926	354.2647	1497	43.9089	2.3926	661.3125	1497	43.9089	2.3926	302.5719	1497	43.9089	2.3926	699.4687
1498	43.9349	2.3912	406.0733	1498	43.9349	2.3912	710.4152	1498	43.9349	2.3912	280.1581	1498	43.9349	2.3912	677.3412
1499	43.9609	2.3899	368.0449	1499	43.9609	2.3899	669.6811	1499	43.9609	2.3899	301.4421	1499	43.9609	2.3899	698.9115
1500	43.9869	2.3885	361.0025	1500	43.9869	2.3885	659.9329	1500	43.9869	2.3885	347.8291	1500	43.9869	2.3885	745.5849
1501	44.0129	2.3872	397.5423	1501	44.0129	2.3872	693.7669	1501	44.0129	2.3872	318.596	1501	44.0129	2.3872	716.6382
1502	44.0389	2.3858	401.0405	1502	44.0389	2.3858	694.5593	1502	44.0389	2.3858	280.5507	1502	44.0389	2.3858	678.8792
1503	44.0649	2.3845	424.8969	1503	44.0649	2.3845	715.7099	1503	44.0649	2.3845	297.5183	1503	44.0649	2.3845	696.1331
1504	44.0909	2.3832	424.6324	1504	44.0909	2.3832	712.7396	1504	44.0909	2.3832	235.3555	1504	44.0909	2.3832	634.2567
1505	44.1169	2.3818	421.37	1505	44.1169	2.3818	706.7714	1505	44.1169	2.3818	262.7329	1505	44.1169	2.3818	661.9205
1506	44.1429	2.3805	386.1747	1506	44.1429	2.3805	668.8703	1506	44.1429	2.3805	305.3083	1506	44.1429	2.3805	704.7822
1507	44.1689	2.3792	399.7556	1507	44.1689	2.3792	679.7454	1507	44.1689	2.3792	247.2663	1507	44.1689	2.3792	647.0265

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1508	44.1949	2.3778	384.3068	1508	44.1949	2.3778	661.5908	1508	44.1949	2.3778	264.3303	1508	44.1949	2.3778	664.3768
1509	44.2209	2.3765	437.6742	1509	44.2209	2.3765	712.2524	1509	44.2209	2.3765	273.3031	1509	44.2209	2.3765	673.636
1510	44.2469	2.3752	396.1908	1510	44.2469	2.3752	668.0632	1510	44.2469	2.3752	315.5716	1510	44.2469	2.3752	716.1908
1511	44.2729	2.3739	437.2148	1511	44.2729	2.3739	706.3814	1511	44.2729	2.3739	320.5513	1511	44.2729	2.3739	721.4569
1512	44.2989	2.3725	460.6567	1512	44.2989	2.3725	727.1175	1512	44.2989	2.3725	233.4903	1512	44.2989	2.3725	634.6823
1513	44.3249	2.3712	345.5432	1513	44.3249	2.3712	609.2983	1513	44.3249	2.3712	324.2911	1513	44.3249	2.3712	725.7694
1514	44.3509	2.3699	453.5866	1514	44.3509	2.3699	719.608	1514	44.3509	2.3699	312.5432	1514	44.3509	2.3699	712.174
1515	44.3769	2.3686	463.4664	1515	44.3769	2.3686	731.7541	1515	44.3769	2.3686	328.8814	1515	44.3769	2.3686	726.6647
1516	44.4029	2.3673	390.8019	1516	44.4029	2.3673	661.3559	1516	44.4029	2.3673	278.8069	1516	44.4029	2.3673	674.7428
1517	44.4289	2.3659	436.9432	1517	44.4289	2.3659	709.7636	1517	44.4289	2.3659	313.3925	1517	44.4289	2.3659	707.481
1518	44.4549	2.3646	398.0501	1518	44.4549	2.3646	673.1368	1518	44.4549	2.3646	241.8764	1518	44.4549	2.3646	634.1173
1519	44.4809	2.3633	397.3987	1519	44.4809	2.3633	674.7518	1519	44.4809	2.3633	269.6212	1519	44.4809	2.3633	660.0147
1520	44.5069	2.362	424.1497	1520	44.5069	2.362	703.7692	1520	44.5069	2.362	282.7344	1520	44.5069	2.362	671.2804
1521	44.5329	2.3607	393.8164	1521	44.5329	2.3607	675.7022	1521	44.5329	2.3607	332.1253	1521	44.5329	2.3607	718.8239
1522	44.5589	2.3594	408.8281	1522	44.5589	2.3594	692.9802	1522	44.5589	2.3594	313.6277	1522	44.5589	2.3594	698.4788
1523	44.5849	2.3581	351.9904	1523	44.5849	2.3581	638.4089	1523	44.5849	2.3581	304.0137	1523	44.5849	2.3581	687.0173
1524	44.6109	2.3568	342.4268	1524	44.6109	2.3568	631.1117	1524	44.6109	2.3568	335.9361	1524	44.6109	2.3568	717.0922
1525	44.6369	2.3555	411.2013	1525	44.6369	2.3555	702.1525	1525	44.6369	2.3555	267.9035	1525	44.6369	2.3555	647.2122
1526	44.6629	2.3542	401.4123	1526	44.6629	2.3542	694.6299	1526	44.6629	2.3542	291.6734	1526	44.6629	2.3542	669.1346
1527	44.6889	2.3529	357.0213	1527	44.6889	2.3529	652.5052	1527	44.6889	2.3529	302.6792	1527	44.6889	2.3529	678.2929
1528	44.7149	2.3516	383.8934	1528	44.7149	2.3516	681.6437	1528	44.7149	2.3516	336.6341	1528	44.7149	2.3516	710.4004
1529	44.7409	2.3503	386.3059	1529	44.7409	2.3503	686.3225	1529	44.7409	2.3503	312.2092	1529	44.7409	2.3503	684.128
1530	44.7669	2.349	398.6356	1530	44.7669	2.349	700.9187	1530	44.7669	2.349	338.5948	1530	44.7669	2.349	708.6661
1531	44.7929	2.3477	366.6949	1531	44.7929	2.3477	671.2443	1531	44.7929	2.3477	337.7683	1531	44.7929	2.3477	705.9922
1532	44.8189	2.3464	393.5879	1532	44.8189	2.3464	700.4037	1532	44.8189	2.3464	358.6568	1532	44.8189	2.3464	725.0332
1533	44.8449	2.3451	404.7122	1533	44.8449	2.3451	713.7943	1533	44.8449	2.3451	301.5473	1533	44.8449	2.3451	666.0762
1534	44.8709	2.3438	353.1475	1534	44.8709	2.3438	664.496	1534	44.8709	2.3438	284.9512	1534	44.8709	2.3438	647.6326
1535	44.8969	2.3425	382.579	1535	44.8969	2.3425	696.1938	1535	44.8969	2.3425	307.2045	1535	44.8969	2.3425	668.0385
1536	44.9229	2.3413	370.8097	1536	44.9229	2.3413	686.6909	1536	44.9229	2.3413	274.2416	1536	44.9229	2.3413	633.2281
1537	44.9489	2.34	381.5958	1537	44.9489	2.34	699.7433	1537	44.9489	2.34	272.2139	1537	44.9489	2.34	629.3529
1538	44.9749	2.3387	351.8615	1538	44.9749	2.3387	672.2754	1538	44.9749	2.3387	296.9432	1538	44.9749	2.3387	652.2348
1539	45.0009	2.3374	358.2867	1539	45.0009	2.3374	680.9669	1539	45.0009	2.3374	301.8583	1539	45.0009	2.3374	655.3024
1540	45.0269	2.3361	345.5432	1540	45.0269	2.3361	670.4898	1540	45.0269	2.3361	324.2911	1540	45.0269	2.3361	675.8878
1541	45.0529	2.3349	348.869	1541	45.0529	2.3349	674.795	1541	45.0529	2.3349	335.8562	1541	45.0529	2.3349	686.8787
1542	45.0789	2.3336	348.5456	1542	45.0789	2.3336	675.4513	1542	45.0789	2.3336	322.647	1542	45.0789	2.3336	673.0953
1543	45.1049	2.3323	382.5057	1543	45.1049	2.3323	710.3909	1543	45.1049	2.3323	334.6215	1543	45.1049	2.3323	684.4956

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1544	45.1309	2.331	366.0897	1544	45.1309	2.331	694.9544	1544	45.1309	2.331	354.4284	1544	45.1309	2.331	703.7283
1545	45.1569	2.3298	316.4768	1545	45.1569	2.3298	646.321	1545	45.1569	2.3298	348.7146	1545	45.1569	2.3298	697.4403
1546	45.1829	2.3285	347.4204	1546	45.1829	2.3285	678.2442	1546	45.1829	2.3285	341.1682	1546	45.1829	2.3285	689.3198
1547	45.2089	2.3272	337.1899	1547	45.2089	2.3272	668.9932	1547	45.2089	2.3272	348.3442	1547	45.2089	2.3272	695.9216
1548	45.2349	2.3259	337.4232	1548	45.2349	2.3259	670.206	1548	45.2349	2.3259	313.984	1548	45.2349	2.3259	660.9872
1549	45.2609	2.3247	356.4823	1549	45.2609	2.3247	690.2447	1549	45.2609	2.3247	291.6501	1549	45.2609	2.3247	638.0791
1550	45.2869	2.3234	349.2811	1550	45.2869	2.3234	684.023	1550	45.2869	2.3234	325.8154	1550	45.2869	2.3234	671.6703
1551	45.3129	2.3222	341.899	1551	45.3129	2.3222	677.6204	1551	45.3129	2.3222	332.449	1551	45.3129	2.3222	677.7297
1552	45.3389	2.3209	338.2464	1552	45.3389	2.3209	674.9474	1552	45.3389	2.3209	299.262	1552	45.3389	2.3209	643.9685
1553	45.3649	2.3196	360.5448	1553	45.3649	2.3196	698.2253	1553	45.3649	2.3196	312.6965	1553	45.3649	2.3196	656.8289
1554	45.3909	2.3184	370.4332	1554	45.3909	2.3184	709.0932	1554	45.3909	2.3184	295.8197	1554	45.3909	2.3184	639.3779
1555	45.4169	2.3171	321.2229	1555	45.4169	2.3171	660.8624	1555	45.4169	2.3171	300.6346	1555	45.4169	2.3171	643.6186
1556	45.4429	2.3159	318.6352	1556	45.4429	2.3159	659.2543	1556	45.4429	2.3159	340.8569	1556	45.4429	2.3159	683.2667
1557	45.4689	2.3146	319.6476	1557	45.4689	2.3146	661.2462	1557	45.4689	2.3146	314.2177	1557	45.4689	2.3146	656.0534
1558	45.4949	2.3134	284.7902	1558	45.4949	2.3134	627.3683	1558	45.4949	2.3134	288.2484	1558	45.4949	2.3134	629.5099
1559	45.5209	2.3121	332.2063	1559	45.5209	2.3121	675.7639	1559	45.5209	2.3121	293.3127	1559	45.5209	2.3121	634
1560	45.5469	2.3109	364.8104	1560	45.5469	2.3109	709.3476	1560	45.5469	2.3109	300.2606	1560	45.5469	2.3109	640.3738
1561	45.5729	2.3096	359.5139	1561	45.5729	2.3096	705.0306	1561	45.5729	2.3096	326.2675	1561	45.5729	2.3096	665.8065
1562	45.5989	2.3084	375.1055	1562	45.5989	2.3084	721.6017	1562	45.5989	2.3084	344.0126	1562	45.5989	2.3084	682.9774
1563	45.6249	2.3071	356.4635	1563	45.6249	2.3071	703.9393	1563	45.6249	2.3071	374.1935	1563	45.6249	2.3071	712.5841
1564	45.6509	2.3059	330.5959	1564	45.6509	2.3059	679.0513	1564	45.6509	2.3059	365.867	1564	45.6509	2.3059	703.6835
1565	45.6769	2.3046	351.1234	1565	45.6769	2.3046	700.5583	1565	45.6769	2.3046	322.8685	1565	45.6769	2.3046	660.1108
1566	45.7029	2.3034	342.1579	1566	45.7029	2.3034	692.5723	1566	45.7029	2.3034	321.2751	1566	45.7029	2.3034	657.9432
1567	45.7289	2.3021	345.5432	1567	45.7289	2.3021	696.9372	1567	45.7289	2.3021	324.2911	1567	45.7289	2.3021	660.3851
1568	45.7549	2.3009	404.5165	1568	45.7549	2.3009	756.0354	1568	45.7549	2.3009	325.7261	1568	45.7549	2.3009	660.6447
1569	45.7809	2.2997	411.3796	1569	45.7809	2.2997	763.0234	1569	45.7809	2.2997	336.3029	1569	45.7809	2.2997	670.0461
1570	45.8069	2.2984	399.7524	1570	45.8069	2.2984	751.5212	1570	45.8069	2.2984	335.8828	1570	45.8069	2.2984	668.4508
1571	45.8329	2.2972	425.2884	1571	45.8329	2.2972	777.1821	1571	45.8329	2.2972	324.6254	1571	45.8329	2.2972	656.018
1572	45.8589	2.296	475.278	1572	45.8589	2.296	827.2966	1572	45.8589	2.296	341.7277	1572	45.8589	2.296	671.9449
1573	45.8849	2.2947	507.2031	1573	45.8849	2.2947	859.3466	1573	45.8849	2.2947	357.1969	1573	45.8849	2.2947	686.2388
1574	45.9109	2.2935	550.0849	1574	45.9109	2.2935	902.3534	1574	45.9109	2.2935	376.9781	1574	45.9109	2.2935	704.8447
1575	45.9369	2.2923	645.7436	1575	45.9369	2.2923	998.1371	1575	45.9369	2.2923	379.604	1575	45.9369	2.2923	706.2953
1576	45.9629	2.2911	886.8341	1576	45.9629	2.2911	1239.3525	1576	45.9629	2.2911	411.1499	1576	45.9629	2.2911	736.6658
1577	45.9889	2.2898	1215.2534	1577	45.9889	2.2898	1567.8967	1577	45.9889	2.2898	495.5592	1577	45.9889	2.2898	819.8997
1578	46.0149	2.2886	1713.1313	1578	46.0149	2.2886	2065.8995	1578	46.0149	2.2886	584.3302	1578	46.0149	2.2886	907.4954
1579	46.0409	2.2874	2106.4526	1579	46.0409	2.2874	2459.3458	1579	46.0409	2.2874	800.7379	1579	46.0409	2.2874	1122.7278

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1580	46.0669	2.2862	2071.1851	1580	46.0669	2.2862	2424.2033	1580	46.0669	2.2862	1039.6324	1580	46.0669	2.2862	1360.4469
1581	46.0929	2.2849	1788.7508	1581	46.0929	2.2849	2141.8939	1581	46.0929	2.2849	1199.7358	1581	46.0929	2.2849	1519.375
1582	46.1189	2.2837	1621.6421	1582	46.1189	2.2837	1974.9101	1582	46.1189	2.2837	956.5566	1582	46.1189	2.2837	1275.0205
1583	46.1449	2.2825	1532.558	1583	46.1449	2.2825	1885.951	1583	46.1449	2.2825	779.0373	1583	46.1449	2.2825	1096.3259
1584	46.1709	2.2813	1345.7562	1584	46.1709	2.2813	1699.2741	1584	46.1709	2.2813	835.0589	1584	46.1709	2.2813	1151.172
1585	46.1969	2.2801	1003.9195	1585	46.1969	2.2801	1357.5624	1585	46.1969	2.2801	799.7128	1585	46.1969	2.2801	1114.6507
1586	46.2229	2.2789	727.4329	1586	46.2229	2.2789	1081.2007	1586	46.2229	2.2789	638.9556	1586	46.2229	2.2789	952.7181
1587	46.2489	2.2777	589.4169	1587	46.2489	2.2777	943.3097	1587	46.2489	2.2777	459.4079	1587	46.2489	2.2777	771.9951
1588	46.2749	2.2765	524.0629	1588	46.2749	2.2765	878.0806	1588	46.2749	2.2765	412.2551	1588	46.2749	2.2765	723.667
1589	46.3009	2.2752	473.9308	1589	46.3009	2.2752	828.0734	1589	46.3009	2.2752	384.7841	1589	46.3009	2.2752	695.0206
1590	46.3269	2.274	415.953	1590	46.3269	2.274	770.2205	1590	46.3269	2.274	357.5071	1590	46.3269	2.274	666.5682
1591	46.3529	2.2728	359.2323	1591	46.3529	2.2728	713.6249	1591	46.3529	2.2728	371.8088	1591	46.3529	2.2728	679.6947
1592	46.3789	2.2716	383.4601	1592	46.3789	2.2716	737.9776	1592	46.3789	2.2716	381.3851	1592	46.3789	2.2716	688.0956
1593	46.4049	2.2704	330.6726	1593	46.4049	2.2704	685.315	1593	46.4049	2.2704	346.335	1593	46.4049	2.2704	651.8701
1594	46.4309	2.2692	345.5432	1594	46.4309	2.2692	700.3106	1594	46.4309	2.2692	324.2911	1594	46.4309	2.2692	628.6509
1595	46.4569	2.268	312.7168	1595	46.4569	2.268	667.1708	1595	46.4569	2.268	346.0082	1595	46.4569	2.268	651.3096
1596	46.4829	2.2668	350.2516	1596	46.4829	2.2668	704.3922	1596	46.4829	2.2668	354.3648	1596	46.4829	2.2668	660.6078
1597	46.5089	2.2656	373.2204	1597	46.5089	2.2656	727.0476	1597	46.5089	2.2656	341.1011	1597	46.5089	2.2656	648.2857
1598	46.5349	2.2644	354.7878	1598	46.5349	2.2644	708.3016	1598	46.5349	2.2644	400.4771	1598	46.5349	2.2644	708.6033
1599	46.5609	2.2632	337.1063	1599	46.5609	2.2632	690.3068	1599	46.5609	2.2632	363.8342	1599	46.5609	2.2632	672.902
1600	46.5869	2.262	351.2471	1600	46.5869	2.262	704.1343	1600	46.5869	2.262	377.3569	1600	46.5869	2.262	687.3663
1601	46.6129	2.2609	350.5613	1601	46.6129	2.2609	703.135	1601	46.6129	2.2609	286.525	1601	46.6129	2.2609	597.4759
1602	46.6389	2.2597	336.1379	1602	46.6389	2.2597	688.3983	1602	46.6389	2.2597	321.5694	1602	46.6389	2.2597	633.462
1603	46.6649	2.2585	324.5754	1603	46.6649	2.2585	676.5224	1603	46.6649	2.2585	351.1953	1603	46.6649	2.2585	664.0295
1604	46.6909	2.2573	322.9359	1604	46.6909	2.2573	674.5696	1604	46.6909	2.2573	319.6286	1604	46.6909	2.2573	633.4043
1605	46.7169	2.2561	270.4826	1605	46.7169	2.2561	621.8028	1605	46.7169	2.2561	349.0819	1605	46.7169	2.2561	663.7993
1606	46.7429	2.2549	365.6942	1606	46.7429	2.2549	716.7011	1606	46.7429	2.2549	324.1169	1606	46.7429	2.2549	639.7758
1607	46.7689	2.2537	357.0578	1607	46.7689	2.2537	707.7513	1607	46.7689	2.2537	320.6586	1607	46.7689	2.2537	637.2592
1608	46.7949	2.2526	284.1441	1608	46.7949	2.2526	634.5243	1608	46.7949	2.2526	323.1834	1608	46.7949	2.2526	640.7256
1609	46.8209	2.2514	328.8772	1609	46.8209	2.2514	678.944	1609	46.8209	2.2514	321.4721	1609	46.8209	2.2514	639.9559
1610	46.8469	2.2502	348.1606	1610	46.8469	2.2502	697.914	1610	46.8469	2.2502	403.2434	1610	46.8469	2.2502	722.6688
1611	46.8729	2.249	319.2128	1611	46.8729	2.249	668.6528	1611	46.8729	2.249	364.0511	1611	46.8729	2.249	684.4181
1612	46.8989	2.2478	344.0228	1612	46.8989	2.2478	693.1495	1612	46.8989	2.2478	302.7241	1612	46.8989	2.2478	624.0327
1613	46.9249	2.2467	289.4341	1613	46.9249	2.2467	638.2474	1613	46.9249	2.2467	368.6393	1613	46.9249	2.2467	690.8894
1614	46.9509	2.2455	336.2811	1614	46.9509	2.2455	684.7811	1614	46.9509	2.2455	346.906	1614	46.9509	2.2455	670.0978
1615	46.9769	2.2443	266.8486	1615	46.9769	2.2443	615.0352	1615	46.9769	2.2443	330.0999	1615	46.9769	2.2443	654.2333

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1616	47.0029	2.2431	343.1911	1616	47.0029	2.2431	691.0643	1616	47.0029	2.2431	313.3171	1616	47.0029	2.2431	638.392
1617	47.0289	2.242	329.9909	1617	47.0289	2.242	677.5508	1617	47.0289	2.242	262.7391	1617	47.0289	2.242	588.7557
1618	47.0549	2.2408	309.6848	1618	47.0549	2.2408	656.9313	1618	47.0549	2.2408	282.0218	1618	47.0549	2.2408	608.98
1619	47.0809	2.2396	311.9041	1619	47.0809	2.2396	658.8372	1619	47.0809	2.2396	335.0611	1619	47.0809	2.2396	662.9609
1620	47.1069	2.2385	294.5999	1620	47.1069	2.2385	641.2196	1620	47.1069	2.2385	326.8647	1620	47.1069	2.2385	655.7061
1621	47.1329	2.2373	345.5432	1621	47.1329	2.2373	691.8496	1621	47.1329	2.2373	324.2911	1621	47.1329	2.2373	654.0741
1622	47.1589	2.2361	320.1975	1622	47.1589	2.2361	663.9413	1622	47.1589	2.2361	321.3679	1622	47.1589	2.2361	650.3361
1623	47.1849	2.235	286.2954	1623	47.1849	2.235	627.4765	1623	47.1849	2.235	299.1956	1623	47.1849	2.235	627.349
1624	47.2109	2.2338	319.4341	1624	47.2109	2.2338	658.0525	1624	47.2109	2.2338	275.2584	1624	47.2109	2.2338	602.597
1625	47.2369	2.2327	318.8547	1625	47.2369	2.2327	654.9104	1625	47.2369	2.2327	328.4204	1625	47.2369	2.2327	654.9442
1626	47.2629	2.2315	313.4967	1626	47.2629	2.2315	646.9898	1626	47.2629	2.2315	305.6214	1626	47.2629	2.2315	631.3304
1627	47.2889	2.2304	334.1293	1627	47.2889	2.2304	665.0598	1627	47.2889	2.2304	270.0507	1627	47.2889	2.2304	594.945
1628	47.3149	2.2292	317.365	1628	47.3149	2.2292	645.7328	1628	47.3149	2.2292	332.7221	1628	47.3149	2.2292	656.8015
1629	47.3409	2.228	342.4366	1629	47.3409	2.228	668.2417	1629	47.3409	2.228	308.3355	1629	47.3409	2.228	631.6002
1630	47.3669	2.2269	363.1429	1630	47.3669	2.2269	686.3854	1630	47.3669	2.2269	337.6867	1630	47.3669	2.2269	660.1366
1631	47.3929	2.2257	360.0535	1631	47.3929	2.2257	680.7334	1631	47.3929	2.2257	311.4717	1631	47.3929	2.2257	633.1068
1632	47.4189	2.2246	292.2766	1632	47.4189	2.2246	610.3938	1632	47.4189	2.2246	310.0802	1632	47.4189	2.2246	630.9004
1633	47.4449	2.2234	337.5364	1633	47.4449	2.2234	653.0909	1633	47.4449	2.2234	317.6422	1633	47.4449	2.2234	637.6477
1634	47.4709	2.2223	334.8826	1634	47.4709	2.2223	647.8745	1634	47.4709	2.2223	316.6217	1634	47.4709	2.2223	635.8124
1635	47.4969	2.2211	327.062	1635	47.4969	2.2211	637.4912	1635	47.4969	2.2211	328.4287	1635	47.4969	2.2211	646.8046
1636	47.5229	2.22	325.0252	1636	47.5229	2.22	632.8918	1636	47.5229	2.22	336.3241	1636	47.5229	2.22	653.8853
1637	47.5489	2.2189	355.847	1637	47.5489	2.2189	661.1509	1637	47.5489	2.2189	339.0208	1637	47.5489	2.2189	655.7671
1638	47.5749	2.2177	343.7853	1638	47.5749	2.2177	646.5266	1638	47.5749	2.2177	318.1095	1638	47.5749	2.2177	634.041
1639	47.6009	2.2166	350.7779	1639	47.6009	2.2166	650.9566	1639	47.6009	2.2166	344.7638	1639	47.6009	2.2166	659.8805
1640	47.6269	2.2154	321.9906	1640	47.6269	2.2154	619.6066	1640	47.6269	2.2154	324.9915	1640	47.6269	2.2154	639.2934
1641	47.6529	2.2143	352.6833	1641	47.6529	2.2143	647.7367	1641	47.6529	2.2143	355.9769	1641	47.6529	2.2143	669.4641
1642	47.6789	2.2132	359.7466	1642	47.6789	2.2132	652.2372	1642	47.6789	2.2132	360.8473	1642	47.6789	2.2132	673.5197
1643	47.7049	2.212	366.5631	1643	47.7049	2.212	656.4911	1643	47.7049	2.212	333.7918	1643	47.7049	2.212	645.6493
1644	47.7309	2.2109	381.0067	1644	47.7309	2.2109	668.3721	1644	47.7309	2.2109	364.0269	1644	47.7309	2.2109	675.0697
1645	47.7569	2.2098	348.6832	1645	47.7569	2.2098	633.4859	1645	47.7569	2.2098	324.6887	1645	47.7569	2.2098	634.9167
1646	47.7829	2.2086	343.9274	1646	47.7829	2.2086	626.1674	1646	47.7829	2.2086	344.3235	1646	47.7829	2.2086	653.7367
1647	47.8089	2.2075	345.3115	1647	47.8089	2.2075	624.9888	1647	47.8089	2.2075	358.3867	1647	47.8089	2.2075	666.9851
1648	47.8349	2.2064	345.5432	1648	47.8349	2.2064	622.658	1648	47.8349	2.2064	324.2911	1648	47.8349	2.2064	632.0747
1649	47.8609	2.2052	340.1581	1649	47.8609	2.2052	618.4636	1649	47.8609	2.2052	331.6687	1649	47.8609	2.2052	638.6822
1650	47.8869	2.2041	379.2591	1650	47.8869	2.2041	658.7554	1650	47.8869	2.2041	349.8617	1650	47.8869	2.2041	656.1051
1651	47.9129	2.203	393.518	1651	47.9129	2.203	674.205	1651	47.9129	2.203	357.9242	1651	47.9129	2.203	663.3975

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1652	47.9389	2.2019	341.3684	1652	47.9389	2.2019	623.2462	1652	47.9389	2.2019	343.9846	1652	47.9389	2.2019	648.6877
1653	47.9649	2.2007	342.3501	1653	47.9649	2.2007	625.4186	1653	47.9649	2.2007	335.2837	1653	47.9649	2.2007	639.2167
1654	47.9909	2.1996	367.9222	1654	47.9909	2.1996	652.1814	1654	47.9909	2.1996	358.3813	1654	47.9909	2.1996	661.5442
1655	48.0169	2.1985	380.3779	1655	48.0169	2.1985	665.8279	1655	48.0169	2.1985	340.0611	1655	48.0169	2.1985	642.4539
1656	48.0429	2.1974	369.7369	1656	48.0429	2.1974	656.3776	1656	48.0429	2.1974	334.1568	1656	48.0429	2.1974	635.7796
1657	48.0689	2.1963	350.913	1657	48.0689	2.1963	638.7445	1657	48.0689	2.1963	353.9716	1657	48.0689	2.1963	654.8242
1658	48.0949	2.1951	377.3859	1658	48.0949	2.1951	666.4082	1658	48.0949	2.1951	368.2989	1658	48.0949	2.1951	668.3814
1659	48.1209	2.194	351.8427	1659	48.1209	2.194	642.0557	1659	48.1209	2.194	346.0503	1659	48.1209	2.194	645.3627
1660	48.1469	2.1929	322.5302	1660	48.1469	2.1929	613.934	1660	48.1469	2.1929	322.4577	1660	48.1469	2.1929	621
1661	48.1729	2.1918	354.0943	1661	48.1729	2.1918	646.6888	1661	48.1729	2.1918	351.7935	1661	48.1729	2.1918	649.5657
1662	48.1989	2.1907	360.7952	1662	48.1989	2.1907	654.5804	1662	48.1989	2.1907	353.0825	1662	48.1989	2.1907	650.0845
1663	48.2249	2.1896	346.4782	1663	48.2249	2.1896	641.4543	1663	48.2249	2.1896	327.204	1663	48.2249	2.1896	623.436
1664	48.2509	2.1885	340.3371	1664	48.2509	2.1885	636.5039	1664	48.2509	2.1885	320.5443	1664	48.2509	2.1885	616.0062
1665	48.2769	2.1874	346.9179	1665	48.2769	2.1874	644.2754	1665	48.2769	2.1874	323.6692	1665	48.2769	2.1874	618.361
1666	48.3029	2.1863	343.9878	1666	48.3029	2.1863	642.536	1666	48.3029	2.1863	342.5836	1666	48.3029	2.1863	636.5052
1667	48.3289	2.1851	337.7113	1667	48.3289	2.1851	637.4503	1667	48.3289	2.1851	331.4365	1667	48.3289	2.1851	624.588
1668	48.3549	2.184	346.0702	1668	48.3549	2.184	647	1668	48.3549	2.184	340.9221	1668	48.3549	2.184	633.3035
1669	48.3809	2.1829	325.546	1669	48.3809	2.1829	627.6665	1669	48.3809	2.1829	349.7683	1669	48.3809	2.1829	641.3796
1670	48.4069	2.1818	323.5528	1670	48.4069	2.1818	626.8641	1670	48.4069	2.1818	327.5054	1670	48.4069	2.1818	618.3465
1671	48.4329	2.1807	351.0682	1671	48.4329	2.1807	655.5702	1671	48.4329	2.1807	341.7549	1671	48.4329	2.1807	631.8259
1672	48.4589	2.1796	334.6125	1672	48.4589	2.1796	640.3053	1672	48.4589	2.1796	320.1418	1672	48.4589	2.1796	609.4427
1673	48.4849	2.1785	341.8114	1673	48.4849	2.1785	648.6949	1673	48.4849	2.1785	329.3258	1673	48.4849	2.1785	617.8566
1674	48.5109	2.1774	371.1256	1674	48.5109	2.1774	679.1999	1674	48.5109	2.1774	351.6392	1674	48.5109	2.1774	639.3999
1675	48.5369	2.1763	345.5432	1675	48.5369	2.1763	654.8083	1675	48.5369	2.1763	368.1945	1675	48.5369	2.1763	655.1851
1676	48.5629	2.1752	329.64	1676	48.5629	2.1752	637.8182	1676	48.5629	2.1752	379.408	1676	48.5629	2.1752	665.6285
1677	48.5889	2.1742	333.1644	1677	48.5889	2.1742	640.2559	1677	48.5889	2.1742	343.3246	1677	48.5889	2.1742	628.775
1678	48.6149	2.1731	334.862	1678	48.6149	2.1731	640.8668	1678	48.6149	2.1731	336.7817	1678	48.6149	2.1731	621.462
1679	48.6409	2.172	312.5859	1679	48.6409	2.172	617.5039	1679	48.6409	2.172	304.2434	1679	48.6409	2.172	588.1535
1680	48.6669	2.1709	320.8496	1680	48.6669	2.1709	624.6809	1680	48.6669	2.1709	320.3931	1680	48.6669	2.1709	603.5332
1681	48.6929	2.1698	328.2137	1681	48.6929	2.1698	630.9582	1681	48.6929	2.1698	338.6384	1681	48.6929	2.1698	621.0084
1682	48.7189	2.1687	339.3422	1682	48.7189	2.1687	641	1682	48.7189	2.1687	354.3934	1682	48.7189	2.1687	635.9932
1683	48.7449	2.1676	346.0216	1683	48.7449	2.1676	646.5927	1683	48.7449	2.1676	353.5751	1683	48.7449	2.1676	634.4048
1684	48.7709	2.1665	360.418	1684	48.7709	2.1665	659.9023	1684	48.7709	2.1665	312.749	1684	48.7709	2.1665	592.8086
1685	48.7969	2.1655	369.4196	1685	48.7969	2.1655	667.8172	1685	48.7969	2.1655	389.1869	1685	48.7969	2.1655	668.4764
1686	48.8229	2.1644	370.3614	1686	48.8229	2.1644	667.6722	1686	48.8229	2.1644	343.6612	1686	48.8229	2.1644	622.1806
1687	48.8489	2.1633	335.3179	1687	48.8489	2.1633	631.542	1687	48.8489	2.1633	344.5319	1687	48.8489	2.1633	622.2811

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1688	48.8749	2.1622	337.8627	1688	48.8749	2.1622	633	1688	48.8749	2.1622	320.2529	1688	48.8749	2.1622	597.2321
1689	48.9009	2.1611	342.4658	1689	48.9009	2.1611	636.5164	1689	48.9009	2.1611	356.4789	1689	48.9009	2.1611	632.688
1690	48.9269	2.1601	350.8999	1690	48.9269	2.1601	643.8638	1690	48.9269	2.1601	323.8335	1690	48.9269	2.1601	599.2724
1691	48.9529	2.159	351.3759	1691	48.9529	2.159	643.253	1691	48.9529	2.159	337.6227	1691	48.9529	2.159	612.2916
1692	48.9789	2.1579	383.431	1692	48.9789	2.1579	674.2214	1692	48.9789	2.1579	326.5072	1692	48.9789	2.1579	600.406
1693	49.0049	2.1568	379.3749	1693	49.0049	2.1568	669.0785	1693	49.0049	2.1568	362.391	1693	49.0049	2.1568	635.5196
1694	49.0309	2.1558	356.7707	1694	49.0309	2.1558	645.3875	1694	49.0309	2.1558	359.8587	1694	49.0309	2.1558	632.2171
1695	49.0569	2.1547	343.996	1695	49.0569	2.1547	631.5262	1695	49.0569	2.1547	362.896	1695	49.0569	2.1547	634.4844
1696	49.0829	2.1536	315.5555	1696	49.0829	2.1536	601.9989	1696	49.0829	2.1536	342.36	1696	49.0829	2.1536	613.1783
1697	49.1089	2.1525	327.8767	1697	49.1089	2.1525	613.2333	1697	49.1089	2.1525	366.4853	1697	49.1089	2.1525	636.5334
1698	49.1349	2.1515	341.3488	1698	49.1349	2.1515	625.6187	1698	49.1349	2.1515	341.8371	1698	49.1349	2.1515	611.1151
1699	49.1609	2.1504	349.4493	1699	49.1609	2.1504	632.6325	1699	49.1609	2.1504	336.6232	1699	49.1609	2.1504	605.1311
1700	49.1869	2.1493	350.857	1700	49.1869	2.1493	632.9534	1700	49.1869	2.1493	407.3146	1700	49.1869	2.1493	675.0524
1701	49.2129	2.1483	392.4605	1701	49.2129	2.1483	673.4701	1701	49.2129	2.1483	349.9371	1701	49.2129	2.1483	616.9048
1702	49.2389	2.1472	345.5432	1702	49.2389	2.1472	625.4662	1702	49.2389	2.1472	324.2911	1702	49.2389	2.1472	590.4887
1703	49.2649	2.1461	358.7368	1703	49.2649	2.1461	638.6942	1703	49.2649	2.1461	334.4301	1703	49.2649	2.1461	601.2968
1704	49.2909	2.1451	377.3474	1704	49.2909	2.1451	657.3393	1704	49.2909	2.1451	389.4175	1704	49.2909	2.1451	656.9533
1705	49.3169	2.144	353.604	1705	49.3169	2.144	633.6303	1705	49.3169	2.144	370.0559	1705	49.3169	2.144	638.2607
1706	49.3429	2.143	350.7641	1706	49.3429	2.143	630.8249	1706	49.3429	2.143	361.7961	1706	49.3429	2.143	630.67
1707	49.3689	2.1419	358.5259	1707	49.3689	2.1419	638.6212	1707	49.3689	2.1419	357.0216	1707	49.3689	2.1419	626.5646
1708	49.3949	2.1409	340.6196	1708	49.3949	2.1409	620.7494	1708	49.3949	2.1409	351.2265	1708	49.3949	2.1409	621.4385
1709	49.4209	2.1398	337.1521	1709	49.4209	2.1398	617.3163	1709	49.4209	2.1398	357.7516	1709	49.4209	2.1398	628.6327
1710	49.4469	2.1387	342.3304	1710	49.4469	2.1387	622.5292	1710	49.4469	2.1387	368.5354	1710	49.4469	2.1387	640.0856
1711	49.4729	2.1377	333.4765	1711	49.4729	2.1377	613.7097	1711	49.4729	2.1377	367.249	1711	49.4729	2.1377	639.4683
1712	49.4989	2.1366	382.9977	1712	49.4989	2.1366	663.2654	1712	49.4989	2.1366	293.9712	1712	49.4989	2.1366	566.8596
1713	49.5249	2.1356	351.9585	1713	49.5249	2.1356	632.2607	1713	49.5249	2.1356	371.3215	1713	49.5249	2.1356	644.879
1714	49.5509	2.1345	371.598	1714	49.5509	2.1345	651.9346	1714	49.5509	2.1345	286.0848	1714	49.5509	2.1345	560.3113
1715	49.5769	2.1335	350.7719	1715	49.5769	2.1335	631.143	1715	49.5769	2.1335	384.4235	1715	49.5769	2.1335	659.3191
1716	49.6029	2.1324	361.4103	1716	49.6029	2.1324	641.816	1716	49.6029	2.1324	320.5229	1716	49.6029	2.1324	596.0876
1717	49.6289	2.1314	330.4128	1717	49.6289	2.1314	610.8529	1717	49.6289	2.1314	341.1532	1717	49.6289	2.1314	617.387
1718	49.6549	2.1303	406.5993	1718	49.6549	2.1303	687.0739	1718	49.6549	2.1303	372.8902	1718	49.6549	2.1303	649.793
1719	49.6809	2.1293	357.0484	1719	49.6809	2.1293	637.5574	1719	49.6809	2.1293	339.102	1719	49.6809	2.1293	616.674
1720	49.7069	2.1283	347.8514	1720	49.7069	2.1283	628.3949	1720	49.7069	2.1283	365.0664	1720	49.7069	2.1283	643.3074
1721	49.7329	2.1272	301.6728	1721	49.7329	2.1272	582.2508	1721	49.7329	2.1272	338.0802	1721	49.7329	2.1272	616.9903
1722	49.7589	2.1262	295.6163	1722	49.7589	2.1262	576.2288	1722	49.7589	2.1262	388.9975	1722	49.7589	2.1262	668.5766
1723	49.7849	2.1251	352.9232	1723	49.7849	2.1251	633.5702	1723	49.7849	2.1251	355.2855	1723	49.7849	2.1251	635.5337

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1724	49.8109	2.1241	340.2408	1724	49.8109	2.1241	620.9222	1724	49.8109	2.1241	326.6777	1724	49.8109	2.1241	607.595
1725	49.8369	2.1231	343.6479	1725	49.8369	2.1231	624.3638	1725	49.8369	2.1231	322.5197	1725	49.8369	2.1231	604.106
1726	49.8629	2.122	370.771	1726	49.8629	2.122	651.5214	1726	49.8629	2.122	339.4255	1726	49.8629	2.122	621.6809
1727	49.8889	2.121	347.9914	1727	49.8889	2.121	628.7763	1727	49.8889	2.121	313.9777	1727	49.8889	2.121	596.9022
1728	49.9149	2.12	337.2671	1728	49.9149	2.12	618.0864	1728	49.9149	2.12	291.2582	1728	49.9149	2.12	574.8518
1729	49.9409	2.1189	345.5432	1729	49.9409	2.1189	626.3971	1729	49.9409	2.1189	360.351	1729	49.9409	2.1189	644.6137
1730	49.9669	2.1179	306.989	1730	49.9669	2.1179	587.4709	1730	49.9669	2.1179	331.5392	1730	49.9669	2.1179	616.4709
1731	49.9929	2.1169	354.1283	1731	49.9929	2.1169	634.2382	1731	49.9929	2.1169	344.26	1731	49.9929	2.1169	629.8608
1732	50.0189	2.1158	374.3316	1732	50.0189	2.1158	654.0696	1732	50.0189	2.1158	318.8722	1732	50.0189	2.1158	605.1421
1733	50.0449	2.1148	396.1841	1733	50.0449	2.1148	675.5501	1733	50.0449	2.1148	298.213	1733	50.0449	2.1148	585.152
1734	50.0709	2.1138	377.6706	1734	50.0709	2.1138	656.6647	1734	50.0709	2.1138	345.086	1734	50.0709	2.1138	632.694
1735	50.0969	2.1127	367.6094	1735	50.0969	2.1127	646.2315	1735	50.0969	2.1127	349.5702	1735	50.0969	2.1127	637.8473
1736	50.1229	2.1117	384.8007	1736	50.1229	2.1117	663.0509	1736	50.1229	2.1117	369.0288	1736	50.1229	2.1117	657.975
1737	50.1489	2.1107	393.2213	1737	50.1489	2.1107	671.0996	1737	50.1489	2.1107	375.1596	1737	50.1489	2.1107	664.7749
1738	50.1749	2.1097	392.9637	1738	50.1749	2.1097	670.47	1738	50.1749	2.1097	306.6326	1738	50.1749	2.1097	596.917
1739	50.2009	2.1087	393.6207	1739	50.2009	2.1087	670.7551	1739	50.2009	2.1087	331.105	1739	50.2009	2.1087	622.0584
1740	50.2269	2.1076	410.6305	1740	50.2269	2.1076	687.3929	1740	50.2269	2.1076	306.6306	1740	50.2269	2.1076	598.2531
1741	50.2529	2.1066	483.5137	1741	50.2529	2.1066	759.9042	1741	50.2529	2.1066	336.0859	1741	50.2529	2.1066	628.3774
1742	50.2789	2.1056	431.1009	1742	50.2789	2.1056	707.1194	1742	50.2789	2.1056	326.3795	1742	50.2789	2.1056	619.3402
1743	50.3049	2.1046	417.3761	1743	50.3049	2.1046	693.0227	1743	50.3049	2.1046	361.4383	1743	50.3049	2.1046	655.0681
1744	50.3309	2.1036	429.3689	1744	50.3309	2.1036	704.6436	1744	50.3309	2.1036	349.778	1744	50.3309	2.1036	644.0768
1745	50.3569	2.1025	452.963	1745	50.3569	2.1025	727.8657	1745	50.3569	2.1025	342.5963	1745	50.3569	2.1025	637.5642
1746	50.3829	2.1015	567.366	1746	50.3829	2.1015	841.8967	1746	50.3829	2.1015	347.791	1746	50.3829	2.1015	643.428
1747	50.4089	2.1005	673.9494	1747	50.4089	2.1005	948.1082	1747	50.4089	2.1005	354.775	1747	50.4089	2.1005	651.0811
1748	50.4349	2.0995	929.9013	1748	50.4349	2.0995	1203.6882	1748	50.4349	2.0995	402.2962	1748	50.4349	2.0995	699.2713
1749	50.4609	2.0985	1341.0214	1749	50.4609	2.0985	1614.4363	1749	50.4609	2.0985	422.3883	1749	50.4609	2.0985	720.0325
1750	50.4869	2.0975	1978.8061	1750	50.4869	2.0975	2251.8491	1750	50.4869	2.0975	514.3437	1750	50.4869	2.0975	812.657
1751	50.5129	2.0965	2352.0829	1751	50.5129	2.0965	2624.754	1751	50.5129	2.0965	577.1014	1751	50.5129	2.0965	876.0838
1752	50.5389	2.0955	2132.3453	1752	50.5389	2.0955	2404.6444	1752	50.5389	2.0955	635.9381	1752	50.5389	2.0955	935.5895
1753	50.5649	2.0945	1779.846	1753	50.5649	2.0945	2051.7731	1753	50.5649	2.0945	735.6876	1753	50.5649	2.0945	1036.0081
1754	50.5909	2.0935	1607.2476	1754	50.5909	2.0935	1878.8028	1754	50.5909	2.0935	679.8026	1754	50.5909	2.0935	980.7922
1755	50.6169	2.0925	1575.1834	1755	50.6169	2.0925	1846.3667	1755	50.6169	2.0925	562.2707	1755	50.6169	2.0925	863.9294
1756	50.6429	2.0914	1494.1641	1756	50.6429	2.0914	1764.9754	1756	50.6429	2.0914	472.8984	1756	50.6429	2.0914	775.2261
1757	50.6689	2.0904	1185.5324	1757	50.6689	2.0904	1455.9718	1757	50.6689	2.0904	477.8434	1757	50.6689	2.0904	779.5047
1758	50.6949	2.0894	849.4024	1758	50.6949	2.0894	1119.4698	1758	50.6949	2.0894	434.7895	1758	50.6949	2.0894	735.7843
1759	50.7209	2.0884	661.0585	1759	50.7209	2.0884	930.754	1759	50.7209	2.0884	399.2662	1759	50.7209	2.0884	699.5946

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1760	50.7469	2.0874	554.3812	1760	50.7469	2.0874	823.7048	1760	50.7469	2.0874	377.5233	1760	50.7469	2.0874	677.1852
1761	50.7729	2.0864	486.2102	1761	50.7729	2.0864	755.1617	1761	50.7729	2.0864	320.2399	1761	50.7729	2.0864	619.2353
1762	50.7989	2.0854	458.1519	1762	50.7989	2.0854	726.7316	1762	50.7989	2.0854	325.5401	1762	50.7989	2.0854	623.869
1763	50.8249	2.0845	459.4784	1763	50.8249	2.0845	727.6861	1763	50.8249	2.0845	334.83	1763	50.8249	2.0845	632.4924
1764	50.8509	2.0835	427.6464	1764	50.8509	2.0835	695.4821	1764	50.8509	2.0835	314.9201	1764	50.8509	2.0835	611.916
1765	50.8769	2.0825	383.0859	1765	50.8769	2.0825	650.5497	1765	50.8769	2.0825	288.7933	1765	50.8769	2.0825	585.1228
1766	50.9029	2.0815	370.0366	1766	50.9029	2.0815	637.1285	1766	50.9029	2.0815	295.6176	1766	50.9029	2.0815	591.2806
1767	50.9289	2.0805	371.4841	1767	50.9289	2.0805	638.204	1767	50.9289	2.0805	311.1638	1767	50.9289	2.0805	606.1603
1768	50.9549	2.0795	397.3444	1768	50.9549	2.0795	663.6924	1768	50.9549	2.0795	311.6238	1768	50.9549	2.0795	605.9539
1769	50.9809	2.0785	400.7285	1769	50.9809	2.0785	666.7045	1769	50.9809	2.0785	331.6234	1769	50.9809	2.0785	625.2869
1770	51.0069	2.0775	386.5554	1770	51.0069	2.0775	652.1594	1770	51.0069	2.0775	347.0844	1770	51.0069	2.0775	640.0815
1771	51.0329	2.0765	382.6416	1771	51.0329	2.0765	647.8737	1771	51.0329	2.0765	330.2912	1771	51.0329	2.0765	622.6219
1772	51.0589	2.0755	357.1598	1772	51.0589	2.0755	622.02	1772	51.0589	2.0755	301.3092	1772	51.0589	2.0755	592.9734
1773	51.0849	2.0746	349.271	1773	51.0849	2.0746	613.7593	1773	51.0849	2.0746	325.9386	1773	51.0849	2.0746	616.9363
1774	51.1109	2.0736	356.9226	1774	51.1109	2.0736	621.0389	1774	51.1109	2.0736	328.29	1774	51.1109	2.0736	618.6212
1775	51.1369	2.0726	398.0517	1775	51.1369	2.0726	661.796	1775	51.1369	2.0726	310.1632	1775	51.1369	2.0726	599.8279
1776	51.1629	2.0716	416.0587	1776	51.1629	2.0716	679.4311	1776	51.1629	2.0716	309.5966	1776	51.1629	2.0716	598.5948
1777	51.1889	2.0706	365.7178	1777	51.1889	2.0706	628.7183	1777	51.1889	2.0706	328.6064	1777	51.1889	2.0706	616.9382
1778	51.2149	2.0696	378.7459	1778	51.2149	2.0696	641.3744	1778	51.2149	2.0696	351.9049	1778	51.2149	2.0696	639.5702
1779	51.2409	2.0687	358.7893	1779	51.2409	2.0687	621.0459	1779	51.2409	2.0687	343.9297	1779	51.2409	2.0687	630.9285
1780	51.2669	2.0677	378.2878	1780	51.2669	2.0677	640.1724	1780	51.2669	2.0677	311.5079	1780	51.2669	2.0677	597.8402
1781	51.2929	2.0667	410.9937	1781	51.2929	2.0667	672.5064	1781	51.2929	2.0667	337.379	1781	51.2929	2.0667	623.0449
1782	51.3189	2.0657	347.8297	1782	51.3189	2.0657	608.9704	1782	51.3189	2.0657	341.7018	1782	51.3189	2.0657	626.7012
1783	51.3449	2.0648	345.5432	1783	51.3449	2.0648	606.312	1783	51.3449	2.0648	324.2911	1783	51.3449	2.0648	608.6241
1784	51.3709	2.0638	330.8391	1784	51.3709	2.0638	592.6171	1784	51.3709	2.0638	304.9917	1784	51.3709	2.0638	588.948
1785	51.3969	2.0628	341.6648	1785	51.3969	2.0628	604.4521	1785	51.3969	2.0628	314.6696	1785	51.3969	2.0628	598.2493
1786	51.4229	2.0618	361.1616	1786	51.4229	2.0618	624.9581	1786	51.4229	2.0618	295.5711	1786	51.4229	2.0618	578.7742
1787	51.4489	2.0609	339.0429	1787	51.4489	2.0609	603.8486	1787	51.4489	2.0609	317.1432	1787	51.4489	2.0609	599.9696
1788	51.4749	2.0599	318.8642	1788	51.4749	2.0599	584.6791	1788	51.4749	2.0599	344.6915	1788	51.4749	2.0599	627.1413
1789	51.5009	2.0589	339.256	1789	51.5009	2.0589	606.0801	1789	51.5009	2.0589	363.7122	1789	51.5009	2.0589	645.7854
1790	51.5269	2.058	332.1352	1790	51.5269	2.058	599.9686	1790	51.5269	2.058	332.6074	1790	51.5269	2.058	614.304
1791	51.5529	2.057	360.8957	1791	51.5529	2.057	629.7383	1791	51.5529	2.057	296.462	1791	51.5529	2.057	577.7819
1792	51.5789	2.056	369.6688	1792	51.5789	2.056	639.5206	1792	51.5789	2.056	301.973	1792	51.5789	2.056	582.9163
1793	51.6049	2.0551	347.3743	1793	51.6049	2.0551	618.2353	1793	51.6049	2.0551	285.0965	1793	51.6049	2.0551	565.6631
1794	51.6309	2.0541	358.5233	1794	51.6309	2.0541	630.3936	1794	51.6309	2.0541	338.3207	1794	51.6309	2.0541	618.5108
1795	51.6569	2.0531	311.3051	1795	51.6569	2.0531	584.1846	1795	51.6569	2.0531	320.9664	1795	51.6569	2.0531	600.7798

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1796	51.6829	2.0522	327.7006	1796	51.6829	2.0522	601.5893	1796	51.6829	2.0522	335.8677	1796	51.6829	2.0522	615.3045
1797	51.7089	2.0512	320.362	1797	51.7089	2.0512	595.2599	1797	51.7089	2.0512	291.4566	1797	51.7089	2.0512	570.5168
1798	51.7349	2.0502	349.2894	1798	51.7349	2.0502	625.1965	1798	51.7349	2.0502	333.6201	1798	51.7349	2.0502	612.3036
1799	51.7609	2.0493	321.4236	1799	51.7609	2.0493	598.34	1799	51.7609	2.0493	324.0959	1799	51.7609	2.0493	602.4028
1800	51.7869	2.0483	374.0826	1800	51.7869	2.0483	652.0082	1800	51.7869	2.0483	323.1101	1800	51.7869	2.0483	601.0404
1801	51.8129	2.0474	345.6393	1801	51.8129	2.0474	624.574	1801	51.8129	2.0474	363.7261	1801	51.8129	2.0474	641.2797
1802	51.8389	2.0464	382.8468	1802	51.8389	2.0464	662.7908	1802	51.8389	2.0464	359.0655	1802	51.8389	2.0464	636.2425
1803	51.8649	2.0455	358.5247	1803	51.8649	2.0455	639.478	1803	51.8649	2.0455	312.8793	1803	51.8649	2.0455	589.6797
1804	51.8909	2.0445	298.5609	1804	51.8909	2.0445	580.5234	1804	51.8909	2.0445	303.2459	1804	51.8909	2.0445	579.6697
1805	51.9169	2.0436	325.1267	1805	51.9169	2.0436	608.0983	1805	51.9169	2.0436	304.7598	1805	51.9169	2.0436	580.807
1806	51.9429	2.0426	315.297	1806	51.9429	2.0426	599.2779	1806	51.9429	2.0426	335.4482	1806	51.9429	2.0426	611.1187
1807	51.9689	2.0417	307.8133	1807	51.9689	2.0417	592.8034	1807	51.9689	2.0417	299.518	1807	51.9689	2.0417	574.8119
1808	51.9949	2.0407	315.0148	1808	51.9949	2.0407	601.0142	1808	51.9949	2.0407	330.6744	1808	51.9949	2.0407	605.5917
1809	52.0209	2.0398	303.9557	1809	52.0209	2.0398	590.9643	1809	52.0209	2.0398	313.1248	1809	52.0209	2.0398	587.6654
1810	52.0469	2.0388	345.5432	1810	52.0469	2.0388	633.5611	1810	52.0469	2.0388	324.2911	1810	52.0469	2.0388	598.4552
1811	52.0729	2.0379	284.2483	1811	52.0729	2.0379	571.8862	1811	52.0729	2.0379	331.5469	1811	52.0729	2.0379	605.3333
1812	52.0989	2.0369	352.8957	1812	52.0989	2.0369	640.1536	1812	52.0989	2.0369	292.7448	1812	52.0989	2.0369	566.1536
1813	52.1249	2.036	357.0193	1813	52.1249	2.036	643.8973	1813	52.1249	2.036	298.0936	1813	52.1249	2.036	571.1248
1814	52.1509	2.035	305.1863	1814	52.1509	2.035	591.6844	1814	52.1509	2.035	304.3355	1814	52.1509	2.035	576.9891
1815	52.1769	2.0341	276.9011	1815	52.1769	2.0341	563.0192	1815	52.1769	2.0341	303.7345	1815	52.1769	2.0341	576.0106
1816	52.2029	2.0331	297.0826	1816	52.2029	2.0331	582.8208	1816	52.2029	2.0331	315.003	1816	52.2029	2.0331	586.9014
1817	52.2289	2.0322	370.2444	1817	52.2289	2.0322	655.6026	1817	52.2289	2.0322	326.2715	1817	52.2289	2.0322	597.7923
1818	52.2549	2.0313	343.8571	1818	52.2549	2.0313	628.8354	1818	52.2549	2.0313	338.5111	1818	52.2549	2.0313	609.6543
1819	52.2809	2.0303	271.3063	1819	52.2809	2.0303	555.9046	1819	52.2809	2.0303	359.4211	1819	52.2809	2.0303	630.1867
1820	52.3069	2.0294	297.3221	1820	52.3069	2.0294	581.5405	1820	52.3069	2.0294	326.3634	1820	52.3069	2.0294	596.7514
1821	52.3329	2.0284	383.8901	1821	52.3329	2.0284	667.7285	1821	52.3329	2.0284	351.3495	1821	52.3329	2.0284	621.36
1822	52.3589	2.0275	296.391	1822	52.3589	2.0275	579.8495	1822	52.3589	2.0275	289.0933	1822	52.3589	2.0275	558.7261
1823	52.3849	2.0266	268.7251	1823	52.3849	2.0266	551.8036	1823	52.3849	2.0266	286.5879	1823	52.3849	2.0266	555.8432
1824	52.4109	2.0256	249.0682	1824	52.4109	2.0256	531.7668	1824	52.4109	2.0256	310.8256	1824	52.4109	2.0256	579.7032
1825	52.4369	2.0247	371.2195	1825	52.4369	2.0247	653.5382	1825	52.4369	2.0247	345.9626	1825	52.4369	2.0247	614.4626
1826	52.4629	2.0238	304.7979	1826	52.4629	2.0238	586.7366	1826	52.4629	2.0238	298.1522	1826	52.4629	2.0238	566.2747
1827	52.4889	2.0228	333.3627	1827	52.4889	2.0228	614.9214	1827	52.4889	2.0228	301.956	1827	52.4889	2.0228	569.7008
1828	52.5149	2.0219	311.7901	1828	52.5149	2.0219	592.9689	1828	52.5149	2.0219	322.8162	1828	52.5149	2.0219	590.1834
1829	52.5409	2.021	326.3042	1829	52.5409	2.021	607.103	1829	52.5409	2.021	347.5616	1829	52.5409	2.021	614.5512
1830	52.5669	2.0201	331.2853	1830	52.5669	2.0201	611.7043	1830	52.5669	2.0201	326.6763	1830	52.5669	2.0201	593.2883
1831	52.5929	2.0191	331.961	1831	52.5929	2.0191	612	1831	52.5929	2.0191	317.7124	1831	52.5929	2.0191	583.9468

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1832	52.6189	2.0182	310.7016	1832	52.6189	2.0182	590.3607	1832	52.6189	2.0182	274.6968	1832	52.6189	2.0182	540.5536
1833	52.6449	2.0173	296.0302	1833	52.6449	2.0173	575.3093	1833	52.6449	2.0173	320.7965	1833	52.6449	2.0173	586.2758
1834	52.6709	2.0163	328.2233	1834	52.6709	2.0163	607.1224	1834	52.6709	2.0163	323.9616	1834	52.6709	2.0163	589.0632
1835	52.6969	2.0154	325.2456	1835	52.6969	2.0154	603.7648	1835	52.6969	2.0154	261.2848	1835	52.6969	2.0154	526.0088
1836	52.7229	2.0145	358.5274	1836	52.7229	2.0145	636.6667	1836	52.7229	2.0145	317.1944	1836	52.7229	2.0145	581.5408
1837	52.7489	2.0136	345.5432	1837	52.7489	2.0136	623.3025	1837	52.7489	2.0136	324.2911	1837	52.7489	2.0136	588.2599
1838	52.7749	2.0127	329.0876	1838	52.7749	2.0127	605.4088	1838	52.7749	2.0127	332.6316	1838	52.7749	2.0127	595.8185
1839	52.8009	2.0117	302.7066	1839	52.8009	2.0117	577.5896	1839	52.8009	2.0117	322.1014	1839	52.8009	2.0117	584.5063
1840	52.8269	2.0108	322.1539	1840	52.8269	2.0108	595.5987	1840	52.8269	2.0108	330.4235	1840	52.8269	2.0108	592.0465
1841	52.8529	2.0099	332.7363	1841	52.8529	2.0099	604.743	1841	52.8529	2.0099	320.2993	1841	52.8529	2.0099	581.1404
1842	52.8789	2.009	339.5628	1842	52.8789	2.009	610.1314	1842	52.8789	2.009	318.8731	1842	52.8789	2.009	578.9322
1843	52.9049	2.0081	317.5598	1843	52.9049	2.0081	586.6902	1843	52.9049	2.0081	339.5244	1843	52.9049	2.0081	598.8016
1844	52.9309	2.0072	337.8363	1844	52.9309	2.0072	605.5286	1844	52.9309	2.0072	363.9087	1844	52.9309	2.0072	622.4039
1845	52.9569	2.0062	353.559	1845	52.9569	2.0062	619.8132	1845	52.9569	2.0062	353.0011	1845	52.9569	2.0062	610.7144
1846	52.9829	2.0053	340.9299	1846	52.9829	2.0053	605.7459	1846	52.9829	2.0053	346.762	1846	52.9829	2.0053	603.6934
1847	53.0089	2.0044	326.7373	1847	53.0089	2.0044	590.1152	1847	53.0089	2.0044	332.8147	1847	53.0089	2.0044	588.9641
1848	53.0349	2.0035	314.6309	1848	53.0349	2.0035	576.5706	1848	53.0349	2.0035	313.8355	1848	53.0349	2.0035	569.203
1849	53.0609	2.0026	347.9966	1849	53.0609	2.0026	608.4982	1849	53.0609	2.0026	327.6589	1849	53.0609	2.0026	582.2445
1850	53.0869	2.0017	357.4777	1850	53.0869	2.0017	616.5411	1850	53.0869	2.0017	327.7374	1850	53.0869	2.0017	581.5411
1851	53.1129	2.0008	357.2373	1851	53.1129	2.0008	614.8626	1851	53.1129	2.0008	314.6094	1851	53.1129	2.0008	567.6311
1852	53.1389	1.9999	337.9948	1852	53.1389	1.9999	594.1819	1852	53.1389	1.9999	319.0001	1852	53.1389	1.9999	571.2399
1853	53.1649	1.999	345.5924	1853	53.1649	1.999	600.3413	1853	53.1649	1.999	350.7465	1853	53.1649	1.999	602.2044
1854	53.1909	1.9981	366.6711	1854	53.1909	1.9981	619.9819	1854	53.1909	1.9981	313.2928	1854	53.1909	1.9981	563.9687
1855	53.2169	1.9971	384.6046	1855	53.2169	1.9971	636.4773	1855	53.2169	1.9971	301.2485	1855	53.2169	1.9971	551.1424
1856	53.2429	1.9962	382.8708	1856	53.2429	1.9962	633.3053	1856	53.2429	1.9962	335.4948	1856	53.2429	1.9962	584.6069
1857	53.2689	1.9953	362.398	1857	53.2689	1.9953	611.3944	1857	53.2689	1.9953	347.9172	1857	53.2689	1.9953	596.2473
1858	53.2949	1.9944	331.044	1858	53.2949	1.9944	578.6022	1858	53.2949	1.9944	330.2227	1858	53.2949	1.9944	577.7709
1859	53.3209	1.9935	341.277	1859	53.3209	1.9935	587.3971	1859	53.3209	1.9935	313.1543	1859	53.3209	1.9935	559.9206
1860	53.3469	1.9926	357.3279	1860	53.3469	1.9926	602.0099	1860	53.3469	1.9926	322.2138	1860	53.3469	1.9926	568.1981
1861	53.3729	1.9917	375.9931	1861	53.3729	1.9917	619.2369	1861	53.3729	1.9917	327.3523	1861	53.3729	1.9917	572.5546
1862	53.3989	1.9908	380.2252	1862	53.3989	1.9908	622.0308	1862	53.3989	1.9908	320.3719	1862	53.3989	1.9908	564.7923
1863	53.4249	1.9899	347.1202	1863	53.4249	1.9899	587.4877	1863	53.4249	1.9899	318.3615	1863	53.4249	1.9899	562
1864	53.4509	1.989	345.5432	1864	53.4509	1.989	584.4726	1864	53.4509	1.989	324.2911	1864	53.4509	1.989	567.1477
1865	53.4769	1.9881	357.7332	1865	53.4769	1.9881	596.9709	1865	53.4769	1.9881	315.3583	1865	53.4769	1.9881	557.3594
1866	53.5029	1.9873	360.8879	1866	53.5029	1.9873	600.434	1866	53.5029	1.9873	322.1463	1866	53.5029	1.9873	563.2919
1867	53.5289	1.9864	366.6604	1867	53.5289	1.9864	606.515	1867	53.5289	1.9864	347.1048	1867	53.5289	1.9864	587.395

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1868	53.5549	1.9855	334.4818	1868	53.5549	1.9855	574.6447	1868	53.5549	1.9855	342.5388	1868	53.5549	1.9855	581.9735
1869	53.5809	1.9846	324.182	1869	53.5809	1.9846	564.6533	1869	53.5809	1.9846	322.7221	1869	53.5809	1.9846	561.3014
1870	53.6069	1.9837	364.0563	1870	53.6069	1.9837	604.8361	1870	53.6069	1.9837	316.2838	1870	53.6069	1.9837	554.0076
1871	53.6329	1.9828	369.4509	1871	53.6329	1.9828	610.5391	1871	53.6329	1.9828	346.288	1871	53.6329	1.9828	583.1563
1872	53.6589	1.9819	366.8758	1872	53.6589	1.9819	608.2724	1872	53.6589	1.9819	346.816	1872	53.6589	1.9819	582.8288
1873	53.6849	1.981	367.9347	1873	53.6849	1.981	609.6397	1873	53.6849	1.981	312.3954	1873	53.6849	1.981	547.5528
1874	53.7109	1.9801	347.9223	1874	53.7109	1.9801	589.9357	1874	53.7109	1.9801	323.3468	1874	53.7109	1.9801	557.6487
1875	53.7369	1.9792	341.3288	1875	53.7369	1.9792	583.6506	1875	53.7369	1.9792	314.8949	1875	53.7369	1.9792	548.3413
1876	53.7629	1.9784	343.2042	1876	53.7629	1.9784	585.8344	1876	53.7629	1.9784	327.9792	1876	53.7629	1.9784	560.5701
1877	53.7889	1.9775	335.3609	1877	53.7889	1.9775	578.2995	1877	53.7889	1.9775	377.3053	1877	53.7889	1.9775	609.0408
1878	53.8149	1.9766	339.7736	1878	53.8149	1.9766	583.0206	1878	53.8149	1.9766	347.4684	1878	53.8149	1.9766	578.3484
1879	53.8409	1.9757	360.2995	1879	53.8409	1.9757	603.855	1879	53.8409	1.9757	335.5622	1879	53.8409	1.9757	565.5868
1880	53.8669	1.9748	364.796	1880	53.8669	1.9748	608.6598	1880	53.8669	1.9748	349.6109	1880	53.8669	1.9748	578.7801
1881	53.8929	1.9739	347.906	1881	53.8929	1.9739	592.0782	1881	53.8929	1.9739	332.5749	1881	53.8929	1.9739	560.8885
1882	53.9189	1.9731	337.5449	1882	53.9189	1.9731	582.0255	1882	53.9189	1.9731	308.6694	1882	53.9189	1.9731	536.1275
1883	53.9449	1.9722	342.8847	1883	53.9449	1.9722	587.6738	1883	53.9449	1.9722	335.4823	1883	53.9449	1.9722	562.0851
1884	53.9709	1.9713	350.4433	1884	53.9709	1.9713	595.5407	1884	53.9709	1.9713	320.661	1884	53.9709	1.9713	546.4082
1885	53.9969	1.9704	367.0622	1885	53.9969	1.9704	612.468	1885	53.9969	1.9704	311.5426	1885	53.9969	1.9704	536.4344
1886	54.0229	1.9695	361.8034	1886	54.0229	1.9695	607.5176	1886	54.0229	1.9695	337.0439	1886	54.0229	1.9695	561.0803
1887	54.0489	1.9687	355.1118	1887	54.0489	1.9687	601.1344	1887	54.0489	1.9687	355.2283	1887	54.0489	1.9687	578.4092
1888	54.0749	1.9678	358.7343	1888	54.0749	1.9678	605.0654	1888	54.0749	1.9678	340.5045	1888	54.0749	1.9678	562.8299
1889	54.1009	1.9669	384.16	1889	54.1009	1.9669	630.7995	1889	54.1009	1.9669	347.7975	1889	54.1009	1.9669	569.2674
1890	54.1269	1.966	363.4966	1890	54.1269	1.966	610.4445	1890	54.1269	1.966	351.9115	1890	54.1269	1.966	572.526
1891	54.1529	1.9652	345.5432	1891	54.1529	1.9652	592.7995	1891	54.1529	1.9652	324.2911	1891	54.1529	1.9652	544.0501
1892	54.1789	1.9643	391.2289	1892	54.1789	1.9643	638.6306	1892	54.1789	1.9643	321.7654	1892	54.1789	1.9643	542.1886
1893	54.2049	1.9634	368.4694	1893	54.2049	1.9634	616.0165	1893	54.2049	1.9634	354.3665	1893	54.2049	1.9634	575.454
1894	54.2309	1.9626	320.781	1894	54.2309	1.9626	568.4736	1894	54.2309	1.9626	352.8601	1894	54.2309	1.9626	574.6119
1895	54.2569	1.9617	346.007	1895	54.2569	1.9617	593.845	1895	54.2569	1.9617	343.7911	1895	54.2569	1.9617	566.2072
1896	54.2829	1.9608	388.7043	1896	54.2829	1.9608	636.6878	1896	54.2829	1.9608	344.3142	1896	54.2829	1.9608	567.3945
1897	54.3089	1.96	366.9924	1897	54.3089	1.96	615.1213	1897	54.3089	1.96	335.8888	1897	54.3089	1.96	559.6333
1898	54.3349	1.9591	378.8711	1898	54.3349	1.9591	627.1454	1898	54.3349	1.9591	294.5912	1898	54.3349	1.9591	519
1899	54.3609	1.9582	355.9349	1899	54.3609	1.9582	604.3547	1899	54.3609	1.9582	310.3408	1899	54.3609	1.9582	535.4139
1900	54.3869	1.9574	374.9137	1900	54.3869	1.9574	623.4789	1900	54.3869	1.9574	384.96	1900	54.3869	1.9574	610.6973
1901	54.4129	1.9565	354.2024	1901	54.4129	1.9565	602.9131	1901	54.4129	1.9565	347.2026	1901	54.4129	1.9565	573.6042
1902	54.4389	1.9556	321.8203	1902	54.4389	1.9556	570.6765	1902	54.4389	1.9556	332.0298	1902	54.4389	1.9556	559.0957
1903	54.4649	1.9548	371.3976	1903	54.4649	1.9548	620.3992	1903	54.4649	1.9548	357.6467	1903	54.4649	1.9548	585.3768

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1904	54.4909	1.9539	339.1457	1904	54.4909	1.9539	588.2927	1904	54.4909	1.9539	323.2028	1904	54.4909	1.9539	551.5972
1905	54.5169	1.953	337.4859	1905	54.5169	1.953	586.7784	1905	54.5169	1.953	356.9413	1905	54.5169	1.953	586
1906	54.5429	1.9522	370.2286	1906	54.5429	1.9522	619.6666	1906	54.5429	1.9522	350.1991	1906	54.5429	1.9522	579.922
1907	54.5689	1.9513	381.8922	1907	54.5689	1.9513	631.4756	1907	54.5689	1.9513	303.2169	1907	54.5689	1.9513	533.604
1908	54.5949	1.9505	348.946	1908	54.5949	1.9505	598.6748	1908	54.5949	1.9505	395.5371	1908	54.5949	1.9505	626.5886
1909	54.6209	1.9496	389.5316	1909	54.6209	1.9496	639.4059	1909	54.6209	1.9496	322.4245	1909	54.6209	1.9496	554.1402
1910	54.6469	1.9488	355.0305	1910	54.6469	1.9488	605.0502	1910	54.6469	1.9488	363.5115	1910	54.6469	1.9488	595.8915
1911	54.6729	1.9479	371.7864	1911	54.6729	1.9479	621.9516	1911	54.6729	1.9479	342.0989	1911	54.6729	1.9479	575.1431
1912	54.6989	1.947	371.3824	1912	54.6989	1.947	621.693	1912	54.6989	1.947	288.6024	1912	54.6989	1.947	522.3109
1913	54.7249	1.9462	386.8865	1913	54.7249	1.9462	637.3426	1913	54.7249	1.9462	370.1986	1913	54.7249	1.9462	604.5714
1914	54.7509	1.9453	330.4918	1914	54.7509	1.9453	581.0933	1914	54.7509	1.9453	355.4853	1914	54.7509	1.9453	590.5223
1915	54.7769	1.9445	335.6984	1915	54.7769	1.9445	586.4453	1915	54.7769	1.9445	381.7574	1915	54.7769	1.9445	617.4586
1916	54.8029	1.9436	386.0469	1916	54.8029	1.9436	636.9393	1916	54.8029	1.9436	319.7083	1916	54.8029	1.9436	556.0738
1917	54.8289	1.9428	333.5511	1917	54.8289	1.9428	584.589	1917	54.8289	1.9428	323.9147	1917	54.8289	1.9428	560.9444
1918	54.8549	1.9419	345.5432	1918	54.8549	1.9419	596.7265	1918	54.8549	1.9419	361.4856	1918	54.8549	1.9419	599.1796
1919	54.8809	1.9411	336.626	1919	54.8809	1.9411	588.2786	1919	54.8809	1.9411	316.0967	1919	54.8809	1.9411	554.455
1920	54.9069	1.9402	403.9756	1920	54.9069	1.9402	656.0976	1920	54.9069	1.9402	320.6913	1920	54.9069	1.9402	559.7138
1921	54.9329	1.9394	336.1681	1921	54.9329	1.9394	588.7593	1921	54.9329	1.9394	313.6688	1921	54.9329	1.9394	553.3556
1922	54.9589	1.9385	356.3606	1922	54.9589	1.9385	609.4212	1922	54.9589	1.9385	287.2885	1922	54.9589	1.9385	527.6395
1923	54.9849	1.9377	384.4214	1923	54.9849	1.9377	637.9513	1923	54.9849	1.9377	347.2514	1923	54.9849	1.9377	588.2667
1924	55.0109	1.9369	352.9013	1924	55.0109	1.9369	606.9005	1924	55.0109	1.9369	333.8512	1924	55.0109	1.9369	575.5308
1925	55.0369	1.936	344.984	1925	55.0369	1.936	599.4525	1925	55.0369	1.936	340.7512	1925	55.0369	1.936	583.0951
1926	55.0629	1.9352	366.5519	1926	55.0629	1.9352	621.4897	1926	55.0629	1.9352	324.7993	1926	55.0629	1.9352	567.8074
1927	55.0889	1.9343	428.2004	1927	55.0889	1.9343	683.6075	1927	55.0889	1.9343	313.431	1927	55.0889	1.9343	557.1034
1928	55.1149	1.9335	431.6046	1928	55.1149	1.9335	687.481	1928	55.1149	1.9335	333.6569	1928	55.1149	1.9335	577.9936
1929	55.1409	1.9326	445.4412	1929	55.1409	1.9326	701.7869	1929	55.1409	1.9326	382.0995	1929	55.1409	1.9326	627.1005
1930	55.1669	1.9318	472.9819	1930	55.1669	1.9318	729.7969	1930	55.1669	1.9318	330.7217	1930	55.1669	1.9318	576.3869
1931	55.1929	1.931	589.7624	1931	55.1929	1.931	847.0467	1931	55.1929	1.931	347.8698	1931	55.1929	1.931	594.1992
1932	55.2189	1.9301	688.2113	1932	55.2189	1.9301	945.965	1932	55.2189	1.9301	327.6448	1932	55.2189	1.9301	574.6385
1933	55.2449	1.9293	786.6203	1933	55.2449	1.9293	1044.8432	1933	55.2449	1.9293	370.4896	1933	55.2449	1.9293	618.1476
1934	55.2709	1.9285	804.9482	1934	55.2709	1.9285	1063.6404	1934	55.2709	1.9285	384.599	1934	55.2709	1.9285	632.9213
1935	55.2969	1.9276	744.067	1935	55.2969	1.9276	1003.2285	1935	55.2969	1.9276	392.3061	1935	55.2969	1.9276	641.2926
1936	55.3229	1.9268	649.3327	1936	55.3229	1.9268	908.9636	1936	55.3229	1.9268	356.5325	1936	55.3229	1.9268	606.1833
1937	55.3489	1.926	655.7748	1937	55.3489	1.926	915.875	1937	55.3489	1.926	356.9607	1937	55.3489	1.926	607.2757
1938	55.3749	1.9251	705.3591	1938	55.3749	1.9251	965.9286	1938	55.3749	1.9251	343.4104	1938	55.3749	1.9251	594.3896
1939	55.4009	1.9243	647.6075	1939	55.4009	1.9243	908.6463	1939	55.4009	1.9243	369.1804	1939	55.4009	1.9243	620.8239

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1940	55.4269	1.9235	605.9537	1940	55.4269	1.9235	867.4618	1940	55.4269	1.9235	398.2304	1940	55.4269	1.9235	650.5382
1941	55.4529	1.9226	547.2207	1941	55.4529	1.9226	809.1981	1941	55.4529	1.9226	386.7607	1941	55.4529	1.9226	639.7327
1942	55.4789	1.9218	520.6633	1942	55.4789	1.9218	783.11	1942	55.4789	1.9218	328.5056	1942	55.4789	1.9218	582.1419
1943	55.5049	1.921	562.4002	1943	55.5049	1.921	825.3163	1943	55.5049	1.921	336.0121	1943	55.5049	1.921	590.3127
1944	55.5309	1.9201	520.2148	1944	55.5309	1.9201	783.6002	1944	55.5309	1.9201	347.9191	1944	55.5309	1.9201	602.8839
1945	55.5569	1.9193	499.2785	1945	55.5569	1.9193	763.1332	1945	55.5569	1.9193	378.9466	1945	55.5569	1.9193	634.5757
1946	55.5829	1.9185	545.2502	1946	55.5829	1.9185	809.5742	1946	55.5829	1.9185	392.7854	1946	55.5829	1.9185	647.7011
1947	55.6089	1.9177	559.3682	1947	55.6089	1.9177	824.1615	1947	55.6089	1.9177	373.061	1947	55.6089	1.9177	627.2634
1948	55.6349	1.9168	657.5693	1948	55.6349	1.9168	922.8319	1948	55.6349	1.9168	498.0449	1948	55.6349	1.9168	751.5341
1949	55.6609	1.916	851.9704	1949	55.6609	1.916	1117.7023	1949	55.6609	1.916	770.0215	1949	55.6609	1.916	1022.7973
1950	55.6869	1.9152	1181.1035	1950	55.6869	1.9152	1447.3048	1950	55.6869	1.9152	1030.363	1950	55.6869	1.9152	1282.4255
1951	55.7129	1.9144	1483.6817	1951	55.7129	1.9144	1750.3523	1951	55.7129	1.9144	1065.3922	1951	55.7129	1.9144	1316.7414
1952	55.7389	1.9135	1592.8252	1952	55.7389	1.9135	1859.965	1952	55.7389	1.9135	901.4937	1952	55.7389	1.9135	1152.1296
1953	55.7649	1.9127	1470.3687	1953	55.7649	1.9127	1737.9779	1953	55.7649	1.9127	851.2399	1953	55.7649	1.9127	1101.1625
1954	55.7909	1.9119	1239.9679	1954	55.7909	1.9119	1508.0464	1954	55.7909	1.9119	915.0447	1954	55.7909	1.9119	1164.254
1955	55.8169	1.9111	1175.2087	1955	55.8169	1.9111	1443.7565	1955	55.8169	1.9111	961.6356	1955	55.8169	1.9111	1210.1315
1956	55.8429	1.9103	1159.2755	1956	55.8429	1.9103	1428.2926	1956	55.8429	1.9103	875.1047	1956	55.8429	1.9103	1122.8874
1957	55.8689	1.9095	1085.602	1957	55.8689	1.9095	1355.0884	1957	55.8689	1.9095	715.0274	1957	55.8689	1.9095	962.0967
1958	55.8949	1.9086	968.554	1958	55.8949	1.9086	1238.5097	1958	55.8949	1.9086	616.4658	1958	55.8949	1.9086	862.8218
1959	55.9209	1.9078	815.7422	1959	55.9209	1.9078	1086.1672	1959	55.9209	1.9078	549.3017	1959	55.9209	1.9078	794.9444
1960	55.9469	1.907	713.0586	1960	55.9469	1.907	983.953	1960	55.9469	1.907	514.8217	1960	55.9469	1.907	759.7511
1961	55.9729	1.9062	587.1166	1961	55.9729	1.9062	858.4802	1961	55.9729	1.9062	483.9594	1961	55.9729	1.9062	728.1754
1962	55.9989	1.9054	441.1657	1962	55.9989	1.9054	712.9987	1962	55.9989	1.9054	419.276	1962	55.9989	1.9054	662.7788
1963	56.0249	1.9046	413.3209	1963	56.0249	1.9046	685.6231	1963	56.0249	1.9046	346.8733	1963	56.0249	1.9046	589.6627
1964	56.0509	1.9038	432.0481	1964	56.0509	1.9038	704.8197	1964	56.0509	1.9038	315.4915	1964	56.0509	1.9038	557.5676
1965	56.0769	1.9029	429.8096	1965	56.0769	1.9029	703.0505	1965	56.0769	1.9029	311.4858	1965	56.0769	1.9029	552.8486
1966	56.1029	1.9021	406.1551	1966	56.1029	1.9021	679.8652	1966	56.1029	1.9021	328.9718	1966	56.1029	1.9021	569.6213
1967	56.1289	1.9013	384.7627	1967	56.1289	1.9013	658.9422	1967	56.1289	1.9013	350.5855	1967	56.1289	1.9013	590.5217
1968	56.1549	1.9005	399.4568	1968	56.1549	1.9005	674.1056	1968	56.1549	1.9005	332.3945	1968	56.1549	1.9005	571.6174
1969	56.1809	1.8997	386.2896	1969	56.1809	1.8997	661.4077	1969	56.1809	1.8997	323.949	1969	56.1809	1.8997	562.4586
1970	56.2069	1.8989	364.4317	1970	56.2069	1.8989	640.0191	1970	56.2069	1.8989	324.0916	1970	56.2069	1.8989	561.8879
1971	56.2329	1.8981	370.4902	1971	56.2329	1.8981	646.5469	1971	56.2329	1.8981	333.6651	1971	56.2329	1.8981	570.748
1972	56.2589	1.8973	345.5432	1972	56.2589	1.8973	622.0693	1972	56.2589	1.8973	324.2911	1972	56.2589	1.8973	560.6608
1973	56.2849	1.8965	303.7208	1973	56.2849	1.8965	579.8693	1973	56.2849	1.8965	273.8587	1973	56.2849	1.8965	510.2344
1974	56.3109	1.8957	322.0943	1974	56.3109	1.8957	597.8653	1974	56.3109	1.8957	279.8946	1974	56.3109	1.8957	516.2762
1975	56.3369	1.8949	360.752	1975	56.3369	1.8949	636.1455	1975	56.3369	1.8949	319.3491	1975	56.3369	1.8949	555.7367

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1976	56.3629	1.8941	356.0361	1976	56.3629	1.8941	631.0521	1976	56.3629	1.8941	344.7474	1976	56.3629	1.8941	581.141
1977	56.3889	1.8933	359.8518	1977	56.3889	1.8933	634.4903	1977	56.3889	1.8933	343.2586	1977	56.3889	1.8933	579.6581
1978	56.4149	1.8925	362.8642	1978	56.4149	1.8925	637.1252	1978	56.4149	1.8925	379.6121	1978	56.4149	1.8925	616.0177
1979	56.4409	1.8917	361.6838	1979	56.4409	1.8917	635.5673	1979	56.4409	1.8917	374.3598	1979	56.4409	1.8917	610.7713
1980	56.4669	1.8909	331.3129	1980	56.4669	1.8909	604.8189	1980	56.4669	1.8909	320.6803	1980	56.4669	1.8909	557.0978
1981	56.4929	1.8901	333.8099	1981	56.4929	1.8901	606.9384	1981	56.4929	1.8901	344.9148	1981	56.4929	1.8901	581.3382
1982	56.5189	1.8893	334.3127	1982	56.5189	1.8893	607.0636	1982	56.5189	1.8893	339.7296	1982	56.5189	1.8893	576.1591
1983	56.5449	1.8885	348.647	1983	56.5449	1.8885	621.0205	1983	56.5449	1.8885	340.5462	1983	56.5449	1.8885	576.9816
1984	56.5709	1.8877	378.4028	1984	56.5709	1.8877	650.3987	1984	56.5709	1.8877	319.6418	1984	56.5709	1.8877	556.0832
1985	56.5969	1.8869	392.4123	1985	56.5969	1.8869	664.0307	1985	56.5969	1.8869	315.1235	1985	56.5969	1.8869	551.5709
1986	56.6229	1.8861	380.3675	1986	56.6229	1.8861	651.6085	1986	56.6229	1.8861	326.1529	1986	56.6229	1.8861	562.6062
1987	56.6489	1.8853	382.1366	1987	56.6489	1.8853	653	1987	56.6489	1.8853	331.1789	1987	56.6489	1.8853	567.6383
1988	56.6749	1.8845	379.1012	1988	56.6749	1.8845	649.5871	1988	56.6749	1.8845	299.2595	1988	56.6749	1.8845	535.7248
1989	56.7009	1.8837	392.3012	1989	56.7009	1.8837	662.4096	1989	56.7009	1.8837	297.097	1989	56.7009	1.8837	533.5683
1990	56.7269	1.8829	444.7716	1990	56.7269	1.8829	714.5025	1990	56.7269	1.8829	306.2582	1990	56.7269	1.8829	542.7354
1991	56.7529	1.8821	450.4712	1991	56.7529	1.8821	719.8246	1991	56.7529	1.8821	315.7023	1991	56.7529	1.8821	552.1855
1992	56.7789	1.8813	505.2265	1992	56.7789	1.8813	774.2024	1992	56.7789	1.8813	335.4774	1992	56.7789	1.8813	571.9667
1993	56.8049	1.8805	544.3335	1993	56.8049	1.8805	812.9319	1993	56.8049	1.8805	320.0012	1993	56.8049	1.8805	556.4964
1994	56.8309	1.8798	690.3802	1994	56.8309	1.8798	958.6011	1994	56.8309	1.8798	363.5278	1994	56.8309	1.8798	600.029
1995	56.8569	1.879	893.4824	1995	56.8569	1.879	1161.3258	1995	56.8569	1.879	348.3057	1995	56.8569	1.879	584.8129
1996	56.8829	1.8782	1179.2179	1996	56.8829	1.8782	1446.6838	1996	56.8829	1.8782	397.9141	1996	56.8829	1.8782	634.4272
1997	56.9089	1.8774	1489.6149	1997	56.9089	1.8774	1756.7033	1997	56.9089	1.8774	487.7227	1997	56.9089	1.8774	724.2419
1998	56.9349	1.8766	1650.6599	1998	56.9349	1.8766	1917.3707	1998	56.9349	1.8766	589.6599	1998	56.9349	1.8766	826.185
1999	56.9609	1.8758	1538.0272	1999	56.9609	1.8758	1804.3606	1999	56.9609	1.8758	622.2008	1999	56.9609	1.8758	858.7318
2000	56.9869	1.875	1391.881	2000	56.9869	1.875	1657.8368	2000	56.9869	1.875	553.0547	2000	56.9869	1.875	789.5917
2001	57.0129	1.8743	1267.0827	2001	57.0129	1.8743	1532.661	2001	57.0129	1.8743	488.1525	2001	57.0129	1.8743	724.6955
2002	57.0389	1.8735	1162.4159	2002	57.0389	1.8735	1427.6168	2002	57.0389	1.8735	446.8506	2002	57.0389	1.8735	683.3996
2003	57.0649	1.8727	1116.1284	2003	57.0649	1.8727	1380.9517	2003	57.0649	1.8727	439.8853	2003	57.0649	1.8727	676.4403
2004	57.0909	1.8719	1010.251	2004	57.0909	1.8719	1274.6969	2004	57.0909	1.8719	463.2292	2004	57.0909	1.8719	699.7902
2005	57.1169	1.8711	910.6946	2005	57.1169	1.8711	1174.7629	2005	57.1169	1.8711	501.5786	2005	57.1169	1.8711	738.1456
2006	57.1429	1.8704	684.7288	2006	57.1429	1.8704	948.4197	2006	57.1429	1.8704	377.5704	2006	57.1429	1.8704	614.1433
2007	57.1689	1.8696	587.1533	2007	57.1689	1.8696	850.4666	2007	57.1689	1.8696	353.9005	2007	57.1689	1.8696	590.4794
2008	57.1949	1.8688	501.5628	2008	57.1949	1.8688	764.4986	2008	57.1949	1.8688	357.9853	2008	57.1949	1.8688	594.5702
2009	57.2209	1.868	442.3012	2009	57.2209	1.868	704.8595	2009	57.2209	1.868	349.6833	2009	57.2209	1.868	586.2742
2010	57.2469	1.8672	423.0673	2010	57.2469	1.8672	685.2481	2010	57.2469	1.8672	307.3783	2010	57.2469	1.8672	543.9751
2011	57.2729	1.8665	346.5235	2011	57.2729	1.8665	608.3268	2011	57.2729	1.8665	345.6885	2011	57.2729	1.8665	582.2913

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2012	57.2989	1.8657	416.798	2012	57.2989	1.8657	678.2238	2012	57.2989	1.8657	284.8256	2012	57.2989	1.8657	521.4344
2013	57.3249	1.8649	361.7691	2013	57.3249	1.8649	622.8174	2013	57.3249	1.8649	314.8214	2013	57.3249	1.8649	551.4362
2014	57.3509	1.8641	409.0344	2014	57.3509	1.8641	669.7052	2014	57.3509	1.8641	326.9077	2014	57.3509	1.8641	563.5285
2015	57.3769	1.8634	361.2942	2015	57.3769	1.8634	621.5874	2015	57.3769	1.8634	346.3073	2015	57.3769	1.8634	582.934
2016	57.4029	1.8626	337.3475	2016	57.4029	1.8626	597.2632	2016	57.4029	1.8626	342.5779	2016	57.4029	1.8626	579.2106
2017	57.4289	1.8618	377.3281	2017	57.4289	1.8618	636.8663	2017	57.4289	1.8618	374.2544	2017	57.4289	1.8618	610.8931
2018	57.4549	1.8611	392.6403	2018	57.4549	1.8611	651.801	2018	57.4549	1.8611	360.541	2018	57.4549	1.8611	597.1857
2019	57.4809	1.8603	305.3035	2019	57.4809	1.8603	564.0868	2019	57.4809	1.8603	342.7667	2019	57.4809	1.8603	579.4174
2020	57.5069	1.8595	318.0976	2020	57.5069	1.8595	576.5034	2020	57.5069	1.8595	319.138	2020	57.5069	1.8595	555.7946
2021	57.5329	1.8587	359.1645	2021	57.5329	1.8587	617.1927	2021	57.5329	1.8587	384.3683	2021	57.5329	1.8587	621.0309
2022	57.5589	1.858	300.7383	2022	57.5589	1.858	558.389	2022	57.5589	1.858	372.1787	2022	57.5589	1.858	608.8473
2023	57.5849	1.8572	338.9603	2023	57.5849	1.8572	596.2335	2023	57.5849	1.8572	334.7776	2023	57.5849	1.8572	571.4521
2024	57.6109	1.8564	332.8323	2024	57.6109	1.8564	589.728	2024	57.6109	1.8564	285.0321	2024	57.6109	1.8564	521.7127
2025	57.6369	1.8557	323.309	2025	57.6369	1.8557	579.8272	2025	57.6369	1.8557	356.5304	2025	57.6369	1.8557	593.2169
2026	57.6629	1.8549	345.5432	2026	57.6629	1.8549	601.6839	2026	57.6629	1.8549	324.2911	2026	57.6629	1.8549	560.9836
2027	57.6889	1.8542	313.0958	2027	57.6889	1.8542	569	2027	57.6889	1.8542	282.7222	2027	57.6889	1.8542	519.3077
2028	57.7149	1.8534	305.7822	2028	57.7149	1.8534	561.4499	2028	57.7149	1.8534	290.0591	2028	57.7149	1.8534	526.5377
2029	57.7409	1.8526	323.1205	2029	57.7409	1.8526	578.5518	2029	57.7409	1.8526	301.2819	2029	57.7409	1.8526	537.6535
2030	57.7669	1.8519	297.1721	2030	57.7669	1.8519	552.3669	2030	57.7669	1.8519	314.8828	2030	57.7669	1.8519	551.1474
2031	57.7929	1.8511	316.2008	2031	57.7929	1.8511	571.1591	2031	57.7929	1.8511	288.5368	2031	57.7929	1.8511	524.6944
2032	57.8189	1.8503	346.5607	2032	57.8189	1.8503	601.2825	2032	57.8189	1.8503	314.471	2032	57.8189	1.8503	550.5217
2033	57.8449	1.8496	343.9735	2033	57.8449	1.8496	598.4589	2033	57.8449	1.8496	313.3531	2033	57.8449	1.8496	549.2968
2034	57.8709	1.8488	334.4713	2034	57.8709	1.8488	588.7202	2034	57.8709	1.8488	284.012	2034	57.8709	1.8488	519.8487
2035	57.8969	1.8481	329.7153	2035	57.8969	1.8481	583.7278	2035	57.8969	1.8481	325.7176	2035	57.8969	1.8481	561.4473
2036	57.9229	1.8473	329.224	2036	57.9229	1.8473	583	2036	57.9229	1.8473	283.8485	2036	57.9229	1.8473	519.4712
2037	57.9489	1.8465	326.2676	2037	57.9489	1.8465	579.8072	2037	57.9489	1.8465	298.6235	2037	57.9489	1.8465	534.1392
2038	57.9749	1.8458	316.2374	2038	57.9749	1.8458	569.5405	2038	57.9749	1.8458	301.6498	2038	57.9749	1.8458	537.0585
2039	58.0009	1.845	313.155	2039	58.0009	1.845	566.2216	2039	58.0009	1.845	279.6823	2039	58.0009	1.845	514.9841
2040	58.0269	1.8443	317.7805	2040	58.0269	1.8443	570.6107	2040	58.0269	1.8443	308.3852	2040	58.0269	1.8443	543.58
2041	58.0529	1.8435	321.6819	2041	58.0529	1.8435	574.2756	2041	58.0529	1.8435	315.1195	2041	58.0529	1.8435	550.2074
2042	58.0789	1.8428	288.9557	2042	58.0789	1.8428	541.313	2042	58.0789	1.8428	325.9967	2042	58.0789	1.8428	560.9776
2043	58.1049	1.842	317.0292	2043	58.1049	1.842	569.15	2043	58.1049	1.842	306.4884	2043	58.1049	1.842	541.3623
2044	58.1309	1.8413	322.3706	2044	58.1309	1.8413	574.2549	2044	58.1309	1.8413	314.2657	2044	58.1309	1.8413	549.0326
2045	58.1569	1.8405	338.7607	2045	58.1569	1.8405	590.4085	2045	58.1569	1.8405	318.1836	2045	58.1569	1.8405	552.8435
2046	58.1829	1.8398	360.7669	2046	58.1829	1.8398	612.1782	2046	58.1829	1.8398	305.3955	2046	58.1829	1.8398	539.9485
2047	58.2089	1.839	343.0595	2047	58.2089	1.839	594.2344	2047	58.2089	1.839	285.8752	2047	58.2089	1.839	520.3212

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2048	58.2349	1.8383	302.7426	2048	58.2349	1.8383	553.681	2048	58.2349	1.8383	294.8205	2048	58.2349	1.8383	529.1595
2049	58.2609	1.8375	310.3516	2049	58.2609	1.8375	561.0535	2049	58.2609	1.8375	282.7519	2049	58.2609	1.8375	516.9839
2050	58.2869	1.8368	345.2958	2050	58.2869	1.8368	595.7612	2050	58.2869	1.8368	299.3054	2050	58.2869	1.8368	533.4305
2051	58.3129	1.836	365.6826	2051	58.3129	1.836	615.9116	2051	58.3129	1.836	326.4865	2051	58.3129	1.836	560.5046
2052	58.3389	1.8353	338.1879	2052	58.3389	1.8353	588.1805	2052	58.3389	1.8353	339.2839	2052	58.3389	1.8353	573.195
2053	58.3649	1.8345	345.5432	2053	58.3649	1.8345	595.2993	2053	58.3649	1.8345	324.2911	2053	58.3649	1.8345	558.0952
2054	58.3909	1.8338	340.5233	2054	58.3909	1.8338	588.8549	2054	58.3909	1.8338	326.1032	2054	58.3909	1.8338	560.5907
2055	58.4169	1.833	319.5595	2055	58.4169	1.833	566.4666	2055	58.4169	1.833	324.7742	2055	58.4169	1.833	559.9451
2056	58.4429	1.8323	332.1983	2056	58.4429	1.8323	577.681	2056	58.4429	1.8323	336.8268	2056	58.4429	1.8323	572.681
2057	58.4689	1.8316	319.7516	2057	58.4689	1.8316	563.8098	2057	58.4689	1.8316	316.8744	2057	58.4689	1.8316	553.4119
2058	58.4949	1.8308	355.0928	2058	58.4949	1.8308	597.7266	2058	58.4949	1.8308	299.908	2058	58.4949	1.8308	537.1289
2059	58.5209	1.8301	368.5938	2059	58.5209	1.8301	609.8031	2059	58.5209	1.8301	287.0178	2059	58.5209	1.8301	524.922
2060	58.5469	1.8293	358.3451	2060	58.5469	1.8293	598.13	2060	58.5469	1.8293	281.1124	2060	58.5469	1.8293	519.7
2061	58.5729	1.8286	356.9187	2061	58.5729	1.8286	595.2791	2061	58.5729	1.8286	290.8899	2061	58.5729	1.8286	530.1609
2062	58.5989	1.8279	350.8634	2062	58.5989	1.8279	587.7994	2062	58.5989	1.8279	285.1429	2062	58.5989	1.8279	525.0972
2063	58.6249	1.8271	337.5229	2063	58.6249	1.8271	573.0344	2063	58.6249	1.8271	312.558	2063	58.6249	1.8271	553.1956
2064	58.6509	1.8264	322.0795	2064	58.6509	1.8264	556.1666	2064	58.6509	1.8264	334.194	2064	58.6509	1.8264	575.515
2065	58.6769	1.8256	353.2034	2065	58.6769	1.8256	585.866	2065	58.6769	1.8256	301.5374	2065	58.6769	1.8256	543.5418
2066	58.7029	1.8249	390.8456	2066	58.7029	1.8249	622.0837	2066	58.7029	1.8249	284.9484	2066	58.7029	1.8249	527.6361
2067	58.7289	1.8242	362.6499	2067	58.7289	1.8242	592.4636	2067	58.7289	1.8242	303.6431	2067	58.7289	1.8242	547.0141
2068	58.7549	1.8234	318.8359	2068	58.7549	1.8234	547.2251	2068	58.7549	1.8234	296.3208	2068	58.7549	1.8234	540.3751
2069	58.7809	1.8227	332.5509	2069	58.7809	1.8227	559.5156	2069	58.7809	1.8227	259.8799	2069	58.7809	1.8227	504.6176
2070	58.8069	1.822	357.1643	2070	58.8069	1.822	582.7046	2070	58.8069	1.822	299.0721	2070	58.8069	1.822	544.4932
2071	58.8329	1.8212	370.5532	2071	58.8329	1.8212	594.669	2071	58.8329	1.8212	323.6446	2071	58.8329	1.8212	569.7491
2072	58.8589	1.8205	370.0167	2072	58.8589	1.8205	592.7081	2072	58.8589	1.8205	290.3874	2072	58.8589	1.8205	537.1752
2073	58.8849	1.8198	342.323	2073	58.8849	1.8198	563.5899	2073	58.8849	1.8198	301.8828	2073	58.8849	1.8198	549.3539
2074	58.9109	1.819	341.6062	2074	58.9109	1.819	561.4487	2074	58.9109	1.819	305.6051	2074	58.9109	1.819	553.7596
2075	58.9369	1.8183	335.3682	2075	58.9369	1.8183	553.7862	2075	58.9369	1.8183	310.5293	2075	58.9369	1.8183	559.3672
2076	58.9629	1.8176	337.2787	2076	58.9629	1.8176	554.2722	2076	58.9629	1.8176	310.4699	2076	58.9629	1.8176	559.9911
2077	58.9889	1.8168	359.4177	2077	58.9889	1.8168	574.9868	2077	58.9889	1.8168	306.1505	2077	58.9889	1.8168	556.3551
2078	59.0149	1.8161	352.507	2078	59.0149	1.8161	566.6516	2078	59.0149	1.8161	292.9401	2078	59.0149	1.8161	543.828
2079	59.0409	1.8154	336.1652	2079	59.0409	1.8154	548.8854	2079	59.0409	1.8154	309.0065	2079	59.0409	1.8154	560.5777
2080	59.0669	1.8147	345.5432	2080	59.0669	1.8147	556.839	2080	59.0669	1.8147	324.2911	2080	59.0669	1.8147	576.5457
2081	59.0929	1.8139	383.6378	2081	59.0929	1.8139	594.8964	2081	59.0929	1.8139	320.4965	2081	59.0929	1.8139	572.5568
2082	59.1189	1.8132	349.9859	2082	59.1189	1.8132	561.2073	2082	59.1189	1.8132	282.155	2082	59.1189	1.8132	534.0209
2083	59.1449	1.8125	335.5248	2083	59.1449	1.8125	546.7089	2083	59.1449	1.8125	273.3791	2083	59.1449	1.8125	525.0507

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2084	59.1709	1.8118	354.1188	2084	59.1709	1.8118	565.2658	2084	59.1709	1.8118	288.1423	2084	59.1709	1.8118	539.6197
2085	59.1969	1.811	382.9585	2085	59.1969	1.811	594.0683	2085	59.1969	1.811	308.1073	2085	59.1969	1.811	559.3903
2086	59.2229	1.8103	373.935	2086	59.2229	1.8103	585.0077	2086	59.2229	1.8103	293.6786	2086	59.2229	1.8103	544.7673
2087	59.2489	1.8096	358.4331	2087	59.2489	1.8096	569.4685	2087	59.2489	1.8096	265.7825	2087	59.2489	1.8096	516.6769
2088	59.2749	1.8089	343.3269	2088	59.2749	1.8089	554.3252	2088	59.2749	1.8089	271.1557	2088	59.2749	1.8089	521.8557
2089	59.3009	1.8081	329.4986	2089	59.3009	1.8081	540.4597	2089	59.3009	1.8081	303.341	2089	59.3009	1.8081	553.8468
2090	59.3269	1.8074	327.7057	2090	59.3269	1.8074	538.6296	2090	59.3269	1.8074	301.3313	2090	59.3269	1.8074	551.6427
2091	59.3529	1.8067	338.5388	2091	59.3529	1.8067	549.4255	2091	59.3529	1.8067	280.4362	2091	59.3529	1.8067	530.5533
2092	59.3789	1.806	332.888	2092	59.3789	1.806	543.7376	2092	59.3789	1.806	254.8347	2092	59.3789	1.806	504.7575
2093	59.4049	1.8053	336.7071	2093	59.4049	1.8053	547.5195	2093	59.4049	1.8053	260.1823	2093	59.4049	1.8053	509.9108
2094	59.4309	1.8046	356.0372	2094	59.4309	1.8046	566.8124	2094	59.4309	1.8046	277.8409	2094	59.4309	1.8046	527.3751
2095	59.4569	1.8038	348.2754	2095	59.4569	1.8038	559.0134	2095	59.4569	1.8038	308.5555	2095	59.4569	1.8038	557.8954
2096	59.4829	1.8031	371.0015	2096	59.4829	1.8031	581.7024	2096	59.4829	1.8031	318.6417	2096	59.4829	1.8031	567.7872
2097	59.5089	1.8024	358.2661	2097	59.5089	1.8024	568.9298	2097	59.5089	1.8024	304.6591	2097	59.5089	1.8024	553.6103
2098	59.5349	1.8017	280.6722	2098	59.5349	1.8017	491.2987	2098	59.5349	1.8017	256.874	2098	59.5349	1.8017	505.6309
2099	59.5609	1.801	275.4507	2099	59.5609	1.801	486.04	2099	59.5609	1.801	267.835	2099	59.5609	1.801	516.3976
2100	59.5869	1.8003	308.5066	2100	59.5869	1.8003	519.0588	2100	59.5869	1.8003	233.6132	2100	59.5869	1.8003	481.9815
2101	59.6129	1.7995	334.0582	2101	59.6129	1.7995	544.5731	2101	59.6129	1.7995	258.048	2101	59.6129	1.7995	506.2219
2102	59.6389	1.7988	321.4267	2102	59.6389	1.7988	531.9044	2102	59.6389	1.7988	282.4149	2102	59.6389	1.7988	530.3945
2103	59.6649	1.7981	349.1328	2103	59.6649	1.7981	559.5734	2103	59.6649	1.7981	266.2079	2103	59.6649	1.7981	513.9932
2104	59.6909	1.7974	350.1951	2104	59.6909	1.7974	560.5985	2104	59.6909	1.7974	258.6784	2104	59.6909	1.7974	506.2694
2105	59.7169	1.7967	336.8567	2105	59.7169	1.7967	547.2229	2105	59.7169	1.7967	289.1968	2105	59.7169	1.7967	536.5934
2106	59.7429	1.796	351.4216	2106	59.7429	1.796	561.7507	2106	59.7429	1.796	310.2963	2106	59.7429	1.796	557.4986
2107	59.7689	1.7953	345.5432	2107	59.7689	1.7953	555.8351	2107	59.7689	1.7953	324.2911	2107	59.7689	1.7953	571.2991
2108	59.7949	1.7946	375.9881	2108	59.7949	1.7946	584.4073	2108	59.7949	1.7946	276.0602	2108	59.7949	1.7946	521.0627
2109	59.8209	1.7939	334.627	2109	59.8209	1.7939	541.1733	2109	59.8209	1.7939	268.3326	2109	59.8209	1.7939	511.3295
2110	59.8469	1.7932	349.1786	2110	59.8469	1.7932	553.8522	2110	59.8469	1.7932	264.4124	2110	59.8469	1.7932	505.4038
2111	59.8729	1.7925	348.7514	2111	59.8729	1.7925	551.5523	2111	59.8729	1.7925	283.5664	2111	59.8729	1.7925	522.5523
2112	59.8989	1.7917	345.0987	2112	59.8989	1.7917	546.0268	2112	59.8989	1.7917	277.7227	2112	59.8989	1.7917	514.703
2113	59.9249	1.791	364.5476	2113	59.9249	1.791	563.6029	2113	59.9249	1.791	257.7311	2113	59.9249	1.791	492.7059
2114	59.9509	1.7903	358.0226	2114	59.9509	1.7903	555.2052	2114	59.9509	1.7903	274.0048	2114	59.9509	1.7903	506.9741
2115	59.9769	1.7896	365.8116	2115	59.9769	1.7896	561.1214	2115	59.9769	1.7896	247.546	2115	59.9769	1.7896	478.5097
2116	60.0029	1.7889	372.3334	2116	60.0029	1.7889	565.7704	2116	60.0029	1.7889	270.0705	2116	60.0029	1.7889	499.0287
2117	60.0289	1.7882	358.5421	2117	60.0289	1.7882	550.1063	2117	60.0289	1.7882	274.3883	2117	60.0289	1.7882	501.341
2118	60.0549	1.7875	384.1767	2118	60.0549	1.7875	573.8682	2118	60.0549	1.7875	352.6299	2118	60.0549	1.7875	577.577
2119	60.0809	1.7868	349.7517	2119	60.0809	1.7868	537.5704	2119	60.0809	1.7868	294.0141	2119	60.0809	1.7868	516.9558

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2120	60.1069	1.7861	356.902	2120	60.1069	1.7861	542.848	2120	60.1069	1.7861	299.9372	2120	60.1069	1.7861	520.8733
2121	60.1329	1.7854	394.6222	2121	60.1329	1.7854	578.6954	2121	60.1329	1.7854	274.092	2121	60.1329	1.7854	493.0225
2122	60.1589	1.7847	405.4381	2122	60.1589	1.7847	587.6385	2122	60.1589	1.7847	292.2617	2122	60.1589	1.7847	509.1867
2123	60.1849	1.784	352.8684	2123	60.1849	1.784	533.1961	2123	60.1849	1.784	304.5295	2123	60.1849	1.784	519.449
2124	60.2109	1.7833	353.4151	2124	60.2109	1.7833	531.8699	2124	60.2109	1.7833	301.4762	2124	60.2109	1.7833	514.3902
2125	60.2369	1.7826	396.1201	2125	60.2369	1.7826	572.7022	2125	60.2369	1.7826	267.9397	2125	60.2369	1.7826	478.8481
2126	60.2629	1.7819	396.715	2126	60.2629	1.7819	571.4244	2126	60.2629	1.7819	301.872	2126	60.2629	1.7819	510.7749
2127	60.2889	1.7812	376.4385	2127	60.2889	1.7812	549.2751	2127	60.2889	1.7812	312.5339	2127	60.2889	1.7812	519.4312
2128	60.3149	1.7805	371.5597	2128	60.3149	1.7805	542.5236	2128	60.3149	1.7805	292.7261	2128	60.3149	1.7805	497.6179
2129	60.3409	1.7798	404.7819	2129	60.3409	1.7798	573.873	2129	60.3409	1.7798	333.7257	2129	60.3409	1.7798	536.612
2130	60.3669	1.7792	357.3799	2130	60.3669	1.7792	524.5982	2130	60.3669	1.7792	293.8455	2130	60.3669	1.7792	494.7263
2131	60.3929	1.7785	350.7889	2131	60.3929	1.7785	516.1345	2131	60.3929	1.7785	316.8213	2131	60.3929	1.7785	515.6965
2132	60.4189	1.7778	404.7185	2132	60.4189	1.7778	568.1913	2132	60.4189	1.7778	346.2314	2132	60.4189	1.7778	543.1011
2133	60.4449	1.7771	373.1164	2133	60.4449	1.7771	534.7164	2133	60.4449	1.7771	331.8397	2133	60.4449	1.7771	526.7039
2134	60.4709	1.7764	345.5432	2134	60.4709	1.7764	505.2705	2134	60.4709	1.7764	324.2911	2134	60.4709	1.7764	517.1498
2135	60.4969	1.7757	353.3689	2135	60.4969	1.7757	513.3874	2135	60.4969	1.7757	307.0126	2135	60.4969	1.7757	499.4834
2136	60.5229	1.775	371.1924	2136	60.5229	1.775	531.5022	2136	60.5229	1.775	268.0172	2136	60.5229	1.775	460.1002
2137	60.5489	1.7743	425.1759	2137	60.5489	1.7743	585.7769	2137	60.5489	1.7743	295.7681	2137	60.5489	1.7743	487.4633
2138	60.5749	1.7736	395.7125	2138	60.5749	1.7736	556.6048	2138	60.5749	1.7736	314.2454	2138	60.5749	1.7736	505.5527
2139	60.6009	1.7729	374.5966	2139	60.6009	1.7729	535.7802	2139	60.6009	1.7729	387.0468	2139	60.6009	1.7729	577.9663
2140	60.6269	1.7722	377.7349	2140	60.6269	1.7722	539.2097	2140	60.6269	1.7722	356.7905	2140	60.6269	1.7722	547.3222
2141	60.6529	1.7716	387.6631	2141	60.6529	1.7716	549.4292	2141	60.6529	1.7716	301.4763	2141	60.6529	1.7716	491.6201
2142	60.6789	1.7709	368.7642	2142	60.6789	1.7709	530.8216	2142	60.6789	1.7709	320.2552	2142	60.6789	1.7709	510.0112
2143	60.7049	1.7702	369.1158	2143	60.7049	1.7702	531.4645	2143	60.7049	1.7702	341.0821	2143	60.7049	1.7702	530.4503
2144	60.7309	1.7695	393.4559	2144	60.7309	1.7695	556.0958	2144	60.7309	1.7695	367.852	2144	60.7309	1.7695	556.8323
2145	60.7569	1.7688	405.4284	2145	60.7569	1.7688	568.3596	2145	60.7569	1.7688	380.0405	2145	60.7569	1.7688	568.633
2146	60.7829	1.7681	353.0264	2146	60.7829	1.7681	516.2488	2146	60.7829	1.7681	323.0273	2146	60.7829	1.7681	511.232
2147	60.8089	1.7674	356.9296	2147	60.8089	1.7674	520.4434	2147	60.8089	1.7674	353.8969	2147	60.8089	1.7674	541.7138
2148	60.8349	1.7668	348.3804	2148	60.8349	1.7668	512.1854	2148	60.8349	1.7668	357.7563	2148	60.8349	1.7668	545.1854
2149	60.8609	1.7661	337.1561	2149	60.8609	1.7661	501.2523	2149	60.8609	1.7661	288.1363	2149	60.8609	1.7661	475.1776
2150	60.8869	1.7654	345.7674	2150	60.8869	1.7654	510.1549	2150	60.8869	1.7654	298.9352	2150	60.8869	1.7654	485.5886
2151	60.9129	1.7647	351.6553	2151	60.9129	1.7647	516.3341	2151	60.9129	1.7647	310.3966	2151	60.9129	1.7647	496.6622
2152	60.9389	1.764	378.3159	2152	60.9389	1.764	543.2859	2152	60.9389	1.764	328.8081	2152	60.9389	1.764	514.6859
2153	60.9649	1.7634	356.1412	2153	60.9649	1.7634	521.4025	2153	60.9649	1.7634	332.7433	2153	60.9649	1.7634	518.2333
2154	60.9909	1.7627	342.8204	2154	60.9909	1.7627	508.373	2154	60.9909	1.7627	323.1621	2154	60.9909	1.7627	508.2643
2155	61.0169	1.762	364.9776	2155	61.0169	1.762	530.8215	2155	61.0169	1.762	307.1107	2155	61.0169	1.762	491.825

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2156	61.0429	1.7613	404.8855	2156	61.0429	1.7613	571.0206	2156	61.0429	1.7613	323.7544	2156	61.0429	1.7613	508.0809
2157	61.0689	1.7606	372.148	2157	61.0689	1.7606	538.5744	2157	61.0689	1.7606	337.2387	2157	61.0689	1.7606	521.1774
2158	61.0949	1.76	333.9038	2158	61.0949	1.76	500.6215	2158	61.0949	1.76	321.5088	2158	61.0949	1.76	505.0596
2159	61.1209	1.7593	324.7018	2159	61.1209	1.7593	491.7108	2159	61.1209	1.7593	310.6616	2159	61.1209	1.7593	493.8246
2160	61.1469	1.7586	354.7883	2160	61.1469	1.7586	522.0885	2160	61.1469	1.7586	314.847	2160	61.1469	1.7586	497.6222
2161	61.1729	1.7579	390.7655	2161	61.1729	1.7579	558.357	2161	61.1729	1.7579	324.2911	2161	61.1729	1.7579	506.6785
2162	61.1989	1.7573	360.0625	2162	61.1989	1.7573	527.9452	2162	61.1989	1.7573	376.1036	2162	61.1989	1.7573	557.8658
2163	61.2249	1.7566	337.0461	2163	61.2249	1.7566	505.2201	2163	61.2249	1.7566	337.6905	2163	61.2249	1.7566	518.8275
2164	61.2509	1.7559	353.2202	2164	61.2509	1.7559	521.6855	2164	61.2509	1.7559	294.321	2164	61.2509	1.7559	474.8328
2165	61.2769	1.7552	368.6377	2165	61.2769	1.7552	537.3942	2165	61.2769	1.7552	296.853	2165	61.2769	1.7552	476.7397
2166	61.3029	1.7546	364.0692	2166	61.3029	1.7546	533.117	2166	61.3029	1.7546	287.8479	2166	61.3029	1.7546	467.1094
2167	61.3289	1.7539	371.9602	2167	61.3289	1.7539	541.2993	2167	61.3289	1.7539	334.5703	2167	61.3289	1.7539	513.2067
2168	61.3549	1.7532	394.852	2168	61.3549	1.7532	564.4823	2168	61.3549	1.7532	366.0241	2168	61.3549	1.7532	544.0354
2169	61.3809	1.7526	385.9128	2169	61.3809	1.7526	555.8344	2169	61.3809	1.7526	373.6873	2169	61.3809	1.7526	551.0734
2170	61.4069	1.7519	356.4307	2170	61.4069	1.7519	526.6436	2170	61.4069	1.7519	363.5691	2170	61.4069	1.7519	540.3301
2171	61.4329	1.7512	351.2742	2171	61.4329	1.7512	521.7784	2171	61.4329	1.7512	349.672	2171	61.4329	1.7512	525.8078
2172	61.4589	1.7506	360.4524	2172	61.4589	1.7506	531.2478	2172	61.4589	1.7506	337.4628	2172	61.4589	1.7506	512.9734
2173	61.4849	1.7499	369.928	2173	61.4849	1.7499	541.0146	2173	61.4849	1.7499	297.7682	2173	61.4849	1.7499	472.6537
2174	61.5109	1.7492	390.4495	2174	61.5109	1.7492	561.8274	2174	61.5109	1.7492	328.7764	2174	61.5109	1.7492	503.0367
2175	61.5369	1.7485	366.7342	2175	61.5369	1.7485	538.4034	2175	61.5369	1.7485	353.2075	2175	61.5369	1.7485	526.8426
2176	61.5629	1.7479	324.9445	2176	61.5629	1.7479	496.9049	2176	61.5629	1.7479	325.1239	2176	61.5629	1.7479	498.1338
2177	61.5889	1.7472	329.1119	2177	61.5889	1.7472	501.3636	2177	61.5889	1.7472	324.1607	2177	61.5889	1.7472	496.5455
2178	61.6149	1.7466	318.301	2178	61.6149	1.7466	490.844	2178	61.6149	1.7466	323.4628	2178	61.6149	1.7466	495.2224
2179	61.6409	1.7459	321.5872	2179	61.6409	1.7459	494.4215	2179	61.6409	1.7459	289.9602	2179	61.6409	1.7459	461.0946
2180	61.6669	1.7452	381.047	2180	61.6669	1.7452	554.1726	2180	61.6669	1.7452	282.2156	2180	61.6669	1.7452	452.7249
2181	61.6929	1.7446	384.9974	2181	61.6929	1.7446	558.4142	2181	61.6929	1.7446	307.3584	2181	61.6929	1.7446	477.2426
2182	61.7189	1.7439	361.599	2182	61.7189	1.7439	535.307	2182	61.7189	1.7439	319.1857	2182	61.7189	1.7439	488.4446
2183	61.7449	1.7432	335.6909	2183	61.7449	1.7432	509.6903	2183	61.7449	1.7432	348.3352	2183	61.7449	1.7432	516.969
2184	61.7709	1.7426	347.6716	2184	61.7709	1.7426	521.9622	2184	61.7709	1.7426	323.7084	2184	61.7709	1.7426	491.7171
2185	61.7969	1.7419	354.2987	2185	61.7969	1.7419	528.8805	2185	61.7969	1.7419	349.0696	2185	61.7969	1.7419	516.4531
2186	61.8229	1.7413	382.8425	2186	61.8229	1.7413	557.7156	2186	61.8229	1.7413	377.7292	2186	61.8229	1.7413	544.4875
2187	61.8489	1.7406	379.1731	2187	61.8489	1.7406	554.3375	2187	61.8489	1.7406	343.0214	2187	61.8489	1.7406	509.1546
2188	61.8749	1.7399	345.5432	2188	61.8749	1.7399	520.9989	2188	61.8749	1.7399	324.2911	2188	61.8749	1.7399	489.7991
2189	61.9009	1.7393	360.4998	2189	61.9009	1.7393	535.29	2189	61.9009	1.7393	325.6446	2189	61.9009	1.7393	490.5591
2190	61.9269	1.7386	355.9931	2190	61.9269	1.7386	530.1179	2190	61.9269	1.7386	295.6371	2190	61.9269	1.7386	459.9582
2191	61.9529	1.738	339.9196	2191	61.9529	1.738	513.3789	2191	61.9529	1.738	297.3217	2191	61.9529	1.738	461.0493

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2192	61.9789	1.7373	340.3702	2192	61.9789	1.7373	513.1641	2192	61.9789	1.7373	346.2761	2192	61.9789	1.7373	509.4103
2193	62.0049	1.7367	358.6292	2193	62.0049	1.7367	530.7577	2193	62.0049	1.7367	363.6922	2193	62.0049	1.7367	526.2329
2194	62.0309	1.736	368.3629	2194	62.0309	1.736	539.826	2194	62.0309	1.736	330.6206	2194	62.0309	1.736	492.5678
2195	62.0569	1.7353	340.667	2195	62.0569	1.7353	511.4646	2195	62.0569	1.7353	345.4157	2195	62.0569	1.7353	506.7695
2196	62.0829	1.7347	338.382	2196	62.0829	1.7347	508.5142	2196	62.0829	1.7347	337.5198	2196	62.0829	1.7347	498.2801
2197	62.1089	1.734	353.6884	2197	62.1089	1.734	523.1552	2197	62.1089	1.734	320.3122	2197	62.1089	1.734	480.479
2198	62.1349	1.7334	338.206	2198	62.1349	1.7334	507.0072	2198	62.1349	1.7334	353.215	2198	62.1349	1.7334	512.7884
2199	62.1609	1.7327	353.1606	2199	62.1609	1.7327	521.2964	2199	62.1609	1.7327	345.7901	2199	62.1609	1.7327	504.77
2200	62.1869	1.7321	370.0386	2200	62.1869	1.7321	537.509	2200	62.1869	1.7321	358.6549	2200	62.1869	1.7321	517.0413
2201	62.2129	1.7314	325.7594	2201	62.2129	1.7314	492.5643	2201	62.2129	1.7314	321.6684	2201	62.2129	1.7314	479.4614
2202	62.2389	1.7308	344.3356	2202	62.2389	1.7308	510.4752	2202	62.2389	1.7308	317.8601	2202	62.2389	1.7308	475.0596
2203	62.2649	1.7301	371.7126	2203	62.2649	1.7301	537.1867	2203	62.2649	1.7301	330.0117	2203	62.2649	1.7301	486.6178
2204	62.2909	1.7295	364.168	2204	62.2909	1.7295	528.9767	2204	62.2909	1.7295	306.8345	2204	62.2909	1.7295	462.8471
2205	62.3169	1.7288	375.2816	2205	62.3169	1.7288	539.4248	2205	62.3169	1.7288	312.7121	2205	62.3169	1.7288	468.1313
2206	62.3429	1.7282	366.129	2206	62.3429	1.7282	529.6067	2206	62.3429	1.7282	318.664	2206	62.3429	1.7282	473.4898
2207	62.3689	1.7275	365.728	2207	62.3689	1.7275	528.5403	2207	62.3689	1.7275	356.0018	2207	62.3689	1.7275	510.2341
2208	62.3949	1.7269	324.5786	2208	62.3949	1.7269	486.7255	2208	62.3949	1.7269	383.9667	2208	62.3949	1.7269	537.6055
2209	62.4209	1.7262	342.3501	2209	62.4209	1.7262	503.8316	2209	62.4209	1.7262	330.1525	2209	62.4209	1.7262	483.1979
2210	62.4469	1.7256	359.4692	2210	62.4469	1.7256	520.2852	2210	62.4469	1.7256	350.8334	2210	62.4469	1.7256	503.2852
2211	62.4729	1.7249	342.2841	2211	62.4729	1.7249	502.4347	2211	62.4729	1.7249	333.0741	2211	62.4729	1.7249	484.9325
2212	62.4989	1.7243	359.9078	2212	62.4989	1.7243	519.3929	2212	62.4989	1.7243	344.437	2212	62.4989	1.7243	495.702
2213	62.5249	1.7237	337.6851	2213	62.5249	1.7237	496.5048	2213	62.5249	1.7237	326.1068	2213	62.5249	1.7237	476.7783
2214	62.5509	1.723	364.9645	2214	62.5509	1.723	523.1187	2214	62.5509	1.723	340.2085	2214	62.5509	1.723	490.2866
2215	62.5769	1.7224	345.5432	2215	62.5769	1.7224	503.032	2215	62.5769	1.7224	324.2911	2215	62.5769	1.7224	473.7757
2216	62.6029	1.7217	347.4031	2216	62.6029	1.7217	504.6415	2216	62.6029	1.7217	317.1411	2216	62.6029	1.7217	467.3761
2217	62.6289	1.7211	375.8533	2217	62.6289	1.7211	532.8414	2217	62.6289	1.7211	332.4412	2217	62.6289	1.7211	483.4266
2218	62.6549	1.7204	363.2166	2218	62.6549	1.7204	519.9545	2218	62.6549	1.7204	285.4509	2218	62.6549	1.7204	437.1867
2219	62.6809	1.7198	343.6654	2219	62.6809	1.7198	500.1529	2219	62.6809	1.7198	365.8868	2219	62.6809	1.7198	518.3731
2220	62.7069	1.7192	371.2709	2220	62.7069	1.7192	527.5081	2220	62.7069	1.7192	314.6768	2220	62.7069	1.7192	467.9135
2221	62.7329	1.7185	360.343	2221	62.7329	1.7185	516.3299	2221	62.7329	1.7185	296.4802	2221	62.7329	1.7185	450.4673
2222	62.7589	1.7179	359.3009	2222	62.7589	1.7179	515.0374	2222	62.7589	1.7179	351.0925	2222	62.7589	1.7179	505.8301
2223	62.7849	1.7172	369.9931	2223	62.7849	1.7172	525.4793	2223	62.7849	1.7172	342.9853	2223	62.7849	1.7172	498.4733
2224	62.8109	1.7166	353.7947	2224	62.8109	1.7166	509.0306	2224	62.8109	1.7166	348.3607	2224	62.8109	1.7166	504.5992
2225	62.8369	1.716	354.8801	2225	62.8369	1.716	509.8656	2225	62.8369	1.716	313.4967	2225	62.8369	1.716	470.4856
2226	62.8629	1.7153	368.1854	2226	62.8629	1.7153	522.9206	2226	62.8629	1.7153	315.7981	2226	62.8629	1.7153	473.5374
2227	62.8889	1.7147	386.8617	2227	62.8889	1.7147	541.3466	2227	62.8889	1.7147	289.0339	2227	62.8889	1.7147	447.5237

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2228	62.9149	1.7141	377.0257	2228	62.9149	1.7141	531.2603	2228	62.9149	1.7141	314.6575	2228	62.9149	1.7141	473.8977
2229	62.9409	1.7134	355.4737	2229	62.9409	1.7134	509.458	2229	62.9409	1.7134	323.2613	2229	62.9409	1.7134	483.2519
2230	62.9669	1.7128	366.5142	2230	62.9669	1.7128	520.2481	2230	62.9669	1.7128	311.7772	2230	62.9669	1.7128	472.5183
2231	62.9929	1.7121	356.2904	2231	62.9929	1.7121	509.774	2231	62.9929	1.7121	321.7345	2231	62.9929	1.7121	483.226
2232	63.0189	1.7115	359.9469	2232	63.0189	1.7115	513.1802	2232	63.0189	1.7115	302.0373	2232	63.0189	1.7115	464.2792
2233	63.0449	1.7109	373.8187	2233	63.0449	1.7109	526.8016	2233	63.0449	1.7109	362.0158	2233	63.0449	1.7109	525.0082
2234	63.0709	1.7102	366.1451	2234	63.0709	1.7102	518.8778	2234	63.0709	1.7102	329.2376	2234	63.0709	1.7102	492.9804
2235	63.0969	1.7096	374.5209	2235	63.0969	1.7096	527.0032	2235	63.0969	1.7096	352.1835	2235	63.0969	1.7096	516.6767
2236	63.1229	1.709	374.297	2236	63.1229	1.709	526.529	2236	63.1229	1.709	347.8722	2236	63.1229	1.709	513.1159
2237	63.1489	1.7084	363.4396	2237	63.1489	1.7084	515.4212	2237	63.1489	1.7084	333.6133	2237	63.1489	1.7084	499.6074
2238	63.1749	1.7077	323.4886	2238	63.1749	1.7077	475.2199	2238	63.1749	1.7077	323.8248	2238	63.1749	1.7077	490.5693
2239	63.2009	1.7071	356.5962	2239	63.2009	1.7071	508.0772	2239	63.2009	1.7071	319.1233	2239	63.2009	1.7071	486.6183
2240	63.2269	1.7065	369.3373	2240	63.2269	1.7065	520.568	2240	63.2269	1.7065	291.883	2240	63.2269	1.7065	460.1284
2241	63.2529	1.7058	328.9942	2241	63.2529	1.7058	479.9746	2241	63.2529	1.7058	293.2929	2241	63.2529	1.7058	462.2888
2242	63.2789	1.7052	345.5432	2242	63.2789	1.7052	496.2733	2242	63.2789	1.7052	324.2911	2242	63.2789	1.7052	494.0374
2243	63.3049	1.7046	358.1449	2243	63.3049	1.7046	509.5253	2243	63.3049	1.7046	315.5195	2243	63.3049	1.7046	484.8987
2244	63.3309	1.704	354.5034	2244	63.3309	1.704	506.5342	2244	63.3309	1.704	282.4487	2244	63.3309	1.704	451.461
2245	63.3569	1.7033	366.2719	2245	63.3569	1.7033	518.9531	2245	63.3569	1.7033	296.1204	2245	63.3569	1.7033	464.7656
2246	63.3829	1.7027	338.0679	2246	63.3829	1.7027	491.3996	2246	63.3829	1.7027	306.8952	2246	63.3829	1.7027	475.1734
2247	63.4089	1.7021	365.7461	2247	63.4089	1.7021	519.7283	2247	63.4089	1.7021	328.0957	2247	63.4089	1.7021	496.0069
2248	63.4349	1.7015	343.3186	2248	63.4349	1.7015	497.9511	2248	63.4349	1.7015	347.7296	2248	63.4349	1.7015	515.2737
2249	63.4609	1.7008	305.8765	2249	63.4609	1.7008	461.1594	2249	63.4609	1.7008	336.1504	2249	63.4609	1.7008	503.3275
2250	63.4869	1.7002	347.4239	2250	63.4869	1.7002	503.3573	2250	63.4869	1.7002	314.8098	2250	63.4869	1.7002	481.62
2251	63.5129	1.6996	332.6251	2251	63.5129	1.6996	489.2089	2251	63.5129	1.6996	304.5079	2251	63.5129	1.6996	470.9509
2252	63.5389	1.699	341.6924	2252	63.5389	1.699	498.9266	2252	63.5389	1.699	317.5522	2252	63.5389	1.699	483.6282
2253	63.5649	1.6983	324.9855	2253	63.5649	1.6983	482.8701	2253	63.5649	1.6983	316.776	2253	63.5649	1.6983	482.485
2254	63.5909	1.6977	334.913	2254	63.5909	1.6977	493.4481	2254	63.5909	1.6977	295.886	2254	63.5909	1.6977	461.2281
2255	63.6169	1.6971	348.1794	2255	63.6169	1.6971	507.3648	2255	63.6169	1.6971	314.3366	2255	63.6169	1.6971	479.3116
2256	63.6429	1.6965	368.4219	2256	63.6429	1.6965	528.2578	2256	63.6429	1.6965	337.2696	2256	63.6429	1.6965	501.8775
2257	63.6689	1.6959	382.3596	2257	63.6689	1.6959	542.8459	2257	63.6689	1.6959	331.9141	2257	63.6689	1.6959	496.1551
2258	63.6949	1.6952	372.5717	2258	63.6949	1.6952	533.7084	2258	63.6949	1.6952	333.3907	2258	63.6949	1.6952	497.2646
2259	63.7209	1.6946	366.4038	2259	63.7209	1.6946	528.1909	2259	63.7209	1.6946	319.4383	2259	63.7209	1.6946	482.9452
2260	63.7469	1.694	357.1938	2260	63.7469	1.694	519.6313	2260	63.7469	1.694	315.6432	2260	63.7469	1.694	478.7831
2261	63.7729	1.6934	359.6975	2261	63.7729	1.6934	522.7855	2261	63.7729	1.6934	322.8027	2261	63.7729	1.6934	485.5756
2262	63.7989	1.6928	358.3418	2262	63.7989	1.6928	522.0802	2262	63.7989	1.6928	324.1598	2262	63.7989	1.6928	486.5657
2263	63.8249	1.6921	360.5036	2263	63.8249	1.6921	524.8924	2263	63.8249	1.6921	300.5071	2263	63.8249	1.6921	462.5459

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2264	63.8509	1.6915	351.1311	2264	63.8509	1.6915	516.1703	2264	63.8509	1.6915	309.1666	2264	63.8509	1.6915	470.8384
2265	63.8769	1.6909	360.3553	2265	63.8769	1.6909	526.045	2265	63.8769	1.6909	325.7281	2265	63.8769	1.6909	487.0329
2266	63.9029	1.6903	341.2614	2266	63.9029	1.6903	507.6015	2266	63.9029	1.6903	326.3743	2266	63.9029	1.6903	487.3121
2267	63.9289	1.6897	326.6529	2267	63.9289	1.6897	493.6434	2267	63.9289	1.6897	350.4922	2267	63.9289	1.6897	511.063
2268	63.9549	1.6891	334.7297	2268	63.9549	1.6891	502.3706	2268	63.9549	1.6891	354.1299	2268	63.9549	1.6891	514.3336
2269	63.9809	1.6885	345.5432	2269	63.9809	1.6885	513.8346	2269	63.9809	1.6885	324.2911	2269	63.9809	1.6885	484.1278
2270	64.0069	1.6878	351.2145	2270	64.0069	1.6878	519.9515	2270	64.0069	1.6878	330.9899	2270	64.0069	1.6878	489.857
2271	64.0329	1.6872	334.7702	2271	64.0329	1.6872	503.9528	2271	64.0329	1.6872	361.3429	2271	64.0329	1.6872	519.2404
2272	64.0589	1.6866	312.0481	2272	64.0589	1.6866	481.6763	2272	64.0589	1.6866	355.4773	2272	64.0589	1.6866	512.4052
2273	64.0849	1.686	311.8627	2273	64.0849	1.686	481.9365	2273	64.0849	1.686	324.6928	2273	64.0849	1.686	480.6511
2274	64.1109	1.6854	343.0339	2274	64.1109	1.6854	513.5534	2274	64.1109	1.6854	309.4776	2274	64.1109	1.6854	464.4663
2275	64.1369	1.6848	345.9653	2275	64.1369	1.6848	516.9304	2275	64.1369	1.6848	347.8605	2275	64.1369	1.6848	501.8796
2276	64.1629	1.6842	350.5893	2276	64.1629	1.6842	522	2276	64.1629	1.6842	375.013	2276	64.1629	1.6842	528.0625
2277	64.1889	1.6836	357.6472	2277	64.1889	1.6836	529.5035	2277	64.1889	1.6836	360.5056	2277	64.1889	1.6836	512.5855
2278	64.2149	1.683	349.7927	2278	64.2149	1.683	522.0946	2278	64.2149	1.683	371.5522	2278	64.2149	1.683	522.6625
2279	64.2409	1.6823	356.6019	2279	64.2409	1.6823	529.3495	2279	64.2409	1.6823	385.4026	2279	64.2409	1.6823	535.5433
2280	64.2669	1.6817	375.8392	2280	64.2669	1.6817	549.0324	2280	64.2669	1.6817	409.8289	2280	64.2669	1.6817	559
2281	64.2929	1.6811	369.7361	2281	64.2929	1.6811	543.3749	2281	64.2929	1.6811	414.7116	2281	64.2929	1.6811	562.9131
2282	64.3189	1.6805	410.0665	2282	64.3189	1.6805	584.1509	2282	64.3189	1.6805	366.8968	2282	64.3189	1.6805	514.1287
2283	64.3449	1.6799	352.8966	2283	64.3449	1.6799	527.4267	2283	64.3449	1.6799	340.6735	2283	64.3449	1.6799	486.9358
2284	64.3709	1.6793	350.888	2284	64.3709	1.6793	525.8637	2284	64.3709	1.6793	361.1488	2284	64.3709	1.6793	506.4415
2285	64.3969	1.6787	344.7294	2285	64.3969	1.6787	520.1507	2285	64.3969	1.6787	357.7516	2285	64.3969	1.6787	502.0747
2286	64.4229	1.6781	318.4087	2286	64.4229	1.6781	494.2756	2286	64.4229	1.6781	366.7158	2286	64.4229	1.6781	510.0693
2287	64.4489	1.6775	318.017	2287	64.4489	1.6775	494.3296	2287	64.4489	1.6775	364.3807	2287	64.4489	1.6775	506.7646
2288	64.4749	1.6769	299.5492	2288	64.4749	1.6769	476.3074	2288	64.4749	1.6769	358.6613	2288	64.4749	1.6769	500.0756
2289	64.5009	1.6763	295.2631	2289	64.5009	1.6763	472.4669	2289	64.5009	1.6763	335.5516	2289	64.5009	1.6763	475.9963
2290	64.5269	1.6757	312.5473	2290	64.5269	1.6757	490.1968	2290	64.5269	1.6757	365.4947	2290	64.5269	1.6757	504.9698
2291	64.5529	1.6751	318.509	2291	64.5529	1.6751	496.604	2291	64.5529	1.6751	356.4945	2291	64.5529	1.6751	495
2292	64.5789	1.6745	298.6443	2292	64.5789	1.6745	477.1851	2292	64.5789	1.6745	352.6396	2292	64.5789	1.6745	490.1755
2293	64.6049	1.6739	321.6259	2293	64.6049	1.6739	500.6122	2293	64.6049	1.6739	335.0135	2293	64.6049	1.6739	471.5798
2294	64.6309	1.6733	315.269	2294	64.6309	1.6733	494.7009	2294	64.6309	1.6733	319.1624	2294	64.6309	1.6733	454.7591
2295	64.6569	1.6727	339.8876	2295	64.6569	1.6727	519.7652	2295	64.6569	1.6727	323.9972	2295	64.6569	1.6727	458.6243
2296	64.6829	1.6721	345.5432	2296	64.6829	1.6721	525.8665	2296	64.6829	1.6721	365.3262	2296	64.6829	1.6721	498.9837
2297	64.7089	1.6715	315.73	2297	64.7089	1.6715	495.2184	2297	64.7089	1.6715	412.8859	2297	64.7089	1.6715	545.5738
2298	64.7349	1.6709	309.2151	2298	64.7349	1.6709	487.8687	2298	64.7349	1.6709	383.3203	2298	64.7349	1.6709	515.0386
2299	64.7609	1.6703	287.7197	2299	64.7609	1.6703	465.5386	2299	64.7609	1.6703	364.4856	2299	64.7609	1.6703	495.2343

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2300	64.7869	1.6697	327.5435	2300	64.7869	1.6697	504.5276	2300	64.7869	1.6697	352.635	2300	64.7869	1.6697	482.4141
2301	64.8129	1.6691	348.5656	2301	64.8129	1.6691	524.7149	2301	64.8129	1.6691	380.1181	2301	64.8129	1.6691	508.9276
2302	64.8389	1.6685	347.9589	2302	64.8389	1.6685	523.2735	2302	64.8389	1.6685	372.6152	2302	64.8389	1.6685	500.4551
2303	64.8649	1.6679	332.3522	2303	64.8649	1.6679	506.8319	2303	64.8649	1.6679	359.4662	2303	64.8649	1.6679	486.3365
2304	64.8909	1.6673	360.1195	2304	64.8909	1.6673	533.7645	2304	64.8909	1.6673	378.5462	2304	64.8909	1.6673	504.4469
2305	64.9169	1.6667	314.8636	2305	64.9169	1.6667	487.6738	2305	64.9169	1.6667	376.0903	2305	64.9169	1.6667	501.0214
2306	64.9429	1.6661	355.217	2306	64.9429	1.6661	527.1924	2306	64.9429	1.6661	345.074	2306	64.9429	1.6661	469.0355
2307	64.9689	1.6655	340.0452	2307	64.9689	1.6655	511.1858	2307	64.9689	1.6655	373.81	2307	64.9689	1.6655	496.8019
2308	64.9949	1.6649	311.1643	2308	64.9949	1.6649	481.4702	2308	64.9949	1.6649	333.6764	2308	64.9949	1.6649	455.6987
2309	65.0209	1.6643	303.8009	2309	65.0209	1.6643	473.272	2309	65.0209	1.6643	371.9538	2309	65.0209	1.6643	493.0065
2310	65.0469	1.6637	346.2253	2310	65.0469	1.6637	514.8616	2310	65.0469	1.6637	359.3561	2310	65.0469	1.6637	479.4392
2311	65.0729	1.6632	374.7674	2311	65.0729	1.6632	542.5689	2311	65.0729	1.6632	318.8158	2311	65.0729	1.6632	437.9293
2312	65.0989	1.6626	354.3017	2312	65.0989	1.6626	521.2684	2312	65.0989	1.6626	374.7686	2312	65.0989	1.6626	492.9125
2313	65.1249	1.662	296.8198	2313	65.1249	1.662	462.9517	2313	65.1249	1.662	347.7064	2313	65.1249	1.662	464.8807
2314	65.1509	1.6614	373.3154	2314	65.1509	1.6614	538.6126	2314	65.1509	1.6614	345.9995	2314	65.1509	1.6614	462.2042
2315	65.1769	1.6608	328.02	2315	65.1769	1.6608	492.4824	2315	65.1769	1.6608	332.6806	2315	65.1769	1.6608	447.9157
2316	65.2029	1.6602	316.7909	2316	65.2029	1.6602	480.4185	2316	65.2029	1.6602	355.4954	2316	65.2029	1.6602	469.7609
2317	65.2289	1.6596	331.307	2317	65.2289	1.6596	494.0999	2317	65.2289	1.6596	348.3846	2317	65.2289	1.6596	461.6805
2318	65.2549	1.659	336.7907	2318	65.2549	1.659	498.7488	2318	65.2549	1.659	334.0756	2318	65.2549	1.659	446.4019
2319	65.2809	1.6584	312.8817	2319	65.2809	1.6584	474.005	2319	65.2809	1.6584	374.6371	2319	65.2809	1.6584	485.9938
2320	65.3069	1.6579	353.3196	2320	65.3069	1.6579	513.6081	2320	65.3069	1.6579	327.0929	2320	65.3069	1.6579	437.48
2321	65.3329	1.6573	347.6843	2321	65.3329	1.6573	507.138	2321	65.3329	1.6573	350.129	2321	65.3329	1.6573	459.5465
2322	65.3589	1.6567	328.9739	2322	65.3589	1.6567	487.5928	2322	65.3589	1.6567	389.3961	2322	65.3589	1.6567	497.844
2323	65.3849	1.6561	345.5432	2323	65.3849	1.6561	503.3274	2323	65.3849	1.6561	324.2911	2323	65.3849	1.6561	431.7694
2324	65.4109	1.6555	323.8553	2324	65.4109	1.6555	480.2371	2324	65.4109	1.6555	338.9232	2324	65.4109	1.6555	447.0598
2325	65.4369	1.6549	353.1788	2325	65.4369	1.6549	508.1584	2325	65.4369	1.6549	330.7398	2325	65.4369	1.6549	439.5347
2326	65.4629	1.6543	353.6307	2326	65.4629	1.6543	507.208	2326	65.4629	1.6543	332.3388	2326	65.4629	1.6543	441.792
2327	65.4889	1.6538	349.3005	2327	65.4889	1.6538	501.4755	2327	65.4889	1.6538	375.1637	2327	65.4889	1.6538	485.2751
2328	65.5149	1.6532	316.5267	2328	65.5149	1.6532	467.2995	2328	65.5149	1.6532	351.8163	2328	65.5149	1.6532	462.5861
2329	65.5409	1.6526	303.8187	2329	65.5409	1.6526	453.1892	2329	65.5409	1.6526	344.9683	2329	65.5409	1.6526	456.3964
2330	65.5669	1.652	312.0507	2330	65.5669	1.652	460.0188	2330	65.5669	1.652	336.7858	2330	65.5669	1.652	448.8722
2331	65.5929	1.6514	358.4871	2331	65.5929	1.6514	505.0529	2331	65.5929	1.6514	341.4228	2331	65.5929	1.6514	454.1674
2332	65.6189	1.6508	334.4755	2332	65.6189	1.6508	479.6391	2332	65.6189	1.6508	352.9219	2332	65.6189	1.6508	466.3248
2333	65.6449	1.6503	338.1284	2333	65.6449	1.6503	481.8897	2333	65.6449	1.6503	383.2201	2333	65.6449	1.6503	497.2813
2334	65.6709	1.6497	325.3178	2334	65.6709	1.6497	467.6768	2334	65.6709	1.6497	349.8237	2334	65.6709	1.6497	464.5432
2335	65.6969	1.6491	364.429	2335	65.6969	1.6491	505.3857	2335	65.6969	1.6491	319.0639	2335	65.6969	1.6491	434.4417

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2336	65.7229	1.6485	348.5022	2336	65.7229	1.6485	488.0566	2336	65.7229	1.6485	338.9073	2336	65.7229	1.6485	454.9434
2337	65.7489	1.6479	357.1707	2337	65.7489	1.6479	495.3229	2337	65.7489	1.6479	318.6599	2337	65.7489	1.6479	435.3543
2338	65.7749	1.6474	338.5253	2338	65.7749	1.6474	475.2751	2338	65.7749	1.6474	336.9954	2338	65.7749	1.6474	454.3481
2339	65.8009	1.6468	315.4121	2339	65.8009	1.6468	450.7597	2339	65.8009	1.6468	305.1118	2339	65.8009	1.6468	423.1227
2340	65.8269	1.6462	338.1827	2340	65.8269	1.6462	472.128	2340	65.8269	1.6462	318.2918	2340	65.8269	1.6462	436.961
2341	65.8529	1.6456	310.4926	2341	65.8529	1.6456	443.0356	2341	65.8529	1.6456	322.8907	2341	65.8529	1.6456	442.2182
2342	65.8789	1.6451	360.5247	2342	65.8789	1.6451	491.6654	2342	65.8789	1.6451	309.6636	2342	65.8789	1.6451	429.6494
2343	65.9049	1.6445	344.972	2343	65.9049	1.6445	474.7104	2343	65.9049	1.6445	312.2138	2343	65.9049	1.6445	432.8579
2344	65.9309	1.6439	321.3746	2344	65.9309	1.6439	449.7107	2344	65.9309	1.6439	321.9704	2344	65.9309	1.6439	443.2728
2345	65.9569	1.6433	347.0099	2345	65.9569	1.6433	473.9437	2345	65.9569	1.6433	322.555	2345	65.9569	1.6433	444.5157
2346	65.9829	1.6428	337.234	2346	65.9829	1.6428	462.7655	2346	65.9829	1.6428	340.4189	2346	65.9829	1.6428	463.0378
2347	66.0089	1.6422	335.9269	2347	66.0089	1.6422	460.0561	2347	66.0089	1.6422	332.999	2347	66.0089	1.6422	456.2763
2348	66.0349	1.6416	358.5073	2348	66.0349	1.6416	481.2342	2348	66.0349	1.6416	319.2283	2348	66.0349	1.6416	443.1638
2349	66.0609	1.641	342.3869	2349	66.0609	1.641	463.7115	2349	66.0609	1.641	311.8939	2349	66.0609	1.641	436.4877
2350	66.0869	1.6405	345.5432	2350	66.0869	1.6405	465.4656	2350	66.0869	1.6405	324.2911	2350	66.0869	1.6405	449.5432
2351	66.1129	1.6399	379.6099	2351	66.1129	1.6399	500.3523	2351	66.1129	1.6399	292.6345	2351	66.1129	1.6399	417.7737
2352	66.1389	1.6393	363.5119	2352	66.1389	1.6393	485.0743	2352	66.1389	1.6393	309.9535	2352	66.1389	1.6393	434.9799
2353	66.1649	1.6388	373.8028	2353	66.1649	1.6388	496.1852	2353	66.1649	1.6388	342.9929	2353	66.1649	1.6388	467.9064
2354	66.1909	1.6382	350.5439	2354	66.1909	1.6382	473.7463	2354	66.1909	1.6382	359.6864	2354	66.1909	1.6382	484.487
2355	66.2169	1.6376	343.836	2355	66.2169	1.6376	467.8585	2355	66.2169	1.6376	346.9533	2355	66.2169	1.6376	471.6411
2356	66.2429	1.637	342.5615	2356	66.2429	1.637	467.404	2356	66.2429	1.637	345.6541	2356	66.2429	1.637	470.229
2357	66.2689	1.6365	314.2836	2357	66.2689	1.6365	439.9461	2357	66.2689	1.6365	323.7456	2357	66.2689	1.6365	448.2076
2358	66.2949	1.6359	341.8253	2358	66.2949	1.6359	468.3078	2358	66.2949	1.6359	356.7034	2358	66.2949	1.6359	481.0525
2359	66.3209	1.6353	333.3132	2359	66.3209	1.6353	460.6157	2359	66.3209	1.6353	344.9341	2359	66.3209	1.6353	469.1704
2360	66.3469	1.6348	327.0836	2360	66.3469	1.6348	455.206	2360	66.3469	1.6348	326.3696	2360	66.3469	1.6348	450.493
2361	66.3729	1.6342	343.8914	2361	66.3729	1.6342	472.8339	2361	66.3729	1.6342	328.3224	2361	66.3729	1.6342	452.3329
2362	66.3989	1.6336	326.5927	2362	66.3989	1.6336	456.3552	2362	66.3989	1.6336	322.235	2362	66.3989	1.6336	446.1327
2363	66.4249	1.6331	338.0312	2363	66.4249	1.6331	468.6137	2363	66.4249	1.6331	311.7621	2363	66.4249	1.6331	435.5468
2364	66.4509	1.6325	353.0613	2364	66.4509	1.6325	484.4638	2364	66.4509	1.6325	314.1861	2364	66.4509	1.6325	437.858
2365	66.4769	1.6319	352.1271	2365	66.4769	1.6319	484.3496	2365	66.4769	1.6319	321.9847	2365	66.4769	1.6319	445.5437
2366	66.5029	1.6314	353.3561	2366	66.5029	1.6314	486.3987	2366	66.5029	1.6314	359.3846	2366	66.5029	1.6314	482.8307
2367	66.5289	1.6308	357.9476	2367	66.5289	1.6308	491.8101	2367	66.5289	1.6308	363.3785	2367	66.5289	1.6308	486.7118
2368	66.5549	1.6302	358.1781	2368	66.5549	1.6302	492.8607	2368	66.5549	1.6302	333.6681	2368	66.5549	1.6302	456.8885
2369	66.5809	1.6297	380.7221	2369	66.5809	1.6297	516.2246	2369	66.5809	1.6297	327.8764	2369	66.5809	1.6297	450.984
2370	66.6069	1.6291	400.7602	2370	66.6069	1.6291	537.0828	2370	66.6069	1.6291	341.3221	2370	66.6069	1.6291	464.3168
2371	66.6329	1.6286	405.4457	2371	66.6329	1.6286	542.5883	2371	66.6329	1.6286	375.5166	2371	66.6329	1.6286	498.3983

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2372	66.6589	1.628	465.9361	2372	66.6589	1.628	603.8987	2372	66.6589	1.628	371.9931	2372	66.6589	1.628	494.762
2373	66.6849	1.6274	543.2908	2373	66.6849	1.6274	682.0734	2373	66.6849	1.6274	364.9169	2373	66.6849	1.6274	487.5729
2374	66.7109	1.6269	580.4854	2374	66.7109	1.6269	720.088	2374	66.7109	1.6269	410.54	2374	66.7109	1.6269	533.0832
2375	66.7369	1.6263	610.5789	2375	66.7369	1.6263	751.0015	2375	66.7369	1.6263	457.7933	2375	66.7369	1.6263	580.2236
2376	66.7629	1.6258	590.8673	2376	66.7629	1.6258	732.1099	2376	66.7629	1.6258	504.5831	2376	66.7629	1.6258	626.9005
2377	66.7889	1.6252	539.7315	2377	66.7889	1.6252	681.7941	2377	66.7889	1.6252	492.0583	2377	66.7889	1.6252	614.2628
2378	66.8149	1.6246	522.4053	2378	66.8149	1.6246	665.2879	2378	66.8149	1.6246	431.6642	2378	66.8149	1.6246	553.7559
2379	66.8409	1.6241	491.3692	2379	66.8409	1.6241	635.0718	2379	66.8409	1.6241	391.5663	2379	66.8409	1.6241	513.5451
2380	66.8669	1.6235	506.9798	2380	66.8669	1.6235	651.5025	2380	66.8669	1.6235	358.0363	2380	66.8669	1.6235	479.9022
2381	66.8929	1.623	484.5522	2381	66.8929	1.623	629.8948	2381	66.8929	1.623	410.9544	2381	66.8929	1.623	532.7074
2382	66.9189	1.6224	425.587	2382	66.9189	1.6224	571.7497	2382	66.9189	1.6224	442.36	2382	66.9189	1.6224	564.0002
2383	66.9449	1.6218	406.5247	2383	66.9449	1.6218	553.5074	2383	66.9449	1.6218	431.7734	2383	66.9449	1.6218	553.3007
2384	66.9709	1.6213	397.7215	2384	66.9709	1.6213	545.5242	2384	66.9709	1.6213	398.5476	2384	66.9709	1.6213	519.962
2385	66.9969	1.6207	398.9124	2385	66.9969	1.6207	547.5351	2385	66.9969	1.6207	370.781	2385	66.9969	1.6207	492.0825
2386	67.0229	1.6202	358.138	2386	67.0229	1.6202	507.5807	2386	67.0229	1.6202	345.518	2386	67.0229	1.6202	466.7066
2387	67.0489	1.6196	319.6258	2387	67.0489	1.6196	469.8885	2387	67.0489	1.6196	357.948	2387	67.0489	1.6196	479.0238
2388	67.0749	1.6191	306.227	2388	67.0749	1.6191	457.3098	2388	67.0749	1.6191	342.7866	2388	67.0749	1.6191	463.7495
2389	67.1009	1.6185	317.2638	2389	67.1009	1.6185	469.1666	2389	67.1009	1.6185	310.7887	2389	67.1009	1.6185	431.6388
2390	67.1269	1.618	320.5552	2390	67.1269	1.618	473.278	2390	67.1269	1.618	312.4278	2390	67.1269	1.618	433.1649
2391	67.1529	1.6174	324.5997	2391	67.1529	1.6174	478.1425	2391	67.1529	1.6174	331.2328	2391	67.1529	1.6174	451.8571
2392	67.1789	1.6169	306.7705	2392	67.1789	1.6169	461.1333	2392	67.1789	1.6169	328.4529	2392	67.1789	1.6169	448.9644
2393	67.2049	1.6163	338.0789	2393	67.2049	1.6163	493.2617	2393	67.2049	1.6163	337.8792	2393	67.2049	1.6163	458.2777
2394	67.2309	1.6157	292.027	2394	67.2309	1.6157	448.0298	2394	67.2309	1.6157	323.3631	2394	67.2309	1.6157	443.6488
2395	67.2569	1.6152	328.8835	2395	67.2569	1.6152	485.7063	2395	67.2569	1.6152	317.7161	2395	67.2569	1.6152	437.8889
2396	67.2829	1.6146	327.385	2396	67.2829	1.6146	485.0278	2396	67.2829	1.6146	328.079	2396	67.2829	1.6146	448.139
2397	67.3089	1.6141	297.5372	2397	67.3089	1.6141	456	2397	67.3089	1.6141	298.2552	2397	67.3089	1.6141	418.2023
2398	67.3349	1.6135	309.9093	2398	67.3349	1.6135	469.1921	2398	67.3349	1.6135	319.626	2398	67.3349	1.6135	439.4602
2399	67.3609	1.613	352.564	2399	67.3609	1.613	512.6668	2399	67.3609	1.613	321.9616	2399	67.3609	1.613	441.6829
2400	67.3869	1.6124	330.1666	2400	67.3869	1.6124	491.0895	2400	67.3869	1.6124	296.141	2400	67.3869	1.6124	415.7494
2401	67.4129	1.6119	318.3955	2401	67.4129	1.6119	480.1384	2401	67.4129	1.6119	340.5686	2401	67.4129	1.6119	460.0641
2402	67.4389	1.6114	353.0227	2402	67.4389	1.6114	515.5856	2402	67.4389	1.6114	293.2083	2402	67.4389	1.6114	412.591
2403	67.4649	1.6108	334.2836	2403	67.4649	1.6108	497.6665	2403	67.4649	1.6108	315.7301	2403	67.4649	1.6108	434.9999
2404	67.4909	1.6103	345.5432	2404	67.4909	1.6103	509.7462	2404	67.4909	1.6103	324.2911	2404	67.4909	1.6103	443.4481
2405	67.5169	1.6097	340.2929	2405	67.5169	1.6097	504.4681	2405	67.5169	1.6097	340.2021	2405	67.5169	1.6097	459.2106
2406	67.5429	1.6092	357.6132	2406	67.5429	1.6092	521.7607	2406	67.5429	1.6092	319.075	2406	67.5429	1.6092	437.9352
2407	67.5689	1.6086	410.5948	2407	67.5689	1.6086	574.7146	2407	67.5689	1.6086	291.732	2407	67.5689	1.6086	410.4437

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2408	67.5949	1.6081	400.4088	2408	67.5949	1.6081	564.501	2408	67.5949	1.6081	322.4366	2408	67.5949	1.6081	441
2409	67.6209	1.6075	445.6847	2409	67.6209	1.6075	609.7492	2409	67.6209	1.6075	322.7993	2409	67.6209	1.6075	441.2142
2410	67.6469	1.607	488.8212	2410	67.6469	1.607	652.8581	2410	67.6469	1.607	328.5241	2410	67.6469	1.607	446.7907
2411	67.6729	1.6064	611.8202	2411	67.6729	1.6064	775.8294	2411	67.6729	1.6064	363.8818	2411	67.6729	1.6064	482
2412	67.6989	1.6059	762.7267	2412	67.6989	1.6059	926.7082	2412	67.6989	1.6059	361.5549	2412	67.6989	1.6059	479.5247
2413	67.7249	1.6054	962.9902	2413	67.7249	1.6054	1126.944	2413	67.7249	1.6054	330.9648	2413	67.7249	1.6054	448.7863
2414	67.7509	1.6048	976.5339	2414	67.7509	1.6048	1140.4601	2414	67.7509	1.6048	316.2247	2414	67.7509	1.6048	433.8978
2415	67.7769	1.6043	978.534	2415	67.7769	1.6043	1142.4325	2415	67.7769	1.6043	349.7119	2415	67.7769	1.6043	467.2365
2416	67.8029	1.6037	862.2329	2416	67.8029	1.6037	1026.1037	2416	67.8029	1.6037	391.9497	2416	67.8029	1.6037	509.3259
2417	67.8289	1.6032	737.3788	2417	67.8289	1.6032	901.2219	2417	67.8289	1.6032	323.5502	2417	67.8289	1.6032	440.7781
2418	67.8549	1.6026	744.5965	2418	67.8549	1.6026	908.412	2418	67.8549	1.6026	316.0987	2418	67.8549	1.6026	433.1782
2419	67.8809	1.6021	713.0335	2419	67.8809	1.6021	876.8212	2419	67.8809	1.6021	326.3295	2419	67.8809	1.6021	443.2606
2420	67.9069	1.6016	816.0292	2420	67.9069	1.6016	979.7893	2420	67.9069	1.6016	359.1505	2420	67.9069	1.6016	475.9332
2421	67.9329	1.601	709.558	2421	67.9329	1.601	873.2904	2421	67.9329	1.601	309.9631	2421	67.9329	1.601	426.5974
2422	67.9589	1.6005	573.3133	2422	67.9589	1.6005	737.0181	2422	67.9589	1.6005	296.7984	2422	67.9589	1.6005	413.2843
2423	67.9849	1.5999	524.8172	2423	67.9849	1.5999	688.4943	2423	67.9849	1.5999	316.9949	2423	67.9849	1.5999	433.3324
2424	68.0109	1.5994	452.4375	2424	68.0109	1.5994	616.0869	2424	68.0109	1.5994	305.3532	2424	68.0109	1.5994	421.5423
2425	68.0369	1.5989	418.0823	2425	68.0369	1.5989	581.704	2425	68.0369	1.5989	358.0676	2425	68.0369	1.5989	474.1083
2426	68.0629	1.5983	406.0831	2426	68.0629	1.5983	569.6772	2426	68.0629	1.5983	320.7548	2426	68.0629	1.5983	436.6471
2427	68.0889	1.5978	367.3644	2427	68.0889	1.5978	530.9308	2427	68.0889	1.5978	342.3976	2427	68.0889	1.5978	458.1415
2428	68.1149	1.5973	336.9034	2428	68.1149	1.5973	500.4421	2428	68.1149	1.5973	355.4276	2428	68.1149	1.5973	471.0232
2429	68.1409	1.5967	328.1283	2429	68.1409	1.5967	491.6393	2429	68.1409	1.5967	315.6626	2429	68.1409	1.5967	431.1097
2430	68.1669	1.5962	329.3142	2430	68.1669	1.5962	492.7975	2430	68.1669	1.5962	282.9412	2430	68.1669	1.5962	398.24
2431	68.1929	1.5957	345.5432	2431	68.1929	1.5957	508.9989	2431	68.1929	1.5957	324.2911	2431	68.1929	1.5957	439.4415
2432	68.2189	1.5951	348.3879	2432	68.2189	1.5951	510.1211	2432	68.2189	1.5951	320.2186	2432	68.2189	1.5951	435.332
2433	68.2449	1.5946	308.2781	2433	68.2449	1.5946	468.2887	2433	68.2449	1.5946	299.8059	2433	68.2449	1.5946	414.8823
2434	68.2709	1.5941	311.4435	2434	68.2709	1.5941	469.7316	2434	68.2709	1.5941	301.2558	2434	68.2709	1.5941	416.2953
2435	68.2969	1.5935	333.9647	2435	68.2969	1.5935	490.5302	2435	68.2969	1.5935	330.8682	2435	68.2969	1.5935	445.8708
2436	68.3229	1.593	337.4785	2436	68.3229	1.593	492.3216	2436	68.3229	1.593	297.4303	2436	68.3229	1.593	412.396
2437	68.3489	1.5925	337.2209	2437	68.3489	1.5925	490.3414	2437	68.3489	1.5925	266.851	2437	68.3489	1.5925	381.7797
2438	68.3749	1.5919	313.2015	2438	68.3749	1.5919	464.5994	2438	68.3749	1.5919	303.8962	2438	68.3749	1.5919	418.788
2439	68.4009	1.5914	337.6553	2439	68.4009	1.5914	487.3308	2439	68.4009	1.5914	326.0964	2439	68.4009	1.5914	440.9512
2440	68.4269	1.5909	315.665	2440	68.4269	1.5909	463.6179	2440	68.4269	1.5909	353.9675	2440	68.4269	1.5909	468.7854
2441	68.4529	1.5903	366.6213	2441	68.4529	1.5903	512.8516	2441	68.4529	1.5903	308.105	2441	68.4529	1.5903	422.886
2442	68.4789	1.5898	300.8457	2442	68.4789	1.5898	445.3535	2442	68.4789	1.5898	330.1214	2442	68.4789	1.5898	444.8655
2443	68.5049	1.5893	341.5654	2443	68.5049	1.5893	484.3507	2443	68.5049	1.5893	373.3926	2443	68.5049	1.5893	488.0997

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2444	68.5309	1.5887	336.8625	2444	68.5309	1.5887	477.9253	2444	68.5309	1.5887	343.8182	2444	68.5309	1.5887	458.4884
2445	68.5569	1.5882	355.407	2445	68.5569	1.5882	494.7473	2445	68.5569	1.5882	328.3671	2445	68.5569	1.5882	443.0003
2446	68.5829	1.5877	357.9823	2446	68.5829	1.5877	495.6001	2446	68.5829	1.5877	317.7837	2446	68.5829	1.5877	432.3801
2447	68.6089	1.5872	342.5034	2447	68.6089	1.5872	478.3986	2447	68.6089	1.5872	337.0729	2447	68.6089	1.5872	451.6322
2448	68.6349	1.5866	400.0401	2448	68.6349	1.5866	534.2128	2448	68.6349	1.5866	357.7201	2448	68.6349	1.5866	472.2426
2449	68.6609	1.5861	399.2714	2449	68.6609	1.5861	531.7216	2449	68.6609	1.5861	330.5542	2449	68.6609	1.5861	445.0397
2450	68.6869	1.5856	343.3519	2450	68.6869	1.5856	474.0795	2450	68.6869	1.5856	306.3465	2450	68.6869	1.5856	420.7951
2451	68.7129	1.585	360.8949	2451	68.7129	1.585	489.8999	2451	68.7129	1.585	314.0152	2451	68.7129	1.585	428.4269
2452	68.7389	1.5845	348.0967	2452	68.7389	1.5845	475.3793	2452	68.7389	1.5845	327.1104	2452	68.7389	1.5845	441.4851
2453	68.7649	1.584	352.2035	2453	68.7649	1.584	477.7635	2453	68.7649	1.584	308.5344	2453	68.7649	1.584	422.8722
2454	68.7909	1.5835	348.9502	2454	68.7909	1.5835	472.7877	2454	68.7909	1.5835	351.2091	2454	68.7909	1.5835	465.5099
2455	68.8169	1.5829	353.6455	2455	68.8169	1.5829	475.7604	2455	68.8169	1.5829	328.6326	2455	68.8169	1.5829	442.8966
2456	68.8429	1.5824	368.9376	2456	68.8429	1.5824	489.33	2456	68.8429	1.5824	308.8215	2456	68.8429	1.5824	423.0485
2457	68.8689	1.5819	342.5259	2457	68.8689	1.5819	461.1958	2457	68.8689	1.5819	326.6886	2457	68.8689	1.5819	440.8787
2458	68.8949	1.5814	345.5432	2458	68.8949	1.5814	462.4906	2458	68.8949	1.5814	324.2911	2458	68.8949	1.5814	438.4442
2459	68.9209	1.5809	361.6868	2459	68.9209	1.5809	478.666	2459	68.9209	1.5809	302.5732	2459	68.9209	1.5809	415.5029
2460	68.9469	1.5803	369.9997	2460	68.9469	1.5803	487.0108	2460	68.9469	1.5803	309.5229	2460	68.9469	1.5803	421.2292
2461	68.9729	1.5798	336.1227	2461	68.9729	1.5798	453.1657	2461	68.9729	1.5798	309.6939	2461	68.9729	1.5798	420.1768
2462	68.9989	1.5793	308.1814	2462	68.9989	1.5793	425.2563	2462	68.9989	1.5793	295.7657	2462	68.9989	1.5793	405.0251
2463	69.0249	1.5788	335.459	2463	69.0249	1.5788	452.5658	2463	69.0249	1.5788	316.5305	2463	69.0249	1.5788	424.5666
2464	69.0509	1.5782	345.6334	2464	69.0509	1.5782	462.7721	2464	69.0509	1.5782	332.819	2464	69.0509	1.5782	439.6316
2465	69.0769	1.5777	359.4397	2465	69.0769	1.5777	476.6103	2465	69.0769	1.5777	339.6828	2465	69.0769	1.5777	445.2721
2466	69.1029	1.5772	355.0525	2466	69.1029	1.5772	472.2549	2466	69.1029	1.5772	331.9293	2466	69.1029	1.5772	436.2951
2467	69.1289	1.5767	334.1708	2467	69.1289	1.5767	451.4051	2467	69.1289	1.5767	310.2883	2467	69.1289	1.5767	413.4307
2468	69.1549	1.5762	340.5593	2468	69.1549	1.5762	457.8256	2468	69.1549	1.5762	318.7321	2468	69.1549	1.5762	420.6511
2469	69.1809	1.5756	373.8028	2469	69.1809	1.5756	491.1009	2469	69.1809	1.5756	320.9981	2469	69.1809	1.5756	421.6937
2470	69.2069	1.5751	383.1123	2470	69.2069	1.5751	500.4424	2470	69.2069	1.5751	297.9851	2470	69.2069	1.5751	397.4572
2471	69.2329	1.5746	351.8961	2471	69.2329	1.5746	469.258	2471	69.2329	1.5746	311.8562	2471	69.2329	1.5746	410.1049
2472	69.2589	1.5741	331.7501	2472	69.2589	1.5741	449.1439	2472	69.2589	1.5741	344.7229	2472	69.2589	1.5741	441.7482
2473	69.2849	1.5736	330.4069	2473	69.2849	1.5736	447.8326	2473	69.2849	1.5736	340.4516	2473	69.2849	1.5736	436.2535
2474	69.3109	1.5731	333.0803	2474	69.3109	1.5731	450.5378	2474	69.3109	1.5731	345.4461	2474	69.3109	1.5731	440.0246
2475	69.3369	1.5725	313.0639	2475	69.3369	1.5725	430.5533	2475	69.3369	1.5725	357.2432	2475	69.3369	1.5725	450.5983
2476	69.3629	1.572	318.6722	2476	69.3629	1.572	436.1935	2476	69.3629	1.572	333.9255	2476	69.3629	1.572	426.0572
2477	69.3889	1.5715	351.1227	2477	69.3889	1.5715	468.676	2477	69.3889	1.5715	317.9297	2477	69.3889	1.5715	408.838
2478	69.4149	1.571	328.5156	2478	69.4149	1.571	446.1007	2478	69.4149	1.571	331.5245	2478	69.4149	1.571	421.2093
2479	69.4409	1.5705	293.8313	2479	69.4409	1.5705	411.4483	2479	69.4409	1.5705	337.8613	2479	69.4409	1.5705	426.3228

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2480	69.4669	1.57	290.2355	2480	69.4669	1.57	407.8844	2480	69.4669	1.57	326.4252	2480	69.4669	1.57	413.6633
2481	69.4929	1.5695	319.9225	2481	69.4929	1.5695	437.6033	2481	69.4929	1.5695	350.6251	2481	69.4929	1.5695	436.6397
2482	69.5189	1.5689	342.412	2482	69.5189	1.5689	460.1247	2482	69.5189	1.5689	349.8971	2482	69.5189	1.5689	434.6883
2483	69.5449	1.5684	336.9678	2483	69.5449	1.5684	454.7123	2483	69.5449	1.5684	324.195	2483	69.5449	1.5684	407.7628
2484	69.5709	1.5679	325.7414	2484	69.5709	1.5679	443.5179	2484	69.5709	1.5679	321.6556	2484	69.5709	1.5679	404
2485	69.5969	1.5674	345.5432	2485	69.5969	1.5674	463.3516	2485	69.5969	1.5674	324.2911	2485	69.5969	1.5674	405.4121
2486	69.6229	1.5669	331.584	2486	69.6229	1.5669	448.1966	2486	69.6229	1.5669	328.7742	2486	69.6229	1.5669	409.3724
2487	69.6489	1.5664	324.5828	2487	69.6489	1.5664	439.9995	2487	69.6489	1.5664	322.5956	2487	69.6489	1.5664	402.6709
2488	69.6749	1.5659	334.2443	2488	69.6749	1.5659	448.4652	2488	69.6749	1.5659	304.1241	2488	69.6749	1.5659	383.6767
2489	69.7009	1.5654	342.7082	2489	69.7009	1.5654	455.7333	2489	69.7009	1.5654	322.7704	2489	69.7009	1.5654	401.8002
2490	69.7269	1.5649	331.9912	2490	69.7269	1.5649	443.8205	2490	69.7269	1.5649	363.8862	2490	69.7269	1.5649	442.3932
2491	69.7529	1.5643	332.0837	2491	69.7529	1.5643	442.7172	2491	69.7529	1.5643	355.6785	2491	69.7529	1.5643	433.6627
2492	69.7789	1.5638	311.4882	2492	69.7789	1.5638	420.9258	2492	69.7789	1.5638	344.21	2492	69.7789	1.5638	421.6714
2493	69.8049	1.5633	295.5048	2493	69.8049	1.5633	403.7466	2493	69.8049	1.5633	356.5986	2493	69.8049	1.5633	433.5372
2494	69.8309	1.5628	327.5138	2494	69.8309	1.5628	434.5598	2494	69.8309	1.5628	346.6283	2494	69.8309	1.5628	423.0441
2495	69.8569	1.5623	357.4293	2495	69.8569	1.5623	463.2795	2495	69.8569	1.5623	336.8684	2495	69.8569	1.5623	412.7614
2496	69.8829	1.5618	318.5161	2496	69.8829	1.5618	423.1704	2496	69.8829	1.5618	342.8002	2496	69.8829	1.5618	418.1704
2497	69.9089	1.5613	332.8169	2497	69.9089	1.5613	436.2754	2497	69.9089	1.5613	354.5563	2497	69.9089	1.5613	429.4037
2498	69.9349	1.5608	345.1854	2498	69.9349	1.5608	447.4481	2498	69.9349	1.5608	352.7303	2498	69.9349	1.5608	427.0549
2499	69.9609	1.5603	348.1473	2499	69.9609	1.5603	449.2141	2499	69.9609	1.5603	329.4123	2499	69.9609	1.5603	403.2141
2500	69.9869	1.5598	350.7415	2500	69.9869	1.5598	450.6126	2500	69.9869	1.5598	327.4539	2500	69.9869	1.5598	400.7329
2501	70.0129	1.5593	348.8853	2501	70.0129	1.5593	447.5605	2501	70.0129	1.5593	322.0431	2501	70.0129	1.5593	394.7994
2502	70.0389	1.5588	326.9676	2502	70.0389	1.5588	424.447	2502	70.0389	1.5588	350.0292	2502	70.0389	1.5588	422.2626
2503	70.0649	1.5583	324.321	2503	70.0649	1.5583	420.6046	2503	70.0649	1.5583	344.4985	2503	70.0649	1.5583	416.2092
2504	70.0909	1.5578	320.8863	2504	70.0909	1.5578	415.974	2504	70.0909	1.5578	334.1151	2504	70.0909	1.5578	405.303
2505	70.1169	1.5573	333.8084	2505	70.1169	1.5573	427.7004	2505	70.1169	1.5573	344.6345	2505	70.1169	1.5573	415.2996
2506	70.1429	1.5567	344.5932	2506	70.1429	1.5567	437.2893	2506	70.1429	1.5567	339.4741	2506	70.1429	1.5567	409.6164
2507	70.1689	1.5562	343.4577	2507	70.1689	1.5562	434.958	2507	70.1689	1.5562	360.0332	2507	70.1689	1.5562	429.6527
2508	70.1949	1.5557	320.0685	2508	70.1949	1.5557	410.3729	2508	70.1949	1.5557	353.9003	2508	70.1949	1.5557	422.997
2509	70.2209	1.5552	334.6827	2509	70.2209	1.5552	423.7914	2509	70.2209	1.5552	368.541	2509	70.2209	1.5552	437.1149
2510	70.2469	1.5547	361.9381	2510	70.2469	1.5547	449.851	2510	70.2469	1.5547	364.9104	2510	70.2469	1.5547	432.9615
2511	70.2729	1.5542	336.7582	2511	70.2729	1.5542	423.4752	2511	70.2729	1.5542	325.9884	2511	70.2729	1.5542	393.5167
2512	70.2989	1.5537	345.5432	2512	70.2989	1.5537	431.0644	2512	70.2989	1.5537	359.7391	2512	70.2989	1.5537	426.7446
2513	70.3249	1.5532	375.5855	2513	70.3249	1.5532	461.368	2513	70.3249	1.5532	357.9685	2513	70.3249	1.5532	424.4512
2514	70.3509	1.5527	342.0423	2514	70.3509	1.5527	428.0861	2514	70.3509	1.5527	360.515	2514	70.3509	1.5527	426.4749
2515	70.3769	1.5522	328.4181	2515	70.3769	1.5522	414.7232	2515	70.3769	1.5522	314.8253	2515	70.3769	1.5522	380.2625

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2516	70.4029	1.5517	325.3419	2516	70.4029	1.5517	411.9082	2516	70.4029	1.5517	385.5413	2516	70.4029	1.5517	450.4557
2517	70.4289	1.5512	364.3911	2517	70.4289	1.5512	451.2187	2517	70.4289	1.5512	333.5673	2517	70.4289	1.5512	397.9588
2518	70.4549	1.5507	341.8619	2518	70.4549	1.5507	428.9508	2518	70.4549	1.5507	360.8222	2518	70.4549	1.5507	424.6909
2519	70.4809	1.5502	302.2294	2519	70.4809	1.5502	389.5797	2519	70.4809	1.5502	386.808	2519	70.4809	1.5502	450.154
2520	70.5069	1.5497	338.3138	2520	70.5069	1.5497	425.9253	2520	70.5069	1.5497	334.2515	2520	70.5069	1.5497	397.0747
2521	70.5329	1.5492	325.1815	2521	70.5329	1.5492	413.0543	2521	70.5329	1.5492	347.6453	2521	70.5329	1.5492	409.9457
2522	70.5589	1.5488	351.4852	2522	70.5589	1.5488	439.6193	2522	70.5589	1.5488	381.743	2522	70.5589	1.5488	443.5206
2523	70.5849	1.5483	384.7878	2523	70.5849	1.5483	473.1833	2523	70.5849	1.5483	348.586	2523	70.5849	1.5483	409.8408
2524	70.6109	1.5478	375.6827	2524	70.6109	1.5478	464.3394	2524	70.6109	1.5478	347.302	2524	70.6109	1.5478	408.0339
2525	70.6369	1.5473	324.4069	2525	70.6369	1.5473	413.3249	2525	70.6369	1.5473	332.4927	2525	70.6369	1.5473	392.7019
2526	70.6629	1.5468	349.2608	2526	70.6629	1.5468	438.4401	2526	70.6629	1.5468	340.8295	2526	70.6629	1.5468	400.5159
2527	70.6889	1.5463	337.4513	2527	70.6889	1.5463	426.892	2527	70.6889	1.5463	350.263	2527	70.6889	1.5463	409.4266
2528	70.7149	1.5458	365.9418	2528	70.7149	1.5458	455.6437	2528	70.7149	1.5458	329.1264	2528	70.7149	1.5458	387.7672
2529	70.7409	1.5453	332.2955	2529	70.7409	1.5453	422.2587	2529	70.7409	1.5453	325.1327	2529	70.7409	1.5453	383.2507
2530	70.7669	1.5448	346.9059	2530	70.7669	1.5448	437.1304	2530	70.7669	1.5448	368.9179	2530	70.7669	1.5448	426.5131
2531	70.7929	1.5443	382.585	2531	70.7929	1.5443	473.0708	2531	70.7929	1.5443	372.1344	2531	70.7929	1.5443	429.2068
2532	70.8189	1.5438	344.5791	2532	70.8189	1.5438	435.3262	2532	70.8189	1.5438	393.7306	2532	70.8189	1.5438	450.2803
2533	70.8449	1.5433	365.2943	2533	70.8449	1.5433	456.3027	2533	70.8449	1.5433	361.903	2533	70.8449	1.5433	417.9298
2534	70.8709	1.5428	334.057	2534	70.8709	1.5428	425.3267	2534	70.8709	1.5428	362.697	2534	70.8709	1.5428	418.201
2535	70.8969	1.5423	348.178	2535	70.8969	1.5423	439.7089	2535	70.8969	1.5423	378.5862	2535	70.8969	1.5423	433.5675
2536	70.9229	1.5418	348.6668	2536	70.9229	1.5418	440.459	2536	70.9229	1.5418	378.1536	2536	70.9229	1.5418	432.612
2537	70.9489	1.5413	344.5982	2537	70.9489	1.5413	436.6517	2537	70.9489	1.5413	342.0705	2537	70.9489	1.5413	396.0062
2538	70.9749	1.5409	301.5008	2538	70.9749	1.5409	393.8157	2538	70.9749	1.5409	389.3515	2538	70.9749	1.5409	442.7643
2539	71.0009	1.5404	345.5432	2539	71.0009	1.5404	438.1194	2539	71.0009	1.5404	324.2911	2539	71.0009	1.5404	377.1812
2540	71.0269	1.5399	314.1532	2540	71.0269	1.5399	408.0204	2540	71.0269	1.5399	345.031	2540	71.0269	1.5399	398.7504
2541	71.0529	1.5394	349.0895	2541	71.0529	1.5394	444.2479	2541	71.0529	1.5394	359.033	2541	71.0529	1.5394	413.5816
2542	71.0789	1.5389	376.0871	2542	71.0789	1.5389	472.5365	2542	71.0789	1.5389	358.8346	2542	71.0789	1.5389	414.2125
2543	71.1049	1.5384	356.711	2543	71.1049	1.5384	454.4516	2543	71.1049	1.5384	359.3478	2543	71.1049	1.5384	415.5551
2544	71.1309	1.5379	357.4121	2544	71.1309	1.5379	456.4437	2544	71.1309	1.5379	371.2452	2544	71.1309	1.5379	428.2818
2545	71.1569	1.5374	346.5542	2545	71.1569	1.5374	446.877	2545	71.1569	1.5374	343.8266	2545	71.1569	1.5374	401.6925
2546	71.1829	1.5369	309.98	2546	71.1829	1.5369	411.5939	2546	71.1829	1.5369	336.2959	2546	71.1829	1.5369	394.9911
2547	71.2089	1.5365	307.687	2547	71.2089	1.5365	410.592	2547	71.2089	1.5365	360.0865	2547	71.2089	1.5365	419.611
2548	71.2349	1.536	312.7156	2548	71.2349	1.536	416.9117	2548	71.2349	1.536	334.8898	2548	71.2349	1.536	395.2436
2549	71.2609	1.5355	318.2568	2549	71.2609	1.5355	423.744	2549	71.2609	1.5355	333.3049	2549	71.2609	1.5355	394.488
2550	71.2869	1.535	320.6379	2550	71.2869	1.535	427.4162	2550	71.2869	1.535	341.9442	2550	71.2869	1.535	403.9565
2551	71.3129	1.5345	321.3269	2551	71.3129	1.5345	429.3963	2551	71.3129	1.5345	329.1953	2551	71.3129	1.5345	392.0369

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2552	71.3389	1.534	330.2748	2552	71.3389	1.534	439.6352	2552	71.3389	1.534	311.3173	2552	71.3389	1.534	374.9883
2553	71.3649	1.5335	354.376	2553	71.3649	1.5335	465.0276	2553	71.3649	1.5335	306.8564	2553	71.3649	1.5335	371.3566
2554	71.3909	1.5331	369.7412	2554	71.3909	1.5331	481.6839	2554	71.3909	1.5331	328.7272	2554	71.3909	1.5331	394.0568
2555	71.4169	1.5326	342.1353	2555	71.4169	1.5326	455.3691	2555	71.4169	1.5326	352.0105	2555	71.4169	1.5326	418.1693
2556	71.4429	1.5321	334.5547	2556	71.4429	1.5321	449.0796	2556	71.4429	1.5321	350.2293	2556	71.4429	1.5321	417.2175
2557	71.4689	1.5316	331.7978	2557	71.4689	1.5316	447.6138	2557	71.4689	1.5316	333.0488	2557	71.4689	1.5316	400.8662
2558	71.4949	1.5311	326.8929	2558	71.4949	1.5311	444	2558	71.4949	1.5311	328.4967	2558	71.4949	1.5311	397.1435
2559	71.5209	1.5306	336.7398	2559	71.5209	1.5306	455.138	2559	71.5209	1.5306	335.0929	2559	71.5209	1.5306	404.569
2560	71.5469	1.5302	336.831	2560	71.5469	1.5302	456.5203	2560	71.5469	1.5302	357.178	2560	71.5469	1.5302	427.4833
2561	71.5729	1.5297	333.8164	2561	71.5729	1.5297	454.7968	2561	71.5729	1.5297	370.0632	2561	71.5729	1.5297	441.1979
2562	71.5989	1.5292	346.0977	2562	71.5989	1.5292	468.3692	2562	71.5989	1.5292	353.5438	2562	71.5989	1.5292	425.5078
2563	71.6249	1.5287	359.2283	2563	71.6249	1.5287	482.7909	2563	71.6249	1.5287	331.9414	2563	71.6249	1.5287	404.7346
2564	71.6509	1.5282	364.9921	2564	71.6509	1.5282	489.8458	2564	71.6509	1.5282	327.2233	2564	71.6509	1.5282	400.8458
2565	71.6769	1.5278	369.2107	2565	71.6769	1.5278	495.3555	2565	71.6769	1.5278	339.1738	2565	71.6769	1.5278	413.6256
2566	71.7029	1.5273	429.8906	2566	71.7029	1.5273	557.3265	2566	71.7029	1.5273	381.8753	2566	71.7029	1.5273	457.1565
2567	71.7289	1.5268	545.6451	2567	71.7289	1.5268	672.3459	2567	71.7289	1.5268	429.8473	2567	71.7289	1.5268	505.9577
2568	71.7549	1.5263	690.3977	2568	71.7549	1.5263	816.3634	2568	71.7549	1.5263	541.8952	2568	71.7549	1.5263	618.835
2569	71.7809	1.5258	747.4677	2569	71.7809	1.5258	872.6983	2569	71.7809	1.5258	675.0689	2569	71.7809	1.5258	752.838
2570	71.8069	1.5254	674.9933	2570	71.8069	1.5254	799.4888	2570	71.8069	1.5254	734.6906	2570	71.8069	1.5254	813.2889
2571	71.8329	1.5249	593.2577	2571	71.8329	1.5249	717.0181	2571	71.8329	1.5249	770.0598	2571	71.8329	1.5249	849.4874
2572	71.8589	1.5244	539.9548	2572	71.8589	1.5244	662.9801	2572	71.8589	1.5244	705.5203	2572	71.8589	1.5244	785.7773
2573	71.8849	1.5239	519.589	2573	71.8849	1.5239	641.8792	2573	71.8849	1.5239	544.894	2573	71.8849	1.5239	625.9802
2574	71.9109	1.5235	532.8437	2574	71.9109	1.5235	654.3988	2574	71.9109	1.5235	479.3029	2574	71.9109	1.5235	561.2185
2575	71.9369	1.523	543.72	2575	71.9369	1.523	664.54	2575	71.9369	1.523	507.8958	2575	71.9369	1.523	590.6406
2576	71.9629	1.5225	553.3671	2576	71.9629	1.5225	673.452	2576	71.9629	1.5225	553.3319	2576	71.9629	1.5225	636.906
2577	71.9889	1.522	547.1629	2577	71.9889	1.522	666.5127	2577	71.9889	1.522	594.9599	2577	71.9889	1.522	679.3633
2578	72.0149	1.5215	492.5466	2578	72.0149	1.5215	611.1613	2578	72.0149	1.5215	580.6732	2578	72.0149	1.5215	665.9059
2579	72.0409	1.5211	442.7138	2579	72.0409	1.5211	560.5934	2579	72.0409	1.5211	489.5121	2579	72.0409	1.5211	575.5742
2580	72.0669	1.5206	420.3641	2580	72.0669	1.5206	537.5086	2580	72.0669	1.5206	406.8775	2580	72.0669	1.5206	493.7688
2581	72.0929	1.5201	434.2265	2581	72.0929	1.5201	550.6359	2581	72.0929	1.5201	423.9031	2581	72.0929	1.5201	511.6238
2582	72.1189	1.5197	468.3899	2582	72.1189	1.5197	584.0642	2582	72.1189	1.5197	489.163	2582	72.1189	1.5197	577.7129
2583	72.1449	1.5192	463.8606	2583	72.1449	1.5192	578.7999	2583	72.1449	1.5192	632.7875	2583	72.1449	1.5192	722.1667
2584	72.1709	1.5187	485.2787	2584	72.1709	1.5187	599.4829	2584	72.1709	1.5187	810.8633	2584	72.1709	1.5187	901.0718
2585	72.1969	1.5182	475.1815	2585	72.1969	1.5182	588.6505	2585	72.1969	1.5182	898.9395	2585	72.1969	1.5182	989.9773
2586	72.2229	1.5178	448.0556	2586	72.2229	1.5178	560.7895	2586	72.2229	1.5178	831.1515	2586	72.2229	1.5178	923.0187
2587	72.2489	1.5173	437.9326	2587	72.2489	1.5173	549.9314	2587	72.2489	1.5173	591.9818	2587	72.2489	1.5173	684.6782

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2588	72.2749	1.5168	427.4398	2588	72.2749	1.5168	538.7035	2588	72.2749	1.5168	517.2608	2588	72.2749	1.5168	610.7865
2589	72.3009	1.5163	418.7558	2589	72.3009	1.5163	529.2844	2589	72.3009	1.5163	490.9571	2589	72.3009	1.5163	585.3121
2590	72.3269	1.5159	424.3848	2590	72.3269	1.5159	534.1783	2590	72.3269	1.5159	524.4414	2590	72.3269	1.5159	619.6257
2591	72.3529	1.5154	417.2885	2591	72.3529	1.5154	526.347	2591	72.3529	1.5154	567.1331	2591	72.3529	1.5154	663.1467
2592	72.3789	1.5149	394.2121	2592	72.3789	1.5149	502.5355	2592	72.3789	1.5149	591.5744	2592	72.3789	1.5149	688.4173
2593	72.4049	1.5145	400.2506	2593	72.4049	1.5145	507.8389	2593	72.4049	1.5145	566.5329	2593	72.4049	1.5145	664.2052
2594	72.4309	1.514	369.83	2594	72.4309	1.514	476.6832	2594	72.4309	1.514	475.6943	2594	72.4309	1.514	572.0631
2595	72.4569	1.5135	346.8056	2595	72.4569	1.5135	452.9236	2595	72.4569	1.5135	373.6407	2595	72.4569	1.5135	468.7061
2596	72.4829	1.5131	354.5906	2596	72.4829	1.5131	459.9736	2596	72.4829	1.5131	337.7216	2596	72.4829	1.5131	431.4835
2597	72.5089	1.5126	349.1536	2597	72.5089	1.5126	453.8015	2597	72.5089	1.5126	348.946	2597	72.5089	1.5126	441.4045
2598	72.5349	1.5121	358.1196	2598	72.5349	1.5121	462.0323	2598	72.5349	1.5121	384.6779	2598	72.5349	1.5121	475.8329
2599	72.5609	1.5117	344.9044	2599	72.5609	1.5117	448.082	2599	72.5609	1.5117	319.8141	2599	72.5609	1.5117	409.6657
2600	72.5869	1.5112	422.7316	2600	72.5869	1.5112	525.1742	2600	72.5869	1.5112	331.7184	2600	72.5869	1.5112	420.2665
2601	72.6129	1.5107	459.2722	2601	72.6129	1.5107	560.9796	2601	72.6129	1.5107	352.0371	2601	72.6129	1.5107	439.2817
2602	72.6389	1.5103	451.4513	2602	72.6389	1.5103	552.4236	2602	72.6389	1.5103	314.7435	2602	72.6389	1.5103	400.6847
2603	72.6649	1.5098	451.0381	2603	72.6649	1.5098	551.2754	2603	72.6649	1.5098	356.3788	2603	72.6649	1.5098	441.0166
2604	72.6909	1.5093	446.8169	2604	72.6909	1.5093	546.3191	2604	72.6909	1.5093	395.5607	2604	72.6909	1.5093	478.895
2605	72.7169	1.5089	407.4351	2605	72.7169	1.5089	506.2022	2605	72.7169	1.5089	403.0469	2605	72.7169	1.5089	485.0777
2606	72.7429	1.5084	458.3466	2606	72.7429	1.5084	556.3786	2606	72.7429	1.5084	379.0599	2606	72.7429	1.5084	459.7873
2607	72.7689	1.5079	413.9955	2607	72.7689	1.5079	511.2924	2607	72.7689	1.5079	324.1461	2607	72.7689	1.5079	403.57
2608	72.7949	1.5075	401.6202	2608	72.7949	1.5075	498.182	2608	72.7949	1.5075	331.6638	2608	72.7949	1.5075	409.7842
2609	72.8209	1.507	420.8428	2609	72.8209	1.507	516.6694	2609	72.8209	1.507	352.5322	2609	72.8209	1.507	429.3493
2610	72.8469	1.5065	404.9084	2610	72.8469	1.5065	500	2610	72.8469	1.5065	366.4176	2610	72.8469	1.5065	441.9312
2611	72.8729	1.5061	409.859	2611	72.8729	1.5061	504.2155	2611	72.8729	1.5061	383.3871	2611	72.8729	1.5061	457.5972
2612	72.8989	1.5056	441.0618	2612	72.8989	1.5056	534.6832	2612	72.8989	1.5056	323.6233	2612	72.8989	1.5056	396.53
2613	72.9249	1.5052	380.0308	2613	72.9249	1.5052	472.917	2613	72.9249	1.5052	358.3181	2613	72.9249	1.5052	429.9214
2614	72.9509	1.5047	377.6573	2614	72.9509	1.5047	469.8085	2614	72.9509	1.5047	348.0654	2614	72.9509	1.5047	418.3652
2615	72.9769	1.5042	348.0588	2615	72.9769	1.5042	439.4749	2615	72.9769	1.5042	354.3824	2615	72.9769	1.5042	423.3788
2616	73.0029	1.5038	312.0639	2616	73.0029	1.5038	402.7449	2616	73.0029	1.5038	360.4558	2616	73.0029	1.5038	428.1487
2617	73.0289	1.5033	327.0063	2617	73.0289	1.5033	416.9522	2617	73.0289	1.5033	347.0001	2617	73.0289	1.5033	413.3895
2618	73.0549	1.5028	347.4882	2618	73.0549	1.5028	436.6989	2618	73.0549	1.5028	357.2142	2618	73.0549	1.5028	422.3002
2619	73.0809	1.5024	311.3212	2619	73.0809	1.5024	399.7969	2619	73.0809	1.5024	366.1862	2619	73.0809	1.5024	429.9687
2620	73.1069	1.5019	345.5432	2620	73.1069	1.5019	433.2838	2620	73.1069	1.5019	324.2911	2620	73.1069	1.5019	386.7702
2621	73.1329	1.5015	366.5251	2621	73.1329	1.5015	453.9569	2621	73.1329	1.5015	308.2954	2621	73.1329	1.5015	369.8347
2622	73.1589	1.501	354.9529	2622	73.1589	1.501	442.0759	2622	73.1589	1.501	263.6917	2622	73.1589	1.501	324.2911
2623	73.1849	1.5005	349.2832	2623	73.1849	1.5005	436.0975	2623	73.1849	1.5005	357.7965	2623	73.1849	1.5005	417.4561

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2624	73.2109	1.5001	360.2065	2624	73.2109	1.5001	446.7121	2624	73.2109	1.5001	307.6936	2624	73.2109	1.5001	366.4134
2625	73.2369	1.4996	346.3446	2625	73.2369	1.4996	432.5414	2625	73.2369	1.4996	392.0436	2625	73.2369	1.4996	449.8236
2626	73.2629	1.4992	357.5597	2626	73.2629	1.4992	443.4478	2626	73.2629	1.4992	336.059	2626	73.2629	1.4992	392.8991
2627	73.2889	1.4987	351.8123	2627	73.2889	1.4987	437.3916	2627	73.2889	1.4987	380.3587	2627	73.2889	1.4987	436.2589
2628	73.3149	1.4983	342.3881	2628	73.3149	1.4983	427.6586	2628	73.3149	1.4983	339.201	2628	73.3149	1.4983	394.1614
2629	73.3409	1.4978	325.4024	2629	73.3409	1.4978	410.3641	2629	73.3409	1.4978	313.874	2629	73.3409	1.4978	367.8946
2630	73.3669	1.4973	368.2331	2630	73.3669	1.4973	452.8861	2630	73.3669	1.4973	341.2623	2630	73.3669	1.4973	394.3431
2631	73.3929	1.4969	357.2815	2631	73.3929	1.4969	441.6257	2631	73.3929	1.4969	342.1459	2631	73.3929	1.4969	394.2869
2632	73.4189	1.4964	295.142	2632	73.4189	1.4964	379.1775	2632	73.4189	1.4964	353.5323	2632	73.4189	1.4964	404.7334
2633	73.4449	1.496	332.4996	2633	73.4449	1.496	416.2263	2633	73.4449	1.496	371.6602	2633	73.4449	1.496	421.9215
2634	73.4709	1.4955	303.5979	2634	73.4709	1.4955	387.0159	2634	73.4709	1.4955	368.5563	2634	73.4709	1.4955	417.8778
2635	73.4969	1.4951	336.9368	2635	73.4969	1.4951	420.046	2635	73.4969	1.4951	360.8363	2635	73.4969	1.4951	409.2179
2636	73.5229	1.4946	328.6686	2636	73.5229	1.4946	411.4691	2636	73.5229	1.4946	374.2344	2636	73.5229	1.4946	421.6761
2637	73.5489	1.4942	355.2328	2637	73.5489	1.4942	437.7245	2637	73.5489	1.4942	360.6013	2637	73.5489	1.4942	407.1033
2638	73.5749	1.4937	314.8968	2638	73.5749	1.4937	397.0797	2638	73.5749	1.4937	342.5745	2638	73.5749	1.4937	388.1366
2639	73.6009	1.4933	330.8756	2639	73.6009	1.4933	412.7498	2639	73.6009	1.4933	332.9528	2639	73.6009	1.4933	377.5751
2640	73.6269	1.4928	332.3592	2640	73.6269	1.4928	413.9247	2640	73.6269	1.4928	342.9135	2640	73.6269	1.4928	386.5959
2641	73.6529	1.4924	330.9382	2641	73.6529	1.4924	412.1949	2641	73.6529	1.4924	353.5037	2641	73.6529	1.4924	396.2463
2642	73.6789	1.4919	336.6187	2642	73.6789	1.4919	417.5666	2642	73.6789	1.4919	336.3166	2642	73.6789	1.4919	378.1194
2643	73.7049	1.4914	303.8075	2643	73.7049	1.4914	384.4467	2643	73.7049	1.4914	377.6846	2643	73.7049	1.4914	418.5476
2644	73.7309	1.491	330.3371	2644	73.7309	1.491	410.6675	2644	73.7309	1.491	356.1847	2644	73.7309	1.491	396.1079
2645	73.7569	1.4905	353.9912	2645	73.7569	1.4905	434.0128	2645	73.7569	1.4905	330.1766	2645	73.7569	1.4905	369.1599
2646	73.7829	1.4901	341.6653	2646	73.7829	1.4901	421.3782	2646	73.7829	1.4901	342.5783	2646	73.7829	1.4901	380.6218
2647	73.8089	1.4896	345.5432	2647	73.8089	1.4896	424.9474	2647	73.8089	1.4896	324.2911	2647	73.8089	1.4896	361.3947
2648	73.8349	1.4892	351.4571	2648	73.8349	1.4892	430.2071	2648	73.8349	1.4892	340.9124	2648	73.8349	1.4892	378.0135
2649	73.8609	1.4887	280.3271	2649	73.8609	1.4887	358.4231	2649	73.8609	1.4887	339.7406	2649	73.8609	1.4887	376.8392
2650	73.8869	1.4883	337.3123	2650	73.8869	1.4883	414.7541	2650	73.8869	1.4883	330.893	2650	73.8869	1.4883	367.9891
2651	73.9129	1.4878	382.5071	2651	73.9129	1.4878	459.2948	2651	73.9129	1.4878	326.0827	2651	73.9129	1.4878	363.1763
2652	73.9389	1.4874	366.9863	2652	73.9389	1.4874	443.1199	2652	73.9389	1.4874	338.133	2652	73.9389	1.4874	375.224
2653	73.9649	1.4869	365.3813	2653	73.9649	1.4869	440.8608	2653	73.9649	1.4869	341.8532	2653	73.9649	1.4869	378.9418
2654	73.9909	1.4865	382.0215	2654	73.9909	1.4865	456.847	2654	73.9909	1.4865	342.2663	2654	73.9909	1.4865	379.3523
2655	74.0169	1.4861	376.8364	2655	74.0169	1.4861	451.0078	2655	74.0169	1.4861	344.249	2655	74.0169	1.4861	381.3325
2656	74.0429	1.4856	347.8555	2656	74.0429	1.4856	421.3727	2656	74.0429	1.4856	350.8258	2656	74.0429	1.4856	387.9068
2657	74.0689	1.4852	325.1482	2657	74.0689	1.4852	398.0114	2657	74.0689	1.4852	366.8494	2657	74.0689	1.4852	403.9278
2658	74.0949	1.4847	343.3403	2658	74.0949	1.4847	415.5493	2658	74.0949	1.4847	358.6488	2658	74.0949	1.4847	395.7248
2659	74.1209	1.4843	363.7105	2659	74.1209	1.4843	435.2655	2659	74.1209	1.4843	338.6487	2659	74.1209	1.4843	375.7222

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2660	74.1469	1.4838	342.2009	2660	74.1469	1.4838	413.1018	2660	74.1469	1.4838	341.1785	2660	74.1469	1.4838	378.2494
2661	74.1729	1.4834	347.9878	2661	74.1729	1.4834	418.2346	2661	74.1729	1.4834	359.0656	2661	74.1729	1.4834	396.134
2662	74.1989	1.4829	349.2782	2662	74.1989	1.4829	418.8709	2662	74.1989	1.4829	358.5792	2662	74.1989	1.4829	395.6451
2663	74.2249	1.4825	324.6294	2663	74.2249	1.4825	393.568	2663	74.2249	1.4825	357.6315	2663	74.2249	1.4825	394.6949
2664	74.2509	1.482	333.9082	2664	74.2509	1.482	402.1927	2664	74.2509	1.482	355.1698	2664	74.2509	1.482	392.2307
2665	74.2769	1.4816	349.9366	2665	74.2769	1.4816	417.567	2665	74.2769	1.4816	348.6736	2665	74.2769	1.4816	385.7319
2666	74.3029	1.4812	364.3939	2666	74.3029	1.4812	431.3702	2666	74.3029	1.4812	348.0584	2666	74.3029	1.4812	385.1142
2667	74.3289	1.4807	358.1684	2667	74.3289	1.4807	424.4906	2667	74.3289	1.4807	374.1164	2667	74.3289	1.4807	411.1697
2668	74.3549	1.4803	342.7202	2668	74.3549	1.4803	408.3883	2668	74.3549	1.4803	351.9696	2668	74.3549	1.4803	389.0203
2669	74.3809	1.4798	362.5516	2669	74.3809	1.4798	427.5656	2669	74.3809	1.4798	314.4244	2669	74.3809	1.4798	351.4727
2670	74.4069	1.4794	390.4359	2670	74.4069	1.4794	454.7958	2670	74.4069	1.4794	334.6503	2670	74.4069	1.4794	371.696
2671	74.4329	1.4789	359.7108	2671	74.4329	1.4789	423.4166	2671	74.4329	1.4789	350.4044	2671	74.4329	1.4789	387.4476
2672	74.4589	1.4785	334.3872	2672	74.4589	1.4785	397.4389	2672	74.4589	1.4785	353.9251	2672	74.4589	1.4785	390.9658
2673	74.4849	1.4781	338.825	2673	74.4849	1.4781	401.2226	2673	74.4849	1.4781	379.4919	2673	74.4849	1.4781	416.5301
2674	74.5109	1.4776	345.5432	2674	74.5109	1.4776	407.2868	2674	74.5109	1.4776	385.1107	2674	74.5109	1.4776	422.1464
2675	74.5369	1.4772	380.0175	2675	74.5369	1.4772	441.776	2675	74.5369	1.4772	372.3058	2675	74.5369	1.4772	409.3389
2676	74.5629	1.4767	388.7798	2676	74.5629	1.4767	450.5533	2676	74.5629	1.4767	373.5958	2676	74.5629	1.4767	410.6264
2677	74.5889	1.4763	366.7005	2677	74.5889	1.4763	428.489	2677	74.5889	1.4763	371.5239	2677	74.5889	1.4763	408.5521
2678	74.6149	1.4759	389.9242	2678	74.6149	1.4759	451.7278	2678	74.6149	1.4759	367.0322	2678	74.6149	1.4759	404.0578
2679	74.6409	1.4754	417.7698	2679	74.6409	1.4754	479.5884	2679	74.6409	1.4754	369.2546	2679	74.6409	1.4754	406.2777
2680	74.6669	1.475	405.9481	2680	74.6669	1.475	467.7817	2680	74.6669	1.475	369.3613	2680	74.6669	1.475	406.3819
2681	74.6929	1.4745	432.8486	2681	74.6929	1.4745	494.6972	2681	74.6929	1.4745	373.5369	2681	74.6929	1.4745	410.555
2682	74.7189	1.4741	450.153	2682	74.7189	1.4741	512.0167	2682	74.7189	1.4741	391.4161	2682	74.7189	1.4741	428.4317
2683	74.7449	1.4737	455.7737	2683	74.7449	1.4737	517.6523	2683	74.7449	1.4737	372.9956	2683	74.7449	1.4737	410.0086
2684	74.7709	1.4732	447.9906	2684	74.7709	1.4732	509.8843	2684	74.7709	1.4732	368.0453	2684	74.7709	1.4732	405.0558
2685	74.7969	1.4728	416.1483	2685	74.7969	1.4728	478.057	2685	74.7969	1.4728	419.64	2685	74.7969	1.4728	456.648
2686	74.8229	1.4724	407.1021	2686	74.8229	1.4724	469.0257	2686	74.8229	1.4724	489.5599	2686	74.8229	1.4724	526.5654
2687	74.8489	1.4719	374.8461	2687	74.8489	1.4719	436.7848	2687	74.8489	1.4719	470.9558	2687	74.8489	1.4719	507.9588
2688	74.8749	1.4715	414.8223	2688	74.8749	1.4715	476.776	2688	74.8749	1.4715	424.3984	2688	74.8749	1.4715	461.3988
2689	74.9009	1.471	422.7693	2689	74.9009	1.471	484.738	2689	74.9009	1.471	379.1758	2689	74.9009	1.471	416.1738
2690	74.9269	1.4706	418.3954	2690	74.9269	1.4706	480.3791	2690	74.9269	1.4706	346.9444	2690	74.9269	1.4706	383.9398
2691	74.9529	1.4702	419.0219	2691	74.9529	1.4702	481.0206	2691	74.9529	1.4702	353.1671	2691	74.9529	1.4702	390.16
2692	74.9789	1.4697	399.5578	2692	74.9789	1.4697	461.5715	2692	74.9789	1.4697	394.5141	2692	74.9789	1.4697	431.5044
2693	75.0049	1.4693	405.4875	2693	75.0049	1.4693	467.5163	2693	75.0049	1.4693	402.8689	2693	75.0049	1.4693	439.8567
2694	75.0309	1.4689	375.2891	2694	75.0309	1.4689	437.3328	2694	75.0309	1.4689	420.2855	2694	75.0309	1.4689	457.2708
2695	75.0569	1.4684	398.7091	2695	75.0569	1.4684	460.7679	2695	75.0569	1.4684	387.3237	2695	75.0569	1.4684	424.3066

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2696	75.0829	1.468	376.6957	2696	75.0829	1.468	438.7695	2696	75.0829	1.468	374.053	2696	75.0829	1.468	411.0333
2697	75.1089	1.4676	348.6417	2697	75.1089	1.4676	410.7305	2697	75.1089	1.4676	357.5212	2697	75.1089	1.4676	394.499
2698	75.1349	1.4671	377.417	2698	75.1349	1.4671	439.5208	2698	75.1349	1.4671	357.1081	2698	75.1349	1.4671	394.0834
2699	75.1609	1.4667	368.9915	2699	75.1609	1.4667	431.1104	2699	75.1609	1.4667	343.6783	2699	75.1609	1.4667	380.6511
2700	75.1869	1.4663	346.3056	2700	75.1869	1.4663	408.4395	2700	75.1869	1.4663	319.9087	2700	75.1869	1.4663	356.8789
2701	75.2129	1.4658	345.5432	2701	75.2129	1.4658	407.6921	2701	75.2129	1.4658	324.2911	2701	75.2129	1.4658	361.2589
2702	75.2389	1.4654	338.0486	2702	75.2389	1.4654	400.1993	2702	75.2389	1.4654	323.9026	2702	75.2389	1.4654	361.2027
2703	75.2649	1.465	346.2668	2703	75.2649	1.465	408.4194	2703	75.2649	1.465	306.6471	2703	75.2649	1.465	344.2796
2704	75.2909	1.4645	360.4854	2704	75.2909	1.4645	422.6399	2704	75.2909	1.4645	315.8552	2704	75.2909	1.4645	353.82
2705	75.3169	1.4641	356.2918	2705	75.3169	1.4641	418.4482	2705	75.3169	1.4641	322.1882	2705	75.3169	1.4641	360.4853
2706	75.3429	1.4637	349.1283	2706	75.3429	1.4637	411.2866	2706	75.3429	1.4637	353.0839	2706	75.3429	1.4637	391.7134
2707	75.3689	1.4633	374.736	2707	75.3689	1.4633	436.8961	2707	75.3689	1.4633	324.5873	2707	75.3689	1.4633	363.5492
2708	75.3949	1.4628	363.3994	2708	75.3949	1.4628	425.5614	2708	75.3949	1.4628	324.3725	2708	75.3949	1.4628	363.6667
2709	75.4209	1.4624	365.0101	2709	75.4209	1.4624	427.174	2709	75.4209	1.4624	336.4605	2709	75.4209	1.4624	376.087
2710	75.4469	1.462	355.7265	2710	75.4469	1.462	417.8922	2710	75.4469	1.462	318.3562	2710	75.4469	1.462	358.3152
2711	75.4729	1.4615	371.9666	2711	75.4729	1.4615	434.1342	2711	75.4729	1.4615	377.824	2711	75.4729	1.4615	418.1153
2712	75.4989	1.4611	337.4611	2712	75.4989	1.4611	399.6306	2712	75.4989	1.4611	369.7724	2712	75.4989	1.4611	410.396
2713	75.5249	1.4607	377.649	2713	75.5249	1.4607	439.8203	2713	75.5249	1.4607	361.231	2713	75.5249	1.4607	402.187
2714	75.5509	1.4603	363.2405	2714	75.5509	1.4603	425.4138	2714	75.5509	1.4603	332.3884	2714	75.5509	1.4603	373.6767
2715	75.5769	1.4598	334.8175	2715	75.5769	1.4598	396.9926	2715	75.5769	1.4598	329.0174	2715	75.5769	1.4598	370.6381
2716	75.6029	1.4594	351.0547	2716	75.6029	1.4594	413.2317	2716	75.6029	1.4594	335.8275	2716	75.6029	1.4594	377.7805
2717	75.6289	1.459	397.5537	2717	75.6289	1.459	459.7326	2717	75.6289	1.459	317.3783	2717	75.6289	1.459	359.6637
2718	75.6549	1.4585	335.5031	2718	75.6549	1.4585	397.6838	2718	75.6549	1.4585	329.1766	2718	75.6549	1.4585	371.7943
2719	75.6809	1.4581	306.9708	2719	75.6809	1.4581	369.1534	2719	75.6809	1.4581	323.8003	2719	75.6809	1.4581	366.7503
2720	75.7069	1.4577	372.7938	2720	75.7069	1.4577	434.9782	2720	75.7069	1.4577	316.5052	2720	75.7069	1.4577	359.7876
2721	75.7329	1.4573	326.6659	2721	75.7329	1.4573	388.8523	2721	75.7329	1.4573	352.8966	2721	75.7329	1.4573	396.5114
2722	75.7589	1.4568	400.7238	2722	75.7589	1.4568	462.912	2722	75.7589	1.4568	396.9635	2722	75.7589	1.4568	440.9106
2723	75.7849	1.4564	340.3272	2723	75.7849	1.4564	402.5173	2723	75.7849	1.4564	335.2463	2723	75.7849	1.4564	379.5258
2724	75.8109	1.456	386.9247	2724	75.8109	1.456	449.1167	2724	75.8109	1.456	347.1489	2724	75.8109	1.456	391.7608
2725	75.8369	1.4556	315.9022	2725	75.8369	1.4556	378.096	2725	75.8369	1.4556	334.424	2725	75.8369	1.4556	379.3682
2726	75.8629	1.4551	332.0775	2726	75.8629	1.4551	394.2733	2726	75.8629	1.4551	345.2645	2726	75.8629	1.4551	390.541
2727	75.8889	1.4547	371.8274	2727	75.8889	1.4547	434.025	2727	75.8889	1.4547	329.21	2727	75.8889	1.4547	374.8189
2728	75.9149	1.4543	345.5432	2728	75.9149	1.4543	407.7428	2728	75.9149	1.4543	324.2911	2728	75.9149	1.4543	370.2324
2729	75.9409	1.4539	386.5882	2729	75.9409	1.4539	448.8714	2729	75.9409	1.4539	315.3511	2729	75.9409	1.4539	361.6121
2730	75.9669	1.4535	318.6344	2730	75.9669	1.4535	381.0011	2730	75.9669	1.4535	306.1205	2730	75.9669	1.4535	352.7014
2731	75.9929	1.453	340.826	2731	75.9929	1.453	403.2764	2731	75.9929	1.453	310.5721	2731	75.9929	1.453	357.4728

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2732	76.0189	1.4526	381.3592	2732	76.0189	1.4526	443.8932	2732	76.0189	1.4526	327.9216	2732	76.0189	1.4526	375.1422
2733	76.0449	1.4522	380.0286	2733	76.0449	1.4522	442.6462	2733	76.0449	1.4522	325.8904	2733	76.0449	1.4522	373.4308
2734	76.0709	1.4518	356.357	2734	76.0709	1.4518	419.0583	2734	76.0709	1.4518	294.2566	2734	76.0709	1.4518	342.1169
2735	76.0969	1.4513	361.0672	2735	76.0969	1.4513	423.8521	2735	76.0969	1.4513	336.0599	2735	76.0969	1.4513	384.24
2736	76.1229	1.4509	354.3688	2736	76.1229	1.4509	417.2372	2736	76.1229	1.4509	320.0743	2736	76.1229	1.4509	368.5742
2737	76.1489	1.4505	336.8484	2737	76.1489	1.4505	399.8005	2737	76.1489	1.4505	309.3594	2737	76.1489	1.4505	358.1791
2738	76.1749	1.4501	370.1998	2738	76.1749	1.4501	433.2355	2738	76.1749	1.4501	333.141	2738	76.1749	1.4501	382.2806
2739	76.2009	1.4497	346.9012	2739	76.2009	1.4497	410.0205	2739	76.2009	1.4497	335.0423	2739	76.2009	1.4497	384.5017
2740	76.2269	1.4492	341.6199	2740	76.2269	1.4492	404.8228	2740	76.2269	1.4492	332.5751	2740	76.2269	1.4492	382.3543
2741	76.2529	1.4488	362.8493	2741	76.2529	1.4488	426.1359	2741	76.2529	1.4488	340.0301	2741	76.2529	1.4488	390.1292
2742	76.2789	1.4484	312.2231	2742	76.2789	1.4484	375.5933	2742	76.2789	1.4484	331.9451	2742	76.2789	1.4484	382.364
2743	76.3049	1.448	337.4068	2743	76.3049	1.448	400.8606	2743	76.3049	1.448	328.4682	2743	76.3049	1.448	379.2069
2744	76.3309	1.4476	359.2099	2744	76.3309	1.4476	422.7473	2744	76.3309	1.4476	302.0974	2744	76.3309	1.4476	353.156
2745	76.3569	1.4472	343.0482	2745	76.3569	1.4472	406.6693	2745	76.3569	1.4472	337.9224	2745	76.3569	1.4472	389.3008
2746	76.3829	1.4467	346.455	2746	76.3829	1.4467	410.1597	2746	76.3829	1.4467	394.5735	2746	76.3829	1.4467	446.2718
2747	76.4089	1.4463	379.3471	2747	76.4089	1.4463	443.1354	2747	76.4089	1.4463	395.1744	2747	76.4089	1.4463	447.1925
2748	76.4349	1.4459	395.0758	2748	76.4349	1.4459	458.9477	2748	76.4349	1.4459	354.9759	2748	76.4349	1.4459	407.3138
2749	76.4609	1.4455	357.4333	2749	76.4609	1.4455	421.3888	2749	76.4609	1.4455	335.0068	2749	76.4609	1.4455	387.6646
2750	76.4869	1.4451	383.4835	2750	76.4869	1.4451	447.5226	2750	76.4869	1.4451	333.4696	2750	76.4869	1.4451	386.4472
2751	76.5129	1.4447	342.4953	2751	76.5129	1.4447	406.6181	2751	76.5129	1.4447	318.715	2751	76.5129	1.4447	372.0124
2752	76.5389	1.4442	368.354	2752	76.5389	1.4442	432.5603	2752	76.5389	1.4442	345.4601	2752	76.5389	1.4442	399.0773
2753	76.5649	1.4438	408.8317	2753	76.5649	1.4438	473.1217	2753	76.5649	1.4438	359.7568	2753	76.5649	1.4438	413.6939
2754	76.5909	1.4434	404.6318	2754	76.5909	1.4434	469.0054	2754	76.5909	1.4434	344.0127	2754	76.5909	1.4434	398.2696
2755	76.6169	1.443	441.0052	2755	76.6169	1.443	505.4624	2755	76.6169	1.443	324.2911	2755	76.6169	1.443	378.8679
2756	76.6429	1.4426	469.4282	2756	76.6429	1.4426	533.969	2756	76.6429	1.4426	328.3143	2756	76.6429	1.4426	381.6331
2757	76.6689	1.4422	517.2044	2757	76.6689	1.4422	581.8288	2757	76.6689	1.4422	354.2181	2757	76.6689	1.4422	406.279
2758	76.6949	1.4418	635.6394	2758	76.6949	1.4418	700.3474	2758	76.6949	1.4418	419.6689	2758	76.6949	1.4418	470.4719
2759	76.7209	1.4413	756.0803	2759	76.7209	1.4413	820.8719	2759	76.7209	1.4413	541.7966	2759	76.7209	1.4413	591.3417
2760	76.7469	1.4409	800.1199	2760	76.7469	1.4409	864.9952	2760	76.7469	1.4409	665.0207	2760	76.7469	1.4409	713.3078
2761	76.7729	1.4405	790.7516	2761	76.7729	1.4405	855.7105	2761	76.7729	1.4405	754.0563	2761	76.7729	1.4405	801.0854
2762	76.7989	1.4401	749.1026	2762	76.7989	1.4401	814.1452	2762	76.7989	1.4401	700.1963	2762	76.7989	1.4401	745.9675
2763	76.8249	1.4397	679.3036	2763	76.8249	1.4397	744.4298	2763	76.8249	1.4397	579.8883	2763	76.8249	1.4397	624.4017
2764	76.8509	1.4393	619.8938	2764	76.8509	1.4393	685.1035	2764	76.8509	1.4393	481.367	2764	76.8509	1.4393	524.6224
2765	76.8769	1.4389	562.7709	2765	76.8769	1.4389	628.0643	2765	76.8769	1.4389	440.5538	2765	76.8769	1.4389	482.5513
2766	76.9029	1.4385	591.674	2766	76.9029	1.4385	657.051	2766	76.9029	1.4385	432.4821	2766	76.9029	1.4385	473.2217
2767	76.9289	1.438	624.9955	2767	76.9289	1.438	690.4562	2767	76.9289	1.438	457.9302	2767	76.9289	1.438	497.4118

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2768	76.9549	1.4376	619.1808	2768	76.9549	1.4376	684.7251	2768	76.9549	1.4376	538.913	2768	76.9549	1.4376	577.1367
2769	76.9809	1.4372	601.0386	2769	76.9809	1.4372	666.6664	2769	76.9809	1.4372	583.8237	2769	76.9809	1.4372	620.7894
2770	77.0069	1.4368	541.7999	2770	77.0069	1.4368	607.5114	2770	77.0069	1.4368	508.7681	2770	77.0069	1.4368	544.4759
2771	77.0329	1.4364	499.0524	2771	77.0329	1.4364	564.8475	2771	77.0329	1.4364	420.8791	2771	77.0329	1.4364	455.329
2772	77.0589	1.436	472.3922	2772	77.0589	1.436	538.2709	2772	77.0589	1.436	376.047	2772	77.0589	1.436	409.239
2773	77.0849	1.4356	439.1479	2773	77.0849	1.4356	505.1103	2773	77.0849	1.4356	367.9281	2773	77.0849	1.4356	399.8622
2774	77.1109	1.4352	434.7218	2774	77.1109	1.4352	500.7677	2774	77.1109	1.4352	385.2949	2774	77.1109	1.4352	415.971
2775	77.1369	1.4348	426.7014	2775	77.1369	1.4348	492.8309	2775	77.1369	1.4348	360.9505	2775	77.1369	1.4348	390.3686
2776	77.1629	1.4344	388.7644	2776	77.1629	1.4344	454.9776	2776	77.1629	1.4344	354.7248	2776	77.1629	1.4344	382.885
2777	77.1889	1.434	364.7918	2777	77.1889	1.434	431.0886	2777	77.1889	1.434	342.8176	2777	77.1889	1.434	369.7199
2778	77.2149	1.4335	351.5831	2778	77.2149	1.4335	417.9636	2778	77.2149	1.4335	315.2958	2778	77.2149	1.4335	340.9402
2779	77.2409	1.4331	330.8696	2779	77.2409	1.4331	397.3337	2779	77.2409	1.4331	337.6136	2779	77.2409	1.4331	362
2780	77.2669	1.4327	327.2859	2780	77.2669	1.4327	393.8335	2780	77.2669	1.4327	349.0943	2780	77.2669	1.4327	372.2228
2781	77.2929	1.4323	347.3457	2781	77.2929	1.4323	413.977	2781	77.2929	1.4323	344.1601	2781	77.2929	1.4323	366.0307
2782	77.3189	1.4319	345.5432	2782	77.3189	1.4319	412.2582	2782	77.3189	1.4319	324.2911	2782	77.3189	1.4319	344.9038
2783	77.3449	1.4315	318.6934	2783	77.3449	1.4315	385.3389	2783	77.3449	1.4315	357.198	2783	77.3449	1.4315	377.9786
2784	77.3709	1.4311	357.7795	2784	77.3709	1.4311	424.3557	2784	77.3709	1.4311	371.5798	2784	77.3709	1.4311	392.5282
2785	77.3969	1.4307	388.3106	2785	77.3969	1.4307	454.8175	2785	77.3969	1.4307	326.4645	2785	77.3969	1.4307	347.5809
2786	77.4229	1.4303	362.6617	2786	77.4229	1.4303	429.0992	2786	77.4229	1.4303	316.3418	2786	77.4229	1.4303	337.626
2787	77.4489	1.4299	362.8494	2787	77.4489	1.4299	429.2175	2787	77.4489	1.4299	345.9556	2787	77.4489	1.4299	367.4078
2788	77.4749	1.4295	356.582	2788	77.4749	1.4295	422.8809	2788	77.4749	1.4295	366.0334	2788	77.4749	1.4295	387.6534
2789	77.5009	1.4291	342.691	2789	77.5009	1.4291	408.9204	2789	77.5009	1.4291	361.5089	2789	77.5009	1.4291	383.2969
2790	77.5269	1.4287	327.1666	2790	77.5269	1.4287	393.3267	2790	77.5269	1.4287	371.6874	2790	77.5269	1.4287	393.6432
2791	77.5529	1.4283	326.0084	2791	77.5529	1.4283	392.0992	2791	77.5529	1.4283	398.689	2791	77.5529	1.4283	420.8127
2792	77.5789	1.4279	328.73	2792	77.5789	1.4279	394.7514	2792	77.5789	1.4279	359.9886	2792	77.5789	1.4279	382.2802
2793	77.6049	1.4275	343.157	2793	77.6049	1.4275	409.1091	2793	77.6049	1.4275	315.4618	2793	77.6049	1.4275	337.9213
2794	77.6309	1.4271	333.6543	2794	77.6309	1.4271	399.537	2794	77.6309	1.4271	313.243	2794	77.6309	1.4271	335.8704
2795	77.6569	1.4267	336.8015	2795	77.6569	1.4267	402.6149	2795	77.6569	1.4267	324.6385	2795	77.6569	1.4267	347.4338
2796	77.6829	1.4263	374.2853	2796	77.6829	1.4263	440.0293	2796	77.6829	1.4263	341.915	2796	77.6829	1.4263	364.8782
2797	77.7089	1.4259	323.8689	2797	77.7089	1.4259	389.5436	2797	77.7089	1.4259	355.8108	2797	77.7089	1.4259	378.9418
2798	77.7349	1.4255	334.8257	2798	77.7349	1.4255	400.431	2798	77.7349	1.4255	343.5173	2798	77.7349	1.4255	366.8163
2799	77.7609	1.4251	352.0897	2799	77.7609	1.4251	417.6257	2799	77.7609	1.4251	323.8208	2799	77.7609	1.4251	347.2877
2800	77.7869	1.4247	354.5435	2800	77.7869	1.4247	420.0101	2800	77.7869	1.4247	330.6929	2800	77.7869	1.4247	354.3276
2801	77.8129	1.4243	366.8446	2801	77.8129	1.4243	432.2419	2801	77.8129	1.4243	366.7665	2801	77.8129	1.4243	390.5692
2802	77.8389	1.4239	302.3775	2802	77.8389	1.4239	367.7055	2802	77.8389	1.4239	376.1767	2802	77.8389	1.4239	400.1473
2803	77.8649	1.4235	370.9558	2803	77.8649	1.4235	436.2144	2803	77.8649	1.4235	353.6185	2803	77.8649	1.4235	377.757

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2804	77.8909	1.4231	436.8107	2804	77.8909	1.4231	502	2804	77.8909	1.4231	376.2062	2804	77.8909	1.4231	400.5126
2805	77.9169	1.4227	437.7695	2805	77.9169	1.4227	502.8895	2805	77.9169	1.4227	403.189	2805	77.9169	1.4227	427.6632
2806	77.9429	1.4223	442.2854	2806	77.9429	1.4223	507.3359	2806	77.9429	1.4223	372.8149	2806	77.9429	1.4223	397.457
2807	77.9689	1.4219	441.9642	2807	77.9689	1.4219	506.9454	2807	77.9689	1.4219	351.3538	2807	77.9689	1.4219	376.1638
2808	77.9949	1.4215	425.9037	2808	77.9949	1.4215	490.8156	2808	77.9949	1.4215	380.9114	2808	77.9949	1.4215	405.8894
2809	78.0209	1.4211	400.0271	2809	78.0209	1.4211	464.8697	2809	78.0209	1.4211	358.1553	2809	78.0209	1.4211	383.3011
2810	78.0469	1.4207	425.4652	2810	78.0469	1.4207	490.2828	2810	78.0469	1.4207	327.3826	2810	78.0469	1.4207	352.5889
2811	78.0729	1.4203	432.1953	2811	78.0729	1.4203	496.9879	2811	78.0729	1.4203	321.5207	2811	78.0729	1.4203	346.7875
2812	78.0989	1.4199	415.7143	2812	78.0989	1.4199	480.4819	2812	78.0989	1.4199	354.1187	2812	78.0989	1.4199	379.4459
2813	78.1249	1.4195	404.4395	2813	78.1249	1.4195	469.1822	2813	78.1249	1.4195	388.051	2813	78.1249	1.4195	413.4387
2814	78.1509	1.4191	411.3843	2814	78.1509	1.4191	476.102	2814	78.1509	1.4191	361.3627	2814	78.1509	1.4191	386.8107
2815	78.1769	1.4187	371.1499	2815	78.1769	1.4187	435.8427	2815	78.1769	1.4187	331.3236	2815	78.1769	1.4187	356.8321
2816	78.2029	1.4183	367.9573	2816	78.2029	1.4183	432.6251	2816	78.2029	1.4183	362.9874	2816	78.2029	1.4183	388.5563
2817	78.2289	1.4179	348.1807	2817	78.2289	1.4179	412.8235	2817	78.2289	1.4179	344.4883	2817	78.2289	1.4179	370.1177
2818	78.2549	1.4175	332.952	2818	78.2549	1.4175	397.5698	2818	78.2549	1.4175	359.2783	2818	78.2549	1.4175	384.9681
2819	78.2809	1.4171	399.4057	2819	78.2809	1.4171	463.9986	2819	78.2809	1.4171	303.6799	2819	78.2809	1.4171	329.4302
2820	78.3069	1.4167	325.374	2820	78.3069	1.4167	389.9419	2820	78.3069	1.4167	386.3587	2820	78.3069	1.4167	412.1694
2821	78.3329	1.4163	323.4188	2821	78.3329	1.4163	387.9617	2821	78.3329	1.4163	325.1097	2821	78.3329	1.4163	350.9809
2822	78.3589	1.4159	321.7768	2822	78.3589	1.4159	386.2948	2822	78.3589	1.4159	324.4369	2822	78.3589	1.4159	350.3685
2823	78.3849	1.4155	353.4843	2823	78.3849	1.4155	417.9773	2823	78.3849	1.4155	363.9796	2823	78.3849	1.4155	389.9716
2824	78.4109	1.4151	311.9785	2824	78.4109	1.4151	376.4465	2824	78.4109	1.4151	325.3622	2824	78.4109	1.4151	351.4146
2825	78.4369	1.4147	359.5497	2825	78.4369	1.4147	423.9928	2825	78.4369	1.4147	391.4894	2825	78.4369	1.4147	417.6023
2826	78.4629	1.4143	333.4352	2826	78.4629	1.4143	397.8533	2826	78.4629	1.4143	307.5086	2826	78.4629	1.4143	333.6819
2827	78.4889	1.4139	314.3744	2827	78.4889	1.4139	378.7676	2827	78.4889	1.4139	344.1098	2827	78.4889	1.4139	370.3437
2828	78.5149	1.4136	334.5247	2828	78.5149	1.4136	398.8929	2828	78.5149	1.4136	341.907	2828	78.5149	1.4136	368.2013
2829	78.5409	1.4132	329.0785	2829	78.5409	1.4132	393.4217	2829	78.5409	1.4132	334.1273	2829	78.5409	1.4132	360.4819
2830	78.5669	1.4128	356.5768	2830	78.5669	1.4128	420.895	2830	78.5669	1.4128	347.5324	2830	78.5669	1.4128	373.9475
2831	78.5929	1.4124	384.4642	2831	78.5929	1.4124	448.7575	2831	78.5929	1.4124	349.4443	2831	78.5929	1.4124	375.9199
2832	78.6189	1.412	331.2223	2832	78.6189	1.412	395.4906	2832	78.6189	1.412	335.8141	2832	78.6189	1.412	362.3502
2833	78.6449	1.4116	347.3582	2833	78.6449	1.4116	411.6016	2833	78.6449	1.4116	342.5041	2833	78.6449	1.4116	369.1006
2834	78.6709	1.4112	314.1758	2834	78.6709	1.4112	378.3942	2834	78.6709	1.4112	362.0361	2834	78.6709	1.4112	388.693
2835	78.6969	1.4108	352.9375	2835	78.6969	1.4108	417.1309	2835	78.6969	1.4108	317.6308	2835	78.6969	1.4108	344.3482
2836	78.7229	1.4104	281.3748	2836	78.7229	1.4104	345.5432	2836	78.7229	1.4104	341.6827	2836	78.7229	1.4104	368.4605
2837	78.7489	1.41	355.0339	2837	78.7489	1.41	419.1775	2837	78.7489	1.41	338.4184	2837	78.7489	1.41	365.2566
2838	78.7749	1.4096	333.1623	2838	78.7749	1.4096	397.2808	2838	78.7749	1.4096	335.4004	2838	78.7749	1.4096	362.2991
2839	78.8009	1.4093	330.2685	2839	78.8009	1.4093	394.3621	2839	78.8009	1.4093	340.9246	2839	78.8009	1.4093	367.8837

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2840	78.8269	1.4089	306.8436	2840	78.8269	1.4089	370.9123	2840	78.8269	1.4089	356.9314	2840	78.8269	1.4089	383.951
2841	78.8529	1.4085	329.8598	2841	78.8529	1.4085	393.9034	2841	78.8529	1.4085	353.3545	2841	78.8529	1.4085	380.4345
2842	78.8789	1.4081	349.7643	2842	78.8789	1.4081	413.783	2842	78.8789	1.4081	355.9134	2842	78.8789	1.4081	383.0538
2843	78.9049	1.4077	320.9725	2843	78.9049	1.4077	384.9662	2843	78.9049	1.4077	352.7949	2843	78.9049	1.4077	379.9958
2844	78.9309	1.4073	285.349	2844	78.9309	1.4073	349.3177	2844	78.9309	1.4073	323.2655	2844	78.9309	1.4073	350.5268
2845	78.9569	1.4069	315.5442	2845	78.9569	1.4069	379.488	2845	78.9569	1.4069	339.1082	2845	78.9569	1.4069	366.43
2846	78.9829	1.4065	319.9125	2846	78.9829	1.4065	383.8314	2846	78.9829	1.4065	338.6781	2846	78.9829	1.4065	366.0603
2847	79.0089	1.4061	346.2689	2847	79.0089	1.4061	410.1627	2847	79.0089	1.4061	337.3185	2847	79.0089	1.4061	364.7612
2848	79.0349	1.4058	319.0719	2848	79.0349	1.4058	382.9408	2848	79.0349	1.4058	320.9698	2848	79.0349	1.4058	348.4729
2849	79.0609	1.4054	323.4649	2849	79.0609	1.4054	387.3088	2849	79.0609	1.4054	347.3128	2849	79.0609	1.4054	374.8764
2850	79.0869	1.405	314.5533	2850	79.0869	1.405	378.3722	2850	79.0869	1.405	327.6577	2850	79.0869	1.405	355.2817
2851	79.1129	1.4046	317.8636	2851	79.1129	1.4046	381.6576	2851	79.1129	1.4046	314.1512	2851	79.1129	1.4046	341.8356
2852	79.1389	1.4042	326.9233	2852	79.1389	1.4042	390.6924	2852	79.1389	1.4042	333.8899	2852	79.1389	1.4042	361.6348
2853	79.1649	1.4038	329.2559	2853	79.1649	1.4038	393	2853	79.1649	1.4038	360.4369	2853	79.1649	1.4038	388.2422
2854	79.1909	1.4034	333.4311	2854	79.1909	1.4034	397.1502	2854	79.1909	1.4034	350.8418	2854	79.1909	1.4034	378.7075
2855	79.2169	1.4031	316.8979	2855	79.2169	1.4031	380.592	2855	79.2169	1.4031	338.3014	2855	79.2169	1.4031	366.2276
2856	79.2429	1.4027	307.659	2856	79.2429	1.4027	371.3281	2856	79.2429	1.4027	326.6074	2856	79.2429	1.4027	354.594
2857	79.2689	1.4023	313.9751	2857	79.2689	1.4023	377.6193	2857	79.2689	1.4023	355.7115	2857	79.2689	1.4023	383.7586
2858	79.2949	1.4019	307.6006	2858	79.2949	1.4019	371.2198	2858	79.2949	1.4019	344.204	2858	79.2949	1.4019	372.3116
2859	79.3209	1.4015	321.6683	2859	79.3209	1.4015	385.2626	2859	79.3209	1.4015	330.1162	2859	79.3209	1.4015	358.2842
2860	79.3469	1.4011	331.7985	2860	79.3469	1.4011	395.3678	2860	79.3469	1.4011	341.5184	2860	79.3469	1.4011	369.7468
2861	79.3729	1.4008	312.7883	2861	79.3729	1.4008	376.3327	2861	79.3729	1.4008	328.4216	2861	79.3729	1.4008	356.7105
2862	79.3989	1.4004	308.2161	2862	79.3989	1.4004	371.7355	2862	79.3989	1.4004	311.1398	2862	79.3989	1.4004	339.4891
2863	79.4249	1.4	340.8183	2863	79.4249	1.4	404.3127	2863	79.4249	1.4	325.0598	2863	79.4249	1.4	353.4696
2864	79.4509	1.3996	364.8628	2864	79.4509	1.3996	428.3323	2864	79.4509	1.3996	348.9718	2864	79.4509	1.3996	377.442
2865	79.4769	1.3992	340.0103	2865	79.4769	1.3992	403.4548	2865	79.4769	1.3992	338.2451	2865	79.4769	1.3992	366.7757
2866	79.5029	1.3988	334.4689	2866	79.5029	1.3988	397.8884	2866	79.5029	1.3988	327.8447	2866	79.5029	1.3988	356.4358
2867	79.5289	1.3985	338.2902	2867	79.5289	1.3985	401.6848	2867	79.5289	1.3985	338.2264	2867	79.5289	1.3985	366.8779
2868	79.5549	1.3981	312.1773	2868	79.5549	1.3981	375.5469	2868	79.5549	1.3981	316.6487	2868	79.5549	1.3981	345.3606
2869	79.5809	1.3977	305.4269	2869	79.5809	1.3977	368.7716	2869	79.5809	1.3977	311.0564	2869	79.5809	1.3977	339.8288
2870	79.6069	1.3973	313.1474	2870	79.6069	1.3973	376.4671	2870	79.6069	1.3973	335.2931	2870	79.6069	1.3973	364.1259
2871	79.6329	1.3969	324.2117	2871	79.6329	1.3969	387.5064	2871	79.6329	1.3969	347.2448	2871	79.6329	1.3969	376.1381
2872	79.6589	1.3966	315.2325	2872	79.6589	1.3966	378.5023	2872	79.6589	1.3966	341.8367	2872	79.6589	1.3966	370.7904
2873	79.6849	1.3962	316.8822	2873	79.6849	1.3962	380.127	2873	79.6849	1.3962	339.0176	2873	79.6849	1.3962	368.0318
2874	79.7109	1.3958	316.0635	2874	79.7109	1.3958	379.2834	2874	79.7109	1.3958	335.0468	2874	79.7109	1.3958	364.1214
2875	79.7369	1.3954	305.4384	2875	79.7369	1.3954	368.6333	2875	79.7369	1.3954	320.5483	2875	79.7369	1.3954	349.6834

Table I. part 1: *Continued*

$CaCO_3$_powderACROS_BackgrdRemoved				CaCO3_powder_ACROS_raw				E007_Crystal_seed_Exp_BackgrdRmovd				E007_Crystal_Seed_Exp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2876	79.7629	1.395	322.9844	2876	79.7629	1.395	386.1543	2876	79.7629	1.395	320.012	2876	79.7629	1.395	349.2075
2877	79.7889	1.3947	322.9028	2877	79.7889	1.3947	386.0477	2877	79.7889	1.3947	335.4773	2877	79.7889	1.3947	364.7332
2878	79.8149	1.3943	317.1479	2878	79.8149	1.3943	380.2678	2878	79.8149	1.3943	348.0443	2878	79.8149	1.3943	377.3607
2879	79.8409	1.3939	326.5596	2879	79.8409	1.3939	389.6546	2879	79.8409	1.3939	338.0885	2879	79.8409	1.3939	367.4653
2880	79.8669	1.3935	317.1475	2880	79.8669	1.3935	380.2175	2880	79.8669	1.3935	332.2371	2880	79.8669	1.3935	361.6744
2881	79.8929	1.3932	291.4121	2881	79.8929	1.3932	354.4572	2881	79.8929	1.3932	339.2643	2881	79.8929	1.3932	368.762
2882	79.9189	1.3928	299.9823	2882	79.9189	1.3928	363.0024	2882	79.9189	1.3928	332.2002	2882	79.9189	1.3928	361.7584
2883	79.9449	1.3924	331.5472	2883	79.9449	1.3924	394.5423	2883	79.9449	1.3924	327.1498	2883	79.9449	1.3924	356.7684
2884	79.9709	1.392	345.5183	2884	79.9709	1.392	408.5134	2884	79.9709	1.392	324.3516	2884	79.9709	1.392	353.9702

APPENDIX I

Table I. part 2: Raw and processed X-ray diffraction data from synthetic samples produced in constant composition experiments shown in Chapter 5.

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1	5.0129	20.4542	360.0713	1	5.0129	20.4542	5529	1	5.0129	20.4542	422.169	1	5.0129	20.4542	5701
2	5.0389	20.3487	469.458	2	5.0389	20.3487	5611.1764	2	5.0389	20.3487	491.6867	2	5.0389	20.3487	5742.5833
3	5.0649	20.2443	542.5789	3	5.0649	20.2443	5657.0871	3	5.0649	20.2443	407.3199	3	5.0649	20.2443	5630.2821
4	5.0909	20.141	370.834	4	5.0909	20.141	5458.132	4	5.0909	20.141	398.0438	4	5.0909	20.141	5593.0716
5	5.1169	20.0387	398.6344	5	5.1169	20.0387	5458.7222	5	5.1169	20.0387	328.8755	5	5.1169	20.0387	5495.9689
6	5.1429	19.9375	271.2092	6	5.1429	19.9375	5304.0867	6	5.1429	19.9375	387.0549	6	5.1429	19.9375	5526.214
7	5.1689	19.8373	243.3094	7	5.1689	19.8373	5248.9767	7	5.1689	19.8373	395.1446	7	5.1689	19.8373	5506.3693
8	5.1949	19.7381	172.6275	8	5.1949	19.7381	5151.0845	8	5.1949	19.7381	315.6277	8	5.1949	19.7381	5398.918
9	5.2209	19.6398	389.7663	9	5.2209	19.6398	5341.013	9	5.2209	19.6398	375.2308	9	5.2209	19.6398	5430.5867
10	5.2469	19.5426	276.4125	10	5.2469	19.5426	5200.449	10	5.2469	19.5426	330.0797	10	5.2469	19.5426	5357.5013
11	5.2729	19.4463	267.4558	11	5.2729	19.4463	5164.2821	11	5.2729	19.4463	355.0168	11	5.2729	19.4463	5354.5039
12	5.2989	19.3509	208.6436	12	5.2989	19.3509	5078.2597	12	5.2989	19.3509	362.9576	12	5.2989	19.3509	5334.5103
13	5.3249	19.2565	301.3544	13	5.3249	19.2565	5143.7602	13	5.3249	19.2565	408.6431	13	5.3249	19.2565	5352.2614
14	5.3509	19.163	281.3177	14	5.3509	19.163	5096.5133	14	5.3509	19.163	318.2456	14	5.3509	19.163	5233.9296
15	5.3769	19.0704	311.2088	15	5.3769	19.0704	5099.1941	15	5.3769	19.0704	339.4445	15	5.3769	19.0704	5227.1941
16	5.4029	18.9787	290.0061	16	5.4029	18.9787	5050.7812	16	5.4029	18.9787	305.3474	16	5.4029	18.9787	5165.1626
17	5.4289	18.8879	219.2634	17	5.4289	18.8879	4952.8282	17	5.4289	18.8879	506.3515	17	5.4289	18.8879	5338.2323
18	5.4549	18.7979	206.3684	18	5.4549	18.7979	4912.723	18	5.4549	18.7979	352.0788	18	5.4549	18.7979	5156.0252
19	5.4809	18.7088	250.212	19	5.4809	18.7088	4929.3564	19	5.4809	18.7088	414.0208	19	5.4809	18.7088	5190.0329
20	5.5069	18.6206	318.5823	20	5.5069	18.6206	4970.5164	20	5.5069	18.6206	403.7419	20	5.5069	18.6206	5151.8196
21	5.5329	18.5331	376.7196	21	5.5329	18.5331	5001.4435	21	5.5329	18.5331	391.6039	21	5.5329	18.5331	5111.7472
22	5.5589	18.4465	404.7366	22	5.5589	18.4465	5002.2502	22	5.5589	18.4465	350.2522	22	5.5589	18.4465	5042.4611
23	5.5849	18.3607	329.0743	23	5.5849	18.3607	4899.3778	23	5.5849	18.3607	324.2034	23	5.5849	18.3607	4988.4779
24	5.6109	18.2757	425.152	24	5.6109	18.2757	4968.2452	24	5.6109	18.2757	354.7802	24	5.6109	18.2757	4991.1204
25	5.6369	18.1915	180.1804	25	5.6369	18.1915	4696.0633	25	5.6369	18.1915	439.1629	25	5.6369	18.1915	5047.5687
26	5.6629	18.108	279.5067	26	5.6629	18.108	4768.1793	26	5.6629	18.108	490.2961	26	5.6629	18.108	5070.7675
27	5.6889	18.0253	365.2477	27	5.6889	18.0253	4826.7101	27	5.6889	18.0253	472.9737	27	5.6889	18.0253	5025.5107
28	5.7149	17.9434	360.0713	28	5.7149	17.9434	4794.3235	28	5.7149	17.9434	422.169	28	5.7149	17.9434	4946.7717
29	5.7409	17.8622	347.6227	29	5.7409	17.8622	4773.3339	29	5.7409	17.8622	515.8623	29	5.7409	17.8622	5030.882
30	5.7669	17.7817	310.8069	30	5.7669	17.7817	4727.977	30	5.7669	17.7817	387.0752	30	5.7669	17.7817	4892.5121
31	5.7929	17.702	395.7809	31	5.7929	17.702	4804.4101	31	5.7929	17.702	489.8961	31	5.7929	17.702	4985.7502

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
32	5.8189	17.623	324.8175	32	5.8189	17.623	4724.9057	32	5.8189	17.623	393.1645	32	5.8189	17.623	4879.4357
33	5.8449	17.5446	260.6608	33	5.8449	17.5446	4652.2079	33	5.8449	17.5446	387.7829	33	5.8449	17.5446	4864.4713
34	5.8709	17.467	301.6929	34	5.8709	17.467	4684.699	34	5.8709	17.467	411.4255	34	5.8709	17.467	4878.531
35	5.8969	17.3901	339.1493	35	5.8969	17.3901	4713.6143	35	5.8969	17.3901	453.2359	35	5.8969	17.3901	4910.7585
36	5.9229	17.3138	332.4943	36	5.9229	17.3138	4698.4184	36	5.9229	17.3138	396.9012	36	5.9229	17.3138	4844.841
37	5.9489	17.2382	354.4004	37	5.9489	17.2382	4711.7835	37	5.9489	17.2382	341.3592	37	5.9489	17.2382	4779.7161
38	5.9749	17.1632	319.8321	38	5.9749	17.1632	4668.6741	38	5.9749	17.1632	485.7872	38	5.9749	17.1632	4914.5613
39	6.0009	17.0889	309.4039	39	6.0009	17.0889	4649.705	39	6.0009	17.0889	472.6609	39	6.0009	17.0889	4891.8521
40	6.0269	17.0153	235.5115	40	6.0269	17.0153	4567.2715	40	6.0269	17.0153	403.905	40	6.0269	17.0153	4813.5133
41	6.0529	16.9423	414.1528	41	6.0529	16.9423	4737.3718	41	6.0529	16.9423	483.3786	41	6.0529	16.9423	4883.4041
42	6.0789	16.8699	358.7751	42	6.0789	16.8699	4673.453	42	6.0789	16.8699	320.3331	42	6.0789	16.8699	4710.7757
43	6.1049	16.7981	250.0262	43	6.1049	16.7981	4556.1632	43	6.1049	16.7981	326.6223	43	6.1049	16.7981	4707.482
44	6.1309	16.7269	318.9646	44	6.1309	16.7269	4616.5606	44	6.1309	16.7269	400.1491	44	6.1309	16.7269	4771.4261
45	6.1569	16.6564	323.7033	45	6.1569	16.6564	4612.7583	45	6.1569	16.6564	426.8868	45	6.1569	16.6564	4788.5809
46	6.1829	16.5864	302.0581	46	6.1829	16.5864	4582.572	46	6.1829	16.5864	492.0472	46	6.1829	16.5864	4844.1584
47	6.2089	16.517	274.9562	47	6.2089	16.517	4546.9291	47	6.2089	16.517	467.0935	47	6.2089	16.517	4809.6219
48	6.2349	16.4482	235.7557	48	6.2349	16.4482	4499.1876	48	6.2349	16.4482	413.1075	48	6.2349	16.4482	4746.053
49	6.2609	16.38	242.3447	49	6.2609	16.38	4497.2356	49	6.2609	16.38	437.2035	49	6.2609	16.38	4760.5662
50	6.2869	16.3123	345.8041	50	6.2869	16.3123	4592.154	50	6.2869	16.3123	460.7508	50	6.2869	16.3123	4774.5305
51	6.3129	16.2452	309.2587	51	6.3129	16.2452	4547.0675	51	6.3129	16.2452	459.3458	51	6.3129	16.2452	4763.5427
52	6.3389	16.1786	185.8891	52	6.3389	16.1786	4415.157	52	6.3389	16.1786	447.218	52	6.3389	16.1786	4741.832
53	6.3649	16.1126	212.2518	53	6.3649	16.1126	4432.9786	53	6.3649	16.1126	450.2666	53	6.3649	16.1126	4735.2978
54	6.3909	16.0471	304.5449	54	6.3909	16.0471	4516.7307	54	6.3909	16.0471	446.5186	54	6.3909	16.0471	4721.967
55	6.4169	15.9821	360.0713	55	6.4169	15.9821	4563.7161	55	6.4169	15.9821	422.169	55	6.4169	15.9821	4688.0346
56	6.4429	15.9177	320.7416	56	6.4429	15.9177	4516.2038	56	6.4429	15.9177	419.8988	56	6.4429	15.9177	4677.7376
57	6.4689	15.8538	270.5012	57	6.4689	15.8538	4457.7807	57	6.4689	15.8538	414.7418	57	6.4689	15.8538	4664.554
58	6.4949	15.7904	266.1162	58	6.4949	15.7904	4445.2132	58	6.4949	15.7904	421.3538	58	6.4949	15.7904	4663.1393
59	6.5209	15.7275	264.1054	59	6.5209	15.7275	4435.0197	59	6.5209	15.7275	392.7423	59	6.5209	15.7275	4626.5011
60	6.5469	15.6651	279.9476	60	6.5469	15.6651	4442.6793	60	6.5469	15.6651	374.4137	60	6.5469	15.6651	4600.1458
61	6.5729	15.6032	297.864	61	6.5729	15.6032	4452.413	61	6.5729	15.6032	399.2204	61	6.5729	15.6032	4616.9259
62	6.5989	15.5418	277.9496	62	6.5989	15.5418	4424.316	62	6.5989	15.5418	411.8737	62	6.5989	15.5418	4621.5525
63	6.6249	15.4809	288.8004	63	6.6249	15.4809	4426.9842	63	6.6249	15.4809	450.0653	63	6.6249	15.4809	4651.7174
64	6.6509	15.4204	250.1235	64	6.6509	15.4204	4380.1247	64	6.6509	15.4204	477.3904	64	6.6509	15.4204	4671.0159
65	6.6769	15.3605	313.1026	65	6.6769	15.3605	4434.9211	65	6.6769	15.3605	402.0803	65	6.6769	15.3605	4587.6791
66	6.7029	15.3009	398.807	66	6.7029	15.3009	4512.4429	66	6.7029	15.3009	386.4015	66	6.7029	15.3009	4563.9737
67	6.7289	15.2419	318.4236	67	6.7289	15.2419	4423.8768	67	6.7289	15.2419	339.9941	67	6.7289	15.2419	4509.5395

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
68	6.7549	15.1833	244.2612	68	6.7549	15.1833	4341.5319	68	6.7549	15.1833	387.0954	68	6.7549	15.1833	4548.6142
69	6.7809	15.1251	315.4304	69	6.7809	15.1251	4404.5185	69	6.7809	15.1251	404.8076	69	6.7809	15.1251	4558.2997
70	6.8069	15.0674	300.8413	70	6.8069	15.0674	4381.7467	70	6.8069	15.0674	454.1897	70	6.8069	15.0674	4599.6551
71	6.8329	15.0102	269.4529	71	6.8329	15.0102	4342.1757	71	6.8329	15.0102	399.5152	71	6.8329	15.0102	4536.954
72	6.8589	14.9533	223.4599	72	6.8589	14.9533	4288	72	6.8589	14.9533	406.7362	72	6.8589	14.9533	4536.1483
73	6.8849	14.8969	265.0571	73	6.8849	14.8969	4321.4146	73	6.8849	14.8969	478.3582	73	6.8849	14.8969	4599.7436
74	6.9109	14.841	353.517	74	6.9109	14.841	4401.6919	74	6.9109	14.841	353.9218	74	6.9109	14.841	4467.2806
75	6.9369	14.7854	388.884	75	6.9369	14.7854	4428.8763	75	6.9369	14.7854	440.0574	75	6.9369	14.7854	4545.3895
76	6.9629	14.7303	456.537	76	6.9629	14.7303	4488.3467	76	6.9629	14.7303	431.3037	76	6.9629	14.7303	4528.6092
77	6.9889	14.6755	343.7171	77	6.9889	14.6755	4367.3442	77	6.9889	14.6755	607.3758	77	6.9889	14.6755	4696.6546
78	7.0149	14.6212	361.2217	78	7.0149	14.6212	4376.6661	78	7.0149	14.6212	392.8366	78	7.0149	14.6212	4474.0887
79	7.0409	14.5673	468.6237	79	7.0409	14.5673	4475.8855	79	7.0409	14.5673	380.9819	79	7.0409	14.5673	4454.2073
80	7.0669	14.5138	498.2263	80	7.0669	14.5138	4497.3054	80	7.0669	14.5138	432.3142	80	7.0669	14.5138	4497.513
81	7.0929	14.4606	409.0497	81	7.0929	14.4606	4399.9462	81	7.0929	14.4606	431.8052	81	7.0929	14.4606	4488.9773
82	7.1189	14.4079	360.0713	82	7.1189	14.4079	4342.7852	82	7.1189	14.4079	422.169	82	7.1189	14.4079	4471.3144
83	7.1449	14.3555	354.1267	83	7.1449	14.3555	4333.3267	83	7.1449	14.3555	540.1952	83	7.1449	14.3555	4582.912
84	7.1709	14.3035	298.079	84	7.1709	14.3035	4273.7652	84	7.1709	14.3035	380.6535	84	7.1709	14.3035	4416.9417
85	7.1969	14.2519	284.8252	85	7.1969	14.2519	4256.9975	85	7.1969	14.2519	389.6226	85	7.1969	14.2519	4419.482
86	7.2229	14.2007	312.268	86	7.2229	14.2007	4280.9265	86	7.2229	14.2007	491.9804	86	7.2229	14.2007	4515.4112
87	7.2489	14.1498	359.3082	87	7.2489	14.1498	4324.4528	87	7.2489	14.1498	447.7324	87	7.2489	14.1498	4464.7346
88	7.2749	14.0993	318.4536	88	7.2749	14.0993	4280.0844	88	7.2749	14.0993	519.828	88	7.2749	14.0993	4530.4015
89	7.3009	14.0492	228.4162	89	7.3009	14.0492	4186.5331	89	7.3009	14.0492	513.2797	89	7.3009	14.0492	4517.4246
90	7.3269	13.9994	369.086	90	7.3269	13.9994	4323.6891	90	7.3269	13.9994	537.9056	90	7.3269	13.9994	4535.6219
91	7.3529	13.95	403.3962	91	7.3529	13.95	4354.4854	91	7.3529	13.95	511.6299	91	7.3529	13.95	4502.9175
92	7.3789	13.9009	472.3894	92	7.3789	13.9009	4419.9648	92	7.3789	13.9009	575.0163	92	7.3789	13.9009	4559.8753
93	7.4049	13.8521	283.6623	93	7.4049	13.8521	4227.7238	93	7.4049	13.8521	494.7395	93	7.4049	13.8521	4473.1699
94	7.4309	13.8037	412.6525	94	7.4309	13.8037	4353.2001	94	7.4309	13.8037	486.0913	94	7.4309	13.8037	4458.093
95	7.4569	13.7557	326.668	95	7.4569	13.7557	4263.7017	95	7.4569	13.7557	536.2445	95	7.4569	13.7557	4501.8176
96	7.4829	13.7079	380.3324	96	7.4829	13.7079	4313.8524	96	7.4829	13.7079	469.8227	96	7.4829	13.7079	4428.9671
97	7.5089	13.6605	359.7733	97	7.5089	13.6605	4289.7794	97	7.5089	13.6605	462.5589	97	7.5089	13.6605	4415.2747
98	7.5349	13.6135	261.9988	98	7.5349	13.6135	4188.491	98	7.5349	13.6135	531.4846	98	7.5349	13.6135	4477.7718
99	7.5609	13.5667	353.7789	99	7.5609	13.5667	4276.7573	99	7.5609	13.5667	457.0193	99	7.5609	13.5667	4396.8778
100	7.5869	13.5203	315.464	100	7.5869	13.5203	4234.9285	100	7.5869	13.5203	529.9063	100	7.5869	13.5203	4463.3362
101	7.6129	13.4742	425.7696	101	7.6129	13.4742	4341.7203	101	7.6129	13.4742	554.7346	101	7.6129	13.4742	4481.7358
102	7.6389	13.4284	393.6406	102	7.6389	13.4284	4306.0775	102	7.6389	13.4284	527.5006	102	7.6389	13.4284	4448.0732
103	7.6649	13.3829	281.4897	103	7.6649	13.3829	4190.4126	103	7.6649	13.3829	463.7133	103	7.6649	13.3829	4377.8572

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
104	7.6909	13.3378	275.7669	104	7.6909	13.3378	4181.176	104	7.6909	13.3378	623.8093	104	7.6909	13.3378	4531.5246
105	7.7169	13.2929	403.0192	105	7.7169	13.2929	4304.9144	105	7.7169	13.2929	565.9476	105	7.7169	13.2929	4467.2343
106	7.7429	13.2483	405.8278	106	7.7429	13.2483	4304.2092	106	7.7429	13.2483	513.6106	106	7.7429	13.2483	4408.4686
107	7.7689	13.204	294.3958	107	7.7689	13.204	4189.2633	107	7.7689	13.204	470.1588	107	7.7689	13.204	4358.5882
108	7.7949	13.1601	352.6368	108	7.7949	13.1601	4243.9905	108	7.7949	13.1601	550.0028	108	7.7949	13.1601	4432.0035
109	7.8209	13.1164	401.9378	109	7.8209	13.1164	4289.7777	109	7.8209	13.1164	422.169	109	7.8209	13.1164	4297.7411
110	7.8469	13.073	204.9627	110	7.8469	13.073	4087.2627	110	7.8469	13.073	555.5403	110	7.8469	13.073	4429.3629
111	7.8729	13.0299	338.5161	111	7.8729	13.0299	4215.2762	111	7.8729	13.0299	459.0842	111	7.8729	13.0299	4331.1572
112	7.8989	12.9871	320.1388	112	7.8989	12.9871	4191.3591	112	7.8989	12.9871	489.2161	112	7.8989	12.9871	4359.5395
113	7.9249	12.9445	219.1187	113	7.9249	12.9445	4084.7991	113	7.9249	12.9445	479.4294	113	7.9249	12.9445	4348.0033
114	7.9509	12.9023	232.0714	114	7.9509	12.9023	4092.212	114	7.9509	12.9023	480.0544	114	7.9509	12.9023	4346.8788
115	7.9769	12.8603	299.4817	115	7.9769	12.8603	4154.0824	115	7.9769	12.8603	611.3851	115	7.9769	12.8603	4476.4599
116	8.0029	12.8186	340.5662	116	8.0029	12.8186	4189.627	116	8.0029	12.8186	563.9598	116	8.0029	12.8186	4427.2851
117	8.0289	12.7771	354.7241	117	8.0289	12.7771	4198.2451	117	8.0289	12.7771	541.689	117	8.0289	12.7771	4403.2648
118	8.0549	12.7359	303.9606	118	8.0549	12.7359	4141.9418	118	8.0549	12.7359	439.6437	118	8.0549	12.7359	4299.4699
119	8.0809	12.695	326.7504	119	8.0809	12.695	4159.1918	119	8.0809	12.695	625.0699	119	8.0809	12.695	4483.1465
120	8.1069	12.6544	408.5538	120	8.1069	12.6544	4235.4553	120	8.1069	12.6544	592.4829	120	8.1069	12.6544	4448.81
121	8.1329	12.614	474.9606	121	8.1329	12.614	4296.3222	121	8.1329	12.614	528.0536	121	8.1329	12.614	4382.6312
122	8.1589	12.5739	463.1991	122	8.1589	12.5739	4279.0209	122	8.1589	12.5739	494.1899	122	8.1589	12.5739	4347.0179
123	8.1849	12.534	288.8219	123	8.1849	12.534	4099.1038	123	8.1849	12.534	528.606	123	8.1849	12.534	4379.6845
124	8.2109	12.4944	343.364	124	8.2109	12.4944	4148.1061	124	8.2109	12.4944	535.9937	124	8.2109	12.4944	4385.3227
125	8.2369	12.455	356.5569	125	8.2369	12.455	4155.7591	125	8.2369	12.455	547.1955	125	8.2369	12.455	4394.7749
126	8.2629	12.4159	365.4542	126	8.2629	12.4159	4159.1166	126	8.2629	12.4159	479.2376	126	8.2629	12.4159	4325.0675
127	8.2889	12.377	493.0943	127	8.2889	12.377	4281.2168	127	8.2889	12.377	478.9138	127	8.2889	12.377	4322.9942
128	8.3149	12.3384	405.241	128	8.3149	12.3384	4187.8236	128	8.3149	12.3384	492.1084	128	8.3149	12.3384	4334.4392
129	8.3409	12.3	404.1043	129	8.3409	12.3	4181.1471	129	8.3409	12.3	503.4482	129	8.3409	12.3	4344.0294
130	8.3669	12.2618	306.4131	130	8.3669	12.2618	4077.916	130	8.3669	12.2618	435.4458	130	8.3669	12.2618	4274.2775
131	8.3929	12.2239	260.3561	131	8.3929	12.2239	4026.3192	131	8.3929	12.2239	476.3775	131	8.3929	12.2239	4313.4597
132	8.4189	12.1862	334.2949	132	8.4189	12.1862	4094.7181	132	8.4189	12.1862	490.2634	132	8.4189	12.1862	4325.596
133	8.4449	12.1488	313.5155	133	8.4449	12.1488	4068.3989	133	8.4449	12.1488	477.1338	133	8.4449	12.1488	4310.7169
134	8.4709	12.1116	409.9938	134	8.4709	12.1116	4159.3373	134	8.4709	12.1116	467.6828	134	8.4709	12.1116	4299.5163
135	8.4969	12.0746	431.9828	135	8.4969	12.0746	4175.7865	135	8.4969	12.0746	514.1857	135	8.4969	12.0746	4344.2697
136	8.5229	12.0378	414.7732	136	8.5229	12.0378	4153.0371	136	8.5229	12.0378	467.0116	136	8.5229	12.0378	4295.346
137	8.5489	12.0013	472.9237	137	8.5489	12.0013	4205.6477	137	8.5489	12.0013	399.8573	137	8.5489	12.0013	4224.821
138	8.5749	11.9649	413.6409	138	8.5749	11.9649	4140.825	138	8.5749	11.9649	448.1903	138	8.5749	11.9649	4269.7833
139	8.6009	11.9288	381.4931	139	8.6009	11.9288	4103.1374	139	8.6009	11.9288	499.3923	139	8.6009	11.9288	4317.6145

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
140	8.6269	11.8929	437.4893	140	8.6269	11.8929	4153.5937	140	8.6269	11.8929	462.3468	140	8.6269	11.8929	4277.1983
141	8.6529	11.8573	414.0672	141	8.6529	11.8573	4124.6318	141	8.6529	11.8573	508.603	141	8.6529	11.8573	4320.0837
142	8.6789	11.8218	517.1858	142	8.6789	11.8218	4222.2105	142	8.6789	11.8218	467.7465	142	8.6789	11.8218	4275.8565
143	8.7049	11.7866	439.7062	143	8.7049	11.7866	4139.191	143	8.7049	11.7866	420.7173	143	8.7049	11.7866	4225.4566
144	8.7309	11.7516	372.3817	144	8.7309	11.7516	4066.3267	144	8.7309	11.7516	493.9727	144	8.7309	11.7516	4295.3412
145	8.7569	11.7167	355.7606	145	8.7569	11.7167	4044.1658	145	8.7569	11.7167	523.5818	145	8.7569	11.7167	4321.5795
146	8.7829	11.6821	322.3797	146	8.7829	11.6821	4005.2451	146	8.7829	11.6821	507.8828	146	8.7829	11.6821	4302.5099
147	8.8089	11.6477	393.6306	147	8.8089	11.6477	4070.9561	147	8.8089	11.6477	534.2083	147	8.8089	11.6477	4325.4646
148	8.8349	11.6135	429.5575	148	8.8349	11.6135	4101.3431	148	8.8349	11.6135	563.9873	148	8.8349	11.6135	4351.8728
149	8.8609	11.5795	458.7428	149	8.8609	11.5795	4124.9886	149	8.8609	11.5795	493.8861	149	8.8609	11.5795	4278.4009
150	8.8869	11.5457	449.1362	150	8.8869	11.5457	4109.8422	150	8.8869	11.5457	460.6722	150	8.8869	11.5457	4241.8163
151	8.9129	11.5121	404.7873	151	8.9129	11.5121	4059.9534	151	8.9129	11.5121	513.1813	151	8.9129	11.5121	4290.9546
152	8.9389	11.4786	413.8929	152	8.9389	11.4786	4063.5191	152	8.9389	11.4786	493.9535	152	8.9389	11.4786	4268.3561
153	8.9649	11.4454	391.4705	153	8.9649	11.4454	4035.5568	153	8.9649	11.4454	465.3126	153	8.9649	11.4454	4236.3444
154	8.9909	11.4124	382.6928	154	8.9909	11.4124	4021.2393	154	8.9909	11.4124	467.2555	154	8.9909	11.4124	4234.9165
155	9.0169	11.3795	323.6234	155	9.0169	11.3795	3956.63	155	9.0169	11.3795	438.4151	155	9.0169	11.3795	4202.7054
156	9.0429	11.3469	334.6451	156	9.0429	11.3469	3962.1119	156	9.0429	11.3469	535.5156	156	9.0429	11.3469	4296.4353
157	9.0689	11.3144	419.2863	157	9.0689	11.3144	4041.2132	157	9.0689	11.3144	537.9102	157	9.0689	11.3144	4295.459
158	9.0949	11.2822	410.6623	158	9.0949	11.2822	4027.0494	158	9.0949	11.2822	396.1631	158	9.0949	11.2822	4150.3412
159	9.1209	11.2501	423.2737	159	9.1209	11.2501	4034.1209	159	9.1209	11.2501	439.0255	159	9.1209	11.2501	4189.8329
160	9.1469	11.2182	374.0902	160	9.1469	11.2182	3979.3976	160	9.1469	11.2182	451.6939	160	9.1469	11.2182	4199.1305
161	9.1729	11.1864	370.4698	161	9.1729	11.1864	3970.2373	161	9.1729	11.1864	398.8037	161	9.1729	11.1864	4142.8696
162	9.1989	11.1549	408.3631	162	9.1989	11.1549	4002.5908	162	9.1989	11.1549	356.2103	162	9.1989	11.1549	4096.9055
163	9.2249	11.1235	433.4013	163	9.2249	11.1235	4022.0892	163	9.2249	11.1235	465.9414	163	9.2249	11.1235	4203.2658
164	9.2509	11.0923	372.9434	164	9.2509	11.0923	3954.0654	164	9.2509	11.0923	564.433	164	9.2509	11.0923	4298.3867
165	9.2769	11.0613	405.5197	165	9.2769	11.0613	3979.0759	165	9.2769	11.0613	514.6896	165	9.2769	11.0613	4245.2726
166	9.3029	11.0304	527.0187	166	9.3029	11.0304	4093.009	166	9.3029	11.0304	549.8841	166	9.3029	11.0304	4277.0963
167	9.3289	10.9998	492.9914	167	9.3289	10.9998	4051.4159	167	9.3289	10.9998	541.462	167	9.3289	10.9998	4265.3034
168	9.3549	10.9693	403.5296	168	9.3549	10.9693	3954.3882	168	9.3549	10.9693	434.141	168	9.3549	10.9693	4154.6118
169	9.3809	10.9389	393.3349	169	9.3809	10.9389	3936.6277	169	9.3809	10.9389	479.5854	169	9.3809	10.9389	4196.6853
170	9.4069	10.9088	453.2353	170	9.4069	10.9088	3988.9622	170	9.4069	10.9088	480.6011	170	9.4069	10.9088	4194.3304
171	9.4329	10.8788	336.9405	171	9.4329	10.8788	3865.1016	171	9.4329	10.8788	558.8603	171	9.4329	10.8788	4269.2187
172	9.4589	10.8489	297.7994	172	9.4589	10.8489	3818.3946	172	9.4589	10.8489	499.8637	172	9.4589	10.8489	4206.8515
173	9.4849	10.8193	396.3048	173	9.4849	10.8193	3909.3341	173	9.4849	10.8193	494.2168	173	9.4849	10.8193	4197.8338
174	9.5109	10.7897	407.6478	174	9.5109	10.7897	3913.1113	174	9.5109	10.7897	632.7789	174	9.5109	10.7897	4333.0252
175	9.5369	10.7604	403.8987	175	9.5369	10.7604	3901.7963	175	9.5369	10.7604	567.8073	175	9.5369	10.7604	4264.6828

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
176	9.5629	10.7312	470.187	176	9.5629	10.7312	3960.5188	176	9.5629	10.7312	535.24	176	9.5629	10.7312	4228.7448
177	9.5889	10.7022	436.0612	177	9.5889	10.7022	3918.8272	177	9.5889	10.7022	539.6895	177	9.5889	10.7022	4229.8235
178	9.6149	10.6733	373.6439	178	9.6149	10.6733	3848.844	178	9.6149	10.6733	503.3366	178	9.6149	10.6733	4190.0999
179	9.6409	10.6446	431.0672	179	9.6409	10.6446	3898.7015	179	9.6409	10.6446	497.6473	179	9.6409	10.6446	4181.0398
180	9.6669	10.616	435.1099	180	9.6669	10.616	3895.1783	180	9.6669	10.616	501.1262	180	9.6669	10.616	4181.148
181	9.6929	10.5876	416.7198	181	9.6929	10.5876	3869.2223	181	9.6929	10.5876	476.3406	181	9.6929	10.5876	4152.9916
182	9.7189	10.5594	401.8389	182	9.7189	10.5594	3846.7756	182	9.7189	10.5594	506.4132	182	9.7189	10.5594	4179.6935
183	9.7449	10.5313	426.5673	183	9.7449	10.5313	3863.9381	183	9.7449	10.5313	526.5373	183	9.7449	10.5313	4196.4469
184	9.7709	10.5033	494.4302	184	9.7709	10.5033	3924.2352	184	9.7709	10.5033	528.2509	184	9.7709	10.5033	4194.7897
185	9.7969	10.4755	373.2557	185	9.7969	10.4755	3795.4948	185	9.7969	10.4755	525.2928	185	9.7969	10.4755	4188.4609
186	9.8229	10.4478	457.4207	186	9.8229	10.4478	3872.094	186	9.8229	10.4478	425.3247	186	9.8229	10.4478	4085.122
187	9.8489	10.4203	637.9049	187	9.8489	10.4203	4045.0123	187	9.8489	10.4203	535.8371	187	9.8489	10.4203	4192.2637
188	9.8749	10.393	459.2982	188	9.8749	10.393	3858.8398	188	9.8749	10.393	390.7449	188	9.8749	10.393	4043.8008
189	9.9009	10.3657	505.987	189	9.9009	10.3657	3897.9627	189	9.9009	10.3657	517.9107	189	9.9009	10.3657	4167.5958
190	9.9269	10.3386	360.0713	190	9.9269	10.3386	3744.4812	190	9.9269	10.3386	561.8153	190	9.9269	10.3386	4208.1297
191	9.9529	10.3117	424.2588	191	9.9529	10.3117	3802.3939	191	9.9529	10.3117	545.4145	191	9.9529	10.3117	4186.737
192	9.9789	10.2849	477.6963	192	9.9789	10.2849	3849.5566	192	9.9789	10.2849	468.2173	192	9.9789	10.2849	4104.5478
193	10.0049	10.2582	523.7259	193	10.0049	10.2582	3889.3115	193	10.0049	10.2582	328.001	193	10.0049	10.2582	3959.3396
194	10.0309	10.2317	454.9892	194	10.0309	10.2317	3814.3	194	10.0309	10.2317	453.7133	194	10.0309	10.2317	4080.0599
195	10.0569	10.2053	449.7207	195	10.0569	10.2053	3802.7568	195	10.0569	10.2053	493.8976	195	10.0569	10.2053	4115.2523
196	10.0829	10.1791	532.5931	196	10.0829	10.1791	3879.3544	196	10.0829	10.1791	519.9917	196	10.0829	10.1791	4136.3544
197	10.1089	10.153	440.0892	197	10.1089	10.153	3780.5757	197	10.1089	10.153	434.5447	197	10.1089	10.153	4045.9155
198	10.1349	10.127	391.2317	198	10.1349	10.127	3725.4434	198	10.1349	10.127	516.4171	198	10.1349	10.127	4122.796
199	10.1609	10.1012	468.223	199	10.1609	10.1012	3796.1599	199	10.1609	10.1012	374.5671	199	10.1609	10.1012	3975.9541
200	10.1869	10.0754	419.9326	200	10.1869	10.0754	3741.5948	200	10.1869	10.0754	512.1096	200	10.1869	10.0754	4108.5045
201	10.2129	10.0499	260.4878	201	10.2129	10.0499	3575.8752	201	10.2129	10.0499	423.664	201	10.2129	10.0499	4015.067
202	10.2389	10.0244	448.8256	202	10.2389	10.0244	3757.9382	202	10.2389	10.0244	558.6617	202	10.2389	10.0244	4145.0728
203	10.2649	9.9991	444.2095	203	10.2649	9.9991	3747.0473	203	10.2649	9.9991	400.2908	203	10.2649	9.9991	3981.71
204	10.2909	9.9739	436.6361	204	10.2909	9.9739	3733.1992	204	10.2909	9.9739	457.8046	204	10.2909	9.9739	4034.2318
205	10.3169	9.9488	496.3836	205	10.3169	9.9488	3786.6719	205	10.3169	9.9488	508.4539	205	10.3169	9.9488	4079.8892
206	10.3429	9.9239	531.0325	206	10.3429	9.9239	3815.046	206	10.3429	9.9239	464.3283	206	10.3429	9.9239	4030.7716
207	10.3689	9.8991	474.2087	207	10.3689	9.8991	3751.9475	207	10.3689	9.8991	455.1205	207	10.3689	9.8991	4016.5719
208	10.3949	9.8744	614.7184	208	10.3949	9.8744	3886.1824	208	10.3949	9.8744	674.3019	208	10.3949	9.8744	4230.7614
209	10.4209	9.8498	457.4929	209	10.4209	9.8498	3722.6821	209	10.4209	9.8498	472.4703	209	10.4209	9.8498	4023.9378
210	10.4469	9.8254	473.3891	210	10.4469	9.8254	3732.3035	210	10.4469	9.8254	489.3854	210	10.4469	9.8254	4035.861
211	10.4729	9.801	455.7034	211	10.4729	9.801	3708.3431	211	10.4729	9.801	441.5372	211	10.4729	9.801	3983.0209

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
212	10.4989	9.7768	413.4089	212	10.4989	9.7768	3659.7738	212	10.4989	9.7768	552.995	212	10.4989	9.7768	4089.4867
213	10.5249	9.7527	506.3502	213	10.5249	9.7527	3746.4403	213	10.5249	9.7527	540.8131	213	10.5249	9.7527	4072.3128
214	10.5509	9.7288	501.0209	214	10.5509	9.7288	3734.8362	214	10.5509	9.7288	446.7446	214	10.5509	9.7288	3973.2524
215	10.5769	9.7049	531.635	215	10.5769	9.7049	3759.1755	215	10.5769	9.7049	472.796	215	10.5769	9.7049	3994.3119
216	10.6029	9.6812	525.2668	216	10.6029	9.6812	3746.5326	216	10.6029	9.6812	398.4055	216	10.6029	9.6812	3914.9294
217	10.6289	9.6576	543.5743	217	10.6289	9.6576	3758.5653	217	10.6289	9.6576	422.169	217	10.6289	9.6576	3933.701
218	10.6549	9.6341	488.7691	218	10.6549	9.6341	3697.4853	218	10.6549	9.6341	427.2309	218	10.6549	9.6341	3934.7657
219	10.6809	9.6107	516.1992	219	10.6809	9.6107	3718.6407	219	10.6809	9.6107	411.2127	219	10.6809	9.6107	3914.7504
220	10.7069	9.5874	491.6175	220	10.7069	9.5874	3687.7842	220	10.7069	9.5874	425.5188	220	10.7069	9.5874	3925.0593
221	10.7329	9.5643	495.0107	221	10.7329	9.5643	3684.9026	221	10.7329	9.5643	443.896	221	10.7329	9.5643	3939.4393
222	10.7589	9.5412	441.8449	222	10.7589	9.5412	3625.462	222	10.7589	9.5412	442.3821	222	10.7589	9.5412	3933.9283
223	10.7849	9.5183	503.8157	223	10.7849	9.5183	3681.1581	223	10.7849	9.5183	410.1692	223	10.7849	9.5183	3897.7182
224	10.8109	9.4955	527.1451	224	10.8109	9.4955	3698.2127	224	10.8109	9.4955	424.344	224	10.8109	9.4955	3907.8959
225	10.8369	9.4728	476.4565	225	10.8369	9.4728	3641.2493	225	10.8369	9.4728	478.5349	225	10.8369	9.4728	3958.0896
226	10.8629	9.4502	394.3384	226	10.8629	9.4502	3552.8565	226	10.8629	9.4502	513.0946	226	10.8629	9.4502	3988.6521
227	10.8889	9.4277	472.6944	227	10.8889	9.4277	3624.9377	227	10.8889	9.4277	548.1967	227	10.8889	9.4277	4019.7571
228	10.9149	9.4053	440.2487	228	10.9149	9.4053	3586.2172	228	10.9149	9.4053	466.9818	228	10.9149	9.4053	3934.5451
229	10.9409	9.383	408.5519	229	10.9409	9.383	3548.2457	229	10.9409	9.383	505.0908	229	10.9409	9.383	3968.6568
230	10.9669	9.3608	382.6526	230	10.9669	9.3608	3516.0716	230	10.9669	9.3608	464.7462	230	10.9669	9.3608	3924.3151
231	10.9929	9.3387	447.7716	231	10.9929	9.3387	3574.9158	231	10.9929	9.3387	401.7917	231	10.9929	9.3387	3857.3634
232	11.0189	9.3168	447.8569	232	11.0189	9.3168	3568.7263	232	11.0189	9.3168	440.3979	232	11.0189	9.3168	3891.9724
233	11.0449	9.2949	452.2719	233	11.0449	9.2949	3566.8665	233	11.0449	9.2949	431.9173	233	11.0449	9.2949	3879.4946
234	11.0709	9.2731	363.2167	234	11.0709	9.2731	3471.5365	234	11.0709	9.2731	465.4585	234	11.0709	9.2731	3909.0388
235	11.0969	9.2515	424.3261	235	11.0969	9.2515	3526.3712	235	11.0969	9.2515	332.0783	235	11.0969	9.2515	3771.6614
236	11.1229	9.2299	512.9793	236	11.1229	9.2299	3608.7496	236	11.1229	9.2299	412.4411	236	11.1229	9.2299	3848.027
237	11.1489	9.2085	469.3539	237	11.1489	9.2085	3558.8494	237	11.1489	9.2085	501.9447	237	11.1489	9.2085	3933.5334
238	11.1749	9.1871	410.9521	238	11.1749	9.1871	3494.1728	238	11.1749	9.1871	387.5608	238	11.1749	9.1871	3815.1524
239	11.2009	9.1659	395.9461	239	11.2009	9.1659	3472.892	239	11.2009	9.1659	390.1705	239	11.2009	9.1659	3813.7649
240	11.2269	9.1447	380.4716	240	11.2269	9.1447	3451.1428	240	11.2269	9.1447	477.2885	240	11.2269	9.1447	3896.8858
241	11.2529	9.1236	396.6377	241	11.2529	9.1236	3461.0341	241	11.2529	9.1236	474.9928	241	11.2529	9.1236	3890.5929
242	11.2789	9.1027	403.0951	242	11.2789	9.1027	3461.2167	242	11.2789	9.1027	399.9592	242	11.2789	9.1027	3811.5622
243	11.3049	9.0818	310.7335	243	11.3049	9.0818	3362.5804	243	11.3049	9.0818	390.3464	243	11.3049	9.0818	3797.9522
244	11.3309	9.061	360.0713	244	11.3309	9.061	3405.6434	244	11.3309	9.061	422.169	244	11.3309	9.061	3825.7777
245	11.3569	9.0404	428.9626	245	11.3569	9.0404	3469.3156	245	11.3569	9.0404	449.0986	245	11.3569	9.0404	3847.8951
246	11.3829	9.0198	315.1965	246	11.3829	9.0198	3350.3304	246	11.3829	9.0198	448.0827	246	11.3829	9.0198	3842.0669
247	11.4089	8.9993	337.4034	247	11.4089	8.9993	3367.3182	247	11.4089	8.9993	465.4291	247	11.4089	8.9993	3854.6011

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
248	11.4349	8.9789	396.3937	248	11.4349	8.9789	3421.0895	248	11.4349	8.9789	470.4184	248	11.4349	8.9789	3854.7782
249	11.4609	8.9586	376.827	249	11.4609	8.9586	3396.3036	249	11.4609	8.9586	444.892	249	11.4609	8.9586	3824.4397
250	11.4869	8.9384	354.863	250	11.4869	8.9384	3369.1206	250	11.4869	8.9384	450.4983	250	11.4869	8.9384	3825.2337
251	11.5129	8.9183	347.8306	251	11.5129	8.9183	3356.8691	251	11.5129	8.9183	508.6309	251	11.5129	8.9183	3878.5541
252	11.5389	8.8982	391.2223	252	11.5389	8.8982	3395.0418	252	11.5389	8.8982	468.8397	252	11.5389	8.8982	3833.9508
253	11.5649	8.8783	448.8792	253	11.5649	8.8783	3447.4795	253	11.5649	8.8783	437.6643	253	11.5649	8.8783	3797.9632
254	11.5909	8.8585	381.6661	254	11.5909	8.8585	3375.0473	254	11.5909	8.8585	548.2105	254	11.5909	8.8585	3903.6972
255	11.6169	8.8387	367.3932	255	11.6169	8.8387	3355.5554	255	11.6169	8.8387	510.8237	255	11.6169	8.8387	3861.4982
256	11.6429	8.819	414.0754	256	11.6429	8.819	3397.0185	256	11.6429	8.819	472.0194	256	11.6429	8.819	3817.8818
257	11.6689	8.7994	394.3295	257	11.6689	8.7994	3372.0535	257	11.6689	8.7994	467.3509	257	11.6689	8.7994	3808.4011
258	11.6949	8.7799	416.7461	258	11.6949	8.7799	3389.251	258	11.6949	8.7799	421.5584	258	11.6949	8.7799	3757.7964
259	11.7209	8.7605	405.3545	259	11.7209	8.7605	3372.6403	259	11.7209	8.7605	422.4063	259	11.7209	8.7605	3753.832
260	11.7469	8.7412	421.6755	260	11.7469	8.7412	3383.7423	260	11.7469	8.7412	338.8275	260	11.7469	8.7412	3665.441
261	11.7729	8.722	395.9724	261	11.7729	8.722	3352.82	261	11.7729	8.722	355.3421	261	11.7729	8.722	3677.1435
262	11.7989	8.7028	351.7565	262	11.7989	8.7028	3303.3851	262	11.7989	8.7028	371.2417	262	11.7989	8.7028	3688.2308
263	11.8249	8.6838	358.7826	263	11.8249	8.6838	3305.1921	263	11.8249	8.6838	395.4388	263	11.8249	8.6838	3707.6158
264	11.8509	8.6648	365.2558	264	11.8509	8.6648	3306.4462	264	11.8509	8.6648	432.8822	264	11.8509	8.6648	3740.247
265	11.8769	8.6459	418.9037	265	11.8769	8.6459	3354.875	265	11.8769	8.6459	432.6073	265	11.8769	8.6459	3735.1599
266	11.9029	8.6271	438.8239	266	11.9029	8.6271	3369.5762	266	11.9029	8.6271	362.859	266	11.9029	8.6271	3660.5994
267	11.9289	8.6083	382.3187	267	11.9289	8.6083	3307.8519	267	11.9289	8.6083	287.8425	267	11.9289	8.6083	3580.7707
268	11.9549	8.5897	353.671	268	11.9549	8.5897	3273.985	268	11.9549	8.5897	344.623	268	11.9549	8.5897	3632.739
269	11.9809	8.5711	360.2197	269	11.9809	8.5711	3275.3147	269	11.9809	8.5711	433.1718	269	11.9809	8.5711	3716.4757
270	12.0069	8.5526	375.2554	270	12.0069	8.5526	3285.1312	270	12.0069	8.5526	492.5331	270	12.0069	8.5526	3771.0247
271	12.0329	8.5342	360.0713	271	12.0329	8.5342	3264.7281	271	12.0329	8.5342	504.3222	271	12.0329	8.5342	3778.0016
272	12.0589	8.5159	384.3823	272	12.0589	8.5159	3281.5139	272	12.0589	8.5159	349.1097	272	12.0589	8.5159	3617.9769
273	12.0849	8.4976	388.8198	273	12.0849	8.4976	3278.4261	273	12.0849	8.4976	349.8881	273	12.0849	8.4976	3613.9432
274	12.1109	8.4794	439.5555	274	12.1109	8.4794	3321.6367	274	12.1109	8.4794	333.7354	274	12.1109	8.4794	3592.9783
275	12.1369	8.4613	357.2556	275	12.1369	8.4613	3231.8116	275	12.1369	8.4613	375.9448	275	12.1369	8.4613	3630.3755
276	12.1629	8.4433	358.4671	276	12.1629	8.4433	3225.4979	276	12.1629	8.4433	379.3408	276	12.1629	8.4433	3628.9593
277	12.1889	8.4254	358.552	277	12.1889	8.4254	3218.0576	277	12.1889	8.4254	382.0312	277	12.1889	8.4254	3626.8375
278	12.2149	8.4075	280.5653	278	12.2149	8.4075	3132.5457	278	12.2149	8.4075	467.0669	278	12.2149	8.4075	3707.061
279	12.2409	8.3897	314.8936	279	12.2409	8.3897	3159.3488	279	12.2409	8.3897	468.9601	279	12.2409	8.3897	3704.142
280	12.2669	8.372	322.1692	280	12.2669	8.372	3159.0992	280	12.2669	8.372	396.5785	280	12.2669	8.372	3626.9482
281	12.2929	8.3544	314.6413	281	12.2929	8.3544	3144.0461	281	12.2929	8.3544	475.911	281	12.2929	8.3544	3701.4686
282	12.3189	8.3368	417.9865	282	12.3189	8.3368	3239.8662	282	12.3189	8.3368	433.8996	282	12.3189	8.3368	3654.6449
283	12.3449	8.3193	356.0504	283	12.3449	8.3193	3170.4048	283	12.3449	8.3193	416.8841	283	12.3449	8.3193	3632.8172

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
284	12.3709	8.3019	293.6902	284	12.3709	8.3019	3100.5195	284	12.3709	8.3019	407.184	284	12.3709	8.3019	3618.305
285	12.3969	8.2845	356.6146	285	12.3969	8.2845	3155.9186	285	12.3969	8.2845	337.8057	285	12.3969	8.2845	3544.1145
286	12.4229	8.2673	397.2869	286	12.4229	8.2673	3189.0658	286	12.4229	8.2673	412.6175	286	12.4229	8.2673	3614.1141
287	12.4489	8.2501	411.0152	287	12.4489	8.2501	3195.2688	287	12.4489	8.2501	375.3933	287	12.4489	8.2501	3572.0777
288	12.4749	8.2329	402.013	288	12.4749	8.2329	3178.7414	288	12.4749	8.2329	341.286	288	12.4749	8.2329	3533.1582
289	12.5009	8.2159	422.3763	289	12.5009	8.2159	3191.5795	289	12.5009	8.2159	370.1358	289	12.5009	8.2159	3557.1958
290	12.5269	8.1989	400.0893	290	12.5269	8.1989	3161.7674	290	12.5269	8.1989	315.5157	290	12.5269	8.1989	3497.7635
291	12.5529	8.182	332.3542	291	12.5529	8.182	3086.507	291	12.5529	8.182	544.5165	291	12.5529	8.182	3721.9521
292	12.5789	8.1652	502.8723	292	12.5789	8.1652	3249.5	292	12.5789	8.1652	468.818	292	12.5789	8.1652	3641.4414
293	12.6049	8.1484	399.472	293	12.6049	8.1484	3138.5744	293	12.6049	8.1484	397.9735	293	12.6049	8.1484	3565.7848
294	12.6309	8.1317	312.1524	294	12.6309	8.1317	3043.7297	294	12.6309	8.1317	336.0104	294	12.6309	8.1317	3499.0095
295	12.6569	8.115	450.8826	295	12.6569	8.115	3174.9347	295	12.6569	8.115	391.3043	295	12.6569	8.115	3549.4912
296	12.6829	8.0985	421.7749	296	12.6829	8.0985	3138.3018	296	12.6829	8.0985	407.4477	296	12.6829	8.0985	3560.8224
297	12.7089	8.082	392.1632	297	12.7089	8.082	3101.1649	297	12.7089	8.082	350.7216	297	12.7089	8.082	3499.2841
298	12.7349	8.0655	360.0713	298	12.7349	8.0655	3061.5478	298	12.7349	8.0655	422.169	298	12.7349	8.0655	3565.9194
299	12.7609	8.0492	409.2983	299	12.7609	8.0492	3106.3526	299	12.7609	8.0492	481.1177	299	12.7609	8.0492	3618
300	12.7869	8.0329	399.3345	300	12.7869	8.0329	3091.9668	300	12.7869	8.0329	483.6653	300	12.7869	8.0329	3613.6795
301	12.8129	8.0166	401.0414	301	12.8129	8.0166	3089.2516	301	12.8129	8.0166	364.5974	301	12.8129	8.0166	3487.7436
302	12.8389	8.0005	332.2388	302	12.8389	8.0005	3016.0268	302	12.8389	8.0005	361.1905	302	12.8389	8.0005	3477.4686
303	12.8649	7.9844	339.0051	303	12.8649	7.9844	3018.371	303	12.8649	7.9844	402.4755	303	12.8649	7.9844	3511.8856
304	12.8909	7.9683	449.3656	304	12.8909	7.9683	3124.3094	304	12.8909	7.9683	376.6709	304	12.8909	7.9683	3479.213
305	12.9169	7.9524	408.2481	305	12.9169	7.9524	3078.7697	305	12.9169	7.9524	499.3935	305	12.9169	7.9524	3595.0675
306	12.9429	7.9365	413.8479	306	12.9429	7.9365	3079.9474	306	12.9429	7.9365	348.5071	306	12.9429	7.9365	3437.3131
307	12.9689	7.9206	354.7132	307	12.9689	7.9206	3016.3906	307	12.9689	7.9206	394.4321	307	12.9689	7.9206	3476.37
308	12.9949	7.9048	314.775	308	12.9949	7.9048	2972.0303	308	12.9949	7.9048	481.1463	308	12.9949	7.9048	3556.2162
309	13.0209	7.8891	403.0648	309	13.0209	7.8891	3055.898	309	13.0209	7.8891	403.0683	309	13.0209	7.8891	3471.2702
310	13.0469	7.8735	408.8529	310	13.0469	7.8735	3057.264	310	13.0469	7.8735	473.783	310	13.0469	7.8735	3535.1169
311	13.0729	7.8579	376.9716	311	13.0729	7.8579	3020.9605	311	13.0729	7.8579	407.9107	311	13.0729	7.8579	3462.3765
312	13.0989	7.8423	352.8365	312	13.0989	7.8423	2992.4033	312	13.0989	7.8423	511.7031	312	13.0989	7.8423	3559.3009
313	13.1249	7.8269	420.8652	313	13.1249	7.8269	3056.0099	313	13.1249	7.8269	379.0699	313	13.1249	7.8269	3419.7996
314	13.1509	7.8115	427.8058	314	13.1509	7.8115	3058.5284	314	13.1509	7.8115	497.1321	314	13.1509	7.8115	3530.9938
315	13.1769	7.7961	421.0868	315	13.1769	7.7961	3047.3872	315	13.1769	7.7961	509.278	315	13.1769	7.7961	3536.2716
316	13.2029	7.7808	365.5317	316	13.2029	7.7808	2987.41	316	13.2029	7.7808	520.1213	316	13.2029	7.7808	3540.2469
317	13.2289	7.7656	375.3767	317	13.2289	7.7656	2992.8329	317	13.2289	7.7656	442.1514	317	13.2289	7.7656	3455.409
318	13.2549	7.7504	359.7455	318	13.2549	7.7504	2972.7795	318	13.2549	7.7504	450.1393	318	13.2549	7.7504	3456.5288
319	13.2809	7.7353	359.5433	319	13.2809	7.7353	2968.1553	319	13.2809	7.7353	487.354	319	13.2809	7.7353	3486.8755

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
320	13.3069	7.7203	376.332	320	13.3069	7.7203	2980.5218	320	13.3069	7.7203	425.0504	320	13.3069	7.7203	3417.7038
321	13.3329	7.7053	415.4021	321	13.3329	7.7053	3015.1698	321	13.3329	7.7053	493.9272	321	13.3329	7.7053	3479.7126
322	13.3589	7.6904	380.2026	322	13.3589	7.6904	2975.5482	322	13.3589	7.6904	495.8941	322	13.3589	7.6904	3474.8115
323	13.3849	7.6755	372.4665	323	13.3849	7.6755	2963.39	323	13.3849	7.6755	322.4559	323	13.3849	7.6755	3294.5052
324	13.4109	7.6607	436.9262	324	13.4109	7.6607	3023.4276	324	13.4109	7.6607	451.4043	324	13.4109	7.6607	3416.5856
325	13.4369	7.6459	401.9584	325	13.4369	7.6459	2984.0376	325	13.4369	7.6459	422.169	325	13.4369	7.6459	3380.4823
326	13.4629	7.6312	436.2679	326	13.4629	7.6312	3012.4143	326	13.4629	7.6312	464.2843	326	13.4629	7.6312	3414.8184
327	13.4889	7.6166	414.9892	327	13.4889	7.6166	2985.2027	327	13.4889	7.6166	428.5491	327	13.4889	7.6166	3371.3041
328	13.5149	7.602	441.9574	328	13.5149	7.602	3006.2381	328	13.5149	7.602	452.7731	328	13.5149	7.602	3387.7489
329	13.5409	7.5875	371.4301	329	13.5409	7.5875	2929.7779	329	13.5409	7.5875	450.1842	329	13.5409	7.5875	3377.3808
330	13.5669	7.573	415.2572	330	13.5669	7.573	2967.672	330	13.5669	7.573	480.7407	330	13.5669	7.573	3400.1582
331	13.5929	7.5586	422.2974	331	13.5929	7.5586	2968.7794	331	13.5929	7.5586	534.1925	331	13.5929	7.5586	3445.8309
332	13.6189	7.5442	386.5277	332	13.6189	7.5442	2927.0768	332	13.6189	7.5442	552.9936	332	13.6189	7.5442	3456.8528
333	13.6449	7.5299	370.2083	333	13.6449	7.5299	2904.8246	333	13.6449	7.5299	481.5762	333	13.6449	7.5299	3377.6563
334	13.6709	7.5157	379.9712	334	13.6709	7.5157	2908.6546	334	13.6709	7.5157	414.9465	334	13.6709	7.5157	3303.2474
335	13.6969	7.5015	313.7945	335	13.6969	7.5015	2836.545	335	13.6969	7.5015	429.8585	335	13.6969	7.5015	3310.3803
336	13.7229	7.4873	356.1657	336	13.7229	7.4873	2872.9834	336	13.7229	7.4873	411.3996	336	13.7229	7.4873	3284.1422
337	13.7489	7.4732	408.1052	337	13.7489	7.4732	2918.99	337	13.7489	7.4732	446.9981	337	13.7489	7.4732	3311.9616
338	13.7749	7.4592	406.2681	338	13.7749	7.4592	2911.2201	338	13.7749	7.4592	482.4089	338	13.7749	7.4592	3339.5933
339	13.8009	7.4452	348.1096	339	13.8009	7.4452	2847.1287	339	13.8009	7.4452	461.5741	339	13.8009	7.4452	3310.9793
340	13.8269	7.4313	372.5485	340	13.8269	7.4313	2865.6347	340	13.8269	7.4313	481.6457	340	13.8269	7.4313	3323.2718
341	13.8529	7.4174	381.1634	341	13.8529	7.4174	2868.3168	341	13.8529	7.4174	454.7866	341	13.8529	7.4174	3288.6335
342	13.8789	7.4036	377.9445	342	13.8789	7.4036	2859.165	342	13.8789	7.4036	479.4026	342	13.8789	7.4036	3305.4704
343	13.9049	7.3898	364.0559	343	13.9049	7.3898	2839.3435	343	13.9049	7.3898	502.7601	343	13.9049	7.3898	3321.0488
344	13.9309	7.3761	397.0077	344	13.9309	7.3761	2866.3624	344	13.9309	7.3761	509.247	344	13.9309	7.3761	3319.7565
345	13.9569	7.3624	428.6445	345	13.9569	7.3624	2892.0663	345	13.9569	7.3624	572.7285	345	13.9569	7.3624	3375.4589
346	13.9829	7.3488	390.9807	346	13.9829	7.3488	2848.4697	346	13.9829	7.3488	550.8694	346	13.9829	7.3488	3345.8206
347	14.0089	7.3352	401.0239	347	14.0089	7.3352	2852.5801	347	14.0089	7.3352	484.1843	347	14.0089	7.3352	3271.3563
348	14.0349	7.3217	415.5539	348	14.0349	7.3217	2861.1771	348	14.0349	7.3217	561.2784	348	14.0349	7.3217	3340.6713
349	14.0609	7.3082	339.4764	349	14.0609	7.3082	2779.1668	349	14.0609	7.3082	527.6955	349	14.0609	7.3082	3299.3093
350	14.0869	7.2948	332.7492	350	14.0869	7.2948	2766.5067	350	14.0869	7.2948	495.8773	350	14.0869	7.2948	3259.712
351	14.1129	7.2814	429.4223	351	14.1129	7.2814	2857.247	351	14.1129	7.2814	505.1327	351	14.1129	7.2814	3261.1882
352	14.1389	7.2681	400.8614	352	14.1389	7.2681	2822.7532	352	14.1389	7.2681	468.0682	352	14.1389	7.2681	3216.3445
353	14.1649	7.2548	385.8499	353	14.1649	7.2548	2801.8088	353	14.1649	7.2548	508.5396	353	14.1649	7.2548	3249.0368
354	14.1909	7.2416	404.1897	354	14.1909	7.2416	2814.2158	354	14.1909	7.2416	534.3744	354	14.1909	7.2416	3267.0925
355	14.2169	7.2284	359.1316	355	14.2169	7.2284	2763.2248	355	14.2169	7.2284	568.4243	355	14.2169	7.2284	3293.3633

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
356	14.2429	7.2153	400.7328	356	14.2429	7.2153	2798.8931	356	14.2429	7.2153	615.1988	356	14.2429	7.2153	3332.3586
357	14.2689	7.2022	425.842	357	14.2689	7.2022	2818.0695	357	14.2689	7.2022	544.4698	357	14.2689	7.2022	3253.8504
358	14.2949	7.1892	409.1489	358	14.2949	7.1892	2795.4435	358	14.2949	7.1892	513.1375	358	14.2949	7.1892	3214.739
359	14.3209	7.1762	387.4389	359	14.3209	7.1762	2767.8006	359	14.3209	7.1762	518.1263	359	14.3209	7.1762	3211.9486
360	14.3469	7.1633	383.2955	360	14.3469	7.1633	2757.7244	360	14.3469	7.1633	477.8453	360	14.3469	7.1633	3163.8885
361	14.3729	7.1504	419.6773	361	14.3729	7.1504	2788.1733	361	14.3729	7.1504	513.7234	361	14.3729	7.1504	3191.9875
362	14.3989	7.1375	369.2635	362	14.3989	7.1375	2731.8266	362	14.3989	7.1375	495.4723	362	14.3989	7.1375	3165.9572
363	14.4249	7.1247	394.5079	363	14.4249	7.1247	2751.1382	363	14.4249	7.1247	510.6975	363	14.4249	7.1247	3173.4033
364	14.4509	7.112	458.2155	364	14.4509	7.112	2808.9129	364	14.4509	7.112	591.7379	364	14.4509	7.112	3246.6645
365	14.4769	7.0993	429.3417	365	14.4769	7.0993	2774.1063	365	14.4769	7.0993	578.6291	365	14.4769	7.0993	3225.7766
366	14.5029	7.0866	417.8449	366	14.5029	7.0866	2756.6766	366	14.5029	7.0866	581.5778	366	14.5029	7.0866	3220.9462
367	14.5289	7.074	356.1522	367	14.5289	7.074	2689.051	367	14.5289	7.074	539.6192	367	14.5289	7.074	3171.2084
368	14.5549	7.0614	322.6578	368	14.5549	7.0614	2649.6237	368	14.5549	7.0614	480.2655	368	14.5549	7.0614	3104.0756
369	14.5809	7.0489	354.0127	369	14.5809	7.0489	2675.0458	369	14.5809	7.0489	492.0607	369	14.5809	7.0489	3108.0916
370	14.6069	7.0364	366.3026	370	14.6069	7.0364	2681.4028	370	14.6069	7.0364	533.2129	370	14.6069	7.0364	3141.4646
371	14.6329	7.024	369.6551	371	14.6329	7.024	2678.8224	371	14.6329	7.024	573.871	371	14.6329	7.024	3174.3436
372	14.6589	7.0116	386.8803	372	14.6589	7.0116	2690.1148	372	14.6589	7.0116	525.5676	372	14.6589	7.0116	3118.2611
373	14.6849	6.9993	439.4413	373	14.6849	6.9993	2736.7429	373	14.6849	6.9993	505.9492	373	14.6849	6.9993	3090.8635
374	14.7109	6.987	383.9404	374	14.7109	6.987	2675.3091	374	14.7109	6.987	492.1232	374	14.7109	6.987	3069.2584
375	14.7369	6.9747	372.8688	375	14.7369	6.9747	2658.3047	375	14.7369	6.9747	527.1986	375	14.7369	6.9747	3096.5547
376	14.7629	6.9625	378.1779	376	14.7629	6.9625	2657.6809	376	14.7629	6.9625	527.5151	376	14.7629	6.9625	3089.092
377	14.7889	6.9503	455.545	377	14.7889	6.9503	2729.1151	377	14.7889	6.9503	534.6249	377	14.7889	6.9503	3088.4226
378	14.8149	6.9382	446.5809	378	14.8149	6.9382	2714.2182	378	14.8149	6.9382	518.7152	378	14.8149	6.9382	3064.7338
379	14.8409	6.9261	360.0713	379	14.8409	6.9261	2621.7757	379	14.8409	6.9261	422.169	379	14.8409	6.9261	2960.4085
380	14.8669	6.9141	351.4014	380	14.8669	6.9141	2610.3955	380	14.8669	6.9141	552.5134	380	14.8669	6.9141	3087.4799
381	14.8929	6.9021	401.0263	381	14.8929	6.9021	2657.3102	381	14.8929	6.9021	575.0409	381	14.8929	6.9021	3106.7344
382	14.9189	6.8901	398.1281	382	14.9189	6.8901	2651.7017	382	14.9189	6.8901	458.3363	382	14.9189	6.8901	2986.7569
383	14.9449	6.8782	507.6995	383	14.9449	6.8782	2758.5629	383	14.9449	6.8782	470.9976	383	14.9449	6.8782	2996.1453
384	14.9709	6.8663	332.0419	384	14.9709	6.8663	2580.195	384	14.9709	6.8663	489.9208	384	14.9709	6.8663	3011.7955
385	14.9969	6.8545	346.4314	385	14.9969	6.8545	2591.8743	385	14.9969	6.8545	498.5267	385	14.9969	6.8545	3017.1283
386	15.0229	6.8427	311.9744	386	15.0229	6.8427	2554.707	386	15.0229	6.8427	474.7843	386	15.0229	6.8427	2990.1131
387	15.0489	6.8309	267.9269	387	15.0489	6.8309	2507.9493	387	15.0489	6.8309	551.3641	387	15.0489	6.8309	3063.4199
388	15.0749	6.8192	383.008	388	15.0749	6.8192	2620.3201	388	15.0749	6.8192	573.9762	388	15.0749	6.8192	3082.759
389	15.1009	6.8075	386.6474	389	15.1009	6.8075	2621.2492	389	15.1009	6.8075	545.2199	389	15.1009	6.8075	3050.7297
390	15.1269	6.7959	386.09	390	15.1269	6.7959	2617.9816	390	15.1269	6.7959	439.0918	390	15.1269	6.7959	2941.3287
391	15.1529	6.7843	389.6064	391	15.1529	6.7843	2618.7878	391	15.1529	6.7843	478.2937	391	15.1529	6.7843	2977.2576

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
392	15.1789	6.7727	353.0747	392	15.1789	6.7727	2579.5458	392	15.1789	6.7727	515.4678	392	15.1789	6.7727	3011.1587
393	15.2049	6.7612	328.7622	393	15.2049	6.7612	2552.5231	393	15.2049	6.7612	595.2104	393	15.2049	6.7612	3087.6283
394	15.2309	6.7498	376.3515	394	15.2309	6.7498	2597.4022	394	15.2309	6.7498	500.4636	394	15.2309	6.7498	2989.6086
395	15.2569	6.7383	380.7567	395	15.2569	6.7383	2599.097	395	15.2569	6.7383	523.6556	395	15.2569	6.7383	3009.5276
396	15.2829	6.7269	368.8888	396	15.2829	6.7269	2584.5189	396	15.2829	6.7269	569.4091	396	15.2829	6.7269	3052.0082
397	15.3089	6.7156	420.3908	397	15.3089	6.7156	2633.3107	397	15.3089	6.7156	436.9175	397	15.3089	6.7156	2916.2436
398	15.3349	6.7043	389.4333	398	15.3349	6.7043	2599.6429	398	15.3349	6.7043	594.0708	398	15.3349	6.7043	3070.124
399	15.3609	6.693	415.4126	399	15.3609	6.693	2622.912	399	15.3609	6.693	488.9281	399	15.3609	6.693	2961.7083
400	15.3869	6.6817	381.9172	400	15.3869	6.6817	2586.7063	400	15.3869	6.6817	452.4452	400	15.3869	6.6817	2921.9524
401	15.4129	6.6705	446.8643	401	15.4129	6.6705	2648.9432	401	15.4129	6.6705	523.7711	401	15.4129	6.6705	2990.0053
402	15.4389	6.6594	415.9119	402	15.4389	6.6594	2615.2805	402	15.4389	6.6594	495.9329	402	15.4389	6.6594	2958.8942
403	15.4649	6.6482	385.2405	403	15.4649	6.6482	2581.8989	403	15.4649	6.6482	494.1543	403	15.4649	6.6482	2953.8427
404	15.4909	6.6371	378.9795	404	15.4909	6.6371	2572.9276	404	15.4909	6.6371	483.5359	404	15.4909	6.6371	2939.9513
405	15.5169	6.6261	327.2355	405	15.5169	6.6261	2518.4733	405	15.5169	6.6261	450.176	405	15.5169	6.6261	2903.3184
406	15.5429	6.6151	402.1013	406	15.5429	6.6151	2590.6289	406	15.5429	6.6151	530.6668	406	15.5429	6.6151	2980.5362
407	15.5689	6.6041	404.2395	407	15.5689	6.6041	2590.0569	407	15.5689	6.6041	545.119	407	15.5689	6.6041	2991.7155
408	15.5949	6.5932	417.4708	408	15.5949	6.5932	2600.5779	408	15.5949	6.5932	527.5207	408	15.5949	6.5932	2970.8442
409	15.6209	6.5823	353.9838	409	15.6209	6.5823	2534.3807	409	15.6209	6.5823	471.8955	409	15.6209	6.5823	2911.946
410	15.6469	6.5714	351.4298	410	15.6469	6.5714	2529.1164	410	15.6469	6.5714	460.921	410	15.6469	6.5714	2897.6986
411	15.6729	6.5605	260.8376	411	15.6729	6.5605	2435.814	411	15.6729	6.5605	403.8563	411	15.6729	6.5605	2837.361
412	15.6989	6.5497	422.6827	412	15.6989	6.5497	2594.9488	412	15.6989	6.5497	371.4225	412	15.6989	6.5497	2801.6541
413	15.7249	6.539	327.2662	413	15.7249	6.539	2496.8221	413	15.7249	6.539	541.6762	413	15.7249	6.539	2968.6349
414	15.7509	6.5283	303.8188	414	15.7509	6.5283	2470.6644	414	15.7509	6.5283	498.1677	414	15.7509	6.5283	2921.8535
415	15.7769	6.5176	392.2974	415	15.7769	6.5176	2556.4327	415	15.7769	6.5176	550.794	415	15.7769	6.5176	2971.2068
416	15.8029	6.5069	408.2216	416	15.8029	6.5069	2569.6467	416	15.8029	6.5069	436.4631	416	15.8029	6.5069	2853.6029
417	15.8289	6.4963	367.6688	417	15.8289	6.4963	2526.3837	417	15.8289	6.4963	532.174	417	15.8289	6.4963	2946.0408
418	15.8549	6.4857	283.7918	418	15.8549	6.4857	2439.7964	418	15.8549	6.4857	448.7801	418	15.8549	6.4857	2859.3739
419	15.8809	6.4752	348.724	419	15.8809	6.4752	2502.0184	419	15.8809	6.4752	419.4819	419	15.8809	6.4752	2826.8028
420	15.9069	6.4646	285.2153	420	15.9069	6.4646	2435.7994	420	15.9069	6.4646	613.7407	420	15.9069	6.4646	3017.7887
421	15.9329	6.4542	313.0927	421	15.9329	6.4542	2460.9666	421	15.9329	6.4542	566.6308	421	15.9329	6.4542	2967.4057
422	15.9589	6.4437	322.191	422	15.9589	6.4437	2467.3546	422	15.9589	6.4437	473.5174	422	15.9589	6.4437	2871.0194
423	15.9849	6.4333	293.6605	423	15.9849	6.4333	2436.1139	423	15.9849	6.4333	474.4012	423	15.9849	6.4333	2868.6303
424	16.0109	6.4229	331.809	424	16.0109	6.4229	2471.5521	424	16.0109	6.4229	541.2592	424	16.0109	6.4229	2932.2153
425	16.0369	6.4126	302.9409	425	16.0369	6.4126	2439.9738	425	16.0369	6.4126	390.419	425	16.0369	6.4126	2778.1021
426	16.0629	6.4023	444.2353	426	16.0629	6.4023	2578.5579	426	16.0629	6.4023	358.2031	426	16.0629	6.4023	2742.6133
427	16.0889	6.392	319.078	427	16.0889	6.392	2450.6904	427	16.0889	6.392	472.8704	427	16.0889	6.392	2854.0076

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
428	16.1149	6.3817	378.9433	428	16.1149	6.3817	2507.8454	428	16.1149	6.3817	427.2386	428	16.1149	6.3817	2805.1028
429	16.1409	6.3715	327.4301	429	16.1409	6.3715	2453.622	429	16.1409	6.3715	485.2542	429	16.1409	6.3715	2859.8454
430	16.1669	6.3614	375.8521	430	16.1669	6.3614	2499.3336	430	16.1669	6.3614	463.3915	430	16.1669	6.3614	2834.7098
431	16.1929	6.3512	377.8257	431	16.1929	6.3512	2498.5971	431	16.1929	6.3512	438.6869	431	16.1929	6.3512	2806.7322
432	16.2189	6.3411	356.4691	432	16.2189	6.3411	2474.5302	432	16.2189	6.3411	391.2007	432	16.2189	6.3411	2755.973
433	16.2449	6.331	360.0713	433	16.2449	6.331	2475.4221	433	16.2449	6.331	422.169	433	16.2449	6.331	2783.6685
434	16.2709	6.321	291.259	434	16.2709	6.321	2401.3024	434	16.2709	6.321	448.8127	434	16.2709	6.321	2804.8146
435	16.2969	6.3109	229.5778	435	16.2969	6.3109	2334.3137	435	16.2969	6.3109	465.9016	435	16.2969	6.3109	2816.4059
436	16.3229	6.301	257.1806	436	16.3229	6.301	2356.6092	436	16.3229	6.301	510.1834	436	16.3229	6.301	2855.1901
437	16.3489	6.291	320.9856	437	16.3489	6.291	2415.1067	437	16.3489	6.291	482.9715	437	16.3489	6.291	2822.4806
438	16.3749	6.2811	326.2675	438	16.3749	6.2811	2415.0813	438	16.3749	6.2811	434.4464	438	16.3749	6.2811	2768.4579
439	16.4009	6.2712	333.9204	439	16.4009	6.2712	2417.4267	439	16.4009	6.2712	459.8039	439	16.4009	6.2712	2788.3179
440	16.4269	6.2613	302.6455	440	16.4269	6.2613	2380.8444	440	16.4269	6.2613	445.9809	440	16.4269	6.2613	2768.9973
441	16.4529	6.2515	357.0406	441	16.4529	6.2515	2429.932	441	16.4529	6.2515	446.9701	441	16.4529	6.2515	2764.489
442	16.4789	6.2417	385.0636	442	16.4789	6.2417	2452.6477	442	16.4789	6.2417	432.0138	442	16.4789	6.2417	2744.0351
443	16.5049	6.232	367.0508	443	16.5049	6.232	2429.3274	443	16.5049	6.232	452.0367	443	16.5049	6.232	2758.5604
444	16.5309	6.2222	337.8317	444	16.5309	6.2222	2394.8009	444	16.5309	6.2222	502.1508	444	16.5309	6.2222	2803.177
445	16.5569	6.2125	327.7163	445	16.5569	6.2125	2379.378	445	16.5569	6.2125	476.5058	445	16.5569	6.2125	2772.0343
446	16.5829	6.2028	367.3822	446	16.5829	6.2028	2413.7365	446	16.5829	6.2028	472.7676	446	16.5829	6.2028	2762.7986
447	16.6089	6.1932	297.6867	447	16.6089	6.1932	2338.7336	447	16.6089	6.1932	469.7563	447	16.6089	6.1932	2754.2897
448	16.6349	6.1836	282.2162	448	16.6349	6.1836	2317.9556	448	16.6349	6.1836	483.5067	448	16.6349	6.1836	2762.5426
449	16.6609	6.174	298.1629	449	16.6609	6.174	2328.5949	449	16.6609	6.174	407.9309	449	16.6609	6.174	2681.4692
450	16.6869	6.1645	386.674	450	16.6869	6.1645	2411.7986	450	16.6869	6.1645	395.7115	450	16.6869	6.1645	2663.7522
451	16.7129	6.1549	406.8222	451	16.7129	6.1549	2426.6394	451	16.7129	6.1549	472.1108	451	16.7129	6.1549	2734.654
452	16.7389	6.1454	320.1878	452	16.7389	6.1454	2334.6976	452	16.7389	6.1454	436.2494	452	16.7389	6.1454	2693.295
453	16.7649	6.136	332.2202	453	16.7649	6.136	2341.4225	453	16.7649	6.136	417.7535	453	16.7649	6.136	2669.3016
454	16.7909	6.1265	311.0277	454	16.7909	6.1265	2314.9226	454	16.7909	6.1265	427.2259	454	16.7909	6.1265	2673.2763
455	16.8169	6.1171	321.3413	455	16.8169	6.1171	2319.9288	455	16.8169	6.1171	423.3338	455	16.8169	6.1171	2663.8867
456	16.8429	6.1078	370.7325	456	16.8429	6.1078	2364.0125	456	16.8429	6.1078	495.3047	456	16.8429	6.1078	2730.36
457	16.8689	6.0984	353.7485	457	16.8689	6.0984	2341.7211	457	16.8689	6.0984	473.3395	457	16.8689	6.0984	2702.8972
458	16.8949	6.0891	352.4727	458	16.8949	6.0891	2335.138	458	16.8949	6.0891	446.3875	458	16.8949	6.0891	2670.4476
459	16.9209	6.0798	402.1124	459	16.9209	6.0798	2379.4702	459	16.9209	6.0798	490.5461	459	16.9209	6.0798	2709.1087
460	16.9469	6.0706	471.863	460	16.9469	6.0706	2443.9134	460	16.9469	6.0706	476.653	460	16.9469	6.0706	2689.718
461	16.9729	6.0613	407.6442	461	16.9729	6.0613	2374.3871	461	16.9729	6.0613	470.5729	461	16.9729	6.0613	2678.1404
462	16.9989	6.0521	316.6551	462	16.9989	6.0521	2278.0906	462	16.9989	6.0521	417.7296	462	16.9989	6.0521	2619.7995
463	17.0249	6.0429	333.7037	463	17.0249	6.0429	2289.8318	463	17.0249	6.0429	395.862	463	17.0249	6.0429	2592.4343

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
464	17.0509	6.0338	353.1707	464	17.0509	6.0338	2303.9913	464	17.0509	6.0338	455.3177	464	17.0509	6.0338	2646.3924
465	17.0769	6.0247	364.813	465	17.0769	6.0247	2310.3262	465	17.0769	6.0247	491.6972	465	17.0769	6.0247	2677.2744
466	17.1029	6.0156	358.903	466	17.1029	6.0156	2299.1088	466	17.1029	6.0156	414.3855	466	17.1029	6.0156	2594.4651
467	17.1289	6.0065	364.6866	467	17.1289	6.0065	2299.585	467	17.1289	6.0065	476.8717	467	17.1289	6.0065	2651.4538
468	17.1549	5.9975	362.9618	468	17.1549	5.9975	2292.5527	468	17.1549	5.9975	492.1472	468	17.1549	5.9975	2661.2317
469	17.1809	5.9885	370.3344	469	17.1809	5.9885	2294.618	469	17.1809	5.9885	443.344	469	17.1809	5.9885	2606.9309
470	17.2069	5.9795	358.8499	470	17.2069	5.9795	2277.826	470	17.2069	5.9795	504.0741	470	17.2069	5.9795	2662.1634
471	17.2329	5.9706	407.687	471	17.2329	5.9706	2321.3557	471	17.2329	5.9706	567.2664	471	17.2329	5.9706	2719.8581
472	17.2589	5.9616	420.9048	472	17.2589	5.9616	2329.266	472	17.2589	5.9616	506.5658	472	17.2589	5.9616	2653.66
473	17.2849	5.9527	441.1798	473	17.2849	5.9527	2344.2336	473	17.2849	5.9527	548.0523	473	17.2849	5.9527	2689.6489
474	17.3109	5.9439	414.5592	474	17.3109	5.9439	2312.3056	474	17.3109	5.9439	511.9752	474	17.3109	5.9439	2648.0742
475	17.3369	5.935	319.4344	475	17.3369	5.935	2211.8733	475	17.3369	5.935	560.3695	475	17.3369	5.935	2690.971
476	17.3629	5.9262	372.0915	476	17.3629	5.9262	2259.223	476	17.3629	5.9262	509.8207	476	17.3629	5.9262	2634.9246
477	17.3889	5.9174	409.6645	477	17.3889	5.9174	2291.4886	477	17.3889	5.9174	482.0272	477	17.3889	5.9174	2601.6335
478	17.4149	5.9086	379.5576	478	17.4149	5.9086	2256.0743	478	17.4149	5.9086	511.4816	478	17.4149	5.9086	2625.5904
479	17.4409	5.8999	414.7337	479	17.4409	5.8999	2285.9429	479	17.4409	5.8999	473.4172	479	17.4409	5.8999	2582.0284
480	17.4669	5.8912	457.9398	480	17.4669	5.8912	2323.8417	480	17.4669	5.8912	428.1141	480	17.4669	5.8912	2531.2277
481	17.4929	5.8825	441.4905	481	17.4929	5.8825	2302.0849	481	17.4929	5.8825	509.7569	481	17.4929	5.8825	2607.373
482	17.5189	5.8738	443.7525	482	17.5189	5.8738	2299.0395	482	17.5189	5.8738	527.8838	482	17.5189	5.8738	2620.0023
483	17.5449	5.8652	404.1506	483	17.5449	5.8652	2254.1302	483	17.5449	5.8652	548.2045	483	17.5449	5.8652	2634.8255
484	17.5709	5.8566	437.8728	484	17.5709	5.8566	2282.545	484	17.5709	5.8566	532.387	484	17.5709	5.8566	2613.5104
485	17.5969	5.848	549.2097	485	17.5969	5.848	2388.5744	485	17.5969	5.848	491.3145	485	17.5969	5.848	2566.9403
486	17.6229	5.8394	466.4757	486	17.6229	5.8394	2300.533	486	17.6229	5.8394	497.1645	486	17.6229	5.8394	2567.2927
487	17.6489	5.8309	360.0713	487	17.6489	5.8309	2188.8212	487	17.6489	5.8309	422.169	487	17.6489	5.8309	2486.7997
488	17.6749	5.8224	435.0103	488	17.6749	5.8224	2261.1608	488	17.6749	5.8224	450.5638	488	17.6749	5.8224	2512.8604
489	17.7009	5.8139	436.7652	489	17.7009	5.8139	2260.3163	489	17.7009	5.8139	476.933	489	17.7009	5.8139	2536.8956
490	17.7269	5.8054	438.2524	490	17.7269	5.8054	2259.2041	490	17.7269	5.8054	517.0634	490	17.7269	5.8054	2574.6919
491	17.7529	5.797	334.8568	491	17.7529	5.797	2153.2092	491	17.7529	5.797	572.3456	491	17.7529	5.797	2627.64
492	17.7789	5.7886	356.245	492	17.7789	5.7886	2171.998	492	17.7789	5.7886	483.6299	492	17.7789	5.7886	2536.5903
493	17.8049	5.7802	395.6839	493	17.8049	5.7802	2208.8376	493	17.8049	5.7802	475.4277	493	17.8049	5.7802	2526.0541
494	17.8309	5.7719	420.2039	494	17.8309	5.7719	2230.7582	494	17.8309	5.7719	466.9168	494	17.8309	5.7719	2515.2092
495	17.8569	5.7635	438.1951	495	17.8569	5.7635	2246.15	495	17.8569	5.7635	435.2868	495	17.8569	5.7635	2481.2452
496	17.8829	5.7552	505.6245	496	17.8829	5.7552	2310.98	496	17.8829	5.7552	410.0756	496	17.8829	5.7552	2453.6999
497	17.9089	5.7469	317.1135	497	17.9089	5.7469	2119.8697	497	17.9089	5.7469	386.8247	497	17.9089	5.7469	2428.115
498	17.9349	5.7387	378.3529	498	17.9349	5.7387	2178.5097	498	17.9349	5.7387	369.5141	498	17.9349	5.7387	2408.4703
499	17.9609	5.7304	401.2665	499	17.9609	5.7304	2198.8239	499	17.9609	5.7304	400.7407	499	17.9609	5.7304	2437.3628

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
500	17.9869	5.7222	401.3346	500	17.9869	5.7222	2196.2927	500	17.9869	5.7222	335.5405	500	17.9869	5.7222	2369.8286
501	18.0129	5.714	407.6209	501	18.0129	5.714	2199.9796	501	18.0129	5.714	468.9867	501	18.0129	5.714	2500.9408
502	18.0389	5.7058	362.4974	502	18.0389	5.7058	2152.2567	502	18.0389	5.7058	420.2932	502	18.0389	5.7058	2449.9132
503	18.0649	5.6977	440.8591	503	18.0649	5.6977	2228.019	503	18.0649	5.6977	420.0752	503	18.0649	5.6977	2447.3612
504	18.0909	5.6896	444.0033	504	18.0909	5.6896	2228.5638	504	18.0909	5.6896	440.8572	504	18.0909	5.6896	2465.8092
505	18.1169	5.6815	399.0789	505	18.1169	5.6815	2181.0401	505	18.1169	5.6815	422.3996	505	18.1169	5.6815	2445.0175
506	18.1429	5.6734	388.778	506	18.1429	5.6734	2168.1399	506	18.1429	5.6734	437.5763	506	18.1429	5.6734	2457.8601
507	18.1689	5.6654	460.7693	507	18.1689	5.6654	2237.5317	507	18.1689	5.6654	416.5465	507	18.1689	5.6654	2434.4963
508	18.1949	5.6573	290.3454	508	18.1949	5.6573	2064.5084	508	18.1949	5.6573	509.5076	508	18.1949	5.6573	2525.1234
509	18.2209	5.6493	383.3839	509	18.2209	5.6493	2154.9475	509	18.2209	5.6493	368.878	509	18.2209	5.6493	2382.1597
510	18.2469	5.6413	409.0267	510	18.2469	5.6413	2177.9911	510	18.2469	5.6413	384.9929	510	18.2469	5.6413	2395.9406
511	18.2729	5.6334	298.0001	511	18.2729	5.6334	2064.365	511	18.2729	5.6334	374.2919	511	18.2729	5.6334	2382.9055
512	18.2989	5.6254	299.7424	512	18.2989	5.6254	2063.508	512	18.2989	5.6254	391.5254	512	18.2989	5.6254	2397.805
513	18.3249	5.6175	365.3793	513	18.3249	5.6175	2126.5455	513	18.3249	5.6175	360.1025	513	18.3249	5.6175	2364.0481
514	18.3509	5.6096	419.8362	514	18.3509	5.6096	2178.4031	514	18.3509	5.6096	422.169	514	18.3509	5.6096	2423.7806
515	18.3769	5.6018	436.032	515	18.3769	5.6018	2191.9994	515	18.3769	5.6018	427.9921	515	18.3769	5.6018	2424.6004
516	18.4029	5.5939	299.8989	516	18.4029	5.5939	2053.267	516	18.4029	5.5939	455.5356	516	18.4029	5.5939	2447.1405
517	18.4289	5.5861	294.9124	517	18.4289	5.5861	2045.6811	517	18.4289	5.5861	347.2256	517	18.4289	5.5861	2333.8272
518	18.4549	5.5783	384.1078	518	18.4549	5.5783	2132.2771	518	18.4549	5.5783	285.0614	518	18.4549	5.5783	2266.6597
519	18.4809	5.5705	392.548	519	18.4809	5.5705	2138.118	519	18.4809	5.5705	343.483	519	18.4809	5.5705	2320.0779
520	18.5069	5.5628	367.6692	520	18.5069	5.5628	2110.6398	520	18.5069	5.5628	414.5301	520	18.5069	5.5628	2386.1218
521	18.5329	5.555	388.3198	521	18.5329	5.555	2128.691	521	18.5329	5.555	427.7308	521	18.5329	5.555	2394.3192
522	18.5589	5.5473	382.7709	522	18.5589	5.5473	2120.5427	522	18.5589	5.5473	453.1771	522	18.5589	5.5473	2414.7621
523	18.5849	5.5396	366.4163	523	18.5849	5.5396	2101.5887	523	18.5849	5.5396	398.4144	523	18.5849	5.5396	2354.9961
524	18.6109	5.532	397.0419	524	18.6109	5.532	2129.615	524	18.6109	5.532	374.8301	524	18.6109	5.532	2326.4085
525	18.6369	5.5243	364.5882	525	18.6369	5.5243	2094.5619	525	18.6369	5.5243	385.2328	525	18.6369	5.5243	2331.8079
526	18.6629	5.5167	270.4288	526	18.6629	5.5167	1997.8032	526	18.6629	5.5167	449.3656	526	18.6629	5.5167	2390.9373
527	18.6889	5.5091	340.0255	527	18.6889	5.5091	2064.8005	527	18.6889	5.5091	350.7387	527	18.6889	5.5091	2287.3071
528	18.7149	5.5015	357.0311	528	18.7149	5.5015	2079.2067	528	18.7149	5.5015	378.7144	528	18.7149	5.5015	2310.2795
529	18.7409	5.4939	374.6885	529	18.7409	5.4939	2094.2647	529	18.7409	5.4939	399.6772	529	18.7409	5.4939	2326.239
530	18.7669	5.4864	459.6361	530	18.7669	5.4864	2176.6129	530	18.7669	5.4864	393.926	530	18.7669	5.4864	2315.4845
531	18.7929	5.4789	475.7635	531	18.7929	5.4789	2190.141	531	18.7929	5.4789	469.5633	531	18.7929	5.4789	2386.1185
532	18.8189	5.4713	404.7519	532	18.8189	5.4713	2116.53	532	18.8189	5.4713	468.2726	532	18.8189	5.4713	2379.8244
533	18.8449	5.4639	389.0347	533	18.8449	5.4639	2098.2134	533	18.8449	5.4639	477.321	533	18.8449	5.4639	2383.8695
534	18.8709	5.4564	364.5411	534	18.8709	5.4564	2071.1204	534	18.8709	5.4564	471.3808	534	18.8709	5.4564	2372.926
535	18.8969	5.449	379.5723	535	18.8969	5.449	2083.5524	535	18.8969	5.449	367.7412	535	18.8969	5.449	2264.2831

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
536	18.9229	5.4415	440.3379	536	18.9229	5.4415	2141.7186	536	18.9229	5.4415	398.6188	536	18.9229	5.4415	2290.1573
537	18.9489	5.4342	413.7765	537	18.9489	5.4342	2112.5578	537	18.9489	5.4342	478.7721	537	18.9489	5.4342	2365.3073
538	18.9749	5.4268	410.2831	538	18.9749	5.4268	2106.465	538	18.9749	5.4268	481.6293	538	18.9749	5.4268	2363.1612
539	19.0009	5.4194	420.0939	539	19.0009	5.4194	2113.6764	539	19.0009	5.4194	429.8067	539	19.0009	5.4194	2306.3353
540	19.0269	5.4121	325.538	540	19.0269	5.4121	2016.5211	540	19.0269	5.4121	404.304	540	19.0269	5.4121	2275.8293
541	19.0529	5.4048	360.0713	541	19.0529	5.4048	2048.4551	541	19.0529	5.4048	422.169	541	19.0529	5.4048	2288.691
542	19.0789	5.3975	363.6058	542	19.0789	5.3975	2048.8611	542	19.0789	5.3975	481.2105	542	19.0789	5.3975	2345.403
543	19.1049	5.3902	403.3292	543	19.1049	5.3902	2085.456	543	19.1049	5.3902	438.3492	543	19.1049	5.3902	2300.2123
544	19.1309	5.3829	433.3701	544	19.1309	5.3829	2112.3683	544	19.1309	5.3829	378.7128	544	19.1309	5.3829	2238.2463
545	19.1569	5.3757	356.2553	545	19.1569	5.3757	2032.125	545	19.1569	5.3757	397.5005	545	19.1569	5.3757	2254.7046
546	19.1829	5.3685	326.0676	546	19.1829	5.3685	1998.8088	546	19.1829	5.3685	427.0107	546	19.1829	5.3685	2281.8853
547	19.2089	5.3613	372.5858	547	19.2089	5.3613	2042.1984	547	19.2089	5.3613	440.6968	547	19.2089	5.3613	2293.2419
548	19.2349	5.3541	417.8361	548	19.2349	5.3541	2084.3202	548	19.2349	5.3541	443.9218	548	19.2349	5.3541	2294.1375
549	19.2609	5.3469	414.954	549	19.2609	5.3469	2078.3096	549	19.2609	5.3469	457.6159	549	19.2609	5.3469	2305.502
550	19.2869	5.3398	391.167	550	19.2869	5.3398	2051.3941	550	19.2869	5.3398	474.8646	550	19.2869	5.3398	2320.4213
551	19.3129	5.3327	365.9056	551	19.3129	5.3327	2023.0041	551	19.3129	5.3327	443.8666	551	19.3129	5.3327	2287.0937
552	19.3389	5.3256	351.9643	552	19.3389	5.3256	2005.9344	552	19.3389	5.3256	420.4305	552	19.3389	5.3256	2261.3282
553	19.3649	5.3185	346.3151	553	19.3649	5.3185	1997.1566	553	19.3649	5.3185	455.1452	553	19.3649	5.3185	2293.7134
554	19.3909	5.3114	369.9875	554	19.3909	5.3114	2017.7005	554	19.3909	5.3114	438.6456	554	19.3909	5.3114	2274.8844
555	19.4169	5.3044	385.8332	555	19.4169	5.3044	2030.4177	555	19.4169	5.3044	416.6975	555	19.4169	5.3044	2250.6067
556	19.4429	5.2974	436.6919	556	19.4429	5.2974	2078.1478	556	19.4429	5.2974	441.3515	556	19.4429	5.2974	2272.9313
557	19.4689	5.2904	453.3856	557	19.4689	5.2904	2091.7131	557	19.4689	5.2904	417.3413	557	19.4689	5.2904	2246.5917
558	19.4949	5.2834	381.5568	558	19.4949	5.2834	2016.7557	558	19.4949	5.2834	396.4914	558	19.4949	5.2834	2223.4122
559	19.5209	5.2764	360.393	559	19.5209	5.2764	1992.4634	559	19.5209	5.2764	419.2125	559	19.5209	5.2764	2243.8039
560	19.5469	5.2694	362.2444	560	19.5469	5.2694	1991.1862	560	19.5469	5.2694	416.7746	560	19.5469	5.2694	2239.0365
561	19.5729	5.2625	350.7682	561	19.5729	5.2625	1976.5815	561	19.5729	5.2625	409.4944	561	19.5729	5.2625	2229.4268
562	19.5989	5.2556	384.2761	562	19.5989	5.2556	2006.961	562	19.5989	5.2556	396.3814	562	19.5989	5.2556	2213.9844
563	19.6249	5.2487	391.0954	563	19.6249	5.2487	2010.6517	563	19.6249	5.2487	377.013	563	19.6249	5.2487	2192.2865
564	19.6509	5.2418	340.7422	564	19.6509	5.2418	1957.17	564	19.6509	5.2418	379.5061	564	19.6509	5.2418	2192.45
565	19.6769	5.235	337.1257	565	19.6769	5.235	1950.425	565	19.6769	5.235	378.5769	565	19.6769	5.235	2189.1913
566	19.7029	5.2281	289.3135	566	19.7029	5.2281	1899.4842	566	19.7029	5.2281	436.7127	566	19.7029	5.2281	2244.9977
567	19.7289	5.2213	322.005	567	19.7289	5.2213	1929.0472	567	19.7289	5.2213	444.1021	567	19.7289	5.2213	2250.0576
568	19.7549	5.2145	360.0713	568	19.7549	5.2145	1963.985	568	19.7549	5.2145	422.169	568	19.7549	5.2145	2225.7951
569	19.7809	5.2077	368.1239	569	19.7809	5.2077	1970.3586	569	19.7809	5.2077	449.7178	569	19.7809	5.2077	2250.9614
570	19.8069	5.201	355.6514	570	19.8069	5.201	1956.2073	570	19.8069	5.201	394.9919	570	19.8069	5.201	2193.853
571	19.8329	5.1942	336.2372	571	19.8329	5.1942	1935.1141	571	19.8329	5.1942	344.649	571	19.8329	5.1942	2141.1277

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
572	19.8589	5.1875	326.8083	572	19.8589	5.1875	1924.0062	572	19.8589	5.1875	320.3781	572	19.8589	5.1875	2114.4744
573	19.8849	5.1808	316.9074	573	19.8849	5.1808	1912.4265	573	19.8849	5.1808	394.4681	573	19.8849	5.1808	2186.182
574	19.9109	5.1741	278.9258	574	19.9109	5.1741	1872.7659	574	19.9109	5.1741	378.7418	574	19.9109	5.1741	2168.0733
575	19.9369	5.1674	302.9143	575	19.9369	5.1674	1895.0755	575	19.9369	5.1674	455.3792	575	19.9369	5.1674	2242.3282
576	19.9629	5.1607	390.339	576	19.9629	5.1607	1980.8213	576	19.9629	5.1607	467.9173	576	19.9629	5.1607	2252.4839
577	19.9889	5.1541	399.448	577	19.9889	5.1541	1988.2513	577	19.9889	5.1541	366.0138	577	19.9889	5.1541	2148.1979
578	20.0149	5.1474	411.4847	578	20.0149	5.1474	1998.6091	578	20.0149	5.1474	425.1287	578	20.0149	5.1474	2204.9304
579	20.0409	5.1408	362.4877	579	20.0409	5.1408	1947.9332	579	20.0409	5.1408	410.2037	579	20.0409	5.1408	2187.6229
580	20.0669	5.1342	341.8433	580	20.0669	5.1342	1925.6098	580	20.0669	5.1342	436.8281	580	20.0669	5.1342	2211.8648
581	20.0929	5.1277	350.3546	581	20.0929	5.1277	1932.4423	581	20.0929	5.1277	441.1513	581	20.0929	5.1277	2213.8056
582	20.1189	5.1211	313.8908	582	20.1189	5.1211	1894.2995	582	20.1189	5.1211	406.8395	582	20.1189	5.1211	2177.1114
583	20.1449	5.1146	307.5405	583	20.1449	5.1146	1886.2703	583	20.1449	5.1146	419.588	583	20.1449	5.1146	2187.4774
584	20.1709	5.108	369.6911	584	20.1709	5.108	1946.742	584	20.1709	5.108	374.2049	584	20.1709	5.108	2139.7119
585	20.1969	5.1015	343.5841	585	20.1969	5.1015	1918.9561	585	20.1969	5.1015	459.6135	585	20.1969	5.1015	2222.7381
586	20.2229	5.095	365.9615	586	20.2229	5.095	1939.6545	586	20.2229	5.095	358.3941	586	20.2229	5.095	2119.1362
587	20.2489	5.0886	350.9355	587	20.2489	5.0886	1922.9496	587	20.2489	5.0886	365.7696	587	20.2489	5.0886	2124.1292
588	20.2749	5.0821	321.3136	588	20.2749	5.0821	1891.6488	588	20.2749	5.0821	471.6124	588	20.2749	5.0821	2227.5896
589	20.3009	5.0757	328.4685	589	20.3009	5.0757	1897.1248	589	20.3009	5.0757	350.1264	589	20.3009	5.0757	2103.7212
590	20.3269	5.0692	354.6515	590	20.3269	5.0692	1921.6288	590	20.3269	5.0692	317.1588	590	20.3269	5.0692	2068.3712
591	20.3529	5.0628	301.8481	591	20.3529	5.0628	1867.1465	591	20.3529	5.0628	383.3578	591	20.3529	5.0628	2132.1877
592	20.3789	5.0564	356.3905	592	20.3789	5.0564	1920.0099	592	20.3789	5.0564	401.5429	592	20.3789	5.0564	2147.9904
593	20.4049	5.0501	411.0491	593	20.4049	5.0501	1972.9896	593	20.4049	5.0501	426.967	593	20.4049	5.0501	2171.0321
594	20.4309	5.0437	301.8193	594	20.4309	5.0437	1862.0809	594	20.4309	5.0437	453.0224	594	20.4309	5.0437	2194.705
595	20.4569	5.0374	360.0713	595	20.4569	5.0374	1918.654	595	20.4569	5.0374	422.169	595	20.4569	5.0374	2161.4692
596	20.4829	5.031	371.563	596	20.4829	5.031	1926.1797	596	20.4829	5.031	425.0524	596	20.4829	5.031	2160.272
597	20.5089	5.0247	245.7575	597	20.5089	5.0247	1796.4082	597	20.5089	5.0247	458.7389	597	20.5089	5.0247	2189.8779
598	20.5349	5.0184	351.7598	598	20.5349	5.0184	1898.4445	598	20.5349	5.0184	444.983	598	20.5349	5.0184	2172.0415
599	20.5609	5.0122	385.0819	599	20.5609	5.0122	1927.8006	599	20.5609	5.0122	378.6838	599	20.5609	5.0122	2101.6617
600	20.5869	5.0059	383.8723	600	20.5869	5.0059	1922.625	600	20.5869	5.0059	405.6503	600	20.5869	5.0059	2124.5476
601	20.6129	4.9997	352.2696	601	20.6129	4.9997	1887.0563	601	20.6129	4.9997	403.582	601	20.6129	4.9997	2118.3987
602	20.6389	4.9934	438.0414	602	20.6389	4.9934	1968.8622	602	20.6389	4.9934	436.5941	602	20.6389	4.9934	2147.3303
603	20.6649	4.9872	414.2608	603	20.6649	4.9872	1941.1156	603	20.6649	4.9872	447.1484	603	20.6649	4.9872	2153.804
604	20.6909	4.981	494.2009	604	20.6909	4.981	2017.0897	604	20.6909	4.981	372.5207	604	20.6909	4.981	2075.0957
605	20.7169	4.9748	444.1756	605	20.7169	4.9748	1963.0984	605	20.7169	4.9748	440.561	605	20.7169	4.9748	2139.0555
606	20.7429	4.9687	319.4315	606	20.7429	4.9687	1834.3883	606	20.7429	4.9687	452.5622	606	20.7429	4.9687	2146.9761
607	20.7689	4.9625	392.1055	607	20.7689	4.9625	1903.0963	607	20.7689	4.9625	358.9446	607	20.7689	4.9625	2049.278

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
608	20.7949	4.9564	295.3496	608	20.7949	4.9564	1802.3745	608	20.7949	4.9564	407.6741	608	20.7949	4.9564	2093.9269
609	20.8209	4.9503	351.1069	609	20.8209	4.9503	1854.1658	609	20.8209	4.9503	455.3866	609	20.8209	4.9503	2137.5588
610	20.8469	4.9441	375.0962	610	20.8469	4.9441	1874.1892	610	20.8469	4.9441	386.2371	610	20.8469	4.9441	2064.3287
611	20.8729	4.9381	354.2932	611	20.8729	4.9381	1849.4202	611	20.8729	4.9381	460.8862	611	20.8729	4.9381	2134.8973
612	20.8989	4.932	333.4021	612	20.8989	4.932	1824.563	612	20.8989	4.932	541.2553	612	20.8989	4.932	2211.1859
613	20.9249	4.9259	420.2127	613	20.9249	4.9259	1907.4077	613	20.9249	4.9259	449.0463	613	20.9249	4.9259	2114.8963
614	20.9509	4.9199	390.3951	614	20.9509	4.9199	1873.6241	614	20.9509	4.9199	425.9602	614	20.9509	4.9199	2087.7297
615	20.9769	4.9138	354.4285	615	20.9769	4.9138	1833.6915	615	20.9769	4.9138	395.6335	615	20.9769	4.9138	2053.3224
616	21.0029	4.9078	418.4461	616	21.0029	4.9078	1893.7431	616	21.0029	4.9078	396.3917	616	21.0029	4.9078	2050
617	21.0289	4.9018	442.987	617	21.0289	4.9018	1914.318	617	21.0289	4.9018	409.3509	617	21.0289	4.9018	2058.8787
618	21.0549	4.8958	489.0204	618	21.0549	4.8958	1956.3855	618	21.0549	4.8958	419.8205	618	21.0549	4.8958	2065.2677
619	21.0809	4.8899	459.5399	619	21.0809	4.8899	1922.939	619	21.0809	4.8899	401.1968	619	21.0809	4.8899	2042.5634
620	21.1069	4.8839	408.6552	620	21.1069	4.8839	1868.0882	620	21.1069	4.8839	369.1061	620	21.1069	4.8839	2006.3922
621	21.1329	4.878	401.1402	621	21.1329	4.878	1856.6073	621	21.1329	4.878	416.1407	621	21.1329	4.878	2049.3462
622	21.1589	4.8721	360.0713	622	21.1589	4.8721	1811.5724	622	21.1589	4.8721	422.169	622	21.1589	4.8721	2051.2939
623	21.1849	4.8661	456.0398	623	21.1849	4.8661	1905.7134	623	21.1849	4.8661	428.3533	623	21.1849	4.8661	2055.7983
624	21.2109	4.8602	345.7528	624	21.2109	4.8602	1793.5989	624	21.2109	4.8602	430.4164	624	21.2109	4.8602	2056.1816
625	21.2369	4.8544	330.1088	625	21.2369	4.8544	1776.1273	625	21.2369	4.8544	349.4488	625	21.2369	4.8544	1973.5341
626	21.2629	4.8485	345.1904	626	21.2629	4.8485	1789.3814	626	21.2629	4.8485	350.7602	626	21.2629	4.8485	1973.1656
627	21.2889	4.8426	344.9047	627	21.2889	4.8426	1787.2681	627	21.2889	4.8426	433.773	627	21.2889	4.8426	2054.4986
628	21.3149	4.8368	363.3747	628	21.3149	4.8368	1803.9106	628	21.3149	4.8368	425.5841	628	21.3149	4.8368	2044.6298
629	21.3409	4.831	374.9045	629	21.3409	4.831	1813.6128	629	21.3409	4.831	397.8765	629	21.3409	4.831	2015.2424
630	21.3669	4.8252	444.1416	630	21.3669	4.8252	1881.0224	630	21.3669	4.8252	375.1009	630	21.3669	4.8252	1990.7869
631	21.3929	4.8194	381.5658	631	21.3929	4.8194	1816.6191	631	21.3929	4.8194	439.1488	631	21.3929	4.8194	2053.155
632	21.4189	4.8136	413.1579	632	21.4189	4.8136	1846.3836	632	21.4189	4.8136	418.5927	632	21.4189	4.8136	2030.919
633	21.4449	4.8078	344.4629	633	21.4449	4.8078	1775.8611	633	21.4449	4.8078	391.2296	633	21.4449	4.8078	2001.876
634	21.4709	4.8021	340.4777	634	21.4709	4.8021	1770.0484	634	21.4709	4.8021	333.3751	634	21.4709	4.8021	1942.3417
635	21.4969	4.7963	404.3241	635	21.4969	4.7963	1832.0672	635	21.4969	4.7963	340.6654	635	21.4969	4.7963	1947.9521
636	21.5229	4.7906	399.1107	636	21.5229	4.7906	1825.0262	636	21.5229	4.7906	353.3932	636	21.5229	4.7906	1959
637	21.5489	4.7849	417.1783	637	21.5489	4.7849	1841.2663	637	21.5489	4.7849	341.974	637	21.5489	4.7849	1945.901
638	21.5749	4.7792	393.6876	638	21.5749	4.7792	1815.948	638	21.5749	4.7792	360.8559	638	21.5749	4.7792	1963.103
639	21.6009	4.7735	319.9834	639	21.6009	4.7735	1740.4163	639	21.6009	4.7735	372.0936	639	21.6009	4.7735	1972.6608
640	21.6269	4.7678	349.4653	640	21.6269	4.7678	1768.0707	640	21.6269	4.7678	361.2388	640	21.6269	4.7678	1960.1262
641	21.6529	4.7622	377.6232	641	21.6529	4.7622	1794.4011	641	21.6529	4.7622	388.6294	641	21.6529	4.7622	1985.8369
642	21.6789	4.7565	374.8507	642	21.6789	4.7565	1789.8009	642	21.6789	4.7565	374.842	642	21.6789	4.7565	1970.3697
643	21.7049	4.7509	340.8633	643	21.7049	4.7509	1753.986	643	21.7049	4.7509	449.486	643	21.7049	4.7509	2043.3338

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
644	21.7309	4.7453	345.6435	644	21.7309	4.7453	1756.9387	644	21.7309	4.7453	426.0964	644	21.7309	4.7453	2018.2643
645	21.7569	4.7397	368.8529	645	21.7569	4.7397	1778.3205	645	21.7569	4.7397	350.8399	645	21.7569	4.7397	1941.328
646	21.7829	4.7341	350.1548	646	21.7829	4.7341	1757.7949	646	21.7829	4.7341	337.7925	646	21.7829	4.7341	1926.6007
647	21.8089	4.7285	371.1896	647	21.8089	4.7285	1777.0021	647	21.8089	4.7285	331.8382	647	21.8089	4.7285	1918.9666
648	21.8349	4.723	357.3956	648	21.8349	4.723	1761.3806	648	21.8349	4.723	317.8473	648	21.8349	4.723	1903.2958
649	21.8609	4.7174	360.0713	649	21.8609	4.7174	1762.2288	649	21.8609	4.7174	422.169	649	21.8609	4.7174	2005.9377
650	21.8869	4.7119	380.2739	650	21.8869	4.7119	1780.5165	650	21.8869	4.7119	403.8496	650	21.8869	4.7119	1983.1992
651	21.9129	4.7064	415.5563	651	21.9129	4.7064	1813.8842	651	21.9129	4.7064	347.5393	651	21.9129	4.7064	1922.4699
652	21.9389	4.7008	367.0395	652	21.9389	4.7008	1763.4525	652	21.9389	4.7008	395.9772	652	21.9389	4.7008	1966.4888
653	21.9649	4.6954	279.8059	653	21.9649	4.6954	1674.3041	653	21.9649	4.6954	397.4355	653	21.9649	4.6954	1963.5281
654	21.9909	4.6899	288.9331	654	21.9909	4.6899	1681.5164	654	21.9909	4.6899	353.2893	654	21.9909	4.6899	1914.9629
655	22.0169	4.6844	323.0155	655	22.0169	4.6844	1713.684	655	22.0169	4.6844	365.4164	655	22.0169	4.6844	1922.6709
656	22.0429	4.6789	348.2734	656	22.0429	4.6789	1737.027	656	22.0429	4.6789	402.1681	656	22.0429	4.6789	1955.0036
657	22.0689	4.6735	353.8688	657	22.0689	4.6735	1740.7076	657	22.0689	4.6735	409.0745	657	22.0689	4.6735	1957.491
658	22.0949	4.6681	351.2919	658	22.0949	4.6681	1736.2158	658	22.0949	4.6681	411.1163	658	22.0949	4.6681	1955.1137
659	22.1209	4.6626	341.6745	659	22.1209	4.6626	1724.6836	659	22.1209	4.6626	404.4124	659	22.1209	4.6626	1943.9908
660	22.1469	4.6572	347.7335	660	22.1469	4.6572	1728.8277	660	22.1469	4.6572	367.556	660	22.1469	4.6572	1902.7154
661	22.1729	4.6519	371.2462	661	22.1729	4.6519	1750.4255	661	22.1729	4.6519	360.4343	661	22.1729	4.6519	1891.1746
662	22.1989	4.6465	345.9636	662	22.1989	4.6465	1723.2281	662	22.1989	4.6465	461.1179	662	22.1989	4.6465	1987.4392
663	22.2249	4.6411	335.7106	663	22.2249	4.6411	1711.0603	663	22.2249	4.6411	479.3613	663	22.2249	4.6411	2001.2636
664	22.2509	4.6357	344.5069	664	22.2509	4.6357	1717.9418	664	22.2509	4.6357	407.1624	664	22.2509	4.6357	1924.6456
665	22.2769	4.6304	318.9001	665	22.2769	4.6304	1690.4201	665	22.2769	4.6304	423.585	665	22.2769	4.6304	1936.6492
666	22.3029	4.6251	341.2026	666	22.3029	4.6251	1710.8078	666	22.3029	4.6251	397.0576	666	22.3029	4.6251	1905.7028
667	22.3289	4.6198	390.2787	667	22.3289	4.6198	1757.969	667	22.3289	4.6198	394.1966	667	22.3289	4.6198	1898.4227
668	22.3549	4.6145	344.4971	668	22.3549	4.6145	1710.2725	668	22.3549	4.6145	452.6478	668	22.3549	4.6145	1952.4549
669	22.3809	4.6092	301.0642	669	22.3809	4.6092	1664.9249	669	22.3809	4.6092	463.3389	669	22.3809	4.6092	1958.727
670	22.4069	4.6039	270.6511	670	22.4069	4.6039	1632.5969	670	22.4069	4.6039	469.4741	670	22.4069	4.6039	1960.4431
671	22.4329	4.5986	317.6881	671	22.4329	4.5986	1677.719	671	22.4329	4.5986	514.8582	671	22.4329	4.5986	2001.4083
672	22.4589	4.5934	285.5918	672	22.4589	4.5934	1643.7079	672	22.4589	4.5934	538.6339	672	22.4589	4.5934	2020.7649
673	22.4849	4.5881	274.6851	673	22.4849	4.5881	1630.8864	673	22.4849	4.5881	530.7706	673	22.4849	4.5881	2008.4826
674	22.5109	4.5829	316.0291	674	22.5109	4.5829	1670.3156	674	22.5109	4.5829	447.3185	674	22.5109	4.5829	1920.6115
675	22.5369	4.5777	300.1114	675	22.5369	4.5777	1652.483	675	22.5369	4.5777	446.3796	675	22.5369	4.5777	1915.2535
676	22.5629	4.5725	397.6604	676	22.5629	4.5725	1748.1172	676	22.5629	4.5725	422.169	676	22.5629	4.5725	1886.624
677	22.5889	4.5673	383.1034	677	22.5889	4.5673	1731.6453	677	22.5889	4.5673	395.3968	677	22.5889	4.5673	1857.9793
678	22.6149	4.5621	356.2642	678	22.6149	4.5621	1702.8912	678	22.6149	4.5621	384.8118	678	22.6149	4.5621	1845.5217
679	22.6409	4.5569	372.9308	679	22.6409	4.5569	1717.643	679	22.6409	4.5569	400.0713	679	22.6409	4.5569	1858.9088

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
680	22.6669	4.5518	278.1216	680	22.6669	4.5518	1620.919	680	22.6669	4.5518	395.4734	680	22.6669	4.5518	1852.4384
681	22.6929	4.5466	330.5891	681	22.6929	4.5466	1671.4716	681	22.6929	4.5466	398.5353	681	22.6929	4.5466	1853.6279
682	22.7189	4.5415	340.0933	682	22.7189	4.5415	1679.061	682	22.7189	4.5415	488.1198	682	22.7189	4.5415	1941.3399
683	22.7449	4.5363	365.4145	683	22.7449	4.5363	1702.4674	683	22.7449	4.5363	461.1083	683	22.7449	4.5363	1912.4559
684	22.7709	4.5312	303.9157	684	22.7709	4.5312	1639.0537	684	22.7709	4.5312	454.0638	684	22.7709	4.5312	1903.5389
685	22.7969	4.5261	363.7292	685	22.7969	4.5261	1696.9524	685	22.7969	4.5261	363.6967	685	22.7969	4.5261	1811.2993
686	22.8229	4.521	378.9784	686	22.8229	4.521	1710.2867	686	22.8229	4.521	448.36	686	22.8229	4.521	1894.0902
687	22.8489	4.516	305.7329	687	22.8489	4.516	1635.1264	687	22.8489	4.516	410.7706	687	22.8489	4.516	1854.6283
688	22.8749	4.5109	313.2205	688	22.8749	4.5109	1640.6991	688	22.8749	4.5109	366.3329	688	22.8749	4.5109	1808.3182
689	22.9009	4.5059	312.2317	689	22.9009	4.5059	1637.7955	689	22.9009	4.5059	389.6322	689	22.9009	4.5059	1829.745
690	22.9269	4.5008	372.6406	690	22.9269	4.5008	1696.2896	690	22.9269	4.5008	380.7597	690	22.9269	4.5008	1819
691	22.9529	4.4958	370.7505	691	22.9529	4.4958	1692.4846	691	22.9529	4.4958	383.4003	691	22.9529	4.4958	1819.7681
692	22.9789	4.4908	290.1984	692	22.9789	4.4908	1610.0176	692	22.9789	4.4908	409.3347	692	22.9789	4.4908	1843.83
693	23.0049	4.4858	300.4639	693	23.0049	4.4858	1618.3683	693	23.0049	4.4858	518.274	693	23.0049	4.4858	1950.8968
694	23.0309	4.4808	245.0884	694	23.0309	4.4808	1561.0779	694	23.0309	4.4808	446.7634	694	23.0309	4.4808	1877.5138
695	23.0569	4.4758	294.3182	695	23.0569	4.4758	1608.3929	695	23.0569	4.4758	430.0332	695	23.0569	4.4758	1858.911
696	23.0829	4.4708	378.1837	696	23.0829	4.4708	1690.3436	696	23.0829	4.4708	376.2751	696	23.0829	4.4708	1803.2805
697	23.1089	4.4658	314.946	697	23.1089	4.4658	1625.191	697	23.1089	4.4658	436.2569	697	23.1089	4.4658	1861.3899
698	23.1349	4.4609	255.7249	698	23.1349	4.4609	1564.0551	698	23.1349	4.4609	395.5911	698	23.1349	4.4609	1818.8516
699	23.1609	4.456	403.6804	699	23.1609	4.456	1710.0957	699	23.1609	4.456	417.5378	699	23.1609	4.456	1838.9258
700	23.1869	4.451	318.6634	700	23.1869	4.451	1623.1639	700	23.1869	4.451	416.6193	700	23.1869	4.451	1836.1348
701	23.2129	4.4461	306.0754	701	23.2129	4.4461	1608.661	701	23.2129	4.4461	393.6416	701	23.2129	4.4461	1811.2846
702	23.2389	4.4412	271.3762	702	23.2389	4.4412	1572.047	702	23.2389	4.4412	434.6068	702	23.2389	4.4412	1850.3774
703	23.2649	4.4363	360.0713	703	23.2649	4.4363	1658.8272	703	23.2649	4.4363	422.169	703	23.2649	4.4363	1836.0671
704	23.2909	4.4314	357.1881	704	23.2909	4.4314	1654.6896	704	23.2909	4.4314	399.3005	704	23.2909	4.4314	1810.4926
705	23.3169	4.4265	385.7088	705	23.3169	4.4265	1681.9559	705	23.3169	4.4265	421.0581	705	23.3169	4.4265	1829.5441
706	23.3429	4.4217	384.3087	706	23.3429	4.4217	1679.3014	706	23.3429	4.4217	393.9185	706	23.3429	4.4217	1799.6984
707	23.3689	4.4168	447.9381	707	23.3689	4.4168	1741.6763	707	23.3689	4.4168	541.1759	707	23.3689	4.4168	1944.2498
708	23.3949	4.412	287.9862	708	23.3949	4.412	1580.47	708	23.3949	4.412	427.4245	708	23.3949	4.412	1827.7922
709	23.4209	4.4072	303.3459	709	23.4209	4.4072	1594.5753	709	23.4209	4.4072	351.3119	709	23.4209	4.4072	1748.9737
710	23.4469	4.4023	366.7911	710	23.4469	4.4023	1656.7661	710	23.4469	4.4023	434.0774	710	23.4469	4.4023	1829.033
711	23.4729	4.3975	311.0588	711	23.4729	4.3975	1599.7793	711	23.4729	4.3975	429.2435	711	23.4729	4.3975	1821.4931
712	23.4989	4.3927	294.41	712	23.4989	4.3927	1581.876	712	23.4989	4.3927	444.69	712	23.4989	4.3927	1834.2335
713	23.5249	4.388	323.7836	713	23.5249	4.388	1609.9952	713	23.5249	4.388	443.4859	713	23.5249	4.388	1830.3234
714	23.5509	4.3832	333.5207	714	23.5509	4.3832	1618.4778	714	23.5509	4.3832	526.3789	714	23.5509	4.3832	1910.5103
715	23.5769	4.3784	275.7909	715	23.5769	4.3784	1559.4936	715	23.5769	4.3784	423.8857	715	23.5769	4.3784	1805.3111

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
716	23.6029	4.3737	332.2243	716	23.6029	4.3737	1614.6726	716	23.6029	4.3737	504.1201	716	23.6029	4.3737	1882.8394
717	23.6289	4.3689	444.5958	717	23.6289	4.3689	1725.7897	717	23.6289	4.3689	563.4556	717	23.6289	4.3689	1939.4688
718	23.6549	4.3642	466.9177	718	23.6549	4.3642	1746.8572	718	23.6549	4.3642	531.8356	718	23.6549	4.3642	1905.1428
719	23.6809	4.3595	384.363	719	23.6809	4.3595	1663.048	719	23.6809	4.3595	437.4405	719	23.6809	4.3595	1808.0416
720	23.7069	4.3547	442.8392	720	23.7069	4.3547	1720.2697	720	23.7069	4.3547	494.6429	720	23.7069	4.3547	1862.538
721	23.7329	4.35	354.6778	721	23.7329	4.35	1630.8539	721	23.7329	4.35	445.3267	721	23.7329	4.35	1810.5157
722	23.7589	4.3453	348.3846	722	23.7589	4.3453	1623.3063	722	23.7589	4.3453	422.2886	722	23.7589	4.3453	1784.7715
723	23.7849	4.3407	375.5798	723	23.7849	4.3407	1649.247	723	23.7849	4.3407	370.3846	723	23.7849	4.3407	1730.1615
724	23.8109	4.336	388.1966	724	23.8109	4.336	1660.6095	724	23.8109	4.336	395.9765	724	23.8109	4.336	1753.0473
725	23.8369	4.3313	268.4026	725	23.8369	4.3313	1539.561	725	23.8369	4.3313	425.2255	725	23.8369	4.3313	1779.5902
726	23.8629	4.3267	339.6629	726	23.8629	4.3267	1609.5669	726	23.8629	4.3267	408.9575	726	23.8629	4.3267	1760.6162
727	23.8889	4.322	350.8114	727	23.8889	4.322	1619.4609	727	23.8889	4.322	436.3112	727	23.8889	4.322	1785.2638
728	23.9149	4.3174	325.0101	728	23.9149	4.3174	1592.4052	728	23.9149	4.3174	397.9908	728	23.9149	4.3174	1744.2374
729	23.9409	4.3128	395.9633	729	23.9409	4.3128	1662.104	729	23.9409	4.3128	425.5115	729	23.9409	4.3128	1769.052
730	23.9669	4.3082	425.247	730	23.9669	4.3082	1690.1332	730	23.9669	4.3082	469.8315	730	23.9669	4.3082	1810.6659
731	23.9929	4.3036	320.1564	731	23.9929	4.3036	1583.7881	731	23.9929	4.3036	435.7113	731	23.9929	4.3036	1773.8397
732	24.0189	4.299	303.0524	732	24.0189	4.299	1565.4297	732	24.0189	4.299	507.2197	732	24.0189	4.299	1842.6421
733	24.0449	4.2944	329.036	733	24.0449	4.2944	1590.1589	733	24.0449	4.2944	508.0716	733	24.0449	4.2944	1840.7878
734	24.0709	4.2898	340.7663	734	24.0709	4.2898	1600.6348	734	24.0709	4.2898	524.7064	734	24.0709	4.2898	1854.7166
735	24.0969	4.2853	322.5919	735	24.0969	4.2853	1581.2059	735	24.0969	4.2853	482.9181	735	24.0969	4.2853	1810.2222
736	24.1229	4.2807	332.6112	736	24.1229	4.2807	1589.9708	736	24.1229	4.2807	528.0423	736	24.1229	4.2807	1852.6403
737	24.1489	4.2762	340.8949	737	24.1489	4.2762	1597	737	24.1489	4.2762	592.6648	737	24.1489	4.2762	1914.5568
738	24.1749	4.2717	288.5422	738	24.1749	4.2717	1543.3929	738	24.1749	4.2717	612.8759	738	24.1749	4.2717	1932.0618
739	24.2009	4.2671	311.4634	739	24.2009	4.2671	1565.0597	739	24.2009	4.2671	673.4173	739	24.2009	4.2671	1989.8972
740	24.2269	4.2626	389.3871	740	24.2269	4.2626	1641.7289	740	24.2269	4.2626	765.2968	740	24.2269	4.2626	2079.0706
741	24.2529	4.2581	424.4876	741	24.2529	4.2581	1675.575	741	24.2529	4.2581	798.9322	741	24.2529	4.2581	2110
742	24.2789	4.2536	367.6468	742	24.2789	4.2536	1617.4798	742	24.2789	4.2536	868.9867	742	24.2789	4.2536	2177.3484
743	24.3049	4.2492	385.1589	743	24.3049	4.2492	1633.7374	743	24.3049	4.2492	1081.7876	743	24.3049	4.2492	2387.4432
744	24.3309	4.2447	389.5664	744	24.3309	4.2447	1636.8905	744	24.3309	4.2447	1328.6853	744	24.3309	4.2447	2631.6349
745	24.3569	4.2402	407.4389	745	24.3569	4.2402	1653.5085	745	24.3569	4.2402	1425.7881	745	24.3569	4.2402	2726.0316
746	24.3829	4.2358	389.8876	746	24.3829	4.2358	1634.7028	746	24.3829	4.2358	1364.1628	746	24.3829	4.2358	2661.7003
747	24.4089	4.2313	365.8412	747	24.4089	4.2313	1609.402	747	24.4089	4.2313	1347.2833	747	24.4089	4.2313	2642.1147
748	24.4349	4.2269	377.2785	748	24.4349	4.2269	1619.5849	748	24.4349	4.2269	1266.3185	748	24.4349	4.2269	2558.4439
749	24.4609	4.2225	418.9012	749	24.4609	4.2225	1659.9531	749	24.4609	4.2225	1050.5807	749	24.4609	4.2225	2340
750	24.4869	4.218	428.861	750	24.4869	4.218	1668.6585	750	24.4869	4.218	846.4195	750	24.4869	4.218	2133.1327
751	24.5129	4.2136	443.0213	751	24.5129	4.2136	1681.5643	751	24.5129	4.2136	699.7415	751	24.5129	4.2136	1983.7487

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
752	24.5389	4.2092	434.6484	752	24.5389	4.2092	1671.937	752	24.5389	4.2092	636.0219	752	24.5389	4.2092	1917.323
753	24.5649	4.2049	402.8124	753	24.5649	4.2049	1638.8466	753	24.5649	4.2049	608.1753	753	24.5649	4.2049	1886.7704
754	24.5909	4.2005	386.1785	754	24.5909	4.2005	1620.9582	754	24.5909	4.2005	555.7576	754	24.5909	4.2005	1831.6466
755	24.6169	4.1961	396.1068	755	24.6169	4.1961	1629.6321	755	24.6169	4.1961	476.4765	755	24.6169	4.1961	1749.6595
756	24.6429	4.1918	403.5557	756	24.6429	4.1918	1635.8266	756	24.6429	4.1918	413.211	756	24.6429	4.1918	1683.6879
757	24.6689	4.1874	360.0713	757	24.6689	4.1874	1591.0877	757	24.6689	4.1874	422.169	757	24.6689	4.1874	1689.9398
758	24.6949	4.1831	395.8637	758	24.6949	4.1831	1623.4578	758	24.6949	4.1831	465.7478	758	24.6949	4.1831	1731.5977
759	24.7209	4.1787	395.5984	759	24.7209	4.1787	1619.7702	759	24.7209	4.1787	441.0543	759	24.7209	4.1787	1704.9832
760	24.7469	4.1744	345.9204	760	24.7469	4.1744	1566.6698	760	24.7469	4.1744	391.1781	760	24.7469	4.1744	1653.1861
761	24.7729	4.1701	383.4273	761	24.7729	4.1701	1600.7543	761	24.7729	4.1701	418.3745	761	24.7729	4.1701	1678.4616
762	24.7989	4.1658	344.7326	762	24.7989	4.1658	1558.6373	762	24.7989	4.1658	474.9432	762	24.7989	4.1658	1733.1094
763	24.8249	4.1615	290.3215	763	24.8249	4.1615	1500.8039	763	24.8249	4.1615	472.8883	763	24.8249	4.1615	1729.1335
764	24.8509	4.1572	286.2177	764	24.8509	4.1572	1493.2778	764	24.8509	4.1572	436.6757	764	24.8509	4.1572	1691
765	24.8769	4.1529	311.8793	765	24.8769	4.1529	1515.5171	765	24.8769	4.1529	451.5971	765	24.8769	4.1529	1704.0004
766	24.9029	4.1487	345.7768	766	24.9029	4.1487	1545.9922	766	24.9029	4.1487	458.4153	766	24.9029	4.1487	1708.8977
767	24.9289	4.1444	312.635	767	24.9289	4.1444	1509.4281	767	24.9289	4.1444	437.4433	767	24.9289	4.1444	1686.0048
768	24.9549	4.1402	293.8757	768	24.9549	4.1402	1487.2465	768	24.9549	4.1402	403.7497	768	24.9549	4.1402	1650.3903
769	24.9809	4.1359	332.0997	769	24.9809	4.1359	1522.0481	769	24.9809	4.1359	401.8045	769	24.9809	4.1359	1646.5241
770	25.0069	4.1317	328.1539	770	25.0069	4.1317	1514.6799	770	25.0069	4.1317	446.5788	770	25.0069	4.1317	1689.3775
771	25.0329	4.1275	284.5741	771	25.0329	4.1275	1467.6779	771	25.0329	4.1275	413.1976	771	25.0329	4.1275	1654.0754
772	25.0589	4.1233	305.0664	772	25.0589	4.1233	1484.7478	772	25.0589	4.1233	407.4996	772	25.0589	4.1233	1646.4564
773	25.0849	4.119	332.2207	773	25.0849	4.119	1508.4798	773	25.0849	4.119	379.6436	773	25.0849	4.119	1616.6795
774	25.1109	4.1148	341.5815	774	25.1109	4.1148	1514.4182	774	25.1109	4.1148	429.0878	774	25.1109	4.1148	1664.2027
775	25.1369	4.1107	321.823	775	25.1369	4.1107	1491.2374	775	25.1369	4.1107	462.9283	775	25.1369	4.1107	1696.1223
776	25.1629	4.1065	326.3475	776	25.1629	4.1065	1492.3396	776	25.1629	4.1065	446.2557	776	25.1629	4.1065	1677.5288
777	25.1889	4.1023	337.8086	777	25.1889	4.1023	1500.3783	777	25.1889	4.1023	399.765	777	25.1889	4.1023	1629.1172
778	25.2149	4.0982	298.4025	778	25.2149	4.0982	1457.5498	778	25.2149	4.0982	440.988	778	25.2149	4.0982	1668.4192
779	25.2409	4.094	316.629	779	25.2409	4.094	1472.3541	779	25.2409	4.094	428.5887	779	25.2409	4.094	1654.099
780	25.2669	4.0899	333.4221	780	25.2669	4.0899	1485.7249	780	25.2669	4.0899	377.6617	780	25.2669	4.0899	1601.251
781	25.2929	4.0857	384.8284	781	25.2929	4.0857	1533.7088	781	25.2929	4.0857	343.7926	781	25.2929	4.0857	1565.461
782	25.3189	4.0816	319.9578	782	25.3189	4.0816	1465.4159	782	25.3189	4.0816	396.2553	782	25.3189	4.0816	1616.0028
783	25.3449	4.0775	267.5978	783	25.3449	4.0775	1409.6335	783	25.3449	4.0775	407.4334	783	25.3449	4.0775	1625.2599
784	25.3709	4.0734	360.0713	784	25.3709	4.0734	1498.6847	784	25.3709	4.0734	422.169	784	25.3709	4.0734	1638.0747
785	25.3969	4.0693	302.7688	785	25.3969	4.0693	1438.4529	785	25.3969	4.0693	405.41	785	25.3969	4.0693	1619.6394
786	25.4229	4.0652	372.0982	786	25.4229	4.0652	1504.853	786	25.4229	4.0652	429.777	786	25.4229	4.0652	1642.33
787	25.4489	4.0611	375.2786	787	25.4489	4.0611	1505.1041	787	25.4489	4.0611	447.4822	787	25.4489	4.0611	1658.359

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
788	25.4749	4.057	302.7073	788	25.4749	4.057	1429.6034	788	25.4749	4.057	434.4743	788	25.4749	4.057	1643.6748
789	25.5009	4.0529	275.253	789	25.5009	4.0529	1399.2198	789	25.5009	4.0529	476.0157	789	25.5009	4.0529	1683.5399
790	25.5269	4.0489	239.1813	790	25.5269	4.0489	1360.2188	790	25.5269	4.0489	372.1996	790	25.5269	4.0489	1578.0475
791	25.5529	4.0448	313.474	791	25.5529	4.0448	1431.5822	791	25.5529	4.0448	432.6291	791	25.5529	4.0448	1636.8008
792	25.5789	4.0408	329.5181	792	25.5789	4.0408	1444.6971	792	25.5789	4.0408	383.3238	792	25.5789	4.0408	1585.8192
793	25.6049	4.0367	323.6731	793	25.6049	4.0367	1435.9228	793	25.6049	4.0367	373.975	793	25.6049	4.0367	1574.7941
794	25.6309	4.0327	291.8402	794	25.6309	4.0327	1401.1606	794	25.6309	4.0327	409.3547	794	25.6309	4.0327	1608.4975
795	25.6569	4.0287	359.6836	795	25.6569	4.0287	1466.0747	795	25.6569	4.0287	370.5392	795	25.6569	4.0287	1568.0058
796	25.6829	4.0247	429.0132	796	25.6829	4.0247	1532.4749	796	25.6829	4.0247	438.6628	796	25.6829	4.0247	1634.4531
797	25.7089	4.0207	330.0696	797	25.7089	4.0207	1430.602	797	25.7089	4.0207	455.4509	797	25.7089	4.0207	1649.5649
798	25.7349	4.0167	377.8002	798	25.7349	4.0167	1475.4034	798	25.7349	4.0167	481.5753	798	25.7349	4.0167	1674.0131
799	25.7609	4.0127	335.8182	799	25.7609	4.0127	1430.4921	799	25.7609	4.0127	416.2888	799	25.7609	4.0127	1607.0503
800	25.7869	4.0087	346.4181	800	25.7869	4.0087	1438.1626	800	25.7869	4.0087	445.0959	800	25.7869	4.0087	1634.1811
801	25.8129	4.0048	373.8278	801	25.8129	4.0048	1462.643	801	25.8129	4.0048	494.4988	801	25.8129	4.0048	1681.9077
802	25.8389	4.0008	324.3901	802	25.8389	4.0008	1410.276	802	25.8389	4.0008	406.0959	802	25.8389	4.0008	1591.8285
803	25.8649	3.9969	294.7738	803	25.8649	3.9969	1377.7304	803	25.8649	3.9969	438.7006	803	25.8649	3.9969	1622.757
804	25.8909	3.9929	270.4631	804	25.8909	3.9929	1350.4904	804	25.8909	3.9929	391.0778	804	25.8909	3.9929	1573.458
805	25.9169	3.989	318.7112	805	25.9169	3.989	1395.8092	805	25.9169	3.989	435.7118	805	25.9169	3.989	1616.4156
806	25.9429	3.985	357.2456	806	25.9429	3.985	1431.4143	806	25.9429	3.985	411.8594	806	25.9429	3.985	1590.887
807	25.9689	3.9811	392.5448	807	25.9689	3.9811	1463.7842	807	25.9689	3.9811	404.7645	807	25.9689	3.9811	1582.1158
808	25.9949	3.9772	314.2877	808	25.9949	3.9772	1382.5978	808	25.9949	3.9772	450.0042	808	25.9949	3.9772	1625.6792
809	26.0209	3.9733	311.7053	809	26.0209	3.9733	1377.0861	809	26.0209	3.9733	483.4504	809	26.0209	3.9733	1657.4492
810	26.0469	3.9694	396.2692	810	26.0469	3.9694	1458.7207	810	26.0469	3.9694	442.8714	810	26.0469	3.9694	1615.1939
811	26.0729	3.9655	360.0713	811	26.0729	3.9655	1419.5934	811	26.0729	3.9655	422.169	811	26.0729	3.9655	1592.8153
812	26.0989	3.9616	404.1555	812	26.0989	3.9616	1461.839	812	26.0989	3.9616	460.6505	812	26.0989	3.9616	1629.1678
813	26.1249	3.9578	306.3007	813	26.1249	3.9578	1362.1454	813	26.1249	3.9578	382.562	813	26.1249	3.9578	1548.9504
814	26.1509	3.9539	301.0609	814	26.1509	3.9539	1355.0668	814	26.1509	3.9539	437.5974	814	26.1509	3.9539	1601.8569
815	26.1769	3.95	331.4537	815	26.1769	3.95	1383.6209	815	26.1769	3.95	436.4834	815	26.1769	3.95	1598.614
816	26.2029	3.9462	374.0315	816	26.2029	3.9462	1424.3599	816	26.2029	3.9462	513.8048	816	26.2029	3.9462	1673.8065
817	26.2289	3.9423	338.8569	817	26.2289	3.9423	1387.3466	817	26.2289	3.9423	404.7806	817	26.2289	3.9423	1562.6534
818	26.2549	3.9385	314.9053	818	26.2549	3.9385	1361.5563	818	26.2549	3.9385	409.4454	818	26.2549	3.9385	1565.1893
819	26.2809	3.9347	321.2563	819	26.2809	3.9347	1366.0685	819	26.2809	3.9347	400.1316	819	26.2809	3.9347	1553.7465
820	26.3069	3.9309	339.7521	820	26.3069	3.9309	1382.7256	820	26.3069	3.9309	426.7232	820	26.3069	3.9309	1578.2093
821	26.3329	3.927	292.9058	821	26.3329	3.927	1334.0405	821	26.3329	3.927	482.7386	821	26.3329	3.927	1632.0958
822	26.3589	3.9232	364.3996	822	26.3589	3.9232	1403.6956	822	26.3589	3.9232	474.842	822	26.3589	3.9232	1622.0702
823	26.3849	3.9194	338.1928	823	26.3849	3.9194	1375.6501	823	26.3849	3.9194	408.0784	823	26.3849	3.9194	1553.1777

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
824	26.4109	3.9156	301.5252	824	26.4109	3.9156	1337.1437	824	26.4109	3.9156	422.2142	824	26.4109	3.9156	1565.1846
825	26.4369	3.9119	328.5334	825	26.4369	3.9119	1362.3132	825	26.4369	3.9119	468.712	825	26.4369	3.9119	1609.5535
826	26.4629	3.9081	398.9312	826	26.4629	3.9081	1430.8723	826	26.4629	3.9081	415.7869	826	26.4629	3.9081	1554.4995
827	26.4889	3.9043	377.1009	827	26.4889	3.9043	1407.2032	827	26.4889	3.9043	465.3387	827	26.4889	3.9043	1601.9223
828	26.5149	3.9006	388.0045	828	26.5149	3.9006	1416.2681	828	26.5149	3.9006	473.8083	828	26.5149	3.9006	1608.2631
829	26.5409	3.8968	432.2236	829	26.5409	3.8968	1458.6484	829	26.5409	3.8968	460.3403	829	26.5409	3.8968	1592.6662
830	26.5669	3.8931	467.6465	830	26.5669	3.8931	1492.2326	830	26.5669	3.8931	485.9077	830	26.5669	3.8931	1616.1047
831	26.5929	3.8893	480.0751	831	26.5929	3.8893	1502.8225	831	26.5929	3.8893	421.7757	831	26.5929	3.8893	1549.8438
832	26.6189	3.8856	494.41	832	26.6189	3.8856	1515.3186	832	26.6189	3.8856	461.4268	832	26.6189	3.8856	1587.366
833	26.6449	3.8819	492.4836	833	26.6449	3.8819	1511.5535	833	26.6449	3.8819	445.9571	833	26.6449	3.8819	1569.7674
834	26.6709	3.8782	543.9347	834	26.6709	3.8782	1561.1659	834	26.6709	3.8782	491.8929	834	26.6709	3.8782	1613.5742
835	26.6969	3.8744	566.0572	835	26.6969	3.8744	1581.4496	835	26.6969	3.8744	594.1764	835	26.6969	3.8744	1713.7289
836	26.7229	3.8707	725.7212	836	26.7229	3.8707	1739.2749	836	26.7229	3.8707	729.52	836	26.7229	3.8707	1846.9435
837	26.7489	3.8671	852.3219	837	26.7489	3.8671	1864.0368	837	26.7489	3.8671	873.5151	837	26.7489	3.8671	1988.8098
838	26.7749	3.8634	939.8974	838	26.7749	3.8634	1949.7735	838	26.7749	3.8634	1090.2045	838	26.7749	3.8634	2203.3702
839	26.8009	3.8597	1109.7822	839	26.8009	3.8597	2117.8196	839	26.8009	3.8597	1363.9072	839	26.8009	3.8597	2474.944
840	26.8269	3.856	1256.4745	840	26.8269	3.856	2262.6732	840	26.8269	3.856	1648.5231	840	26.8269	3.856	2757.431
841	26.8529	3.8524	1339.2176	841	26.8529	3.8524	2343.5776	841	26.8529	3.8524	1664.7186	841	26.8529	3.8524	2771.4976
842	26.8789	3.8487	1420.1498	842	26.8789	3.8487	2422.671	842	26.8789	3.8487	1563.1254	842	26.8789	3.8487	2667.7755
843	26.9049	3.845	1434.2455	843	26.9049	3.845	2434.928	843	26.9049	3.845	1393.3569	843	26.9049	3.845	2495.8781
844	26.9309	3.8414	1368.3251	844	26.9309	3.8414	2367.1688	844	26.9309	3.8414	1168.357	844	26.9309	3.8414	2268.7492
845	26.9569	3.8378	1321.3554	845	26.9569	3.8378	2318.3604	845	26.9569	3.8378	993.0268	845	26.9569	3.8378	2091.2902
846	26.9829	3.8341	1303.9831	846	26.9829	3.8341	2299.1494	846	26.9829	3.8341	854.0571	846	26.9829	3.8341	1950.1915
847	27.0089	3.8305	1257.2707	847	27.0089	3.8305	2250.5982	847	27.0089	3.8305	680.2406	847	27.0089	3.8305	1774.2462
848	27.0349	3.8269	1199.337	848	27.0349	3.8269	2190.8258	848	27.0349	3.8269	584.653	848	27.0349	3.8269	1676.5296
849	27.0609	3.8233	1154.1564	849	27.0609	3.8233	2143.8065	849	27.0609	3.8233	547.301	849	27.0609	3.8233	1637.0488
850	27.0869	3.8197	1111.6939	850	27.0869	3.8197	2099.5052	850	27.0869	3.8197	502.1585	850	27.0869	3.8197	1589.7773
851	27.1129	3.8161	1108.1787	851	27.1129	3.8161	2094.1513	851	27.1129	3.8161	482.378	851	27.1129	3.8161	1567.8679
852	27.1389	3.8125	1034.6662	852	27.1389	3.8125	2018.8	852	27.1389	3.8125	486.4196	852	27.1389	3.8125	1569.7806
853	27.1649	3.8089	950.7725	853	27.1649	3.8089	1933.0676	853	27.1649	3.8089	493.4989	853	27.1649	3.8089	1574.731
854	27.1909	3.8053	895.1046	854	27.1909	3.8053	1875.561	854	27.1909	3.8053	491.4614	854	27.1909	3.8053	1570.5646
855	27.2169	3.8018	842.5388	855	27.2169	3.8018	1821.1564	855	27.2169	3.8018	423.2832	855	27.2169	3.8018	1500.2575
856	27.2429	3.7982	781.1922	856	27.2429	3.7982	1757.9711	856	27.2429	3.7982	414.6671	856	27.2429	3.7982	1489.5125
857	27.2689	3.7947	658.0301	857	27.2689	3.7947	1632.9702	857	27.2689	3.7947	448.6206	857	27.2689	3.7947	1521.3371
858	27.2949	3.7911	584.8782	858	27.2949	3.7911	1557.9796	858	27.2949	3.7911	406.1337	858	27.2949	3.7911	1476.7213
859	27.3209	3.7876	564.4304	859	27.3209	3.7876	1535.693	859	27.3209	3.7876	404.7417	859	27.3209	3.7876	1473.2004

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
860	27.3469	3.7841	510.9711	860	27.3469	3.7841	1480.395	860	27.3469	3.7841	426.705	860	27.3469	3.7841	1493.0347
861	27.3729	3.7805	468.3437	861	27.3729	3.7805	1435.9288	861	27.3729	3.7805	417.7328	861	27.3729	3.7805	1481.9337
862	27.3989	3.777	426.4685	862	27.3989	3.777	1392.2149	862	27.3989	3.777	411.7899	862	27.3989	3.777	1473.8619
863	27.4249	3.7735	397.6682	863	27.4249	3.7735	1361.5759	863	27.4249	3.7735	418.2544	863	27.4249	3.7735	1478.1974
864	27.4509	3.77	386.0116	864	27.4509	3.77	1348.0805	864	27.4509	3.77	430.4446	864	27.4509	3.77	1488.2588
865	27.4769	3.7665	360.0713	865	27.4769	3.7665	1320.3015	865	27.4769	3.7665	422.169	865	27.4769	3.7665	1477.8543
866	27.5029	3.763	386.5758	866	27.5029	3.763	1344.8741	866	27.5029	3.763	405.7803	866	27.5029	3.763	1461.4769
867	27.5289	3.7595	412.0836	867	27.5289	3.7595	1368.4499	867	27.5289	3.7595	394.7328	867	27.5289	3.7595	1450.4407
868	27.5549	3.756	412.587	868	27.5549	3.756	1367.0213	868	27.5549	3.756	415.4728	868	27.5549	3.756	1471.1921
869	27.5809	3.7526	432.638	869	27.5809	3.7526	1385.1404	869	27.5809	3.7526	411.4575	869	27.5809	3.7526	1467.1882
870	27.6069	3.7491	362.9419	870	27.6069	3.7491	1313.5124	870	27.6069	3.7491	423.0219	870	27.6069	3.7491	1478.764
871	27.6329	3.7456	328.7854	871	27.6329	3.7456	1277.4239	871	27.6329	3.7456	421.9564	871	27.6329	3.7456	1477.7099
872	27.6589	3.7422	363.5705	872	27.6589	3.7422	1310.2771	872	27.6589	3.7422	354.7969	872	27.6589	3.7422	1410.5617
873	27.6849	3.7387	377.1343	873	27.6849	3.7387	1321.9089	873	27.6849	3.7387	353.6566	873	27.6849	3.7387	1409.4328
874	27.7109	3.7353	428.2654	874	27.7109	3.7353	1371.1081	874	27.7109	3.7353	373.2124	874	27.7109	3.7353	1429
875	27.7369	3.7319	416.5768	875	27.7369	3.7319	1357.4875	875	27.7369	3.7319	391.5644	875	27.7369	3.7319	1447.3633
876	27.7629	3.7284	363.4271	876	27.7629	3.7284	1302.4059	876	27.7629	3.7284	432.0517	876	27.7629	3.7284	1487.8619
877	27.7889	3.725	386.1953	877	27.7889	3.725	1323.2422	877	27.7889	3.725	444.0317	877	27.7889	3.725	1499.8534
878	27.8149	3.7216	403.8165	878	27.8149	3.7216	1338.9315	878	27.8149	3.7216	447.0299	878	27.8149	3.7216	1502.8629
879	27.8409	3.7182	380.8468	879	27.8409	3.7182	1314.0298	879	27.8409	3.7182	428.3437	879	27.8409	3.7182	1484.1881
880	27.8669	3.7148	343.7913	880	27.8669	3.7148	1275.0424	880	27.8669	3.7148	432.2385	880	27.8669	3.7148	1488.0942
881	27.8929	3.7114	338.6846	881	27.8929	3.7114	1268.0037	881	27.8929	3.7114	410.2064	881	27.8929	3.7114	1466.0735
882	27.9189	3.708	390.2558	882	27.9189	3.708	1317.643	882	27.9189	3.708	421.9091	882	27.9189	3.708	1477.7876
883	27.9449	3.7046	428.9103	883	27.9449	3.7046	1354.3655	883	27.9449	3.7046	433.4405	883	27.9449	3.7046	1489.3304
884	27.9709	3.7013	379.1124	884	27.9709	3.7013	1302.6357	884	27.9709	3.7013	382.0769	884	27.9709	3.7013	1437.9781
885	27.9969	3.6979	396.4896	885	27.9969	3.6979	1318.081	885	27.9969	3.6979	367.0107	885	27.9969	3.6979	1422.9233
886	28.0229	3.6945	384.9672	886	28.0229	3.6945	1304.6266	886	28.0229	3.6945	429.5453	886	28.0229	3.6945	1485.4693
887	28.0489	3.6912	438.9629	887	28.0489	3.6912	1356.6903	887	28.0489	3.6912	435.6983	887	28.0489	3.6912	1491.6337
888	28.0749	3.6878	413.4034	888	28.0749	3.6878	1329.1989	888	28.0749	3.6878	400.1717	888	28.0749	3.6878	1456.1184
889	28.1009	3.6845	412.5454	889	28.1009	3.6845	1326.4089	889	28.1009	3.6845	478.2413	889	28.1009	3.6845	1534.1994
890	28.1269	3.6811	404.799	890	28.1269	3.6811	1316.7306	890	28.1269	3.6811	550.5979	890	28.1269	3.6811	1606.5673
891	28.1529	3.6778	428.433	891	28.1529	3.6778	1338.4327	891	28.1529	3.6778	540.2977	891	28.1529	3.6778	1596.2785
892	28.1789	3.6745	408.41	892	28.1789	3.6745	1316.4777	892	28.1789	3.6745	515.9568	892	28.1789	3.6745	1571.949
893	28.2049	3.6712	420.6286	893	28.2049	3.6712	1326.7644	893	28.2049	3.6712	483.0456	893	28.2049	3.6712	1537.3123
894	28.2309	3.6679	461.4992	894	28.2309	3.6679	1365.7031	894	28.2309	3.6679	472.1071	894	28.2309	3.6679	1524.6485
895	28.2569	3.6645	436.4248	895	28.2569	3.6645	1338.6967	895	28.2569	3.6645	474.6477	895	28.2569	3.6645	1525.4635

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
896	28.2829	3.6612	477.1382	896	28.2829	3.6612	1377.4782	896	28.2829	3.6612	385.0599	896	28.2829	3.6612	1434.1503
897	28.3089	3.658	476.0144	897	28.3089	3.658	1374.4224	897	28.3089	3.658	476.3997	897	28.3089	3.658	1523.7647
898	28.3349	3.6547	413.9554	898	28.3349	3.6547	1310.4314	898	28.3349	3.6547	428.932	898	28.3349	3.6547	1474.5715
899	28.3609	3.6514	328.1771	899	28.3609	3.6514	1222.7212	899	28.3609	3.6514	508.1975	899	28.3609	3.6514	1552.1117
900	28.3869	3.6481	409.0267	900	28.3869	3.6481	1301.6389	900	28.3869	3.6481	422.6862	900	28.3869	3.6481	1464.8749
901	28.4129	3.6448	419.2289	901	28.4129	3.6448	1309.9092	901	28.4129	3.6448	462.3624	901	28.4129	3.6448	1502.8256
902	28.4389	3.6416	433.9119	902	28.4389	3.6416	1322.6602	902	28.4389	3.6416	527.1219	902	28.4389	3.6416	1565.8597
903	28.4649	3.6383	445.7328	903	28.4649	3.6383	1332.5492	903	28.4649	3.6383	514.0933	903	28.4649	3.6383	1551.1057
904	28.4909	3.6351	442.53	904	28.4909	3.6351	1327.4144	904	28.4909	3.6351	572.0619	904	28.4909	3.6351	1607.3488
905	28.5169	3.6318	523.4462	905	28.5169	3.6318	1406.3987	905	28.5169	3.6318	513.9472	905	28.5169	3.6318	1547.5087
906	28.5429	3.6286	442.4266	906	28.5429	3.6286	1323.4472	906	28.5429	3.6286	627.168	906	28.5429	3.6286	1659.0041
907	28.5689	3.6253	465.1936	907	28.5689	3.6253	1344.2822	907	28.5689	3.6253	580.7021	907	28.5689	3.6253	1610.8127
908	28.5949	3.6221	398.7972	908	28.5949	3.6221	1275.9539	908	28.5949	3.6221	564.6547	908	28.5949	3.6221	1593.0399
909	28.6209	3.6189	305.6817	909	28.6209	3.6189	1180.9064	909	28.6209	3.6189	648.5566	909	28.6209	3.6189	1675.2163
910	28.6469	3.6157	393.9839	910	28.6469	3.6157	1267.2766	910	28.6469	3.6157	750.11	910	28.6469	3.6157	1775.0442
911	28.6729	3.6125	464.6184	911	28.6729	3.6125	1335.9793	911	28.6729	3.6125	803.2976	911	28.6729	3.6125	1826.5064
912	28.6989	3.6093	455.1201	912	28.6989	3.6093	1324.5489	912	28.6989	3.6093	1001.5573	912	28.6989	3.6093	2023.0407
913	28.7249	3.6061	413.714	913	28.7249	3.6061	1281.2109	913	28.7249	3.6061	1077.8029	913	28.7249	3.6061	2097.5608
914	28.7509	3.6029	366.3877	914	28.7509	3.6029	1231.9527	914	28.7509	3.6029	1180.826	914	28.7509	3.6029	2198.8585
915	28.7769	3.5997	427.7456	915	28.7769	3.5997	1291.3786	915	28.7769	3.5997	1427.9662	915	28.7769	3.5997	2444.2733
916	28.8029	3.5965	380.875	916	28.8029	3.5965	1242.5761	916	28.8029	3.5965	1668.4829	916	28.8029	3.5965	2683.0646
917	28.8289	3.5933	390.0762	917	28.8289	3.5933	1249.8453	917	28.8289	3.5933	1942.4518	917	28.8289	3.5933	2955.308
918	28.8549	3.5902	405.7804	918	28.8549	3.5902	1263.6176	918	28.8549	3.5902	2503.3151	918	28.8549	3.5902	3514.4458
919	28.8809	3.587	360.0713	919	28.8809	3.587	1215.9766	919	28.8809	3.587	3002.1317	919	28.8809	3.587	4011.537
920	28.9069	3.5838	468.2514	920	28.9069	3.5838	1324.5837	920	28.9069	3.5838	3535.046	920	28.9069	3.5838	4542.7259
921	28.9329	3.5807	396.0916	921	28.9329	3.5807	1252.8509	921	28.9329	3.5807	3956.6138	921	28.9329	3.5807	4962.5683
922	28.9589	3.5775	362.136	922	28.9589	3.5775	1219.3224	922	28.9589	3.5775	4255.4565	922	28.9589	3.5775	5259.6855
923	28.9849	3.5744	379.6778	923	28.9849	3.5744	1237.2912	923	28.9849	3.5744	4525.5893	923	28.9849	3.5744	5528.0928
924	29.0109	3.5713	369.492	924	29.0109	3.5713	1227.5324	924	29.0109	3.5713	4150.5685	924	29.0109	3.5713	5151.3466
925	29.0369	3.5681	382.3368	925	29.0369	3.5681	1240.8042	925	29.0369	3.5681	3768.6761	925	29.0369	3.5681	4767.7288
926	29.0629	3.565	390.0368	926	29.0629	3.565	1248.9313	926	29.0629	3.565	3162.9449	926	29.0629	3.565	4160.2721
927	29.0889	3.5619	379.3111	927	29.0889	3.5619	1238.6326	927	29.0889	3.5619	2531.6174	927	29.0889	3.5619	3527.2192
928	29.1149	3.5588	383.4698	928	29.1149	3.5588	1243.2183	928	29.1149	3.5588	2042.7815	928	29.1149	3.5588	3036.6579
929	29.1409	3.5557	387.2008	929	29.1409	3.5557	1247.3763	929	29.1409	3.5557	1627.2909	929	29.1409	3.5557	2619.4418
930	29.1669	3.5526	376.4468	930	29.1669	3.5526	1237.0493	930	29.1669	3.5526	1358.1955	930	29.1669	3.5526	2348.6209
931	29.1929	3.5495	406.9502	931	29.1929	3.5495	1267.9798	931	29.1929	3.5495	1105.9658	931	29.1929	3.5495	2094.6658

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
932	29.2189	3.5464	391.386	932	29.2189	3.5464	1252.8426	932	29.2189	3.5464	947.3958	932	29.2189	3.5464	1934.3704
933	29.2449	3.5433	350.7622	933	29.2449	3.5433	1212.6458	933	29.2449	3.5433	787.5816	933	29.2449	3.5433	1772.8308
934	29.2709	3.5402	341.9168	934	29.2709	3.5402	1204.2275	934	29.2709	3.5402	721.2313	934	29.2709	3.5402	1704.755
935	29.2969	3.5372	329.8085	935	29.2969	3.5372	1192.5462	935	29.2969	3.5372	634.3506	935	29.2969	3.5372	1616.1489
936	29.3229	3.5341	359.5228	936	29.3229	3.5341	1222.6875	936	29.3229	3.5341	593.9194	936	29.3229	3.5341	1573.9922
937	29.3489	3.531	410.8959	937	29.3489	3.531	1274.4876	937	29.3489	3.531	576.3979	937	29.3489	3.531	1554.7453
938	29.3749	3.528	381.0013	938	29.3749	3.528	1245.02	938	29.3749	3.528	541.4543	938	29.3749	3.528	1518.0763
939	29.4009	3.5249	364.3258	939	29.4009	3.5249	1228.7716	939	29.4009	3.5249	504.4666	939	29.4009	3.5249	1479.3631
940	29.4269	3.5219	345.3211	940	29.4269	3.5219	1210.1939	940	29.4269	3.5219	518.7328	940	29.4269	3.5219	1491.9039
941	29.4529	3.5188	336.3732	941	29.4529	3.5188	1201.673	941	29.4529	3.5188	493.1908	941	29.4529	3.5188	1464.6364
942	29.4789	3.5158	362.1349	942	29.4789	3.5158	1227.8618	942	29.4789	3.5158	465.0067	942	29.4789	3.5158	1434.7269
943	29.5049	3.5128	333.6945	943	29.5049	3.5128	1199.8484	943	29.5049	3.5128	471.4565	943	29.5049	3.5128	1439.4512
944	29.5309	3.5097	342.2964	944	29.5309	3.5097	1208.8773	944	29.5309	3.5097	467.1517	944	29.5309	3.5097	1433.421
945	29.5569	3.5067	361.5255	945	29.5569	3.5067	1228.5334	945	29.5569	3.5067	432.6884	945	29.5569	3.5067	1397.2323
946	29.5829	3.5037	360.0713	946	29.5829	3.5037	1227.5063	946	29.5829	3.5037	422.169	946	29.5829	3.5037	1384.9875
947	29.6089	3.5007	415.7234	947	29.6089	3.5007	1284.2836	947	29.6089	3.5007	397.0808	947	29.6089	3.5007	1358.5515
948	29.6349	3.4977	453.7289	948	29.6349	3.4977	1323.4144	948	29.6349	3.4977	420.9211	948	29.6349	3.4977	1381.044
949	29.6609	3.4947	401.353	949	29.6609	3.4947	1272.1637	949	29.6609	3.4947	490.1878	949	29.6609	3.4947	1448.963
950	29.6869	3.4917	319.1158	950	29.6869	3.4917	1191.0517	950	29.6869	3.4917	443.6858	950	29.6869	3.4917	1401.1132
951	29.7129	3.4887	319.2206	951	29.7129	3.4887	1192.2817	951	29.7129	3.4887	397.2324	951	29.7129	3.4887	1353.312
952	29.7389	3.4857	362.5502	952	29.7389	3.4857	1236.7365	952	29.7389	3.4857	397.0652	952	29.7389	3.4857	1351.7971
953	29.7649	3.4828	371.7027	953	29.7649	3.4828	1247.0142	953	29.7649	3.4828	420.2067	953	29.7649	3.4828	1373.5909
954	29.7909	3.4798	379.6206	954	29.7909	3.4798	1256.0573	954	29.7909	3.4798	404.3356	954	29.7909	3.4798	1356.3721
955	29.8169	3.4768	388.9039	955	29.8169	3.4768	1266.4659	955	29.8169	3.4768	416.5761	955	29.8169	3.4768	1367.2648
956	29.8429	3.4739	399.8939	956	29.8429	3.4739	1278.5811	956	29.8429	3.4739	468.2401	956	29.8429	3.4739	1417.5811
957	29.8689	3.4709	368.5303	957	29.8689	3.4709	1248.3426	957	29.8689	3.4709	475.3496	957	29.8689	3.4709	1423.3428
958	29.8949	3.468	371.4379	958	29.8949	3.468	1252.3755	958	29.8949	3.468	433.0227	958	29.8949	3.468	1379.6682
959	29.9209	3.465	392.1706	959	29.9209	3.465	1274.2334	959	29.9209	3.465	410.5467	959	29.9209	3.465	1355.8444
960	29.9469	3.4621	355.7609	960	29.9469	3.4621	1238.9489	960	29.9469	3.4621	396.4942	960	29.9469	3.4621	1340.4442
961	29.9729	3.4592	364.3659	961	29.9729	3.4592	1248.6792	961	29.9729	3.4592	381.1104	961	29.9729	3.4592	1323.7126
962	29.9989	3.4562	381.7327	962	29.9989	3.4562	1267.1711	962	29.9989	3.4562	399.2102	962	29.9989	3.4562	1340.4647
963	30.0249	3.4533	376.3481	963	30.0249	3.4533	1262.9118	963	30.0249	3.4533	419.2835	963	30.0249	3.4533	1359.1902
964	30.0509	3.4504	372.9696	964	30.0509	3.4504	1260.6585	964	30.0509	3.4504	418.8649	964	30.0509	3.4504	1357.4239
965	30.0769	3.4475	346.7037	965	30.0769	3.4475	1235.5178	965	30.0769	3.4475	365.564	965	30.0769	3.4475	1302.7752
966	30.1029	3.4446	346.3351	966	30.1029	3.4446	1236.2745	966	30.1029	3.4446	340.9363	966	30.1029	3.4446	1276.7998
967	30.1289	3.4417	379.0669	967	30.1289	3.4417	1270.1314	967	30.1289	3.4417	380.1238	967	30.1289	3.4417	1314.6395

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
968	30.1549	3.4388	398.508	968	30.1549	3.4388	1290.6977	968	30.1549	3.4388	414.1343	968	30.1549	3.4388	1347.3023
969	30.1809	3.4359	410.2659	969	30.1809	3.4359	1303.5809	969	30.1809	3.4359	423.1504	969	30.1809	3.4359	1354.9706
970	30.2069	3.433	407.7068	970	30.2069	3.433	1302.147	970	30.2069	3.433	423.4742	970	30.2069	3.433	1353.9467
971	30.2329	3.4301	391.8009	971	30.2329	3.4301	1287.3663	971	30.2329	3.4301	390.0134	971	30.2329	3.4301	1319.1382
972	30.2589	3.4272	413.2202	972	30.2589	3.4272	1309.9108	972	30.2589	3.4272	406.6448	972	30.2589	3.4272	1334.4218
973	30.2849	3.4243	481.1616	973	30.2849	3.4243	1378.9774	973	30.2849	3.4243	422.169	973	30.2849	3.4243	1348.5983
974	30.3109	3.4215	504.5754	974	30.3109	3.4215	1401.4788	974	30.3109	3.4215	437.4258	974	30.3109	3.4215	1364.2408
975	30.3369	3.4186	554.1715	975	30.3369	3.4186	1450.1624	975	30.3369	3.4186	403.3044	975	30.3369	3.4186	1330.5052
976	30.3629	3.4157	611.0203	976	30.3629	3.4157	1506.0987	976	30.3629	3.4157	472.914	976	30.3629	3.4157	1400.5005
977	30.3889	3.4129	633.4658	977	30.3889	3.4129	1527.6317	977	30.3889	3.4129	507.2366	977	30.3889	3.4129	1435.2089
978	30.4149	3.41	699.6839	978	30.4149	3.41	1592.9373	978	30.4149	3.41	527.5531	978	30.4149	3.41	1455.9111
979	30.4409	3.4072	846.8431	979	30.4409	3.4072	1739.184	979	30.4409	3.4072	600.3524	979	30.4409	3.4072	1529.0962
980	30.4669	3.4044	863.731	980	30.4669	3.4044	1755.1595	980	30.4669	3.4044	580.197	980	30.4669	3.4044	1509.3265
981	30.4929	3.4015	910.4633	981	30.4929	3.4015	1800.9792	981	30.4929	3.4015	678.987	981	30.4929	3.4015	1608.5023
982	30.5189	3.3987	971.4872	982	30.5189	3.3987	1861.0906	982	30.5189	3.3987	709.794	982	30.5189	3.3987	1639.695
983	30.5449	3.3959	1043.0275	983	30.5449	3.3959	1931.7185	983	30.5449	3.3959	644.0279	983	30.5449	3.3959	1574.3147
984	30.5709	3.3931	1023.4672	984	30.5709	3.3931	1911.2457	984	30.5709	3.3931	588.8781	984	30.5709	3.3931	1519.5506
985	30.5969	3.3902	985.6666	985	30.5969	3.3902	1872.5326	985	30.5969	3.3902	542.945	985	30.5969	3.3902	1474.0033
986	30.6229	3.3874	1019.1175	986	30.6229	3.3874	1905.071	986	30.6229	3.3874	435.6726	986	30.6229	3.3874	1367.1166
987	30.6489	3.3846	965.8815	987	30.6489	3.3846	1850.9226	987	30.6489	3.3846	441.8733	987	30.6489	3.3846	1373.7031
988	30.6749	3.3818	842.0008	988	30.6749	3.3818	1726.1294	988	30.6749	3.3818	399.4992	988	30.6749	3.3818	1331.7148
989	30.7009	3.379	732.5033	989	30.7009	3.379	1615.7193	989	30.7009	3.379	436.5955	989	30.7009	3.379	1369.1968
990	30.7269	3.3762	678.4713	990	30.7269	3.3762	1560.7749	990	30.7269	3.3762	434.7707	990	30.7269	3.3762	1367.7578
991	30.7529	3.3735	572.2629	991	30.7529	3.3735	1453.654	991	30.7529	3.3735	435.5969	991	30.7529	3.3735	1368.9697
992	30.7789	3.3707	573.4968	992	30.7789	3.3707	1453.9754	992	30.7789	3.3707	472.8808	992	30.7789	3.3707	1406.6394
993	30.8049	3.3679	514.2768	993	30.8049	3.3679	1393.8429	993	30.8049	3.3679	413.8671	993	30.8049	3.3679	1348.0114
994	30.8309	3.3651	498.0113	994	30.8309	3.3651	1376.6649	994	30.8309	3.3651	467.6544	994	30.8309	3.3651	1402.1844
995	30.8569	3.3624	410.1603	995	30.8569	3.3624	1287.9014	995	30.8569	3.3624	535.1035	995	30.8569	3.3624	1470.0193
996	30.8829	3.3596	461.7945	996	30.8829	3.3596	1338.6231	996	30.8829	3.3596	555.6082	996	30.8829	3.3596	1490.9098
997	30.9089	3.3568	544.579	997	30.9089	3.3568	1420.4951	997	30.9089	3.3568	567.6083	997	30.9089	3.3568	1503.2956
998	30.9349	3.3541	468.9915	998	30.9349	3.3541	1343.9951	998	30.9349	3.3541	559.2401	998	30.9349	3.3541	1495.3131
999	30.9609	3.3513	550.6651	999	30.9609	3.3513	1424.7563	999	30.9609	3.3513	539.7604	999	30.9609	3.3513	1476.2192
1000	30.9869	3.3486	525.1254	1000	30.9869	3.3486	1398.3041	1000	30.9869	3.3486	568.3668	1000	30.9869	3.3486	1505.2113
1001	31.0129	3.3459	467.744	1001	31.0129	3.3459	1340.0102	1001	31.0129	3.3459	570.5586	1001	31.0129	3.3459	1505.0816
1002	31.0389	3.3431	478.3416	1002	31.0389	3.3431	1349.6953	1002	31.0389	3.3431	670.3577	1002	31.0389	3.3431	1602.5591
1003	31.0649	3.3404	446.3437	1003	31.0649	3.3404	1316.7849	1003	31.0649	3.3404	693.1944	1003	31.0649	3.3404	1623.0742

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1004	31.0909	3.3377	430.8271	1004	31.0909	3.3377	1300.3558	1004	31.0909	3.3377	685.6194	1004	31.0909	3.3377	1613.1776
1005	31.1169	3.3349	491.5025	1005	31.1169	3.3349	1360.1187	1005	31.1169	3.3349	793.2347	1005	31.1169	3.3349	1718.4712
1006	31.1429	3.3322	323.0445	1006	31.1429	3.3322	1190.7482	1006	31.1429	3.3322	858.928	1006	31.1429	3.3322	1781.8429
1007	31.1689	3.3295	486.2823	1007	31.1689	3.3295	1353.0736	1007	31.1689	3.3295	892.2059	1007	31.1689	3.3295	1812.7992
1008	31.1949	3.3268	383.5255	1008	31.1949	3.3268	1249.4043	1008	31.1949	3.3268	993.7664	1008	31.1949	3.3268	1912.0381
1009	31.2209	3.3241	432.9518	1009	31.2209	3.3241	1297.9181	1009	31.2209	3.3241	1240.6372	1009	31.2209	3.3241	2156.5873
1010	31.2469	3.3214	385.5143	1010	31.2469	3.3214	1249.5681	1010	31.2469	3.3214	1393.6094	1010	31.2469	3.3214	2307.2378
1011	31.2729	3.3187	438.6969	1011	31.2729	3.3187	1301.8382	1011	31.2729	3.3187	1642.3143	1011	31.2729	3.3187	2553.6211
1012	31.2989	3.316	374.909	1012	31.2989	3.316	1237.1378	1012	31.2989	3.316	1823.3874	1012	31.2989	3.316	2732.3726
1013	31.3249	3.3134	493.5137	1013	31.3249	3.3134	1354.83	1013	31.3249	3.3134	2211.9164	1013	31.3249	3.3134	3118.5801
1014	31.3509	3.3107	510.0321	1014	31.3509	3.3107	1370.4359	1014	31.3509	3.3107	2768.5809	1014	31.3509	3.3107	3672.9229
1015	31.3769	3.308	442.9766	1015	31.3769	3.308	1302.4679	1015	31.3769	3.308	3280.6428	1015	31.3769	3.308	4182.6632
1016	31.4029	3.3053	401.3373	1016	31.4029	3.3053	1259.9162	1016	31.4029	3.3053	3931.0729	1016	31.4029	3.3053	4830.7717
1017	31.4289	3.3027	432.4158	1017	31.4289	3.3027	1290.0822	1017	31.4289	3.3027	4739.6761	1017	31.4289	3.3027	5637.0533
1018	31.4549	3.3	488.9698	1018	31.4549	3.3	1345.7237	1018	31.4549	3.3	5679.7937	1018	31.4549	3.3	6574.8493
1019	31.4809	3.2973	472.6809	1019	31.4809	3.2973	1328.5223	1019	31.4809	3.2973	6376.1627	1019	31.4809	3.2973	7268.8967
1020	31.5069	3.2947	455.955	1020	31.5069	3.2947	1310.8839	1020	31.5069	3.2947	6678.6646	1020	31.5069	3.2947	7569.077
1021	31.5329	3.292	429.485	1021	31.5329	3.292	1283.5014	1021	31.5329	3.292	6765.3027	1021	31.5329	3.292	7653.3935
1022	31.5589	3.2894	509.4833	1022	31.5589	3.2894	1362.5872	1022	31.5589	3.2894	6392.7216	1022	31.5589	3.2894	7278.4907
1023	31.5849	3.2868	515.0738	1023	31.5849	3.2868	1367.2652	1023	31.5849	3.2868	5694.7086	1023	31.5849	3.2868	6578.1561
1024	31.6109	3.2841	549.5503	1024	31.6109	3.2841	1400.8293	1024	31.6109	3.2841	4923.3217	1024	31.6109	3.2841	5804.4477
1025	31.6369	3.2815	618.7619	1025	31.6369	3.2815	1469.1284	1025	31.6369	3.2815	4094.3987	1025	31.6369	3.2815	4973.203
1026	31.6629	3.2789	600.0193	1026	31.6629	3.2789	1449.4733	1026	31.6629	3.2789	3341.5983	1026	31.6629	3.2789	4218.081
1027	31.6889	3.2763	617.4109	1027	31.6889	3.2763	1465.9524	1027	31.6889	3.2763	2675.8186	1027	31.6889	3.2763	3549.9796
1028	31.7149	3.2736	665.0892	1028	31.7149	3.2736	1510.6805	1028	31.7149	3.2736	2227.9501	1028	31.7149	3.2736	3099.7895
1029	31.7409	3.271	627.7661	1029	31.7409	3.271	1470.4072	1029	31.7409	3.271	1820.5306	1029	31.7409	3.271	2690.0485
1030	31.7669	3.2684	674.3963	1030	31.7669	3.2684	1514.0872	1030	31.7669	3.2684	1458.5777	1030	31.7669	3.2684	2325.7739
1031	31.7929	3.2658	632.1963	1031	31.7929	3.2658	1468.937	1031	31.7929	3.2658	1214.5169	1031	31.7929	3.2658	2079.3915
1032	31.8189	3.2632	674.428	1032	31.8189	3.2632	1508.2185	1032	31.8189	3.2632	1019.0444	1032	31.8189	3.2632	1881.5974
1033	31.8449	3.2606	631.8237	1033	31.8449	3.2606	1462.6641	1033	31.8449	3.2606	888.5861	1033	31.8449	3.2606	1748.8175
1034	31.8709	3.258	606.8569	1034	31.8709	3.258	1434.747	1034	31.8709	3.258	868.3421	1034	31.8709	3.258	1726.2519
1035	31.8969	3.2554	501.1901	1035	31.8969	3.2554	1326.13	1035	31.8969	3.2554	814.6646	1035	31.8969	3.2554	1670.2527
1036	31.9229	3.2529	518.1401	1036	31.9229	3.2529	1340.1299	1036	31.9229	3.2529	769.7076	1036	31.9229	3.2529	1622.9742
1037	31.9489	3.2503	541.4014	1037	31.9489	3.2503	1360.441	1037	31.9489	3.2503	686.402	1037	31.9489	3.2503	1537.347
1038	31.9749	3.2477	465.3254	1038	31.9749	3.2477	1281.4147	1038	31.9749	3.2477	639.4803	1038	31.9749	3.2477	1488.1037
1039	32.0009	3.2451	453.3773	1039	32.0009	3.2451	1266.5165	1039	32.0009	3.2451	647.7115	1039	32.0009	3.2451	1494.0132

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1040	32.0269	3.2426	371.2521	1040	32.0269	3.2426	1181.4411	1040	32.0269	3.2426	614.5756	1040	32.0269	3.2426	1458.5557
1041	32.0529	3.24	338.2077	1041	32.0529	3.24	1145.4465	1041	32.0529	3.24	562.2582	1041	32.0529	3.24	1403.9168
1042	32.0789	3.2374	347.7368	1042	32.0789	3.2374	1152.0254	1042	32.0789	3.2374	582.5495	1042	32.0789	3.2374	1421.8865
1043	32.1049	3.2349	326.2227	1043	32.1049	3.2349	1127.5612	1043	32.1049	3.2349	522.6682	1043	32.1049	3.2349	1359.6835
1044	32.1309	3.2323	336.4453	1044	32.1309	3.2323	1134.8336	1044	32.1309	3.2323	505.1399	1044	32.1309	3.2323	1339.8336
1045	32.1569	3.2298	360.82	1045	32.1569	3.2298	1156.258	1045	32.1569	3.2298	526.3214	1045	32.1569	3.2298	1358.6935
1046	32.1829	3.2273	369.5122	1046	32.1829	3.2273	1162	1046	32.1829	3.2273	503.9141	1046	32.1829	3.2273	1333.9646
1047	32.2089	3.2247	376.8113	1047	32.2089	3.2247	1166.349	1047	32.2089	3.2247	520.9565	1047	32.2089	3.2247	1348.6854
1048	32.2349	3.2222	335.9492	1048	32.2349	3.2222	1122.5367	1048	32.2349	3.2222	477.7886	1048	32.2349	3.2222	1303.1959
1049	32.2609	3.2197	332.8188	1049	32.2609	3.2197	1116.4561	1049	32.2609	3.2197	469.5877	1049	32.2609	3.2197	1292.6733
1050	32.2869	3.2171	351.9045	1050	32.2869	3.2171	1132.5915	1050	32.2869	3.2171	486.3208	1050	32.2869	3.2171	1307.0848
1051	32.3129	3.2146	419.2383	1051	32.3129	3.2146	1196.9752	1051	32.3129	3.2146	481.6496	1051	32.3129	3.2146	1300.092
1052	32.3389	3.2121	420.193	1052	32.3389	3.2121	1194.9797	1052	32.3389	3.2121	493.8843	1052	32.3389	3.2121	1310.0051
1053	32.3649	3.2096	394.4662	1053	32.3649	3.2096	1166.3027	1053	32.3649	3.2096	483.2926	1053	32.3649	3.2096	1297.0918
1054	32.3909	3.2071	360.0713	1054	32.3909	3.2071	1128.9576	1054	32.3909	3.2071	422.169	1054	32.3909	3.2071	1233.6466
1055	32.4169	3.2046	359.4976	1055	32.4169	3.2046	1128.1399	1055	32.4169	3.2046	421.4813	1055	32.4169	3.2046	1232.3075
1056	32.4429	3.2021	346.575	1056	32.4429	3.2021	1114.9735	1056	32.4429	3.2021	450.6972	1056	32.4429	3.2021	1260.8721
1057	32.4689	3.1996	315.0661	1057	32.4689	3.1996	1083.2206	1057	32.4689	3.1996	437.9911	1057	32.4689	3.1996	1247.5147
1058	32.4949	3.1971	360.5482	1058	32.4949	3.1971	1128.4588	1058	32.4949	3.1971	449.6375	1058	32.4949	3.1971	1258.5097
1059	32.5209	3.1946	392.8045	1059	32.5209	3.1946	1160.4712	1059	32.5209	3.1946	435.1219	1059	32.5209	3.1946	1243.3428
1060	32.5469	3.1921	379.6852	1060	32.5469	3.1921	1147.1079	1060	32.5469	3.1921	430.4603	1060	32.5469	3.1921	1238.0298
1061	32.5729	3.1896	377.6449	1061	32.5729	3.1896	1144.8237	1061	32.5729	3.1896	457.2581	1061	32.5729	3.1896	1264.1763
1062	32.5989	3.1872	355.6631	1062	32.5989	3.1872	1122.598	1062	32.5989	3.1872	428.1659	1062	32.5989	3.1872	1234.4327
1063	32.6249	3.1847	350.7479	1063	32.6249	3.1847	1117.4389	1063	32.6249	3.1847	415.7227	1063	32.6249	3.1847	1221.3383
1064	32.6509	3.1822	386.4368	1064	32.6509	3.1822	1152.8838	1064	32.6509	3.1822	432.5832	1064	32.6509	3.1822	1237.5474
1065	32.6769	3.1798	380.0738	1065	32.6769	3.1798	1146.2769	1065	32.6769	3.1798	416.7506	1065	32.6769	3.1798	1221.0635
1066	32.7029	3.1773	368.2339	1066	32.7029	3.1773	1134.1931	1066	32.7029	3.1773	419.4092	1066	32.7029	3.1773	1223.0707
1067	32.7289	3.1749	363.0225	1067	32.7289	3.1749	1128.7378	1067	32.7289	3.1749	432.0764	1067	32.7289	3.1749	1235.0866
1068	32.7549	3.1724	341.9866	1068	32.7549	3.1724	1107.4579	1068	32.7549	3.1724	418.7253	1068	32.7549	3.1724	1221.0841
1069	32.7809	3.17	329.7277	1069	32.7809	3.17	1094.9551	1069	32.7809	3.17	448.4122	1069	32.7809	3.17	1250.1197
1070	32.8069	3.1675	313.5482	1070	32.8069	3.1675	1078.5317	1070	32.8069	3.1675	465.0824	1070	32.8069	3.1675	1266.1386
1071	32.8329	3.1651	290.3829	1071	32.8329	3.1651	1055.1224	1071	32.8329	3.1651	454.3615	1071	32.8329	3.1651	1254.7663
1072	32.8589	3.1626	292.7781	1072	32.8589	3.1626	1057.2738	1072	32.8589	3.1626	446.1694	1072	32.8589	3.1626	1245.9229
1073	32.8849	3.1602	329.4749	1073	32.8849	3.1602	1093.7266	1073	32.8849	3.1602	439.707	1073	32.8849	3.1602	1238.8092
1074	32.9109	3.1578	316.5036	1074	32.9109	3.1578	1080.5114	1074	32.9109	3.1578	427.5119	1074	32.9109	3.1578	1225.9627
1075	32.9369	3.1554	307.409	1075	32.9369	3.1554	1071.1729	1075	32.9369	3.1554	376.6351	1075	32.9369	3.1554	1174.4346

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1076	32.9629	3.1529	314.4643	1076	32.9629	3.1529	1077.9842	1076	32.9629	3.1529	383.1848	1076	32.9629	3.1529	1180.3329
1077	32.9889	3.1505	288.2894	1077	32.9889	3.1505	1051.5654	1077	32.9889	3.1505	381.856	1077	32.9889	3.1505	1178.3528
1078	33.0149	3.1481	319.0684	1078	33.0149	3.1481	1082.1006	1078	33.0149	3.1481	382.723	1078	33.0149	3.1481	1178.5685
1079	33.0409	3.1457	294.1208	1079	33.0409	3.1457	1056.909	1079	33.0409	3.1457	391.0586	1079	33.0409	3.1457	1186.2528
1080	33.0669	3.1433	357.9203	1080	33.0669	3.1433	1120.4646	1080	33.0669	3.1433	403.5141	1080	33.0669	3.1433	1198.0569
1081	33.0929	3.1409	360.0713	1081	33.0929	3.1409	1122.3716	1081	33.0929	3.1409	422.169	1081	33.0929	3.1409	1216.0605
1082	33.1189	3.1385	315.6579	1082	33.1189	3.1385	1079.5059	1082	33.1189	3.1385	451.7404	1082	33.1189	3.1385	1245.438
1083	33.1449	3.1361	289.2275	1083	33.1449	3.1361	1054.6233	1083	33.1449	3.1361	426.6515	1083	33.1449	3.1361	1220.1552
1084	33.1709	3.1337	307.743	1084	33.1709	3.1337	1074.6865	1084	33.1709	3.1337	380.4027	1084	33.1709	3.1337	1173.7126
1085	33.1969	3.1313	352.2698	1085	33.1969	3.1313	1120.761	1085	33.1969	3.1313	360.9395	1085	33.1969	3.1313	1154.0556
1086	33.2229	3.129	250.2581	1086	33.2229	3.129	1020.2971	1086	33.2229	3.129	322.718	1086	33.2229	3.129	1115.6402
1087	33.2489	3.1266	257.8572	1087	33.2489	3.1266	1029.4439	1087	33.2489	3.1266	343.979	1087	33.2489	3.1266	1136.7073
1088	33.2749	3.1242	295.6511	1088	33.2749	3.1242	1068.7855	1088	33.2749	3.1242	395.034	1088	33.2749	3.1242	1187.5685
1089	33.3009	3.1218	288.2042	1089	33.3009	3.1218	1062.8864	1089	33.3009	3.1218	383.6821	1089	33.3009	3.1218	1176.0227
1090	33.3269	3.1195	269.6895	1090	33.3269	3.1195	1045.9194	1090	33.3269	3.1195	390.5779	1090	33.3269	3.1195	1182.7247
1091	33.3529	3.1171	292.7821	1091	33.3529	3.1171	1070.5597	1091	33.3529	3.1171	395.0284	1091	33.3529	3.1171	1186.9814
1092	33.3789	3.1147	350.1703	1092	33.3789	3.1147	1129.4956	1092	33.3789	3.1147	369.3095	1092	33.3789	3.1147	1161.0686
1093	33.4049	3.1124	351.7736	1093	33.4049	3.1124	1132.6466	1093	33.4049	3.1124	400.029	1093	33.4049	3.1124	1191.5943
1094	33.4309	3.11	294.0444	1094	33.4309	3.11	1076.4651	1094	33.4309	3.11	429.2904	1094	33.4309	3.11	1220.6618
1095	33.4569	3.1077	347.0559	1095	33.4569	3.1077	1131.0243	1095	33.4569	3.1077	408.5777	1095	33.4569	3.1077	1199.7552
1096	33.4829	3.1053	295.3768	1096	33.4829	3.1053	1080.8929	1096	33.4829	3.1053	418.1267	1096	33.4829	3.1053	1209.1104
1097	33.5089	3.103	288.0801	1097	33.5089	3.103	1075.1439	1097	33.5089	3.103	379.4672	1097	33.5089	3.103	1170.257
1098	33.5349	3.1007	382.853	1098	33.5349	3.1007	1171.4646	1098	33.5349	3.1007	418.9394	1098	33.5349	3.1007	1209.5354
1099	33.5609	3.0983	362.7886	1099	33.5609	3.0983	1152.9479	1099	33.5609	3.0983	436.2808	1099	33.5609	3.0983	1226.6829
1100	33.5869	3.096	367.7666	1100	33.5869	3.096	1159.4736	1100	33.5869	3.096	416.1239	1100	33.5869	3.096	1206.3322
1101	33.6129	3.0937	348.3261	1101	33.6129	3.0937	1141.5809	1101	33.6129	3.0937	416.6529	1101	33.6129	3.0937	1206.6673
1102	33.6389	3.0914	314.0509	1102	33.6389	3.0914	1108.8534	1102	33.6389	3.0914	487.1972	1102	33.6389	3.0914	1277.0178
1103	33.6649	3.089	353.6115	1103	33.6649	3.089	1149.9617	1103	33.6649	3.089	480.624	1103	33.6649	3.089	1270.2507
1104	33.6909	3.0867	270.8933	1104	33.6909	3.0867	1068.7912	1104	33.6909	3.0867	550.4974	1104	33.6909	3.0867	1339.9303
1105	33.7169	3.0844	353.2559	1105	33.7169	3.0844	1152.7016	1105	33.7169	3.0844	463.9368	1105	33.7169	3.0844	1253.1758
1106	33.7429	3.0821	406.4644	1106	33.7429	3.0821	1207.4577	1106	33.7429	3.0821	446.2734	1106	33.7429	3.0821	1235.3185
1107	33.7689	3.0798	365.1713	1107	33.7689	3.0798	1167.7123	1107	33.7689	3.0798	427.9411	1107	33.7689	3.0798	1216.7924
1108	33.7949	3.0775	427.4466	1108	33.7949	3.0775	1231.5354	1108	33.7949	3.0775	422.169	1108	33.7949	3.0775	1210.8265
1109	33.8209	3.0752	399.8229	1109	33.8209	3.0752	1203.1403	1109	33.8209	3.0752	535.1391	1109	33.8209	3.0752	1322.8658
1110	33.8469	3.0729	423.366	1110	33.8469	3.0729	1225.9121	1110	33.8469	3.0729	514.2881	1110	33.8469	3.0729	1301.0841
1111	33.8729	3.0706	434.0878	1111	33.8729	3.0706	1235.8626	1111	33.8729	3.0706	489.4921	1111	33.8729	3.0706	1275.3574

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1112	33.8989	3.0683	438.9019	1112	33.8989	3.0683	1239.9053	1112	33.8989	3.0683	547.6691	1112	33.8989	3.0683	1332.6036
1113	33.9249	3.066	518.0472	1113	33.9249	3.066	1318.2793	1113	33.9249	3.066	558.6939	1113	33.9249	3.066	1342.6977
1114	33.9509	3.0638	517.7133	1114	33.9509	3.0638	1317.174	1114	33.9509	3.0638	614.4468	1114	33.9509	3.0638	1397.5198
1115	33.9769	3.0615	586.4633	1115	33.9769	3.0615	1385.1528	1115	33.9769	3.0615	661.3997	1115	33.9769	3.0615	1443.542
1116	34.0029	3.0592	644.4706	1116	34.0029	3.0592	1442.3887	1116	34.0029	3.0592	709.7473	1116	34.0029	3.0592	1490.9589
1117	34.0289	3.057	749.8659	1117	34.0289	3.057	1547.0126	1117	34.0289	3.057	713.7192	1117	34.0289	3.057	1494
1118	34.0549	3.0547	861.3061	1118	34.0549	3.0547	1657.6815	1118	34.0549	3.0547	894.3425	1118	34.0549	3.0547	1673.6926
1119	34.0809	3.0524	1035.5406	1119	34.0809	3.0524	1831.1447	1119	34.0809	3.0524	1104.7454	1119	34.0809	3.0524	1883.1648
1120	34.1069	3.0502	1352.75	1120	34.1069	3.0502	2147.5828	1120	34.1069	3.0502	1239.4246	1120	34.1069	3.0502	2016.9132
1121	34.1329	3.0479	1845.6472	1121	34.1329	3.0479	2639.7087	1121	34.1329	3.0479	1635.753	1121	34.1329	3.0479	2412.3109
1122	34.1589	3.0457	2670.4269	1122	34.1589	3.0457	3463.7171	1122	34.1589	3.0457	2246.7233	1122	34.1589	3.0457	3022.3504
1123	34.1849	3.0434	3864.2003	1123	34.1849	3.0434	4656.7191	1123	34.1849	3.0434	3128.4522	1123	34.1849	3.0434	3903.1487
1124	34.2109	3.0412	5352.2986	1124	34.2109	3.0412	6144.0461	1124	34.2109	3.0412	4811.6002	1124	34.2109	3.0412	5585.3659
1125	34.2369	3.0389	6531.369	1125	34.2369	3.0389	7322.3451	1125	34.2369	3.0389	7038.0012	1125	34.2369	3.0389	7810.8361
1126	34.2629	3.0367	7915.7058	1126	34.2629	3.0367	8705.9106	1126	34.2629	3.0367	9387.8323	1126	34.2629	3.0367	10159.7365
1127	34.2889	3.0345	9295.997	1127	34.2889	3.0345	10085.4305	1127	34.2889	3.0345	11501.3611	1127	34.2889	3.0345	12272.3345
1128	34.3149	3.0322	10231.9128	1128	34.3149	3.0322	11020.575	1128	34.3149	3.0322	12167.7308	1128	34.3149	3.0322	12937.7735
1129	34.3409	3.03	10928.4297	1129	34.3409	3.03	11716.3205	1129	34.3409	3.03	12162.5838	1129	34.3409	3.03	12931.6958
1130	34.3669	3.0278	10808.1905	1130	34.3669	3.0278	11595.31	1130	34.3669	3.0278	11234.0114	1130	34.3669	3.0278	12002.1927
1131	34.3929	3.0256	9933.4203	1131	34.3929	3.0256	10719.7685	1131	34.3929	3.0256	9773.979	1131	34.3929	3.0256	10541.2295
1132	34.4189	3.0233	8637.2716	1132	34.4189	3.0233	9422.8485	1132	34.4189	3.0233	8027.9256	1132	34.4189	3.0233	8794.2454
1133	34.4449	3.0211	7519.9916	1133	34.4449	3.0211	8304.7971	1133	34.4449	3.0211	6338.2699	1133	34.4449	3.0211	7103.6589
1134	34.4709	3.0189	6491.3918	1134	34.4709	3.0189	7275.426	1134	34.4709	3.0189	4911.2654	1134	34.4709	3.0189	5675.7237
1135	34.4969	3.0167	5781.6432	1135	34.4969	3.0167	6564.9061	1135	34.4969	3.0167	3913.1492	1135	34.4969	3.0167	4676.6767
1136	34.5229	3.0145	5414.1693	1136	34.5229	3.0145	6196.6608	1136	34.5229	3.0145	3097.3684	1136	34.5229	3.0145	3859.9652
1137	34.5489	3.0123	5616.7528	1137	34.5489	3.0123	6398.473	1137	34.5489	3.0123	2324.6485	1137	34.5489	3.0123	3086.3146
1138	34.5749	3.0101	6133.386	1138	34.5749	3.0101	6914.3348	1138	34.5749	3.0101	1805.6543	1138	34.5749	3.0101	2566.3897
1139	34.6009	3.0079	6847.6903	1139	34.6009	3.0079	7627.8678	1139	34.6009	3.0079	1401.8229	1139	34.6009	3.0079	2161.6276
1140	34.6269	3.0057	7574.3291	1140	34.6269	3.0057	8353.7353	1140	34.6269	3.0057	1108.0064	1140	34.6269	3.0057	1866.8803
1141	34.6529	3.0036	8220.0431	1141	34.6529	3.0036	8998.678	1141	34.6529	3.0036	922.5716	1141	34.6529	3.0036	1680.5147
1142	34.6789	3.0014	8379.1673	1142	34.6789	3.0014	9157.0308	1142	34.6789	3.0014	768.116	1142	34.6789	3.0014	1525.1284
1143	34.7049	2.9992	8399.6886	1143	34.7049	2.9992	9176.7808	1143	34.7049	2.9992	749.0117	1143	34.7049	2.9992	1505.0934
1144	34.7309	2.997	8163.0571	1144	34.7309	2.997	8939.378	1144	34.7309	2.997	701.6024	1144	34.7309	2.997	1456.7533
1145	34.7569	2.9948	7588.9025	1145	34.7569	2.9948	8364.452	1145	34.7569	2.9948	625.0059	1145	34.7569	2.9948	1379.2261
1146	34.7829	2.9927	6689.5216	1146	34.7829	2.9927	7464.2998	1146	34.7829	2.9927	587.6531	1146	34.7829	2.9927	1340.9425
1147	34.8089	2.9905	5757.1362	1147	34.8089	2.9905	6531.1431	1147	34.8089	2.9905	585.0446	1147	34.8089	2.9905	1337.4034

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1148	34.8349	2.9883	4785.107	1148	34.8349	2.9883	5558.3426	1148	34.8349	2.9883	540.2798	1148	34.8349	2.9883	1291.7078
1149	34.8609	2.9862	3769.1435	1149	34.8609	2.9862	4541.6077	1149	34.8609	2.9862	547.446	1149	34.8609	2.9862	1297.9433
1150	34.8869	2.984	2992.5584	1150	34.8869	2.984	3764.2513	1150	34.8869	2.984	555.852	1150	34.8869	2.984	1305.4186
1151	34.9129	2.9819	2381.156	1151	34.9129	2.9819	3152.0776	1151	34.9129	2.9819	498.0364	1151	34.9129	2.9819	1246.6722
1152	34.9389	2.9797	1856.0357	1152	34.9389	2.9797	2626.186	1152	34.9389	2.9797	485.5754	1152	34.9389	2.9797	1233.2804
1153	34.9649	2.9776	1373.5702	1153	34.9649	2.9776	2142.9491	1153	34.9649	2.9776	497.239	1153	34.9649	2.9776	1244.0134
1154	34.9909	2.9754	1060.2246	1154	34.9909	2.9754	1828.8322	1154	34.9909	2.9754	498.514	1154	34.9909	2.9754	1244.3576
1155	35.0169	2.9733	818.9105	1155	35.0169	2.9733	1586.7467	1155	35.0169	2.9733	511.9813	1155	35.0169	2.9733	1256.8941
1156	35.0429	2.9712	649.2319	1156	35.0429	2.9712	1416.2969	1156	35.0429	2.9712	510.7626	1156	35.0429	2.9712	1254.7447
1157	35.0689	2.969	628.2433	1157	35.0689	2.969	1394.5369	1157	35.0689	2.969	499.7696	1157	35.0689	2.969	1242.821
1158	35.0949	2.9669	594.8453	1158	35.0949	2.9669	1360.3676	1158	35.0949	2.9669	476.5631	1158	35.0949	2.9669	1218.6838
1159	35.1209	2.9648	496.0708	1159	35.1209	2.9648	1260.8217	1159	35.1209	2.9648	451.6903	1159	35.1209	2.9648	1192.8802
1160	35.1469	2.9626	444.5211	1160	35.1469	2.9626	1208.5007	1160	35.1469	2.9626	485.7457	1160	35.1469	2.9626	1226.0049
1161	35.1729	2.9605	432.6565	1161	35.1729	2.9605	1195.8648	1161	35.1729	2.9605	520.28	1161	35.1729	2.9605	1259.6085
1162	35.1989	2.9584	417.9246	1162	35.1989	2.9584	1180.3615	1162	35.1989	2.9584	500.7155	1162	35.1989	2.9584	1239.1132
1163	35.2249	2.9563	431.2376	1163	35.2249	2.9563	1190.5841	1163	35.2249	2.9563	498.2747	1163	35.2249	2.9563	1234.2871
1164	35.2509	2.9542	408.1365	1164	35.2509	2.9542	1164.3927	1164	35.2509	2.9542	527.1841	1164	35.2509	2.9542	1260.8112
1165	35.2769	2.9521	361.9243	1165	35.2769	2.9521	1115.0901	1165	35.2769	2.9521	513.7761	1165	35.2769	2.9521	1245.0179
1166	35.3029	2.95	350.7219	1166	35.3029	2.95	1100.7974	1166	35.3029	2.95	466.5708	1166	35.3029	2.95	1195.4273
1167	35.3289	2.9479	346.7089	1167	35.3289	2.9479	1093.6939	1167	35.3289	2.9479	445.1942	1167	35.3289	2.9479	1171.6654
1168	35.3549	2.9458	353.7811	1168	35.3549	2.9458	1097.6757	1168	35.3549	2.9458	398.5766	1168	35.3549	2.9458	1122.6625
1169	35.3809	2.9437	379.6432	1169	35.3809	2.9437	1120.4475	1169	35.3809	2.9437	390.0895	1169	35.3809	2.9437	1111.7901
1170	35.4069	2.9416	401.497	1170	35.4069	2.9416	1139.2109	1170	35.4069	2.9416	439.8704	1170	35.4069	2.9416	1159.1857
1171	35.4329	2.9395	362.339	1171	35.4329	2.9395	1096.9625	1171	35.4329	2.9395	413.306	1171	35.4329	2.9395	1130.236
1172	35.4589	2.9374	295.8487	1172	35.4589	2.9374	1027.3819	1172	35.4589	2.9374	391.7892	1172	35.4589	2.9374	1106.3339
1173	35.4849	2.9353	324.8026	1173	35.4849	2.9353	1053.2454	1173	35.4849	2.9353	421.0232	1173	35.4849	2.9353	1133.1826
1174	35.5109	2.9332	362.3713	1174	35.5109	2.9332	1087.7237	1174	35.5109	2.9332	447.7252	1174	35.5109	2.9332	1157.4993
1175	35.5369	2.9312	371.8253	1175	35.5369	2.9312	1094.0873	1175	35.5369	2.9312	453.0116	1175	35.5369	2.9312	1160.4004
1176	35.5629	2.9291	349.6784	1176	35.5629	2.9291	1068.85	1176	35.5629	2.9291	475.1704	1176	35.5629	2.9291	1180.1739
1177	35.5889	2.927	372.5581	1177	35.5889	2.927	1088.6394	1177	35.5889	2.927	422.6274	1177	35.5889	2.927	1125.2456
1178	35.6149	2.9249	396.2603	1178	35.6149	2.9249	1109.2512	1178	35.6149	2.9249	381.9142	1178	35.6149	2.9249	1082.1471
1179	35.6409	2.9229	387.584	1179	35.6409	2.9229	1097.4845	1179	35.6409	2.9229	477.0717	1179	35.6409	2.9229	1174.9192
1180	35.6669	2.9208	336.0176	1180	35.6669	2.9208	1042.8277	1180	35.6669	2.9208	475.0439	1180	35.6669	2.9208	1170.5062
1181	35.6929	2.9188	379.4038	1181	35.6929	2.9188	1083.1236	1181	35.6929	2.9188	444.7988	1181	35.6929	2.9188	1137.8758
1182	35.7189	2.9167	323.2653	1182	35.7189	2.9167	1023.8947	1182	35.7189	2.9167	468.2807	1182	35.7189	2.9167	1158.9724
1183	35.7449	2.9147	277.7913	1183	35.7449	2.9147	975.3303	1183	35.7449	2.9147	452.8582	1183	35.7449	2.9147	1141.1646

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1184	35.7709	2.9126	310.1229	1184	35.7709	2.9126	1004.5716	1184	35.7709	2.9126	391.7216	1184	35.7709	2.9126	1077.6426
1185	35.7969	2.9106	335.5341	1185	35.7969	2.9106	1026.8924	1185	35.7969	2.9106	413.1688	1185	35.7969	2.9106	1096.7046
1186	35.8229	2.9085	375.5125	1186	35.8229	2.9085	1063.7804	1186	35.8229	2.9085	467.3991	1186	35.8229	2.9085	1148.5496
1187	35.8489	2.9065	336.8768	1187	35.8489	2.9065	1022.0543	1187	35.8489	2.9065	417.6117	1187	35.8489	2.9065	1096.3769
1188	35.8749	2.9044	365.2459	1188	35.8749	2.9044	1047.333	1188	35.8749	2.9044	479.7297	1188	35.8749	2.9044	1156.1096
1189	35.9009	2.9024	360.0713	1189	35.9009	2.9024	1039.068	1189	35.9009	2.9024	422.169	1189	35.9009	2.9024	1096.1636
1190	35.9269	2.9004	388.2215	1190	35.9269	2.9004	1067.3808	1190	35.9269	2.9004	467.4337	1190	35.9269	2.9004	1142.1665
1191	35.9529	2.8983	388.992	1191	35.9529	2.8983	1068.3139	1191	35.9529	2.8983	449.9473	1191	35.9529	2.8983	1125.4183
1192	35.9789	2.8963	412.2135	1192	35.9789	2.8963	1091.698	1192	35.9789	2.8963	422.87	1192	35.9789	2.8963	1099.0792
1193	36.0049	2.8943	374.0014	1193	36.0049	2.8943	1053.6486	1193	36.0049	2.8943	421.1365	1193	36.0049	2.8943	1098.0839
1194	36.0309	2.8923	354.373	1194	36.0309	2.8923	1034.1828	1194	36.0309	2.8923	466.2742	1194	36.0309	2.8923	1143.9598
1195	36.0569	2.8903	371.8188	1195	36.0569	2.8903	1051.7912	1195	36.0569	2.8903	408.7708	1195	36.0569	2.8903	1087.1946
1196	36.0829	2.8882	301.2938	1196	36.0829	2.8882	981.4288	1196	36.0829	2.8882	438.6952	1196	36.0829	2.8882	1117.8572
1197	36.1089	2.8862	357.8176	1197	36.1089	2.8862	1038.1152	1197	36.1089	2.8862	445.1116	1197	36.1089	2.8862	1125.0119
1198	36.1349	2.8842	388.5597	1198	36.1349	2.8842	1069.0198	1198	36.1349	2.8842	430.5401	1198	36.1349	2.8842	1111.1786
1199	36.1609	2.8822	328.901	1199	36.1609	2.8822	1009.5237	1199	36.1609	2.8822	510.2901	1199	36.1609	2.8822	1191.6668
1200	36.1869	2.8802	360.81	1200	36.1869	2.8802	1041.5953	1200	36.1869	2.8802	461.1232	1200	36.1869	2.8802	1143.2381
1201	36.2129	2.8782	332.6372	1201	36.2129	2.8782	1013.5852	1201	36.2129	2.8782	466.5778	1201	36.2129	2.8782	1149.4308
1202	36.2389	2.8762	344.3897	1202	36.2389	2.8762	1025.5003	1202	36.2389	2.8762	423.242	1202	36.2389	2.8762	1106.8332
1203	36.2649	2.8742	305.6534	1203	36.2649	2.8742	986.9266	1203	36.2649	2.8742	440.3216	1203	36.2649	2.8742	1124.6511
1204	36.2909	2.8722	308.5636	1204	36.2909	2.8722	989.9994	1204	36.2909	2.8722	406.8217	1204	36.2909	2.8722	1091.8894
1205	36.3169	2.8703	368.5799	1205	36.3169	2.8703	1050.1783	1205	36.3169	2.8703	361.1582	1205	36.3169	2.8703	1046.9641
1206	36.3429	2.8683	389.1081	1206	36.3429	2.8683	1070.8691	1206	36.3429	2.8683	381.9506	1206	36.3429	2.8683	1068.4947
1207	36.3689	2.8663	383.6489	1207	36.3689	2.8663	1065.5725	1207	36.3689	2.8663	475.1662	1207	36.3689	2.8663	1162.4485
1208	36.3949	2.8643	313.9852	1208	36.3949	2.8643	996.0714	1208	36.3949	2.8643	344.3602	1208	36.3949	2.8643	1032.3807
1209	36.4209	2.8623	317.2783	1209	36.4209	2.8623	999.5271	1209	36.4209	2.8623	360.9058	1209	36.4209	2.8623	1049.6645
1210	36.4469	2.8604	354.7386	1210	36.4469	2.8604	1037.15	1210	36.4469	2.8604	478.4557	1210	36.4469	2.8604	1167.9526
1211	36.4729	2.8584	392.199	1211	36.4729	2.8584	1074.773	1211	36.4729	2.8584	465.8366	1211	36.4729	2.8584	1156.0717
1212	36.4989	2.8564	360.7721	1212	36.4989	2.8564	1043.5087	1212	36.4989	2.8564	381.3779	1212	36.4989	2.8564	1072.3512
1213	36.5249	2.8545	326.9786	1213	36.5249	2.8545	1009.8778	1213	36.5249	2.8545	420.2041	1213	36.5249	2.8545	1111.9156
1214	36.5509	2.8525	355.8302	1214	36.5509	2.8525	1038.892	1214	36.5509	2.8525	377.1586	1214	36.5509	2.8525	1069.6083
1215	36.5769	2.8505	435.0312	1215	36.5769	2.8505	1118.2556	1215	36.5769	2.8505	427.3006	1215	36.5769	2.8505	1120.4885
1216	36.6029	2.8486	462.2233	1216	36.6029	2.8486	1145.6104	1216	36.6029	2.8486	498.9606	1216	36.6029	2.8486	1192.8867
1217	36.6289	2.8466	496.1576	1217	36.6289	2.8466	1179.7072	1217	36.6289	2.8466	520.091	1217	36.6289	2.8466	1214.7554
1218	36.6549	2.8447	494.5895	1218	36.6549	2.8447	1178.3017	1218	36.6549	2.8447	555.7311	1218	36.6549	2.8447	1251.1337
1219	36.6809	2.8427	554.4919	1219	36.6809	2.8427	1238.3667	1219	36.6809	2.8427	635.6043	1219	36.6809	2.8427	1331.7451

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1220	36.7069	2.8408	560.8673	1220	36.7069	2.8408	1244.9047	1220	36.7069	2.8408	607.7415	1220	36.7069	2.8408	1304.6204
1221	36.7329	2.8389	492.7949	1221	36.7329	2.8389	1176.995	1221	36.7329	2.8389	620.3841	1221	36.7329	2.8389	1318.0013
1222	36.7589	2.8369	526.2267	1222	36.7589	2.8369	1210.5894	1222	36.7589	2.8369	688.8956	1222	36.7589	2.8369	1387.2509
1223	36.7849	2.835	518.3503	1223	36.7849	2.835	1202.8756	1223	36.7849	2.835	609.4106	1223	36.7849	2.835	1308.5042
1224	36.8109	2.833	432.4036	1224	36.8109	2.833	1117.0915	1224	36.8109	2.833	545.1311	1224	36.8109	2.833	1244.9629
1225	36.8369	2.8311	461.0501	1225	36.8369	2.8311	1145.9006	1225	36.8369	2.8311	586.0267	1225	36.8369	2.8311	1286.5966
1226	36.8629	2.8292	440.0956	1226	36.8629	2.8292	1125.1087	1226	36.8629	2.8292	556.5034	1226	36.8629	2.8292	1257.8116
1227	36.8889	2.8273	393.8961	1227	36.8889	2.8273	1079.0718	1227	36.8889	2.8273	481.2968	1227	36.8889	2.8273	1183.3432
1228	36.9149	2.8253	316.3326	1228	36.9149	2.8253	1001.6708	1228	36.9149	2.8253	457.3113	1228	36.9149	2.8253	1160.0958
1229	36.9409	2.8234	346.3475	1229	36.9409	2.8234	1031.8484	1229	36.9409	2.8234	419.414	1229	36.9409	2.8234	1122.9367
1230	36.9669	2.8215	328.1439	1230	36.9669	2.8215	1013.8074	1230	36.9669	2.8215	481.6232	1230	36.9669	2.8215	1185.8842
1231	36.9929	2.8196	369.7043	1231	36.9929	2.8196	1055.5304	1231	36.9929	2.8196	427.1942	1231	36.9929	2.8196	1132.1934
1232	37.0189	2.8177	328.5866	1232	37.0189	2.8177	1014.5753	1232	37.0189	2.8177	505.6842	1232	37.0189	2.8177	1211.4216
1233	37.0449	2.8158	354.9627	1233	37.0449	2.8158	1041.114	1233	37.0449	2.8158	463.2597	1233	37.0449	2.8158	1169.7353
1234	37.0709	2.8139	372.0468	1234	37.0709	2.8139	1058.3607	1234	37.0709	2.8139	419.8118	1234	37.0709	2.8139	1127.0256
1235	37.0969	2.812	400.7356	1235	37.0969	2.812	1087.2121	1235	37.0969	2.812	402.2214	1235	37.0969	2.812	1110.1734
1236	37.1229	2.8101	442.1835	1236	37.1229	2.8101	1128.8226	1236	37.1229	2.8101	419.9429	1236	37.1229	2.8101	1128.6331
1237	37.1489	2.8082	476.7518	1237	37.1489	2.8082	1163.5535	1237	37.1489	2.8082	430.9879	1237	37.1489	2.8082	1140.4163
1238	37.1749	2.8063	510.45	1238	37.1749	2.8063	1197.4143	1238	37.1749	2.8063	470.318	1238	37.1749	2.8063	1180.4846
1239	37.2009	2.8044	509.13	1239	37.2009	2.8044	1196.257	1239	37.2009	2.8044	433.2449	1239	37.2009	2.8044	1144.1497
1240	37.2269	2.8025	537.9056	1240	37.2269	2.8025	1225.1951	1240	37.2269	2.8025	464.6217	1240	37.2269	2.8025	1176.2647
1241	37.2529	2.8006	484.6976	1241	37.2529	2.8006	1172.1497	1241	37.2529	2.8006	477.9588	1241	37.2529	2.8006	1190.3401
1242	37.2789	2.7987	454.6988	1242	37.2789	2.7987	1142.3136	1242	37.2789	2.7987	469.0755	1242	37.2789	2.7987	1182.195
1243	37.3049	2.7968	435.2803	1243	37.3049	2.7968	1123.0576	1243	37.3049	2.7968	422.169	1243	37.3049	2.7968	1136.0267
1244	37.3309	2.795	428.786	1244	37.3309	2.795	1115.3332	1244	37.3309	2.795	425.763	1244	37.3309	2.795	1140.3304
1245	37.3569	2.7931	379.4628	1245	37.3569	2.7931	1064.7799	1245	37.3569	2.7931	480.4062	1245	37.3569	2.7931	1195.6834
1246	37.3829	2.7912	324.8096	1246	37.3829	2.7912	1008.8964	1246	37.3829	2.7912	473.5562	1246	37.3829	2.7912	1189.5432
1247	37.4089	2.7893	317.7852	1247	37.4089	2.7893	1000.6419	1247	37.4089	2.7893	487.8708	1247	37.4089	2.7893	1204.5675
1248	37.4349	2.7875	327.1348	1248	37.4349	2.7875	1008.7614	1248	37.4349	2.7875	458.2028	1248	37.4349	2.7875	1175.6093
1249	37.4609	2.7856	307.1584	1249	37.4609	2.7856	987.5548	1249	37.4609	2.7856	434.2026	1249	37.4609	2.7856	1152.3189
1250	37.4869	2.7837	290.7985	1250	37.4869	2.7837	969.9647	1250	37.4869	2.7837	478.6679	1250	37.4869	2.7837	1197.494
1251	37.5129	2.7819	296.0352	1251	37.5129	2.7819	973.9713	1251	37.5129	2.7819	516.2126	1251	37.5129	2.7819	1235.7484
1252	37.5389	2.78	307.1662	1252	37.5389	2.78	983.8721	1252	37.5389	2.78	492.8066	1252	37.5389	2.78	1213.0522
1253	37.5649	2.7782	307.3286	1253	37.5649	2.7782	982.8044	1253	37.5649	2.7782	460.0761	1253	37.5649	2.7782	1181.0315
1254	37.5909	2.7763	292.2723	1254	37.5909	2.7763	966.5179	1254	37.5909	2.7763	466.6537	1254	37.5909	2.7763	1188.3189
1255	37.6169	2.7745	314.0865	1255	37.6169	2.7745	987.102	1255	37.6169	2.7745	492.6761	1255	37.6169	2.7745	1215.051

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1256	37.6429	2.7726	286.105	1256	37.6429	2.7726	957.8903	1256	37.6429	2.7726	537.8617	1256	37.6429	2.7726	1260.9464
1257	37.6689	2.7708	267.6368	1257	37.6689	2.7708	938.192	1257	37.6689	2.7708	586.1719	1257	37.6689	2.7708	1309.9664
1258	37.6949	2.7689	289.675	1258	37.6949	2.7689	959	1258	37.6949	2.7689	605.0787	1258	37.6949	2.7689	1329.583
1259	37.7209	2.7671	275.3725	1259	37.7209	2.7671	943.4673	1259	37.7209	2.7671	653.4195	1259	37.7209	2.7671	1378.6335
1260	37.7469	2.7653	279.9095	1260	37.7469	2.7653	946.7742	1260	37.7469	2.7653	675.2393	1260	37.7469	2.7653	1401.1632
1261	37.7729	2.7634	309.3195	1261	37.7729	2.7634	974.9541	1261	37.7729	2.7634	653.8643	1261	37.7729	2.7634	1380.4979
1262	37.7989	2.7616	337.2113	1262	37.7989	2.7616	1001.6157	1262	37.7989	2.7616	699.5276	1262	37.7989	2.7616	1426.871
1263	37.8249	2.7598	366.7774	1263	37.8249	2.7598	1029.9517	1263	37.8249	2.7598	778.9773	1263	37.8249	2.7598	1507.0305
1264	37.8509	2.7579	355.7761	1264	37.8509	2.7579	1017.7202	1264	37.8509	2.7579	843.6664	1264	37.8509	2.7579	1572.4294
1265	37.8769	2.7561	333.7847	1265	37.8769	2.7561	994.4987	1265	37.8769	2.7561	949.9264	1265	37.8769	2.7561	1679.3991
1266	37.9029	2.7543	324.0325	1266	37.9029	2.7543	983.5163	1266	37.9029	2.7543	1070.2332	1266	37.9029	2.7543	1800.4157
1267	37.9289	2.7525	308.1302	1267	37.9289	2.7525	966.3838	1267	37.9289	2.7525	1214.3729	1267	37.9289	2.7525	1945.2652
1268	37.9549	2.7507	334.257	1268	37.9549	2.7507	991.2805	1268	37.9549	2.7507	1365.2491	1268	37.9549	2.7507	2096.8512
1269	37.9809	2.7488	359.5326	1269	37.9809	2.7488	1015.3259	1269	37.9809	2.7488	1486.6025	1269	37.9809	2.7488	2218.9143
1270	38.0069	2.747	360.0713	1270	38.0069	2.747	1014.6344	1270	38.0069	2.747	1725.7119	1270	38.0069	2.747	2458.7335
1271	38.0329	2.7452	376.3247	1271	38.0329	2.7452	1028.562	1271	38.0329	2.7452	2017.6965	1271	38.0329	2.7452	2748.5737
1272	38.0589	2.7434	366.9312	1272	38.0589	2.7434	1016.8425	1272	38.0589	2.7434	2367.6634	1272	38.0589	2.7434	3096.3963
1273	38.0849	2.7416	309.3974	1273	38.0849	2.7416	956.9828	1273	38.0849	2.7416	2765.1163	1273	38.0849	2.7416	3491.7048
1274	38.1109	2.7398	309.0312	1274	38.1109	2.7398	954.2907	1274	38.1109	2.7398	3256.821	1274	38.1109	2.7398	3981.2652
1275	38.1369	2.738	353.9644	1275	38.1369	2.738	996.898	1275	38.1369	2.738	3875.8178	1275	38.1369	2.738	4598.1176
1276	38.1629	2.7362	374.5813	1276	38.1629	2.7362	1015.1889	1276	38.1629	2.7362	4454.0915	1276	38.1629	2.7362	5174.247
1277	38.1889	2.7344	362.6732	1277	38.1889	2.7344	1000.9549	1277	38.1889	2.7344	4942.581	1277	38.1889	2.7344	5660.592
1278	38.2149	2.7326	331.2627	1278	38.2149	2.7326	967.2185	1278	38.2149	2.7326	5358.5064	1278	38.2149	2.7326	6074.3731
1279	38.2409	2.7309	369.6128	1279	38.2409	2.7309	1003.2427	1279	38.2409	2.7309	5637.5322	1279	38.2409	2.7309	6351.2545
1280	38.2669	2.7291	397.558	1280	38.2669	2.7291	1028.862	1280	38.2669	2.7291	5412.4571	1280	38.2669	2.7291	6124.0351
1281	38.2929	2.7273	362.1449	1281	38.2929	2.7273	991.123	1281	38.2929	2.7273	5016.7428	1281	38.2929	2.7273	5726.1764
1282	38.3189	2.7255	354.3263	1282	38.3189	2.7255	980.9785	1282	38.3189	2.7255	4608.4835	1282	38.3189	2.7255	5315.7727
1283	38.3449	2.7237	391.4131	1283	38.3449	2.7237	1015.7393	1283	38.3449	2.7237	4036.0779	1283	38.3449	2.7237	4741.2227
1284	38.3709	2.7219	390.712	1284	38.3709	2.7219	1012.7123	1284	38.3709	2.7219	3484.9498	1284	38.3709	2.7219	4187.9502
1285	38.3969	2.7202	461.4652	1285	38.3969	2.7202	1081.1397	1285	38.3969	2.7202	2824.7138	1285	38.3969	2.7202	3525.5699
1286	38.4229	2.7184	412.8931	1286	38.4229	2.7184	1030.2417	1286	38.4229	2.7184	2415.8545	1286	38.4229	2.7184	3114.5663
1287	38.4489	2.7166	457.2576	1287	38.4489	2.7166	1072.2802	1287	38.4489	2.7166	2010.0118	1287	38.4489	2.7166	2706.5792
1288	38.4749	2.7149	461.2135	1288	38.4749	2.7149	1073.9102	1288	38.4749	2.7149	1751.8851	1288	38.4749	2.7149	2446.3081
1289	38.5009	2.7131	488.0737	1289	38.5009	2.7131	1098.4445	1289	38.5009	2.7131	1540.4987	1289	38.5009	2.7131	2232.7773
1290	38.5269	2.7113	528.0128	1290	38.5269	2.7113	1136.0577	1290	38.5269	2.7113	1331.4592	1290	38.5269	2.7113	2021.5934
1291	38.5529	2.7096	543.5104	1291	38.5529	2.7096	1149.2294	1291	38.5529	2.7096	1281.9859	1291	38.5529	2.7096	1969.9757

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1292	38.5789	2.7078	644.5102	1292	38.5789	2.7078	1247.9032	1292	38.5789	2.7078	1191.974	1292	38.5789	2.7078	1877.8195
1293	38.6049	2.7061	657.4584	1293	38.6049	2.7061	1258.5256	1293	38.6049	2.7061	1138.5105	1293	38.6049	2.7061	1822.2116
1294	38.6309	2.7043	677.3959	1294	38.6309	2.7043	1276.1371	1294	38.6309	2.7043	1083.7224	1294	38.6309	2.7043	1765.2792
1295	38.6569	2.7026	705.2497	1295	38.6569	2.7026	1301.6651	1295	38.6569	2.7026	886.6471	1295	38.6569	2.7026	1566.0595
1296	38.6829	2.7008	681.898	1296	38.6829	2.7008	1275.9874	1296	38.6829	2.7008	851.5561	1296	38.6829	2.7008	1528.8241
1297	38.7089	2.6991	676.8047	1297	38.7089	2.6991	1268.5682	1297	38.7089	2.6991	807.4789	1297	38.7089	2.6991	1482.6026
1298	38.7349	2.6973	730.3692	1298	38.7349	2.6973	1319.8067	1298	38.7349	2.6973	728.7731	1298	38.7349	2.6973	1401.7524
1299	38.7609	2.6956	682.9545	1299	38.7609	2.6956	1270.0662	1299	38.7609	2.6956	652.7809	1299	38.7609	2.6956	1323.6158
1300	38.7869	2.6939	658.8997	1300	38.7869	2.6939	1243.6854	1300	38.7869	2.6939	627.7578	1300	38.7869	2.6939	1296.4483
1301	38.8129	2.6921	561.1259	1301	38.8129	2.6921	1143.5857	1301	38.8129	2.6921	612.0803	1301	38.8129	2.6921	1278.6265
1302	38.8389	2.6904	548.3154	1302	38.8389	2.6904	1128.4493	1302	38.8389	2.6904	639.6023	1302	38.8389	2.6904	1304.0041
1303	38.8649	2.6887	526.3285	1303	38.8649	2.6887	1104.1365	1303	38.8649	2.6887	653.4627	1303	38.8649	2.6887	1315.7201
1304	38.8909	2.6869	538.169	1304	38.8909	2.6869	1113.6511	1304	38.8909	2.6869	561.8157	1304	38.8909	2.6869	1221.9287
1305	38.9169	2.6852	496.2919	1305	38.9169	2.6852	1069.448	1305	38.9169	2.6852	565.6072	1305	38.9169	2.6852	1223.5759
1306	38.9429	2.6835	489.2958	1306	38.9429	2.6835	1060.1261	1306	38.9429	2.6835	604.2968	1306	38.9429	2.6835	1260.1211
1307	38.9689	2.6818	470.6003	1307	38.9689	2.6818	1039.1047	1307	38.9689	2.6818	552.9467	1307	38.9689	2.6818	1206.6266
1308	38.9949	2.68	362.4098	1308	38.9949	2.68	928.5882	1308	38.9949	2.68	544.4443	1308	38.9949	2.68	1195.9799
1309	39.0209	2.6783	442.5893	1309	39.0209	2.6783	1006.4418	1309	39.0209	2.6783	485.2147	1309	39.0209	2.6783	1134.606
1310	39.0469	2.6766	374.6843	1310	39.0469	2.6766	936.2109	1310	39.0469	2.6766	514.5305	1310	39.0469	2.6766	1161.7773
1311	39.0729	2.6749	394.6951	1311	39.0729	2.6749	953.8958	1311	39.0729	2.6749	497.9478	1311	39.0729	2.6749	1143.0503
1312	39.0989	2.6732	339.5965	1312	39.0989	2.6732	896.4713	1312	39.0989	2.6732	527.8144	1312	39.0989	2.6732	1170.7725
1313	39.1249	2.6715	339.4872	1313	39.1249	2.6715	894.0361	1313	39.1249	2.6715	481.0886	1313	39.1249	2.6715	1121.9024
1314	39.1509	2.6698	299.9798	1314	39.1509	2.6698	852.2027	1314	39.1509	2.6698	459.0019	1314	39.1509	2.6698	1097.6713
1315	39.1769	2.6681	339.5873	1315	39.1769	2.6681	889.4843	1315	39.1769	2.6681	534.5573	1315	39.1769	2.6681	1171.0823
1316	39.2029	2.6664	382.4685	1316	39.2029	2.6664	930.0396	1316	39.2029	2.6664	497.7232	1316	39.2029	2.6664	1132.1038
1317	39.2289	2.6647	350.9488	1317	39.2289	2.6647	896.194	1317	39.2289	2.6647	526.0316	1317	39.2289	2.6647	1158.2679
1318	39.2549	2.663	379.0509	1318	39.2549	2.663	921.9702	1318	39.2549	2.663	456.2532	1318	39.2549	2.663	1086.3451
1319	39.2809	2.6613	392.6308	1319	39.2809	2.6613	933.2242	1319	39.2809	2.6613	409.6988	1319	39.2809	2.6613	1037.6463
1320	39.3069	2.6596	356.4952	1320	39.3069	2.6596	894.7627	1320	39.3069	2.6596	417.3218	1320	39.3069	2.6596	1043.125
1321	39.3329	2.6579	369.4996	1321	39.3329	2.6579	905.4412	1321	39.3329	2.6579	490.742	1321	39.3329	2.6579	1114.4008
1322	39.3589	2.6562	366.2432	1322	39.3589	2.6562	899.8588	1322	39.3589	2.6562	468.3501	1322	39.3589	2.6562	1089.8645
1323	39.3849	2.6545	371.2412	1323	39.3849	2.6545	902.5309	1323	39.3849	2.6545	476.34	1323	39.3849	2.6545	1095.71
1324	39.4109	2.6529	360.0713	1324	39.4109	2.6529	889.0351	1324	39.4109	2.6529	422.169	1324	39.4109	2.6529	1039.3947
1325	39.4369	2.6512	358.1015	1325	39.4369	2.6512	886.1371	1325	39.4369	2.6512	422.5607	1325	39.4369	2.6512	1037.0402
1326	39.4629	2.6495	340.9805	1326	39.4629	2.6495	868.0878	1326	39.4629	2.6495	369.9711	1326	39.4629	2.6495	981.7045
1327	39.4889	2.6478	380.9729	1327	39.4889	2.6478	907.152	1327	39.4889	2.6478	417.8104	1327	39.4889	2.6478	1026.7976

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1328	39.5149	2.6462	381.418	1328	39.5149	2.6462	906.6688	1328	39.5149	2.6462	434.9246	1328	39.5149	2.6462	1041.1656
1329	39.5409	2.6445	369.9758	1329	39.5409	2.6445	894.2985	1329	39.5409	2.6445	429.45	1329	39.5409	2.6445	1032.9448
1330	39.5669	2.6428	379.9914	1330	39.5669	2.6428	903.3858	1330	39.5669	2.6428	392.8408	1330	39.5669	2.6428	993.5894
1331	39.5929	2.6412	352.2031	1331	39.5929	2.6412	874.6693	1331	39.5929	2.6412	378.964	1331	39.5929	2.6412	976.9665
1332	39.6189	2.6395	343.8752	1332	39.6189	2.6395	865.4131	1332	39.6189	2.6395	450.3589	1332	39.6189	2.6395	1045.6151
1333	39.6449	2.6378	374.947	1333	39.6449	2.6378	895.5567	1333	39.6449	2.6378	453.4693	1333	39.6449	2.6378	1045.9794
1334	39.6709	2.6362	369.6204	1334	39.6709	2.6362	889.3019	1334	39.6709	2.6362	403.2739	1334	39.6709	2.6362	993.0378
1335	39.6969	2.6345	363.1921	1335	39.6969	2.6345	881.9454	1335	39.6969	2.6345	424.8197	1335	39.6969	2.6345	1011.8375
1336	39.7229	2.6329	357.8988	1336	39.7229	2.6329	875.7238	1336	39.7229	2.6329	464.8631	1336	39.7229	2.6329	1049.1346
1337	39.7489	2.6312	308.7551	1337	39.7489	2.6312	825.6519	1337	39.7489	2.6312	440.7714	1337	39.7489	2.6312	1022.2968
1338	39.7749	2.6296	335.5974	1338	39.7749	2.6296	851.5659	1338	39.7749	2.6296	395.9938	1338	39.7749	2.6296	974.773
1339	39.8009	2.6279	371.507	1339	39.8009	2.6279	886.5473	1339	39.8009	2.6279	417.0978	1339	39.8009	2.6279	993.1308
1340	39.8269	2.6263	364.1788	1340	39.8269	2.6263	878.2909	1340	39.8269	2.6263	443.138	1340	39.8269	2.6263	1016.4248
1341	39.8529	2.6246	336.9882	1341	39.8529	2.6246	850.172	1341	39.8529	2.6246	472.9914	1341	39.8529	2.6246	1043.5321
1342	39.8789	2.623	334.9923	1342	39.8789	2.623	847.2479	1342	39.8789	2.623	453.9662	1342	39.8789	2.623	1021.7607
1343	39.9049	2.6213	357.8326	1343	39.9049	2.6213	869.1599	1343	39.9049	2.6213	479.903	1343	39.9049	2.6213	1044.9513
1344	39.9309	2.6197	387.8317	1344	39.9309	2.6197	898.2308	1344	39.9309	2.6197	431.5874	1344	39.9309	2.6197	993.8895
1345	39.9569	2.6181	381.2537	1345	39.9569	2.6181	890.7246	1345	39.9569	2.6181	446.6259	1345	39.9569	2.6181	1006.1818
1346	39.9829	2.6164	384.5841	1346	39.9829	2.6164	893.1268	1346	39.9829	2.6164	453.2092	1346	39.9829	2.6164	1010.019
1347	40.0089	2.6148	401.6991	1347	40.0089	2.6148	909.3135	1347	40.0089	2.6148	457.5391	1347	40.0089	2.6148	1011.6027
1348	40.0349	2.6132	363.8868	1348	40.0349	2.6132	870.573	1348	40.0349	2.6132	430.5063	1348	40.0349	2.6132	981.8237
1349	40.0609	2.6115	341.741	1349	40.0609	2.6115	847.499	1349	40.0609	2.6115	408.0555	1349	40.0609	2.6115	956.6268
1350	40.0869	2.6099	325.1106	1350	40.0869	2.6099	829.9404	1350	40.0869	2.6099	426.6197	1350	40.0869	2.6099	972.4448
1351	40.1129	2.6083	360.0713	1351	40.1129	2.6083	863.9728	1351	40.1129	2.6083	422.169	1351	40.1129	2.6083	965.2479
1352	40.1389	2.6067	396.4925	1352	40.1389	2.6067	900.5448	1352	40.1389	2.6067	421.6456	1352	40.1389	2.6067	964.8997
1353	40.1649	2.6051	392.6061	1353	40.1649	2.6051	896.8092	1353	40.1649	2.6051	442.4421	1353	40.1649	2.6051	985.8713
1354	40.1909	2.6034	386.071	1354	40.1909	2.6034	890.4249	1354	40.1909	2.6034	438.7425	1354	40.1909	2.6034	982.347
1355	40.2169	2.6018	392.2779	1355	40.2169	2.6018	896.7826	1355	40.2169	2.6018	394.177	1355	40.2169	2.6018	937.9566
1356	40.2429	2.6002	351.2552	1356	40.2429	2.6002	855.9106	1356	40.2429	2.6002	391.4781	1356	40.2429	2.6002	935.4329
1357	40.2689	2.5986	349.0975	1357	40.2689	2.5986	853.9038	1357	40.2689	2.5986	399.4172	1357	40.2689	2.5986	943.5472
1358	40.2949	2.597	369.4758	1358	40.2949	2.597	874.4328	1358	40.2949	2.597	419.1445	1358	40.2949	2.597	963.4497
1359	40.3209	2.5954	352.9583	1359	40.3209	2.5954	858.066	1359	40.3209	2.5954	422.973	1359	40.3209	2.5954	967.4534
1360	40.3469	2.5938	345.7726	1360	40.3469	2.5938	851.0312	1360	40.3469	2.5938	443.5616	1360	40.3469	2.5938	988.2171
1361	40.3729	2.5922	327.3747	1361	40.3729	2.5922	832.7841	1361	40.3729	2.5922	475.1011	1361	40.3729	2.5922	1019.9318
1362	40.3989	2.5906	312.4059	1362	40.3989	2.5906	817.9661	1362	40.3989	2.5906	439.2485	1362	40.3989	2.5906	984.2544
1363	40.4249	2.589	334.7509	1363	40.4249	2.589	840.4618	1363	40.4249	2.589	422.4223	1363	40.4249	2.589	967.6035

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1364	40.4509	2.5874	369.3676	1364	40.4509	2.5874	875.2293	1364	40.4509	2.5874	447.5897	1364	40.4509	2.5874	992.9461
1365	40.4769	2.5858	385.9875	1365	40.4769	2.5858	892	1365	40.4769	2.5858	429.6449	1365	40.4769	2.5858	975.1765
1366	40.5029	2.5842	382.1881	1366	40.5029	2.5842	888.3514	1366	40.5029	2.5842	393.9251	1366	40.5029	2.5842	939.6318
1367	40.5289	2.5826	356.2708	1367	40.5289	2.5826	862.5849	1367	40.5289	2.5826	391.672	1367	40.5289	2.5826	937.5539
1368	40.5549	2.581	361.8158	1368	40.5549	2.581	868.2807	1368	40.5549	2.581	400.9761	1368	40.5549	2.581	947.0332
1369	40.5809	2.5795	408.5	1369	40.5809	2.5795	915.1156	1369	40.5809	2.5795	425.2779	1369	40.5809	2.5795	971.5102
1370	40.6069	2.5779	373.5954	1370	40.6069	2.5779	880.3619	1370	40.6069	2.5779	449.3366	1370	40.6069	2.5779	995.744
1371	40.6329	2.5763	323.6184	1371	40.6329	2.5763	830.5356	1371	40.6329	2.5763	444.3461	1371	40.6329	2.5763	990.9287
1372	40.6589	2.5747	333.5528	1372	40.6589	2.5747	840.6208	1372	40.6589	2.5747	401.398	1372	40.6589	2.5747	948.1558
1373	40.6849	2.5731	331.7143	1373	40.6849	2.5731	838.9331	1373	40.6849	2.5731	401.13	1373	40.6849	2.5731	948.063
1374	40.7109	2.5716	324.083	1374	40.7109	2.5716	831.4526	1374	40.7109	2.5716	437.488	1374	40.7109	2.5716	984.5962
1375	40.7369	2.57	316.3824	1375	40.7369	2.57	823.9028	1375	40.7369	2.57	420.4815	1375	40.7369	2.57	967.7649
1376	40.7629	2.5684	335.1131	1376	40.7629	2.5684	842.7842	1376	40.7629	2.5684	396.3381	1376	40.7629	2.5684	943.7966
1377	40.7889	2.5669	344.4227	1377	40.7889	2.5669	852.2447	1377	40.7889	2.5669	390.4064	1377	40.7889	2.5669	938.0401
1378	40.8149	2.5653	360.0713	1378	40.8149	2.5653	868.044	1378	40.8149	2.5653	422.169	1378	40.8149	2.5653	969.978
1379	40.8409	2.5637	369.3447	1379	40.8409	2.5637	876.3271	1379	40.8409	2.5637	413.4342	1379	40.8409	2.5637	960.7667
1380	40.8669	2.5622	351.9784	1380	40.8669	2.5622	857.9705	1380	40.8669	2.5622	420.2706	1380	40.8669	2.5622	967.1266
1381	40.8929	2.5606	331.0469	1381	40.8929	2.5606	836.0486	1381	40.8929	2.5606	435.8067	1381	40.8929	2.5606	982.1862
1382	40.9189	2.5591	362.2041	1382	40.9189	2.5591	866.2155	1382	40.9189	2.5591	391.5567	1382	40.9189	2.5591	937.4597
1383	40.9449	2.5575	341.6007	1383	40.9449	2.5575	844.6218	1383	40.9449	2.5575	395.1012	1383	40.9449	2.5575	940.5278
1384	40.9709	2.5559	356.755	1384	40.9709	2.5559	858.7858	1384	40.9709	2.5559	388.4261	1384	40.9709	2.5559	933.3762
1385	40.9969	2.5544	344.043	1385	40.9969	2.5544	845.0834	1385	40.9969	2.5544	416.386	1385	40.9969	2.5544	960.8596
1386	41.0229	2.5528	356.8889	1386	41.0229	2.5528	856.939	1386	41.0229	2.5528	412.5486	1386	41.0229	2.5528	956.5457
1387	41.0489	2.5513	345.0046	1387	41.0489	2.5513	844.0643	1387	41.0489	2.5513	410.0482	1387	41.0489	2.5513	953.5689
1388	41.0749	2.5498	326.3573	1388	41.0749	2.5498	824.4267	1388	41.0749	2.5498	395.327	1388	41.0749	2.5498	938.3712
1389	41.1009	2.5482	345.3645	1389	41.1009	2.5482	842.4436	1389	41.1009	2.5482	419.888	1389	41.1009	2.5482	962.4557
1390	41.1269	2.5467	380.3607	1390	41.1269	2.5467	876.4494	1390	41.1269	2.5467	413.8451	1390	41.1269	2.5467	955.9364
1391	41.1529	2.5451	340.1096	1391	41.1529	2.5451	835.208	1391	41.1529	2.5451	383.5131	1391	41.1529	2.5451	925.1279
1392	41.1789	2.5436	345.4575	1392	41.1789	2.5436	839.5656	1392	41.1789	2.5436	385.3796	1392	41.1789	2.5436	926.5179
1393	41.2049	2.5421	348.0868	1393	41.2049	2.5421	841.2045	1393	41.2049	2.5421	419.0209	1393	41.2049	2.5421	959.6828
1394	41.2309	2.5405	305.2803	1394	41.2309	2.5405	797.4078	1394	41.2309	2.5405	424.3311	1394	41.2309	2.5405	964.5165
1395	41.2569	2.539	359.0312	1395	41.2569	2.539	850.1683	1395	41.2569	2.539	479.5191	1395	41.2569	2.539	1019.228
1396	41.2829	2.5375	350.8739	1396	41.2829	2.5375	841.0207	1396	41.2829	2.5375	491.9177	1396	41.2829	2.5375	1031.1502
1397	41.3089	2.5359	308.1978	1397	41.3089	2.5359	797.3542	1397	41.3089	2.5359	391.7986	1397	41.3089	2.5359	930.5546
1398	41.3349	2.5344	361.7254	1398	41.3349	2.5344	849.8915	1398	41.3349	2.5344	382.7926	1398	41.3349	2.5344	921.0721
1399	41.3609	2.5329	359.1687	1399	41.3609	2.5329	846.3445	1399	41.3609	2.5329	348.4296	1399	41.3609	2.5329	886.2326

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1400	41.3869	2.5314	381.2713	1400	41.3869	2.5314	867.4567	1400	41.3869	2.5314	402.774	1400	41.3869	2.5314	940.1006
1401	41.4129	2.5298	368.9555	1401	41.4129	2.5298	854.1506	1401	41.4129	2.5298	388.4971	1401	41.4129	2.5298	925.3473
1402	41.4389	2.5283	351.5326	1402	41.4389	2.5283	835.7374	1402	41.4389	2.5283	387.9766	1402	41.4389	2.5283	924.3502
1403	41.4649	2.5268	326.0766	1403	41.4649	2.5268	809.291	1403	41.4649	2.5268	427.836	1403	41.4649	2.5268	963.7332
1404	41.4909	2.5253	360.8549	1404	41.4909	2.5253	843.079	1404	41.4909	2.5253	430.3997	1404	41.4909	2.5253	965.8204
1405	41.5169	2.5238	360.0713	1405	41.5169	2.5238	841.3051	1405	41.5169	2.5238	482.1496	1405	41.5169	2.5238	1017.0938
1406	41.5429	2.5223	323.436	1406	41.5429	2.5223	804.1123	1406	41.5429	2.5223	415.7037	1406	41.5429	2.5223	950.1715
1407	41.5689	2.5208	313.9202	1407	41.5689	2.5208	794.039	1407	41.5689	2.5208	403.058	1407	41.5689	2.5208	937.0493
1408	41.5949	2.5193	391.1406	1408	41.5949	2.5193	870.702	1408	41.5949	2.5193	402.5578	1408	41.5949	2.5193	936.0726
1409	41.6209	2.5178	361.0844	1409	41.6209	2.5178	840.0882	1409	41.6209	2.5178	358.8146	1409	41.6209	2.5178	891.853
1410	41.6469	2.5163	397.8849	1410	41.6469	2.5163	876.3313	1410	41.6469	2.5163	454.1982	1410	41.6469	2.5163	986.7601
1411	41.6729	2.5148	414.7284	1411	41.6729	2.5148	892.6173	1411	41.6729	2.5148	492.0344	1411	41.6729	2.5148	1024.1198
1412	41.6989	2.5133	375.6828	1412	41.6989	2.5133	853.0142	1412	41.6989	2.5133	401.4237	1412	41.6989	2.5133	933.0326
1413	41.7249	2.5118	410.8663	1413	41.7249	2.5118	887.6403	1413	41.7249	2.5118	402.8573	1413	41.7249	2.5118	933.9897
1414	41.7509	2.5103	407.8643	1414	41.7509	2.5103	884.0808	1414	41.7509	2.5103	458.2128	1414	41.7509	2.5103	988.8688
1415	41.7769	2.5088	416.1	1415	41.7769	2.5088	891.759	1415	41.7769	2.5088	461.7602	1415	41.7769	2.5088	991.9398
1416	41.8029	2.5073	429.3779	1416	41.8029	2.5073	904.4794	1416	41.8029	2.5073	465.1768	1416	41.8029	2.5073	994.8799
1417	41.8289	2.5058	436.1561	1417	41.8289	2.5058	910.7002	1417	41.8289	2.5058	498.0746	1417	41.8289	2.5058	1027.3011
1418	41.8549	2.5043	469.9173	1418	41.8549	2.5043	943.9039	1418	41.8549	2.5043	470.1663	1418	41.8549	2.5043	998.9164
1419	41.8809	2.5028	558.1483	1419	41.8809	2.5028	1031.5774	1419	41.8809	2.5028	563.6056	1419	41.8809	2.5028	1091.8793
1420	41.9069	2.5013	628.6268	1420	41.9069	2.5013	1101.4984	1420	41.9069	2.5013	650.3458	1420	41.9069	2.5013	1178.1429
1421	41.9329	2.4999	827.6789	1421	41.9329	2.4999	1299.993	1421	41.9329	2.4999	780.5758	1421	41.9329	2.4999	1307.8965
1422	41.9589	2.4984	1048.9379	1422	41.9589	2.4984	1520.6946	1422	41.9589	2.4984	1043.4732	1422	41.9589	2.4984	1570.3174
1423	41.9849	2.4969	1179.5513	1423	41.9849	2.4969	1650.7505	1423	41.9849	2.4969	1263.9802	1423	41.9849	2.4969	1790.348
1424	42.0109	2.4954	1387.9659	1424	42.0109	2.4954	1858.6077	1424	42.0109	2.4954	1594.5497	1424	42.0109	2.4954	2120.441
1425	42.0369	2.494	1578.599	1425	42.0369	2.494	2048.6832	1425	42.0369	2.494	1774.1487	1425	42.0369	2.494	2299.5636
1426	42.0629	2.4925	1781.645	1426	42.0629	2.4925	2251.1718	1426	42.0629	2.4925	1877.692	1426	42.0629	2.4925	2402.6304
1427	42.0889	2.491	1884.2004	1427	42.0889	2.491	2353.1697	1427	42.0889	2.491	1824.3241	1427	42.0889	2.491	2348.7859
1428	42.1149	2.4895	1899.2699	1428	42.1149	2.4895	2367.6818	1428	42.1149	2.4895	1713.7897	1428	42.1149	2.4895	2237.7752
1429	42.1409	2.4881	1851.9496	1429	42.1409	2.4881	2319.804	1429	42.1409	2.4881	1593.2822	1429	42.1409	2.4881	2116.7912
1430	42.1669	2.4866	1846.8083	1430	42.1669	2.4866	2314.1052	1430	42.1669	2.4866	1411.2219	1430	42.1669	2.4866	1934.2543
1431	42.1929	2.4852	1681.9806	1431	42.1929	2.4852	2148.7201	1431	42.1929	2.4852	1181.7748	1431	42.1929	2.4852	1704.3308
1432	42.2189	2.4837	1551.6801	1432	42.2189	2.4837	2017.8621	1432	42.2189	2.4837	999.1142	1432	42.2189	2.4837	1521.1937
1433	42.2449	2.4822	1419.388	1433	42.2449	2.4822	1885.0125	1433	42.2449	2.4822	901.1512	1433	42.2449	2.4822	1420.5327
1434	42.2709	2.4808	1378.4313	1434	42.2709	2.4808	1843.4983	1434	42.2709	2.4808	760.5183	1434	42.2709	2.4808	1277.2019
1435	42.2969	2.4793	1336.1474	1435	42.2969	2.4793	1800.6569	1435	42.2969	2.4793	658.5855	1435	42.2969	2.4793	1172.5711

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1436	42.3229	2.4779	1263.3656	1436	42.3229	2.4779	1727.3177	1436	42.3229	2.4779	631.5742	1436	42.3229	2.4779	1142.8619
1437	42.3489	2.4764	1310.7452	1437	42.3489	2.4764	1774.1397	1437	42.3489	2.4764	581.0539	1437	42.3489	2.4764	1089.6436
1438	42.3749	2.475	1310.9129	1438	42.3749	2.475	1773.75	1438	42.3749	2.475	507.0334	1438	42.3749	2.475	1012.9251
1439	42.4009	2.4735	1286.8903	1439	42.4009	2.4735	1749.1699	1439	42.4009	2.4735	468.3175	1439	42.4009	2.4735	971.5112
1440	42.4269	2.4721	1252.405	1440	42.4269	2.4721	1714.1272	1440	42.4269	2.4721	399.2622	1440	42.4269	2.4721	899.7579
1441	42.4529	2.4706	1212.6475	1441	42.4529	2.4706	1673.8122	1441	42.4529	2.4706	416.3566	1441	42.4529	2.4706	914.1544
1442	42.4789	2.4692	1222.4521	1442	42.4789	2.4692	1683.0593	1442	42.4789	2.4692	422.9666	1442	42.4789	2.4692	918.0664
1443	42.5049	2.4677	1150.98	1443	42.5049	2.4677	1611.0297	1443	42.5049	2.4677	418.522	1443	42.5049	2.4677	910.9238
1444	42.5309	2.4663	1049.341	1444	42.5309	2.4663	1508.8332	1444	42.5309	2.4663	399.8322	1444	42.5309	2.4663	889.536
1445	42.5569	2.4649	957.8942	1445	42.5569	2.4649	1416.8289	1445	42.5569	2.4649	420.5547	1445	42.5569	2.4649	907.5606
1446	42.5829	2.4634	883.5872	1446	42.5829	2.4634	1341.9645	1446	42.5829	2.4634	430.7315	1446	42.5829	2.4634	915.0394
1447	42.6089	2.462	825.3001	1447	42.6089	2.462	1283.1199	1447	42.6089	2.462	421.2569	1447	42.6089	2.462	902.8669
1448	42.6349	2.4606	734.7841	1448	42.6349	2.4606	1192.0464	1448	42.6349	2.4606	440.9311	1448	42.6349	2.4606	919.8431
1449	42.6609	2.4591	635.2057	1449	42.6609	2.4591	1091.9106	1449	42.6609	2.4591	442.5031	1449	42.6609	2.4591	918.7171
1450	42.6869	2.4577	618.2854	1450	42.6869	2.4577	1074.4327	1450	42.6869	2.4577	398.8829	1450	42.6869	2.4577	872.3989
1451	42.7129	2.4563	547.3115	1451	42.7129	2.4563	1002.9014	1451	42.7129	2.4563	407.5904	1451	42.7129	2.4563	878.4084
1452	42.7389	2.4549	516.4612	1452	42.7389	2.4549	971.4936	1452	42.7389	2.4549	433.0992	1452	42.7389	2.4549	901.2193
1453	42.7649	2.4534	464.7208	1453	42.7649	2.4534	919.1957	1453	42.7649	2.4534	449.8417	1453	42.7649	2.4534	915.2638
1454	42.7909	2.452	446.8963	1454	42.7909	2.452	900.8138	1454	42.7909	2.452	428.2159	1454	42.7909	2.452	890.94
1455	42.8169	2.4506	427.1039	1455	42.8169	2.4506	880.4639	1455	42.8169	2.4506	429.1743	1455	42.8169	2.4506	889.2005
1456	42.8429	2.4492	375.1118	1456	42.8429	2.4492	827.9144	1456	42.8429	2.4492	425.1492	1456	42.8429	2.4492	882.4774
1457	42.8689	2.4478	389.8372	1457	42.8689	2.4478	842.0822	1457	42.8689	2.4478	426.4109	1457	42.8689	2.4478	881.0411
1458	42.8949	2.4464	396.7565	1458	42.8949	2.4464	848.4441	1458	42.8949	2.4464	456.7347	1458	42.8949	2.4464	908.6669
1459	42.9209	2.4449	360.0713	1459	42.9209	2.4449	811.2014	1459	42.9209	2.4449	422.169	1459	42.9209	2.4449	871.4033
1460	42.9469	2.4435	374.2705	1460	42.9469	2.4435	825.4493	1460	42.9469	2.4435	407.1118	1460	42.9469	2.4435	858.8791
1461	42.9729	2.4421	373.9922	1461	42.9729	2.4421	825.2197	1461	42.9729	2.4421	411.1346	1461	42.9729	2.4421	865.435
1462	42.9989	2.4407	339.1779	1462	42.9989	2.4407	790.4541	1462	42.9989	2.4407	409.3148	1462	42.9989	2.4407	866.1483
1463	43.0249	2.4393	313.918	1463	43.0249	2.4393	765.2429	1463	43.0249	2.4393	418.7485	1463	43.0249	2.4393	878.1151
1464	43.0509	2.4379	312.0391	1464	43.0509	2.4379	763.4127	1464	43.0509	2.4379	388.2366	1464	43.0509	2.4379	850.1362
1465	43.0769	2.4365	351.4233	1465	43.0769	2.4365	802.8456	1465	43.0769	2.4365	346.143	1465	43.0769	2.4365	810.5757
1466	43.1029	2.4351	342.0601	1466	43.1029	2.4351	793.5311	1466	43.1029	2.4351	354.5031	1466	43.1029	2.4351	821.4689
1467	43.1289	2.4337	327.1763	1467	43.1289	2.4337	778.696	1467	43.1289	2.4337	386.3237	1467	43.1289	2.4337	855.8226
1468	43.1549	2.4323	345.9957	1468	43.1549	2.4323	797.5641	1468	43.1549	2.4323	394.62	1468	43.1549	2.4323	866.6519
1469	43.1809	2.4309	321.0585	1469	43.1809	2.4309	772.6755	1469	43.1809	2.4309	395.2424	1469	43.1809	2.4309	869.8074
1470	43.2069	2.4295	293.8512	1470	43.2069	2.4295	745.517	1470	43.2069	2.4295	390.7163	1470	43.2069	2.4295	867.8144
1471	43.2329	2.4281	306.7251	1471	43.2329	2.4281	758.4396	1471	43.2329	2.4281	387.9293	1471	43.2329	2.4281	867.5604

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1472	43.2589	2.4267	336.3852	1472	43.2589	2.4267	788.1483	1472	43.2589	2.4267	376.7115	1472	43.2589	2.4267	858.8757
1473	43.2849	2.4254	351.6682	1473	43.2849	2.4254	803.48	1473	43.2849	2.4254	394.5554	1473	43.2849	2.4254	879.2527
1474	43.3109	2.424	388.8307	1474	43.3109	2.424	840.6912	1474	43.3109	2.424	352.8513	1474	43.3109	2.424	840.0816
1475	43.3369	2.4226	386.3491	1475	43.3369	2.4226	838.2583	1475	43.3369	2.4226	364.9453	1475	43.3369	2.4226	854.7087
1476	43.3629	2.4212	348.0603	1476	43.3629	2.4212	800.0182	1476	43.3629	2.4212	400.8372	1476	43.3629	2.4212	893.1337
1477	43.3889	2.4198	341.0741	1477	43.3889	2.4198	793.0807	1477	43.3889	2.4198	368.2346	1477	43.3889	2.4198	863.0641
1478	43.4149	2.4184	388.7762	1478	43.4149	2.4184	840.8315	1478	43.4149	2.4184	385.5656	1478	43.4149	2.4184	882.9282
1479	43.4409	2.4171	352.9507	1479	43.4409	2.4171	805.0547	1479	43.4409	2.4171	394.6693	1479	43.4409	2.4171	894.5649
1480	43.4669	2.4157	382.3711	1480	43.4669	2.4157	834.5238	1480	43.4669	2.4157	370.9662	1480	43.4669	2.4157	873.3949
1481	43.4929	2.4143	380.2533	1481	43.4929	2.4143	832.4547	1481	43.4929	2.4143	401.6029	1481	43.4929	2.4143	906.5647
1482	43.5189	2.4129	365.394	1482	43.5189	2.4129	817.6441	1482	43.5189	2.4129	369.4712	1482	43.5189	2.4129	876.9661
1483	43.5449	2.4116	422.0191	1483	43.5449	2.4116	874.3178	1483	43.5449	2.4116	369.1833	1483	43.5449	2.4116	879.2113
1484	43.5709	2.4102	453.6924	1484	43.5709	2.4102	906.0398	1484	43.5709	2.4102	366.4124	1484	43.5709	2.4102	878.9734
1485	43.5969	2.4088	379.5627	1485	43.5969	2.4088	831.9588	1485	43.5969	2.4088	409.4123	1485	43.5969	2.4088	924.5064
1486	43.6229	2.4075	360.0713	1486	43.6229	2.4075	812.5161	1486	43.6229	2.4075	422.169	1486	43.6229	2.4075	939.7962
1487	43.6489	2.4061	407.2663	1487	43.6489	2.4061	859.7226	1487	43.6489	2.4061	413.9821	1487	43.6489	2.4061	933.0584
1488	43.6749	2.4047	408.6888	1488	43.6749	2.4047	861.1566	1488	43.6749	2.4047	378.3713	1488	43.6749	2.4047	898.8968
1489	43.7009	2.4034	426.1701	1489	43.7009	2.4034	878.6494	1489	43.7009	2.4034	340.2438	1489	43.7009	2.4034	862.2186
1490	43.7269	2.402	415.9355	1490	43.7269	2.402	868.4263	1490	43.7269	2.402	311.1842	1490	43.7269	2.402	834.6082
1491	43.7529	2.4007	377.3869	1491	43.7529	2.4007	829.8891	1491	43.7529	2.4007	342.4585	1491	43.7529	2.4007	867.3317
1492	43.7789	2.3993	420.9873	1492	43.7789	2.3993	873.501	1492	43.7789	2.3993	326.4424	1492	43.7789	2.3993	852.7648
1493	43.8049	2.398	389.0961	1493	43.8049	2.398	841.6213	1493	43.8049	2.398	325.3228	1493	43.8049	2.398	853.0944
1494	43.8309	2.3966	401.3972	1494	43.8309	2.3966	853.9339	1494	43.8309	2.3966	341.6169	1494	43.8309	2.3966	870.8377
1495	43.8569	2.3953	312.6024	1495	43.8569	2.3953	765.1505	1495	43.8569	2.3953	349.3984	1495	43.8569	2.3953	880.0684
1496	43.8829	2.3939	363.1258	1496	43.8829	2.3939	815.6854	1496	43.8829	2.3939	437.2694	1496	43.8829	2.3939	969.3887
1497	43.9089	2.3926	328.1476	1497	43.9089	2.3926	780.7187	1497	43.9089	2.3926	333.2128	1497	43.9089	2.3926	866.7812
1498	43.9349	2.3912	309.5394	1498	43.9349	2.3912	762.122	1498	43.9349	2.3912	297.3468	1498	43.9349	2.3912	832.3644
1499	43.9609	2.3899	316.1368	1499	43.9609	2.3899	768.7309	1499	43.9609	2.3899	372.029	1499	43.9609	2.3899	908.4958
1500	43.9869	2.3885	389.8885	1500	43.9869	2.3885	842.4941	1500	43.9869	2.3885	290.9022	1500	43.9869	2.3885	828.8182
1501	44.0129	2.3872	376.2421	1501	44.0129	2.3872	828.8592	1501	44.0129	2.3872	331.4997	1501	44.0129	2.3872	870.865
1502	44.0389	2.3858	310.2486	1502	44.0389	2.3858	762.8772	1502	44.0389	2.3858	336.8274	1502	44.0389	2.3858	877.6419
1503	44.0649	2.3845	403.7779	1503	44.0649	2.3845	856.4179	1503	44.0649	2.3845	279.8295	1503	44.0649	2.3845	822.0931
1504	44.0909	2.3832	423.1371	1504	44.0909	2.3832	875.7886	1504	44.0909	2.3832	334.506	1504	44.0909	2.3832	878.2189
1505	44.1169	2.3818	391.1819	1505	44.1169	2.3818	843.8449	1505	44.1169	2.3818	324.761	1505	44.1169	2.3818	869.9231
1506	44.1429	2.3805	415.8696	1506	44.1429	2.3805	868.5441	1506	44.1429	2.3805	323.5268	1506	44.1429	2.3805	870.1381
1507	44.1689	2.3792	449.204	1507	44.1689	2.3792	901.89	1507	44.1689	2.3792	341.9884	1507	44.1689	2.3792	890.0489

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1508	44.1949	2.3778	420.2849	1508	44.1949	2.3778	872.9823	1508	44.1949	2.3778	408.3853	1508	44.1949	2.3778	957.895
1509	44.2209	2.3765	540.2871	1509	44.2209	2.3765	992.9961	1509	44.2209	2.3765	426.6771	1509	44.2209	2.3765	977.636
1510	44.2469	2.3752	514.9611	1510	44.2469	2.3752	967.6815	1510	44.2469	2.3752	465.5746	1510	44.2469	2.3752	1017.9827
1511	44.2729	2.3739	540.031	1511	44.2729	2.3739	992.7629	1511	44.2729	2.3739	392.1947	1511	44.2729	2.3739	946.052
1512	44.2989	2.3725	583.5755	1512	44.2989	2.3725	1036.3189	1512	44.2989	2.3725	393.9159	1512	44.2989	2.3725	949.2225
1513	44.3249	2.3712	626.1374	1513	44.3249	2.3712	1078.8922	1513	44.3249	2.3712	422.169	1513	44.3249	2.3712	978.9248
1514	44.3509	2.3699	555.1285	1514	44.3509	2.3699	1007.8949	1514	44.3509	2.3699	350.1931	1514	44.3509	2.3699	907.8949
1515	44.3769	2.3686	565.954	1515	44.3769	2.3686	1018.7318	1515	44.3769	2.3686	315.1122	1515	44.3769	2.3686	873.7599
1516	44.4029	2.3673	567.1784	1516	44.4029	2.3673	1019.9677	1516	44.4029	2.3673	333.7286	1516	44.4029	2.3673	893.3223
1517	44.4289	2.3659	570.0726	1517	44.4289	2.3659	1022.8734	1517	44.4289	2.3659	282.6968	1517	44.4289	2.3659	843.2364
1518	44.4549	2.3646	536.064	1518	44.4549	2.3646	988.8762	1518	44.4549	2.3646	292.7848	1518	44.4549	2.3646	854.2704
1519	44.4809	2.3633	494.7819	1519	44.4809	2.3633	947.6057	1519	44.4809	2.3633	363.8534	1519	44.4809	2.3633	926.285
1520	44.5069	2.362	439.2666	1520	44.5069	2.362	892.1019	1520	44.5069	2.362	326.7889	1520	44.5069	2.362	890.1663
1521	44.5329	2.3607	457.188	1521	44.5329	2.3607	910.0348	1521	44.5329	2.3607	295.1331	1521	44.5329	2.3607	859.4565
1522	44.5589	2.3594	456.4172	1522	44.5589	2.3594	909.2754	1522	44.5589	2.3594	331.6911	1522	44.5589	2.3594	896.9605
1523	44.5849	2.3581	459.7234	1523	44.5849	2.3581	912.5931	1523	44.5849	2.3581	382.393	1523	44.5849	2.3581	948.6083
1524	44.6109	2.3568	406.8179	1524	44.6109	2.3568	859.6991	1524	44.6109	2.3568	319.3242	1524	44.6109	2.3568	886.4855
1525	44.6369	2.3555	351.7939	1525	44.6369	2.3555	804.6866	1525	44.6369	2.3555	299.3516	1525	44.6369	2.3555	867.4589
1526	44.6629	2.3542	338.1478	1526	44.6629	2.3542	791.052	1526	44.6629	2.3542	277.8397	1526	44.6629	2.3542	846.8929
1527	44.6889	2.3529	404.9123	1527	44.6889	2.3529	857.8279	1527	44.6889	2.3529	307.4855	1527	44.6889	2.3529	877.4847
1528	44.7149	2.3516	401.6457	1528	44.7149	2.3516	854.5728	1528	44.7149	2.3516	323.936	1528	44.7149	2.3516	894.8812
1529	44.7409	2.3503	424.2235	1529	44.7409	2.3503	877.1621	1529	44.7409	2.3503	367.8844	1529	44.7409	2.3503	939.7756
1530	44.7669	2.349	424.077	1530	44.7669	2.349	877.0271	1530	44.7669	2.349	359.4154	1530	44.7669	2.349	932.2525
1531	44.7929	2.3477	434.5029	1531	44.7929	2.3477	887.4645	1531	44.7929	2.3477	350.3036	1531	44.7929	2.3477	924.0866
1532	44.8189	2.3464	423.2745	1532	44.8189	2.3464	876.2475	1532	44.8189	2.3464	374.158	1532	44.8189	2.3464	948.887
1533	44.8449	2.3451	460.7669	1533	44.8449	2.3451	913.7514	1533	44.8449	2.3451	429.665	1533	44.8449	2.3451	1005.34
1534	44.8709	2.3438	493.0995	1534	44.8709	2.3438	946.0955	1534	44.8709	2.3438	449.2703	1534	44.8709	2.3438	1025.8913
1535	44.8969	2.3425	507.5637	1535	44.8969	2.3425	960.5712	1535	44.8969	2.3425	452.7707	1535	44.8969	2.3425	1030.3376
1536	44.9229	2.3413	499.2111	1536	44.9229	2.3413	952.2301	1536	44.9229	2.3413	435.5629	1536	44.9229	2.3413	1014.0758
1537	44.9489	2.34	535.4562	1537	44.9489	2.34	988.4866	1537	44.9489	2.34	465.231	1537	44.9489	2.34	1044.6899
1538	44.9749	2.3387	516.4817	1538	44.9749	2.3387	969.5237	1538	44.9749	2.3387	504.0738	1538	44.9749	2.3387	1084.4786
1539	45.0009	2.3374	455.6596	1539	45.0009	2.3374	908.713	1539	45.0009	2.3374	457.1857	1539	45.0009	2.3374	1038.5364
1540	45.0269	2.3361	495.5728	1540	45.0269	2.3361	948.6377	1540	45.0269	2.3361	464.4278	1540	45.0269	2.3361	1046.7245
1541	45.0529	2.3349	510.7968	1541	45.0529	2.3349	961.364	1541	45.0529	2.3349	450.7279	1541	45.0529	2.3349	1033.9706
1542	45.0789	2.3336	505.6722	1542	45.0789	2.3336	953.7415	1542	45.0789	2.3336	469.2012	1542	45.0789	2.3336	1053.3899
1543	45.1049	2.3323	536.521	1543	45.1049	2.3323	982.0925	1543	45.1049	2.3323	482.6647	1543	45.1049	2.3323	1067.7993

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1544	45.1309	2.331	529.8494	1544	45.1309	2.331	972.9231	1544	45.1309	2.331	509.1357	1544	45.1309	2.331	1095.2163
1545	45.1569	2.3298	507.4645	1545	45.1569	2.3298	948.0404	1545	45.1569	2.3298	505.6939	1545	45.1569	2.3298	1092.7204
1546	45.1829	2.3285	498.9016	1546	45.1829	2.3285	936.9797	1546	45.1829	2.3285	516.1191	1546	45.1829	2.3285	1104.0916
1547	45.2089	2.3272	471.0339	1547	45.2089	2.3272	906.6142	1547	45.2089	2.3272	528.0424	1547	45.2089	2.3272	1116.9608
1548	45.2349	2.3259	468.6707	1548	45.2349	2.3259	901.7532	1548	45.2349	2.3259	535.6377	1548	45.2349	2.3259	1125.5021
1549	45.2609	2.3247	458.4872	1549	45.2609	2.3247	889.0718	1549	45.2609	2.3247	557.3984	1549	45.2609	2.3247	1148.2087
1550	45.2869	2.3234	445.2398	1550	45.2869	2.3234	873.3267	1550	45.2869	2.3234	569.1348	1550	45.2869	2.3234	1160.8911
1551	45.3129	2.3222	430.1407	1551	45.3129	2.3222	855.7297	1551	45.3129	2.3222	522.7642	1551	45.3129	2.3222	1115.4665
1552	45.3389	2.3209	407.4246	1552	45.3389	2.3209	830.5158	1552	45.3389	2.3209	522.6569	1552	45.3389	2.3209	1116.3052
1553	45.3649	2.3196	407.2144	1553	45.3649	2.3196	827.8078	1553	45.3649	2.3196	569.2347	1553	45.3649	2.3196	1163.8289
1554	45.3909	2.3184	403.0907	1554	45.3909	2.3184	821.1864	1554	45.3909	2.3184	585.6878	1554	45.3909	2.3184	1181.228
1555	45.4169	2.3171	403.2097	1555	45.4169	2.3171	818.8076	1555	45.4169	2.3171	575.964	1555	45.4169	2.3171	1172.4502
1556	45.4429	2.3159	401.3374	1556	45.4429	2.3159	814.4375	1556	45.4429	2.3159	549.0178	1556	45.4429	2.3159	1146.4499
1557	45.4689	2.3146	400.2023	1557	45.4689	2.3146	810.8046	1557	45.4689	2.3146	561.2285	1557	45.4689	2.3146	1159.6066
1558	45.4949	2.3134	397.1817	1558	45.4949	2.3134	805.2861	1558	45.4949	2.3134	577.1661	1558	45.4949	2.3134	1176.4901
1559	45.5209	2.3121	377.1613	1559	45.5209	2.3121	782.768	1559	45.5209	2.3121	567.9425	1559	45.5209	2.3121	1168.2125
1560	45.5469	2.3109	377.5764	1560	45.5469	2.3109	780.6852	1560	45.5469	2.3109	569.6267	1560	45.5469	2.3109	1170.8426
1561	45.5729	2.3096	389.3465	1561	45.5729	2.3096	789.9576	1561	45.5729	2.3096	552.9892	1561	45.5729	2.3096	1155.1511
1562	45.5989	2.3084	383.7286	1562	45.5989	2.3084	781.8418	1562	45.5989	2.3084	502.2141	1562	45.5989	2.3084	1105.3219
1563	45.6249	2.3071	366.8501	1563	45.6249	2.3071	762.4655	1563	45.6249	2.3071	472.9489	1563	45.6249	2.3071	1077.0028
1564	45.6509	2.3059	361.3055	1564	45.6509	2.3059	754.4231	1564	45.6509	2.3059	493.6414	1564	45.6509	2.3059	1098.6412
1565	45.6769	2.3046	378.9739	1565	45.6769	2.3046	769.5938	1565	45.6769	2.3046	496.2375	1565	45.6769	2.3046	1102.1832
1566	45.7029	2.3034	371.6554	1566	45.7029	2.3034	759.7775	1566	45.7029	2.3034	487.8986	1566	45.7029	2.3034	1094.7903
1567	45.7289	2.3021	360.0713	1567	45.7289	2.3021	745.6955	1567	45.7289	2.3021	491.8519	1567	45.7289	2.3021	1099.6896
1568	45.7549	2.3009	376.1258	1568	45.7549	2.3009	761.5177	1568	45.7549	2.3009	490.4616	1568	45.7549	2.3009	1097.68
1569	45.7809	2.2997	394.6539	1569	45.7809	2.2997	779.8135	1569	45.7809	2.2997	501.7262	1569	45.7809	2.2997	1108.3255
1570	45.8069	2.2984	414.0962	1570	45.8069	2.2984	799.0235	1570	45.8069	2.2984	486.311	1570	45.8069	2.2984	1092.2912
1571	45.8329	2.2972	442.7811	1571	45.8329	2.2972	827.476	1571	45.8329	2.2972	494.4451	1571	45.8329	2.2972	1099.806
1572	45.8589	2.296	490.136	1572	45.8589	2.296	874.5986	1572	45.8589	2.296	535.6099	1572	45.8589	2.296	1140.3517
1573	45.8849	2.2947	521.8344	1573	45.8849	2.2947	906.0647	1573	45.8849	2.2947	557.6046	1573	45.8849	2.2947	1161.7272
1574	45.9109	2.2935	529.4117	1574	45.9109	2.2935	913.4097	1574	45.9109	2.2935	582.514	1574	45.9109	2.2935	1186.0175
1575	45.9369	2.2923	554.1417	1575	45.9369	2.2923	937.9073	1575	45.9369	2.2923	589.0544	1575	45.9369	2.2923	1191.9387
1576	45.9629	2.2911	646.9063	1576	45.9629	2.2911	1030.4396	1576	45.9629	2.2911	657.6432	1576	45.9629	2.2911	1259.9083
1577	45.9889	2.2898	759.1178	1577	45.9889	2.2898	1142.4188	1577	45.9889	2.2898	740.8013	1577	45.9889	2.2898	1342.4472
1578	46.0149	2.2886	1015.4237	1578	46.0149	2.2886	1398.4924	1578	46.0149	2.2886	916.2486	1578	46.0149	2.2886	1517.2754
1579	46.0409	2.2874	1337.3733	1579	46.0409	2.2874	1720.2097	1579	46.0409	2.2874	1241.0087	1579	46.0409	2.2874	1841.4162

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1580	46.0669	2.2862	1544.2553	1580	46.0669	2.2862	1926.8594	1580	46.0669	2.2862	1581.9343	1580	46.0669	2.2862	2181.7226
1581	46.0929	2.2849	1758.4749	1581	46.0929	2.2849	2140.8467	1581	46.0929	2.2849	2026.8591	1581	46.0929	2.2849	2626.0283
1582	46.1189	2.2837	1985.3986	1582	46.1189	2.2837	2367.5381	1582	46.1189	2.2837	2384.9312	1582	46.1189	2.2837	2983.4812
1583	46.1449	2.2825	2234.3179	1583	46.1449	2.2825	2616.225	1583	46.1449	2.2825	2455.5284	1583	46.1449	2.2825	3053.4592
1584	46.1709	2.2813	2351.9999	1584	46.1709	2.2813	2733.6747	1584	46.1709	2.2813	2386.648	1584	46.1709	2.2813	2983.9597
1585	46.1969	2.2801	2287.8479	1585	46.1969	2.2801	2669.2904	1585	46.1969	2.2801	2269.4509	1585	46.1969	2.2801	2866.1433
1586	46.2229	2.2789	2118.9809	1586	46.2229	2.2789	2500.1911	1586	46.2229	2.2789	2165.7027	1586	46.2229	2.2789	2761.776
1587	46.2489	2.2777	1936.9015	1587	46.2489	2.2777	2317.8793	1587	46.2489	2.2777	2029.4187	1587	46.2489	2.2777	2624.8728
1588	46.2749	2.2765	1771.056	1588	46.2749	2.2765	2151.8016	1588	46.2749	2.2765	1779.0879	1588	46.2749	2.2765	2373.9229
1589	46.3009	2.2752	1616.9389	1589	46.3009	2.2752	1997.4521	1589	46.3009	2.2752	1529.5268	1589	46.3009	2.2752	2123.7426
1590	46.3269	2.274	1426.204	1590	46.3269	2.274	1806.4849	1590	46.3269	2.274	1265.7302	1590	46.3269	2.274	1859.3268
1591	46.3529	2.2728	1318.007	1591	46.3529	2.2728	1698.0556	1591	46.3529	2.2728	1025.4076	1591	46.3529	2.2728	1618.385
1592	46.3789	2.2716	1244.256	1592	46.3789	2.2716	1624.0723	1592	46.3789	2.2716	900.5786	1592	46.3789	2.2716	1492.9368
1593	46.4049	2.2704	1325.1381	1593	46.4049	2.2704	1704.7221	1593	46.4049	2.2704	777.5563	1593	46.4049	2.2704	1369.2954
1594	46.4309	2.2692	1321.0508	1594	46.4309	2.2692	1700.4024	1594	46.4309	2.2692	668.3298	1594	46.4309	2.2692	1259.4497
1595	46.4569	2.268	1390.5318	1595	46.4569	2.268	1769.6511	1595	46.4569	2.268	660.8512	1595	46.4569	2.268	1248.7711
1596	46.4829	2.2668	1480.0714	1596	46.4829	2.2668	1858.9584	1596	46.4829	2.2668	621.276	1596	46.4829	2.2668	1205.9958
1597	46.5089	2.2656	1551.5358	1597	46.5089	2.2656	1930.1905	1597	46.5089	2.2656	510.1521	1597	46.5089	2.2656	1091.672
1598	46.5349	2.2644	1657.1285	1598	46.5349	2.2644	2035.5508	1598	46.5349	2.2644	492.1097	1598	46.5349	2.2644	1070.4295
1599	46.5609	2.2632	1691.8895	1599	46.5609	2.2632	2070.0795	1599	46.5609	2.2632	390.1871	1599	46.5609	2.2632	965.3068
1600	46.5869	2.262	1652.9218	1600	46.5869	2.262	2030.8796	1600	46.5869	2.262	414.33	1600	46.5869	2.262	986.2497
1601	46.6129	2.2609	1663.7826	1601	46.6129	2.2609	2041.508	1601	46.6129	2.2609	457.5664	1601	46.6129	2.2609	1026.2861
1602	46.6389	2.2597	1638.4048	1602	46.6389	2.2597	2015.8979	1602	46.6389	2.2597	423.7772	1602	46.6389	2.2597	989.2969
1603	46.6649	2.2585	1518.8136	1603	46.6649	2.2585	1896.0744	1603	46.6649	2.2585	496.5451	1603	46.6649	2.2585	1058.8647
1604	46.6909	2.2573	1477.99	1604	46.6909	2.2573	1855.0185	1604	46.6909	2.2573	413.3532	1604	46.6909	2.2573	972.4728
1605	46.7169	2.2561	1309.6296	1605	46.7169	2.2561	1686.4257	1605	46.7169	2.2561	418.8797	1605	46.7169	2.2561	974.7993
1606	46.7429	2.2549	1135.2344	1606	46.7429	2.2549	1511.7982	1606	46.7429	2.2549	400.2231	1606	46.7429	2.2549	952.9427
1607	46.7689	2.2537	1053.5494	1607	46.7689	2.2537	1429.8809	1607	46.7689	2.2537	427.8044	1607	46.7689	2.2537	977.324
1608	46.7949	2.2526	975.6205	1608	46.7949	2.2526	1351.7197	1608	46.7949	2.2526	434.8024	1608	46.7949	2.2526	981.122
1609	46.8209	2.2514	898.8065	1609	46.8209	2.2514	1274.6734	1609	46.8209	2.2514	421.9364	1609	46.8209	2.2514	965.056
1610	46.8469	2.2502	822.5502	1610	46.8469	2.2502	1198.1848	1610	46.8469	2.2502	403.7843	1610	46.8469	2.2502	943.7038
1611	46.8729	2.249	662.4722	1611	46.8729	2.249	1037.8745	1611	46.8729	2.249	371.0796	1611	46.8729	2.249	907.7991
1612	46.8989	2.2478	656.0532	1612	46.8989	2.2478	1031.2232	1612	46.8989	2.2478	366.7995	1612	46.8989	2.2478	900.3189
1613	46.9249	2.2467	540.9623	1613	46.9249	2.2467	915.9	1613	46.9249	2.2467	390.6279	1613	46.9249	2.2467	920.9474
1614	46.9509	2.2455	522.3832	1614	46.9509	2.2455	897.0885	1614	46.9509	2.2455	383.9272	1614	46.9509	2.2455	911.0466
1615	46.9769	2.2443	519.5707	1615	46.9769	2.2443	894.0437	1615	46.9769	2.2443	384.1244	1615	46.9769	2.2443	908.0437

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1616	47.0029	2.2431	452.45	1616	47.0029	2.2431	826.6907	1616	47.0029	2.2431	405.8151	1616	47.0029	2.2431	926.5345
1617	47.0289	2.242	430.7146	1617	47.0289	2.242	804.7229	1617	47.0289	2.242	353.4773	1617	47.0289	2.242	870.9966
1618	47.0549	2.2408	415.8892	1618	47.0549	2.2408	789.6652	1618	47.0549	2.2408	368.0598	1618	47.0549	2.2408	882.3791
1619	47.0809	2.2396	416.402	1619	47.0809	2.2396	789.9457	1619	47.0809	2.2396	395.524	1619	47.0809	2.2396	906.6433
1620	47.1069	2.2385	412.0095	1620	47.1069	2.2385	785.321	1620	47.1069	2.2385	404.7598	1620	47.1069	2.2385	912.679
1621	47.1329	2.2373	360.0713	1621	47.1329	2.2373	733.1504	1621	47.1329	2.2373	422.169	1621	47.1329	2.2373	926.8883
1622	47.1589	2.2361	368.0223	1622	47.1589	2.2361	740.9075	1622	47.1589	2.2361	404.4084	1622	47.1589	2.2361	907.8488
1623	47.1849	2.235	372.0268	1623	47.1849	2.235	744.7181	1623	47.1849	2.235	373.9391	1623	47.1849	2.235	876.1006
1624	47.2109	2.2338	312.4626	1624	47.2109	2.2338	684.96	1624	47.2109	2.2338	404.3776	1624	47.2109	2.2338	905.2603
1625	47.2369	2.2327	374.8199	1625	47.2369	2.2327	747.1234	1625	47.2369	2.2327	447.5027	1625	47.2369	2.2327	947.1065
1626	47.2629	2.2315	361.1073	1626	47.2629	2.2315	733.2169	1626	47.2629	2.2315	345.017	1626	47.2629	2.2315	843.342
1627	47.2889	2.2304	374.545	1627	47.2889	2.2304	746.4607	1627	47.2889	2.2304	367.3407	1627	47.2889	2.2304	864.3868
1628	47.3149	2.2292	319.041	1628	47.3149	2.2292	690.7628	1628	47.3149	2.2292	427.3314	1628	47.3149	2.2292	923.0987
1629	47.3409	2.228	379.7323	1629	47.3409	2.228	751.2601	1629	47.3409	2.228	424.814	1629	47.3409	2.228	919.3024
1630	47.3669	2.2269	358.366	1630	47.3669	2.2269	729.7	1630	47.3669	2.2269	438.849	1630	47.3669	2.2269	932.0585
1631	47.3929	2.2257	322.1	1631	47.3929	2.2257	693.2401	1631	47.3929	2.2257	422.4028	1631	47.3929	2.2257	914.3334
1632	47.4189	2.2246	341.3728	1632	47.4189	2.2246	712.319	1632	47.4189	2.2246	443.8505	1632	47.4189	2.2246	934.5022
1633	47.4449	2.2234	325.4636	1633	47.4449	2.2234	696.2159	1633	47.4449	2.2234	440.1385	1633	47.4449	2.2234	929.5114
1634	47.4709	2.2223	328.4106	1634	47.4709	2.2223	698.969	1634	47.4709	2.2223	424.5618	1634	47.4709	2.2223	912.6559
1635	47.4969	2.2211	333.7834	1635	47.4969	2.2211	704.1479	1635	47.4969	2.2211	474.9121	1635	47.4969	2.2211	961.7273
1636	47.5229	2.22	321.6195	1636	47.5229	2.22	691.7901	1636	47.5229	2.22	439.9553	1636	47.5229	2.22	925.4916
1637	47.5489	2.2189	346.4071	1637	47.5489	2.2189	716.3838	1637	47.5489	2.2189	541.0448	1637	47.5489	2.2189	1025.3023
1638	47.5749	2.2177	372.633	1638	47.5749	2.2177	742.4158	1638	47.5749	2.2177	585.3507	1638	47.5749	2.2177	1068.3293
1639	47.6009	2.2166	314.1446	1639	47.6009	2.2166	683.7335	1639	47.6009	2.2166	504.8571	1639	47.6009	2.2166	986.5568
1640	47.6269	2.2154	347.9072	1640	47.6269	2.2154	717.3022	1640	47.6269	2.2154	560.1637	1640	47.6269	2.2154	1040.5846
1641	47.6529	2.2143	351.7952	1641	47.6529	2.2143	720.9963	1641	47.6529	2.2143	571.9445	1641	47.6529	2.2143	1051.0866
1642	47.6789	2.2132	314.422	1642	47.6789	2.2132	683.4292	1642	47.6789	2.2132	548.1989	1642	47.6789	2.2132	1026.0621
1643	47.7049	2.212	339.6893	1643	47.7049	2.212	708.5026	1643	47.7049	2.212	565.7664	1643	47.7049	2.212	1042.3507
1644	47.7309	2.2109	312.8225	1644	47.7309	2.2109	681.4419	1644	47.7309	2.2109	520.183	1644	47.7309	2.2109	995.4885
1645	47.7569	2.2098	309.705	1645	47.7569	2.2098	678.1305	1645	47.7569	2.2098	494.9102	1645	47.7569	2.2098	968.9367
1646	47.7829	2.2086	355.4047	1646	47.7829	2.2086	723.6362	1646	47.7829	2.2086	491.8632	1646	47.7829	2.2086	964.6109
1647	47.8089	2.2075	393.9995	1647	47.8089	2.2075	762.0372	1647	47.8089	2.2075	454.7963	1647	47.8089	2.2075	926.2651
1648	47.8349	2.2064	360.0713	1648	47.8349	2.2064	727.9151	1648	47.8349	2.2064	464.7874	1648	47.8349	2.2064	934.9774
1649	47.8609	2.2052	309.9917	1649	47.8609	2.2052	677.1333	1649	47.8609	2.2052	481.385	1649	47.8609	2.2052	950.2961
1650	47.8869	2.2041	309.5996	1650	47.8869	2.2041	676.0391	1650	47.8869	2.2041	464.2236	1650	47.8869	2.2041	931.8558
1651	47.9129	2.203	332.7117	1651	47.9129	2.203	698.449	1651	47.9129	2.203	416.9536	1651	47.9129	2.203	883.307

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1652	47.9389	2.2019	333.927	1652	47.9389	2.2019	698.9622	1652	47.9389	2.2019	410.7646	1652	47.9389	2.2019	875.8391
1653	47.9649	2.2007	376.5117	1653	47.9649	2.2007	740.8447	1653	47.9649	2.2007	424.8546	1653	47.9649	2.2007	888.6502
1654	47.9909	2.1996	372.659	1654	47.9909	2.1996	736.2899	1654	47.9909	2.1996	420.7033	1654	47.9909	2.1996	883.2201
1655	48.0169	2.1985	380.0862	1655	48.0169	2.1985	743.0149	1655	48.0169	2.1985	400.8718	1655	48.0169	2.1985	862.1097
1656	48.0429	2.1974	380.365	1656	48.0429	2.1974	742.5916	1656	48.0429	2.1974	396.827	1656	48.0429	2.1974	856.7861
1657	48.0689	2.1963	364.9069	1657	48.0689	2.1963	726.4313	1657	48.0689	2.1963	375.5917	1657	48.0689	2.1963	834.2719
1658	48.0949	2.1951	326.6232	1658	48.0949	2.1951	687.4455	1658	48.0949	2.1951	333.6894	1658	48.0949	2.1951	791.0908
1659	48.1209	2.194	342.4335	1659	48.1209	2.194	702.5536	1659	48.1209	2.194	394.2638	1659	48.1209	2.194	850.3863
1660	48.1469	2.1929	369.2648	1660	48.1469	2.1929	728.6828	1660	48.1469	2.1929	390.175	1660	48.1469	2.1929	845.0187
1661	48.1729	2.1918	349.7043	1661	48.1729	2.1918	708.4201	1661	48.1729	2.1918	393.7986	1661	48.1729	2.1918	847.3633
1662	48.1989	2.1907	334.7574	1662	48.1989	2.1907	692.7711	1662	48.1989	2.1907	441.4089	1662	48.1989	2.1907	893.6948
1663	48.2249	2.1896	380.0943	1663	48.2249	2.1896	737.4058	1663	48.2249	2.1896	421.7551	1663	48.2249	2.1896	872.7621
1664	48.2509	2.1885	422.4014	1664	48.2509	2.1885	779.0108	1664	48.2509	2.1885	411.7695	1664	48.2509	2.1885	861.4977
1665	48.2769	2.1874	407.7746	1665	48.2769	2.1874	763.6818	1665	48.2769	2.1874	386.171	1665	48.2769	2.1874	834.6203
1666	48.3029	2.1863	387.8103	1666	48.3029	2.1863	743.0154	1666	48.3029	2.1863	382.2781	1666	48.3029	2.1863	829.4485
1667	48.3289	2.1851	358.5965	1667	48.3289	2.1851	713.0994	1667	48.3289	2.1851	425.6006	1667	48.3289	2.1851	871.4922
1668	48.3549	2.184	364.0952	1668	48.3549	2.184	717.896	1668	48.3549	2.184	418.1936	1668	48.3549	2.184	862.8063
1669	48.3809	2.1829	394.6998	1669	48.3809	2.1829	747.7985	1669	48.3809	2.1829	385.0692	1669	48.3809	2.1829	828.4031
1670	48.4069	2.1818	377.3776	1670	48.4069	2.1818	729.7741	1670	48.4069	2.1818	373.5908	1670	48.4069	2.1818	815.6458
1671	48.4329	2.1807	360.4713	1671	48.4329	2.1807	712.1657	1671	48.4329	2.1807	380.1254	1671	48.4329	2.1807	820.9015
1672	48.4589	2.1796	370.3284	1672	48.4589	2.1796	721.3206	1672	48.4589	2.1796	426.854	1672	48.4589	2.1796	866.3512
1673	48.4849	2.1785	364.6107	1673	48.4849	2.1785	714.9007	1673	48.4849	2.1785	447.8441	1673	48.4849	2.1785	886.0625
1674	48.5109	2.1774	365.0122	1674	48.5109	2.1774	714.6001	1674	48.5109	2.1774	426.2604	1674	48.5109	2.1774	863.2
1675	48.5369	2.1763	360.0713	1675	48.5369	2.1763	708.957	1675	48.5369	2.1763	422.169	1675	48.5369	2.1763	857.8298
1676	48.5629	2.1752	331.3874	1676	48.5629	2.1752	678.2563	1676	48.5629	2.1752	391.9081	1676	48.5629	2.1752	829.769
1677	48.5889	2.1742	328.7741	1677	48.5889	2.1742	673.6262	1677	48.5889	2.1742	379.8901	1677	48.5889	2.1742	819.9512
1678	48.6149	2.1731	338.8776	1678	48.6149	2.1731	681.7127	1678	48.6149	2.1731	431.9371	1678	48.6149	2.1731	874.1984
1679	48.6409	2.172	337.0439	1679	48.6409	2.172	677.8622	1679	48.6409	2.172	389.3969	1679	48.6409	2.172	833.8583
1680	48.6669	2.1709	376.5625	1680	48.6669	2.1709	715.364	1680	48.6669	2.1709	337.4047	1680	48.6669	2.1709	784.0664
1681	48.6929	2.1698	392.0519	1681	48.6929	2.1698	728.8365	1681	48.6929	2.1698	390.3183	1681	48.6929	2.1698	839.1802
1682	48.7189	2.1687	339.1247	1682	48.7189	2.1687	673.8924	1682	48.7189	2.1687	425.2586	1682	48.7189	2.1687	876.3206
1683	48.7449	2.1676	335.1733	1683	48.7449	2.1676	667.9242	1683	48.7449	2.1676	431.816	1683	48.7449	2.1676	885.0783
1684	48.7709	2.1665	378.2347	1684	48.7709	2.1665	708.9687	1684	48.7709	2.1665	446.936	1684	48.7709	2.1665	902.3984
1685	48.7969	2.1655	336.5764	1685	48.7969	2.1655	665.2936	1685	48.7969	2.1655	428.2127	1685	48.7969	2.1655	885.8753
1686	48.8229	2.1644	312.099	1686	48.8229	2.1644	638.7994	1686	48.8229	2.1644	388.5753	1686	48.8229	2.1644	848.4381
1687	48.8489	2.1633	346.4847	1687	48.8489	2.1633	671.1681	1687	48.8489	2.1633	397.4037	1687	48.8489	2.1633	859.4667

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1688	48.8749	2.1622	360.3385	1688	48.8749	2.1622	683.0051	1688	48.8749	2.1622	437.3528	1688	48.8749	2.1622	901.6161
1689	48.9009	2.1611	370.3081	1689	48.9009	2.1611	690.9579	1689	48.9009	2.1611	443.964	1689	48.9009	2.1611	910.4274
1690	48.9269	2.1601	355.017	1690	48.9269	2.1601	673.6499	1690	48.9269	2.1601	400.1614	1690	48.9269	2.1601	868.825
1691	48.9529	2.159	372.1165	1691	48.9529	2.159	688.7325	1691	48.9529	2.159	406.4278	1691	48.9529	2.159	877.2916
1692	48.9789	2.1579	332.257	1692	48.9789	2.1579	646.8561	1692	48.9789	2.1579	403.4121	1692	48.9789	2.1579	876.4761
1693	49.0049	2.1568	372.8195	1693	49.0049	2.1568	685.4018	1693	49.0049	2.1568	464.2584	1693	49.0049	2.1568	939.5226
1694	49.0309	2.1558	392.3566	1694	49.0309	2.1558	702.9221	1694	49.0309	2.1558	412.9154	1694	49.0309	2.1558	890.3797
1695	49.0569	2.1547	353.4932	1695	49.0569	2.1547	662.0418	1695	49.0569	2.1547	408.3842	1695	49.0569	2.1547	888.0487
1696	49.0829	2.1536	359.4637	1696	49.0829	2.1536	665.9954	1696	49.0829	2.1536	429.7775	1696	49.0829	2.1536	911.6423
1697	49.1089	2.1525	388.8955	1697	49.1089	2.1525	693.4104	1697	49.1089	2.1525	383.3401	1697	49.1089	2.1525	867.4051
1698	49.1349	2.1515	351.2825	1698	49.1349	2.1515	653.7806	1698	49.1349	2.1515	385.6126	1698	49.1349	2.1515	871.8777
1699	49.1609	2.1504	357.8085	1699	49.1609	2.1504	658.2896	1699	49.1609	2.1504	355.9554	1699	49.1609	2.1504	844.4207
1700	49.1869	2.1493	338.5066	1700	49.1869	2.1493	636.9709	1700	49.1869	2.1493	387.7292	1700	49.1869	2.1493	878.3947
1701	49.2129	2.1483	369.6278	1701	49.2129	2.1483	666.0753	1701	49.2129	2.1483	293.7423	1701	49.2129	2.1483	786.608
1702	49.2389	2.1472	360.0713	1702	49.2389	2.1472	654.5019	1702	49.2389	2.1472	422.169	1702	49.2389	2.1472	917.235
1703	49.2649	2.1461	325.8381	1703	49.2649	2.1461	622.6335	1703	49.2649	2.1461	380.1557	1703	49.2649	2.1461	876.9381
1704	49.2909	2.1451	382.9188	1704	49.2909	2.1451	682.079	1704	49.2909	2.1451	327.7381	1704	49.2909	2.1451	826.2369
1705	49.3169	2.144	371.2736	1705	49.3169	2.144	672.7986	1705	49.3169	2.144	306.1282	1705	49.3169	2.144	806.3434
1706	49.3429	2.143	361.8947	1706	49.3429	2.143	665.7845	1706	49.3429	2.143	342.5313	1706	49.3429	2.143	844.463
1707	49.3689	2.1419	405.1256	1707	49.3689	2.1419	711.3803	1707	49.3689	2.1419	292.3838	1707	49.3689	2.1419	796.0319
1708	49.3949	2.1409	308.325	1708	49.3949	2.1409	616.9444	1708	49.3949	2.1409	317.8258	1708	49.3949	2.1409	823.1903
1709	49.4209	2.1398	349.8576	1709	49.4209	2.1398	660.8418	1709	49.4209	2.1398	334.2354	1709	49.4209	2.1398	841.3163
1710	49.4469	2.1387	346.3631	1710	49.4469	2.1387	659.7121	1710	49.4469	2.1387	338.6306	1710	49.4469	2.1387	847.428
1711	49.4729	2.1377	381.6943	1711	49.4729	2.1377	697.4082	1711	49.4729	2.1377	345.5984	1711	49.4729	2.1377	856.1122
1712	49.4989	2.1366	362.0132	1712	49.4989	2.1366	680.0918	1712	49.4989	2.1366	317.4024	1712	49.4989	2.1366	829.6327
1713	49.5249	2.1356	362.9309	1713	49.5249	2.1356	683.3743	1713	49.5249	2.1356	299.9099	1713	49.5249	2.1356	813.8566
1714	49.5509	2.1345	313.4097	1714	49.5509	2.1345	636.2179	1714	49.5509	2.1345	287.533	1714	49.5509	2.1345	803.1961
1715	49.5769	2.1335	380.3503	1715	49.5769	2.1335	705.5233	1715	49.5769	2.1335	348.1914	1715	49.5769	2.1335	865.571
1716	49.6029	2.1324	365.6797	1716	49.6029	2.1324	693.2175	1716	49.6029	2.1324	266.276	1716	49.6029	2.1324	785.372
1717	49.6289	2.1314	284.2563	1717	49.6289	2.1314	614.159	1717	49.6289	2.1314	288.4946	1717	49.6289	2.1314	809.307
1718	49.6549	2.1303	345.2453	1718	49.6549	2.1303	677.5128	1718	49.6549	2.1303	356.8376	1718	49.6549	2.1303	879.3665
1719	49.6809	2.1293	379.6938	1719	49.6809	2.1293	714.326	1719	49.6809	2.1293	326.2891	1719	49.6809	2.1293	850.5345
1720	49.7069	2.1283	383.7208	1720	49.7069	2.1283	720.7179	1720	49.7069	2.1283	372.1044	1720	49.7069	2.1283	898.0661
1721	49.7329	2.1272	350.8274	1721	49.7329	2.1272	690.1893	1721	49.7329	2.1272	366.7862	1721	49.7329	2.1272	894.4644
1722	49.7589	2.1262	359.2056	1722	49.7589	2.1262	700.9323	1722	49.7589	2.1262	330.4272	1722	49.7589	2.1262	859.8218
1723	49.7849	2.1251	352.4256	1723	49.7849	2.1251	696.5171	1723	49.7849	2.1251	367.0105	1723	49.7849	2.1251	898.1215

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1724	49.8109	2.1241	339.6009	1724	49.8109	2.1241	686.0572	1724	49.8109	2.1241	367.3647	1724	49.8109	2.1241	900.1922
1725	49.8369	2.1231	341.5427	1725	49.8369	2.1231	690.3638	1725	49.8369	2.1231	467.3684	1725	49.8369	2.1231	1001.9123
1726	49.8629	2.122	391.9728	1726	49.8629	2.122	743.1587	1726	49.8629	2.122	454.7545	1726	49.8629	2.122	991.0148
1727	49.8889	2.121	336.1348	1727	49.8889	2.121	689.6855	1727	49.8889	2.121	488.4846	1727	49.8889	2.121	1026.4614
1728	49.9149	2.12	374.3439	1728	49.9149	2.12	730.2594	1728	49.9149	2.12	576.9984	1728	49.9149	2.12	1116.6917
1729	49.9409	2.1189	360.0713	1729	49.9409	2.1189	718.3516	1729	49.9409	2.1189	633.0128	1729	49.9409	2.1189	1174.4225
1730	49.9669	2.1179	355.4498	1730	49.9669	2.1179	714.1556	1730	49.9669	2.1179	688.6376	1730	49.9669	2.1179	1229.2839
1731	49.9929	2.1169	340.6832	1731	49.9929	2.1169	699.8146	1731	49.9929	2.1169	748.183	1731	49.9929	2.1169	1288.066
1732	50.0189	2.1158	362.1783	1732	50.0189	2.1158	721.7353	1732	50.0189	2.1158	666.535	1732	50.0189	2.1158	1205.6547
1733	50.0449	2.1148	392.2696	1733	50.0449	2.1148	752.2523	1733	50.0449	2.1148	639.4977	1733	50.0449	2.1148	1177.8541
1734	50.0709	2.1138	350.1164	1734	50.0709	2.1138	710.5246	1734	50.0709	2.1138	699.5616	1734	50.0709	2.1138	1237.1547
1735	50.0969	2.1127	369.956	1735	50.0969	2.1127	730.7898	1735	50.0969	2.1127	630.1325	1735	50.0969	2.1127	1166.9623
1736	50.1229	2.1117	395.7915	1736	50.1229	2.1117	757.0509	1736	50.1229	2.1117	582.2495	1736	50.1229	2.1117	1118.316
1737	50.1489	2.1107	404.9644	1737	50.1489	2.1107	766.6494	1737	50.1489	2.1107	523.7785	1737	50.1489	2.1107	1059.0817
1738	50.1749	2.1097	441.0784	1738	50.1749	2.1097	803.189	1738	50.1749	2.1097	480.391	1738	50.1749	2.1097	1014.9308
1739	50.2009	2.1087	434.8527	1739	50.2009	2.1087	797.3888	1739	50.2009	2.1087	561.32	1739	50.2009	2.1087	1095.0966
1740	50.2269	2.1076	487.1587	1740	50.2269	2.1076	850.1204	1740	50.2269	2.1076	478.4716	1740	50.2269	2.1076	1011.4849
1741	50.2529	2.1066	501.4662	1741	50.2529	2.1066	864.8535	1741	50.2529	2.1066	420.8993	1741	50.2529	2.1066	953.1493
1742	50.2789	2.1056	541.2539	1742	50.2789	2.1056	905.0667	1742	50.2789	2.1056	414.5133	1742	50.2789	2.1056	946
1743	50.3049	2.1046	480.2174	1743	50.3049	2.1046	844.4558	1743	50.3049	2.1046	390.2388	1743	50.3049	2.1046	920.9622
1744	50.3309	2.1036	526.2294	1744	50.3309	2.1036	890.8934	1744	50.3309	2.1036	425.4829	1744	50.3309	2.1036	955.443
1745	50.3569	2.1025	541.2179	1745	50.3569	2.1025	906.3075	1745	50.3569	2.1025	412.8093	1745	50.3569	2.1025	942.006
1746	50.3829	2.1015	585.5904	1746	50.3829	2.1015	951.1056	1746	50.3829	2.1015	455.7857	1746	50.3829	2.1015	984.2192
1747	50.4089	2.1005	596.2214	1747	50.4089	2.1005	962.1621	1747	50.4089	2.1005	483.0056	1747	50.4089	2.1005	1010.6757
1748	50.4349	2.0995	622.9214	1748	50.4349	2.0995	989.2877	1748	50.4349	2.0995	499.4056	1748	50.4349	2.0995	1026.3124
1749	50.4609	2.0985	778.9004	1749	50.4609	2.0985	1145.6923	1749	50.4609	2.0985	589.8356	1749	50.4609	2.0985	1115.9791
1750	50.4869	2.0975	906.6849	1750	50.4869	2.0975	1273.9024	1750	50.4869	2.0975	733.7359	1750	50.4869	2.0975	1259.1161
1751	50.5129	2.0965	1081.9982	1751	50.5129	2.0965	1449.6413	1751	50.5129	2.0965	940.7483	1751	50.5129	2.0965	1465.3651
1752	50.5389	2.0955	1313.935	1752	50.5389	2.0955	1682.0036	1752	50.5389	2.0955	1345.5617	1752	50.5389	2.0955	1869.4153
1753	50.5649	2.0945	1515.8761	1753	50.5649	2.0945	1884.3704	1753	50.5649	2.0945	1677.6227	1753	50.5649	2.0945	2200.713
1754	50.5909	2.0935	1750.9723	1754	50.5909	2.0935	2119.8922	1754	50.5909	2.0935	1826.6889	1754	50.5909	2.0935	2349.0159
1755	50.6169	2.0925	1992.4181	1755	50.6169	2.0925	2361.7635	1755	50.6169	2.0925	1915.9292	1755	50.6169	2.0925	2437.4928
1756	50.6429	2.0914	2152.4214	1756	50.6429	2.0914	2522.1924	1756	50.6429	2.0914	1862.2432	1756	50.6429	2.0914	2383.0435
1757	50.6689	2.0904	2111.0356	1757	50.6689	2.0904	2478.7673	1757	50.6689	2.0904	1774.4461	1757	50.6689	2.0904	2294.4831
1758	50.6949	2.0894	1858.9186	1758	50.6949	2.0894	2224.611	1758	50.6949	2.0894	1772.7222	1758	50.6949	2.0894	2291.996
1759	50.7209	2.0884	1699.4222	1759	50.7209	2.0884	2063.0753	1759	50.7209	2.0884	1667.9317	1759	50.7209	2.0884	2186.4421

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1760	50.7469	2.0874	1577.5955	1760	50.7469	2.0874	1939.2092	1760	50.7469	2.0874	1424.4605	1760	50.7469	2.0874	1942.2077
1761	50.7729	2.0864	1413.2049	1761	50.7729	2.0864	1772.7794	1761	50.7729	2.0864	1244.6559	1761	50.7729	2.0864	1761.6397
1762	50.7989	2.0854	1260.9553	1762	50.7989	2.0854	1618.4904	1762	50.7989	2.0854	1097.7331	1762	50.7989	2.0854	1613.9536
1763	50.8249	2.0845	1132.846	1763	50.8249	2.0845	1488.3418	1763	50.8249	2.0845	968.7061	1763	50.8249	2.0845	1484.1633
1764	50.8509	2.0835	1011.4938	1764	50.8509	2.0835	1364.9503	1764	50.8509	2.0835	950.5721	1764	50.8509	2.0835	1465.2659
1765	50.8769	2.0825	980.343	1765	50.8769	2.0825	1331.7602	1765	50.8769	2.0825	882.087	1765	50.8769	2.0825	1396.0176
1766	50.9029	2.0815	1052.3642	1766	50.9029	2.0815	1401.7421	1766	50.9029	2.0815	757.2962	1766	50.9029	2.0815	1270.4635
1767	50.9289	2.0805	1132.3846	1767	50.9289	2.0805	1479.7231	1767	50.9289	2.0805	733.913	1767	50.9289	2.0805	1246.3169
1768	50.9549	2.0795	1212.87	1768	50.9549	2.0795	1558.1693	1768	50.9549	2.0795	749.4247	1768	50.9549	2.0795	1261.0654
1769	50.9809	2.0785	1249.7713	1769	50.9809	2.0785	1593.0313	1769	50.9809	2.0785	736.3158	1769	50.9809	2.0785	1247.1932
1770	51.0069	2.0775	1304.7631	1770	51.0069	2.0775	1645.9838	1770	51.0069	2.0775	714.7265	1770	51.0069	2.0775	1224.8406
1771	51.0329	2.0765	1349.5047	1771	51.0329	2.0765	1688.686	1771	51.0329	2.0765	746.0281	1771	51.0329	2.0765	1255.3788
1772	51.0589	2.0755	1335.2789	1772	51.0589	2.0755	1672.421	1772	51.0589	2.0755	819.6488	1772	51.0589	2.0755	1328.2362
1773	51.0849	2.0746	1331.0372	1773	51.0849	2.0746	1666.1399	1773	51.0849	2.0746	884.0094	1773	51.0849	2.0746	1391.8335
1774	51.1109	2.0736	1257.9936	1774	51.1109	2.0736	1591.057	1774	51.1109	2.0736	1024.5042	1774	51.1109	2.0736	1531.565
1775	51.1369	2.0726	1174.9652	1775	51.1369	2.0726	1505.9893	1775	51.1369	2.0726	1202.2728	1775	51.1369	2.0726	1708.5703
1776	51.1629	2.0716	1150.1446	1776	51.1629	2.0716	1479.1293	1776	51.1629	2.0716	1341.9485	1776	51.1629	2.0716	1847.4827
1777	51.1889	2.0706	1084.2641	1777	51.1889	2.0706	1411.2095	1777	51.1889	2.0706	1524.8686	1777	51.1889	2.0706	2029.6394
1778	51.2149	2.0696	1013.8129	1778	51.2149	2.0696	1338.719	1778	51.2149	2.0696	1686.4692	1778	51.2149	2.0696	2190.4767
1779	51.2409	2.0687	961.2362	1779	51.2409	2.0687	1284.1031	1779	51.2409	2.0687	1905.0386	1779	51.2409	2.0687	2408.2828
1780	51.2669	2.0677	919.4443	1780	51.2669	2.0677	1240.2718	1780	51.2669	2.0677	2231.5985	1780	51.2669	2.0677	2734.0795
1781	51.2929	2.0667	801.1968	1781	51.2929	2.0667	1119.985	1781	51.2929	2.0667	2565.3465	1781	51.2929	2.0667	3067.0642
1782	51.3189	2.0657	766.441	1782	51.3189	2.0657	1083.1899	1782	51.3189	2.0657	2897.5151	1782	51.3189	2.0657	3398.4695
1783	51.3449	2.0648	692.8318	1783	51.3449	2.0648	1007.5414	1783	51.3449	2.0648	3050.5227	1783	51.3449	2.0648	3550.7137
1784	51.3709	2.0638	658.1771	1784	51.3709	2.0638	970.8474	1784	51.3709	2.0638	3170.0151	1784	51.3709	2.0638	3666.9631
1785	51.3969	2.0628	603.2512	1785	51.3969	2.0628	913.8822	1785	51.3969	2.0628	3268.4896	1785	51.3969	2.0628	3762.1945
1786	51.4229	2.0618	589.2908	1786	51.4229	2.0618	897.8824	1786	51.4229	2.0618	3193.6999	1786	51.4229	2.0618	3684.1618
1787	51.4489	2.0609	519.4114	1787	51.4489	2.0609	825.9637	1787	51.4489	2.0609	2922.5091	1787	51.4489	2.0609	3409.7279
1788	51.4749	2.0599	504.0906	1788	51.4749	2.0599	808.6036	1788	51.4749	2.0599	2693.3834	1788	51.4749	2.0599	3177.3592
1789	51.5009	2.0589	516.5792	1789	51.5009	2.0589	819.053	1789	51.5009	2.0589	2493.5393	1789	51.5009	2.0589	2974.272
1790	51.5269	2.058	474.5931	1790	51.5269	2.058	775.0275	1790	51.5269	2.058	2170.6595	1790	51.5269	2.058	2648.1492
1791	51.5529	2.057	441.7373	1791	51.5529	2.057	740.1324	1791	51.5529	2.057	1998.0665	1791	51.5529	2.057	2472.3131
1792	51.5789	2.056	407.6653	1792	51.5789	2.056	704.0211	1792	51.5789	2.056	1731.2024	1792	51.5789	2.056	2202.206
1793	51.6049	2.0551	421.5552	1793	51.6049	2.0551	715.8716	1793	51.6049	2.0551	1459.4908	1793	51.6049	2.0551	1927.2513
1794	51.6309	2.0541	375.7934	1794	51.6309	2.0541	668.0706	1794	51.6309	2.0541	1319.9647	1794	51.6309	2.0541	1784.4822
1795	51.6569	2.0531	395.9764	1795	51.6569	2.0531	686.2142	1795	51.6569	2.0531	1111.2222	1795	51.6569	2.0531	1572.4966

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1796	51.6829	2.0522	381.8332	1796	51.6829	2.0522	670.0318	1796	51.6829	2.0522	966.915	1796	51.6829	2.0522	1424.9464
1797	51.7089	2.0512	393.07	1797	51.7089	2.0512	679.2292	1797	51.7089	2.0512	880.5124	1797	51.7089	2.0512	1335.3007
1798	51.7349	2.0502	373.6391	1798	51.7349	2.0502	657.759	1798	51.7349	2.0502	796.5978	1798	51.7349	2.0502	1248.143
1799	51.7609	2.0493	357.1554	1799	51.7609	2.0493	639.2361	1799	51.7609	2.0493	726.733	1799	51.7609	2.0493	1175.0353
1800	51.7869	2.0483	374.1044	1800	51.7869	2.0483	654.1457	1800	51.7869	2.0483	622.9935	1800	51.7869	2.0483	1068.0527
1801	51.8129	2.0474	387.1442	1801	51.8129	2.0474	665.1462	1801	51.8129	2.0474	608.0503	1801	51.8129	2.0474	1049.8665
1802	51.8389	2.0464	351.4557	1802	51.8389	2.0464	627.4183	1802	51.8389	2.0464	564.568	1802	51.8389	2.0464	1003.1411
1803	51.8649	2.0455	379.7158	1803	51.8649	2.0455	653.6392	1803	51.8649	2.0455	551.4306	1803	51.8649	2.0455	986.7607
1804	51.8909	2.0445	360.7495	1804	51.8909	2.0445	632.6335	1804	51.8909	2.0445	563.3518	1804	51.8909	2.0445	995.4388
1805	51.9169	2.0436	389.1497	1805	51.9169	2.0436	658.9945	1805	51.9169	2.0436	466.2434	1805	51.9169	2.0436	895.0873
1806	51.9429	2.0426	367.0829	1806	51.9429	2.0426	634.8884	1806	51.9429	2.0426	409.8362	1806	51.9429	2.0426	835.4371
1807	51.9689	2.0417	399.2783	1807	51.9689	2.0417	665.0444	1807	51.9689	2.0417	442.7036	1807	51.9689	2.0417	865.0614
1808	51.9949	2.0407	412.7803	1808	51.9949	2.0407	676.5071	1808	51.9949	2.0407	500.7165	1808	51.9949	2.0407	919.8312
1809	52.0209	2.0398	405.1668	1809	52.0209	2.0398	666.8543	1809	52.0209	2.0398	459.527	1809	52.0209	2.0398	875.3987
1810	52.0469	2.0388	360.0713	1810	52.0469	2.0388	619.7195	1810	52.0469	2.0388	422.169	1810	52.0469	2.0388	834.7977
1811	52.0729	2.0379	390.5327	1811	52.0729	2.0379	650.1301	1811	52.0729	2.0379	419.8138	1811	52.0729	2.0379	830.065
1812	52.0989	2.0369	348.6967	1812	52.0989	2.0369	608.2432	1812	52.0989	2.0369	400.1261	1812	52.0989	2.0369	808
1813	52.1249	2.036	418.2144	1813	52.1249	2.036	677.71	1813	52.1249	2.036	403.6062	1813	52.1249	2.036	809.1027
1814	52.1509	2.035	357.9905	1814	52.1509	2.035	617.4353	1814	52.1509	2.035	457.1082	1814	52.1509	2.035	860.2273
1815	52.1769	2.0341	397.607	1815	52.1769	2.0341	657.001	1815	52.1769	2.0341	389.2429	1815	52.1769	2.0341	789.9846
1816	52.2029	2.0331	398.6479	1816	52.2029	2.0331	657.991	1816	52.2029	2.0331	375.7791	1816	52.2029	2.0331	774.1434
1817	52.2289	2.0322	381.0476	1817	52.2289	2.0322	640.3399	1817	52.2289	2.0322	456.5025	1817	52.2289	2.0322	852.4893
1818	52.2549	2.0313	371.0467	1818	52.2549	2.0313	630.2881	1818	52.2549	2.0313	375.8966	1818	52.2549	2.0313	769.5061
1819	52.2809	2.0303	372.732	1819	52.2809	2.0303	631.9225	1819	52.2809	2.0303	380.5743	1819	52.2809	2.0303	771.8064
1820	52.3069	2.0294	373.8116	1820	52.3069	2.0294	632.9513	1820	52.3069	2.0294	361.2643	1820	52.3069	2.0294	750.119
1821	52.3329	2.0284	358.8483	1821	52.3329	2.0284	617.9372	1821	52.3329	2.0284	317.3342	1821	52.3329	2.0284	703.8115
1822	52.3589	2.0275	316.9758	1822	52.3589	2.0275	576.0138	1822	52.3589	2.0275	333.6672	1822	52.3589	2.0275	717.7671
1823	52.3849	2.0266	389.5826	1823	52.3849	2.0266	648.5698	1823	52.3849	2.0266	360.3171	1823	52.3849	2.0266	742.0396
1824	52.4109	2.0256	342.2757	1824	52.4109	2.0256	601.212	1824	52.4109	2.0256	364.6549	1824	52.4109	2.0256	744
1825	52.4369	2.0247	358.7563	1825	52.4369	2.0247	617.6417	1825	52.4369	2.0247	376.9514	1825	52.4369	2.0247	753.9191
1826	52.4629	2.0238	360.2736	1826	52.4629	2.0238	619.1082	1826	52.4629	2.0238	409.8396	1826	52.4629	2.0238	784.4299
1827	52.4889	2.0228	395.492	1827	52.4889	2.0228	654.2758	1827	52.4889	2.0228	396.3854	1827	52.4889	2.0228	768.5983
1828	52.5149	2.0219	378.4678	1828	52.5149	2.0219	637.2007	1828	52.5149	2.0219	397.9085	1828	52.5149	2.0219	767.7439
1829	52.5409	2.021	383.9384	1829	52.5409	2.021	642.6205	1829	52.5409	2.021	403.9901	1829	52.5409	2.021	771.4482
1830	52.5669	2.0201	391.3337	1830	52.5669	2.0201	649.9649	1830	52.5669	2.0201	400.1023	1830	52.5669	2.0201	765.183
1831	52.5929	2.0191	373.0489	1831	52.5929	2.0191	631.6293	1831	52.5929	2.0191	432.4583	1831	52.5929	2.0191	795.1616

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1832	52.6189	2.0182	381.9547	1832	52.6189	2.0182	640.4842	1832	52.6189	2.0182	397.3954	1832	52.6189	2.0182	757.7213
1833	52.6449	2.0173	354.094	1833	52.6449	2.0173	612.5727	1833	52.6449	2.0173	392.6962	1833	52.6449	2.0173	750.6447
1834	52.6709	2.0163	349.197	1834	52.6709	2.0163	607.6249	1834	52.6709	2.0163	443.3627	1834	52.6709	2.0163	798.9338
1835	52.6969	2.0154	417.8368	1835	52.6969	2.0154	676.2138	1835	52.6969	2.0154	377.3573	1835	52.6969	2.0154	730.551
1836	52.7229	2.0145	387.9109	1836	52.7229	2.0145	646.237	1836	52.7229	2.0145	414.8726	1836	52.7229	2.0145	765.6889
1837	52.7489	2.0136	360.0713	1837	52.7489	2.0136	618.3466	1837	52.7489	2.0136	422.169	1837	52.7489	2.0136	770.6079
1838	52.7749	2.0127	387.103	1838	52.7749	2.0127	646.4554	1838	52.7749	2.0127	400.2887	1838	52.7749	2.0127	747.1358
1839	52.8009	2.0117	395.5704	1839	52.8009	2.0117	656	1839	52.8009	2.0117	397.2704	1839	52.8009	2.0117	742.5257
1840	52.8269	2.0108	368.8945	1840	52.8269	2.0108	630.4013	1840	52.8269	2.0108	418.1592	1840	52.8269	2.0108	761.8226
1841	52.8529	2.0099	347.5284	1841	52.8529	2.0099	610.1123	1841	52.8529	2.0099	422.9565	1841	52.8529	2.0099	765.0281
1842	52.8789	2.009	373.1274	1842	52.8789	2.009	636.7885	1842	52.8789	2.009	397.1301	1842	52.8789	2.009	737.6099
1843	52.9049	2.0081	376.7536	1843	52.9049	2.0081	641.4918	1843	52.9049	2.0081	392.0046	1843	52.9049	2.0081	730.8925
1844	52.9309	2.0072	372.4714	1844	52.9309	2.0072	638.2868	1844	52.9309	2.0072	446.0553	1844	52.9309	2.0072	783.3515
1845	52.9569	2.0062	346.4922	1845	52.9569	2.0062	613.3848	1845	52.9569	2.0062	416.2521	1845	52.9569	2.0062	751.9564
1846	52.9829	2.0053	366.9254	1846	52.9829	2.0053	634.895	1846	52.9829	2.0053	382.0201	1846	52.9829	2.0053	716.1326
1847	53.0089	2.0044	373.8021	1847	53.0089	2.0044	642.849	1847	53.0089	2.0044	386.3642	1847	53.0089	2.0044	718.8848
1848	53.0349	2.0035	345.6291	1848	53.0349	2.0035	615.7531	1848	53.0349	2.0035	397.4594	1848	53.0349	2.0035	728.3882
1849	53.0609	2.0026	356.025	1849	53.0609	2.0026	627.2261	1849	53.0609	2.0026	391.709	1849	53.0609	2.0026	721.0459
1850	53.0869	2.0017	361.4923	1850	53.0869	2.0017	633.7706	1850	53.0869	2.0017	403.2895	1850	53.0869	2.0017	731.0347
1851	53.1129	2.0008	333.8255	1851	53.1129	2.0008	607.1809	1851	53.1129	2.0008	386.4526	1851	53.1129	2.0008	712.6059
1852	53.1389	1.9999	343.0194	1852	53.1389	1.9999	617.4519	1852	53.1389	1.9999	412.1025	1852	53.1389	1.9999	736.664
1853	53.1649	1.999	369.2164	1853	53.1649	1.999	644.7261	1853	53.1649	1.999	447.2608	1853	53.1649	1.999	770.2305
1854	53.1909	1.9981	386.851	1854	53.1909	1.9981	663.4379	1854	53.1909	1.9981	425.5365	1854	53.1909	1.9981	746.9144
1855	53.2169	1.9971	388.7115	1855	53.2169	1.9971	666.3756	1855	53.2169	1.9971	390.696	1855	53.2169	1.9971	710.482
1856	53.2429	1.9962	410.213	1856	53.2429	1.9962	688.9542	1856	53.2429	1.9962	401.0068	1856	53.2429	1.9962	719.201
1857	53.2689	1.9953	375.3541	1857	53.2689	1.9953	655.1724	1857	53.2689	1.9953	421.6557	1857	53.2689	1.9953	738.258
1858	53.2949	1.9944	347.8676	1858	53.2949	1.9944	628.7631	1858	53.2949	1.9944	395.9771	1858	53.2949	1.9944	710.9877
1859	53.3209	1.9935	371.5231	1859	53.3209	1.9935	653.4958	1859	53.3209	1.9935	375.1457	1859	53.3209	1.9935	688.5644
1860	53.3469	1.9926	349.0193	1860	53.3469	1.9926	632.0691	1860	53.3469	1.9926	391.0346	1860	53.3469	1.9926	702.8615
1861	53.3729	1.9917	377.0493	1861	53.3729	1.9917	661.1763	1861	53.3729	1.9917	392.8742	1861	53.3729	1.9917	703.1093
1862	53.3989	1.9908	395.996	1862	53.3989	1.9908	681.2001	1862	53.3989	1.9908	408.3451	1862	53.3989	1.9908	716.9884
1863	53.4249	1.9899	374.3916	1863	53.4249	1.9899	660.6728	1863	53.4249	1.9899	440.9671	1863	53.4249	1.9899	748.0185
1864	53.4509	1.989	396.2028	1864	53.4509	1.989	683.5612	1864	53.4509	1.989	422.169	1864	53.4509	1.989	727.6286
1865	53.4769	1.9881	412.0499	1865	53.4769	1.9881	700.4855	1865	53.4769	1.9881	388.5874	1865	53.4769	1.9881	692.9418
1866	53.5029	1.9873	414.9314	1866	53.5029	1.9873	704.4442	1866	53.5029	1.9873	426.8091	1866	53.5029	1.9873	730.0584
1867	53.5289	1.9864	415.5301	1867	53.5289	1.9864	706.12	1867	53.5289	1.9864	430.1456	1867	53.5289	1.9864	732.2898

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1868	53.5549	1.9855	421.2598	1868	53.5549	1.9855	712.9268	1868	53.5549	1.9855	373.6586	1868	53.5549	1.9855	674.6978
1869	53.5809	1.9846	450.8621	1869	53.5809	1.9846	743.6063	1869	53.5809	1.9846	379.6026	1869	53.5809	1.9846	679.5366
1870	53.6069	1.9837	489.8433	1870	53.6069	1.9837	783.6646	1870	53.6069	1.9837	431.8509	1870	53.6069	1.9837	730.6798
1871	53.6329	1.9828	560.5312	1871	53.6329	1.9828	855.4297	1871	53.6329	1.9828	456.1433	1871	53.6329	1.9828	753.8672
1872	53.6589	1.9819	612.3165	1872	53.6589	1.9819	908.2922	1872	53.6589	1.9819	462.9739	1872	53.6589	1.9819	759.5926
1873	53.6849	1.981	580.3757	1873	53.6849	1.981	877.4285	1873	53.6849	1.981	497.5703	1873	53.6849	1.981	793.0839
1874	53.7109	1.9801	589.0226	1874	53.7109	1.9801	887.1525	1874	53.7109	1.9801	529.9532	1874	53.7109	1.9801	824.3618
1875	53.7369	1.9792	634.7367	1875	53.7369	1.9792	933.9438	1875	53.7369	1.9792	592.5521	1875	53.7369	1.9792	885.8555
1876	53.7629	1.9784	674.8042	1876	53.7629	1.9784	975.0885	1876	53.7629	1.9784	633.8877	1876	53.7629	1.9784	926.086
1877	53.7889	1.9775	747.1817	1877	53.7889	1.9775	1048.5431	1877	53.7889	1.9775	598.2169	1877	53.7889	1.9775	889.3101
1878	53.8149	1.9766	753.8234	1878	53.8149	1.9766	1056.262	1878	53.8149	1.9766	558.8843	1878	53.8149	1.9766	848.8724
1879	53.8409	1.9757	774.6579	1879	53.8409	1.9757	1078.1736	1879	53.8409	1.9757	537.2588	1879	53.8409	1.9757	826.1417
1880	53.8669	1.9748	786.7948	1880	53.8669	1.9748	1091.3877	1880	53.8669	1.9748	491.5418	1880	53.8669	1.9748	779.3196
1881	53.8929	1.9739	767.6378	1881	53.8929	1.9739	1073.3078	1881	53.8929	1.9739	487.863	1881	53.8929	1.9739	774.5358
1882	53.9189	1.9731	748.7806	1882	53.9189	1.9731	1055.5278	1882	53.9189	1.9731	492.5644	1882	53.9189	1.9731	778.1321
1883	53.9449	1.9722	686.7923	1883	53.9449	1.9722	994.6166	1883	53.9449	1.9722	430.8777	1883	53.9449	1.9722	715.3402
1884	53.9709	1.9713	630.8944	1884	53.9709	1.9713	939.7959	1884	53.9709	1.9713	411.3465	1884	53.9709	1.9713	694.704
1885	53.9969	1.9704	623.3141	1885	53.9969	1.9704	933.2928	1885	53.9969	1.9704	447.5525	1885	53.9969	1.9704	729.8048
1886	54.0229	1.9695	567.3013	1886	54.0229	1.9695	878.3571	1886	54.0229	1.9695	467.295	1886	54.0229	1.9695	748.4423
1887	54.0489	1.9687	509.4225	1887	54.0489	1.9687	821.5554	1887	54.0489	1.9687	450.7881	1887	54.0489	1.9687	730.8302
1888	54.0749	1.9678	495.6198	1888	54.0749	1.9678	808.8299	1888	54.0749	1.9678	418.5509	1888	54.0749	1.9678	697.4879
1889	54.1009	1.9669	484.444	1889	54.1009	1.9669	798.7313	1889	54.1009	1.9669	402.3031	1889	54.1009	1.9669	680.135
1890	54.1269	1.966	451.1763	1890	54.1269	1.966	766.5407	1890	54.1269	1.966	429.4757	1890	54.1269	1.966	706.2025
1891	54.1529	1.9652	436.0434	1891	54.1529	1.9652	752.485	1891	54.1529	1.9652	422.169	1891	54.1529	1.9652	697.7907
1892	54.1789	1.9643	382.8998	1892	54.1789	1.9643	699.0803	1892	54.1789	1.9643	409.732	1892	54.1789	1.9643	685.8675
1893	54.2049	1.9634	388.5401	1893	54.2049	1.9634	704.4596	1893	54.2049	1.9634	415.9721	1893	54.2049	1.9634	692.6213
1894	54.2309	1.9626	375.0784	1894	54.2309	1.9626	690.7368	1894	54.2309	1.9626	454.4555	1894	54.2309	1.9626	731.6186
1895	54.2569	1.9617	374.5586	1895	54.2569	1.9617	689.956	1895	54.2569	1.9617	427.5303	1895	54.2569	1.9617	705.2072
1896	54.2829	1.9608	345.2994	1896	54.2829	1.9608	660.4357	1896	54.2829	1.9608	419.7218	1896	54.2829	1.9608	697.9125
1897	54.3089	1.96	339.6208	1897	54.3089	1.96	654.496	1897	54.3089	1.96	395.8495	1897	54.3089	1.96	674.554
1898	54.3349	1.9591	353.3538	1898	54.3349	1.9591	667.968	1898	54.3349	1.9591	442.104	1898	54.3349	1.9591	721.3223
1899	54.3609	1.9582	328.8291	1899	54.3609	1.9582	643.1823	1899	54.3609	1.9582	459.0659	1899	54.3609	1.9582	738.798
1900	54.3869	1.9574	346.1684	1900	54.3869	1.9574	660.2605	1900	54.3869	1.9574	423.5419	1900	54.3869	1.9574	703.7878
1901	54.4129	1.9565	347.7061	1901	54.4129	1.9565	661.5372	1901	54.4129	1.9565	427.9785	1901	54.4129	1.9565	708.7382
1902	54.4389	1.9556	319.7353	1902	54.4389	1.9556	633.3053	1902	54.4389	1.9556	432.8282	1902	54.4389	1.9556	714.1018
1903	54.4649	1.9548	341.8413	1903	54.4649	1.9548	655.1502	1903	54.4649	1.9548	436.9123	1903	54.4649	1.9548	718.6996

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1904	54.4909	1.9539	347.7124	1904	54.4909	1.9539	660.7603	1904	54.4909	1.9539	423.0564	1904	54.4909	1.9539	705.3575
1905	54.5169	1.953	328.0825	1905	54.5169	1.953	640.8693	1905	54.5169	1.953	436.5146	1905	54.5169	1.953	719.3295
1906	54.5429	1.9522	304.2388	1906	54.5429	1.9522	616.7646	1906	54.5429	1.9522	408.3181	1906	54.5429	1.9522	691.6469
1907	54.5689	1.9513	318.1801	1907	54.5689	1.9513	630.4448	1907	54.5689	1.9513	430.9239	1907	54.5689	1.9513	714.7665
1908	54.5949	1.9505	294.8893	1908	54.5949	1.9505	606.893	1908	54.5949	1.9505	421.3967	1908	54.5949	1.9505	705.753
1909	54.6209	1.9496	326.9363	1909	54.6209	1.9496	638.679	1909	54.6209	1.9496	464.1741	1909	54.6209	1.9496	749.0443
1910	54.6469	1.9488	295.6935	1910	54.6469	1.9488	607.175	1910	54.6469	1.9488	446.5903	1910	54.6469	1.9488	731.9743
1911	54.6729	1.9479	298.3437	1911	54.6729	1.9479	609.5642	1911	54.6729	1.9479	383.2812	1911	54.6729	1.9479	669.179
1912	54.6989	1.947	292.543	1912	54.6989	1.947	603.5024	1912	54.6989	1.947	424.78	1912	54.6989	1.947	711.1915
1913	54.7249	1.9462	352.9583	1913	54.7249	1.9462	663.6567	1913	54.7249	1.9462	404.2175	1913	54.7249	1.9462	691.1429
1914	54.7509	1.9453	274.7938	1914	54.7509	1.9453	585.2312	1914	54.7509	1.9453	408.9339	1914	54.7509	1.9453	696.3731
1915	54.7769	1.9445	340.3301	1915	54.7769	1.9445	650.5065	1915	54.7769	1.9445	428.5185	1915	54.7769	1.9445	716.4715
1916	54.8029	1.9436	398.0157	1916	54.8029	1.9436	707.931	1916	54.8029	1.9436	481.4689	1916	54.8029	1.9436	769.9357
1917	54.8289	1.9428	289.5682	1917	54.8289	1.9428	599.2224	1917	54.8289	1.9428	407.8417	1917	54.8289	1.9428	696.8223
1918	54.8549	1.9419	360.0713	1918	54.8549	1.9419	669.4645	1918	54.8549	1.9419	422.169	1918	54.8549	1.9419	711.6634
1919	54.8809	1.9411	342.1933	1919	54.8809	1.9411	654.5263	1919	54.8809	1.9411	409.8691	1919	54.8809	1.9411	703.2786
1920	54.9069	1.9402	308.9944	1920	54.9069	1.9402	624.2673	1920	54.9069	1.9402	421.9804	1920	54.9069	1.9402	719.305
1921	54.9329	1.9394	316.1777	1921	54.9329	1.9394	634.3904	1921	54.9329	1.9394	358.0115	1921	54.9329	1.9394	659.2513
1922	54.9589	1.9385	284.7299	1922	54.9589	1.9385	605.8824	1922	54.9589	1.9385	416.5944	1922	54.9589	1.9385	721.7493
1923	54.9849	1.9377	326.3753	1923	54.9849	1.9377	650.4677	1923	54.9849	1.9377	376.9678	1923	54.9849	1.9377	686.0378
1924	55.0109	1.9369	318.6929	1924	55.0109	1.9369	645.7251	1924	55.0109	1.9369	419.6641	1924	55.0109	1.9369	732.6493
1925	55.0369	1.936	378.6936	1925	55.0369	1.936	708.6656	1925	55.0369	1.936	393.724	1925	55.0369	1.936	710.6242
1926	55.0629	1.9352	350.6026	1926	55.0629	1.9352	683.5145	1926	55.0629	1.9352	430.3648	1926	55.0629	1.9352	751.1802
1927	55.0889	1.9343	321.017	1927	55.0889	1.9343	656.8687	1927	55.0889	1.9343	436.6074	1927	55.0889	1.9343	761.338
1928	55.1149	1.9335	345.1197	1928	55.1149	1.9335	683.9112	1928	55.1149	1.9335	438.6328	1928	55.1149	1.9335	767.2785
1929	55.1409	1.9326	381.9312	1929	55.1409	1.9326	723.6626	1929	55.1409	1.9326	463.2734	1929	55.1409	1.9326	795.8342
1930	55.1669	1.9318	349.9329	1930	55.1669	1.9318	694.6041	1930	55.1669	1.9318	457.5048	1930	55.1669	1.9318	793.9807
1931	55.1929	1.931	383.8877	1931	55.1929	1.931	731.4988	1931	55.1929	1.931	471.3084	1931	55.1929	1.931	811.6995
1932	55.2189	1.9301	472.4544	1932	55.2189	1.9301	823.0053	1932	55.2189	1.9301	463.1333	1932	55.2189	1.9301	807.4395
1933	55.2449	1.9293	546.9389	1933	55.2449	1.9293	900.4297	1933	55.2449	1.9293	562.3752	1933	55.2449	1.9293	910.5965
1934	55.2709	1.9285	593.4788	1934	55.2709	1.9285	949.9094	1934	55.2709	1.9285	675.828	1934	55.2709	1.9285	1027.9644
1935	55.2969	1.9276	694.2434	1935	55.2969	1.9276	1053.6138	1935	55.2969	1.9276	715.6365	1935	55.2969	1.9276	1071.688
1936	55.3229	1.9268	740.9021	1936	55.3229	1.9268	1103.2124	1936	55.3229	1.9268	853.0952	1936	55.3229	1.9268	1213.0619
1937	55.3489	1.926	757.397	1937	55.3489	1.926	1122.6471	1937	55.3489	1.926	864.938	1937	55.3489	1.926	1228.8198
1938	55.3749	1.9251	784.3477	1938	55.3749	1.9251	1152.5377	1938	55.3749	1.9251	843.7148	1938	55.3749	1.9251	1211.5117
1939	55.4009	1.9243	864.3888	1939	55.4009	1.9243	1235.5185	1939	55.4009	1.9243	881.7532	1939	55.4009	1.9243	1253.4652

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1940	55.4269	1.9235	850.4607	1940	55.4269	1.9235	1224.5303	1940	55.4269	1.9235	860.1851	1940	55.4269	1.9235	1235.8123
1941	55.4529	1.9226	787.4409	1941	55.4529	1.9226	1164.4503	1941	55.4529	1.9226	832.9441	1941	55.4529	1.9226	1212.4865
1942	55.4789	1.9218	756.9383	1942	55.4789	1.9218	1136.8875	1942	55.4789	1.9218	776.3886	1942	55.4789	1.9218	1159.846
1943	55.5049	1.921	726.7218	1943	55.5049	1.921	1109.6109	1943	55.5049	1.921	776.0929	1943	55.5049	1.921	1163.4654
1944	55.5309	1.9201	670.47	1944	55.5309	1.9201	1056.2989	1944	55.5309	1.9201	780.4333	1944	55.5309	1.9201	1171.721
1945	55.5569	1.9193	618.2334	1945	55.5569	1.9193	1007.0022	1945	55.5569	1.9193	725.6006	1945	55.5569	1.9193	1120.8034
1946	55.5829	1.9185	609.3887	1946	55.5829	1.9185	998.908	1946	55.5829	1.9185	618.3112	1946	55.5829	1.9185	1015.8631
1947	55.6089	1.9177	611.4214	1947	55.6089	1.9177	1001.6912	1947	55.6089	1.9177	629.1757	1947	55.6089	1.9177	1029.0765
1948	55.6349	1.9168	705.6798	1948	55.6349	1.9168	1096.7002	1948	55.6349	1.9168	647.3875	1948	55.6349	1.9168	1049.6374
1949	55.6609	1.916	790.1829	1949	55.6609	1.916	1181.9538	1949	55.6609	1.916	655.8145	1949	55.6609	1.916	1060.4134
1950	55.6869	1.9152	890.1756	1950	55.6869	1.9152	1282.6971	1950	55.6869	1.9152	665.6666	1950	55.6869	1.9152	1072.6145
1951	55.7129	1.9144	1123.5807	1951	55.7129	1.9144	1516.8527	1951	55.7129	1.9144	781.3723	1951	55.7129	1.9144	1190.6692
1952	55.7389	1.9135	1351.0908	1952	55.7389	1.9135	1745.1134	1952	55.7389	1.9135	950.7105	1952	55.7389	1.9135	1362.3564
1953	55.7649	1.9127	1561.0926	1953	55.7649	1.9127	1955.8657	1953	55.7649	1.9127	1166.6629	1953	55.7649	1.9127	1580.6579
1954	55.7909	1.9119	1759.9895	1954	55.7909	1.9119	2155.5131	1954	55.7909	1.9119	1343.9463	1954	55.7909	1.9119	1760.2903
1955	55.8169	1.9111	1995.3109	1955	55.8169	1.9111	2391.5851	1955	55.8169	1.9111	1452.82	1955	55.8169	1.9111	1871.513
1956	55.8429	1.9103	2228.9896	1956	55.8429	1.9103	2626.0143	1956	55.8429	1.9103	1567.615	1956	55.8429	1.9103	1988.657
1957	55.8689	1.9095	2327.2487	1957	55.8689	1.9095	2725.0239	1957	55.8689	1.9095	1658.2727	1957	55.8689	1.9095	2081.6637
1958	55.8949	1.9086	2246.999	1958	55.8949	1.9086	2645.5248	1958	55.8949	1.9086	1694.3193	1958	55.8949	1.9086	2120.0594
1959	55.9209	1.9078	2124.9364	1959	55.9209	1.9078	2524.2127	1959	55.9209	1.9078	1674.1641	1959	55.9209	1.9078	2102.2532
1960	55.9469	1.907	1934.2314	1960	55.9469	1.907	2334.2583	1960	55.9469	1.907	1577.7855	1960	55.9469	1.907	2008.2236
1961	55.9729	1.9062	1740.7951	1961	55.9729	1.9062	2141.5725	1961	55.9729	1.9062	1558.0836	1961	55.9729	1.9062	1990.8707
1962	55.9989	1.9054	1562.029	1962	55.9989	1.9054	1963.5569	1962	55.9989	1.9054	1479.3023	1962	55.9989	1.9054	1914.4384
1963	56.0249	1.9046	1371.0082	1963	56.0249	1.9046	1773.2867	1963	56.0249	1.9046	1357.8918	1963	56.0249	1.9046	1795.3769
1964	56.0509	1.9038	1186.5983	1964	56.0509	1.9038	1589.6273	1964	56.0509	1.9038	1282.5246	1964	56.0509	1.9038	1722.3587
1965	56.0769	1.9029	997.8736	1965	56.0769	1.9029	1401.6532	1965	56.0769	1.9029	1173.8154	1965	56.0769	1.9029	1615.9985
1966	56.1029	1.9021	871.7839	1966	56.1029	1.9021	1276.314	1966	56.1029	1.9021	1070.236	1966	56.1029	1.9021	1514.7682
1967	56.1289	1.9013	792.8626	1967	56.1289	1.9013	1198.1432	1967	56.1289	1.9013	1018.22	1967	56.1289	1.9013	1465.1012
1968	56.1549	1.9005	688.061	1968	56.1549	1.9005	1094.0922	1968	56.1549	1.9005	914.1311	1968	56.1549	1.9005	1363.3613
1969	56.1809	1.8997	600.5719	1969	56.1809	1.8997	1007.3536	1969	56.1809	1.8997	749.8859	1969	56.1809	1.8997	1201.4652
1970	56.2069	1.8989	572.0787	1970	56.2069	1.8989	979.611	1970	56.2069	1.8989	647.6613	1970	56.2069	1.8989	1101.5896
1971	56.2329	1.8981	561.1086	1971	56.2329	1.8981	969.3914	1971	56.2329	1.8981	581.4439	1971	56.2329	1.8981	1037.7211
1972	56.2589	1.8973	591.6238	1972	56.2589	1.8973	1000.6572	1972	56.2589	1.8973	552.2485	1972	56.2589	1.8973	1010.8748
1973	56.2849	1.8965	668.4021	1973	56.2849	1.8965	1076.3949	1973	56.2849	1.8965	523.0135	1973	56.2849	1.8965	982.3409
1974	56.3109	1.8957	718.6737	1974	56.3109	1.8957	1125.6259	1974	56.3109	1.8957	462.1554	1974	56.3109	1.8957	922.1839
1975	56.3369	1.8949	745.5016	1975	56.3369	1.8949	1151.4134	1975	56.3369	1.8949	409.0257	1975	56.3369	1.8949	869.7552

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1976	56.3629	1.8941	808.0531	1976	56.3629	1.8941	1212.9243	1976	56.3629	1.8941	388.795	1976	56.3629	1.8941	850.2257
1977	56.3889	1.8933	961.3502	1977	56.3889	1.8933	1365.1809	1977	56.3889	1.8933	411.9133	1977	56.3889	1.8933	874.0451
1978	56.4149	1.8925	1062.4297	1978	56.4149	1.8925	1465.2199	1978	56.4149	1.8925	350.188	1978	56.4149	1.8925	813.0209
1979	56.4409	1.8917	1116.2161	1979	56.4409	1.8917	1517.9658	1979	56.4409	1.8917	306.7776	1979	56.4409	1.8917	770.3116
1980	56.4669	1.8909	1237.9449	1980	56.4669	1.8909	1638.654	1980	56.4669	1.8909	350.2249	1980	56.4669	1.8909	814.46
1981	56.4929	1.8901	1370.1799	1981	56.4929	1.8901	1769.8484	1981	56.4929	1.8901	351.8322	1981	56.4929	1.8901	816.7684
1982	56.5189	1.8893	1455.2069	1982	56.5189	1.8893	1853.8349	1982	56.5189	1.8893	315.8021	1982	56.5189	1.8893	781.4394
1983	56.5449	1.8885	1420.4023	1983	56.5449	1.8885	1817.9898	1983	56.5449	1.8885	319.3235	1983	56.5449	1.8885	785.6619
1984	56.5709	1.8877	1437.3805	1984	56.5709	1.8877	1833.9275	1984	56.5709	1.8877	304.5618	1984	56.5709	1.8877	771.6013
1985	56.5969	1.8869	1476.1566	1985	56.5969	1.8869	1871.6631	1985	56.5969	1.8869	281.1177	1985	56.5969	1.8869	748.8583
1986	56.6229	1.8861	1436.9704	1986	56.6229	1.8861	1831.4363	1986	56.6229	1.8861	295.7686	1986	56.6229	1.8861	764.2102
1987	56.6489	1.8853	1420.2165	1987	56.6489	1.8853	1813.6418	1987	56.6489	1.8853	339.6764	1987	56.6489	1.8853	808.8191
1988	56.6749	1.8845	1366.6426	1988	56.6749	1.8845	1759.0274	1988	56.6749	1.8845	324.725	1988	56.6749	1.8845	794.5688
1989	56.7009	1.8837	1271.3619	1989	56.7009	1.8837	1662.7062	1989	56.7009	1.8837	341.924	1989	56.7009	1.8837	812.4689
1990	56.7269	1.8829	1243.8542	1990	56.7269	1.8829	1634.158	1990	56.7269	1.8829	374.7007	1990	56.7269	1.8829	845.9467
1991	56.7529	1.8821	1187.6997	1991	56.7529	1.8821	1576.9629	1991	56.7529	1.8821	365.4054	1991	56.7529	1.8821	837.3525
1992	56.7789	1.8813	1164.6683	1992	56.7789	1.8813	1552.8911	1992	56.7789	1.8813	438.2372	1992	56.7789	1.8813	910.8854
1993	56.8049	1.8805	1099.2521	1993	56.8049	1.8805	1486.4343	1993	56.8049	1.8805	492.9378	1993	56.8049	1.8805	966.2871
1994	56.8309	1.8798	1055.7392	1994	56.8309	1.8798	1441.8808	1994	56.8309	1.8798	516.6667	1994	56.8309	1.8798	990.7171
1995	56.8569	1.879	1058.0103	1995	56.8569	1.879	1443.1114	1995	56.8569	1.879	580.0145	1995	56.8569	1.879	1054.766
1996	56.8829	1.8782	1198.3204	1996	56.8829	1.8782	1582.3809	1996	56.8829	1.8782	669.2511	1996	56.8829	1.8782	1144.7037
1997	56.9089	1.8774	1265.0497	1997	56.9089	1.8774	1648.0698	1997	56.9089	1.8774	824.9153	1997	56.9089	1.8774	1301.069
1998	56.9349	1.8766	1447.3533	1998	56.9349	1.8766	1829.3328	1998	56.9349	1.8766	1062.922	1998	56.9349	1.8766	1539.7768
1999	56.9609	1.8758	1622.6595	1999	56.9609	1.8758	2003.5984	1999	56.9609	1.8758	1313.1969	1999	56.9609	1.8758	1790.7528
2000	56.9869	1.875	1879.9181	2000	56.9869	1.875	2259.8165	2000	56.9869	1.875	1446.7068	2000	56.9869	1.875	1924.9637
2001	57.0129	1.8743	2024.1168	2001	57.0129	1.8743	2402.9747	2001	57.0129	1.8743	1699.6446	2001	57.0129	1.8743	2178.6027
2002	57.0389	1.8735	2173.3998	2002	57.0389	1.8735	2551.2172	2002	57.0389	1.8735	1815.1769	2002	57.0389	1.8735	2294.8361
2003	57.0649	1.8727	2166.1869	2003	57.0649	1.8727	2542.9637	2003	57.0649	1.8727	1813.876	2003	57.0649	1.8727	2294.2362
2004	57.0909	1.8719	2227.7416	2004	57.0909	1.8719	2603.4779	2004	57.0909	1.8719	1845.2741	2004	57.0909	1.8719	2326.3355
2005	57.1169	1.8711	2009.5893	2005	57.1169	1.8711	2384.2851	2005	57.1169	1.8711	1785.567	2005	57.1169	1.8711	2267.3294
2006	57.1429	1.8704	1844.1979	2006	57.1429	1.8704	2217.8531	2006	57.1429	1.8704	1751.482	2006	57.1429	1.8704	2233.9455
2007	57.1689	1.8696	1752.2232	2007	57.1689	1.8696	2124.838	2007	57.1689	1.8696	1814.6044	2007	57.1689	1.8696	2297.7691
2008	57.1949	1.8688	1506.3429	2008	57.1949	1.8688	1877.9171	2008	57.1949	1.8688	1608.1774	2008	57.1949	1.8688	2092.0432
2009	57.2209	1.868	1289.7153	2009	57.2209	1.868	1660.2489	2009	57.2209	1.868	1442.1221	2009	57.2209	1.868	1926.689
2010	57.2469	1.8672	1100.2013	2010	57.2469	1.8672	1469.6945	2010	57.2469	1.8672	1352.1042	2010	57.2469	1.8672	1837.3722
2011	57.2729	1.8665	936.0406	2011	57.2729	1.8665	1304.4932	2011	57.2729	1.8665	1169.9966	2011	57.2729	1.8665	1655.9656

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2012	57.2989	1.8657	838.4341	2012	57.2989	1.8657	1205.8461	2012	57.2989	1.8657	1116.803	2012	57.2989	1.8657	1603.4731
2013	57.3249	1.8649	713.2464	2013	57.3249	1.8649	1079.6179	2013	57.3249	1.8649	1080.4852	2013	57.3249	1.8649	1567.8564
2014	57.3509	1.8641	729.5856	2014	57.3509	1.8641	1094.9166	2014	57.3509	1.8641	968.7385	2014	57.3509	1.8641	1456.8109
2015	57.3769	1.8634	690.3795	2015	57.3769	1.8634	1054.6699	2015	57.3769	1.8634	924.5566	2015	57.3769	1.8634	1413.3301
2016	57.4029	1.8626	672.52	2016	57.4029	1.8626	1035.7699	2016	57.4029	1.8626	942.8477	2016	57.4029	1.8626	1432.3222
2017	57.4289	1.8618	789.3996	2017	57.4289	1.8618	1151.609	2017	57.4289	1.8618	840.1686	2017	57.4289	1.8618	1330.3442
2018	57.4549	1.8611	825.3669	2018	57.4549	1.8611	1186.5358	2018	57.4549	1.8611	885.4999	2018	57.4549	1.8611	1376.3766
2019	57.4809	1.8603	959.7183	2019	57.4809	1.8603	1319.8467	2019	57.4809	1.8603	919.6107	2019	57.4809	1.8603	1411.1885
2020	57.5069	1.8595	1101.2108	2020	57.5069	1.8595	1460.2986	2020	57.5069	1.8595	871.3765	2020	57.5069	1.8595	1363.6554
2021	57.5329	1.8587	1135.6618	2021	57.5329	1.8587	1493.7091	2021	57.5329	1.8587	960.889	2021	57.5329	1.8587	1453.869
2022	57.5589	1.858	1219.4393	2022	57.5589	1.858	1576.446	2022	57.5589	1.858	1023.9828	2022	57.5589	1.858	1517.6639
2023	57.5849	1.8572	1378.7222	2023	57.5849	1.8572	1734.6884	2023	57.5849	1.8572	1080.0339	2023	57.5849	1.8572	1574.4161
2024	57.6109	1.8564	1350.2046	2024	57.6109	1.8564	1705.1303	2024	57.6109	1.8564	1109.8056	2024	57.6109	1.8564	1604.8889
2025	57.6369	1.8557	1373.7987	2025	57.6369	1.8557	1727.6838	2025	57.6369	1.8557	1160.7487	2025	57.6369	1.8557	1656.5331
2026	57.6629	1.8549	1318.1771	2026	57.6629	1.8549	1671.0218	2026	57.6629	1.8549	1087.3891	2026	57.6629	1.8549	1583.8746
2027	57.6889	1.8542	1426.269	2027	57.6889	1.8542	1776.282	2027	57.6889	1.8542	1134.3075	2027	57.6889	1.8542	1629.8461
2028	57.7149	1.8534	1338.8671	2028	57.7149	1.8534	1686.0485	2028	57.7149	1.8534	1073.9572	2028	57.7149	1.8534	1568.549
2029	57.7409	1.8526	1304.0777	2029	57.7409	1.8526	1648.4275	2029	57.7409	1.8526	1066.355	2029	57.7409	1.8526	1560
2030	57.7669	1.8519	1227.127	2030	57.7669	1.8519	1568.6452	2030	57.7669	1.8519	1078.5815	2030	57.7669	1.8519	1571.2797
2031	57.7929	1.8511	1190.8655	2031	57.7929	1.8511	1529.5521	2031	57.7929	1.8511	1040.9346	2031	57.7929	1.8511	1532.6859
2032	57.8189	1.8503	1031.4498	2032	57.8189	1.8503	1367.3048	2032	57.8189	1.8503	968.2174	2032	57.8189	1.8503	1459.0219
2033	57.8449	1.8496	959.892	2033	57.8449	1.8496	1292.9154	2033	57.8449	1.8496	887.5965	2033	57.8449	1.8496	1377.4542
2034	57.8709	1.8488	914.8932	2034	57.8709	1.8488	1245.085	2034	57.8709	1.8488	822.0984	2034	57.8709	1.8488	1311.0093
2035	57.8969	1.8481	858.1022	2035	57.8969	1.8481	1185.4624	2035	57.8969	1.8481	744.9553	2035	57.8969	1.8481	1232.9193
2036	57.9229	1.8473	767.8498	2036	57.9229	1.8473	1092.3784	2036	57.9229	1.8473	669.5645	2036	57.9229	1.8473	1156.5818
2037	57.9489	1.8465	696.2264	2037	57.9489	1.8465	1017.9233	2037	57.9489	1.8465	637.5707	2037	57.9489	1.8465	1123.6411
2038	57.9749	1.8458	633.1075	2038	57.9749	1.8458	951.9729	2038	57.9749	1.8458	592.8853	2038	57.9749	1.8458	1078.0089
2039	58.0009	1.845	555.0266	2039	58.0009	1.845	871.0604	2039	58.0009	1.845	529.8942	2039	58.0009	1.845	1014.071
2040	58.0269	1.8443	527.2712	2040	58.0269	1.8443	840.4733	2040	58.0269	1.8443	512.6963	2040	58.0269	1.8443	995.9262
2041	58.0529	1.8435	506.1493	2041	58.0529	1.8435	816.5199	2041	58.0529	1.8435	467.2055	2041	58.0529	1.8435	949.4886
2042	58.0789	1.8428	422.3608	2042	58.0789	1.8428	729.8997	2042	58.0789	1.8428	421.4739	2042	58.0789	1.8428	902.8102
2043	58.1049	1.842	399.0313	2043	58.1049	1.842	703.7387	2043	58.1049	1.842	418.9973	2043	58.1049	1.842	899.3868
2044	58.1309	1.8413	399.2092	2044	58.1309	1.8413	701.085	2044	58.1309	1.8413	415.9986	2044	58.1309	1.8413	895.4412
2045	58.1569	1.8405	421.8021	2045	58.1569	1.8405	720.8462	2045	58.1569	1.8405	408.0347	2045	58.1569	1.8405	886.5305
2046	58.1829	1.8398	376.0745	2046	58.1829	1.8398	672.2871	2046	58.1829	1.8398	364.6252	2046	58.1829	1.8398	842.1742
2047	58.2089	1.839	387.7726	2047	58.2089	1.839	681.1535	2047	58.2089	1.839	350.4948	2047	58.2089	1.839	827.097

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2048	58.2349	1.8383	346.569	2048	58.2349	1.8383	637.1184	2048	58.2349	1.8383	375.7729	2048	58.2349	1.8383	851.4283
2049	58.2609	1.8375	280.4962	2049	58.2609	1.8375	568.2139	2049	58.2609	1.8375	388.6498	2049	58.2609	1.8375	863.3583
2050	58.2869	1.8368	307.2826	2050	58.2869	1.8368	592.1687	2050	58.2869	1.8368	398.9382	2050	58.2869	1.8368	872.6999
2051	58.3129	1.836	330.6269	2051	58.3129	1.836	612.6814	2051	58.3129	1.836	409.4595	2051	58.3129	1.836	882.2744
2052	58.3389	1.8353	335.3746	2052	58.3389	1.8353	614.5975	2052	58.3389	1.8353	439.7565	2052	58.3389	1.8353	911.6245
2053	58.3649	1.8345	360.0713	2053	58.3649	1.8345	636.4626	2053	58.3649	1.8345	474.9019	2053	58.3649	1.8345	945.8231
2054	58.3909	1.8338	317.1922	2054	58.3909	1.8338	591.342	2054	58.3909	1.8338	479.9419	2054	58.3909	1.8338	948.1865
2055	58.4169	1.833	288.5702	2055	58.4169	1.833	560.4784	2055	58.4169	1.833	533.8165	2055	58.4169	1.833	999.3846
2056	58.4429	1.8323	303.3077	2056	58.4429	1.8323	572.9744	2056	58.4429	1.8323	546.7209	2056	58.4429	1.8323	1009.6124
2057	58.4689	1.8316	332.9668	2057	58.4689	1.8316	600.3921	2057	58.4689	1.8316	614.1537	2057	58.4689	1.8316	1074.3687
2058	58.4949	1.8308	329.3514	2058	58.4949	1.8308	594.5351	2058	58.4949	1.8308	667.5123	2058	58.4949	1.8308	1125.0508
2059	58.5209	1.8301	330.2362	2059	58.5209	1.8301	593.1784	2059	58.5209	1.8301	705.2531	2059	58.5209	1.8301	1160.115
2060	58.5469	1.8293	344.7193	2060	58.5469	1.8293	605.42	2060	58.5469	1.8293	800.9346	2060	58.5469	1.8293	1253.12
2061	58.5729	1.8286	306.4149	2061	58.5729	1.8286	564.874	2061	58.5729	1.8286	892.6967	2061	58.5729	1.8286	1342.2054
2062	58.5989	1.8279	319.3449	2062	58.5989	1.8279	575.5626	2062	58.5989	1.8279	1002.0892	2062	58.5989	1.8279	1448.9214
2063	58.6249	1.8271	336.4146	2063	58.6249	1.8271	590.3907	2063	58.6249	1.8271	1125.1895	2063	58.6249	1.8271	1569.3451
2064	58.6509	1.8264	339.8869	2064	58.6509	1.8264	591.6215	2064	58.6509	1.8264	1257.5978	2064	58.6509	1.8264	1699.0769
2065	58.6769	1.8256	349.0992	2065	58.6769	1.8256	598.5922	2065	58.6769	1.8256	1435.7955	2065	58.6769	1.8256	1874.598
2066	58.7029	1.8249	343.2799	2066	58.7029	1.8249	590.5314	2066	58.7029	1.8249	1665.5533	2066	58.7029	1.8249	2101.6793
2067	58.7289	1.8242	375.521	2067	58.7289	1.8242	620.531	2067	58.7289	1.8242	1846.6082	2067	58.7289	1.8242	2280.0576
2068	58.7549	1.8234	419.4783	2068	58.7549	1.8234	662.2468	2068	58.7549	1.8234	1972.8766	2068	58.7549	1.8234	2403.6495
2069	58.7809	1.8227	409.5153	2069	58.7809	1.8227	650.0423	2069	58.7809	1.8227	2163.3101	2069	58.7809	1.8227	2591.4064
2070	58.8069	1.822	391.247	2070	58.8069	1.822	629.5324	2070	58.8069	1.822	2368.2	2070	58.8069	1.822	2793.6197
2071	58.8329	1.8212	413.9383	2071	58.8329	1.8212	649.9822	2071	58.8329	1.8212	2504.4205	2071	58.8329	1.8212	2927.1637
2072	58.8589	1.8205	406.2982	2072	58.8589	1.8205	640.1006	2072	58.8589	1.8205	2519.8004	2072	58.8589	1.8205	2939.867
2073	58.8849	1.8198	375.029	2073	58.8849	1.8198	606.5899	2073	58.8849	1.8198	2470.5229	2073	58.8849	1.8198	2887.9129
2074	58.9109	1.819	394.5283	2074	58.9109	1.819	623.8476	2074	58.9109	1.819	2417.556	2074	58.9109	1.819	2832.2695
2075	58.9369	1.8183	413.4449	2075	58.9369	1.8183	640.5227	2075	58.9369	1.8183	2283.7343	2075	58.9369	1.8183	2695.7712
2076	58.9629	1.8176	439.1104	2076	58.9629	1.8176	663.9468	2076	58.9629	1.8176	2111.6247	2076	58.9629	1.8176	2520.9851
2077	58.9889	1.8168	512.6422	2077	58.9889	1.8168	735.237	2077	58.9889	1.8168	1951.3616	2077	58.9889	1.8168	2358.0455
2078	59.0149	1.8161	503.0746	2078	59.0149	1.8161	723.4279	2078	59.0149	1.8161	1824.1088	2078	59.0149	1.8161	2228.1161
2079	59.0409	1.8154	486.0656	2079	59.0409	1.8154	704.1774	2079	59.0409	1.8154	1651.2704	2079	59.0409	1.8154	2052.6012
2080	59.0669	1.8147	507.5796	2080	59.0669	1.8147	723.4499	2080	59.0669	1.8147	1443.8058	2080	59.0669	1.8147	1842.4599
2081	59.0929	1.8139	493.261	2081	59.0929	1.8139	706.8897	2081	59.0929	1.8139	1271.2401	2081	59.0929	1.8139	1665.2646
2082	59.1189	1.8132	524.282	2082	59.1189	1.8132	735.6692	2082	59.1189	1.8132	1137.4419	2082	59.1189	1.8132	1526.8368
2083	59.1449	1.8125	516.5632	2083	59.1449	1.8125	725.7089	2083	59.1449	1.8125	1000.8785	2083	59.1449	1.8125	1385.6438

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2084	59.1709	1.8118	514.7948	2084	59.1709	1.8118	721.699	2084	59.1709	1.8118	892.6779	2084	59.1709	1.8118	1272.8135
2085	59.1969	1.811	498.474	2085	59.1969	1.811	703.1367	2085	59.1969	1.811	808.9238	2085	59.1969	1.811	1184.4299
2086	59.2229	1.8103	475.1057	2086	59.2229	1.8103	677.5269	2086	59.2229	1.8103	723.8167	2086	59.2229	1.8103	1094.6932
2087	59.2489	1.8096	438.5183	2087	59.2489	1.8096	638.6979	2087	59.2489	1.8096	629.5448	2087	59.2489	1.8096	995.7916
2088	59.2749	1.8089	435.3871	2088	59.2749	1.8089	633.3252	2088	59.2749	1.8089	603.334	2088	59.2749	1.8089	964.9512
2089	59.3009	1.8081	417.8358	2089	59.3009	1.8081	613.5324	2089	59.3009	1.8081	540.0125	2089	59.3009	1.8081	897
2090	59.3269	1.8074	420.8761	2090	59.3269	1.8074	614.3311	2090	59.3269	1.8074	539.4678	2090	59.3269	1.8074	891.8257
2091	59.3529	1.8067	469.666	2091	59.3529	1.8067	660.8796	2091	59.3529	1.8067	511.6407	2091	59.3529	1.8067	859.369
2092	59.3789	1.806	423.6661	2092	59.3789	1.806	612.6381	2092	59.3789	1.806	465.1638	2092	59.3789	1.806	808.2624
2093	59.4049	1.8053	409.7341	2093	59.4049	1.8053	596.4646	2093	59.4049	1.8053	479.8376	2093	59.4049	1.8053	818.3067
2094	59.4309	1.8046	444.6427	2094	59.4309	1.8046	629.1317	2094	59.4309	1.8046	489.5042	2094	59.4309	1.8046	823.3436
2095	59.4569	1.8038	370.7436	2095	59.4569	1.8038	552.9911	2095	59.4569	1.8038	437.3269	2095	59.4569	1.8038	766.5367
2096	59.4829	1.8031	368.9955	2096	59.4829	1.8031	549.0015	2096	59.4829	1.8031	418.8038	2096	59.4829	1.8031	743.3839
2097	59.5089	1.8024	402.1493	2097	59.5089	1.8024	579.9138	2097	59.5089	1.8024	439.5431	2097	59.5089	1.8024	759.4936
2098	59.5349	1.8017	382.4066	2098	59.5349	1.8017	557.9295	2098	59.5349	1.8017	414.8721	2098	59.5349	1.8017	730.193
2099	59.5609	1.801	389.058	2099	59.5609	1.801	562.3394	2099	59.5609	1.801	430.0093	2099	59.5609	1.801	740.7006
2100	59.5869	1.8003	380.4996	2100	59.5869	1.8003	551.5395	2100	59.5869	1.8003	469.8023	2100	59.5869	1.8003	775.8639
2101	59.6129	1.7995	404.6325	2101	59.6129	1.7995	573.4308	2101	59.6129	1.7995	426.5928	2101	59.6129	1.7995	728.0248
2102	59.6389	1.7988	377.6192	2102	59.6389	1.7988	544.176	2102	59.6389	1.7988	392.0945	2102	59.6389	1.7988	688.8969
2103	59.6649	1.7981	353.1317	2103	59.6649	1.7981	517.447	2103	59.6649	1.7981	429.2369	2103	59.6649	1.7981	721.4097
2104	59.6909	1.7974	389.7941	2104	59.6909	1.7974	551.8679	2104	59.6909	1.7974	407.1278	2104	59.6909	1.7974	694.6709
2105	59.7169	1.7967	399.7219	2105	59.7169	1.7967	559.5541	2105	59.7169	1.7967	449.8996	2105	59.7169	1.7967	732.8131
2106	59.7429	1.796	368.5921	2106	59.7429	1.796	526.1828	2106	59.7429	1.796	417.9433	2106	59.7429	1.796	696.2271
2107	59.7689	1.7953	360.0713	2107	59.7689	1.7953	515.4205	2107	59.7689	1.7953	422.169	2107	59.7689	1.7953	695.8233
2108	59.7949	1.7946	388.7975	2108	59.7949	1.7946	544.5314	2108	59.7949	1.7946	413.9265	2108	59.7949	1.7946	685.1545
2109	59.8209	1.7939	384.7195	2109	59.8209	1.7939	540.8381	2109	59.8209	1.7939	494.2764	2109	59.8209	1.7939	763.0781
2110	59.8469	1.7932	393.2751	2110	59.8469	1.7932	549.7783	2110	59.8469	1.7932	483.5214	2110	59.8469	1.7932	749.8968
2111	59.8729	1.7925	391.5832	2111	59.8729	1.7925	548.4711	2111	59.8729	1.7925	449.8652	2111	59.8729	1.7925	713.8144
2112	59.8989	1.7917	411.8628	2112	59.8989	1.7917	569.1354	2112	59.8989	1.7917	492.2882	2112	59.8989	1.7917	753.8111
2113	59.9249	1.791	397.0927	2113	59.9249	1.791	554.75	2113	59.9249	1.791	475.0504	2113	59.9249	1.791	734.1471
2114	59.9509	1.7903	411.2825	2114	59.9509	1.7903	569.3244	2114	59.9509	1.7903	503.3555	2114	59.9509	1.7903	760.0259
2115	59.9769	1.7896	364.4472	2115	59.9769	1.7896	522.8738	2115	59.9769	1.7896	535.387	2115	59.9769	1.7896	789.6311
2116	60.0029	1.7889	399.0739	2116	60.0029	1.7889	557.8852	2116	60.0029	1.7889	562.6655	2116	60.0029	1.7889	814.4834
2117	60.0289	1.7882	390.6977	2117	60.0289	1.7882	549.8937	2117	60.0289	1.7882	529.635	2117	60.0289	1.7882	779.0266
2118	60.0549	1.7875	366.5512	2118	60.0549	1.7875	526.1318	2118	60.0549	1.7875	538.0018	2118	60.0549	1.7875	784.967
2119	60.0809	1.7868	388.6801	2119	60.0809	1.7868	548.6454	2119	60.0809	1.7868	574.9214	2119	60.0809	1.7868	819.4605

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2120	60.1069	1.7861	386.7007	2120	60.1069	1.7861	547.0507	2120	60.1069	1.7861	638.3163	2120	60.1069	1.7861	880.429
2121	60.1329	1.7854	399.7717	2121	60.1329	1.7854	560.5064	2121	60.1329	1.7854	586.3586	2121	60.1329	1.7854	826.0451
2122	60.1589	1.7847	342.5916	2122	60.1589	1.7847	503.711	2122	60.1589	1.7847	611.5651	2122	60.1589	1.7847	848.8253
2123	60.1849	1.784	353.6694	2123	60.1849	1.784	515.1734	2123	60.1849	1.784	542.4091	2123	60.1849	1.784	777.2431
2124	60.2109	1.7833	394.3151	2124	60.2109	1.7833	556.2038	2124	60.2109	1.7833	562.0967	2124	60.2109	1.7833	794.5044
2125	60.2369	1.7826	398.5767	2125	60.2369	1.7826	560.8501	2125	60.2369	1.7826	506.8154	2125	60.2369	1.7826	736.7968
2126	60.2629	1.7819	360.8217	2126	60.2629	1.7819	523.4797	2126	60.2629	1.7819	551.1164	2126	60.2629	1.7819	778.6715
2127	60.2889	1.7812	383.2082	2127	60.2889	1.7812	546.251	2127	60.2889	1.7812	523.4733	2127	60.2889	1.7812	748.6022
2128	60.3149	1.7805	371.248	2128	60.3149	1.7805	534.6755	2128	60.3149	1.7805	520.5069	2128	60.3149	1.7805	743.2094
2129	60.3409	1.7798	352.366	2129	60.3409	1.7798	516.1781	2129	60.3409	1.7798	493.5068	2129	60.3409	1.7798	713.7831
2130	60.3669	1.7792	347.1769	2130	60.3669	1.7792	511.3737	2130	60.3669	1.7792	486.0219	2130	60.3669	1.7792	703.8719
2131	60.3929	1.7785	362.8634	2131	60.3929	1.7785	527.4448	2131	60.3929	1.7785	468.5349	2131	60.3929	1.7785	683.9586
2132	60.4189	1.7778	402.68	2132	60.4189	1.7778	567.6462	2132	60.4189	1.7778	441.4791	2132	60.4189	1.7778	654.4766
2133	60.4449	1.7771	375.668	2133	60.4449	1.7771	541.0188	2133	60.4449	1.7771	428.435	2133	60.4449	1.7771	639.0063
2134	60.4709	1.7764	360.0713	2134	60.4709	1.7764	525.8068	2134	60.4709	1.7764	422.169	2134	60.4709	1.7764	630.314
2135	60.4969	1.7757	370.7259	2135	60.4969	1.7757	536.3874	2135	60.4969	1.7757	406.3209	2135	60.4969	1.7757	613.3093
2136	60.5229	1.775	380.7556	2136	60.5229	1.775	546.3431	2136	60.5229	1.775	415.5909	2136	60.5229	1.775	621.4227
2137	60.5489	1.7743	346.2172	2137	60.5489	1.7743	511.7308	2137	60.5489	1.7743	453.1762	2137	60.5489	1.7743	657.8513
2138	60.5749	1.7736	356.6658	2138	60.5749	1.7736	522.1055	2138	60.5749	1.7736	445.7642	2138	60.5749	1.7736	649.2827
2139	60.6009	1.7729	395.4383	2139	60.6009	1.7729	560.804	2139	60.6009	1.7729	437.9213	2139	60.6009	1.7729	640.2832
2140	60.6269	1.7722	346.4921	2140	60.6269	1.7722	511.7838	2140	60.6269	1.7722	460.305	2140	60.6269	1.7722	661.5103
2141	60.6529	1.7716	342.0429	2141	60.6529	1.7716	507.2607	2141	60.6529	1.7716	426.5714	2141	60.6529	1.7716	626.6201
2142	60.6789	1.7709	367.791	2142	60.6789	1.7709	532.9348	2142	60.6789	1.7709	402.2496	2142	60.6789	1.7709	601.1417
2143	60.7049	1.7702	372.6908	2143	60.7049	1.7702	537.7607	2143	60.7049	1.7702	424.6438	2143	60.7049	1.7702	622.3793
2144	60.7309	1.7695	392.6269	2144	60.7309	1.7695	557.6228	2144	60.7309	1.7695	465.3553	2144	60.7309	1.7695	661.9341
2145	60.7569	1.7688	376.1001	2145	60.7569	1.7688	541.022	2145	60.7569	1.7688	439.0677	2145	60.7569	1.7688	634.4899
2146	60.7829	1.7681	374.3189	2146	60.7829	1.7681	539.1668	2146	60.7829	1.7681	437.2013	2146	60.7829	1.7681	631.4669
2147	60.8089	1.7674	356.0232	2147	60.8089	1.7674	520.7972	2147	60.8089	1.7674	425.222	2147	60.8089	1.7674	618.331
2148	60.8349	1.7668	377.9608	2148	60.8349	1.7668	542.6609	2148	60.8349	1.7668	442.7401	2148	60.8349	1.7668	634.6925
2149	60.8609	1.7661	394.1216	2149	60.8609	1.7661	558.7477	2149	60.8609	1.7661	455.578	2149	60.8609	1.7661	646.3738
2150	60.8869	1.7654	359.5672	2150	60.8869	1.7654	524.1194	2150	60.8869	1.7654	417.4182	2150	60.8869	1.7654	607.0574
2151	60.9129	1.7647	331.8487	2151	60.9129	1.7647	496.3269	2151	60.9129	1.7647	433.538	2151	60.9129	1.7647	622.0206
2152	60.9389	1.764	385.082	2152	60.9389	1.764	549.4862	2152	60.9389	1.764	428.0166	2152	60.9389	1.764	615.3426
2153	60.9649	1.7634	384.6029	2153	60.9649	1.7634	548.9331	2153	60.9649	1.7634	433.0113	2153	60.9649	1.7634	619.1807
2154	60.9909	1.7627	366.4691	2154	60.9909	1.7627	530.7254	2154	60.9909	1.7627	446.811	2154	60.9909	1.7627	631.8238
2155	61.0169	1.762	363.3081	2155	61.0169	1.762	527.4905	2155	61.0169	1.762	457.045	2155	61.0169	1.762	640.9012

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2156	61.0429	1.7613	383.5027	2156	61.0429	1.7613	547.6111	2156	61.0429	1.7613	445.0116	2156	61.0429	1.7613	627.7111
2157	61.0689	1.7606	370.8415	2157	61.0689	1.7606	534.8759	2157	61.0689	1.7606	448.2153	2157	61.0689	1.7606	629.7583
2158	61.0949	1.76	395.275	2158	61.0949	1.76	559.2354	2158	61.0949	1.76	434.3067	2158	61.0949	1.76	614.693
2159	61.1209	1.7593	419.5873	2159	61.1209	1.7593	583.4738	2159	61.1209	1.7593	451.5057	2159	61.1209	1.7593	630.7354
2160	61.1469	1.7586	353.6327	2160	61.1469	1.7586	517.4453	2160	61.1469	1.7586	438.5273	2160	61.1469	1.7586	616.6005
2161	61.1729	1.7579	360.0713	2161	61.1729	1.7579	523.8099	2161	61.1729	1.7579	422.169	2161	61.1729	1.7579	599.0856
2162	61.1989	1.7573	395.1092	2162	61.1989	1.7573	558.9787	2162	61.1989	1.7573	450.6532	2162	61.1989	1.7573	627.2012
2163	61.2249	1.7566	381.1356	2163	61.2249	1.7566	545.1359	2163	61.2249	1.7566	478.2326	2163	61.2249	1.7566	654.4121
2164	61.2509	1.7559	384.1684	2164	61.2509	1.7559	548.2997	2164	61.2509	1.7559	470.5085	2164	61.2509	1.7559	646.3195
2165	61.2769	1.7552	378.4212	2165	61.2769	1.7552	542.6834	2165	61.2769	1.7552	462.3673	2165	61.2769	1.7552	637.8097
2166	61.3029	1.7546	364.0887	2166	61.3029	1.7546	528.4818	2166	61.3029	1.7546	476.7361	2166	61.3029	1.7546	651.81
2167	61.3289	1.7539	369.0675	2167	61.3289	1.7539	533.5915	2167	61.3289	1.7539	498.0024	2167	61.3289	1.7539	672.7079
2168	61.3549	1.7532	383.3162	2168	61.3549	1.7532	547.9711	2168	61.3549	1.7532	515.647	2168	61.3549	1.7532	689.9839
2169	61.3809	1.7526	387.3295	2169	61.3809	1.7526	552.1153	2169	61.3809	1.7526	491.235	2169	61.3809	1.7526	665.2033
2170	61.4069	1.7519	387.3474	2170	61.4069	1.7519	552.264	2170	61.4069	1.7519	465.6642	2170	61.4069	1.7519	639.264
2171	61.4329	1.7512	398.5759	2171	61.4329	1.7512	563.6235	2171	61.4329	1.7512	468.4883	2171	61.4329	1.7512	641.7196
2172	61.4589	1.7506	420.8761	2172	61.4589	1.7506	586.0546	2172	61.4589	1.7506	473.8525	2172	61.4589	1.7506	646.7154
2173	61.4849	1.7499	431.1638	2173	61.4849	1.7499	596.4732	2173	61.4849	1.7499	478.2228	2173	61.4849	1.7499	650.7171
2174	61.5109	1.7492	417.0489	2174	61.5109	1.7492	582.4891	2174	61.5109	1.7492	490.184	2174	61.5109	1.7492	662.3098
2175	61.5369	1.7485	443.3122	2175	61.5369	1.7485	608.8834	2175	61.5369	1.7485	518.2453	2175	61.5369	1.7485	690.0026
2176	61.5629	1.7479	463.3473	2176	61.5629	1.7479	629.0493	2176	61.5629	1.7479	514.65	2176	61.5629	1.7479	686.0387
2177	61.5889	1.7472	445.6216	2177	61.5889	1.7472	611.4546	2177	61.5889	1.7472	511.3434	2177	61.5889	1.7472	682.3636
2178	61.6149	1.7466	470.0195	2178	61.6149	1.7466	635.9834	2178	61.6149	1.7466	514.3649	2178	61.6149	1.7466	685.0166
2179	61.6409	1.7459	480.7375	2179	61.6409	1.7459	646.8323	2179	61.6409	1.7459	510.5017	2179	61.6409	1.7459	680.7849
2180	61.6669	1.7452	481.0503	2180	61.6669	1.7452	647.2759	2180	61.6669	1.7452	529.1545	2180	61.6669	1.7452	699.0692
2181	61.6929	1.7446	514.565	2181	61.6929	1.7446	680.9216	2181	61.6929	1.7446	563.465	2181	61.6929	1.7446	733.0111
2182	61.7189	1.7439	543.5843	2182	61.7189	1.7439	710.0717	2182	61.7189	1.7439	571.3907	2182	61.7189	1.7439	740.5684
2183	61.7449	1.7432	518.0144	2183	61.7449	1.7432	684.6327	2183	61.7449	1.7432	520.2307	2183	61.7449	1.7432	689.0398
2184	61.7709	1.7426	525.5897	2184	61.7709	1.7426	692.339	2184	61.7709	1.7426	511.1056	2184	61.7709	1.7426	679.5463
2185	61.7969	1.7419	502.3301	2185	61.7969	1.7419	669.2102	2185	61.7969	1.7419	461.9496	2185	61.7969	1.7419	630.0217
2186	61.8229	1.7413	539.0598	2186	61.8229	1.7413	706.0708	2186	61.8229	1.7413	473.3266	2186	61.8229	1.7413	641.0302
2187	61.8489	1.7406	563.9002	2187	61.8489	1.7406	731.0421	2187	61.8489	1.7406	497.9182	2187	61.8489	1.7406	665.2533
2188	61.8749	1.7399	535.9302	2188	61.8749	1.7399	703.203	2188	61.8749	1.7399	492.1315	2188	61.8749	1.7399	659.098
2189	61.9009	1.7393	494.5661	2189	61.9009	1.7393	661.9698	2189	61.9009	1.7393	487.3694	2189	61.9009	1.7393	653.9674
2190	61.9269	1.7386	482.1827	2190	61.9269	1.7386	649.7174	2190	61.9269	1.7386	428.8567	2190	61.9269	1.7386	595.0862
2191	61.9529	1.738	462.7941	2191	61.9529	1.738	630.4596	2191	61.9529	1.738	466.3845	2191	61.9529	1.738	632.2455

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2192	61.9789	1.7373	457.56	2192	61.9789	1.7373	625.3564	2192	61.9789	1.7373	438.0972	2192	61.9789	1.7373	603.5897
2193	62.0049	1.7367	451.5787	2193	62.0049	1.7367	619.506	2193	62.0049	1.7367	413.1317	2193	62.0049	1.7367	578.2557
2194	62.0309	1.736	453.6424	2194	62.0309	1.736	621.7006	2194	62.0309	1.736	435.861	2194	62.0309	1.736	600.6165
2195	62.0569	1.7353	425.4171	2195	62.0569	1.7353	593.6062	2195	62.0569	1.7353	450.7092	2195	62.0569	1.7353	615.0962
2196	62.0829	1.7347	449.136	2196	62.0829	1.7347	617.456	2196	62.0829	1.7347	404.378	2196	62.0829	1.7347	568.3965
2197	62.1089	1.734	440.1788	2197	62.1089	1.734	608.6297	2197	62.1089	1.734	432.1949	2197	62.1089	1.734	595.8448
2198	62.1349	1.7334	434.6442	2198	62.1349	1.7334	603.226	2198	62.1349	1.7334	438.4745	2198	62.1349	1.7334	601.7559
2199	62.1609	1.7327	454.8921	2199	62.1609	1.7327	623.6048	2199	62.1609	1.7327	402.1076	2199	62.1609	1.7327	565.0205
2200	62.1869	1.7321	408.1228	2200	62.1869	1.7321	576.9664	2200	62.1869	1.7321	456.7115	2200	62.1869	1.7321	619.2558
2201	62.2129	1.7314	363.6671	2201	62.2129	1.7314	532.6416	2201	62.2129	1.7314	471.6532	2201	62.2129	1.7314	633.829
2202	62.2389	1.7308	395.8867	2202	62.2389	1.7308	564.9921	2202	62.2389	1.7308	470.3875	2202	62.2389	1.7308	632.1948
2203	62.2649	1.7301	433.7015	2203	62.2649	1.7301	602.9378	2203	62.2649	1.7301	463.0856	2203	62.2649	1.7301	624.5244
2204	62.2909	1.7295	490.6084	2204	62.2909	1.7295	659.9755	2204	62.2909	1.7295	448.1654	2204	62.2909	1.7295	609.2357
2205	62.3169	1.7288	430.8146	2205	62.3169	1.7288	600.3127	2205	62.3169	1.7288	474.167	2205	62.3169	1.7288	634.8687
2206	62.3429	1.7282	446.1663	2206	62.3429	1.7282	615.7953	2206	62.3429	1.7282	467.8422	2206	62.3429	1.7282	628.1754
2207	62.3689	1.7275	493.1231	2207	62.3689	1.7275	662.883	2207	62.3689	1.7275	431.6064	2207	62.3689	1.7275	591.5711
2208	62.3949	1.7269	477.5302	2208	62.3949	1.7269	647.421	2208	62.3949	1.7269	473.0543	2208	62.3949	1.7269	632.6505
2209	62.4209	1.7262	485.5826	2209	62.4209	1.7262	655.6043	2209	62.4209	1.7262	445.146	2209	62.4209	1.7262	604.3737
2210	62.4469	1.7256	442.2557	2210	62.4469	1.7256	612.4083	2210	62.4469	1.7256	459.9574	2210	62.4469	1.7256	618.8166
2211	62.4729	1.7249	449.2989	2211	62.4729	1.7249	619.5824	2211	62.4729	1.7249	469.7963	2211	62.4729	1.7249	628.2869
2212	62.4989	1.7243	479.4333	2212	62.4989	1.7243	649.8476	2212	62.4989	1.7243	471.529	2212	62.4989	1.7243	629.6512
2213	62.5249	1.7237	431.7661	2213	62.5249	1.7237	602.3113	2213	62.5249	1.7237	437.6993	2213	62.5249	1.7237	595.4529
2214	62.5509	1.723	437.3658	2214	62.5509	1.723	608.042	2214	62.5509	1.723	462.7684	2214	62.5509	1.723	620.1535
2215	62.5769	1.7224	437.4239	2215	62.5769	1.7224	608.2309	2215	62.5769	1.7224	422.169	2215	62.5769	1.7224	579.1856
2216	62.6029	1.7217	414.5211	2216	62.6029	1.7217	584.0266	2216	62.6029	1.7217	456.5621	2216	62.6029	1.7217	614.1151
2217	62.6289	1.7211	372.6984	2217	62.6289	1.7211	540.9024	2217	62.6289	1.7211	417.3375	2217	62.6289	1.7211	575.427
2218	62.6549	1.7204	366.1431	2218	62.6549	1.7204	533.0455	2218	62.6549	1.7204	451.4105	2218	62.6549	1.7204	610.0364
2219	62.6809	1.7198	387.2463	2219	62.6809	1.7198	552.8471	2219	62.6809	1.7198	466.7152	2219	62.6809	1.7198	625.8777
2220	62.7069	1.7192	376.9115	2220	62.7069	1.7192	541.2108	2220	62.7069	1.7192	445.67	2220	62.7069	1.7192	605.3689
2221	62.7329	1.7185	325.4867	2221	62.7329	1.7185	488.4844	2221	62.7329	1.7185	408.7817	2221	62.7329	1.7185	569.0171
2222	62.7589	1.7179	350.3311	2222	62.7589	1.7179	512.0273	2222	62.7589	1.7179	410.1159	2222	62.7589	1.7179	570.8878
2223	62.7849	1.7172	355.4634	2223	62.7849	1.7172	515.858	2223	62.7849	1.7172	457.325	2223	62.7849	1.7172	618.6333
2224	62.8109	1.7166	322.0254	2224	62.8109	1.7166	481.1185	2224	62.8109	1.7166	473.2964	2224	62.8109	1.7166	635.1412
2225	62.8369	1.716	361.3198	2225	62.8369	1.716	519.1113	2225	62.8369	1.716	428.8433	2225	62.8369	1.716	591.2246
2226	62.8629	1.7153	362.7414	2226	62.8629	1.7153	519.2313	2226	62.8629	1.7153	434.3113	2226	62.8629	1.7153	597.229
2227	62.8889	1.7147	349.204	2227	62.8889	1.7147	504.3924	2227	62.8889	1.7147	466.5	2227	62.8889	1.7147	629.9542

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2228	62.9149	1.7141	315.7002	2228	62.9149	1.7141	469.587	2228	62.9149	1.7141	474.4277	2228	62.9149	1.7141	638.4183
2229	62.9409	1.7134	332.1705	2229	62.9409	1.7134	484.7558	2229	62.9409	1.7134	439.6408	2229	62.9409	1.7134	604.1678
2230	62.9669	1.7128	341.8988	2230	62.9669	1.7128	493.1825	2230	62.9669	1.7128	397.8416	2230	62.9669	1.7128	562.9052
2231	62.9929	1.7121	371.963	2231	62.9929	1.7121	521.9452	2231	62.9929	1.7121	443.924	2231	62.9929	1.7121	609.524
2232	63.0189	1.7115	321.2007	2232	63.0189	1.7115	469.8813	2232	63.0189	1.7115	408.5586	2232	63.0189	1.7115	574.6951
2233	63.0449	1.7109	327.276	2233	63.0449	1.7109	474.6551	2233	63.0449	1.7109	429.4907	2233	63.0449	1.7109	596.1636
2234	63.0709	1.7102	321.6438	2234	63.0709	1.7102	467.7213	2234	63.0709	1.7102	448.974	2234	63.0709	1.7102	616.1834
2235	63.0969	1.7096	377.0752	2235	63.0969	1.7096	521.8511	2235	63.0969	1.7096	439.5838	2235	63.0969	1.7096	607.3296
2236	63.1229	1.709	380.4652	2236	63.1229	1.709	523.9396	2236	63.1229	1.709	447.4255	2236	63.1229	1.709	615.7078
2237	63.1489	1.7084	346.4633	2237	63.1489	1.7084	488.6361	2237	63.1489	1.7084	401.1697	2237	63.1489	1.7084	569.9885
2238	63.1749	1.7077	373.8897	2238	63.1749	1.7077	514.7609	2238	63.1749	1.7077	449.1283	2238	63.1749	1.7077	618.4835
2239	63.2009	1.7071	380.2547	2239	63.2009	1.7071	519.8244	2239	63.2009	1.7071	437.7032	2239	63.2009	1.7071	607.5949
2240	63.2269	1.7065	334.4766	2240	63.2269	1.7065	472.7448	2240	63.2269	1.7065	417.244	2240	63.2269	1.7065	587.6722
2241	63.2529	1.7058	382.6364	2241	63.2529	1.7058	519.603	2241	63.2529	1.7058	444.772	2241	63.2529	1.7058	615.7367
2242	63.2789	1.7052	360.0713	2242	63.2789	1.7052	495.7363	2242	63.2789	1.7052	422.169	2242	63.2789	1.7052	593.6702
2243	63.3049	1.7046	353.7299	2243	63.3049	1.7046	489.0338	2243	63.3049	1.7046	446.3465	2243	63.3049	1.7046	618.6941
2244	63.3309	1.704	353.0801	2244	63.3309	1.704	488.0228	2244	63.3309	1.704	410.6594	2244	63.3309	1.704	583.8535
2245	63.3569	1.7033	322.3091	2245	63.3569	1.7033	456.8906	2245	63.3569	1.7033	422.6	2245	63.3569	1.7033	596.6406
2246	63.3829	1.7027	360.318	2246	63.3829	1.7027	494.5384	2246	63.3829	1.7027	459.642	2246	63.3829	1.7027	634.5292
2247	63.4089	1.7021	354.8467	2247	63.4089	1.7021	488.7059	2247	63.4089	1.7021	441.3996	2247	63.4089	1.7021	617.1333
2248	63.4349	1.7015	360.2987	2248	63.4349	1.7015	493.7968	2248	63.4349	1.7015	411.8045	2248	63.4349	1.7015	588.3848
2249	63.4609	1.7008	354.3587	2249	63.4609	1.7008	487.4956	2249	63.4609	1.7008	404.2679	2249	63.4609	1.7008	581.6947
2250	63.4869	1.7002	356.0719	2250	63.4869	1.7002	488.8476	2250	63.4869	1.7002	420.8458	2250	63.4869	1.7002	599.1191
2251	63.5129	1.6996	401.4256	2251	63.5129	1.6996	533.8402	2251	63.5129	1.6996	424.506	2251	63.5129	1.6996	603.6258
2252	63.5389	1.699	407.3184	2252	63.5389	1.699	539.3718	2252	63.5389	1.699	463.9236	2252	63.5389	1.699	643.8899
2253	63.5649	1.6983	345.288	2253	63.5649	1.6983	476.9802	2253	63.5649	1.6983	428.5124	2253	63.5649	1.6983	609.3252
2254	63.5909	1.6977	341.8268	2254	63.5909	1.6977	473.1579	2254	63.5909	1.6977	420.2731	2254	63.5909	1.6977	601.9325
2255	63.6169	1.6971	369.3683	2255	63.6169	1.6971	500.3382	2255	63.6169	1.6971	453.7244	2255	63.6169	1.6971	636.2303
2256	63.6429	1.6965	359.2596	2256	63.6429	1.6965	489.8683	2256	63.6429	1.6965	463.1466	2256	63.6429	1.6965	646.4991
2257	63.6689	1.6959	369.0576	2257	63.6689	1.6959	499.3052	2257	63.6689	1.6959	430.0356	2257	63.6689	1.6959	614.2346
2258	63.6949	1.6952	342.7635	2258	63.6949	1.6952	472.6499	2258	63.6949	1.6952	409.3491	2258	63.6949	1.6952	594.3946
2259	63.7209	1.6946	361.539	2259	63.7209	1.6946	491.0643	2259	63.7209	1.6946	395.0078	2259	63.7209	1.6946	580.8998
2260	63.7469	1.694	377.7829	2260	63.7469	1.694	506.947	2260	63.7469	1.694	433.2758	2260	63.7469	1.694	620.0144
2261	63.7729	1.6934	363.0165	2261	63.7729	1.6934	491.8194	2261	63.7729	1.6934	415.1848	2261	63.7729	1.6934	602.7699
2262	63.7989	1.6928	371.4378	2262	63.7989	1.6928	499.8796	2262	63.7989	1.6928	387.3166	2262	63.7989	1.6928	575.7482
2263	63.8249	1.6921	349.2402	2263	63.8249	1.6921	477.3209	2263	63.8249	1.6921	416.9528	2263	63.8249	1.6921	606.231

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2264	63.8509	1.6915	347.2063	2264	63.8509	1.6915	474.9258	2264	63.8509	1.6915	400.0325	2264	63.8509	1.6915	590.1572
2265	63.8769	1.6909	374.1447	2265	63.8769	1.6909	501.503	2265	63.8769	1.6909	397.2894	2265	63.8769	1.6909	588.2606
2266	63.9029	1.6903	395.205	2266	63.9029	1.6903	522.2022	2266	63.9029	1.6903	403.4021	2266	63.9029	1.6903	595.2198
2267	63.9289	1.6897	385.6563	2267	63.9289	1.6897	512.2923	2267	63.9289	1.6897	401.2379	2267	63.9289	1.6897	593.9021
2268	63.9549	1.6891	361.182	2268	63.9549	1.6891	487.4569	2268	63.9549	1.6891	419.5755	2268	63.9549	1.6891	613.0863
2269	63.9809	1.6885	360.0713	2269	63.9809	1.6885	485.985	2269	63.9809	1.6885	422.169	2269	63.9809	1.6885	616.5263
2270	64.0069	1.6878	352.0675	2270	64.0069	1.6878	476.8147	2270	64.0069	1.6878	427.3897	2270	64.0069	1.6878	620.7811
2271	64.0329	1.6872	352.3765	2271	64.0329	1.6872	475.9571	2271	64.0329	1.6872	409.8962	2271	64.0329	1.6872	602.3218
2272	64.0589	1.6866	342.2623	2272	64.0589	1.6866	464.6763	2272	64.0589	1.6866	401.1322	2272	64.0589	1.6866	592.5919
2273	64.0849	1.686	318.5787	2273	64.0849	1.686	439.8262	2273	64.0849	1.686	438.6592	2273	64.0849	1.686	629.1531
2274	64.1109	1.6854	318.7926	2274	64.1109	1.6854	438.8736	2274	64.1109	1.6854	460.4916	2274	64.1109	1.6854	650.0197
2275	64.1369	1.6848	328.7501	2275	64.1369	1.6848	447.6645	2275	64.1369	1.6848	452.8999	2275	64.1369	1.6848	641.4621
2276	64.1629	1.6842	359.4824	2276	64.1629	1.6842	477.2303	2276	64.1629	1.6842	445.3661	2276	64.1629	1.6842	632.9625
2277	64.1889	1.6836	365.4959	2277	64.1889	1.6836	482.0773	2277	64.1889	1.6836	486.2992	2277	64.1889	1.6836	672.9298
2278	64.2149	1.683	352.6546	2278	64.2149	1.683	468.0694	2278	64.2149	1.683	516.5688	2278	64.2149	1.683	702.2334
2279	64.2409	1.6823	346.2532	2279	64.2409	1.6823	460.5014	2279	64.2409	1.6823	519.5789	2279	64.2409	1.6823	704.2777
2280	64.2669	1.6817	331.1764	2280	64.2669	1.6817	444.258	2280	64.2669	1.6817	526.2993	2280	64.2669	1.6817	710.0323
2281	64.2929	1.6811	353.7946	2281	64.2929	1.6811	465.7097	2281	64.2929	1.6811	474.9797	2281	64.2929	1.6811	657.7468
2282	64.3189	1.6805	374.4771	2282	64.3189	1.6805	485.2257	2282	64.3189	1.6805	440.6677	2282	64.3189	1.6805	622.469
2283	64.3449	1.6799	366.7033	2283	64.3449	1.6799	476.2853	2283	64.3449	1.6799	442.3779	2283	64.3449	1.6799	623.2134
2284	64.3709	1.6793	360.3312	2284	64.3709	1.6793	468.7467	2284	64.3709	1.6793	427.6238	2284	64.3709	1.6793	607.4934
2285	64.3969	1.6787	356.8382	2285	64.3969	1.6787	464.0872	2285	64.3969	1.6787	418.9331	2285	64.3969	1.6787	597.8368
2286	64.4229	1.6781	377.8137	2286	64.4229	1.6781	483.8961	2286	64.4229	1.6781	452.3031	2286	64.4229	1.6781	630.241
2287	64.4489	1.6775	389.1783	2287	64.4489	1.6775	494.0942	2287	64.4489	1.6775	463.7103	2287	64.4489	1.6775	640.6824
2288	64.4749	1.6769	389.6355	2288	64.4749	1.6769	493.3849	2288	64.4749	1.6769	463.0706	2288	64.4749	1.6769	639.0768
2289	64.5009	1.6763	382.3363	2289	64.5009	1.6763	484.9191	2289	64.5009	1.6763	463.1508	2289	64.5009	1.6763	638.1912
2290	64.5269	1.6757	353.6442	2290	64.5269	1.6757	455.0604	2290	64.5269	1.6757	461.4559	2290	64.5269	1.6757	635.5304
2291	64.5529	1.6751	397.8201	2291	64.5529	1.6751	498.0699	2291	64.5529	1.6751	449.4472	2291	64.5529	1.6751	622.5559
2292	64.5789	1.6745	436.9386	2292	64.5789	1.6745	536.0217	2292	64.5789	1.6745	447.3007	2292	64.5789	1.6745	619.4435
2293	64.6049	1.6739	363.8876	2293	64.6049	1.6739	461.8042	2293	64.6049	1.6739	425.2407	2293	64.6049	1.6739	596.4177
2294	64.6309	1.6733	344.1046	2294	64.6309	1.6733	440.8547	2294	64.6309	1.6733	412.9135	2294	64.6309	1.6733	583.1246
2295	64.6569	1.6727	394.933	2295	64.6569	1.6727	490.5165	2295	64.6569	1.6727	453.1268	2295	64.6569	1.6727	622.3722
2296	64.6829	1.6721	360.0713	2296	64.6829	1.6721	454.4883	2296	64.6829	1.6721	422.169	2296	64.6829	1.6721	590.4485
2297	64.7089	1.6715	358.4415	2297	64.7089	1.6715	453.6446	2297	64.7089	1.6715	452.7875	2297	64.7089	1.6715	622.7131
2298	64.7349	1.6709	383.9684	2298	64.7349	1.6709	479.9575	2298	64.7349	1.6709	459.633	2298	64.7349	1.6709	631.2046
2299	64.7609	1.6703	373.6648	2299	64.7609	1.6703	470.44	2299	64.7609	1.6703	451.1009	2299	64.7609	1.6703	624.3186

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2300	64.7869	1.6697	349.4955	2300	64.7869	1.6697	447.0568	2300	64.7869	1.6697	490.7973	2300	64.7869	1.6697	665.6611
2301	64.8129	1.6691	349.4783	2301	64.8129	1.6691	447.8256	2301	64.8129	1.6691	473.7073	2301	64.8129	1.6691	650.2171
2302	64.8389	1.6685	368.1657	2302	64.8389	1.6685	467.2991	2302	64.8389	1.6685	489.2074	2302	64.8389	1.6685	667.3633
2303	64.8649	1.6679	351.2206	2303	64.8649	1.6679	451.1401	2303	64.8649	1.6679	493.6371	2303	64.8649	1.6679	673.4391
2304	64.8909	1.6673	337.2309	2304	64.8909	1.6673	437.9365	2304	64.8909	1.6673	456.2956	2304	64.8909	1.6673	637.7437
2305	64.9169	1.6667	344.0324	2305	64.9169	1.6667	445.5241	2305	64.9169	1.6667	418.3497	2305	64.9169	1.6667	601.4438
2306	64.9429	1.6661	322.8844	2306	64.9429	1.6661	425.162	2306	64.9429	1.6661	417.908	2306	64.9429	1.6661	602.6482
2307	64.9689	1.6655	330.6514	2307	64.9689	1.6655	433.7152	2307	64.9689	1.6655	448.8057	2307	64.9689	1.6655	635.1919
2308	64.9949	1.6649	339.1932	2308	64.9949	1.6649	443.043	2308	64.9949	1.6649	450.2856	2308	64.9949	1.6649	638.3179
2309	65.0209	1.6643	369.7745	2309	65.0209	1.6643	474.4104	2309	65.0209	1.6643	407.7858	2309	65.0209	1.6643	597.4642
2310	65.0469	1.6637	350.8221	2310	65.0469	1.6637	456.2441	2310	65.0469	1.6637	450.0417	2310	65.0469	1.6637	641.3661
2311	65.0729	1.6632	314.2566	2311	65.0729	1.6632	420.4646	2311	65.0729	1.6632	399.4569	2311	65.0729	1.6632	592.4274
2312	65.0989	1.6626	341.8667	2312	65.0989	1.6626	448.8608	2312	65.0989	1.6626	491.8347	2312	65.0989	1.6626	686.4513
2313	65.1249	1.662	340.1147	2313	65.1249	1.662	447.8949	2313	65.1249	1.662	440.9475	2313	65.1249	1.662	637.2102
2314	65.1509	1.6614	352.5385	2314	65.1509	1.6614	461.1047	2314	65.1509	1.6614	413.4786	2314	65.1509	1.6614	611.3874
2315	65.1769	1.6608	334.6875	2315	65.1769	1.6608	444.0398	2315	65.1769	1.6608	457.485	2315	65.1769	1.6608	657.0398
2316	65.2029	1.6602	335.3399	2316	65.2029	1.6602	445.4783	2316	65.2029	1.6602	456.5301	2316	65.2029	1.6602	657.731
2317	65.2289	1.6596	350.4151	2317	65.2289	1.6596	461.3395	2317	65.2289	1.6596	445.7936	2317	65.2289	1.6596	648.6405
2318	65.2549	1.659	366.0383	2318	65.2549	1.659	477.7488	2318	65.2549	1.659	427.0998	2318	65.2549	1.659	631.5928
2319	65.2809	1.6584	340.5034	2319	65.2809	1.6584	453	2319	65.2809	1.6584	483.8585	2319	65.2809	1.6584	689.9976
2320	65.3069	1.6579	339.7174	2320	65.3069	1.6579	453	2320	65.3069	1.6579	463.4009	2320	65.3069	1.6579	671.1861
2321	65.3329	1.6573	361.4778	2321	65.3329	1.6573	475.5465	2321	65.3329	1.6573	464.5096	2321	65.3329	1.6573	673.9408
2322	65.3589	1.6567	377.6413	2322	65.3589	1.6567	492.4961	2322	65.3589	1.6567	479.4188	2322	65.3589	1.6567	690.4961
2323	65.3849	1.6561	360.0713	2323	65.3849	1.6561	475.7121	2323	65.3849	1.6561	515.7336	2323	65.3849	1.6561	728.457
2324	65.4109	1.6555	321.613	2324	65.4109	1.6555	436.9794	2324	65.4109	1.6555	539.4316	2324	65.4109	1.6555	751.8618
2325	65.4369	1.6549	327.4328	2325	65.4369	1.6549	442.5247	2325	65.4369	1.6549	542.7442	2325	65.4369	1.6549	754.8812
2326	65.4629	1.6543	350.5186	2326	65.4629	1.6543	465.3361	2326	65.4629	1.6543	518.0281	2326	65.4629	1.6543	729.8719
2327	65.4889	1.6538	350.6155	2327	65.4889	1.6538	465.1585	2327	65.4889	1.6538	590.1092	2327	65.4889	1.6538	801.6598
2328	65.5149	1.6532	358.0181	2328	65.5149	1.6532	472.2866	2328	65.5149	1.6532	591.2776	2328	65.5149	1.6532	802.535
2329	65.5409	1.6526	331.078	2329	65.5409	1.6526	445.072	2329	65.5409	1.6526	624.3692	2329	65.5409	1.6526	835.3334
2330	65.5669	1.652	328.2804	2330	65.5669	1.652	442	2330	65.5669	1.652	715.6451	2330	65.5669	1.652	926.3161
2331	65.5929	1.6514	340.8897	2331	65.5929	1.6514	454.3348	2331	65.5929	1.6514	726.6221	2331	65.5929	1.6514	937
2332	65.6189	1.6508	304.4994	2332	65.6189	1.6508	417.67	2332	65.6189	1.6508	735.6267	2332	65.6189	1.6508	945.7114
2333	65.6449	1.6503	353.3603	2333	65.6449	1.6503	466.2565	2333	65.6449	1.6503	820.7463	2333	65.6449	1.6503	1030.5377
2334	65.6709	1.6497	349.6089	2334	65.6709	1.6497	462.2306	2334	65.6709	1.6497	883.0253	2334	65.6709	1.6497	1092.5236
2335	65.6969	1.6491	340.9218	2335	65.6969	1.6491	453.269	2335	65.6969	1.6491	940.5943	2335	65.6969	1.6491	1149.7994

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2336	65.7229	1.6485	314.1523	2336	65.7229	1.6485	426.2251	2336	65.7229	1.6485	965.0542	2336	65.7229	1.6485	1173.966
2337	65.7489	1.6479	331.3828	2337	65.7489	1.6479	443.1812	2337	65.7489	1.6479	1061.2136	2337	65.7489	1.6479	1269.8323
2338	65.7749	1.6474	354.3314	2338	65.7749	1.6474	465.8553	2338	65.7749	1.6474	1106.8342	2338	65.7749	1.6474	1315.1597
2339	65.8009	1.6468	342.717	2339	65.8009	1.6468	453.9664	2339	65.8009	1.6468	1106.5542	2339	65.8009	1.6468	1314.5866
2340	65.8269	1.6462	343.7756	2340	65.8269	1.6462	454.7505	2340	65.8269	1.6462	1147.224	2340	65.8269	1.6462	1354.9632
2341	65.8529	1.6456	354.6816	2341	65.8529	1.6456	465.382	2341	65.8529	1.6456	1203.9005	2341	65.8529	1.6456	1411.3465
2342	65.8789	1.6451	372.2403	2342	65.8789	1.6451	482.6663	2342	65.8789	1.6451	1165.901	2342	65.8789	1.6451	1373.0537
2343	65.9049	1.6445	364.6566	2343	65.9049	1.6445	474.8081	2343	65.9049	1.6445	1106.945	2343	65.9049	1.6445	1313.8045
2344	65.9309	1.6439	384.4371	2344	65.9309	1.6439	494.3141	2344	65.9309	1.6439	1035.5244	2344	65.9309	1.6439	1242.0907
2345	65.9569	1.6433	385.7181	2345	65.9569	1.6433	495.3207	2345	65.9569	1.6433	1027.859	2345	65.9569	1.6433	1234.1322
2346	65.9829	1.6428	371.9563	2346	65.9829	1.6428	481.2844	2346	65.9829	1.6428	1016.6433	2346	65.9829	1.6428	1222.6233
2347	66.0089	1.6422	352.778	2347	66.0089	1.6422	461.8317	2347	66.0089	1.6422	987.4773	2347	66.0089	1.6422	1193.164
2348	66.0349	1.6416	330.1237	2348	66.0349	1.6416	438.9029	2348	66.0349	1.6416	942.9875	2348	66.0349	1.6416	1148.381
2349	66.0609	1.641	362.1304	2349	66.0609	1.641	470.6351	2349	66.0609	1.641	836.1753	2349	66.0609	1.641	1041.2757
2350	66.0869	1.6405	360.0713	2350	66.0869	1.6405	468.3016	2350	66.0869	1.6405	815.8913	2350	66.0869	1.6405	1020.6984
2351	66.1129	1.6399	368.0805	2351	66.1129	1.6399	479.7958	2351	66.1129	1.6399	801.2772	2351	66.1129	1.6399	1005.7912
2352	66.1389	1.6393	334.7837	2352	66.1389	1.6393	449.984	2352	66.1389	1.6393	704.0022	2352	66.1389	1.6393	908.223
2353	66.1649	1.6388	360.034	2353	66.1649	1.6388	478.7193	2353	66.1649	1.6388	649.4798	2353	66.1649	1.6388	853.4074
2354	66.1909	1.6382	360.5915	2354	66.1909	1.6382	482.7618	2354	66.1909	1.6382	628.3501	2354	66.1909	1.6382	831.9846
2355	66.2169	1.6376	354.7027	2355	66.2169	1.6376	480.358	2355	66.2169	1.6376	617.4442	2355	66.2169	1.6376	820.7854
2356	66.2429	1.637	355.2266	2356	66.2429	1.637	484.367	2356	66.2429	1.637	591.8979	2356	66.2429	1.637	794.946
2357	66.2689	1.6365	357.6054	2357	66.2689	1.6365	490.2308	2357	66.2689	1.6365	542.7297	2357	66.2689	1.6365	745.4845
2358	66.2949	1.6359	362.1817	2358	66.2949	1.6359	498.2921	2358	66.2949	1.6359	536.8673	2358	66.2949	1.6359	739.3289
2359	66.3209	1.6353	353.5626	2359	66.3209	1.6353	493.158	2359	66.3209	1.6353	515.4634	2359	66.3209	1.6353	717.6318
2360	66.3469	1.6348	349.6661	2360	66.3469	1.6348	492.7465	2360	66.3469	1.6348	512.9241	2360	66.3469	1.6348	714.7994
2361	66.3729	1.6342	351.7681	2361	66.3729	1.6342	498.3336	2361	66.3729	1.6342	479.9136	2361	66.3729	1.6342	681.4956
2362	66.3989	1.6336	348.2292	2362	66.3989	1.6336	498.2796	2362	66.3989	1.6336	462.0478	2362	66.3989	1.6336	663.3367
2363	66.4249	1.6331	332.7572	2363	66.4249	1.6331	486.2926	2363	66.4249	1.6331	455.5344	2363	66.4249	1.6331	656.5301
2364	66.4509	1.6325	355.3041	2364	66.4509	1.6325	512.3246	2364	66.4509	1.6325	432.3323	2364	66.4509	1.6325	633.0348
2365	66.4769	1.6319	368.0768	2365	66.4769	1.6319	528.5823	2365	66.4769	1.6319	422.9596	2365	66.4769	1.6319	623.3689
2366	66.5029	1.6314	327.253	2366	66.5029	1.6314	491.2435	2366	66.5029	1.6314	426.6879	2366	66.5029	1.6314	626.804
2367	66.5289	1.6308	307.9062	2367	66.5289	1.6308	475.3817	2367	66.5289	1.6308	417.5568	2367	66.5289	1.6308	617.3797
2368	66.5549	1.6302	318.2067	2368	66.5549	1.6302	489.1672	2368	66.5549	1.6302	433.2227	2368	66.5549	1.6302	632.7524
2369	66.5809	1.6297	324.0825	2369	66.5809	1.6297	498.5281	2369	66.5809	1.6297	476.3959	2369	66.5809	1.6297	675.6324
2370	66.6069	1.6291	324.0694	2370	66.6069	1.6291	502	2370	66.6069	1.6291	479.7163	2370	66.6069	1.6291	678.6596
2371	66.6329	1.6286	340.9194	2371	66.6329	1.6286	522.335	2371	66.6329	1.6286	477.0015	2371	66.6329	1.6286	675.6517

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2372	66.6589	1.628	372.3783	2372	66.6589	1.628	557.2788	2372	66.6589	1.628	487.6946	2372	66.6589	1.628	686.0515
2373	66.6849	1.6274	402.6516	2373	66.6849	1.6274	591.0372	2373	66.6849	1.6274	524.082	2373	66.6849	1.6274	722.1458
2374	66.7109	1.6269	411.587	2374	66.7109	1.6269	603.4576	2374	66.7109	1.6269	552.6887	2374	66.7109	1.6269	750.4592
2375	66.7369	1.6263	461.0936	2375	66.7369	1.6263	656.4492	2375	66.7369	1.6263	584.4152	2375	66.7369	1.6263	781.8925
2376	66.7629	1.6258	525.1227	2376	66.7629	1.6258	723.9633	2376	66.7629	1.6258	634.952	2376	66.7629	1.6258	832.1361
2377	66.7889	1.6252	512.7424	2377	66.7889	1.6252	715.068	2377	66.7889	1.6252	642.7653	2377	66.7889	1.6252	839.6563
2378	66.8149	1.6246	553.8251	2378	66.8149	1.6246	757.518	2378	66.8149	1.6246	668.9503	2378	66.8149	1.6246	863.6088
2379	66.8409	1.6241	572.6526	2379	66.8409	1.6241	777.7127	2379	66.8409	1.6241	629.1669	2379	66.8409	1.6241	821.593
2380	66.8669	1.6235	558.0801	2380	66.8669	1.6235	764.5074	2380	66.8669	1.6235	584.3602	2380	66.8669	1.6235	774.5538
2381	66.8929	1.623	581.5819	2381	66.8929	1.623	789.3764	2381	66.8929	1.623	593.9636	2381	66.8929	1.623	781.9247
2382	66.9189	1.6224	559.588	2382	66.9189	1.6224	768.7497	2382	66.9189	1.6224	615.7723	2382	66.9189	1.6224	801.5009
2383	66.9449	1.6218	535.2322	2383	66.9449	1.6218	745.7611	2383	66.9449	1.6218	641.1226	2383	66.9449	1.6218	824.6188
2384	66.9709	1.6213	492.0554	2384	66.9709	1.6213	703.9515	2384	66.9709	1.6213	616.9119	2384	66.9709	1.6213	798.1756
2385	66.9969	1.6207	458.7009	2385	66.9969	1.6207	671.9642	2385	66.9969	1.6207	578.0636	2385	66.9969	1.6207	757.0949
2386	67.0229	1.6202	463.0821	2386	67.0229	1.6202	677.7126	2386	67.0229	1.6202	548.4225	2386	67.0229	1.6202	725.2214
2387	67.0489	1.6196	452.9219	2387	67.0489	1.6196	668.9197	2387	67.0489	1.6196	528.0771	2387	67.0489	1.6196	702.6434
2388	67.0749	1.6191	399.1111	2388	67.0749	1.6191	616.4761	2388	67.0749	1.6191	538.8974	2388	67.0749	1.6191	711.2314
2389	67.1009	1.6185	386.1565	2389	67.1009	1.6185	604.8887	2389	67.1009	1.6185	496.343	2389	67.1009	1.6185	666.4445
2390	67.1269	1.618	365.579	2390	67.1269	1.618	585.6784	2390	67.1269	1.618	492.6009	2390	67.1269	1.618	660.4699
2391	67.1529	1.6174	356.9621	2391	67.1529	1.6174	578.4287	2391	67.1529	1.6174	484.221	2391	67.1529	1.6174	649.8575
2392	67.1789	1.6169	371.9241	2392	67.1789	1.6169	594.758	2392	67.1789	1.6169	500.7403	2392	67.1789	1.6169	664.1444
2393	67.2049	1.6163	372.7473	2393	67.2049	1.6163	596.9484	2393	67.2049	1.6163	445.2492	2393	67.2049	1.6163	606.4208
2394	67.2309	1.6157	373.3009	2394	67.2309	1.6157	598.8691	2394	67.2309	1.6157	492.3644	2394	67.2309	1.6157	651.3036
2395	67.2569	1.6152	406.7471	2395	67.2569	1.6152	633.6825	2395	67.2569	1.6152	500.8012	2395	67.2569	1.6152	657.5079
2396	67.2829	1.6146	368.3362	2396	67.2829	1.6146	596.6389	2396	67.2829	1.6146	492.3175	2396	67.2829	1.6146	646.7917
2397	67.3089	1.6141	364.9848	2397	67.3089	1.6141	594.6547	2397	67.3089	1.6141	448.4727	2397	67.3089	1.6141	600.7145
2398	67.3349	1.6135	380.8002	2398	67.3349	1.6135	611.8374	2398	67.3349	1.6135	399.0997	2398	67.3349	1.6135	549.109
2399	67.3609	1.613	371.802	2399	67.3609	1.613	604.2063	2399	67.3609	1.613	420.5563	2399	67.3609	1.613	568.3332
2400	67.3869	1.6124	373.1927	2400	67.3869	1.6124	606.9642	2400	67.3869	1.6124	441.2233	2400	67.3869	1.6124	586.7678
2401	67.4129	1.6119	381.7262	2401	67.4129	1.6119	616.865	2401	67.4129	1.6119	453.8585	2401	67.4129	1.6119	597.1705
2402	67.4389	1.6114	393.6147	2402	67.4389	1.6114	630.1207	2402	67.4389	1.6114	468.5079	2402	67.4389	1.6114	609.5874
2403	67.4649	1.6108	416.9601	2403	67.4649	1.6108	654.8333	2403	67.4649	1.6108	456.6535	2403	67.4649	1.6108	595.5006
2404	67.4909	1.6103	417.2519	2404	67.4909	1.6103	656.4923	2404	67.4909	1.6103	422.169	2404	67.4909	1.6103	558.7837
2405	67.5169	1.6097	401.6844	2405	67.5169	1.6097	640.0638	2405	67.5169	1.6097	436.2951	2405	67.5169	1.6097	574.0107
2406	67.5429	1.6092	389.4512	2406	67.5429	1.6092	626.9697	2406	67.5429	1.6092	491.7916	2406	67.5429	1.6092	630.6081
2407	67.5689	1.6086	412.6762	2407	67.5689	1.6086	649.3338	2407	67.5689	1.6086	448.9072	2407	67.5689	1.6086	588.8246

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2408	67.5949	1.6081	394.7353	2408	67.5949	1.6081	630.5318	2408	67.5949	1.6081	479.46	2408	67.5949	1.6081	620.4785
2409	67.6209	1.6075	399.1343	2409	67.6209	1.6075	634.0699	2409	67.6209	1.6075	471.5939	2409	67.6209	1.6075	613.7133
2410	67.6469	1.607	462.5217	2410	67.6469	1.607	696.5963	2410	67.6469	1.607	509.2937	2410	67.6469	1.607	652.514
2411	67.6729	1.6064	499.4918	2411	67.6729	1.6064	732.7055	2411	67.6729	1.6064	509.0025	2411	67.6729	1.6064	653.3238
2412	67.6989	1.6059	534.7581	2412	67.6989	1.6059	767.1109	2412	67.6989	1.6059	564.8154	2412	67.6989	1.6059	710.2376
2413	67.7249	1.6054	617.6788	2413	67.7249	1.6054	849.1705	2413	67.7249	1.6054	589.8726	2413	67.7249	1.6054	736.3957
2414	67.7509	1.6048	747.842	2414	67.7509	1.6048	978.4728	2414	67.7509	1.6048	755.0596	2414	67.7509	1.6048	902.6837
2415	67.7769	1.6043	795.6066	2415	67.7769	1.6043	1025.3765	2415	67.7769	1.6043	899.6535	2415	67.7769	1.6043	1048.3786
2416	67.8029	1.6037	927.5185	2416	67.8029	1.6037	1156.4274	2416	67.8029	1.6037	967.1532	2416	67.8029	1.6037	1116.9793
2417	67.8289	1.6032	1015.9798	2417	67.8289	1.6032	1244.0277	2417	67.8289	1.6032	991.1563	2417	67.8289	1.6032	1142.0832
2418	67.8549	1.6026	1018.0447	2418	67.8549	1.6026	1245.2316	2418	67.8549	1.6026	994.9322	2418	67.8549	1.6026	1146.9601
2419	67.8809	1.6021	1031.5792	2419	67.8809	1.6021	1257.9052	2419	67.8809	1.6021	1100.9078	2419	67.8809	1.6021	1254.0366
2420	67.9069	1.6016	1020.5592	2420	67.9069	1.6016	1246.0243	2420	67.9069	1.6016	979.0173	2420	67.9069	1.6016	1133.2471
2421	67.9329	1.601	918.6385	2421	67.9329	1.601	1143.2426	2421	67.9329	1.601	1067.582	2421	67.9329	1.601	1222.9127
2422	67.9589	1.6005	914.3443	2422	67.9589	1.6005	1138.0875	2422	67.9589	1.6005	1020.6181	2422	67.9589	1.6005	1177.0498
2423	67.9849	1.5999	865.7392	2423	67.9849	1.5999	1088.6214	2423	67.9849	1.5999	987.4847	2423	67.9849	1.5999	1145.0174
2424	68.0109	1.5994	748.068	2424	68.0109	1.5994	970.0892	2424	68.0109	1.5994	910.6201	2424	68.0109	1.5994	1069.2538
2425	68.0369	1.5989	715.3888	2425	68.0369	1.5989	936.5491	2425	68.0369	1.5989	874.0211	2425	68.0369	1.5989	1033.7557
2426	68.0629	1.5983	675.2862	2426	68.0629	1.5983	895.5855	2426	68.0629	1.5983	767.936	2426	68.0629	1.5983	928.7715
2427	68.0889	1.5978	592.7805	2427	68.0889	1.5978	812.2189	2427	68.0889	1.5978	760.0635	2427	68.0889	1.5978	922
2428	68.1149	1.5973	536.8998	2428	68.1149	1.5973	755.4772	2428	68.1149	1.5973	649.6497	2428	68.1149	1.5973	812.6871
2429	68.1409	1.5967	512.3841	2429	68.1409	1.5967	730.1005	2429	68.1409	1.5967	634.3183	2429	68.1409	1.5967	798.4566
2430	68.1669	1.5962	520.132	2430	68.1669	1.5962	736.9875	2430	68.1669	1.5962	601.3044	2430	68.1669	1.5962	766.5437
2431	68.1929	1.5957	487.3411	2431	68.1929	1.5957	703.3357	2431	68.1929	1.5957	583.3273	2431	68.1929	1.5957	749.6676
2432	68.2189	1.5951	482.1086	2432	68.2189	1.5951	697.2422	2432	68.2189	1.5951	537.0978	2432	68.2189	1.5951	702.2968
2433	68.2449	1.5946	506.19	2433	68.2449	1.5946	720.4626	2433	68.2449	1.5946	513.6935	2433	68.2449	1.5946	677.7513
2434	68.2709	1.5941	529.4877	2434	68.2709	1.5941	742.8994	2434	68.2709	1.5941	535.278	2434	68.2709	1.5941	698.1947
2435	68.2969	1.5935	557.2252	2435	68.2969	1.5935	769.7759	2435	68.2969	1.5935	473.9916	2435	68.2969	1.5935	635.7671
2436	68.3229	1.593	595.879	2436	68.3229	1.593	807.5687	2436	68.3229	1.593	461.6873	2436	68.3229	1.593	622.3216
2437	68.3489	1.5925	613.952	2437	68.3489	1.5925	824.7808	2437	68.3489	1.5925	423.53	2437	68.3489	1.5925	583.0231
2438	68.3749	1.5919	672.7495	2438	68.3749	1.5919	882.7174	2438	68.3749	1.5919	471.5461	2438	68.3749	1.5919	629.898
2439	68.4009	1.5914	659.9907	2439	68.4009	1.5914	869.0976	2439	68.4009	1.5914	451.6018	2439	68.4009	1.5914	608.8125
2440	68.4269	1.5909	643.5607	2440	68.4269	1.5909	851.8066	2440	68.4269	1.5909	459.322	2440	68.4269	1.5909	615.3915
2441	68.4529	1.5903	620.2957	2441	68.4529	1.5903	827.6806	2441	68.4529	1.5903	415.1161	2441	68.4529	1.5903	570.0444
2442	68.4789	1.5898	634.9681	2442	68.4789	1.5898	841.4921	2442	68.4789	1.5898	402.4332	2442	68.4789	1.5898	556.2203
2443	68.5049	1.5893	633.6393	2443	68.5049	1.5893	839.3024	2443	68.5049	1.5893	441.8422	2443	68.5049	1.5893	594.4881

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2444	68.5309	1.5887	630.6782	2444	68.5309	1.5887	835.4803	2444	68.5309	1.5887	437.7788	2444	68.5309	1.5887	589.2835
2445	68.5569	1.5882	596.5627	2445	68.5569	1.5882	800.5038	2445	68.5569	1.5882	405.8896	2445	68.5569	1.5882	556.2531
2446	68.5829	1.5877	609.5997	2446	68.5829	1.5877	812.6798	2446	68.5829	1.5877	467.3372	2446	68.5829	1.5877	616.5595
2447	68.6089	1.5872	539.933	2447	68.6089	1.5872	742.1522	2447	68.6089	1.5872	440.3537	2447	68.6089	1.5872	588.4348
2448	68.6349	1.5866	560.6119	2448	68.6349	1.5866	761.9702	2448	68.6349	1.5866	450.8661	2448	68.6349	1.5866	597.806
2449	68.6609	1.5861	554.9345	2449	68.6609	1.5861	755.4318	2449	68.6609	1.5861	467.4626	2449	68.6609	1.5861	613.2614
2450	68.6869	1.5856	547.4646	2450	68.6869	1.5856	747.1009	2450	68.6869	1.5856	479.4464	2450	68.6869	1.5856	624.104
2451	68.7129	1.585	554.7477	2451	68.7129	1.585	753.5231	2451	68.7129	1.585	445.8222	2451	68.7129	1.585	589.3385
2452	68.7389	1.5845	573.7362	2452	68.7389	1.5845	771.6506	2452	68.7389	1.5845	493.5882	2452	68.7389	1.5845	635.9633
2453	68.7649	1.584	504.164	2453	68.7649	1.584	701.2175	2453	68.7649	1.584	496.6034	2453	68.7649	1.584	637.8374
2454	68.7909	1.5835	445.6678	2454	68.7909	1.5835	641.8603	2454	68.7909	1.5835	483.9073	2454	68.7909	1.5835	624
2455	68.8169	1.5829	436.9698	2455	68.8169	1.5829	632.3014	2455	68.8169	1.5829	459.6714	2455	68.8169	1.5829	598.6229
2456	68.8429	1.5824	443.6556	2456	68.8429	1.5824	638.1262	2456	68.8429	1.5824	490.1214	2456	68.8429	1.5824	627.9317
2457	68.8689	1.5819	439.8202	2457	68.8689	1.5819	633.4298	2457	68.8689	1.5819	504.6064	2457	68.8689	1.5819	641.2756
2458	68.8949	1.5814	423.2118	2458	68.8949	1.5814	615.9605	2458	68.8949	1.5814	482.707	2458	68.8949	1.5814	618.235
2459	68.9209	1.5809	397.5663	2459	68.9209	1.5809	587.2258	2459	68.9209	1.5809	462.6151	2459	68.9209	1.5809	597.0019
2460	68.9469	1.5803	407.8664	2460	68.9469	1.5803	594.4368	2460	68.9469	1.5803	455.5523	2460	68.9469	1.5803	588.7978
2461	68.9729	1.5798	391.4137	2461	68.9729	1.5798	574.895	2461	68.9729	1.5798	489.0006	2461	68.9729	1.5798	621.105
2462	68.9989	1.5793	342.5459	2462	68.9989	1.5793	522.9381	2462	68.9989	1.5793	473.5126	2462	68.9989	1.5793	604.4758
2463	69.0249	1.5788	320.6977	2463	69.0249	1.5788	498.0008	2463	69.0249	1.5788	446.178	2463	69.0249	1.5788	576
2464	69.0509	1.5782	302.2601	2464	69.0509	1.5782	476.474	2464	69.0509	1.5782	447.3192	2464	69.0509	1.5782	576
2465	69.0769	1.5777	301.3532	2465	69.0769	1.5777	472.478	2465	69.0769	1.5777	408.7545	2465	69.0769	1.5777	536.2941
2466	69.1029	1.5772	325.9615	2466	69.1029	1.5772	493.9972	2466	69.1029	1.5772	365.146	2466	69.1029	1.5772	491.5444
2467	69.1289	1.5767	329.4209	2467	69.1289	1.5767	494.3675	2467	69.1289	1.5767	392.9567	2467	69.1289	1.5767	518.2139
2468	69.1549	1.5762	327.3162	2468	69.1549	1.5762	489.1736	2468	69.1549	1.5762	423.7538	2468	69.1549	1.5762	547.8698
2469	69.1809	1.5756	329.6257	2469	69.1809	1.5756	488.394	2469	69.1809	1.5756	433.2844	2469	69.1809	1.5756	556.2592
2470	69.2069	1.5751	317.2799	2470	69.2069	1.5751	472.9591	2470	69.2069	1.5751	394.9804	2470	69.2069	1.5751	516.814
2471	69.2329	1.5746	302.0309	2471	69.2329	1.5746	454.6209	2471	69.2329	1.5746	362.0496	2471	69.2329	1.5746	482.742
2472	69.2589	1.5741	306.1754	2472	69.2589	1.5741	455.6763	2472	69.2589	1.5741	406.4416	2472	69.2589	1.5741	525.9928
2473	69.2849	1.5736	311.5068	2473	69.2849	1.5736	457.9186	2473	69.2849	1.5736	447.9202	2473	69.2849	1.5736	566.3302
2474	69.3109	1.5731	332.5589	2474	69.3109	1.5731	475.8815	2474	69.3109	1.5731	439.547	2474	69.3109	1.5731	556.8158
2475	69.3369	1.5725	353.1035	2475	69.3369	1.5725	493.3371	2475	69.3369	1.5725	419.8471	2475	69.3369	1.5725	535.9747
2476	69.3629	1.572	316.0854	2476	69.3629	1.572	453.2297	2476	69.3629	1.572	423.9173	2476	69.3629	1.572	538.9037
2477	69.3889	1.5715	324.699	2477	69.3889	1.5715	458.7543	2477	69.3889	1.5715	431.9649	2477	69.3889	1.5715	545.8101
2478	69.4149	1.571	346.8827	2478	69.4149	1.571	477.8488	2478	69.4149	1.571	431.6642	2478	69.4149	1.571	544.3682
2479	69.4409	1.5705	316.7239	2479	69.4409	1.5705	444.6009	2479	69.4409	1.5705	413.9125	2479	69.4409	1.5705	525.4754

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2480	69.4669	1.57	333.6411	2480	69.4669	1.57	458.429	2480	69.4669	1.57	423.41	2480	69.4669	1.57	533.8316
2481	69.4929	1.5695	342.9085	2481	69.4929	1.5695	464.6073	2481	69.4929	1.5695	437.2176	2481	69.4929	1.5695	546.498
2482	69.5189	1.5689	354.5774	2482	69.5189	1.5689	473.187	2482	69.5189	1.5689	439.5877	2482	69.5189	1.5689	547.7269
2483	69.5449	1.5684	368.3779	2483	69.5449	1.5684	483.8984	2483	69.5449	1.5684	424.1546	2483	69.5449	1.5684	531.1527
2484	69.5709	1.5679	359.1244	2484	69.5709	1.5679	471.5558	2484	69.5709	1.5679	414.9655	2484	69.5709	1.5679	520.8223
2485	69.5969	1.5674	360.0713	2485	69.5969	1.5674	469.4135	2485	69.5969	1.5674	422.169	2485	69.5969	1.5674	526.8847
2486	69.6229	1.5669	360.1131	2486	69.6229	1.5669	467.9035	2486	69.6229	1.5669	447.5687	2486	69.6229	1.5669	552.2052
2487	69.6489	1.5664	331.0956	2487	69.6489	1.5664	437.3341	2487	69.6489	1.5664	445.1169	2487	69.6489	1.5664	549.6741
2488	69.6749	1.5659	352.2648	2488	69.6749	1.5659	456.9513	2488	69.6749	1.5659	421.5733	2488	69.6749	1.5659	526.0512
2489	69.7009	1.5654	386.8252	2489	69.7009	1.5654	489.9599	2489	69.7009	1.5654	439.6613	2489	69.7009	1.5654	544.06
2490	69.7269	1.5649	355.1138	2490	69.7269	1.5649	456.6966	2490	69.7269	1.5649	437.9839	2490	69.7269	1.5649	542.3034
2491	69.7529	1.5643	361.2519	2491	69.7529	1.5643	461.2828	2491	69.7529	1.5643	434.6509	2491	69.7529	1.5643	538.8911
2492	69.7789	1.5638	361.3425	2492	69.7789	1.5638	459.8215	2492	69.7789	1.5638	421.1526	2492	69.7789	1.5638	525.3136
2493	69.8049	1.5633	339.6606	2493	69.8049	1.5633	436.5878	2493	69.8049	1.5633	410.8236	2493	69.8049	1.5633	514.9054
2494	69.8309	1.5628	380.6904	2494	69.8309	1.5628	476.0657	2494	69.8309	1.5628	412.217	2494	69.8309	1.5628	516.2196
2495	69.8569	1.5623	387.7555	2495	69.8569	1.5623	481.5789	2495	69.8569	1.5623	424.3305	2495	69.8569	1.5623	528.2538
2496	69.8829	1.5618	355.9724	2496	69.8829	1.5618	448.2439	2496	69.8829	1.5618	418.5711	2496	69.8829	1.5618	522.4152
2497	69.9089	1.5613	355.9408	2497	69.9089	1.5613	446.6604	2497	69.9089	1.5613	406.8916	2497	69.9089	1.5613	510.6564
2498	69.9349	1.5608	354.0889	2498	69.9349	1.5608	443.2567	2498	69.9349	1.5608	435.5384	2498	69.9349	1.5608	539.224
2499	69.9609	1.5603	363.5325	2499	69.9609	1.5603	451.1484	2499	69.9609	1.5603	430.3984	2499	69.9609	1.5603	534.0048
2500	69.9869	1.5598	347.6953	2500	69.9869	1.5598	433.7593	2500	69.9869	1.5598	410.7189	2500	69.9869	1.5598	514.2461
2501	70.0129	1.5593	373.6599	2501	70.0129	1.5593	458.1719	2501	70.0129	1.5593	424.603	2501	70.0129	1.5593	528.051
2502	70.0389	1.5588	349.565	2502	70.0389	1.5588	432.5252	2502	70.0389	1.5588	439.3635	2502	70.0389	1.5588	542.7322
2503	70.0649	1.5583	350.1733	2503	70.0649	1.5583	431.5816	2503	70.0649	1.5583	413.8036	2503	70.0649	1.5583	517.0931
2504	70.0909	1.5578	382.7496	2504	70.0909	1.5578	462.606	2504	70.0909	1.5578	419.8417	2504	70.0909	1.5578	523.052
2505	70.1169	1.5573	401.6669	2505	70.1169	1.5573	479.9714	2505	70.1169	1.5573	401.7239	2505	70.1169	1.5573	504.855
2506	70.1429	1.5567	372.2725	2506	70.1429	1.5567	449.0252	2506	70.1429	1.5567	422.5082	2506	70.1429	1.5567	525.56
2507	70.1689	1.5562	385.1256	2507	70.1689	1.5562	460.3263	2507	70.1689	1.5562	481.2549	2507	70.1689	1.5562	584.2274
2508	70.1949	1.5557	380.9782	2508	70.1949	1.5557	454.6271	2508	70.1949	1.5557	457.4811	2508	70.1949	1.5557	560.3744
2509	70.2209	1.5552	375.2008	2509	70.2209	1.5552	447.2978	2509	70.2209	1.5552	462.5986	2509	70.2209	1.5552	565.4127
2510	70.2469	1.5547	391.9357	2510	70.2469	1.5547	462.4808	2510	70.2469	1.5547	473.2876	2510	70.2469	1.5547	576.0224
2511	70.2729	1.5542	374.573	2511	70.2729	1.5542	443.5662	2511	70.2729	1.5542	406.58	2511	70.2729	1.5542	509.2356
2512	70.2989	1.5537	400.6438	2512	70.2989	1.5537	468.0851	2512	70.2989	1.5537	422.169	2512	70.2989	1.5537	524.7454
2513	70.3249	1.5532	400.7793	2513	70.3249	1.5532	466.6688	2513	70.3249	1.5532	460.5151	2513	70.3249	1.5532	565.752
2514	70.3509	1.5527	371.9652	2514	70.3509	1.5527	436.3028	2514	70.3509	1.5527	462.9247	2514	70.3509	1.5527	570.8222
2515	70.3769	1.5522	348.3286	2515	70.3769	1.5522	411.1143	2515	70.3769	1.5522	402.6009	2515	70.3769	1.5522	513.1589

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2516	70.4029	1.5517	334.9934	2516	70.4029	1.5517	396.2272	2516	70.4029	1.5517	436.0545	2516	70.4029	1.5517	549.2731
2517	70.4289	1.5512	342.7031	2517	70.4289	1.5512	402.385	2517	70.4289	1.5512	419.5059	2517	70.4289	1.5512	535.385
2518	70.4549	1.5507	382.1003	2518	70.4549	1.5507	440.2303	2518	70.4549	1.5507	454.1277	2518	70.4549	1.5507	572.6673
2519	70.4809	1.5502	392.3749	2519	70.4809	1.5502	448.953	2519	70.4809	1.5502	439.2542	2519	70.4809	1.5502	560.4544
2520	70.5069	1.5497	390.9967	2520	70.5069	1.5497	446.023	2520	70.5069	1.5497	465.0991	2520	70.5069	1.5497	588.9598
2521	70.5329	1.5492	396.5089	2521	70.5329	1.5492	449.9833	2521	70.5329	1.5492	455.508	2521	70.5329	1.5492	582.0292
2522	70.5589	1.5488	357.6556	2522	70.5589	1.5488	409.5781	2522	70.5589	1.5488	440.0015	2522	70.5589	1.5488	569.1833
2523	70.5849	1.5483	413.2842	2523	70.5849	1.5483	463.6548	2523	70.5849	1.5483	456.6772	2523	70.5849	1.5483	588.5196
2524	70.6109	1.5478	406.5207	2524	70.6109	1.5478	455.3394	2524	70.6109	1.5478	421.6512	2524	70.6109	1.5478	556.1541
2525	70.6369	1.5473	366.6194	2525	70.6369	1.5473	413.8863	2525	70.6369	1.5473	415.9243	2525	70.6369	1.5473	553.0877
2526	70.6629	1.5468	354.9305	2526	70.6629	1.5468	400.6455	2526	70.6629	1.5468	491.7116	2526	70.6629	1.5468	631.5355
2527	70.6889	1.5463	383.9256	2527	70.6889	1.5463	428.0887	2527	70.6889	1.5463	478.5349	2527	70.6889	1.5463	621.0194
2528	70.7149	1.5458	400.358	2528	70.7149	1.5458	442.9691	2528	70.7149	1.5458	455.4013	2528	70.7149	1.5458	600.5463
2529	70.7409	1.5453	356.202	2529	70.7409	1.5453	397.2613	2529	70.7409	1.5453	433.782	2529	70.7409	1.5453	581.5876
2530	70.7669	1.5448	374.3426	2530	70.7669	1.5448	413.85	2530	70.7669	1.5448	455.823	2530	70.7669	1.5448	606.2891
2531	70.7929	1.5443	361.9057	2531	70.7929	1.5443	399.8612	2531	70.7929	1.5443	437.0447	2531	70.7929	1.5443	590.1714
2532	70.8189	1.5438	420.1171	2532	70.8189	1.5438	456.5207	2532	70.8189	1.5438	469.4533	2532	70.8189	1.5438	625.2405
2533	70.8449	1.5433	404.5991	2533	70.8449	1.5433	439.4509	2533	70.8449	1.5433	429.468	2533	70.8449	1.5433	587.9157
2534	70.8709	1.5428	396.6323	2534	70.8709	1.5428	429.9322	2534	70.8709	1.5428	486.771	2534	70.8709	1.5428	647.8793
2535	70.8969	1.5423	374.1154	2535	70.8969	1.5423	405.8634	2535	70.8969	1.5423	525.9369	2535	70.8969	1.5423	689.7057
2536	70.9229	1.5418	435.328	2536	70.9229	1.5418	465.5241	2536	70.9229	1.5418	452.3417	2536	70.9229	1.5418	618.771
2537	70.9489	1.5413	405.6654	2537	70.9489	1.5413	434.3096	2537	70.9489	1.5413	435.073	2537	70.9489	1.5413	604.1629
2538	70.9749	1.5409	412.142	2538	70.9749	1.5409	439.2343	2538	70.9749	1.5409	450.4467	2538	70.9749	1.5409	622.1972
2539	71.0009	1.5404	360.0713	2539	71.0009	1.5404	385.6117	2539	71.0009	1.5404	422.169	2539	71.0009	1.5404	596.58
2540	71.0269	1.5399	372.2157	2540	71.0269	1.5399	401.2555	2540	71.0269	1.5399	414.9769	2540	71.0269	1.5399	589.1927
2541	71.0529	1.5394	369.8792	2541	71.0529	1.5394	402.4184	2541	71.0529	1.5394	456.443	2541	71.0529	1.5394	630.4636
2542	71.0789	1.5389	412.9962	2542	71.0789	1.5389	449.0347	2542	71.0789	1.5389	491.5857	2542	71.0789	1.5389	665.4111
2543	71.1049	1.5384	394.4709	2543	71.1049	1.5384	434.0088	2543	71.1049	1.5384	449.3853	2543	71.1049	1.5384	623.0155
2544	71.1309	1.5379	377.5894	2544	71.1309	1.5379	420.6267	2544	71.1309	1.5379	420.2128	2544	71.1309	1.5379	593.6478
2545	71.1569	1.5374	376.2517	2545	71.1569	1.5374	422.7884	2545	71.1569	1.5374	425.6102	2545	71.1569	1.5374	598.8499
2546	71.1829	1.5369	379.1983	2546	71.1829	1.5369	429.2344	2546	71.1829	1.5369	408.7658	2546	71.1829	1.5369	581.8103
2547	71.2089	1.5365	384.843	2547	71.2089	1.5365	438.3784	2547	71.2089	1.5365	439.7806	2547	71.2089	1.5365	612.63
2548	71.2349	1.536	373.7743	2548	71.2349	1.536	430.8091	2548	71.2349	1.536	462.0809	2548	71.2349	1.536	634.7351
2549	71.2609	1.5355	363.5938	2549	71.2609	1.5355	424.128	2549	71.2609	1.5355	462.6691	2549	71.2609	1.5355	635.128
2550	71.2869	1.535	341.2645	2550	71.2869	1.535	405.2981	2550	71.2869	1.535	407.9225	2550	71.2869	1.535	580.1862
2551	71.3129	1.5345	343.0338	2551	71.3129	1.5345	410.5668	2551	71.3129	1.5345	363.5905	2551	71.3129	1.5345	535.6591

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2552	71.3389	1.534	365.6146	2552	71.3389	1.534	436.647	2552	71.3389	1.534	402.9911	2552	71.3389	1.534	574.8644
2553	71.3649	1.5335	338.9094	2553	71.3649	1.5335	413.4411	2553	71.3649	1.5335	421.252	2553	71.3649	1.5335	592.9301
2554	71.3909	1.5331	352.0514	2554	71.3909	1.5331	430.0826	2554	71.3909	1.5331	404.8126	2554	71.3909	1.5331	576.2955
2555	71.4169	1.5326	371.7126	2555	71.4169	1.5326	453.2431	2555	71.4169	1.5326	387.8353	2555	71.4169	1.5326	559.123
2556	71.4429	1.5321	360.2963	2556	71.4429	1.5321	445.3262	2556	71.4429	1.5321	401.0667	2556	71.4429	1.5321	572.1592
2557	71.4689	1.5316	321.7328	2557	71.4689	1.5316	410.2621	2557	71.4689	1.5316	428.9841	2557	71.4689	1.5316	599.8814
2558	71.4949	1.5311	321.461	2558	71.4949	1.5311	413.4896	2558	71.4949	1.5311	402.8334	2558	71.4949	1.5311	573.5355
2559	71.5209	1.5306	331.9471	2559	71.5209	1.5306	427.4751	2559	71.5209	1.5306	408.1004	2559	71.5209	1.5306	578.6074
2560	71.5469	1.5302	365.2861	2560	71.5469	1.5302	464.3135	2560	71.5469	1.5302	413.1201	2560	71.5469	1.5302	583.4318
2561	71.5729	1.5297	388.0668	2561	71.5729	1.5297	490.5936	2561	71.5729	1.5297	395.7017	2561	71.5729	1.5297	565.8182
2562	71.5989	1.5292	374.6046	2562	71.5989	1.5292	480.6308	2562	71.5989	1.5292	415.5841	2562	71.5989	1.5292	585.5054
2563	71.6249	1.5287	360.1581	2563	71.6249	1.5287	469.6837	2563	71.6249	1.5287	391.4215	2563	71.6249	1.5287	561.1476
2564	71.6509	1.5282	362.3742	2564	71.6509	1.5282	475.3991	2564	71.6509	1.5282	406.0022	2564	71.6509	1.5282	575.5331
2565	71.6769	1.5278	384.0491	2565	71.6769	1.5278	500.5735	2565	71.6769	1.5278	434.5127	2565	71.6769	1.5278	603.8483
2566	71.7029	1.5273	420.1464	2566	71.7029	1.5273	540.1701	2566	71.7029	1.5273	422.169	2566	71.7029	1.5273	591.3095
2567	71.7289	1.5268	446.414	2567	71.7289	1.5268	567.5516	2567	71.7289	1.5268	452.5004	2567	71.7289	1.5268	621.1396
2568	71.7549	1.5263	484.0465	2568	71.7549	1.5263	606.298	2568	71.7549	1.5263	483.3325	2568	71.7549	1.5263	651.4705
2569	71.7809	1.5258	531.8972	2569	71.7809	1.5258	655.2626	2569	71.7809	1.5258	521.2905	2569	71.7809	1.5258	688.9273
2570	71.8069	1.5254	609.1475	2570	71.8069	1.5254	733.6268	2570	71.8069	1.5254	588.9711	2570	71.8069	1.5254	756.1067
2571	71.8329	1.5249	687.3941	2571	71.8329	1.5249	812.9872	2571	71.8329	1.5249	657.3441	2571	71.8329	1.5249	823.9784
2572	71.8589	1.5244	729.3538	2572	71.8589	1.5244	856.0608	2572	71.8589	1.5244	712.4992	2572	71.8589	1.5244	878.6323
2573	71.8849	1.5239	734.8235	2573	71.8849	1.5239	862.6444	2573	71.8849	1.5239	724.65	2573	71.8849	1.5239	890.2819
2574	71.9109	1.5235	719.415	2574	71.9109	1.5235	848.3497	2574	71.9109	1.5235	712.7	2574	71.9109	1.5235	877.8306
2575	71.9369	1.523	707.1508	2575	71.9369	1.523	837.1994	2575	71.9369	1.523	714.7309	2575	71.9369	1.523	879.3603
2576	71.9629	1.5225	656.9805	2576	71.9629	1.5225	788.1429	2576	71.9629	1.5225	705.4178	2576	71.9629	1.5225	869.546
2577	71.9889	1.522	658.8607	2577	71.9889	1.522	791.1371	2577	71.9889	1.522	704.5014	2577	71.9889	1.522	868.1284
2578	72.0149	1.5215	664.8518	2578	72.0149	1.5215	798.242	2578	72.0149	1.5215	724.56	2578	72.0149	1.5215	887.6857
2579	72.0409	1.5211	597.5536	2579	72.0409	1.5211	732.0577	2579	72.0409	1.5211	700.2436	2579	72.0409	1.5211	862.8681
2580	72.0669	1.5206	623.1626	2580	72.0669	1.5206	758.7806	2580	72.0669	1.5206	674.9518	2580	72.0669	1.5206	837.0751
2581	72.0929	1.5201	631.8264	2581	72.0929	1.5201	768.5583	2581	72.0929	1.5201	662.7711	2581	72.0929	1.5201	824.3932
2582	72.1189	1.5197	563.5317	2582	72.1189	1.5197	701.3775	2582	72.1189	1.5197	636.9133	2582	72.1189	1.5197	798.0341
2583	72.1449	1.5192	537.6597	2583	72.1449	1.5192	676.6194	2583	72.1449	1.5192	612.4255	2583	72.1449	1.5192	773.0451
2584	72.1709	1.5187	516.2784	2584	72.1709	1.5187	656.3519	2584	72.1709	1.5187	590.0777	2584	72.1709	1.5187	750.1961
2585	72.1969	1.5182	486.503	2585	72.1969	1.5182	627.6903	2585	72.1969	1.5182	550.9595	2585	72.1969	1.5182	710.5767
2586	72.2229	1.5178	514.0494	2586	72.2229	1.5178	656.3507	2586	72.2229	1.5178	571.9015	2586	72.2229	1.5178	731.0175
2587	72.2489	1.5173	550.2439	2587	72.2489	1.5173	693.659	2587	72.2489	1.5173	562.2006	2587	72.2489	1.5173	720.8153

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2588	72.2749	1.5168	558.7329	2588	72.2749	1.5168	703.2619	2588	72.2749	1.5168	533.1138	2588	72.2749	1.5168	691.2273
2589	72.3009	1.5163	571.935	2589	72.3009	1.5163	717.5779	2589	72.3009	1.5163	560.2133	2589	72.3009	1.5163	717.8256
2590	72.3269	1.5159	554.4426	2590	72.3269	1.5159	701.1993	2590	72.3269	1.5159	557.8015	2590	72.3269	1.5159	714.9125
2591	72.3529	1.5154	568.2177	2591	72.3529	1.5154	716.0884	2591	72.3529	1.5154	571.0889	2591	72.3529	1.5154	727.6987
2592	72.3789	1.5149	610.1887	2592	72.3789	1.5149	759.1732	2592	72.3789	1.5149	554.5764	2592	72.3789	1.5149	710.685
2593	72.4049	1.5145	589.8361	2593	72.4049	1.5145	739.9345	2593	72.4049	1.5145	530.5892	2593	72.4049	1.5145	686.1966
2594	72.4309	1.514	589.634	2594	72.4309	1.514	740.8463	2594	72.4309	1.514	553.0612	2594	72.4309	1.514	708.1673
2595	72.4569	1.5135	620.1808	2595	72.4569	1.5135	772.507	2595	72.4569	1.5135	511.0108	2595	72.4569	1.5135	665.6157
2596	72.4829	1.5131	598.0237	2596	72.4829	1.5131	751.4637	2596	72.4829	1.5131	526.4458	2596	72.4829	1.5131	680.5495
2597	72.5089	1.5126	591.3239	2597	72.5089	1.5126	745.8778	2597	72.5089	1.5126	553.5069	2597	72.5089	1.5126	707.1094
2598	72.5349	1.5121	625.0277	2598	72.5349	1.5121	780.6954	2598	72.5349	1.5121	558.3219	2598	72.5349	1.5121	711.4232
2599	72.5609	1.5117	620.8931	2599	72.5609	1.5117	777.6748	2599	72.5609	1.5117	532.8407	2599	72.5609	1.5117	685.4407
2600	72.5869	1.5112	598.137	2600	72.5869	1.5112	756.0325	2600	72.5869	1.5112	538.0859	2600	72.5869	1.5112	690.1847
2601	72.6129	1.5107	587.0008	2601	72.6129	1.5107	746.0102	2601	72.6129	1.5107	529.4534	2601	72.6129	1.5107	681.051
2602	72.6389	1.5103	593.3348	2602	72.6389	1.5103	753.4581	2602	72.6389	1.5103	553.3618	2602	72.6389	1.5103	704.4581
2603	72.6649	1.5098	605.4875	2603	72.6649	1.5098	766.7246	2603	72.6649	1.5098	559.8418	2603	72.6649	1.5098	710.4368
2604	72.6909	1.5093	602.6112	2604	72.6909	1.5093	764.9623	2604	72.6909	1.5093	521.9061	2604	72.6909	1.5093	672
2605	72.7169	1.5089	622.4833	2605	72.7169	1.5089	785.9482	2605	72.7169	1.5089	514.4522	2605	72.7169	1.5089	664.0448
2606	72.7429	1.5084	633.0979	2606	72.7429	1.5084	797.6767	2606	72.7429	1.5084	486.5601	2606	72.7429	1.5084	635.6515
2607	72.7689	1.5079	641.4499	2607	72.7689	1.5079	807.1425	2607	72.7689	1.5079	555.8423	2607	72.7689	1.5079	704.4324
2608	72.7949	1.5075	637.3486	2608	72.7949	1.5075	804.1551	2608	72.7949	1.5075	551.1537	2608	72.7949	1.5075	699.2427
2609	72.8209	1.507	606.6638	2609	72.8209	1.507	774.5842	2609	72.8209	1.507	579.2896	2609	72.8209	1.507	726.8773
2610	72.8469	1.5065	574.9804	2610	72.8469	1.5065	744.0146	2610	72.8469	1.5065	575.3059	2610	72.8469	1.5065	722.3924
2611	72.8729	1.5061	579.1786	2611	72.8729	1.5061	749.3268	2611	72.8729	1.5061	542.4795	2611	72.8729	1.5061	689.0648
2612	72.8989	1.5056	559.6614	2612	72.8989	1.5056	730.9234	2612	72.8989	1.5056	502.3312	2612	72.8989	1.5056	648.4152
2613	72.9249	1.5052	598.4099	2613	72.9249	1.5052	770.7858	2613	72.9249	1.5052	527.3299	2613	72.9249	1.5052	672.9127
2614	72.9509	1.5047	509.4322	2614	72.9509	1.5047	682.922	2614	72.9509	1.5047	533.9737	2614	72.9509	1.5047	679.0553
2615	72.9769	1.5042	544.7019	2615	72.9769	1.5042	719.3056	2615	72.9769	1.5042	485.8716	2615	72.9769	1.5042	630.4519
2616	73.0029	1.5038	531.5799	2616	73.0029	1.5038	707.2974	2616	73.0029	1.5038	507.2824	2616	73.0029	1.5038	651.3615
2617	73.0289	1.5033	499.6059	2617	73.0289	1.5033	676.4373	2617	73.0289	1.5033	494.6475	2617	73.0289	1.5033	638.2254
2618	73.0549	1.5028	484.4868	2618	73.0549	1.5028	662.4321	2618	73.0549	1.5028	454.6556	2618	73.0549	1.5028	597.7323
2619	73.0809	1.5024	437.7533	2619	73.0809	1.5024	616.8125	2619	73.0809	1.5024	418.4948	2619	73.0809	1.5024	561.0703
2620	73.1069	1.5019	428.8134	2620	73.1069	1.5019	608.9865	2620	73.1069	1.5019	422.169	2620	73.1069	1.5019	564.2433
2621	73.1329	1.5015	429.0662	2621	73.1329	1.5015	607.9677	2621	73.1329	1.5015	442.8113	2621	73.1329	1.5015	582
2622	73.1589	1.501	421.4272	2622	73.1589	1.501	599.057	2622	73.1589	1.501	445.6969	2622	73.1589	1.501	582
2623	73.1849	1.5005	421.6581	2623	73.1849	1.5005	598.0163	2623	73.1849	1.5005	455.4687	2623	73.1849	1.5005	588.8862

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2624	73.2109	1.5001	443.3638	2624	73.2109	1.5001	618.4504	2624	73.2109	1.5001	444.8344	2624	73.2109	1.5001	575.3664
2625	73.2369	1.4996	411.4484	2625	73.2369	1.4996	585.2633	2625	73.2369	1.4996	427.1115	2625	73.2369	1.4996	554.758
2626	73.2629	1.4992	373.2974	2626	73.2629	1.4992	545.8407	2626	73.2629	1.4992	417.7913	2626	73.2629	1.4992	542.5522
2627	73.2889	1.4987	394.4417	2627	73.2889	1.4987	565.7134	2627	73.2889	1.4987	352.1523	2627	73.2889	1.4987	474.0277
2628	73.3149	1.4983	340.0176	2628	73.3149	1.4983	510.0176	2628	73.3149	1.4983	411.7291	2628	73.3149	1.4983	530.7189
2629	73.3409	1.4978	389.0276	2629	73.3409	1.4978	557.756	2629	73.3409	1.4978	424.441	2629	73.3409	1.4978	540.5453
2630	73.3669	1.4973	368.0287	2630	73.3669	1.4973	535.4855	2630	73.3669	1.4973	414.9812	2630	73.3669	1.4973	528.1999
2631	73.3929	1.4969	360.4843	2631	73.3929	1.4969	526.6694	2631	73.3929	1.4969	429.328	2631	73.3929	1.4969	539.6612
2632	73.4189	1.4964	395.97	2632	73.4189	1.4964	560.8835	2632	73.4189	1.4964	377.2022	2632	73.4189	1.4964	484.6498
2633	73.4449	1.496	417.2796	2633	73.4449	1.496	580.9215	2633	73.4449	1.496	420.3178	2633	73.4449	1.496	524.8799
2634	73.4709	1.4955	413.6329	2634	73.4709	1.4955	576.0032	2634	73.4709	1.4955	445.941	2634	73.4709	1.4955	547.6175
2635	73.4969	1.4951	400.0665	2635	73.4969	1.4951	561.1651	2635	73.4969	1.4951	443.4269	2635	73.4969	1.4951	542.2179
2636	73.5229	1.4946	382.9326	2636	73.5229	1.4946	542.7596	2636	73.5229	1.4946	428.8542	2636	73.5229	1.4946	524.7596
2637	73.5489	1.4942	400.031	2637	73.5489	1.4942	558.5864	2637	73.5489	1.4942	432.3595	2637	73.5489	1.4942	525.3793
2638	73.5749	1.4937	391.3576	2638	73.5749	1.4937	548.6414	2638	73.5749	1.4937	389.1105	2638	73.5749	1.4937	479.2448
2639	73.6009	1.4933	378.438	2639	73.6009	1.4933	534.4501	2639	73.6009	1.4933	438.0258	2639	73.6009	1.4933	525.2745
2640	73.6269	1.4928	397.6362	2640	73.6269	1.4928	552.3767	2640	73.6269	1.4928	418.4039	2640	73.6269	1.4928	502.7671
2641	73.6529	1.4924	401.9208	2641	73.6529	1.4924	555.3897	2641	73.6529	1.4924	376.4856	2641	73.6529	1.4924	457.9632
2642	73.6789	1.4919	370.1985	2642	73.6789	1.4919	522.3958	2642	73.6789	1.4919	399.8313	2642	73.6789	1.4919	478.4233
2643	73.7049	1.4914	376.4245	2643	73.7049	1.4914	527.3502	2643	73.7049	1.4914	381.2373	2643	73.7049	1.4914	456.9438
2644	73.7309	1.491	376.6937	2644	73.7309	1.491	526.3477	2644	73.7309	1.491	382.3821	2644	73.7309	1.491	455.203
2645	73.7569	1.4905	349.0611	2645	73.7569	1.4905	497.4435	2645	73.7569	1.4905	379.41	2645	73.7569	1.4905	449.3454
2646	73.7829	1.4901	412.1541	2646	73.7829	1.4901	559.2649	2646	73.7829	1.4901	388.2611	2646	73.7829	1.4901	455.3109
2647	73.8089	1.4896	435.4153	2647	73.8089	1.4896	581.2544	2647	73.8089	1.4896	422.169	2647	73.8089	1.4896	486.3333
2648	73.8349	1.4892	411.0222	2648	73.8349	1.4892	553.0437	2648	73.8349	1.4892	445.456	2648	73.8349	1.4892	511.4495
2649	73.8609	1.4887	384.4746	2649	73.8609	1.4887	522.6785	2649	73.8609	1.4887	417.2434	2649	73.8609	1.4887	485.0662
2650	73.8869	1.4883	378.4662	2650	73.8869	1.4883	512.8525	2650	73.8869	1.4883	421.9601	2650	73.8869	1.4883	491.612
2651	73.9129	1.4878	339.0759	2651	73.9129	1.4878	469.6445	2651	73.9129	1.4878	425.401	2651	73.9129	1.4878	496.8822
2652	73.9389	1.4874	341.9531	2652	73.9389	1.4874	468.7041	2652	73.9389	1.4874	413.6415	2652	73.9389	1.4874	486.952
2653	73.9649	1.4869	344.8337	2653	73.9649	1.4869	467.767	2653	73.9649	1.4869	421.5819	2653	73.9649	1.4869	496.7216
2654	73.9909	1.4865	357.7313	2654	73.9909	1.4865	476.847	2654	73.9909	1.4865	440.2304	2654	73.9909	1.4865	517.1993
2655	74.0169	1.4861	361.0396	2655	74.0169	1.4861	476.3376	2655	74.0169	1.4861	423.2161	2655	74.0169	1.4861	502.0142
2656	74.0429	1.4856	327.3913	2656	74.0429	1.4856	438.8717	2656	74.0429	1.4856	437.9378	2656	74.0429	1.4856	518.5652
2657	74.0689	1.4852	328.2042	2657	74.0689	1.4852	435.867	2657	74.0689	1.4852	406.5888	2657	74.0689	1.4852	489.0454
2658	74.0949	1.4847	341.4278	2658	74.0949	1.4847	445.2729	2658	74.0949	1.4847	387.0789	2658	74.0949	1.4847	471.3647
2659	74.1209	1.4843	342.2132	2659	74.1209	1.4843	442.2407	2659	74.1209	1.4843	394.5239	2659	74.1209	1.4843	480.6389

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2660	74.1469	1.4838	353.0395	2660	74.1469	1.4838	449.2494	2660	74.1469	1.4838	448.4688	2660	74.1469	1.4838	536.413
2661	74.1729	1.4834	357.7541	2661	74.1729	1.4834	450.1464	2661	74.1729	1.4834	467.6992	2661	74.1729	1.4834	557.4727
2662	74.1989	1.4829	340.522	2662	74.1989	1.4829	429.0966	2662	74.1989	1.4829	426.1712	2662	74.1989	1.4829	517.7739
2663	74.2249	1.4825	318.1584	2663	74.2249	1.4825	402.9154	2663	74.2249	1.4825	426.6292	2663	74.2249	1.4825	520.0611
2664	74.2509	1.482	318.4069	2664	74.2509	1.482	399.3463	2664	74.2509	1.482	438.8541	2664	74.2509	1.482	534.1153
2665	74.2769	1.4816	343.3216	2665	74.2769	1.4816	420.4434	2665	74.2769	1.4816	471.7654	2665	74.2769	1.4816	568.8558
2666	74.3029	1.4812	335.1839	2666	74.3029	1.4812	408.488	2666	74.3029	1.4812	478.0251	2666	74.3029	1.4812	576.9447
2667	74.3289	1.4807	317.872	2667	74.3289	1.4807	387.3585	2667	74.3289	1.4807	453.1379	2667	74.3289	1.4807	553.8868
2668	74.3549	1.4803	333.2251	2668	74.3549	1.4803	398.8939	2668	74.3549	1.4803	457.2413	2668	74.3549	1.4803	559.8194
2669	74.3809	1.4798	353.9494	2669	74.3809	1.4798	415.8006	2669	74.3809	1.4798	493.0135	2669	74.3809	1.4798	597.4208
2670	74.4069	1.4794	359.862	2670	74.4069	1.4794	417.8956	2670	74.4069	1.4794	509.0372	2670	74.4069	1.4794	615.2738
2671	74.4329	1.4789	370.9336	2671	74.4329	1.4789	425.1496	2671	74.4329	1.4789	503.9791	2671	74.4329	1.4789	612.0449
2672	74.4589	1.4785	396.0455	2672	74.4589	1.4785	446.4438	2672	74.4589	1.4785	509.583	2672	74.4589	1.4785	619.478
2673	74.4849	1.4781	388.0129	2673	74.4849	1.4781	434.5936	2673	74.4849	1.4781	508.8623	2673	74.4849	1.4781	620.5866
2674	74.5109	1.4776	360.0713	2674	74.5109	1.4776	402.8343	2674	74.5109	1.4776	520.1664	2674	74.5109	1.4776	633.7199
2675	74.5369	1.4772	373.6208	2675	74.5369	1.4772	417.9217	2675	74.5369	1.4772	549.7419	2675	74.5369	1.4772	662.7592
2676	74.5629	1.4767	396.3297	2676	74.5629	1.4767	442.1685	2676	74.5629	1.4767	538.252	2676	74.5629	1.4767	650.733
2677	74.5889	1.4763	409.1973	2677	74.5889	1.4763	456.574	2677	74.5889	1.4763	527.9729	2677	74.5889	1.4763	639.9178
2678	74.6149	1.4759	407.4984	2678	74.6149	1.4759	456.4129	2678	74.6149	1.4759	555.4096	2678	74.6149	1.4759	666.8183
2679	74.6409	1.4754	388.9658	2679	74.6409	1.4754	439.4182	2679	74.6409	1.4754	556.1341	2679	74.6409	1.4754	667.0066
2680	74.6669	1.475	384.9553	2680	74.6669	1.475	436.9456	2680	74.6669	1.475	552.8455	2680	74.6669	1.475	663.1818
2681	74.6929	1.4745	397.9901	2681	74.6929	1.4745	451.5183	2681	74.6929	1.4745	544.911	2681	74.6929	1.4745	654.711
2682	74.7189	1.4741	455.104	2682	74.7189	1.4741	510.17	2682	74.7189	1.4741	553.8145	2682	74.7189	1.4741	663.0784
2683	74.7449	1.4737	486.9239	2683	74.7449	1.4737	543.5279	2683	74.7449	1.4737	580.017	2683	74.7449	1.4737	688.7447
2684	74.7709	1.4732	512.153	2684	74.7709	1.4732	570.2948	2684	74.7709	1.4732	559.3783	2684	74.7709	1.4732	667.5698
2685	74.7969	1.4728	504.0602	2685	74.7969	1.4728	563.7399	2685	74.7969	1.4728	586.7188	2685	74.7969	1.4728	694.3741
2686	74.8229	1.4724	501.7953	2686	74.8229	1.4724	563.0129	2686	74.8229	1.4724	601.8389	2686	74.8229	1.4724	708.958
2687	74.8489	1.4719	479.0805	2687	74.8489	1.4719	541.8359	2687	74.8489	1.4719	571.8631	2687	74.8489	1.4719	678.446
2688	74.8749	1.4715	492.4991	2688	74.8749	1.4715	556.7924	2688	74.8749	1.4715	541.4998	2688	74.8749	1.4715	647.5464
2689	74.9009	1.471	521.2972	2689	74.9009	1.471	587.1284	2689	74.9009	1.471	534.0671	2689	74.9009	1.471	639.5776
2690	74.9269	1.4706	521.2871	2690	74.9269	1.4706	588.6561	2690	74.9269	1.4706	553.448	2690	74.9269	1.4706	658.4222
2691	74.9529	1.4702	469.4544	2691	74.9529	1.4702	538.3613	2691	74.9529	1.4702	558.4542	2691	74.9529	1.4702	662.8922
2692	74.9789	1.4697	502.4348	2692	74.9789	1.4697	572.8795	2692	74.9789	1.4697	542.2008	2692	74.9789	1.4697	646.1027
2693	75.0049	1.4693	502.8471	2693	75.0049	1.4693	574.8298	2693	75.0049	1.4693	543.5262	2693	75.0049	1.4693	646.8919
2694	75.0309	1.4689	464.8039	2694	75.0309	1.4689	538.3244	2694	75.0309	1.4689	565.1339	2694	75.0309	1.4689	667.9633
2695	75.0569	1.4684	451.9386	2695	75.0569	1.4684	526.9971	2695	75.0569	1.4684	571.8096	2695	75.0569	1.4684	674.1028

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2696	75.0829	1.468	428.2906	2696	75.0829	1.468	504.8869	2696	75.0829	1.468	500.8416	2696	75.0829	1.468	602.5986
2697	75.1089	1.4676	420.3608	2697	75.1089	1.4676	498.495	2697	75.1089	1.4676	517.5517	2697	75.1089	1.4676	618.7725
2698	75.1349	1.4671	410.7554	2698	75.1349	1.4671	490.4275	2698	75.1349	1.4671	482.6383	2698	75.1349	1.4671	583.323
2699	75.1609	1.4667	378.1625	2699	75.1609	1.4667	459.3724	2699	75.1609	1.4667	476.244	2699	75.1609	1.4667	576.3924
2700	75.1869	1.4663	420.6736	2700	75.1869	1.4663	503.4214	2700	75.1869	1.4663	474.9035	2700	75.1869	1.4663	574.5157
2701	75.2129	1.4658	360.0713	2701	75.2129	1.4658	444.357	2701	75.2129	1.4658	486.0357	2701	75.2129	1.4658	585.1117
2702	75.2389	1.4654	374.418	2702	75.2389	1.4654	458.799	2702	75.2389	1.4654	474.2631	2702	75.2389	1.4654	572.8029
2703	75.2649	1.465	373.1653	2703	75.2649	1.465	457.6415	2703	75.2649	1.465	442.9784	2703	75.2649	1.465	540.982
2704	75.2909	1.4645	340.1291	2704	75.2909	1.4645	424.7006	2704	75.2909	1.4645	403.9143	2704	75.2909	1.4645	501.3818
2705	75.3169	1.4641	360.8393	2705	75.3169	1.4641	445.506	2705	75.3169	1.4641	440.9608	2705	75.3169	1.4641	537.8921
2706	75.3429	1.4637	399.5146	2706	75.3429	1.4637	484.2766	2706	75.3429	1.4637	452.0806	2706	75.3429	1.4637	548.4756
2707	75.3689	1.4633	388.1482	2707	75.3689	1.4633	473.0055	2707	75.3689	1.4633	432.0373	2707	75.3689	1.4633	527.8961
2708	75.3949	1.4628	408.4159	2708	75.3949	1.4628	493.3685	2708	75.3949	1.4628	418.5721	2708	75.3949	1.4628	513.8947
2709	75.4209	1.4624	433.6476	2709	75.4209	1.4624	518.6955	2709	75.4209	1.4624	405.0397	2709	75.4209	1.4624	499.8261
2710	75.4469	1.462	459.4339	2710	75.4469	1.462	544.5771	2710	75.4469	1.462	397.5088	2710	75.4469	1.462	491.759
2711	75.4729	1.4615	419.4298	2711	75.4729	1.4615	504.6682	2711	75.4729	1.4615	400.0459	2711	75.4729	1.4615	493.76
2712	75.4989	1.4611	412.841	2712	75.4989	1.4611	498.1747	2712	75.4989	1.4611	423.071	2712	75.4989	1.4611	516.2488
2713	75.5249	1.4607	382.2914	2713	75.5249	1.4607	467.7204	2713	75.5249	1.4607	356.8992	2713	75.5249	1.4607	449.5408
2714	75.5509	1.4603	416.8086	2714	75.5509	1.4603	502.3329	2714	75.5509	1.4603	384.8343	2714	75.5509	1.4603	476.9397
2715	75.5769	1.4598	389.8544	2715	75.5769	1.4598	475.474	2715	75.5769	1.4598	406.1546	2715	75.5769	1.4598	497.7238
2716	75.6029	1.4594	436.6876	2716	75.6029	1.4594	522.4024	2716	75.6029	1.4594	388.5646	2716	75.6029	1.4594	479.5976
2717	75.6289	1.459	455.1267	2717	75.6289	1.459	540.9368	2717	75.6289	1.459	368.269	2717	75.6289	1.459	458.7658
2718	75.6549	1.4585	397.5599	2718	75.6549	1.4585	483.4653	2718	75.6549	1.4585	382.8337	2718	75.6549	1.4585	472.7943
2719	75.6809	1.4581	385.3114	2719	75.6809	1.4581	471.3121	2719	75.6809	1.4581	378.9189	2719	75.6809	1.4581	468.3433
2720	75.7069	1.4577	394.8189	2720	75.7069	1.4577	480.9149	2720	75.7069	1.4577	390.0267	2720	75.7069	1.4577	478.9149
2721	75.7329	1.4573	390.8429	2721	75.7329	1.4573	477.0341	2721	75.7329	1.4573	386.9207	2721	75.7329	1.4573	475.2727
2722	75.7589	1.4568	393.6645	2722	75.7589	1.4568	479.951	2722	75.7589	1.4568	411.1208	2722	75.7589	1.4568	498.9366
2723	75.7849	1.4564	359.9065	2723	75.7849	1.4564	446.2883	2723	75.7849	1.4564	368.0935	2723	75.7849	1.4564	455.3731
2724	75.8109	1.456	443.9403	2724	75.8109	1.456	530.4174	2724	75.8109	1.456	378.0726	2724	75.8109	1.456	464.816
2725	75.8369	1.4556	365.7503	2725	75.8369	1.4556	452.3226	2725	75.8369	1.4556	377.8211	2725	75.8369	1.4556	464.0283
2726	75.8629	1.4551	351.7913	2726	75.8629	1.4551	438.459	2726	75.8629	1.4551	375.4438	2726	75.8629	1.4551	461.1147
2727	75.8889	1.4547	374.081	2727	75.8889	1.4547	460.8439	2727	75.8889	1.4547	415.8421	2727	75.8889	1.4547	500.9769
2728	75.9149	1.4543	360.0713	2728	75.9149	1.4543	446.9295	2728	75.9149	1.4543	422.169	2728	75.9149	1.4543	506.7676
2729	75.9409	1.4539	399.8137	2729	75.9409	1.4539	486.0754	2729	75.9409	1.4539	356.2619	2729	75.9409	1.4539	440.829
2730	75.9669	1.4535	407.9451	2730	75.9669	1.4535	493.6103	2730	75.9669	1.4535	337.6335	2730	75.9669	1.4535	422.169
2731	75.9929	1.453	377.0064	2731	75.9929	1.453	462.0751	2731	75.9929	1.453	356.5631	2731	75.9929	1.453	441.0671

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2732	76.0189	1.4526	331.2213	2732	76.0189	1.4526	415.6935	2732	76.0189	1.4526	408.1496	2732	76.0189	1.4526	492.622
2733	76.0449	1.4522	338.7242	2733	76.0449	1.4522	422.5999	2733	76.0449	1.4522	343.9599	2733	76.0449	1.4522	428.4009
2734	76.0709	1.4518	375.1334	2734	76.0709	1.4518	458.4126	2734	76.0709	1.4518	370.8856	2734	76.0709	1.4518	455.295
2735	76.0969	1.4513	325.3529	2735	76.0969	1.4513	408.0355	2735	76.0969	1.4513	375.6222	2735	76.0969	1.4513	460
2736	76.1229	1.4509	349.8275	2736	76.1229	1.4509	431.9136	2736	76.1229	1.4509	395.4919	2736	76.1229	1.4509	479.8382
2737	76.1489	1.4505	332.49	2737	76.1489	1.4505	413.9796	2737	76.1489	1.4505	372.2544	2737	76.1489	1.4505	456.5692
2738	76.1749	1.4501	324.0508	2738	76.1749	1.4501	404.9439	2738	76.1749	1.4501	418.2779	2738	76.1749	1.4501	502.5611
2739	76.2009	1.4497	342.8569	2739	76.2009	1.4497	423.1535	2739	76.2009	1.4497	402.7654	2739	76.2009	1.4497	487.0171
2740	76.2269	1.4492	306.1578	2740	76.2269	1.4492	385.858	2740	76.2269	1.4492	384.6144	2740	76.2269	1.4492	468.8345
2741	76.2529	1.4488	322.2839	2741	76.2529	1.4488	401.3876	2741	76.2529	1.4488	374.4951	2741	76.2529	1.4488	458.6837
2742	76.2789	1.4484	333.3109	2742	76.2789	1.4484	411.818	2742	76.2789	1.4484	372.8429	2742	76.2789	1.4484	457
2743	76.3049	1.448	313.6764	2743	76.3049	1.448	391.587	2743	76.3049	1.448	358.5991	2743	76.3049	1.448	442.7247
2744	76.3309	1.4476	334.5299	2744	76.3309	1.4476	411.844	2744	76.3309	1.4476	405.0277	2744	76.3309	1.4476	489.1217
2745	76.3569	1.4472	326.0446	2745	76.3569	1.4472	402.7622	2745	76.3569	1.4472	356.3059	2745	76.3569	1.4472	440.3684
2746	76.3829	1.4467	324.1688	2746	76.3829	1.4467	400.2899	2746	76.3829	1.4467	373.0811	2746	76.3829	1.4467	457.1121
2747	76.4089	1.4463	309.6543	2747	76.4089	1.4463	385.1789	2747	76.4089	1.4463	418.6563	2747	76.4089	1.4463	502.6557
2748	76.4349	1.4459	312.5065	2748	76.4349	1.4459	387.4346	2748	76.4349	1.4459	377.2463	2748	76.4349	1.4459	461.2142
2749	76.4609	1.4455	325.2044	2749	76.4609	1.4455	399.536	2749	76.4609	1.4455	374.468	2749	76.4609	1.4455	458.4043
2750	76.4869	1.4451	322.7524	2750	76.4869	1.4451	396.4874	2750	76.4869	1.4451	384.4369	2750	76.4869	1.4451	468.3417
2751	76.5129	1.4447	333.7079	2751	76.5129	1.4447	406.8465	2751	76.5129	1.4447	391.8363	2751	76.5129	1.4447	475.7096
2752	76.5389	1.4442	360.5711	2752	76.5389	1.4442	433.1132	2752	76.5389	1.4442	401.8997	2752	76.5389	1.4442	485.7415
2753	76.5649	1.4438	359.6467	2753	76.5649	1.4438	431.5922	2753	76.5649	1.4438	409.3529	2753	76.5649	1.4438	493.1631
2754	76.5909	1.4434	369.3295	2754	76.5909	1.4434	440.6786	2754	76.5909	1.4434	403.0142	2754	76.5909	1.4434	486.7929
2755	76.6169	1.443	360.0713	2755	76.6169	1.443	430.8238	2755	76.6169	1.443	422.169	2755	76.6169	1.443	505.9162
2756	76.6429	1.4426	363.2689	2756	76.6429	1.4426	434.9535	2756	76.6429	1.4426	411.5915	2756	76.6429	1.4426	495.0852
2757	76.6689	1.4422	411.5581	2757	76.6689	1.4422	484.1747	2757	76.6689	1.4422	426.9262	2757	76.6689	1.4422	510.1665
2758	76.6949	1.4418	481.1252	2758	76.6949	1.4418	554.6737	2758	76.6949	1.4418	495.7736	2758	76.6949	1.4418	578.7604
2759	76.7209	1.4413	528.0862	2759	76.7209	1.4413	602.5668	2759	76.7209	1.4413	532.6099	2759	76.7209	1.4413	615.3432
2760	76.7469	1.4409	597.0318	2760	76.7469	1.4409	672.4443	2760	76.7469	1.4409	567.1155	2760	76.7469	1.4409	649.5953
2761	76.7729	1.4405	616.5226	2761	76.7729	1.4405	692.8671	2761	76.7729	1.4405	642.3051	2761	76.7729	1.4405	724.5315
2762	76.7989	1.4401	687.7332	2762	76.7989	1.4401	765.0097	2762	76.7989	1.4401	675.6089	2762	76.7989	1.4401	757.5818
2763	76.8249	1.4397	805.2005	2763	76.8249	1.4397	883.4091	2763	76.8249	1.4397	737.9058	2763	76.8249	1.4397	819.6252
2764	76.8509	1.4393	824.3018	2764	76.8509	1.4393	903.4424	2764	76.8509	1.4393	778.6105	2764	76.8509	1.4393	860.0765
2765	76.8769	1.4389	791.5578	2765	76.8769	1.4389	871.6304	2765	76.8769	1.4389	746.324	2765	76.8769	1.4389	827.5365
2766	76.9029	1.4385	794.117	2766	76.9029	1.4385	875.1215	2766	76.9029	1.4385	737.0328	2766	76.9029	1.4385	817.9918
2767	76.9289	1.438	776.8714	2767	76.9289	1.438	858.808	2767	76.9289	1.438	755.0636	2767	76.9289	1.438	835.7691

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2768	76.9549	1.4376	743.7761	2768	76.9549	1.4376	826.6447	2768	76.9549	1.4376	755.0077	2768	76.9549	1.4376	835.4598
2769	76.9809	1.4372	711.1904	2769	76.9809	1.4372	794.9909	2769	76.9809	1.4372	766.9244	2769	76.9809	1.4372	847.123
2770	77.0069	1.4368	689.2171	2770	77.0069	1.4368	773.9497	2770	77.0069	1.4368	775.7528	2770	77.0069	1.4368	855.6979
2771	77.0329	1.4364	670.8474	2771	77.0329	1.4364	756.512	2771	77.0329	1.4364	704.8717	2771	77.0329	1.4364	784.5633
2772	77.0589	1.436	645.8129	2772	77.0589	1.436	732.4094	2772	77.0589	1.436	686.5146	2772	77.0589	1.436	765.9528
2773	77.0849	1.4356	615.169	2773	77.0849	1.4356	702.6976	2773	77.0849	1.4356	663.4218	2773	77.0849	1.4356	742.6065
2774	77.1109	1.4352	578.9459	2774	77.1109	1.4352	667.4065	2774	77.1109	1.4352	582.5043	2774	77.1109	1.4352	661.4355
2775	77.1369	1.4348	558.3763	2775	77.1369	1.4348	647.7688	2775	77.1369	1.4348	590.1491	2775	77.1369	1.4348	668.8269
2776	77.1629	1.4344	522.3402	2776	77.1629	1.4344	612.6648	2776	77.1629	1.4344	588.5687	2776	77.1629	1.4344	666.993
2777	77.1889	1.434	490.022	2777	77.1889	1.434	581.2786	2777	77.1889	1.434	542.7906	2777	77.1889	1.434	620.9614
2778	77.2149	1.4335	463.2806	2778	77.2149	1.4335	555.4692	2778	77.2149	1.4335	510.3715	2778	77.2149	1.4335	588.2888
2779	77.2409	1.4331	445.6219	2779	77.2409	1.4331	538.7425	2779	77.2409	1.4331	493.6437	2779	77.2409	1.4331	571.3076
2780	77.2669	1.4327	460.0025	2780	77.2669	1.4327	554.0551	2780	77.2669	1.4327	492.182	2780	77.2669	1.4327	569.5924
2781	77.2929	1.4323	463.2405	2781	77.2929	1.4323	558.225	2781	77.2929	1.4323	493.6674	2781	77.2929	1.4323	570.8244
2782	77.3189	1.4319	483.0529	2782	77.3189	1.4319	578.9695	2782	77.3189	1.4319	468.796	2782	77.3189	1.4319	545.6994
2783	77.3449	1.4315	469.5434	2783	77.3449	1.4315	564.1145	2783	77.3449	1.4315	427.0851	2783	77.3449	1.4315	503.7351
2784	77.3709	1.4311	492.1728	2784	77.3709	1.4311	585.3985	2784	77.3709	1.4311	460.0065	2784	77.3709	1.4311	536.4031
2785	77.3969	1.4307	534.2921	2785	77.3969	1.4307	626.1724	2785	77.3969	1.4307	464.6209	2785	77.3969	1.4307	540.764
2786	77.4229	1.4303	519.618	2786	77.4229	1.4303	610.1528	2786	77.4229	1.4303	425.5685	2786	77.4229	1.4303	501.4581
2787	77.4489	1.4299	565.4359	2787	77.4489	1.4299	654.6253	2787	77.4489	1.4299	446.6509	2787	77.4489	1.4299	522.287
2788	77.4749	1.4295	578.2643	2788	77.4749	1.4295	666.1083	2788	77.4749	1.4295	436.6065	2788	77.4749	1.4295	511.9892
2789	77.5009	1.4291	562.4418	2789	77.5009	1.4291	648.9403	2789	77.5009	1.4291	427.9504	2789	77.5009	1.4291	503.0796
2790	77.5269	1.4287	556.4211	2790	77.5269	1.4287	641.5742	2790	77.5269	1.4287	432.3621	2790	77.5269	1.4287	507.2379
2791	77.5529	1.4283	550.4017	2791	77.5529	1.4283	634.2094	2791	77.5529	1.4283	417.5651	2791	77.5529	1.4283	492.1873
2792	77.5789	1.4279	531.1887	2792	77.5789	1.4279	613.651	2792	77.5789	1.4279	427.811	2792	77.5789	1.4279	502.1798
2793	77.6049	1.4275	550.6596	2793	77.6049	1.4275	631.7764	2793	77.6049	1.4275	408.5573	2793	77.6049	1.4275	482.6726
2794	77.6309	1.4271	519.5527	2794	77.6309	1.4271	599.3241	2794	77.6309	1.4271	415.1382	2794	77.6309	1.4271	489
2795	77.6569	1.4267	533.2606	2795	77.6569	1.4267	611.6866	2795	77.6569	1.4267	413.4518	2795	77.6569	1.4267	487.0602
2796	77.6829	1.4263	509.9804	2796	77.6829	1.4263	587.0609	2796	77.6829	1.4263	407.042	2796	77.6829	1.4263	480.3968
2797	77.7089	1.4259	500.9495	2797	77.7089	1.4259	576.6846	2797	77.7089	1.4259	406.5004	2797	77.7089	1.4259	479.6018
2798	77.7349	1.4255	505.2569	2798	77.7349	1.4255	579.6466	2798	77.7349	1.4255	416.9047	2798	77.7349	1.4255	489.7527
2799	77.7609	1.4251	523.3723	2799	77.7609	1.4251	596.4165	2799	77.7609	1.4251	407.1459	2799	77.7609	1.4251	479.7404
2800	77.7869	1.4247	480.2062	2800	77.7869	1.4247	551.9049	2800	77.7869	1.4247	388.1241	2800	77.7869	1.4247	460.4651
2801	77.8129	1.4243	476.7851	2801	77.8129	1.4243	547.1384	2801	77.8129	1.4243	419.5608	2801	77.8129	1.4243	491.6484
2802	77.8389	1.4239	513.2764	2802	77.8389	1.4239	582.2842	2802	77.8389	1.4239	414.1335	2802	77.8389	1.4239	485.9676
2803	77.8649	1.4235	515.0326	2803	77.8649	1.4235	582.6951	2803	77.8649	1.4235	446.4873	2803	77.8649	1.4235	518.0679

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2804	77.8909	1.4231	492.825	2804	77.8909	1.4231	559.142	2804	77.8909	1.4231	428.1195	2804	77.8909	1.4231	499.4466
2805	77.9169	1.4227	545.4999	2805	77.9169	1.4227	610.4715	2805	77.9169	1.4227	450.859	2805	77.9169	1.4227	521.9326
2806	77.9429	1.4223	588.2606	2806	77.9429	1.4223	651.8867	2806	77.9429	1.4223	447.8595	2806	77.9429	1.4223	518.6797
2807	77.9689	1.4219	624.3515	2807	77.9689	1.4219	686.6322	2807	77.9689	1.4219	463.3874	2807	77.9689	1.4219	533.9541
2808	77.9949	1.4215	626.8429	2808	77.9949	1.4215	687.7781	2808	77.9949	1.4215	501.5755	2808	77.9949	1.4215	571.8887
2809	78.0209	1.4211	615.6866	2809	78.0209	1.4211	675.2764	2809	78.0209	1.4211	508.7369	2809	78.0209	1.4211	578.7966
2810	78.0469	1.4207	627.7721	2810	78.0469	1.4207	686.8776	2810	78.0469	1.4207	521.1663	2810	78.0469	1.4207	590.5131
2811	78.0729	1.4203	687.5673	2811	78.0729	1.4203	746.1884	2811	78.0729	1.4203	524.8927	2811	78.0729	1.4203	593.5266
2812	78.0989	1.4199	633.1163	2812	78.0989	1.4199	691.2531	2812	78.0989	1.4199	522.9465	2812	78.0989	1.4199	590.8675
2813	78.1249	1.4195	657.2937	2813	78.1249	1.4195	714.9461	2813	78.1249	1.4195	537.6879	2813	78.1249	1.4195	604.8959
2814	78.1509	1.4191	628.0601	2814	78.1509	1.4191	685.2282	2814	78.1509	1.4191	597.6955	2814	78.1509	1.4191	664.1906
2815	78.1769	1.4187	606.6976	2815	78.1769	1.4187	663.3812	2815	78.1769	1.4187	563.23	2815	78.1769	1.4187	629.0121
2816	78.2029	1.4183	560.6071	2816	78.2029	1.4183	616.8065	2816	78.2029	1.4183	610.6558	2816	78.2029	1.4183	675.725
2817	78.2289	1.4179	505.6968	2817	78.2289	1.4179	561.4118	2817	78.2289	1.4179	609.1732	2817	78.2289	1.4179	673.5294
2818	78.2549	1.4175	526.7155	2818	78.2549	1.4175	581.9461	2818	78.2549	1.4175	632.8407	2818	78.2549	1.4175	696.484
2819	78.2809	1.4171	488.657	2819	78.2809	1.4171	543.4033	2819	78.2809	1.4171	605.1221	2819	78.2809	1.4171	668.0524
2820	78.3069	1.4167	523.0698	2820	78.3069	1.4167	577.3317	2820	78.3069	1.4167	630.1554	2820	78.3069	1.4167	692.3728
2821	78.3329	1.4163	499.9404	2821	78.3329	1.4163	553.718	2821	78.3329	1.4163	575.6153	2821	78.3329	1.4163	637.1198
2822	78.3589	1.4159	434.541	2822	78.3589	1.4159	487.8342	2822	78.3589	1.4159	531.623	2822	78.3589	1.4159	592.4146
2823	78.3849	1.4155	417.2039	2823	78.3849	1.4155	470.0128	2823	78.3849	1.4155	576.8895	2823	78.3849	1.4155	636.9681
2824	78.4109	1.4151	451.314	2824	78.4109	1.4151	503.6385	2824	78.4109	1.4151	532.1234	2824	78.4109	1.4151	591.4891
2825	78.4369	1.4147	456.0777	2825	78.4369	1.4147	507.9178	2825	78.4369	1.4147	556.8334	2825	78.4369	1.4147	615.4861
2826	78.4629	1.4143	417.8633	2826	78.4629	1.4143	469.2191	2826	78.4629	1.4143	560.9688	2826	78.4629	1.4143	618.9086
2827	78.4889	1.4139	429.6034	2827	78.4889	1.4139	480.4748	2827	78.4889	1.4139	564.652	2827	78.4889	1.4139	621.8788
2828	78.5149	1.4136	387.8774	2828	78.5149	1.4136	438.2644	2828	78.5149	1.4136	576.8823	2828	78.5149	1.4136	633.3961
2829	78.5409	1.4132	395.4949	2829	78.5409	1.4132	445.3976	2829	78.5409	1.4132	522.7534	2829	78.5409	1.4132	578.5544
2830	78.5669	1.4128	386.3535	2830	78.5669	1.4128	435.7718	2830	78.5669	1.4128	501.3153	2830	78.5669	1.4128	556.4033
2831	78.5929	1.4124	376.8669	2831	78.5929	1.4124	425.8009	2831	78.5929	1.4124	484.0665	2831	78.5929	1.4124	538.4416
2832	78.6189	1.412	380.1903	2832	78.6189	1.412	428.64	2832	78.6189	1.412	472.418	2832	78.6189	1.412	526.0801
2833	78.6449	1.4116	372.9341	2833	78.6449	1.4116	420.8994	2833	78.6449	1.4116	521.5545	2833	78.6449	1.4116	574.5037
2834	78.6709	1.4112	342.2542	2834	78.6709	1.4112	389.7351	2834	78.6709	1.4112	539.3356	2834	78.6709	1.4112	591.5719
2835	78.6969	1.4108	390.9366	2835	78.6969	1.4108	437.9332	2835	78.6969	1.4108	511.5491	2835	78.6969	1.4108	563.0724
2836	78.7229	1.4104	354.9728	2836	78.7229	1.4104	401.485	2836	78.7229	1.4104	507.3193	2836	78.7229	1.4104	558.1297
2837	78.7489	1.41	406.6175	2837	78.7489	1.41	452.6453	2837	78.7489	1.41	470.0459	2837	78.7489	1.41	520.1434
2838	78.7749	1.4096	386.6906	2838	78.7749	1.4096	432.234	2838	78.7749	1.4096	499.4842	2838	78.7749	1.4096	548.8687
2839	78.8009	1.4093	358.4059	2839	78.8009	1.4093	403.4651	2839	78.8009	1.4093	460.9396	2839	78.8009	1.4093	509.6112

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2840	78.8269	1.4089	427.5191	2840	78.8269	1.4089	472.0938	2840	78.8269	1.4089	455.5332	2840	78.8269	1.4089	503.4918
2841	78.8529	1.4085	376.4338	2841	78.8529	1.4085	420.5242	2841	78.8529	1.4085	458.3957	2841	78.8529	1.4085	505.6414
2842	78.8789	1.4081	363.2047	2842	78.8789	1.4081	406.8108	2842	78.8789	1.4081	478.1149	2842	78.8789	1.4081	524.6476
2843	78.9049	1.4077	403.9205	2843	78.9049	1.4077	447.0422	2843	78.9049	1.4077	457.5532	2843	78.9049	1.4077	503.373
2844	78.9309	1.4073	411.199	2844	78.9309	1.4073	453.8363	2844	78.9309	1.4073	425.7927	2844	78.9309	1.4073	470.8996
2845	78.9569	1.4069	399.913	2845	78.9569	1.4069	442.066	2845	78.9569	1.4069	414.1391	2845	78.9569	1.4069	458.533
2846	78.9829	1.4065	415.0662	2846	78.9829	1.4065	456.7348	2846	78.9829	1.4065	428.7406	2846	78.9829	1.4065	472.4216
2847	79.0089	1.4061	455.8289	2847	79.0089	1.4061	497.0131	2847	79.0089	1.4061	421.0924	2847	79.0089	1.4061	464.0604
2848	79.0349	1.4058	461.2902	2848	79.0349	1.4058	501.9901	2848	79.0349	1.4058	423.7548	2848	79.0349	1.4058	466.0099
2849	79.0609	1.4054	436.0625	2849	79.0609	1.4054	476.2781	2849	79.0609	1.4054	426.4579	2849	79.0609	1.4054	468
2850	79.0869	1.405	472.1521	2850	79.0869	1.405	511.8833	2850	79.0869	1.405	430.0964	2850	79.0869	1.405	470.9256
2851	79.1129	1.4046	481.5385	2851	79.1129	1.4046	520.7853	2851	79.1129	1.4046	438.377	2851	79.1129	1.4046	478.4932
2852	79.1389	1.4042	490.6222	2852	79.1389	1.4042	529.3847	2852	79.1389	1.4042	440.8852	2852	79.1389	1.4042	480.2885
2853	79.1649	1.4038	523.7867	2853	79.1649	1.4038	562.0649	2853	79.1649	1.4038	416.0513	2853	79.1649	1.4038	454.7416
2854	79.1909	1.4034	525.1391	2854	79.1909	1.4034	562.9328	2854	79.1909	1.4034	421.24	2854	79.1909	1.4034	459.2174
2855	79.2169	1.4031	484.5564	2855	79.2169	1.4031	521.8658	2855	79.2169	1.4031	448.5071	2855	79.2169	1.4031	485.7715
2856	79.2429	1.4027	503.1114	2856	79.2429	1.4027	539.9364	2856	79.2429	1.4027	410.7468	2856	79.2429	1.4027	447.2983
2857	79.2689	1.4023	545.8127	2857	79.2689	1.4023	582.1534	2857	79.2689	1.4023	423.2438	2857	79.2689	1.4023	459.0824
2858	79.2949	1.4019	550.6675	2858	79.2949	1.4019	586.5239	2858	79.2949	1.4019	418.402	2858	79.2949	1.4019	453.5276
2859	79.3209	1.4015	518.3762	2859	79.3209	1.4015	553.7481	2859	79.3209	1.4015	419.4291	2859	79.3209	1.4015	453.8418
2860	79.3469	1.4011	518.2844	2860	79.3469	1.4011	553.172	2860	79.3469	1.4011	456.3799	2860	79.3469	1.4011	490.0796
2861	79.3729	1.4008	487.1509	2861	79.3729	1.4008	521.5542	2861	79.3729	1.4008	441.0343	2861	79.3729	1.4008	474.0211
2862	79.3989	1.4004	464.9181	2862	79.3989	1.4004	498.837	2862	79.3989	1.4004	448.6682	2862	79.3989	1.4004	480.9421
2863	79.4249	1.4	452.1079	2863	79.4249	1.4	485.5424	2863	79.4249	1.4	463.4271	2863	79.4249	1.4	494.988
2864	79.4509	1.3996	478.0059	2864	79.4509	1.3996	510.9561	2864	79.4509	1.3996	451.4874	2864	79.4509	1.3996	482.3354
2865	79.4769	1.3992	462.3379	2865	79.4769	1.3992	494.8038	2865	79.4769	1.3992	443.6998	2865	79.4769	1.3992	473.8349
2866	79.5029	1.3988	424.8564	2866	79.5029	1.3988	456.8379	2866	79.5029	1.3988	438.9968	2866	79.5029	1.3988	468.4189
2867	79.5289	1.3985	450.0146	2867	79.5289	1.3985	481.5117	2867	79.5289	1.3985	409.2808	2867	79.5289	1.3985	437.9899
2868	79.5549	1.3981	456.1925	2868	79.5549	1.3981	487.2052	2868	79.5549	1.3981	403.929	2868	79.5549	1.3981	431.9253
2869	79.5809	1.3977	428.4428	2869	79.5809	1.3977	458.9712	2869	79.5809	1.3977	452.0029	2869	79.5809	1.3977	479.2862
2870	79.6069	1.3973	454.1961	2870	79.6069	1.3973	484.2401	2870	79.6069	1.3973	462.7108	2870	79.6069	1.3973	489.2811
2871	79.6329	1.3969	462.3814	2871	79.6329	1.3969	491.9411	2871	79.6329	1.3969	408.4851	2871	79.6329	1.3969	434.3425
2872	79.6589	1.3966	419.8876	2872	79.6589	1.3966	448.963	2872	79.6589	1.3966	405.1283	2872	79.6589	1.3966	430.2728
2873	79.6849	1.3962	383.301	2873	79.6849	1.3962	411.892	2873	79.6849	1.3962	418.97	2873	79.6849	1.3962	443.4016
2874	79.7109	1.3958	373.3057	2874	79.7109	1.3958	401.4123	2874	79.7109	1.3958	424.0116	2874	79.7109	1.3958	447.7301
2875	79.7369	1.3954	379.8944	2875	79.7369	1.3954	407.5167	2875	79.7369	1.3954	424.6944	2875	79.7369	1.3954	447.7001

Table I. part 2: *Continued*

E033_ConstCompExp_BackgroundRemoved				E033_ConstCompExp_raw				E016_vial2_ConstCompExp_BackgrdRmovd				E016_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2876	79.7629	1.395	378.4419	2876	79.7629	1.395	405.5798	2876	79.7629	1.395	413.1755	2876	79.7629	1.395	435.4682
2877	79.7889	1.3947	352.7817	2877	79.7889	1.3947	379.4352	2877	79.7889	1.3947	440.6423	2877	79.7889	1.3947	462.222
2878	79.8149	1.3943	333.9021	2878	79.8149	1.3943	360.0713	2878	79.8149	1.3943	451.0619	2878	79.8149	1.3943	471.9287
2879	79.8409	1.3939	343.9842	2879	79.8409	1.3939	369.6691	2879	79.8409	1.3939	440.8461	2879	79.8409	1.3939	461
2880	79.8669	1.3935	342.7995	2880	79.8669	1.3935	368	2880	79.8669	1.3935	430.2824	2880	79.8669	1.3935	449.7233
2881	79.8929	1.3932	353.8788	2881	79.8929	1.3932	378.5949	2881	79.8929	1.3932	430.6811	2881	79.8929	1.3932	449.4091
2882	79.9189	1.3928	368.7682	2882	79.9189	1.3928	393	2882	79.9189	1.3928	450.5711	2882	79.9189	1.3928	468.5861
2883	79.9449	1.3924	363.5973	2883	79.9449	1.3924	387.3447	2883	79.9449	1.3924	437.7714	2883	79.9449	1.3924	455.0735
2884	79.9709	1.392	359.5869	2884	79.9709	1.392	383.3343	2884	79.9709	1.392	421.4561	2884	79.9709	1.392	438.7582

APPENDIX I

Table I. part 3: Raw and processed X-ray diffraction data from synthetic samples produced in constant composition experiments shown in Chapter 5.

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1	5.0129	20.4542	397.6509	1	5.0129	20.4542	5439	1	5.0129	20.4542	402.0807	1	5.0129	20.4542	5863
2	5.0389	20.3487	308.3328	2	5.0389	20.3487	5323.1609	2	5.0389	20.3487	423.7021	2	5.0389	20.3487	5864.9802
3	5.0649	20.2443	328.7921	3	5.0649	20.2443	5317.0992	3	5.0649	20.2443	385.534	3	5.0649	20.2443	5807.1708
4	5.0909	20.141	381.4101	4	5.0909	20.141	5343.1963	4	5.0909	20.141	332.2071	4	5.0909	20.141	5734.2027
5	5.1169	20.0387	330.9497	5	5.1169	20.0387	5266.2148	5	5.1169	20.0387	177.75	5	5.1169	20.0387	5560.1044
6	5.1429	19.9375	343.8015	6	5.1429	19.9375	5252.5457	6	5.1429	19.9375	158.924	6	5.1429	19.9375	5521.6372
7	5.1689	19.8373	401.7527	7	5.1689	19.8373	5283.9759	7	5.1689	19.8373	317.0576	7	5.1689	19.8373	5660.1295
8	5.1949	19.7381	434.02	8	5.1949	19.7381	5289.7222	8	5.1949	19.7381	246.0011	8	5.1949	19.7381	5569.4318
9	5.2209	19.6398	402.8196	9	5.2209	19.6398	5232.0008	9	5.2209	19.6398	240.7188	9	5.2209	19.6398	5544.5082
10	5.2469	19.5426	457.1249	10	5.2469	19.5426	5259.7852	10	5.2469	19.5426	127.7111	10	5.2469	19.5426	5411.8593
11	5.2729	19.4463	247.254	11	5.2729	19.4463	5023.3933	11	5.2729	19.4463	131.7907	11	5.2729	19.4463	5396.2977
12	5.2989	19.3509	413.0807	12	5.2989	19.3509	5162.699	12	5.2989	19.3509	216.1667	12	5.2989	19.3509	5461.0324
13	5.3249	19.2565	231.7412	13	5.3249	19.2565	4954.8385	13	5.3249	19.2565	170.6581	13	5.3249	19.2565	5395.8826
14	5.3509	19.163	264.0061	14	5.3509	19.163	4960.5824	14	5.3509	19.163	90.7027	14	5.3509	19.163	5296.2859
15	5.3769	19.0704	304.5556	15	5.3769	19.0704	4974.6109	15	5.3769	19.0704	122.0296	15	5.3769	19.0704	5307.9715
16	5.4029	18.9787	287.3539	16	5.4029	18.9787	4930.8882	16	5.4029	18.9787	93.7781	16	5.4029	18.9787	5260.0789
17	5.4289	18.8879	265.607	17	5.4289	18.8879	4882.6203	17	5.4289	18.8879	26.1049	17	5.4289	18.8879	5172.7644
18	5.4549	18.7979	202.2069	18	5.4549	18.7979	4792.6992	18	5.4549	18.7979	109.1259	18	5.4549	18.7979	5236.1442
19	5.4809	18.7088	362.3446	19	5.4809	18.7088	4926.316	19	5.4809	18.7088	178.3003	19	5.4809	18.7088	5285.6773
20	5.5069	18.6206	412.6234	20	5.5069	18.6206	4950.0738	20	5.5069	18.6206	170.3707	20	5.5069	18.6206	5258.1065
21	5.5329	18.5331	375.3509	21	5.5329	18.5331	4886.2803	21	5.5329	18.5331	117.7811	21	5.5329	18.5331	5185.8757
22	5.5589	18.4465	430.923	22	5.5589	18.4465	4915.3314	22	5.5589	18.4465	22.5927	22	5.5589	18.4465	5071.046
23	5.5849	18.3607	405.0124	23	5.5849	18.3607	4862.8998	23	5.5849	18.3607	196.7628	23	5.5849	18.3607	5225.5749
24	5.6109	18.2757	378.9031	24	5.6109	18.2757	4810.2696	24	5.6109	18.2757	129.451	24	5.6109	18.2757	5138.6219
25	5.6369	18.1915	475.1504	25	5.6369	18.1915	4879.9958	25	5.6369	18.1915	125.9933	25	5.6369	18.1915	5115.5229
26	5.6629	18.108	429.6749	26	5.6629	18.108	4807.9994	26	5.6629	18.108	148.8558	26	5.6629	18.108	5118.7442
27	5.6889	18.0253	443.489	27	5.6889	18.0253	4795.2925	27	5.6889	18.0253	100.971	27	5.6889	18.0253	5051.2182
28	5.7149	17.9434	397.6509	28	5.7149	17.9434	4722.9334	28	5.7149	17.9434	97.3941	28	5.7149	17.9434	5028
29	5.7409	17.8622	485.9412	29	5.7409	17.8622	4803.7707	29	5.7409	17.8622	160.3659	29	5.7409	17.8622	5071.3305
30	5.7669	17.7817	405.9933	30	5.7669	17.7817	4716.3699	30	5.7669	17.7817	253.6569	30	5.7669	17.7817	5144.9803
31	5.7929	17.702	351.2437	31	5.7929	17.702	4654.1674	31	5.7929	17.702	129.163	31	5.7929	17.702	5000.8452

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
32	5.8189	17.623	380.8409	32	5.8189	17.623	4676.3115	32	5.8189	17.623	129.1973	32	5.8189	17.623	4981.2383
33	5.8449	17.5446	462.771	33	5.8449	17.5446	4750.7888	33	5.8449	17.5446	173.6478	33	5.8449	17.5446	5006.0475
34	5.8709	17.467	412.6744	34	5.8709	17.467	4693.2392	34	5.8709	17.467	155.9054	34	5.8709	17.467	4968.6638
35	5.8969	17.3901	428.249	35	5.8969	17.3901	4701.3608	35	5.8969	17.3901	188.027	35	5.8969	17.3901	4981.1442
36	5.9229	17.3138	365.3913	36	5.9229	17.3138	4631.0502	36	5.9229	17.3138	200.6788	36	5.9229	17.3138	4974.1548
37	5.9489	17.2382	376.4319	37	5.9489	17.2382	4634.6378	37	5.9489	17.2382	165.7406	37	5.9489	17.2382	4919.5754
38	5.9749	17.1632	421.2087	38	5.9749	17.1632	4671.9616	38	5.9749	17.1632	174.464	38	5.9749	17.1632	4908.6575
39	6.0009	17.0889	473.192	39	6.0009	17.0889	4716.4919	39	6.0009	17.0889	206.4314	39	6.0009	17.0889	4920.9836
40	6.0269	17.0153	387.4511	40	6.0269	17.0153	4623.2981	40	6.0269	17.0153	211.9241	40	6.0269	17.0153	4906.8351
41	6.0529	16.9423	394.7883	41	6.0529	16.9423	4623.1823	41	6.0529	16.9423	165.2443	41	6.0529	16.9423	4840.514
42	6.0789	16.8699	382.8425	42	6.0789	16.8699	4603.7836	42	6.0789	16.8699	187.5217	42	6.0789	16.8699	4843.1503
43	6.1049	16.7981	353.4273	43	6.1049	16.7981	4566.9155	43	6.1049	16.7981	351.832	43	6.1049	16.7981	4987.8193
44	6.1309	16.7269	440.2058	44	6.1309	16.7269	4646.241	44	6.1309	16.7269	288.8116	44	6.1309	16.7269	4905.1576
45	6.1569	16.6564	409.017	45	6.1569	16.6564	4607.5993	45	6.1569	16.6564	213.593	45	6.1569	16.6564	4810.2978
46	6.1829	16.5864	383.062	46	6.1829	16.5864	4574.1913	46	6.1829	16.5864	280.8438	46	6.1829	16.5864	4857.9074
47	6.2089	16.517	473.5068	47	6.2089	16.517	4657.1832	47	6.2089	16.517	321.1212	47	6.2089	16.517	4878.5436
48	6.2349	16.4482	414.8443	48	6.2349	16.4482	4591.0676	48	6.2349	16.4482	308.1325	48	6.2349	16.4482	4845.9136
49	6.2609	16.38	355.5585	49	6.2609	16.38	4524.3289	49	6.2609	16.38	304.6212	49	6.2609	16.38	4822.761
50	6.2869	16.3123	360.3955	50	6.2869	16.3123	4521.713	50	6.2869	16.3123	413.252	50	6.2869	16.3123	4911.7506
51	6.3129	16.2452	436.8815	51	6.3129	16.2452	4590.746	51	6.3129	16.2452	451.6764	51	6.3129	16.2452	4930.5338
52	6.3389	16.1786	466.4819	52	6.3389	16.1786	4612.8935	52	6.3389	16.1786	414.7476	52	6.3389	16.1786	4873.9638
53	6.3649	16.1126	421.3073	53	6.3649	16.1126	4560.2659	53	6.3649	16.1126	377.8881	53	6.3649	16.1126	4817.463
54	6.3909	16.0471	396.5484	54	6.3909	16.0471	4528.054	54	6.3909	16.0471	396.1759	54	6.3909	16.0471	4816.1095
55	6.4169	15.9821	397.6509	55	6.4169	15.9821	4521.7035	55	6.4169	15.9821	402.0807	55	6.4169	15.9821	4802.3731
56	6.4429	15.9177	415.9613	56	6.4429	15.9177	4534.667	56	6.4429	15.9177	276.2077	56	6.4429	15.9177	4671.5666
57	6.4689	15.8538	331.647	57	6.4689	15.8538	4445.0058	57	6.4689	15.8538	343.8859	57	6.4689	15.8538	4734.3113
58	6.4949	15.7904	317.1931	58	6.4949	15.7904	4425.205	58	6.4949	15.7904	439.6717	58	6.4949	15.7904	4825.1636
59	6.5209	15.7275	284.602	59	6.5209	15.7275	4387.267	59	6.5209	15.7275	468.2774	59	6.5209	15.7275	4848.8358
60	6.5469	15.6651	283.4051	60	6.5469	15.6651	4380.7232	60	6.5469	15.6651	562.8646	60	6.5469	15.6651	4938.4895
61	6.5729	15.6032	377.0796	61	6.5729	15.6032	4469.0508	61	6.5729	15.6032	467.1854	61	6.5729	15.6032	4837.8768
62	6.5989	15.5418	303.3752	62	6.5989	15.5418	4389.9995	62	6.5989	15.5418	378.716	62	6.5989	15.5418	4744.4739
63	6.6249	15.4809	285.9898	63	6.6249	15.4809	4367.2672	63	6.6249	15.4809	397.7017	63	6.6249	15.4809	4758.5261
64	6.6509	15.4204	401.3197	64	6.6509	15.4204	4477.2502	64	6.6509	15.4204	374.1066	64	6.6509	15.4204	4729.9975
65	6.6769	15.3605	385.7079	65	6.6769	15.3605	4456.2914	65	6.6769	15.3605	403.8969	65	6.6769	15.3605	4754.8543
66	6.7029	15.3009	379.8417	66	6.7029	15.3009	4445.0783	66	6.7029	15.3009	438.7579	66	6.7029	15.3009	4784.7818
67	6.7289	15.2419	401.2256	67	6.7289	15.2419	4461.1153	67	6.7289	15.2419	468.2901	67	6.7289	15.2419	4809.3805

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
68	6.7549	15.1833	333.6575	68	6.7549	15.1833	4388.2003	68	6.7549	15.1833	448.6914	68	6.7549	15.1833	4784.8483
69	6.7809	15.1251	280.0938	69	6.7809	15.1251	4329.2898	69	6.7809	15.1251	392.9456	69	6.7809	15.1251	4724.169
70	6.8069	15.0674	280.7034	70	6.8069	15.0674	4324.5524	70	6.8069	15.0674	384.0255	70	6.8069	15.0674	4710.3154
71	6.8329	15.0102	351.1004	71	6.8329	15.0102	4389.6025	71	6.8329	15.0102	388.7273	71	6.8329	15.0102	4710.0837
72	6.8589	14.9533	424.0982	72	6.8589	14.9533	4457.2534	72	6.8589	14.9533	342.8168	72	6.8589	14.9533	4659.2397
73	6.8849	14.8969	428.2084	73	6.8849	14.8969	4456.0167	73	6.8849	14.8969	274.3498	73	6.8849	14.8969	4585.8392
74	6.9109	14.841	342.9115	74	6.9109	14.841	4365.3729	74	6.9109	14.841	403.8115	74	6.9109	14.841	4710.3674
75	6.9369	14.7854	377.1375	75	6.9369	14.7854	4394.252	75	6.9369	14.7854	464.2104	75	6.9369	14.7854	4765.8328
76	6.9629	14.7303	386.5576	76	6.9629	14.7303	4398.3252	76	6.9629	14.7303	478.1473	76	6.9629	14.7303	4774.8362
77	6.9889	14.6755	370.563	77	6.9889	14.6755	4376.9836	77	6.9889	14.6755	427.2937	77	6.9889	14.6755	4719.0491
78	7.0149	14.6212	378.2183	78	7.0149	14.6212	4379.292	78	7.0149	14.6212	412.3229	78	7.0149	14.6212	4699.1448
79	7.0409	14.5673	388.055	79	7.0409	14.5673	4383.7818	79	7.0409	14.5673	399.2923	79	7.0409	14.5673	4681.1806
80	7.0669	14.5138	379.6603	80	7.0669	14.5138	4370.0403	80	7.0669	14.5138	448.9961	80	7.0669	14.5138	4725.951
81	7.0929	14.4606	279.4249	81	7.0929	14.4606	4264.4579	81	7.0929	14.4606	382.3569	81	7.0929	14.4606	4654.3783
82	7.1189	14.4079	397.6509	82	7.1189	14.4079	4377.337	82	7.1189	14.4079	313.4083	82	7.1189	14.4079	4580.4962
83	7.1449	14.3555	402.1547	83	7.1449	14.3555	4377.0221	83	7.1449	14.3555	332.2725	83	7.1449	14.3555	4594.4269
84	7.1709	14.3035	380.3589	84	7.1709	14.3035	4350.4077	84	7.1709	14.3035	324.4821	84	7.1709	14.3035	4581.703
85	7.1969	14.2519	514.7958	85	7.1969	14.2519	4480.0259	85	7.1969	14.2519	439.3837	85	7.1969	14.2519	4691.6711
86	7.2229	14.2007	346.4224	86	7.2229	14.2007	4306.8338	86	7.2229	14.2007	415.297	86	7.2229	14.2007	4662.6509
87	7.2489	14.1498	258.9812	87	7.2489	14.1498	4214.5739	87	7.2489	14.1498	384.4037	87	7.2489	14.1498	4626.8241
88	7.2749	14.0993	299.5082	88	7.2749	14.0993	4250.2823	88	7.2749	14.0993	285.0107	88	7.2749	14.0993	4522.4976
89	7.3009	14.0492	334.938	89	7.3009	14.0492	4280.8934	89	7.3009	14.0492	482.0661	89	7.3009	14.0492	4714.6195
90	7.3269	13.9994	409.5001	90	7.3269	13.9994	4350.6368	90	7.3269	13.9994	477.7159	90	7.3269	13.9994	4705.3358
91	7.3529	13.95	413.2008	91	7.3529	13.95	4349.5188	91	7.3529	13.95	420.1163	91	7.3529	13.95	4642.8027
92	7.3789	13.9009	318.8965	92	7.3789	13.9009	4250.3959	92	7.3789	13.9009	336.0605	92	7.3789	13.9009	4553.8134
93	7.4049	13.8521	451.5439	93	7.4049	13.8521	4378.2245	93	7.4049	13.8521	448.5026	93	7.4049	13.8521	4661.322
94	7.4309	13.8037	484.1143	94	7.4309	13.8037	4405.9763	94	7.4309	13.8037	339.8407	94	7.4309	13.8037	4547.7266
95	7.4569	13.7557	413.7934	95	7.4569	13.7557	4330.8367	95	7.4569	13.7557	439.9615	95	7.4569	13.7557	4642.9139
96	7.4829	13.7079	372.3079	96	7.4829	13.7079	4284.5326	96	7.4829	13.7079	320.5304	96	7.4829	13.7079	4518.5493
97	7.5089	13.6605	338.7297	97	7.5089	13.6605	4246.1357	97	7.5089	13.6605	356.2776	97	7.5089	13.6605	4549.363
98	7.5349	13.6135	387.4262	98	7.5349	13.6135	4290.0135	98	7.5349	13.6135	465.8827	98	7.5349	13.6135	4654.0345
99	7.5609	13.5667	414.5309	99	7.5609	13.5667	4312.2995	99	7.5609	13.5667	395.3063	99	7.5609	13.5667	4578.5247
100	7.5869	13.5203	291.1732	100	7.5869	13.5203	4184.1232	100	7.5869	13.5203	420.1483	100	7.5869	13.5203	4598.4331
101	7.6129	13.4742	414.1174	101	7.6129	13.4742	4302.2487	101	7.6129	13.4742	502.6438	101	7.6129	13.4742	4675.9951
102	7.6389	13.4284	450.6186	102	7.6389	13.4284	4333.9312	102	7.6389	13.4284	252.1372	102	7.6389	13.4284	4420.5551
103	7.6649	13.3829	428.8321	103	7.6649	13.3829	4307.326	103	7.6649	13.3829	472.8715	103	7.6649	13.3829	4636.3558

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
104	7.6909	13.3378	383.4466	104	7.6909	13.3378	4257.1218	104	7.6909	13.3378	445.241	104	7.6909	13.3378	4603.7919
105	7.7169	13.2929	371.6542	105	7.7169	13.2929	4240.5107	105	7.7169	13.2929	358.383	105	7.7169	13.2929	4512.0003
106	7.7429	13.2483	233.1964	106	7.7429	13.2483	4097.2343	106	7.7429	13.2483	450.3831	106	7.7429	13.2483	4599.067
107	7.7689	13.204	337.0351	107	7.7689	13.204	4196.2543	107	7.7689	13.204	404.2519	107	7.7689	13.204	4548.0023
108	7.7949	13.1601	376.6872	108	7.7949	13.1601	4231.0878	108	7.7949	13.1601	366.7739	108	7.7949	13.1601	4505.5908
109	7.8209	13.1164	432.623	109	7.8209	13.1164	4282.2048	109	7.8209	13.1164	428.5337	109	7.8209	13.1164	4562.4171
110	7.8469	13.073	297.037	110	7.8469	13.073	4141.8002	110	7.8469	13.073	440.8055	110	7.8469	13.073	4569.7554
111	7.8729	13.0299	321.7632	111	7.8729	13.0299	4161.7077	111	7.8729	13.0299	467.7888	111	7.8729	13.0299	4591.8051
112	7.8989	12.9871	343.3536	112	7.8989	12.9871	4178.4794	112	7.8989	12.9871	329.3398	112	7.8989	12.9871	4448.4227
113	7.9249	12.9445	329.2527	113	7.9249	12.9445	4159.5598	113	7.9249	12.9445	458.2657	113	7.9249	12.9445	4572.4151
114	7.9509	12.9023	383.3596	114	7.9509	12.9023	4208.8481	114	7.9509	12.9023	523.8444	114	7.9509	12.9023	4633.0603
115	7.9769	12.8603	477.8718	115	7.9769	12.8603	4298.5416	115	7.9769	12.8603	347.0442	115	7.9769	12.8603	4451.3265
116	8.0029	12.8186	447.9074	116	8.0029	12.8186	4263.7585	116	8.0029	12.8186	382.9177	116	8.0029	12.8186	4482.2666
117	8.0289	12.7771	395.7248	117	8.0289	12.7771	4206.7572	117	8.0289	12.7771	457.0156	117	8.0289	12.7771	4551.431
118	8.0549	12.7359	482.4082	118	8.0549	12.7359	4288.6219	118	8.0549	12.7359	522.0246	118	8.0549	12.7359	4611.5064
119	8.0809	12.695	459.8298	119	8.0809	12.695	4261.2248	119	8.0809	12.695	500.7974	119	8.0809	12.695	4585.3457
120	8.1069	12.6544	323.5248	120	8.1069	12.6544	4120.1012	120	8.1069	12.6544	462.3383	120	8.1069	12.6544	4541.9531
121	8.1329	12.614	372.8909	121	8.1329	12.614	4164.6486	121	8.1329	12.614	393.7633	121	8.1329	12.614	4468.4447
122	8.1589	12.5739	392.6628	122	8.1589	12.5739	4179.6018	122	8.1589	12.5739	436.0127	122	8.1589	12.5739	4505.7606
123	8.1849	12.534	465.5644	123	8.1849	12.534	4247.6848	123	8.1849	12.534	376.8166	123	8.1849	12.534	4441.6309
124	8.2109	12.4944	353.8348	124	8.2109	12.4944	4131.1365	124	8.2109	12.4944	409.4517	124	8.2109	12.4944	4469.3326
125	8.2369	12.455	373.6219	125	8.2369	12.455	4146.1049	125	8.2369	12.455	419.5867	125	8.2369	12.455	4474.534
126	8.2629	12.4159	347.9932	126	8.2629	12.4159	4115.6575	126	8.2629	12.4159	514.6712	126	8.2629	12.4159	4564.685
127	8.2889	12.377	383.1418	127	8.2889	12.377	4145.9875	127	8.2889	12.377	474.6903	127	8.2889	12.377	4519.7707
128	8.3149	12.3384	363.0201	128	8.3149	12.3384	4121.0471	128	8.3149	12.3384	542.8975	128	8.3149	12.3384	4583.0444
129	8.3409	12.3	340.6527	129	8.3409	12.3	4093.861	129	8.3409	12.3	551.7786	129	8.3409	12.3	4586.992
130	8.3669	12.2618	415.4929	130	8.3669	12.2618	4163.8825	130	8.3669	12.2618	499.1986	130	8.3669	12.2618	4529.4784
131	8.3929	12.2239	386.9401	131	8.3929	12.2239	4130.511	131	8.3929	12.2239	450.8587	131	8.3929	12.2239	4476.205
132	8.4189	12.1862	359.9461	132	8.4189	12.1862	4098.6984	132	8.4189	12.1862	502.5028	132	8.4189	12.1862	4522.9156
133	8.4449	12.1488	415.2162	133	8.4449	12.1488	4149.1498	133	8.4449	12.1488	494.176	133	8.4449	12.1488	4509.6553
134	8.4709	12.1116	443.8851	134	8.4709	12.1116	4173	134	8.4709	12.1116	483.4952	134	8.4709	12.1116	4494.041
135	8.4969	12.0746	399.7636	135	8.4969	12.0746	4124.0599	135	8.4969	12.0746	534.3053	135	8.4969	12.0746	4539.9177
136	8.5229	12.0378	469.6887	136	8.5229	12.0378	4189.1662	136	8.5229	12.0378	522.3522	136	8.5229	12.0378	4523.0311
137	8.5489	12.0013	409.0881	137	8.5489	12.0013	4122.4517	137	8.5489	12.0013	419.428	137	8.5489	12.0013	4415.1733
138	8.5749	11.9649	345.7813	138	8.5749	11.9649	4053.031	138	8.5749	11.9649	429.7211	138	8.5749	11.9649	4420.533
139	8.6009	11.9288	385.3384	139	8.6009	11.9288	4086.4741	139	8.6009	11.9288	481.7819	139	8.6009	11.9288	4467.6603

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
140	8.6269	11.8929	415.8406	140	8.6269	11.8929	4110.8624	140	8.6269	11.8929	484.6391	140	8.6269	11.8929	4465.584
141	8.6529	11.8573	346.7323	141	8.6529	11.8573	4035.6401	141	8.6529	11.8573	490.541	141	8.6529	11.8573	4466.5523
142	8.6789	11.8218	288.5812	142	8.6789	11.8218	3971.3751	142	8.6789	11.8218	532.7729	142	8.6789	11.8218	4503.8507
143	8.7049	11.7866	349.3338	143	8.7049	11.7866	4026.0138	143	8.7049	11.7866	497.3881	143	8.7049	11.7866	4463.5324
144	8.7309	11.7516	419.0295	144	8.7309	11.7516	4089.5956	144	8.7309	11.7516	470.2492	144	8.7309	11.7516	4431.46
145	8.7569	11.7167	407.7036	145	8.7569	11.7167	4072.1557	145	8.7569	11.7167	523.8483	145	8.7569	11.7167	4480.1257
146	8.7829	11.6821	426.0217	146	8.7829	11.6821	4084.3599	146	8.7829	11.6821	511.3872	146	8.7829	11.6821	4462.731
147	8.8089	11.6477	454.8137	147	8.8089	11.6477	4107.0379	147	8.8089	11.6477	540.3404	147	8.8089	11.6477	4486.7507
148	8.8349	11.6135	392.4604	148	8.8349	11.6135	4038.5707	148	8.8349	11.6135	518.0997	148	8.8349	11.6135	4459.5765
149	8.8609	11.5795	400.8742	149	8.8609	11.5795	4040.8706	149	8.8609	11.5795	554.1898	149	8.8609	11.5795	4490.7331
150	8.8869	11.5457	446.1644	150	8.8869	11.5457	4080.0469	150	8.8869	11.5457	600.056	150	8.8869	11.5457	4531.6658
151	8.9129	11.5121	386.461	151	8.9129	11.5121	4014.2295	151	8.9129	11.5121	572.5102	151	8.9129	11.5121	4499.1865
152	8.9389	11.4786	377.979	152	8.9389	11.4786	3999.6335	152	8.9389	11.4786	536.589	152	8.9389	11.4786	4458.3318
153	8.9649	11.4454	440.1646	153	8.9649	11.4454	4055.7052	153	8.9649	11.4454	501.5515	153	8.9649	11.4454	4418.3608
154	8.9909	11.4124	427.4679	154	8.9909	11.4124	4036.8945	154	8.9909	11.4124	571.9871	154	8.9909	11.4124	4483.8629
155	9.0169	11.3795	434.2764	155	9.0169	11.3795	4037.5892	155	9.0169	11.3795	592.7489	155	9.0169	11.3795	4499.6912
156	9.0429	11.3469	401.2471	156	9.0429	11.3469	3998.4458	156	9.0429	11.3469	576.1	156	9.0429	11.3469	4478.1088
157	9.0689	11.3144	362.2656	157	9.0689	11.3144	3953.3504	157	9.0689	11.3144	548.9148	157	9.0689	11.3144	4445.9901
158	9.0949	11.2822	401.6329	158	9.0949	11.2822	3986.6038	158	9.0949	11.2822	499.5058	158	9.0949	11.2822	4391.6476
159	9.1209	11.2501	437.7398	159	9.1209	11.2501	4016.5967	159	9.1209	11.2501	540.6822	159	9.1209	11.2501	4427.8905
160	9.1469	11.2182	543.7041	160	9.1469	11.2182	4116.4471	160	9.1469	11.2182	532.9863	160	9.1469	11.2182	4415.2611
161	9.1729	11.1864	511.0541	161	9.1729	11.1864	4077.6832	161	9.1729	11.1864	522.7322	161	9.1729	11.1864	4400.0735
162	9.1989	11.1549	433.4095	162	9.1989	11.1549	3993.9247	162	9.1989	11.1549	518.8566	162	9.1989	11.1549	4391.2644
163	9.2249	11.1235	397.6509	163	9.2249	11.1235	3952.0521	163	9.2249	11.1235	480.9258	163	9.2249	11.1235	4348.4001
164	9.2509	11.0923	408.8491	164	9.2509	11.0923	3957.0933	164	9.2509	11.0923	439.2286	164	9.2509	11.0923	4301.7694
165	9.2769	11.0613	483.2855	165	9.2769	11.0613	4025.3727	165	9.2769	11.0613	444.5949	165	9.2769	11.0613	4302.2022
166	9.3029	11.0304	455.2388	166	9.3029	11.0304	3991.1691	166	9.3029	11.0304	513.0967	166	9.3029	11.0304	4365.7704
167	9.3289	10.9998	440.4572	167	9.3289	10.9998	3970.2305	167	9.3289	10.9998	545.3113	167	9.3289	10.9998	4393.0516
168	9.3549	10.9693	489.8587	168	9.3549	10.9693	4013.475	168	9.3549	10.9693	614.8624	168	9.3549	10.9693	4457.6692
169	9.3809	10.9389	433.8771	169	9.3809	10.9389	3951.3364	169	9.3809	10.9389	546.4456	169	9.3809	10.9389	4384.3189
170	9.4069	10.9088	463.7184	170	9.4069	10.9088	3975.0207	170	9.4069	10.9088	596.7236	170	9.4069	10.9088	4429.6634
171	9.4329	10.8788	493.8241	171	9.4329	10.8788	3998.9695	171	9.4329	10.8788	603.0086	171	9.4329	10.8788	4431.0149
172	9.4589	10.8489	397.2735	172	9.4589	10.8489	3896.2619	172	9.4589	10.8489	562.5338	172	9.4589	10.8489	4385.6066
173	9.4849	10.8193	396.7577	173	9.4849	10.8193	3889.5892	173	9.4849	10.8193	549.4986	173	9.4849	10.8193	4367.6379
174	9.5109	10.7897	470.3639	174	9.5109	10.7897	3957.0384	174	9.5109	10.7897	525.0843	174	9.5109	10.7897	4338.29
175	9.5369	10.7604	501.8239	175	9.5369	10.7604	3982.3414	175	9.5369	10.7604	536.2553	175	9.5369	10.7604	4344.5276

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
176	9.5629	10.7312	459.9616	176	9.5629	10.7312	3934.3221	176	9.5629	10.7312	475.6655	176	9.5629	10.7312	4279.0042
177	9.5889	10.7022	391.5869	177	9.5889	10.7022	3859.7904	177	9.5889	10.7022	587.0102	177	9.5889	10.7022	4385.4154
178	9.6149	10.6733	429.3538	178	9.6149	10.6733	3891.4004	178	9.6149	10.6733	612.853	178	9.6149	10.6733	4406.3248
179	9.6409	10.6446	504.6029	179	9.6409	10.6446	3960.4925	179	9.6409	10.6446	574.7204	179	9.6409	10.6446	4363.2587
180	9.6669	10.616	499.2674	180	9.6669	10.616	3949	180	9.6669	10.616	568.5148	180	9.6669	10.616	4352.1195
181	9.6929	10.5876	487.4494	181	9.6929	10.5876	3931.0251	181	9.6929	10.5876	598.0855	181	9.6929	10.5876	4376.7568
182	9.7189	10.5594	406.1545	182	9.7189	10.5594	3843.5732	182	9.7189	10.5594	655.5907	182	9.7189	10.5594	4429.3285
183	9.7449	10.5313	361.7426	183	9.7449	10.5313	3793.0043	183	9.7449	10.5313	554.0233	183	9.7449	10.5313	4322.8276
184	9.7709	10.5033	514.1063	184	9.7709	10.5033	3939.211	184	9.7709	10.5033	517.0775	184	9.7709	10.5033	4280.9483
185	9.7969	10.4755	551.2916	185	9.7969	10.4755	3970.2393	185	9.7969	10.4755	590.0908	185	9.7969	10.4755	4349.0281
186	9.8229	10.4478	517.2912	186	9.8229	10.4478	3930.0819	186	9.8229	10.4478	554.5993	186	9.8229	10.4478	4308.6031
187	9.8489	10.4203	532.5883	187	9.8489	10.4203	3939.222	187	9.8489	10.4203	526.8723	187	9.8489	10.4203	4275.9425
188	9.8749	10.393	446.9842	188	9.8749	10.393	3847.4609	188	9.8749	10.393	558.4296	188	9.8749	10.393	4302.5664
189	9.9009	10.3657	619.8531	189	9.9009	10.3657	4014.1729	189	9.9009	10.3657	558.643	189	9.9009	10.3657	4297.8463
190	9.9269	10.3386	618.1743	190	9.9269	10.3386	4006.3371	190	9.9269	10.3386	542.1244	190	9.9269	10.3386	4276.3941
191	9.9529	10.3117	382.027	191	9.9529	10.3117	3764.0329	191	9.9529	10.3117	505.4845	191	9.9529	10.3117	4234.8207
192	9.9789	10.2849	390.5945	192	9.9789	10.2849	3766.4434	192	9.9789	10.2849	601.7021	192	9.9789	10.2849	4326.1048
193	10.0049	10.2582	352.4404	193	10.0049	10.2582	3722.1324	193	10.0049	10.2582	595.0013	193	10.0049	10.2582	4314.4706
194	10.0309	10.2317	394.1599	194	10.0309	10.2317	3757.6948	194	10.0309	10.2317	483.0142	194	10.0309	10.2317	4197.5499
195	10.0569	10.2053	463.1986	195	10.0569	10.2053	3820.5766	195	10.0569	10.2053	511.9443	195	10.0569	10.2053	4221.5465
196	10.0829	10.1791	491.4503	196	10.0829	10.1791	3842.6713	196	10.0829	10.1791	479.2177	196	10.0829	10.1791	4183.8865
197	10.1089	10.153	526.6572	197	10.1089	10.153	3871.7212	197	10.1089	10.153	556.5292	197	10.1089	10.153	4256.2645
198	10.1349	10.127	375.8147	198	10.1349	10.127	3714.7217	198	10.1349	10.127	593.7192	198	10.1349	10.127	4288.5209
199	10.1609	10.1012	420.9747	199	10.1609	10.1012	3753.7247	199	10.1609	10.1012	465.635	199	10.1609	10.1012	4155.5032
200	10.1869	10.0754	497.2818	200	10.1869	10.0754	3823.8749	200	10.1869	10.0754	566.218	200	10.1869	10.0754	4251.1528
201	10.2129	10.0499	345.1287	201	10.2129	10.0499	3665.5648	201	10.2129	10.0499	575.8953	201	10.2129	10.0499	4255.8966
202	10.2389	10.0244	323.7715	202	10.2389	10.0244	3638.0506	202	10.2389	10.0244	511.1458	202	10.2389	10.0244	4186.2135
203	10.2649	9.9991	338.8391	203	10.2649	9.9991	3646.9613	203	10.2649	9.9991	553.7022	203	10.2649	9.9991	4223.8365
204	10.2909	9.9739	453.47	204	10.2909	9.9739	3755.4352	204	10.2909	9.9739	477.9657	204	10.2909	9.9739	4143.1665
205	10.3169	9.9488	470.9503	205	10.3169	9.9488	3766.7585	205	10.3169	9.9488	537.3563	205	10.3169	9.9488	4197.6236
206	10.3429	9.9239	467.6895	206	10.3429	9.9239	3757.3407	206	10.3429	9.9239	715.6018	206	10.3429	9.9239	4370.9355
207	10.3689	9.8991	423.7934	207	10.3689	9.8991	3707.2876	207	10.3689	9.8991	567.9025	207	10.3689	9.8991	4218.3027
208	10.3949	9.8744	498.6191	208	10.3949	9.8744	3775.9564	208	10.3949	9.8744	608.1071	208	10.3949	9.8744	4253.5738
209	10.4209	9.8498	445.1606	209	10.4209	9.8498	3716.3409	209	10.4209	9.8498	643.5517	209	10.4209	9.8498	4284.0849
210	10.4469	9.8254	509.0348	210	10.4469	9.8254	3774.0581	210	10.4469	9.8254	743.0244	210	10.4469	9.8254	4378.6241
211	10.4729	9.801	368.9411	211	10.4729	9.801	3627.8074	211	10.4729	9.801	579.4006	211	10.4729	9.801	4210.0668

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
212	10.4989	9.7768	383.9505	212	10.4989	9.7768	3636.6599	212	10.4989	9.7768	723.261	212	10.4989	9.7768	4348.9938
213	10.5249	9.7527	500.921	213	10.5249	9.7527	3747.4734	213	10.5249	9.7527	680.5511	213	10.5249	9.7527	4301.3503
214	10.5509	9.7288	459.3191	214	10.5509	9.7288	3699.7145	214	10.5509	9.7288	641.7857	214	10.5509	9.7288	4257.6514
215	10.5769	9.7049	309.6112	215	10.5769	9.7049	3543.8496	215	10.5769	9.7049	668.3667	215	10.5769	9.7049	4279.2989
216	10.6029	9.6812	386.7895	216	10.6029	9.6812	3614.871	216	10.6029	9.6812	559.1291	216	10.6029	9.6812	4165.1278
217	10.6289	9.6576	397.6509	217	10.6289	9.6576	3619.5754	217	10.6289	9.6576	534.7966	217	10.6289	9.6576	4135.8618
218	10.6549	9.6341	372.9268	218	10.6549	9.6341	3588.3598	218	10.6549	9.6341	416.7669	218	10.6549	9.6341	4012.8987
219	10.6809	9.6107	430.1334	219	10.6809	9.6107	3639.075	219	10.6809	9.6107	461.7354	219	10.6809	9.6107	4052.9336
220	10.7069	9.5874	411.1611	220	10.7069	9.5874	3613.6112	220	10.7069	9.5874	580.4585	220	10.7069	9.5874	4166.7232
221	10.7329	9.5643	468.0552	221	10.7329	9.5643	3664.0138	221	10.7329	9.5643	606.6688	221	10.7329	9.5643	4188
222	10.7589	9.5412	514.1695	222	10.7589	9.5412	3703.6367	222	10.7589	9.5412	525.2347	222	10.7589	9.5412	4101.6325
223	10.7849	9.5183	444.9074	223	10.7849	9.5183	3627.8831	223	10.7849	9.5183	543.8176	223	10.7849	9.5183	4115.2818
224	10.8109	9.4955	326.5883	224	10.8109	9.4955	3503.0726	224	10.8109	9.4955	607.071	224	10.8109	9.4955	4173.6017
225	10.8369	9.4728	399.8508	225	10.8369	9.4728	3569.8436	225	10.8369	9.4728	658.8313	225	10.8369	9.4728	4220.4285
226	10.8629	9.4502	430.4287	226	10.8629	9.4502	3593.9301	226	10.8629	9.4502	572.7959	226	10.8629	9.4502	4129.4596
227	10.8889	9.4277	432.9599	227	10.8889	9.4277	3589.9698	227	10.8889	9.4277	563.9362	227	10.8889	9.4277	4115.6664
228	10.9149	9.4053	368.9511	228	10.9149	9.4053	3519.4695	228	10.9149	9.4053	551.0265	228	10.9149	9.4053	4097.8232
229	10.9409	9.383	359.3502	229	10.9409	9.383	3503.3772	229	10.9409	9.383	505.3492	229	10.9409	9.383	4047.2124
230	10.9669	9.3608	361.1866	230	10.9669	9.3608	3498.722	230	10.9669	9.3608	483.4256	230	10.9669	9.3608	4020.3553
231	10.9929	9.3387	367.8275	231	10.9929	9.3387	3498.8715	231	10.9929	9.3387	476.1072	231	10.9929	9.3387	4008.1034
232	11.0189	9.3168	346.4215	232	11.0189	9.3168	3470.974	232	11.0189	9.3168	591.9173	232	11.0189	9.3168	4118.98
233	11.0449	9.2949	354.2014	233	11.0449	9.2949	3472.2625	233	11.0449	9.2949	634.7965	233	11.0449	9.2949	4156.9256
234	11.0709	9.2731	365.0541	234	11.0709	9.2731	3476.6238	234	11.0709	9.2731	555.2959	234	11.0709	9.2731	4072.4916
235	11.0969	9.2515	343.1163	235	11.0969	9.2515	3448.1945	235	11.0969	9.2515	519.6687	235	11.0969	9.2515	4031.9309
236	11.1229	9.2299	381.1868	236	11.1229	9.2299	3479.7735	236	11.1229	9.2299	527.3492	236	11.1229	9.2299	4034.6778
237	11.1489	9.2085	340.7791	237	11.1489	9.2085	3432.8744	237	11.1489	9.2085	458.8958	237	11.1489	9.2085	3961.291
238	11.1749	9.1871	439.7827	238	11.1749	9.1871	3525.3865	238	11.1749	9.1871	539.3081	238	11.1749	9.1871	4036.7697
239	11.2009	9.1659	427.7754	239	11.2009	9.1659	3506.8878	239	11.2009	9.1659	567.5237	239	11.2009	9.1659	4060.0518
240	11.2269	9.1447	431.522	240	11.2269	9.1447	3504.1429	240	11.2269	9.1447	530.291	240	11.2269	9.1447	4017.8857
241	11.2529	9.1236	486.9047	241	11.2529	9.1236	3553.0341	241	11.2529	9.1236	562.9324	241	11.2529	9.1236	4045.5936
242	11.2789	9.1027	460.0987	242	11.2789	9.1027	3519.7367	242	11.2789	9.1027	631.8396	242	11.2789	9.1027	4109.5673
243	11.3049	9.0818	424.8774	243	11.3049	9.0818	3478.0239	243	11.3049	9.0818	566.397	243	11.3049	9.0818	4039.1912
244	11.3309	9.061	492.8331	244	11.3309	9.061	3539.4882	244	11.3309	9.061	531.2835	244	11.3309	9.061	3999.1442
245	11.3569	9.0404	440.7287	245	11.3569	9.0404	3480.8923	245	11.3569	9.0404	528.7565	245	11.3569	9.0404	3991.6837
246	11.3829	9.0198	352.2567	246	11.3829	9.0198	3385.9289	246	11.3829	9.0198	531.3704	246	11.3829	9.0198	3989.364
247	11.4089	8.9993	347.4967	247	11.4089	8.9993	3374.6773	247	11.4089	8.9993	508.2426	247	11.4089	8.9993	3961.3028

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
248	11.4349	8.9789	398.1479	248	11.4349	8.9789	3418.8371	248	11.4349	8.9789	554.3669	248	11.4349	8.9789	4002.4936
249	11.4609	8.9586	470.5407	249	11.4609	8.9586	3484.7385	249	11.4609	8.9586	558.4084	249	11.4609	8.9586	4001.6016
250	11.4869	8.9384	423.8913	250	11.4869	8.9384	3431.5976	250	11.4869	8.9384	544.0306	250	11.4869	8.9384	3982.2903
251	11.5129	8.9183	395.6256	251	11.5129	8.9183	3396.8405	251	11.5129	8.9183	525.2117	251	11.5129	8.9183	3958.5379
252	11.5389	8.8982	394.5163	252	11.5389	8.8982	3389.2396	252	11.5389	8.8982	500.9685	252	11.5389	8.8982	3929.3612
253	11.5649	8.8783	390.2443	253	11.5649	8.8783	3378.4762	253	11.5649	8.8783	536.5308	253	11.5649	8.8783	3959.99
254	11.5909	8.8585	426.7285	254	11.5909	8.8585	3408.469	254	11.5909	8.8585	508.4256	254	11.5909	8.8585	3926.9513
255	11.6169	8.8387	445.785	255	11.6169	8.8387	3421.034	255	11.6169	8.8387	469.766	255	11.6169	8.8387	3883.3582
256	11.6429	8.819	461.4236	256	11.6429	8.819	3430.1811	256	11.6429	8.819	433.2391	256	11.6429	8.819	3841.8977
257	11.6689	8.7994	420.1243	257	11.6689	8.7994	3382.3904	257	11.6689	8.7994	467.2963	257	11.6689	8.7994	3871.0214
258	11.6949	8.7799	417.4226	258	11.6949	8.7799	3373.1972	258	11.6949	8.7799	522.5612	258	11.6949	8.7799	3921.3528
259	11.7209	8.7605	464.3955	259	11.7209	8.7605	3413.6786	259	11.7209	8.7605	493.9441	259	11.7209	8.7605	3887.8022
260	11.7469	8.7412	416.0668	260	11.7469	8.7412	3358.8585	260	11.7469	8.7412	505.1498	260	11.7469	8.7412	3894.0744
261	11.7729	8.722	422.3849	261	11.7729	8.722	3358.6851	261	11.7729	8.722	522.407	261	11.7729	8.722	3906.3982
262	11.7989	8.7028	473.5229	262	11.7989	8.7028	3403.3317	262	11.7989	8.7028	537.9142	262	11.7989	8.7028	3916.9718
263	11.8249	8.6838	399.645	263	11.8249	8.6838	3322.9623	263	11.8249	8.6838	518.7071	263	11.8249	8.6838	3892.8313
264	11.8509	8.6648	382.2179	264	11.8509	8.6648	3299.0437	264	11.8509	8.6648	531.2996	264	11.8509	8.6648	3900.4902
265	11.8769	8.6459	431.4009	265	11.8769	8.6459	3341.7353	265	11.8769	8.6459	515.0683	265	11.8769	8.6459	3879.3254
266	11.9029	8.6271	412.9748	266	11.9029	8.6271	3316.8177	266	11.9029	8.6271	579.7762	266	11.9029	8.6271	3939.0998
267	11.9289	8.6083	392.6635	267	11.9289	8.6083	3290.015	267	11.9289	8.6083	530.2483	267	11.9289	8.6083	3884.6384
268	11.9549	8.5897	365.1998	268	11.9549	8.5897	3256.0598	268	11.9549	8.5897	481.5135	268	11.9549	8.5897	3830.9701
269	11.9809	8.5711	413.7475	269	11.9809	8.5711	3298.1161	269	11.9809	8.5711	524.8929	269	11.9809	8.5711	3869.416
270	12.0069	8.5526	389.5413	270	12.0069	8.5526	3267.4184	270	12.0069	8.5526	616.0256	270	12.0069	8.5526	3955.6152
271	12.0329	8.5342	397.6509	271	12.0329	8.5342	3269.0365	271	12.0329	8.5342	502.2583	271	12.0329	8.5342	3836.9144
272	12.0589	8.5159	438.908	272	12.0589	8.5159	3303.3365	272	12.0589	8.5159	457.9155	272	12.0589	8.5159	3787.6381
273	12.0849	8.4976	423.1992	273	12.0849	8.4976	3280.6705	273	12.0849	8.4976	527.5404	273	12.0849	8.4976	3852.3295
274	12.1109	8.4794	471.7386	274	12.1109	8.4794	3322.2527	274	12.1109	8.4794	519.7219	274	12.1109	8.4794	3839.5775
275	12.1369	8.4613	453.0649	275	12.1369	8.4613	3296.6218	275	12.1369	8.4613	585.5759	275	12.1369	8.4613	3900.498
276	12.1629	8.4433	425.753	276	12.1629	8.4433	3262.3527	276	12.1629	8.4433	553.2977	276	12.1629	8.4433	3863.2863
277	12.1889	8.4254	482.1285	277	12.1889	8.4254	3311.7711	277	12.1889	8.4254	555.9124	277	12.1889	8.4254	3860.9675
278	12.2149	8.4075	436.0828	278	12.2149	8.4075	3258.7682	278	12.2149	8.4075	555.0079	278	12.2149	8.4075	3855.1295
279	12.2409	8.3897	324.6813	279	12.2409	8.3897	3140.4095	279	12.2409	8.3897	515.3081	279	12.2409	8.3897	3810.4962
280	12.2669	8.372	341.3237	280	12.2669	8.372	3150.0948	280	12.2669	8.372	541.8823	280	12.2669	8.372	3832.1369
281	12.2929	8.3544	426.4121	281	12.2929	8.3544	3228.2259	281	12.2929	8.3544	471.6706	281	12.2929	8.3544	3756.9916
282	12.3189	8.3368	423.3302	282	12.3189	8.3368	3218.187	282	12.3189	8.3368	504.5936	282	12.3189	8.3368	3784.9812
283	12.3449	8.3193	428.2153	283	12.3449	8.3193	3216.1148	283	12.3449	8.3193	560.9402	283	12.3449	8.3193	3836.3943

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
284	12.3709	8.3019	463.8585	284	12.3709	8.3019	3244.8009	284	12.3709	8.3019	551.576	284	12.3709	8.3019	3822.0965
285	12.3969	8.2845	401.121	285	12.3969	8.2845	3175.1062	285	12.3969	8.2845	496.035	285	12.3969	8.2845	3761.6221
286	12.4229	8.2673	441.7902	286	12.4229	8.2673	3208.8182	286	12.4229	8.2673	444.3619	286	12.4229	8.2673	3705.0155
287	12.4489	8.2501	374.4981	287	12.4489	8.2501	3134.5689	287	12.4489	8.2501	420.7468	287	12.4489	8.2501	3676.4669
288	12.4749	8.2329	399.4294	288	12.4749	8.2329	3152.5431	288	12.4749	8.2329	527.2795	288	12.4749	8.2329	3778.0661
289	12.5009	8.2159	406.1216	289	12.5009	8.2159	3152.2781	289	12.5009	8.2159	531.0279	289	12.5009	8.2159	3776.881
290	12.5269	8.1989	425.8735	290	12.5269	8.1989	3165.0728	290	12.5269	8.1989	515.2008	290	12.5269	8.1989	3756.1204
291	12.5529	8.182	418.548	291	12.5529	8.182	3150.7901	291	12.5529	8.182	652.6379	291	12.5529	8.182	3888.6239
292	12.5789	8.1652	364.3502	292	12.5789	8.1652	3089.6351	292	12.5789	8.1652	562.3033	292	12.5789	8.1652	3793.3558
293	12.6049	8.1484	348.77	293	12.6049	8.1484	3067.0978	293	12.6049	8.1484	514.3675	293	12.6049	8.1484	3740.4865
294	12.6309	8.1317	333.782	294	12.6309	8.1317	3045.1526	294	12.6309	8.1317	512.2169	294	12.6309	8.1317	3733.4025
295	12.6569	8.115	454.3673	295	12.6569	8.115	3158.7807	295	12.6569	8.115	490.2567	295	12.6569	8.115	3706.5088
296	12.6829	8.0985	399.7517	296	12.6829	8.0985	3097.208	296	12.6829	8.0985	482.4006	296	12.6829	8.0985	3693.7191
297	12.7089	8.082	366.5021	297	12.7089	8.082	3057.0012	297	12.7089	8.082	535.434	297	12.7089	8.082	3741.819
298	12.7349	8.0655	484.6555	298	12.7349	8.0655	3168.1974	298	12.7349	8.0655	553.3977	298	12.7349	8.0655	3754.8493
299	12.7609	8.0492	353.7963	299	12.7609	8.0492	3030.381	299	12.7609	8.0492	572.8778	299	12.7609	8.0492	3769.3958
300	12.7869	8.0329	390.9072	300	12.7869	8.0329	3060.5347	300	12.7869	8.0329	568.7027	300	12.7869	8.0329	3760.2873
301	12.8129	8.0166	385.0523	301	12.8129	8.0166	3047.7227	301	12.8129	8.0166	694.0828	301	12.8129	8.0166	3880.7339
302	12.8389	8.0005	422.7956	302	12.8389	8.0005	3078.5088	302	12.8389	8.0005	520.5235	302	12.8389	8.0005	3702.241
303	12.8649	7.9844	466.8868	303	12.8649	7.9844	3115.6428	303	12.8649	7.9844	542.8657	303	12.8649	7.9844	3719.6498
304	12.8909	7.9683	371.866	304	12.8909	7.9683	3013.6648	304	12.8909	7.9683	447.8014	304	12.8909	7.9683	3619.6519
305	12.9169	7.9524	435.2084	305	12.9169	7.9524	3070.0501	305	12.9169	7.9524	545.5272	305	12.9169	7.9524	3712.4442
306	12.9429	7.9365	371.0616	306	12.9429	7.9365	2998.9461	306	12.9429	7.9365	433.225	306	12.9429	7.9365	3595.2085
307	12.9689	7.9206	416.5514	307	12.9689	7.9206	3037.4787	307	12.9689	7.9206	622.8868	307	12.9689	7.9206	3779.9368
308	12.9949	7.9048	447.9224	308	12.9949	7.9048	3061.8925	308	12.9949	7.9048	593.8677	308	12.9949	7.9048	3745.9842
309	13.0209	7.8891	432.3887	309	13.0209	7.8891	3039.4017	309	13.0209	7.8891	518.4705	309	13.0209	7.8891	3665.6535
310	13.0469	7.8735	461.2945	310	13.0469	7.8735	3061.3503	310	13.0469	7.8735	476.72	310	13.0469	7.8735	3618.9695
311	13.0729	7.8579	381.1888	311	13.0729	7.8579	2974.2874	311	13.0729	7.8579	560.0038	311	13.0729	7.8579	3697.3199
312	13.0989	7.8423	496.9577	312	13.0989	7.8423	3083.0992	312	13.0989	7.8423	459.1749	312	13.0989	7.8423	3591.5575
313	13.1249	7.8269	422.5827	313	13.1249	7.8269	3001.767	313	13.1249	7.8269	516.8481	313	13.1249	7.8269	3644.2971
314	13.1509	7.8115	614.7352	314	13.1509	7.8115	3186.9623	314	13.1509	7.8115	498.0775	314	13.1509	7.8115	3620.593
315	13.1769	7.7961	410.364	315	13.1769	7.7961	2975.634	315	13.1769	7.7961	502.0712	315	13.1769	7.7961	3619.6532
316	13.2029	7.7808	454.8965	316	13.2029	7.7808	3013.2093	316	13.2029	7.7808	467.1255	316	13.2029	7.7808	3579.774
317	13.2289	7.7656	462.9988	317	13.2289	7.7656	3014.3544	317	13.2289	7.7656	505.19	317	13.2289	7.7656	3612.905
318	13.2549	7.7504	444.6718	318	13.2549	7.7504	2989.0703	318	13.2549	7.7504	503.399	318	13.2549	7.7504	3606.1805
319	13.2809	7.7353	499.0861	319	13.2809	7.7353	3036.5274	319	13.2809	7.7353	555.1452	319	13.2809	7.7353	3652.9932

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
320	13.3069	7.7203	483.794	320	13.3069	7.7203	3014.278	320	13.3069	7.7203	428.841	320	13.3069	7.7203	3521.7555
321	13.3329	7.7053	452.3033	321	13.3329	7.7053	2975.8302	321	13.3329	7.7053	567.6928	321	13.3329	7.7053	3655.6738
322	13.3589	7.6904	467.0993	322	13.3589	7.6904	2983.669	322	13.3589	7.6904	546.6466	322	13.3589	7.6904	3629.6941
323	13.3849	7.6755	395.2752	323	13.3849	7.6755	2904.8878	323	13.3849	7.6755	574.112	323	13.3849	7.6755	3652.226
324	13.4109	7.6607	462.6497	324	13.4109	7.6607	2965.305	324	13.4109	7.6607	532.9577	324	13.4109	7.6607	3606.1381
325	13.4369	7.6459	397.6509	325	13.4369	7.6459	2893.3491	325	13.4369	7.6459	421.68	325	13.4369	7.6459	3489.927
326	13.4629	7.6312	500.077	326	13.4629	7.6312	2990.4903	326	13.4629	7.6312	494.0429	326	13.4629	7.6312	3557.3564
327	13.4889	7.6166	539.341	327	13.4889	7.6166	3024.4693	327	13.4889	7.6166	482.2307	327	13.4889	7.6166	3540.6107
328	13.5149	7.602	489.0117	328	13.5149	7.602	2968.855	328	13.5149	7.602	490.1726	328	13.5149	7.602	3543.619
329	13.5409	7.5875	530.8622	329	13.5409	7.5875	3005.4206	329	13.5409	7.5875	510.1784	329	13.5409	7.5875	3558.6913
330	13.5669	7.573	518.6838	330	13.5669	7.573	2987.9573	330	13.5669	7.573	591.9771	330	13.5669	7.573	3635.5566
331	13.5929	7.5586	466.7472	331	13.5929	7.5586	2930.7357	331	13.5929	7.5586	549.3384	331	13.5929	7.5586	3587.9844
332	13.6189	7.5442	519.7113	332	13.6189	7.5442	2978.4149	332	13.6189	7.5442	529.8661	332	13.6189	7.5442	3563.5786
333	13.6449	7.5299	451.7695	333	13.6449	7.5299	2905.1882	333	13.6449	7.5299	498.1079	333	13.6449	7.5299	3526.8869
334	13.6709	7.5157	424.2168	334	13.6709	7.5157	2872.3505	334	13.6709	7.5157	487.1545	334	13.6709	7.5157	3511
335	13.6969	7.5015	400.9113	335	13.6969	7.5015	2843.7601	335	13.6969	7.5015	560.6835	335	13.6969	7.5015	3579.5954
336	13.7229	7.4873	477.2922	336	13.7229	7.4873	2914.8561	336	13.7229	7.4873	458.435	336	13.7229	7.4873	3472.4134
337	13.7489	7.4732	486.4189	337	13.7489	7.4732	2918.6979	337	13.7489	7.4732	466.2305	337	13.7489	7.4732	3475.2754
338	13.7749	7.4592	464.4756	338	13.7749	7.4592	2891.4696	338	13.7749	7.4592	516.3876	338	13.7749	7.4592	3520.499
339	13.8009	7.4452	533.1488	339	13.8009	7.4452	2954.8578	339	13.8009	7.4452	513.8968	339	13.8009	7.4452	3513.0747
340	13.8269	7.4313	523.3958	340	13.8269	7.4313	2939.8199	340	13.8269	7.4313	507.3012	340	13.8269	7.4313	3501.5456
341	13.8529	7.4174	501.9929	341	13.8529	7.4174	2913.1321	341	13.8529	7.4174	528.4817	341	13.8529	7.4174	3517.7926
342	13.8789	7.4036	468.4569	342	13.8789	7.4036	2874.3111	342	13.8789	7.4036	572.9815	342	13.8789	7.4036	3557.3589
343	13.9049	7.3898	406.577	343	13.9049	7.3898	2807.1463	343	13.9049	7.3898	550.6694	343	13.9049	7.3898	3530.1134
344	13.9309	7.3761	409.1784	344	13.9309	7.3761	2804.4628	344	13.9309	7.3761	526.4896	344	13.9309	7.3761	3501
345	13.9569	7.3624	471.485	345	13.9569	7.3624	2861.4845	345	13.9569	7.3624	533.1833	345	13.9569	7.3624	3502.7602
346	13.9829	7.3488	464.3321	346	13.9829	7.3488	2849.0466	346	13.9829	7.3488	458.6033	346	13.9829	7.3488	3423.2467
347	14.0089	7.3352	419.7294	347	14.0089	7.3352	2799.159	347	14.0089	7.3352	488.1893	347	14.0089	7.3352	3447.8992
348	14.0349	7.3217	416.539	348	14.0349	7.3217	2790.6836	348	14.0349	7.3217	487.0461	348	14.0349	7.3217	3441.8225
349	14.0609	7.3082	382.2829	349	14.0609	7.3082	2751.1425	349	14.0609	7.3082	466.7914	349	14.0609	7.3082	3416.6344
350	14.0869	7.2948	422.3993	350	14.0869	7.2948	2785.9741	350	14.0869	7.2948	513.7413	350	14.0869	7.2948	3458.6507
351	14.1129	7.2814	474.9487	351	14.1129	7.2814	2833.2385	351	14.1129	7.2814	508.773	351	14.1129	7.2814	3448.7489
352	14.1389	7.2681	488.2034	352	14.1389	7.2681	2841.2083	352	14.1389	7.2681	480.5775	352	14.1389	7.2681	3415.6199
353	14.1649	7.2548	449.3536	353	14.1649	7.2548	2797.0735	353	14.1649	7.2548	474.3837	353	14.1649	7.2548	3404.4926
354	14.1909	7.2416	383.6113	354	14.1909	7.2416	2726.0462	354	14.1909	7.2416	441.0199	354	14.1909	7.2416	3366.1953
355	14.2169	7.2284	365.2247	355	14.2169	7.2284	2702.3747	355	14.2169	7.2284	418.9708	355	14.2169	7.2284	3339.2127

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
356	14.2429	7.2153	382.8349	356	14.2429	7.2153	2714.7	356	14.2429	7.2153	423.2744	356	14.2429	7.2153	3338.5828
357	14.2689	7.2022	424.9671	357	14.2689	7.2022	2751.5473	357	14.2689	7.2022	457.6502	357	14.2689	7.2022	3368.0251
358	14.2949	7.1892	470.6622	358	14.2949	7.1892	2791.9574	358	14.2949	7.1892	488.6715	358	14.2949	7.1892	3394.1129
359	14.3209	7.1762	496.1813	359	14.3209	7.1762	2812.1916	359	14.3209	7.1762	493.3613	359	14.3209	7.1762	3393.8692
360	14.3469	7.1633	455.0661	360	14.3469	7.1633	2765.7915	360	14.3469	7.1633	503.4002	360	14.3469	7.1633	3398.9746
361	14.3729	7.1504	461.3738	361	14.3729	7.1504	2766.8142	361	14.3729	7.1504	492.4739	361	14.3729	7.1504	3383.1148
362	14.3989	7.1375	487.36	362	14.3989	7.1375	2787.5154	362	14.3989	7.1375	495.447	362	14.3989	7.1375	3381.1544
363	14.4249	7.1247	475.9652	363	14.4249	7.1247	2770.8358	363	14.4249	7.1247	478.592	363	14.4249	7.1247	3359.3659
364	14.4509	7.112	470.9381	364	14.4509	7.112	2760.5237	364	14.4509	7.112	488.6564	364	14.4509	7.112	3364.4968
365	14.4769	7.0993	442.8533	365	14.4769	7.0993	2727.154	365	14.4769	7.0993	454.8806	365	14.4769	7.0993	3325.7874
366	14.5029	7.0866	460.9843	366	14.5029	7.0866	2740	366	14.5029	7.0866	468.5664	366	14.5029	7.0866	3334.5398
367	14.5289	7.074	402.5289	367	14.5289	7.074	2676.2597	367	14.5289	7.074	505.8023	367	14.5289	7.074	3366.8422
368	14.5549	7.0614	377.0697	368	14.5549	7.0614	2645.5156	368	14.5549	7.0614	466.9277	368	14.5549	7.0614	3323.0341
369	14.5809	7.0489	470.5496	369	14.5809	7.0489	2733.7105	369	14.5809	7.0489	409.4401	369	14.5809	7.0489	3260.613
370	14.6069	7.0364	383.5428	370	14.6069	7.0364	2641.4188	370	14.6069	7.0364	413.4424	370	14.6069	7.0364	3259.6818
371	14.6329	7.024	431.9554	371	14.6329	7.024	2684.5464	371	14.6329	7.024	362.0218	371	14.6329	7.024	3203.3276
372	14.6589	7.0116	479.4629	372	14.6589	7.0116	2726.769	372	14.6589	7.0116	429.6997	372	14.6589	7.0116	3266.072
373	14.6849	6.9993	421.5493	373	14.6849	6.9993	2663.5704	373	14.6849	6.9993	483.5668	373	14.6849	6.9993	3315.0057
374	14.7109	6.987	389.6034	374	14.7109	6.987	2626.3396	374	14.7109	6.987	510.9779	374	14.7109	6.987	3337.4832
375	14.7369	6.9747	416.6894	375	14.7369	6.9747	2648.1406	375	14.7369	6.9747	459.5844	375	14.7369	6.9747	3281.1563
376	14.7629	6.9625	511.2908	376	14.7629	6.9625	2737.4571	376	14.7629	6.9625	485.7849	376	14.7629	6.9625	3302.4233
377	14.7889	6.9503	399.3126	377	14.7889	6.9503	2620.194	377	14.7889	6.9503	501.9507	377	14.7889	6.9503	3313.6556
378	14.8149	6.9382	325.5542	378	14.8149	6.9382	2541.1507	378	14.8149	6.9382	456.9763	378	14.8149	6.9382	3263.7476
379	14.8409	6.9261	397.6509	379	14.8409	6.9261	2607.9624	379	14.8409	6.9261	558.7687	379	14.8409	6.9261	3360.6065
380	14.8669	6.9141	439.5763	380	14.8669	6.9141	2643.9009	380	14.8669	6.9141	437.7718	380	14.8669	6.9141	3234.6762
381	14.8929	6.9021	422.4006	381	14.8929	6.9021	2620.7382	381	14.8929	6.9021	479.2451	381	14.8929	6.9021	3271.2159
382	14.9189	6.8901	455.1159	382	14.9189	6.8901	2647.4666	382	14.9189	6.8901	556.6805	382	14.9189	6.8901	3343.7178
383	14.9449	6.8782	479.6682	383	14.9449	6.8782	2666.032	383	14.9449	6.8782	450.4608	383	14.9449	6.8782	3232.5646
384	14.9709	6.8663	461.8157	384	14.9709	6.8663	2642.1926	384	14.9709	6.8663	456.0449	384	14.9709	6.8663	3233.2152
385	14.9969	6.8545	496.5966	385	14.9969	6.8545	2670.9866	385	14.9969	6.8545	419.445	385	14.9969	6.8545	3191.6818
386	15.0229	6.8427	503.0445	386	15.0229	6.8427	2671.4476	386	15.0229	6.8427	465.6967	386	15.0229	6.8427	3233
387	15.0489	6.8309	445.8235	387	15.0489	6.8309	2608.2396	387	15.0489	6.8309	458.5605	387	15.0489	6.8309	3220.9303
388	15.0749	6.8192	512.6913	388	15.0749	6.8192	2669.1205	388	15.0749	6.8192	385.1949	388	15.0749	6.8192	3142.6312
389	15.1009	6.8075	514.6478	389	15.1009	6.8075	2665.0901	389	15.1009	6.8075	307.1159	389	15.1009	6.8075	3059.6187
390	15.1269	6.7959	463.4228	390	15.1269	6.7959	2607.8782	390	15.1269	6.7959	413.3641	390	15.1269	6.7959	3160.9334
391	15.1529	6.7843	458.6224	391	15.1529	6.7843	2597.0908	391	15.1529	6.7843	403.7887	391	15.1529	6.7843	3146.4245

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
392	15.1789	6.7727	434.6662	392	15.1789	6.7727	2567.1477	392	15.1789	6.7727	483.2334	392	15.1789	6.7727	3220.9357
393	15.2049	6.7612	409.7439	393	15.2049	6.7612	2536.2385	393	15.2049	6.7612	519.2604	393	15.2049	6.7612	3252.0292
394	15.2309	6.7498	399.4241	394	15.2309	6.7498	2519.9318	394	15.2309	6.7498	479.8415	394	15.2309	6.7498	3207.6768
395	15.2569	6.7383	452.7704	395	15.2569	6.7383	2567.2911	395	15.2569	6.7383	441.3861	395	15.2569	6.7383	3164.2879
396	15.2829	6.7269	402.5959	396	15.2829	6.7269	2511.1297	396	15.2829	6.7269	407.1819	396	15.2829	6.7269	3125.1501
397	15.3089	6.7156	427.1856	397	15.3089	6.7156	2529.7325	397	15.3089	6.7156	501.5682	397	15.3089	6.7156	3214.6029
398	15.3349	6.7043	499.921	398	15.3349	6.7043	2596.481	398	15.3349	6.7043	457.7001	398	15.3349	6.7043	3165.8014
399	15.3609	6.693	379.4687	399	15.3609	6.693	2470.0418	399	15.3609	6.693	401.9574	399	15.3609	6.693	3105.1251
400	15.3869	6.6817	477.3636	400	15.3869	6.6817	2561.9497	400	15.3869	6.6817	480.9364	400	15.3869	6.6817	3179.1706
401	15.4129	6.6705	438.3226	401	15.4129	6.6705	2516.9218	401	15.4129	6.6705	420.5696	401	15.4129	6.6705	3113.8703
402	15.4389	6.6594	532.2136	402	15.4389	6.6594	2604.8259	402	15.4389	6.6594	456.0184	402	15.4389	6.6594	3144.3857
403	15.4649	6.6482	391.6218	403	15.4649	6.6482	2458.2472	403	15.4649	6.6482	615.386	403	15.4649	6.6482	3298.8198
404	15.4909	6.6371	419.4089	404	15.4909	6.6371	2480.0474	404	15.4909	6.6371	428.5484	404	15.4909	6.6371	3107.0487
405	15.5169	6.6261	461.0386	405	15.5169	6.6261	2515.6902	405	15.5169	6.6261	470.1148	405	15.5169	6.6261	3143.6816
406	15.5429	6.6151	397.6509	406	15.5429	6.6151	2446.3155	406	15.5429	6.6151	368.3863	406	15.5429	6.6151	3037.0196
407	15.5689	6.6041	441.5887	407	15.5689	6.6041	2486.7766	407	15.5689	6.6041	447.0811	407	15.5689	6.6041	3110.7808
408	15.5949	6.5932	386.6678	408	15.5949	6.5932	2428.3791	408	15.5949	6.5932	448.464	408	15.5949	6.5932	3107.2302
409	15.6209	6.5823	512.4387	409	15.6209	6.5823	2550.6733	409	15.6209	6.5823	404.6303	409	15.6209	6.5823	3058.4631
410	15.6469	6.5714	482.6872	410	15.6469	6.5714	2517.4451	410	15.6469	6.5714	460.7823	410	15.6469	6.5714	3109.6816
411	15.6729	6.5605	411.9655	411	15.6729	6.5605	2443.2468	411	15.6729	6.5605	349.7562	411	15.6729	6.5605	2993.7219
412	15.6989	6.5497	479.3407	412	15.6989	6.5497	2507.1453	412	15.6989	6.5497	340.4361	412	15.6989	6.5497	2979.4684
413	15.7249	6.539	547.041	413	15.7249	6.539	2571.369	413	15.7249	6.539	366.7896	413	15.7249	6.539	3000.8884
414	15.7509	6.5283	452.408	414	15.7509	6.5283	2473.2593	414	15.7509	6.5283	454.1211	414	15.7509	6.5283	3083.2863
415	15.7769	6.5176	437.488	415	15.7769	6.5176	2454.8626	415	15.7769	6.5176	386.5807	415	15.7769	6.5176	3010.8124
416	15.8029	6.5069	451.5713	416	15.8029	6.5069	2465.4692	416	15.8029	6.5069	417.874	416	15.8029	6.5069	3037.1722
417	15.8289	6.4963	473.1529	417	15.8289	6.4963	2483.5742	417	15.8289	6.4963	475.6132	417	15.8289	6.4963	3089.9779
418	15.8549	6.4857	453.1833	418	15.8549	6.4857	2460.1279	418	15.8549	6.4857	399.6036	418	15.8549	6.4857	3009.0348
419	15.8809	6.4752	415.8754	419	15.8809	6.4752	2419.3433	419	15.8809	6.4752	452.7334	419	15.8809	6.4752	3057.2312
420	15.9069	6.4646	451.7665	420	15.9069	6.4646	2451.7577	420	15.9069	6.4646	429.6781	420	15.9069	6.4646	3029.2423
421	15.9329	6.4542	413.3598	421	15.9329	6.4542	2409.8744	421	15.9329	6.4542	509.8004	421	15.9329	6.4542	3104.4311
422	15.9589	6.4437	503.2197	422	15.9589	6.4437	2496.2576	422	15.9589	6.4437	440.8042	422	15.9589	6.4437	3030.5014
423	15.9849	6.4333	496.5526	423	15.9849	6.4333	2486.1139	423	15.9849	6.4333	463.6247	423	15.9849	6.4333	3048.3885
424	16.0109	6.4229	447.9547	424	16.0109	6.4229	2434.0393	424	16.0109	6.4229	420.9689	424	16.0109	6.4229	3000.7991
425	16.0369	6.4126	450.7004	425	16.0369	6.4126	2433.3083	425	16.0369	6.4126	389.9008	425	16.0369	6.4126	2964.7975
426	16.0629	6.4023	503.0673	426	16.0629	6.4023	2482.1985	426	16.0629	6.4023	407.8294	426	16.0629	6.4023	2977.7926
427	16.0889	6.392	435.0772	427	16.0889	6.392	2410.7317	427	16.0889	6.392	432.6593	427	16.0889	6.392	2997.689

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
428	16.1149	6.3817	397.0321	428	16.1149	6.3817	2369.21	428	16.1149	6.3817	393.8234	428	16.1149	6.3817	2953.9196
429	16.1409	6.3715	494.7289	429	16.1409	6.3715	2463.4302	429	16.1409	6.3715	485.5272	429	16.1409	6.3715	3040.6899
430	16.1669	6.3614	403.6649	430	16.1669	6.3614	2368.8895	430	16.1669	6.3614	447.2072	430	16.1669	6.3614	2997.4363
431	16.1929	6.3512	358.1182	431	16.1929	6.3512	2319.8661	431	16.1929	6.3512	463.1084	431	16.1929	6.3512	3008.4041
432	16.2189	6.3411	432.078	432	16.2189	6.3411	2390.3492	432	16.2189	6.3411	515.6419	432	16.2189	6.3411	3056.0041
433	16.2449	6.331	429.6677	433	16.2449	6.331	2384.4622	433	16.2449	6.331	453.6515	433	16.2449	6.331	2989.0802
434	16.2709	6.321	423.904	434	16.2709	6.321	2375.2219	434	16.2709	6.321	403.9881	434	16.2709	6.321	2934.4833
435	16.2969	6.3109	465.9262	435	16.2969	6.3109	2413.7674	435	16.2969	6.3109	425.1062	435	16.2969	6.3109	2950.6678
436	16.3229	6.301	468.5404	436	16.3229	6.301	2412.9049	436	16.3229	6.301	423.593	436	16.3229	6.301	2944.2211
437	16.3489	6.291	444.5696	437	16.3489	6.291	2385.4575	437	16.3489	6.291	420.9792	437	16.3489	6.291	2936.6739
438	16.3749	6.2811	483.074	438	16.3749	6.2811	2420.4852	438	16.3749	6.2811	446.8215	438	16.3749	6.2811	2957.5827
439	16.4009	6.2712	463.937	439	16.4009	6.2712	2397.8715	439	16.4009	6.2712	494.8741	439	16.4009	6.2712	3000.7018
440	16.4269	6.2613	468.6626	440	16.4269	6.2613	2399.1204	440	16.4269	6.2613	475.8826	440	16.4269	6.2613	2976.7767
441	16.4529	6.2515	499.3368	441	16.4529	6.2515	2426.318	441	16.4529	6.2515	401.5963	441	16.4529	6.2515	2897.557
442	16.4789	6.2417	481.7791	442	16.4789	6.2417	2405.2836	442	16.4789	6.2417	441.3939	442	16.4789	6.2417	2932.4211
443	16.5049	6.232	434.1831	443	16.5049	6.232	2354.2109	443	16.5049	6.232	410.113	443	16.5049	6.232	2896.2067
444	16.5309	6.2222	463.5939	444	16.5309	6.2222	2380.1451	444	16.5309	6.2222	398.2699	444	16.5309	6.2222	2879.4301
445	16.5569	6.2125	436.0973	445	16.5569	6.2125	2349.1718	445	16.5569	6.2125	474.9005	445	16.5569	6.2125	2951.1272
446	16.5829	6.2028	412.6012	446	16.5829	6.2028	2322.1991	446	16.5829	6.2028	412.99	446	16.5829	6.2028	2884.2831
447	16.6089	6.1932	441.2453	447	16.6089	6.1932	2347.3664	447	16.6089	6.1932	408.278	447	16.6089	6.1932	2874.6377
448	16.6349	6.1836	486.9807	448	16.6349	6.1836	2389.6252	448	16.6349	6.1836	391.2409	448	16.6349	6.1836	2852.667
449	16.6609	6.174	412.7466	449	16.6609	6.174	2311.9144	449	16.6609	6.174	367.3643	449	16.6609	6.174	2823.857
450	16.6869	6.1645	383.8939	450	16.6869	6.1645	2279.585	450	16.6869	6.1645	383.8124	450	16.6869	6.1645	2835.3715
451	16.7129	6.1549	394.0126	451	16.7129	6.1549	2286.2271	451	16.7129	6.1549	413.4025	451	16.7129	6.1549	2860.0282
452	16.7389	6.1454	448.1193	452	16.7389	6.1454	2336.8571	452	16.7389	6.1454	415.3803	452	16.7389	6.1454	2857.0724
453	16.7649	6.136	463.9542	453	16.7649	6.136	2349.2154	453	16.7649	6.136	408.18	453	16.7649	6.136	2844.9386
454	16.7909	6.1265	429.4132	454	16.7909	6.1265	2311.1977	454	16.7909	6.1265	457.9922	454	16.7909	6.1265	2889.8173
455	16.8169	6.1171	430.3952	455	16.8169	6.1171	2308.703	455	16.8169	6.1171	473.2972	455	16.8169	6.1171	2900.1888
456	16.8429	6.1078	405.8592	456	16.8429	6.1078	2280.6904	456	16.8429	6.1078	432.8033	456	16.8429	6.1078	2854.7614
457	16.8689	6.0984	414.0559	457	16.8689	6.0984	2285.4104	457	16.8689	6.0984	401.4667	457	16.8689	6.0984	2818.4913
458	16.8949	6.0891	455.2598	458	16.8949	6.0891	2323.1377	458	16.8949	6.0891	456.4255	458	16.8949	6.0891	2868.5166
459	16.9209	6.0798	490.3324	459	16.9209	6.0798	2354.7335	459	16.9209	6.0798	469.7933	459	16.9209	6.0798	2876.9509
460	16.9469	6.0706	472.1181	460	16.9469	6.0706	2333.0426	460	16.9469	6.0706	441.886	460	16.9469	6.0706	2844.1101
461	16.9729	6.0613	430.0512	461	16.9729	6.0613	2286.3132	461	16.9729	6.0613	484.9443	461	16.9729	6.0613	2882.2349
462	16.9989	6.0521	431.4334	462	16.9989	6.0521	2283.0329	462	16.9989	6.0521	468.2556	462	16.9989	6.0521	2860.6127
463	17.0249	6.0429	477.3626	463	17.0249	6.0429	2324.2996	463	17.0249	6.0429	462.4969	463	17.0249	6.0429	2849.9205

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
464	17.0509	6.0338	466.7216	464	17.0509	6.0338	2308.9962	464	17.0509	6.0338	436.0914	464	17.0509	6.0338	2818.5815
465	17.0769	6.0247	396.7338	465	17.0769	6.0247	2234.3459	465	17.0769	6.0247	428.3555	465	17.0769	6.0247	2805.9121
466	17.1029	6.0156	379.0504	466	17.1029	6.0156	2212	466	17.1029	6.0156	484.3273	466	17.1029	6.0156	2856.9504
467	17.1289	6.0065	429.9869	467	17.1289	6.0065	2258.274	467	17.1289	6.0065	462.6893	467	17.1289	6.0065	2830.3788
468	17.1549	5.9975	488.6654	468	17.1549	5.9975	2312.2901	468	17.1549	5.9975	456.1582	468	17.1549	5.9975	2818.9142
469	17.1809	5.9885	430.1612	469	17.1809	5.9885	2249.1234	469	17.1809	5.9885	521.0244	469	17.1809	5.9885	2878.847
470	17.2069	5.9795	389.2752	470	17.2069	5.9795	2203.5749	470	17.2069	5.9795	428.6873	470	17.2069	5.9795	2781.5764
471	17.2329	5.9706	397.1028	471	17.2329	5.9706	2206.74	471	17.2329	5.9706	371.9567	471	17.2329	5.9706	2719.9122
472	17.2589	5.9616	406.2474	472	17.2589	5.9616	2211.2222	472	17.2589	5.9616	438.7557	472	17.2589	5.9616	2781.7778
473	17.2849	5.9527	380.1374	473	17.2849	5.9527	2180.4497	473	17.2849	5.9527	457.3611	473	17.2849	5.9527	2795.4497
474	17.3109	5.9439	371.565	474	17.3109	5.9439	2167.2148	474	17.3109	5.9439	461.0233	474	17.3109	5.9439	2794.1783
475	17.3369	5.935	408.1973	475	17.3369	5.935	2199.1847	475	17.3369	5.935	459.0661	475	17.3369	5.935	2787.2877
476	17.3629	5.9262	460.9621	476	17.3629	5.9262	2247.2869	476	17.3629	5.9262	389.2805	476	17.3629	5.9262	2712.5686
477	17.3889	5.9174	492.0976	477	17.3889	5.9174	2273.76	477	17.3889	5.9174	482.3543	477	17.3889	5.9174	2800.7088
478	17.4149	5.9086	549.0444	478	17.4149	5.9086	2326.0443	478	17.4149	5.9086	475.2759	478	17.4149	5.9086	2788.697
479	17.4409	5.8999	497.2339	479	17.4409	5.8999	2269.5714	479	17.4409	5.8999	391.3981	479	17.4409	5.8999	2699.8856
480	17.4669	5.8912	465.2362	480	17.4669	5.8912	2232.9111	480	17.4669	5.8912	380.9014	480	17.4669	5.8912	2684.4555
481	17.4929	5.8825	501.5811	481	17.4929	5.8825	2264.5936	481	17.4929	5.8825	494.225	481	17.4929	5.8825	2792.8456
482	17.5189	5.8738	504.729	482	17.5189	5.8738	2263.079	482	17.5189	5.8738	391.9579	482	17.5189	5.8738	2685.6449
483	17.5449	5.8652	416.0936	483	17.5449	5.8652	2169.7811	483	17.5449	5.8652	463.5083	483	17.5449	5.8652	2752.2618
484	17.5709	5.8566	411.5215	484	17.5709	5.8566	2160.5465	484	17.5709	5.8566	480.595	484	17.5709	5.8566	2764.4151
485	17.5969	5.848	442.9545	485	17.5969	5.848	2187.3171	485	17.5969	5.848	474.4664	485	17.5969	5.848	2753.3529
486	17.6229	5.8394	404.3585	486	17.6229	5.8394	2144.0585	486	17.6229	5.8394	434.2407	486	17.6229	5.8394	2708.1937
487	17.6489	5.8309	397.6509	487	17.6489	5.8309	2132.6885	487	17.6489	5.8309	449.626	487	17.6489	5.8309	2718.6455
488	17.6749	5.8224	422.5408	488	17.6749	5.8224	2157.1537	488	17.6749	5.8224	399.7266	488	17.6749	5.8224	2663.8126
489	17.7009	5.8139	407.179	489	17.7009	5.8139	2141.3673	489	17.7009	5.8139	494.8979	489	17.7009	5.8139	2754.0505
490	17.7269	5.8054	387.3322	490	17.7269	5.8054	2121.0959	490	17.7269	5.8054	421.6051	490	17.7269	5.8054	2675.8241
491	17.7529	5.797	457.6776	491	17.7529	5.797	2191.0166	491	17.7529	5.797	390.1456	491	17.7529	5.797	2639.4311
492	17.7789	5.7886	362.2099	492	17.7789	5.7886	2095.1242	492	17.7789	5.7886	493.4189	492	17.7789	5.7886	2737.7709
493	17.8049	5.7802	435.6484	493	17.8049	5.7802	2168.1381	493	17.8049	5.7802	459.7682	493	17.8049	5.7802	2699.1867
494	17.8309	5.7719	463.3608	494	17.8309	5.7719	2195.4258	494	17.8309	5.7719	395.3058	494	17.8309	5.7719	2629.7908
495	17.8569	5.7635	430.4241	495	17.8569	5.7635	2162.0645	495	17.8569	5.7635	434.6953	495	17.8569	5.7635	2664.2468
496	17.8829	5.7552	393.2804	496	17.8829	5.7552	2124.4961	496	17.8829	5.7552	457.7046	496	17.8829	5.7552	2682.3226
497	17.9089	5.7469	378.4446	497	17.9089	5.7469	2109.2356	497	17.9089	5.7469	345.7714	497	17.9089	5.7469	2565.4559
498	17.9349	5.7387	377.2419	498	17.9349	5.7387	2107.6083	498	17.9349	5.7387	397.0131	498	17.9349	5.7387	2611.7641
499	17.9609	5.7304	323.3998	499	17.9609	5.7304	2053.3415	499	17.9609	5.7304	476.1323	499	17.9609	5.7304	2685.9498

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
500	17.9869	5.7222	412.4095	500	17.9869	5.7222	2141.9266	500	17.9869	5.7222	410.9458	500	17.9869	5.7222	2615.8297
501	18.0129	5.714	465.3228	501	18.0129	5.714	2194.4153	501	18.0129	5.714	319.5177	501	18.0129	5.714	2519.4682
502	18.0389	5.7058	352.4769	502	18.0389	5.7058	2081.1447	502	18.0389	5.7058	435.4459	502	18.0389	5.7058	2630.4629
503	18.0649	5.6977	355.97	503	18.0649	5.6977	2084.2131	503	18.0649	5.6977	454.6619	503	18.0649	5.6977	2644.7454
504	18.0909	5.6896	264.9448	504	18.0909	5.6896	1992.7633	504	18.0909	5.6896	395.1681	504	18.0909	5.6896	2580.318
505	18.1169	5.6815	348.536	505	18.1169	5.6815	2075.9298	505	18.1169	5.6815	434.7543	505	18.1169	5.6815	2614.9708
506	18.1429	5.6734	369.8049	506	18.1429	5.6734	2096.7741	506	18.1429	5.6734	479.2867	506	18.1429	5.6734	2654.5697
507	18.1689	5.6654	345.9725	507	18.1689	5.6654	2072.517	507	18.1689	5.6654	425.8913	507	18.1689	5.6654	2596.2408
508	18.1949	5.6573	351.6966	508	18.1949	5.6573	2077.8164	508	18.1949	5.6573	423.7677	508	18.1949	5.6573	2589.1836
509	18.2209	5.6493	343.6695	509	18.2209	5.6493	2069.3647	509	18.2209	5.6493	347.9216	509	18.2209	5.6493	2508.4041
510	18.2469	5.6413	376.0143	510	18.2469	5.6413	2101.2848	510	18.2469	5.6413	427.3144	510	18.2469	5.6413	2582.8634
511	18.2729	5.6334	285.1307	511	18.2729	5.6334	2009.9766	511	18.2729	5.6334	395.0408	511	18.2729	5.6334	2545.6562
512	18.2989	5.6254	422.7539	512	18.2989	5.6254	2147.1751	512	18.2989	5.6254	335.9573	512	18.2989	5.6254	2481.6392
513	18.3249	5.6175	355.8216	513	18.3249	5.6175	2079.8182	513	18.3249	5.6175	496.2944	513	18.3249	5.6175	2637.0428
514	18.3509	5.6096	397.6509	514	18.3509	5.6096	2121.2228	514	18.3509	5.6096	566.1374	514	18.3509	5.6096	2701.9524
515	18.3769	5.6018	313.5719	515	18.3769	5.6018	2035.1059	515	18.3769	5.6018	440.2274	515	18.3769	5.6018	2571.1088
516	18.4029	5.5939	361.5752	516	18.4029	5.5939	2081.0712	516	18.4029	5.5939	388.2212	516	18.4029	5.5939	2514.1691
517	18.4289	5.5861	334.4579	517	18.4289	5.5861	2051.916	517	18.4289	5.5861	496.2375	517	18.4289	5.5861	2617.2519
518	18.4549	5.5783	326.3588	518	18.4549	5.5783	2041.779	518	18.4549	5.5783	471.5402	518	18.4549	5.5783	2587.6211
519	18.4809	5.5705	405.9007	519	18.4809	5.5705	2119.283	519	18.4809	5.5705	444.9053	519	18.4809	5.5705	2556.0527
520	18.5069	5.5628	333.0716	520	18.5069	5.5628	2044.416	520	18.5069	5.5628	461.9424	520	18.5069	5.5628	2568.1563
521	18.5329	5.555	287.7581	521	18.5329	5.555	1997.0645	521	18.5329	5.555	378.9555	521	18.5329	5.555	2480.236
522	18.5589	5.5473	322.7643	522	18.5589	5.5473	2030.0328	522	18.5589	5.5473	318.4849	522	18.5589	5.5473	2414.8318
523	18.5849	5.5396	313.0759	523	18.5849	5.5396	2018.3065	523	18.5849	5.5396	426.8243	523	18.5849	5.5396	2518.2377
524	18.6109	5.532	358.6352	524	18.6109	5.532	2061.8278	524	18.6109	5.532	471.1116	524	18.6109	5.532	2557.5915
525	18.6369	5.5243	375.8489	525	18.6369	5.5243	2077.0036	525	18.6369	5.5243	399.3817	525	18.6369	5.5243	2480.9281
526	18.6629	5.5167	409.7243	526	18.6629	5.5167	2108.8411	526	18.6629	5.5167	458.722	526	18.6629	5.5167	2535.3349
527	18.6889	5.5091	364.4791	527	18.6889	5.5091	2061.5579	527	18.6889	5.5091	421.6315	527	18.6889	5.5091	2493.3109
528	18.7149	5.5015	329.3724	528	18.7149	5.5015	2024.4133	528	18.7149	5.5015	389.2094	528	18.7149	5.5015	2455.9553
529	18.7409	5.4939	360.7654	529	18.7409	5.4939	2053.7684	529	18.7409	5.4939	362.3126	529	18.7409	5.4939	2424.125
530	18.7669	5.4864	300.4264	530	18.7669	5.4864	1991.3915	530	18.7669	5.4864	445.4984	530	18.7669	5.4864	2502.3773
531	18.7929	5.4789	343.2971	531	18.7929	5.4789	2032.2243	531	18.7929	5.4789	470.9016	531	18.7929	5.4789	2522.847
532	18.8189	5.4713	350.5605	532	18.8189	5.4713	2037.4497	532	18.8189	5.4713	437.8875	532	18.8189	5.4713	2484.8994
533	18.8449	5.4639	310.803	533	18.8449	5.4639	1995.6543	533	18.8449	5.4639	515.7611	533	18.8449	5.4639	2557.8395
534	18.8709	5.4564	395.9395	534	18.8709	5.4564	2078.7529	534	18.8709	5.4564	484.1362	534	18.8709	5.4564	2521.281
535	18.8969	5.449	441.4335	535	18.8969	5.449	2122.209	535	18.8969	5.449	467.1021	535	18.8969	5.449	2499.3135

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
536	18.9229	5.4415	366.4231	536	18.9229	5.4415	2045.1606	536	18.9229	5.4415	447.7508	536	18.9229	5.4415	2475.0286
537	18.9489	5.4342	314.8958	537	18.9489	5.4342	1991.5954	537	18.9489	5.4342	439.2923	537	18.9489	5.4342	2461.6367
538	18.9749	5.4268	343.2682	538	18.9749	5.4268	2017.9299	538	18.9749	5.4268	478.519	538	18.9749	5.4268	2495.9299
539	19.0009	5.4194	376.2742	539	19.0009	5.4194	2048.8979	539	19.0009	5.4194	470.0795	539	19.0009	5.4194	2482.5569
540	19.0269	5.4121	444.7356	540	19.0269	5.4121	2115.3215	540	19.0269	5.4121	407.9573	540	19.0269	5.4121	2415.5011
541	19.0529	5.4048	423.8853	541	19.0529	5.4048	2092.4332	541	19.0529	5.4048	402.0807	541	19.0529	5.4048	2404.691
542	19.0789	5.3975	462.0762	542	19.0789	5.3975	2127.1001	542	19.0789	5.3975	350.5656	542	19.0789	5.3975	2350.164
543	19.1049	5.3902	421.3805	543	19.1049	5.3902	2082.8805	543	19.1049	5.3902	389.8233	543	19.1049	5.3902	2386.4099
544	19.1309	5.3829	488.8923	544	19.1309	5.3829	2146.8683	544	19.1309	5.3829	445.9961	544	19.1309	5.3829	2439.5707
545	19.1569	5.3757	569.9684	545	19.1569	5.3757	2224.4205	545	19.1569	5.3757	410.4714	545	19.1569	5.3757	2401.0341
546	19.1829	5.3685	619.1288	546	19.1829	5.3685	2270.0569	546	19.1829	5.3685	484.5565	546	19.1829	5.3685	2472.1072
547	19.2089	5.3613	761.6749	547	19.2089	5.3613	2409.0789	547	19.2089	5.3613	526.7573	547	19.2089	5.3613	2511.2962
548	19.2349	5.3541	848.1274	548	19.2349	5.3541	2492.0075	548	19.2349	5.3541	485.0003	548	19.2349	5.3541	2466.5273
549	19.2609	5.3469	887.8363	549	19.2609	5.3469	2528.1924	549	19.2609	5.3469	489.0503	549	19.2609	5.3469	2467.5653
550	19.2869	5.3398	993.4351	550	19.2869	5.3398	2630.2673	550	19.2869	5.3398	447.9148	550	19.2869	5.3398	2423.4179
551	19.3129	5.3327	1188.9492	551	19.3129	5.3327	2822.2574	551	19.3129	5.3327	397.5387	551	19.3129	5.3327	2370.0299
552	19.3389	5.3256	1387.9993	552	19.3389	5.3256	3017.7835	552	19.3389	5.3256	385.9301	552	19.3389	5.3256	2355.4093
553	19.3649	5.3185	1555.6318	553	19.3649	5.3185	3181.8921	553	19.3649	5.3185	388.3761	553	19.3649	5.3185	2354.8434
554	19.3909	5.3114	1799.7981	554	19.3909	5.3114	3422.5344	554	19.3909	5.3114	400.5965	554	19.3909	5.3114	2364.0519
555	19.4169	5.3044	1951.2663	555	19.4169	5.3044	3570.4787	555	19.4169	5.3044	435.7395	555	19.4169	5.3044	2396.183
556	19.4429	5.2974	1865.0143	556	19.4429	5.2974	3480.7027	556	19.4429	5.2974	440.4602	556	19.4429	5.2974	2397.8917
557	19.4689	5.2904	1718.9517	557	19.4689	5.2904	3331.1161	557	19.4689	5.2904	459.0352	557	19.4689	5.2904	2413.4549
558	19.4949	5.2834	1424.9776	558	19.4949	5.2834	3033.618	558	19.4949	5.2834	465.1037	558	19.4949	5.2834	2416.5114
559	19.5209	5.2764	1045.2395	559	19.5209	5.2764	2650.356	559	19.5209	5.2764	404.7034	559	19.5209	5.2764	2353.0992
560	19.5469	5.2694	840.4727	560	19.5469	5.2694	2442.0652	560	19.5469	5.2694	388.8955	560	19.5469	5.2694	2334.2794
561	19.5729	5.2625	753.626	561	19.5729	5.2625	2351.6945	561	19.5729	5.2625	393.5067	561	19.5729	5.2625	2335.8787
562	19.5989	5.2556	654.1703	562	19.5989	5.2556	2248.7148	562	19.5989	5.2556	401.3392	562	19.5989	5.2556	2340.6992
563	19.6249	5.2487	563.621	563	19.6249	5.2487	2154.6415	563	19.6249	5.2487	421.2934	563	19.6249	5.2487	2357.6415
564	19.6509	5.2418	551.956	564	19.6509	5.2418	2139.4526	564	19.6509	5.2418	472.0062	564	19.6509	5.2418	2405.3425
565	19.6769	5.235	477.0284	565	19.6769	5.235	2061.001	565	19.6769	5.235	459.0241	565	19.6769	5.235	2389.3484
566	19.7029	5.2281	478.7003	566	19.7029	5.2281	2059.1489	566	19.7029	5.2281	390.5059	566	19.7029	5.2281	2317.8183
567	19.7289	5.2213	499.0446	567	19.7289	5.2213	2075.9693	567	19.7289	5.2213	380.948	567	19.7289	5.2213	2305.2485
568	19.7549	5.2145	437.7741	568	19.7549	5.2145	2011.1748	568	19.7549	5.2145	367.8336	568	19.7549	5.2145	2289.1222
569	19.7809	5.2077	383.3619	569	19.7809	5.2077	1953.2386	569	19.7809	5.2077	401.4903	569	19.7809	5.2077	2319.7669
570	19.8069	5.201	362.7749	570	19.8069	5.201	1929.1276	570	19.8069	5.201	446.5883	570	19.8069	5.201	2361.853
571	19.8329	5.1942	393.5967	571	19.8329	5.1942	1956.4255	571	19.8329	5.1942	447.8304	571	19.8329	5.1942	2360.0831

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
572	19.8589	5.1875	365.6423	572	19.8589	5.1875	1924.9471	572	19.8589	5.1875	487.7965	572	19.8589	5.1875	2397.0374
573	19.8849	5.1808	402.0556	573	19.8849	5.1808	1957.8364	573	19.8849	5.1808	467.726	573	19.8849	5.1808	2373.9549
574	19.9109	5.1741	490.0155	574	19.9109	5.1741	2042.2724	574	19.9109	5.1741	392.9127	574	19.9109	5.1741	2296.1297
575	19.9369	5.1674	351.7264	575	19.9369	5.1674	1900.4593	575	19.9369	5.1674	421.214	575	19.9369	5.1674	2321.4192
576	19.9629	5.1607	315.873	576	19.9629	5.1607	1861.082	576	19.9629	5.1607	405.0867	576	19.9629	5.1607	2302.2799
577	19.9889	5.1541	348.5998	577	19.9889	5.1541	1890.2848	577	19.9889	5.1541	443.8856	577	19.9889	5.1541	2338.0668
578	20.0149	5.1474	374.826	578	20.0149	5.1474	1912.987	578	20.0149	5.1474	411.9467	578	20.0149	5.1474	2303.116
579	20.0409	5.1408	426.0313	579	20.0409	5.1408	1960.6683	579	20.0409	5.1408	452.1934	579	20.0409	5.1408	2340.3509
580	20.0669	5.1342	379.2126	580	20.0669	5.1342	1910.3256	580	20.0669	5.1342	431.28	580	20.0669	5.1342	2316.4255
581	20.0929	5.1277	332.8898	581	20.0929	5.1277	1860.4789	581	20.0929	5.1277	395.6692	581	20.0929	5.1277	2277.8028
582	20.1189	5.1211	378.6403	582	20.1189	5.1211	1902.7054	582	20.1189	5.1211	433.111	582	20.1189	5.1211	2312.2327
583	20.1449	5.1146	378.1525	583	20.1449	5.1146	1898.6937	583	20.1449	5.1146	443.8092	583	20.1449	5.1146	2319.9189
584	20.1709	5.108	367.3031	584	20.1709	5.108	1884.3203	584	20.1709	5.108	434.9449	584	20.1709	5.108	2308.0427
585	20.1969	5.1015	393.1938	585	20.1969	5.1015	1906.687	585	20.1969	5.1015	460.4397	585	20.1969	5.1015	2330.5256
586	20.2229	5.095	389.8037	586	20.2229	5.095	1899.7729	586	20.2229	5.095	416.6713	586	20.2229	5.095	2283.7453
587	20.2489	5.0886	424.8345	587	20.2489	5.0886	1931.2798	587	20.2489	5.0886	399.3185	587	20.2489	5.0886	2263.3806
588	20.2749	5.0821	374.0978	588	20.2749	5.0821	1877.0191	588	20.2749	5.0821	445.443	588	20.2749	5.0821	2306.4932
589	20.3009	5.0757	320.0003	589	20.3009	5.0757	1819.3977	589	20.3009	5.0757	532.6713	589	20.3009	5.0757	2390.7096
590	20.3269	5.0692	411.7497	590	20.3269	5.0692	1907.6231	590	20.3269	5.0692	486.2006	590	20.3269	5.0692	2341.2269
591	20.3529	5.0628	399.2529	591	20.3529	5.0628	1891.6023	591	20.3529	5.0628	422.465	591	20.3529	5.0628	2274.4794
592	20.3789	5.0564	292.3009	592	20.3789	5.0564	1781.1263	592	20.3789	5.0564	424.7739	592	20.3789	5.0564	2273.7764
593	20.4049	5.0501	328.8028	593	20.4049	5.0501	1814.1043	593	20.4049	5.0501	350.5399	593	20.4049	5.0501	2196.5304
594	20.4309	5.0437	420.4366	594	20.4309	5.0437	1902.2141	594	20.4309	5.0437	481.0118	594	20.4309	5.0437	2323.9904
595	20.4569	5.0374	397.6509	595	20.4569	5.0374	1875.9044	595	20.4569	5.0374	435.2415	595	20.4569	5.0374	2275.2082
596	20.4829	5.031	363.2362	596	20.4829	5.031	1836.5607	596	20.4829	5.031	536.7146	596	20.4829	5.031	2373.6694
597	20.5089	5.0247	400.0507	597	20.5089	5.0247	1868.4464	597	20.5089	5.0247	486.1101	597	20.5089	5.0247	2320.053
598	20.5349	5.0184	391.6654	598	20.5349	5.0184	1855.132	598	20.5349	5.0184	361.9235	598	20.5349	5.0184	2192.8545
599	20.5609	5.0122	428.4801	599	20.5609	5.0122	1887.0178	599	20.5609	5.0122	475.44	599	20.5609	5.0122	2303.359
600	20.5869	5.0059	353.3495	600	20.5869	5.0059	1806.9583	600	20.5869	5.0059	363.1434	600	20.5869	5.0059	2188.0505
601	20.6129	4.9997	419.1449	601	20.6129	4.9997	1867.8247	601	20.6129	4.9997	462.8153	601	20.6129	4.9997	2284.7105
602	20.6389	4.9934	320.5614	602	20.6389	4.9934	1764.3122	602	20.6389	4.9934	377.5295	602	20.6389	4.9934	2196.4128
603	20.6649	4.9872	385.8835	603	20.6649	4.9872	1824.7054	603	20.6649	4.9872	366.0391	603	20.6649	4.9872	2181.9105
604	20.6909	4.981	381.2533	604	20.6909	4.981	1815.1463	604	20.6909	4.981	403.1183	604	20.6909	4.981	2215.9777
605	20.7169	4.9748	452.5089	605	20.7169	4.9748	1881.4729	605	20.7169	4.9748	462.4728	605	20.7169	4.9748	2272.3203
606	20.7429	4.9687	382.1919	606	20.7429	4.9687	1806.227	606	20.7429	4.9687	368.4571	606	20.7429	4.9687	2175.2927
607	20.7689	4.9625	411.5711	607	20.7689	4.9625	1830.6773	607	20.7689	4.9625	479.7563	607	20.7689	4.9625	2283.58

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
608	20.7949	4.9564	295.6539	608	20.7949	4.9564	1709.8311	608	20.7949	4.9564	413.8321	608	20.7949	4.9564	2214.6439
609	20.8209	4.9503	414.7886	609	20.8209	4.9503	1824.0368	609	20.8209	4.9503	495.4816	609	20.8209	4.9503	2293.2814
610	20.8469	4.9441	363.3693	610	20.8469	4.9441	1767.6886	610	20.8469	4.9441	532.8038	610	20.8469	4.9441	2327.5917
611	20.8729	4.9381	498.2459	611	20.8729	4.9381	1897.6362	611	20.8729	4.9381	562.8038	611	20.8729	4.9381	2354.5798
612	20.8989	4.932	373.6667	612	20.8989	4.932	1768.128	612	20.8989	4.932	471.613	612	20.8989	4.932	2260.3771
613	20.9249	4.9259	400.077	613	20.9249	4.9259	1789.6094	613	20.9249	4.9259	417.2322	613	20.9249	4.9259	2202.9844
614	20.9509	4.9199	331.2328	614	20.9509	4.9199	1715.8363	614	20.9509	4.9199	405.2481	614	20.9509	4.9199	2187.9884
615	20.9769	4.9138	454.5898	615	20.9769	4.9138	1834.2643	615	20.9769	4.9138	394.5637	615	20.9769	4.9138	2174.292
616	21.0029	4.9078	465.0721	616	21.0029	4.9078	1839.8177	616	21.0029	4.9078	399.8747	616	21.0029	4.9078	2176.5912
617	21.0289	4.9018	347.5455	617	21.0289	4.9018	1717.3621	617	21.0289	4.9018	392.6411	617	21.0289	4.9018	2166.3456
618	21.0549	4.8958	402.9582	618	21.0549	4.8958	1767.8459	618	21.0549	4.8958	335.4851	618	21.0549	4.8958	2106.1777
619	21.0809	4.8899	368.432	619	21.0809	4.8899	1728.3907	619	21.0809	4.8899	475.2792	619	21.0809	4.8899	2242.9599
620	21.1069	4.8839	414.882	620	21.1069	4.8839	1769.9118	620	21.1069	4.8839	436.8318	620	21.1069	4.8839	2201.5005
621	21.1329	4.878	423.6583	621	21.1329	4.878	1773.7591	621	21.1329	4.878	387.7824	621	21.1329	4.878	2149.4392
622	21.1589	4.8721	397.6509	622	21.1589	4.8721	1742.8228	622	21.1589	4.8721	376.649	622	21.1589	4.8721	2135.2939
623	21.1849	4.8661	478.4264	623	21.1849	4.8661	1822.3184	623	21.1849	4.8661	367.5987	623	21.1849	4.8661	2123.2317
624	21.2109	4.8602	497.3879	624	21.2109	4.8602	1840	624	21.2109	4.8602	392.1129	624	21.2109	4.8602	2144.7339
625	21.2369	4.8544	411.3509	625	21.2369	4.8544	1752.6831	625	21.2369	4.8544	427.8795	625	21.2369	4.8544	2177.4886
626	21.2629	4.8485	373.5805	626	21.2629	4.8485	1713.633	626	21.2629	4.8485	359.1432	626	21.2629	4.8485	2105.7404
627	21.2889	4.8426	421.4894	627	21.2889	4.8426	1760.2619	627	21.2889	4.8426	382.6356	627	21.2889	4.8426	2126.2209
628	21.3149	4.8368	391.3414	628	21.3149	4.8368	1728.8341	628	21.3149	4.8368	366.0564	628	21.3149	4.8368	2106.6298
629	21.3409	4.831	419.7648	629	21.3409	4.831	1755.9776	629	21.3409	4.831	389.6529	629	21.3409	4.831	2127.2144
630	21.3669	4.8252	498.3306	630	21.3669	4.8252	1833.2635	630	21.3669	4.8252	383.9963	630	21.3669	4.8252	2118.5458
631	21.3929	4.8194	431.9701	631	21.3929	4.8194	1765.6232	631	21.3929	4.8194	385.9561	631	21.3929	4.8194	2117.4937
632	21.4189	4.8136	411.0171	632	21.4189	4.8136	1743.3903	632	21.4189	4.8136	422.2527	632	21.4189	4.8136	2150.7784
633	21.4449	4.8078	420.7395	633	21.4449	4.8078	1751.8329	633	21.4449	4.8078	466.3798	633	21.4449	4.8078	2191.8936
634	21.4709	4.8021	389.6655	634	21.4709	4.8021	1719.4789	634	21.4709	4.8021	448.8538	634	21.4709	4.8021	2171.3557
635	21.4969	4.7963	390.2332	635	21.4969	4.7963	1718.7668	635	21.4969	4.7963	370.7112	635	21.4969	4.7963	2090.2011
636	21.5229	4.7906	434.5108	636	21.5229	4.7906	1761.7646	636	21.5229	4.7906	346.2213	636	21.5229	4.7906	2062.6993
637	21.5489	4.7849	389.9781	637	21.5489	4.7849	1715.952	637	21.5489	4.7849	341.2608	637	21.5489	4.7849	2054.7269
638	21.5749	4.7792	388.4475	638	21.5749	4.7792	1713.1415	638	21.5749	4.7792	353.4563	638	21.5749	4.7792	2063.9105
639	21.6009	4.7735	418.9949	639	21.6009	4.7735	1742.409	639	21.6009	4.7735	379.9667	639	21.6009	4.7735	2087.409
640	21.6269	4.7678	437.4412	640	21.6269	4.7678	1759.5755	640	21.6269	4.7678	373.0993	640	21.6269	4.7678	2077.5297
641	21.6529	4.7622	467.1857	641	21.6529	4.7622	1788.0401	641	21.6529	4.7622	425.0575	641	21.6529	4.7622	2126.4759
642	21.6789	4.7565	440.4776	642	21.6789	4.7565	1760.0521	642	21.6789	4.7565	354.0248	642	21.6789	4.7565	2052.4313
643	21.7049	4.7509	404.8478	643	21.7049	4.7509	1723.1425	643	21.7049	4.7509	254.1431	643	21.7049	4.7509	1949.5377

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
644	21.7309	4.7453	400.465	644	21.7309	4.7453	1717.4799	644	21.7309	4.7453	353.1306	644	21.7309	4.7453	2045.5133
645	21.7569	4.7397	440.4777	645	21.7569	4.7397	1756.2127	645	21.7569	4.7397	419.6485	645	21.7569	4.7397	2109.0192
646	21.7829	4.7341	427.1371	646	21.7829	4.7341	1741.5922	646	21.7829	4.7341	394.0368	646	21.7829	4.7341	2080.3956
647	21.8089	4.7285	372.1344	647	21.8089	4.7285	1685.3097	647	21.8089	4.7285	457.0181	647	21.8089	4.7285	2140.3651
648	21.8349	4.723	371.8341	648	21.8349	4.723	1683.7294	648	21.8349	4.723	437.3896	648	21.8349	4.723	2117.7246
649	21.8609	4.7174	397.6509	649	21.8609	4.7174	1708.2664	649	21.8609	4.7174	404.9283	649	21.8609	4.7174	2082.2513
650	21.8869	4.7119	364.4552	650	21.8869	4.7119	1672.2863	650	21.8869	4.7119	389.1838	650	21.8869	4.7119	2063.4949
651	21.9129	4.7064	363.7819	651	21.9129	4.7064	1668.8286	651	21.9129	4.7064	445.4237	651	21.9129	4.7064	2116.7229
652	21.9389	4.7008	403.0901	652	21.9389	4.7008	1705.3523	652	21.9389	4.7008	447.3016	652	21.9389	4.7008	2115.5889
653	21.9649	4.6954	391.1116	653	21.9649	4.6954	1690.5894	653	21.9649	4.6954	365.0073	653	21.9649	4.6954	2030.2827
654	21.9909	4.6899	382.2007	654	21.9909	4.6899	1678.8941	654	21.9909	4.6899	351.1099	654	21.9909	4.6899	2013.3734
655	22.0169	4.6844	380.8097	655	22.0169	4.6844	1674.7187	655	22.0169	4.6844	362.2376	655	22.0169	4.6844	2021.4892
656	22.0429	4.6789	368.8718	656	22.0429	4.6789	1659.9964	656	22.0429	4.6789	364.2594	656	22.0429	4.6789	2020.4991
657	22.0689	4.6735	353.9486	657	22.0689	4.6735	1642.2888	657	22.0689	4.6735	369.2271	657	22.0689	4.6735	2022.4549
658	22.0949	4.6681	309.1757	658	22.0949	4.6681	1594.7315	658	22.0949	4.6681	400.7611	658	22.0949	4.6681	2050.9769
659	22.1209	4.6626	359.7344	659	22.1209	4.6626	1642.5057	659	22.1209	4.6626	375.7315	659	22.1209	4.6626	2022.9354
660	22.1469	4.6572	447.5561	660	22.1469	4.6572	1727.5431	660	22.1469	4.6572	359.1617	660	22.1469	4.6572	2003.3537
661	22.1729	4.6519	456.7874	661	22.1729	4.6519	1733.9899	661	22.1729	4.6519	430.4201	661	22.1729	4.6519	2071.6002
662	22.1989	4.6465	419.6459	662	22.1989	4.6465	1694.064	662	22.1989	4.6465	436.2945	662	22.1989	4.6465	2074.4627
663	22.2249	4.6411	353.3864	663	22.2249	4.6411	1625.0201	663	22.2249	4.6411	389.5258	663	22.2249	4.6411	2024.682
664	22.2509	4.6357	391.7647	664	22.2509	4.6357	1660.614	664	22.2509	4.6357	354.9051	664	22.2509	4.6357	1987.0494
665	22.2769	4.6304	444.5207	665	22.2769	4.6304	1710.5856	665	22.2769	4.6304	366.6271	665	22.2769	4.6304	1995.7595
666	22.3029	4.6251	444.6693	666	22.3029	4.6251	1707.9497	666	22.3029	4.6251	370.2058	666	22.3029	4.6251	1996.3263
667	22.3289	4.6198	414.2256	667	22.3289	4.6198	1674.7216	667	22.3289	4.6198	387.6338	667	22.3289	4.6198	2010.7423
668	22.3549	4.6145	401.3068	668	22.3549	4.6145	1659.0184	668	22.3549	4.6145	406.1745	668	22.3549	4.6145	2026.2711
669	22.3809	4.6092	441.2469	669	22.3809	4.6092	1696.1741	669	22.3809	4.6092	347.9074	669	22.3809	4.6092	1964.9921
670	22.4069	4.6039	456.6223	670	22.4069	4.6039	1708.7651	670	22.4069	4.6039	409.42	670	22.4069	4.6039	2023.4928
671	22.4329	4.5986	429.3572	671	22.4329	4.5986	1678.7156	671	22.4329	4.5986	453.5045	671	22.4329	4.5986	2064.5654
672	22.4589	4.5934	474.9267	672	22.4589	4.5934	1721.5007	672	22.4589	4.5934	437.4782	672	22.4589	4.5934	2045.5271
673	22.4849	4.5881	459.9785	673	22.4849	4.5881	1703.768	673	22.4849	4.5881	428.7176	673	22.4849	4.5881	2033.7547
674	22.5109	4.5829	408.7631	674	22.5109	4.5829	1649.7682	674	22.5109	4.5829	391.8668	674	22.5109	4.5829	1993.8919
675	22.5369	4.5777	420.4689	675	22.5369	4.5777	1658.6896	675	22.5369	4.5777	414.1774	675	22.5369	4.5777	2013.1906
676	22.5629	4.5725	397.6509	676	22.5629	4.5725	1633.0872	676	22.5629	4.5725	423.8925	676	22.5629	4.5725	2019.8937
677	22.5889	4.5673	379.4586	677	22.5889	4.5673	1613.8713	677	22.5889	4.5673	466.5065	677	22.5889	4.5673	2059.4959
678	22.6149	4.5621	409.0674	678	22.6149	4.5621	1642.4565	678	22.6149	4.5621	421.2835	678	22.6149	4.5621	2011.2609
679	22.6409	4.5569	398.9988	679	22.6409	4.5569	1631.3643	679	22.6409	4.5569	415.3044	679	22.6409	4.5569	2002.2699

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
680	22.6669	4.5518	411.3067	680	22.6669	4.5518	1642.6487	680	22.6669	4.5518	448.653	680	22.6669	4.5518	2032.6066
681	22.6929	4.5466	471.3492	681	22.6929	4.5466	1701.6676	681	22.6929	4.5466	398.5413	681	22.6929	4.5466	1979.483
682	22.7189	4.5415	446.0897	682	22.7189	4.5415	1675.3845	682	22.7189	4.5415	370.1063	682	22.7189	4.5415	1948.036
683	22.7449	4.5363	442.9806	683	22.7449	4.5363	1671.2518	683	22.7449	4.5363	311.6828	683	22.7449	4.5363	1886.6007
684	22.7709	4.5312	457.4526	684	22.7709	4.5312	1684.7002	684	22.7709	4.5312	387.5326	684	22.7709	4.5312	1959.4385
685	22.7969	4.5261	394.3836	685	22.7969	4.5261	1620.6077	685	22.7969	4.5261	389.369	685	22.7969	4.5261	1958.263
686	22.8229	4.521	433.2126	686	22.8229	4.521	1658.4132	686	22.8229	4.521	401.0049	686	22.8229	4.521	1966.887
687	22.8489	4.516	470.1986	687	22.8489	4.516	1694.3756	687	22.8489	4.516	389.8547	687	22.8489	4.516	1952.7248
688	22.8749	4.5109	405.1476	688	22.8749	4.5109	1628.3009	688	22.8749	4.5109	446.8408	688	22.8749	4.5109	2006.6991
689	22.9009	4.5059	423.6456	689	22.9009	4.5059	1645.7754	689	22.9009	4.5059	408.6139	689	22.9009	4.5059	1965.4602
690	22.9269	4.5008	442.4729	690	22.9269	4.5008	1663.5791	690	22.9269	4.5008	294.6509	690	22.9269	4.5008	1848.4853
691	22.9529	4.4958	469.9897	691	22.9529	4.4958	1690.0724	691	22.9529	4.4958	373.3679	691	22.9529	4.4958	1924.1904
692	22.9789	4.4908	482.7679	692	22.9789	4.4908	1701.8269	692	22.9789	4.4908	512.682	692	22.9789	4.4908	2060.4926
693	23.0049	4.4858	447.2123	693	23.0049	4.4858	1665.2477	693	23.0049	4.4858	435.4689	693	23.0049	4.4858	1980.2675
694	23.0309	4.4808	415.6945	694	23.0309	4.4808	1632.7063	694	23.0309	4.4808	435.7546	694	23.0309	4.4808	1977.5414
695	23.0569	4.4758	449.7838	695	23.0569	4.4758	1665.7721	695	23.0569	4.4758	414.5166	695	23.0569	4.4758	1953.2915
696	23.0829	4.4708	455.4837	696	23.0829	4.4708	1670.4484	696	23.0829	4.4708	466.8526	696	23.0829	4.4708	2002.6155
697	23.1089	4.4658	502.9327	697	23.1089	4.4658	1716.8738	697	23.1089	4.4658	410.3887	697	23.1089	4.4658	1943.1397
698	23.1349	4.4609	420.7955	698	23.1349	4.4609	1633.7131	698	23.1349	4.4609	446.8646	698	23.1349	4.4609	1976.6037
699	23.1609	4.456	477.3377	699	23.1609	4.456	1689.2317	699	23.1609	4.456	378.9366	699	23.1609	4.456	1905.6637
700	23.1869	4.451	531.0009	700	23.1869	4.451	1741.8714	700	23.1869	4.451	361.6187	700	23.1869	4.451	1885.3339
701	23.2129	4.4461	532.7097	701	23.2129	4.4461	1742.5566	701	23.2129	4.4461	316.7362	701	23.2129	4.4461	1837.4395
702	23.2389	4.4412	576.9315	702	23.2389	4.4412	1785.7548	702	23.2389	4.4412	413.5971	702	23.2389	4.4412	1931.2884
703	23.2649	4.4363	551.4076	703	23.2649	4.4363	1759.2073	703	23.2649	4.4363	402.0807	703	23.2649	4.4363	1916.7601
704	23.2909	4.4314	559.0151	704	23.2909	4.4314	1764.6552	704	23.2909	4.4314	427.4185	704	23.2909	4.4314	1939.3792
705	23.3169	4.4265	548.3283	705	23.3169	4.4265	1751.8088	705	23.3169	4.4265	483.9199	705	23.3169	4.4265	1993.1618
706	23.3429	4.4217	605.0474	706	23.3429	4.4217	1806.3683	706	23.3429	4.4217	430.1612	706	23.3429	4.4217	1936.6843
707	23.3689	4.4168	683.4429	707	23.3689	4.4168	1882.6043	707	23.3689	4.4168	367.5349	707	23.3689	4.4168	1871.3391
708	23.3949	4.412	603.2633	708	23.3949	4.412	1800.2651	708	23.3949	4.412	415.2218	708	23.3949	4.412	1916.3072
709	23.4209	4.4072	804.0362	709	23.4209	4.4072	1998.8785	709	23.4209	4.4072	365.9824	709	23.4209	4.4072	1864.3491
710	23.4469	4.4023	871.1532	710	23.4469	4.4023	2063.8359	710	23.4469	4.4023	413.6767	710	23.4469	4.4023	1909.3245
711	23.4729	4.3975	878.3424	711	23.4729	4.3975	2068.8655	711	23.4729	4.3975	430.4882	711	23.4729	4.3975	1923.4172
712	23.4989	4.3927	954.3659	712	23.4989	4.3927	2142.7295	712	23.4989	4.3927	427.173	712	23.4989	4.3927	1917.3833
713	23.5249	4.388	997.2738	713	23.5249	4.388	2183.4778	713	23.5249	4.388	459.439	713	23.5249	4.388	1946.9305
714	23.5509	4.3832	1284.2042	714	23.5509	4.3832	2468.2486	714	23.5509	4.3832	483.6609	714	23.5509	4.3832	1968.4335
715	23.5769	4.3784	1471.1556	715	23.5769	4.3784	2653.0405	715	23.5769	4.3784	499.8474	715	23.5769	4.3784	1981.9013

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
716	23.6029	4.3737	1707.4204	716	23.6029	4.3737	2887.1457	716	23.6029	4.3737	515.4372	716	23.6029	4.3737	1994.7723
717	23.6289	4.3689	2017.2473	717	23.6289	4.3689	3194.8131	717	23.6289	4.3689	531.0271	717	23.6289	4.3689	2007.6433
718	23.6549	4.3642	2488.3662	718	23.6549	4.3642	3663.7724	718	23.6549	4.3642	596.217	718	23.6549	4.3642	2070.1144
719	23.6809	4.3595	3056.4655	719	23.6809	4.3595	4229.7121	719	23.6809	4.3595	494.7197	719	23.6809	4.3595	1965.8984
720	23.7069	4.3547	3698.0589	720	23.7069	4.3547	4869.1459	720	23.7069	4.3547	517.0409	720	23.7069	4.3547	1985.5007
721	23.7329	4.35	4519.0533	721	23.7329	4.35	5687.9808	721	23.7329	4.35	405.4261	721	23.7329	4.35	1871.1671
722	23.7589	4.3453	5520.7162	722	23.7589	4.3453	6687.484	722	23.7589	4.3453	448.8917	722	23.7589	4.3453	1911.9139
723	23.7849	4.3407	6198.2683	723	23.7849	4.3407	7362.8766	723	23.7849	4.3407	440.1217	723	23.7849	4.3407	1900.4252
724	23.8109	4.336	6145.4028	724	23.8109	4.336	7307.8515	724	23.8109	4.336	441.7201	724	23.8109	4.336	1899.3047
725	23.8369	4.3313	5483.7417	725	23.8369	4.3313	6644.0309	725	23.8369	4.3313	454.113	725	23.8369	4.3313	1908.9789
726	23.8629	4.3267	4398.0361	726	23.8629	4.3267	5556.1656	726	23.8629	4.3267	448.3706	726	23.8629	4.3267	1900.5176
727	23.8889	4.322	3241.2237	727	23.8889	4.322	4397.1937	727	23.8889	4.322	445.3861	727	23.8889	4.322	1894.8143
728	23.9149	4.3174	2541.1585	728	23.9149	4.3174	3694.9689	728	23.9149	4.3174	479.5368	728	23.9149	4.3174	1926.2462
729	23.9409	4.3128	2149.4321	729	23.9409	4.3128	3301.083	729	23.9409	4.3128	371.4174	729	23.9409	4.3128	1815.4081
730	23.9669	4.3082	1757.1161	730	23.9669	4.3082	2906.6074	730	23.9669	4.3082	395.6935	730	23.9669	4.3082	1836.9654
731	23.9929	4.3036	1483.3241	731	23.9929	4.3036	2630.6558	731	23.9929	4.3036	460.0938	731	23.9929	4.3036	1898.6469
732	24.0189	4.299	1240.38	732	24.0189	4.299	2385.5522	732	24.0189	4.299	510.772	732	24.0189	4.299	1946.6062
733	24.0449	4.2944	1083.1928	733	24.0449	4.2944	2226.2054	733	24.0449	4.2944	437.1956	733	24.0449	4.2944	1870.3111
734	24.0709	4.2898	1040.9695	734	24.0709	4.2898	2181.8226	734	24.0709	4.2898	439.1357	734	24.0709	4.2898	1869.5323
735	24.0969	4.2853	872.9539	735	24.0969	4.2853	2011.6474	735	24.0969	4.2853	402.4125	735	24.0969	4.2853	1830.0904
736	24.1229	4.2807	801.6878	736	24.1229	4.2807	1938.2217	736	24.1229	4.2807	469.1877	736	24.1229	4.2807	1894.1467
737	24.1489	4.2762	706.5047	737	24.1489	4.2762	1840.879	737	24.1489	4.2762	476.0833	737	24.1489	4.2762	1898.3235
738	24.1749	4.2717	655.4144	738	24.1749	4.2717	1787.6291	738	24.1749	4.2717	498.4676	738	24.1749	4.2717	1917.989
739	24.2009	4.2671	656.6862	739	24.2009	4.2671	1786.7414	739	24.2009	4.2671	542.614	739	24.2009	4.2671	1959.4166
740	24.2269	4.2626	585.6853	740	24.2269	4.2626	1713.5809	740	24.2269	4.2626	565.2579	740	24.2269	4.2626	1979.3417
741	24.2529	4.2581	551.579	741	24.2529	4.2581	1677.315	741	24.2529	4.2581	604.5102	741	24.2529	4.2581	2015.8752
742	24.2789	4.2536	569.3179	742	24.2789	4.2536	1692.8944	742	24.2789	4.2536	582.261	742	24.2789	4.2536	1990.9072
743	24.3049	4.2492	573.8442	743	24.3049	4.2492	1695.2611	743	24.3049	4.2492	550.5947	743	24.3049	4.2492	1956.5221
744	24.3309	4.2447	534.4507	744	24.3309	4.2447	1653.7081	744	24.3309	4.2447	600.149	744	24.3309	4.2447	2003.3576
745	24.3569	4.2402	513.9022	745	24.3569	4.2402	1631	745	24.3569	4.2402	624.0073	745	24.3569	4.2402	2024.4972
746	24.3829	4.2358	471.6857	746	24.3829	4.2358	1586.6239	746	24.3829	4.2358	652.4473	746	24.3829	4.2358	2050.2183
747	24.4089	4.2313	478.7077	747	24.4089	4.2313	1591.4863	747	24.4089	4.2313	611.965	747	24.4089	4.2313	2007.0172
748	24.4349	4.2269	485.1515	748	24.4349	4.2269	1595.7705	748	24.4349	4.2269	532.2674	748	24.4349	4.2269	1924.6008
749	24.4609	4.2225	447.3686	749	24.4609	4.2225	1555.8281	749	24.4609	4.2225	512.5885	749	24.4609	4.2225	1902.2031
750	24.4869	4.218	446.7462	750	24.4869	4.218	1553.0461	750	24.4869	4.218	478.7618	750	24.4869	4.218	1865.6576
751	24.5129	4.2136	490.332	751	24.5129	4.2136	1594.4723	751	24.5129	4.2136	453.6144	751	24.5129	4.2136	1837.7914

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
752	24.5389	4.2092	505.1488	752	24.5389	4.2092	1607.1296	752	24.5389	4.2092	465.6705	752	24.5389	4.2092	1847.1287
753	24.5649	4.2049	480.3335	753	24.5649	4.2049	1580.1547	753	24.5649	4.2049	431.1857	753	24.5649	4.2049	1809.9251
754	24.5909	4.2005	503.3343	754	24.5909	4.2005	1600.996	754	24.5909	4.2005	383.7666	754	24.5909	4.2005	1759.7872
755	24.6169	4.1961	488.1946	755	24.6169	4.1961	1583.6966	755	24.6169	4.1961	435.3734	755	24.6169	4.1961	1808.6752
756	24.6429	4.1918	419.75	756	24.6429	4.1918	1513.0926	756	24.6429	4.1918	434.9027	756	24.6429	4.1918	1805.4857
757	24.6689	4.1874	428.2431	757	24.6689	4.1874	1519.4261	757	24.6689	4.1874	402.0807	757	24.6689	4.1874	1769.9449
758	24.6949	4.1831	435.2049	758	24.6949	4.1831	1523.0923	758	24.6949	4.1831	387.7755	758	24.6949	4.1831	1753.3829
759	24.7209	4.1787	430.0854	759	24.7209	4.1787	1514.6772	759	24.7209	4.1787	374.0735	759	24.7209	4.1787	1737.424
760	24.7469	4.1744	451.8278	760	24.7469	4.1744	1533.1241	760	24.7469	4.1744	429.1692	760	24.7469	4.1744	1790.2629
761	24.7729	4.1701	453.9174	761	24.7729	4.1701	1531.9181	761	24.7729	4.1701	405.1582	761	24.7729	4.1701	1763.995
762	24.7989	4.1658	415.1779	762	24.7989	4.1658	1489.883	762	24.7989	4.1658	341.8692	762	24.7989	4.1658	1698.4491
763	24.8249	4.1615	374.3747	763	24.8249	4.1615	1445.7843	763	24.8249	4.1615	371.0297	763	24.8249	4.1615	1725.3528
764	24.8509	4.1572	415.0727	764	24.8509	4.1572	1483.1867	764	24.8509	4.1572	387.6157	764	24.8509	4.1572	1739.6819
765	24.8769	4.1529	409.9866	765	24.8769	4.1529	1474.805	765	24.8769	4.1529	387.6753	765	24.8769	4.1529	1737.4846
766	24.9029	4.1487	371.4928	766	24.9029	4.1487	1433.0156	766	24.9029	4.1487	438.0065	766	24.9029	4.1487	1785.559
767	24.9289	4.1444	429.1389	767	24.9289	4.1444	1487.3662	767	24.9289	4.1444	453.5153	767	24.9289	4.1444	1798.811
768	24.9549	4.1402	453.6402	768	24.9549	4.1402	1508.5719	768	24.9549	4.1402	423.2603	768	24.9549	4.1402	1766.2991
769	24.9809	4.1359	416.5296	769	24.9809	4.1359	1468.1658	769	24.9809	4.1359	382.5496	769	24.9809	4.1359	1723.3315
770	25.0069	4.1317	411.9872	770	25.0069	4.1317	1460.3278	770	25.0069	4.1317	365.433	770	25.0069	4.1317	1703.9581
771	25.0329	4.1275	427.0721	771	25.0329	4.1275	1472.1172	771	25.0329	4.1275	383.8867	771	25.0329	4.1275	1720.1549
772	25.0589	4.1233	412.9076	772	25.0589	4.1233	1454.6571	772	25.0589	4.1233	394.4415	772	25.0589	4.1233	1728.4529
773	25.0849	4.119	363.2061	773	25.0849	4.119	1401.66	773	25.0849	4.119	393.9449	773	25.0849	4.119	1725.6995
774	25.1109	4.1148	391.2568	774	25.1109	4.1148	1426.4152	774	25.1109	4.1148	401.806	774	25.1109	4.1148	1731.3037
775	25.1369	4.1107	443.2559	775	25.1369	4.1107	1475.1187	775	25.1369	4.1107	334.0757	775	25.1369	4.1107	1661.3165
776	25.1629	4.1065	453.1519	776	25.1629	4.1065	1481.7192	776	25.1629	4.1065	334.9068	776	25.1629	4.1065	1659.8907
777	25.1889	4.1023	473.3169	777	25.1889	4.1023	1498.5886	777	25.1889	4.1023	383.7865	777	25.1889	4.1023	1706.5135
778	25.2149	4.0982	433.1819	778	25.2149	4.0982	1455.158	778	25.2149	4.0982	436.114	778	25.2149	4.0982	1756.5842
779	25.2409	4.094	412.4273	779	25.2409	4.094	1431.1078	779	25.2409	4.094	449.8514	779	25.2409	4.094	1768.0648
780	25.2669	4.0899	451.2284	780	25.2669	4.0899	1466.6134	780	25.2669	4.0899	382.0871	780	25.2669	4.0899	1698.0436
781	25.2929	4.0857	436.8622	781	25.2929	4.0857	1448.9516	781	25.2929	4.0857	425.8699	781	25.2929	4.0857	1739.5696
782	25.3189	4.0816	450.9472	782	25.3189	4.0816	1459.741	782	25.3189	4.0816	423.0779	782	25.3189	4.0816	1734.5207
783	25.3449	4.0775	426.9257	783	25.3449	4.0775	1432.424	783	25.3449	4.0775	433.8495	783	25.3449	4.0775	1743.0355
784	25.3709	4.0734	397.6509	784	25.3709	4.0734	1399.8536	784	25.3709	4.0734	416.0788	784	25.3709	4.0734	1723.0079
785	25.3969	4.0693	454.1385	785	25.3969	4.0693	1455.2333	785	25.3969	4.0693	475.3518	785	25.3969	4.0693	1780.024
786	25.4229	4.0652	402.0583	786	25.4229	4.0652	1402.045	786	25.4229	4.0652	394.2636	786	25.4229	4.0652	1696.679
787	25.4489	4.0611	460.0242	787	25.4489	4.0611	1458.903	787	25.4489	4.0611	391.4609	787	25.4489	4.0611	1691.6194

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
788	25.4749	4.057	394.1993	788	25.4749	4.057	1391.97	788	25.4749	4.057	425.1112	788	25.4749	4.057	1723.0129
789	25.5009	4.0529	425.2177	789	25.5009	4.0529	1421.8804	789	25.5009	4.0529	469.6329	789	25.5009	4.0529	1765.2777
790	25.5269	4.0489	467.987	790	25.5269	4.0489	1463.5418	790	25.5269	4.0489	344.2932	790	25.5269	4.0489	1637.6811
791	25.5529	4.0448	476.3918	791	25.5529	4.0448	1470.8386	791	25.5529	4.0448	370.9608	791	25.5529	4.0448	1662.0919
792	25.5789	4.0408	473.7834	792	25.5789	4.0408	1467.1221	792	25.5789	4.0408	350.3017	792	25.5789	4.0408	1639.176
793	25.6049	4.0367	456.6461	793	25.6049	4.0367	1448.8768	793	25.6049	4.0367	449.5701	793	25.6049	4.0367	1736.1875
794	25.6309	4.0327	443.9559	794	25.6309	4.0327	1435.0786	794	25.6309	4.0327	416.8481	794	25.6309	4.0327	1701.2086
795	25.6569	4.0287	438.255	795	25.6569	4.0287	1428.2698	795	25.6569	4.0287	382.6001	795	25.6569	4.0287	1664.7038
796	25.6829	4.0247	430.5163	796	25.6829	4.0247	1419.4231	796	25.6829	4.0247	401.5125	796	25.6829	4.0247	1681.3593
797	25.7089	4.0207	403.6086	797	25.7089	4.0207	1391.4074	797	25.7089	4.0207	433.6228	797	25.7089	4.0207	1711.2128
798	25.7349	4.0167	413.1817	798	25.7349	4.0167	1399.8724	798	25.7349	4.0167	398.1716	798	25.7349	4.0167	1673.5047
799	25.7609	4.0127	461.4331	799	25.7609	4.0127	1447.0159	799	25.7609	4.0127	435.7386	799	25.7609	4.0127	1708.8148
800	25.7869	4.0087	450.5881	800	25.7869	4.0087	1435.0629	800	25.7869	4.0087	338.8571	800	25.7869	4.0087	1609.6765
801	25.8129	4.0048	438.1412	801	25.8129	4.0048	1421.508	801	25.8129	4.0048	389.8051	801	25.8129	4.0048	1658.3677
802	25.8389	4.0008	414.7037	802	25.8389	4.0008	1396.9625	802	25.8389	4.0008	415.411	802	25.8389	4.0008	1681.7167
803	25.8649	3.9969	380.4574	803	25.8649	3.9969	1361.6082	803	25.8649	3.9969	467.5437	803	25.8649	3.9969	1731.5925
804	25.8909	3.9929	418.2164	804	25.8909	3.9929	1398.2592	804	25.8909	3.9929	480.5189	804	25.8909	3.9929	1742.3109
805	25.9169	3.989	426.773	805	25.9169	3.989	1405.7078	805	25.9169	3.989	402.9369	805	25.9169	3.989	1662.472
806	25.9429	3.985	414.8468	806	25.9429	3.985	1392.6736	806	25.9429	3.985	425.0061	806	25.9429	3.985	1682.2844
807	25.9689	3.9811	390.1733	807	25.9689	3.9811	1366.8921	807	25.9689	3.9811	371.1734	807	25.9689	3.9811	1626.1948
808	25.9949	3.9772	350.6881	808	25.9949	3.9772	1326.2989	808	25.9949	3.9772	446.696	808	25.9949	3.9772	1699.4605
809	26.0209	3.9733	426.1891	809	26.0209	3.9733	1400.6919	809	26.0209	3.9733	451.4579	809	26.0209	3.9733	1701.9656
810	26.0469	3.9694	394.5549	810	26.0469	3.9694	1367.9497	810	26.0469	3.9694	428.4547	810	26.0469	3.9694	1676.7055
811	26.0729	3.9655	434.1939	811	26.0729	3.9655	1406.4807	811	26.0729	3.9655	402.0807	811	26.0729	3.9655	1648.0747
812	26.0989	3.9616	429.197	812	26.0989	3.9616	1400.3758	812	26.0989	3.9616	405.7994	812	26.0989	3.9616	1649.8591
813	26.1249	3.9578	412.0103	813	26.1249	3.9578	1382.0811	813	26.1249	3.9578	394.6713	813	26.1249	3.9578	1636.7966
814	26.1509	3.9539	387.7746	814	26.1509	3.9539	1356.7374	814	26.1509	3.9539	484.4608	814	26.1509	3.9539	1724.6517
815	26.1769	3.95	362.2173	815	26.1769	3.95	1330.0721	815	26.1769	3.95	402.2645	815	26.1769	3.95	1640.5211
816	26.2029	3.9462	420.6197	816	26.2029	3.9462	1387.3666	816	26.2029	3.9462	457.871	816	26.2029	3.9462	1694.1932
817	26.2289	3.9423	360.5089	817	26.2289	3.9423	1326.1477	817	26.2289	3.9423	429.4757	817	26.2289	3.9423	1663.8636
818	26.2549	3.9385	382.1673	818	26.2549	3.9385	1346.6981	818	26.2549	3.9385	450.7771	818	26.2549	3.9385	1683.2307
819	26.2809	3.9347	341.5154	819	26.2809	3.9347	1304.9382	819	26.2809	3.9347	389.2135	819	26.2809	3.9347	1619.7326
820	26.3069	3.9309	375.1254	820	26.3069	3.9309	1337.4403	820	26.3069	3.9309	438.3283	820	26.3069	3.9309	1666.9131
821	26.3329	3.927	424.1155	821	26.3329	3.927	1385.3223	821	26.3329	3.927	513.1285	821	26.3329	3.927	1739.779
822	26.3589	3.9232	395.1879	822	26.3589	3.9232	1355.2867	822	26.3589	3.9232	509.0617	822	26.3589	3.9232	1733.7778
823	26.3849	3.9194	359.6297	823	26.3849	3.9194	1318.6205	823	26.3849	3.9194	433.9572	823	26.3849	3.9194	1656.739

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
824	26.4109	3.9156	405.1544	824	26.4109	3.9156	1363.0372	824	26.4109	3.9156	443.0014	824	26.4109	3.9156	1663.8488
825	26.4369	3.9119	385.736	825	26.4369	3.9119	1342.5109	825	26.4369	3.9119	433.4303	825	26.4369	3.9119	1652.3434
826	26.4629	3.9081	330.6725	826	26.4629	3.9081	1286.3394	826	26.4629	3.9081	536.2272	826	26.4629	3.9081	1753.2059
827	26.4889	3.9043	433.0273	827	26.4889	3.9043	1387.5861	827	26.4889	3.9043	514.5086	827	26.4889	3.9043	1729.553
828	26.5149	3.9006	400.3908	828	26.5149	3.9006	1353.8417	828	26.5149	3.9006	565.254	828	26.5149	3.9006	1778.3641
829	26.5409	3.8968	371.539	829	26.5409	3.8968	1323.8818	829	26.5409	3.8968	633.0222	829	26.5409	3.8968	1844.1979
830	26.5669	3.8931	393.5466	830	26.5669	3.8931	1344.7814	830	26.5669	3.8931	594.5493	830	26.5669	3.8931	1803.7906
831	26.5929	3.8893	369.7643	831	26.5929	3.8893	1319.8911	831	26.5929	3.8893	627.3273	831	26.5929	3.8893	1834.6343
832	26.6189	3.8856	419.0834	832	26.6189	3.8856	1368.1023	832	26.6189	3.8856	799.0698	832	26.6189	3.8856	2004.4424
833	26.6449	3.8819	477.8111	833	26.6449	3.8819	1425.7219	833	26.6449	3.8819	876.8799	833	26.6449	3.8819	2080.3182
834	26.6709	3.8782	461.3385	834	26.6709	3.8782	1408.1413	834	26.6709	3.8782	1011.6655	834	26.6709	3.8782	2213.1694
835	26.6969	3.8744	462.9021	835	26.6969	3.8744	1408.5969	835	26.6969	3.8744	1140.3337	835	26.6969	3.8744	2339.9033
836	26.7229	3.8707	509.1616	836	26.7229	3.8707	1453.7485	836	26.7229	3.8707	1393.5496	836	26.7229	3.8707	2591.1848
837	26.7489	3.8671	587.853	837	26.7489	3.8671	1531.3318	837	26.7489	3.8671	1784.3185	837	26.7489	3.8671	2980.0194
838	26.7749	3.8634	615.3242	838	26.7749	3.8634	1557.695	838	26.7749	3.8634	2247.2433	838	26.7749	3.8634	3441.0098
839	26.8009	3.8597	552.3192	839	26.8009	3.8597	1492.2286	839	26.8009	3.8597	2717.4885	839	26.8009	3.8597	3909.3207
840	26.8269	3.856	540.7567	840	26.8269	3.856	1478.2047	840	26.8269	3.856	2987.2871	840	26.8269	3.856	4177.185
841	26.8529	3.8524	625.5242	841	26.8529	3.8524	1560.5107	841	26.8529	3.8524	2895.354	841	26.8529	3.8524	4083.3175
842	26.8789	3.8487	566.5168	842	26.8789	3.8487	1499.0419	842	26.8789	3.8487	2547.0337	842	26.8789	3.8487	3733.0629
843	26.9049	3.845	606.0056	843	26.9049	3.845	1536.0693	843	26.9049	3.845	2051.2097	843	26.9049	3.845	3235.3045
844	26.9309	3.8414	598.9311	844	26.9309	3.8414	1526.5333	844	26.9309	3.8414	1605.9076	844	26.9309	3.8414	2788.0681
845	26.9569	3.8378	617.2805	845	26.9569	3.8378	1542.4212	845	26.9569	3.8378	1176.8815	845	26.9569	3.8378	2357.1076
846	26.9829	3.8341	688.1074	846	26.9829	3.8341	1610.7868	846	26.9829	3.8341	944.9106	846	26.9829	3.8341	2123.2024
847	27.0089	3.8305	685.1008	847	27.0089	3.8305	1605.3187	847	27.0089	3.8305	802.2438	847	27.0089	3.8305	1978.6012
848	27.0349	3.8269	622.3656	848	27.0349	3.8269	1540.122	848	27.0349	3.8269	755.8348	848	27.0349	3.8269	1930.2578
849	27.0609	3.8233	562.6525	849	27.0609	3.8233	1477.9475	849	27.0609	3.8233	714.0935	849	27.0609	3.8233	1886.5822
850	27.0869	3.8197	571.9651	850	27.0869	3.8197	1484.7987	850	27.0869	3.8197	670.2619	850	27.0869	3.8197	1840.8162
851	27.1129	3.8161	569.0235	851	27.1129	3.8161	1479.3956	851	27.1129	3.8161	631.0206	851	27.1129	3.8161	1799.6406
852	27.1389	3.8125	483.7977	852	27.1389	3.8125	1391.7084	852	27.1389	3.8125	573.7273	852	27.1389	3.8125	1740.4129
853	27.1649	3.8089	455.4914	853	27.1649	3.8089	1360.9407	853	27.1649	3.8089	539.2322	853	27.1649	3.8089	1703.9835
854	27.1909	3.8053	460.3874	854	27.1909	3.8053	1363.3752	854	27.1909	3.8053	496.8608	854	27.1909	3.8053	1659.6778
855	27.2169	3.8018	453.2109	855	27.2169	3.8018	1353.7373	855	27.2169	3.8018	477.0128	855	27.2169	3.8018	1637.8954
856	27.2429	3.7982	429.4651	856	27.2429	3.7982	1327.53	856	27.2429	3.7982	488.1175	856	27.2429	3.7982	1647.0658
857	27.2689	3.7947	423.6572	857	27.2689	3.7947	1319.2607	857	27.2689	3.7947	514.2729	857	27.2689	3.7947	1671.2868
858	27.2949	3.7911	434.4363	858	27.2949	3.7911	1327.5783	858	27.2949	3.7911	477.3358	858	27.2949	3.7911	1632.4154
859	27.3209	3.7876	425.3194	859	27.3209	3.7876	1316	859	27.3209	3.7876	430.5083	859	27.3209	3.7876	1583.6535

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
860	27.3469	3.7841	401.5596	860	27.3469	3.7841	1289.7787	860	27.3469	3.7841	421.9516	860	27.3469	3.7841	1573.1625
861	27.3729	3.7805	393.4486	861	27.3729	3.7805	1279.2063	861	27.3729	3.7805	439.2712	861	27.3729	3.7805	1588.5477
862	27.3989	3.777	413.0485	862	27.3989	3.777	1296.3448	862	27.3989	3.777	437.0275	862	27.3989	3.777	1584.3696
863	27.4249	3.7735	399.5436	863	27.4249	3.7735	1280.3784	863	27.4249	3.7735	365.9706	863	27.4249	3.7735	1511.3784
864	27.4509	3.77	389.8119	864	27.4509	3.77	1268.1853	864	27.4509	3.77	390.6768	864	27.4509	3.77	1534.1502
865	27.4769	3.7665	397.6509	865	27.4769	3.7665	1273.5628	865	27.4769	3.7665	438.7523	865	27.4769	3.7665	1580.2914
866	27.5029	3.763	389.9118	866	27.5029	3.763	1264.9007	866	27.5029	3.763	418.786	866	27.5029	3.763	1558.3908
867	27.5289	3.7595	389.8187	867	27.5289	3.7595	1263.8845	867	27.5289	3.7595	391.2931	867	27.5289	3.7595	1528.9635
868	27.5549	3.756	415.4467	868	27.5549	3.756	1288.5895	868	27.5549	3.756	386.2902	868	27.5549	3.756	1522.0263
869	27.5809	3.7526	412.5811	869	27.5809	3.7526	1284.8008	869	27.5809	3.7526	384.9104	869	27.5809	3.7526	1518.7122
870	27.6069	3.7491	395.0202	870	27.6069	3.7491	1266.3169	870	27.6069	3.7491	346.5844	870	27.6069	3.7491	1478.4517
871	27.6329	3.7456	407.7264	871	27.6329	3.7456	1278.1	871	27.6329	3.7456	294.5501	871	27.6329	3.7456	1424.4831
872	27.6589	3.7422	419.2118	872	27.6589	3.7422	1288.6624	872	27.6589	3.7422	351.1047	872	27.6589	3.7422	1479.1033
873	27.6849	3.7387	376.9038	873	27.6849	3.7387	1245.4313	873	27.6849	3.7387	377.7208	873	27.6849	3.7387	1503.7851
874	27.7109	3.7353	397.1928	874	27.7109	3.7353	1264.7973	874	27.7109	3.7353	401.1539	874	27.7109	3.7353	1525.2839
875	27.7369	3.7319	371.5977	875	27.7369	3.7319	1238.2792	875	27.7369	3.7319	443.6332	875	27.7369	3.7319	1565.8288
876	27.7629	3.7284	373.1997	876	27.7629	3.7284	1238.9581	876	27.7629	3.7284	372.9482	876	27.7629	3.7284	1493.2094
877	27.7889	3.725	369.7907	877	27.7889	3.725	1234.626	877	27.7889	3.725	422.4211	877	27.7889	3.725	1540.748
878	27.8149	3.7216	399.9267	878	27.8149	3.7216	1263.8389	878	27.8149	3.7216	396.0427	878	27.8149	3.7216	1512.4352
879	27.8409	3.7182	423.1461	879	27.8409	3.7182	1286.1353	879	27.8409	3.7182	432.0533	879	27.8409	3.7182	1546.5115
880	27.8669	3.7148	429.1698	880	27.8669	3.7148	1291.2359	880	27.8669	3.7148	450.7968	880	27.8669	3.7148	1563.3207
881	27.8929	3.7114	428.9966	881	27.8929	3.7114	1290.1397	881	27.8929	3.7114	432.1899	881	27.8929	3.7114	1542.7794
882	27.9189	3.708	389.2199	882	27.9189	3.708	1249.4399	882	27.9189	3.708	432.8402	882	27.9189	3.708	1541.4953
883	27.9449	3.7046	407.8258	883	27.9449	3.7046	1267.1228	883	27.9449	3.7046	452.7997	883	27.9449	3.7046	1559.5205
884	27.9709	3.7013	371.3965	884	27.9709	3.7013	1229.7705	884	27.9709	3.7013	410.8073	884	27.9709	3.7013	1515.5938
885	27.9969	3.6979	450.4326	885	27.9969	3.6979	1307.8835	885	27.9969	3.6979	340.4519	885	27.9969	3.6979	1443.304
886	28.0229	3.6945	447.7544	886	28.0229	3.6945	1304.2822	886	28.0229	3.6945	453.7068	886	28.0229	3.6945	1554.6246
887	28.0489	3.6912	478.9209	887	28.0489	3.6912	1334.5257	887	28.0489	3.6912	456.9333	887	28.0489	3.6912	1555.9168
888	28.0749	3.6878	452.9311	888	28.0749	3.6878	1307.6129	888	28.0749	3.6878	519.3703	888	28.0749	3.6878	1616.4193
889	28.1009	3.6845	435.9251	889	28.1009	3.6845	1289.6838	889	28.1009	3.6845	504.2392	889	28.1009	3.6845	1599.3539
890	28.1269	3.6811	414.0582	890	28.1269	3.6811	1266.8939	890	28.1269	3.6811	496.2523	890	28.1269	3.6811	1589.4327
891	28.1529	3.6778	470.535	891	28.1529	3.6778	1322.4476	891	28.1529	3.6778	497.4801	891	28.1529	3.6778	1588.7261
892	28.1789	3.6745	460.0615	892	28.1789	3.6745	1311.051	892	28.1789	3.6745	454.9303	892	28.1789	3.6745	1544.2419
893	28.2049	3.6712	487.8568	893	28.2049	3.6712	1337.9233	893	28.2049	3.6712	415.8487	893	28.2049	3.6712	1503.226
894	28.2309	3.6679	452.19	894	28.2309	3.6679	1301.3334	894	28.2309	3.6679	437.242	894	28.2309	3.6679	1522.6849
895	28.2569	3.6645	409.9227	895	28.2569	3.6645	1258.1431	895	28.2569	3.6645	388.8268	895	28.2569	3.6645	1472.3355

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
896	28.2829	3.6612	431.0516	896	28.2829	3.6612	1278.3489	896	28.2829	3.6612	475.8829	896	28.2829	3.6612	1557.4572
897	28.3089	3.658	383.2995	897	28.3089	3.658	1229.6738	897	28.3089	3.658	447.32	897	28.3089	3.658	1526.9599
898	28.3349	3.6547	445.8508	898	28.3349	3.6547	1291.3021	898	28.3349	3.6547	466.4149	898	28.3349	3.6547	1544.1205
899	28.3609	3.6514	437.9579	899	28.3609	3.6514	1282.4861	899	28.3609	3.6514	408.4733	899	28.3609	3.6514	1484.2445
900	28.3869	3.6481	413.2351	900	28.3869	3.6481	1256.8403	900	28.3869	3.6481	430.5278	900	28.3869	3.6481	1504.3647
901	28.4129	3.6448	415.1154	901	28.4129	3.6448	1257.7975	901	28.4129	3.6448	394.8241	901	28.4129	3.6448	1466.7266
902	28.4389	3.6416	449.8802	902	28.4389	3.6416	1291.6392	902	28.4389	3.6416	307.4736	902	28.4389	3.6416	1377.4418
903	28.4649	3.6383	397.4627	903	28.4649	3.6383	1238.2987	903	28.4649	3.6383	422.7102	903	28.4649	3.6383	1490.744
904	28.4909	3.6351	385.8905	904	28.4909	3.6351	1225.8034	904	28.4909	3.6351	366.0338	904	28.4909	3.6351	1432.1332
905	28.5169	3.6318	406.2824	905	28.5169	3.6318	1245.2722	905	28.5169	3.6318	441.6552	905	28.5169	3.6318	1505.8203
906	28.5429	3.6286	415.3844	906	28.5429	3.6286	1253.4512	906	28.5429	3.6286	406.5822	906	28.5429	3.6286	1468.813
907	28.5689	3.6253	389.6378	907	28.5689	3.6253	1226.7815	907	28.5689	3.6253	447.4331	907	28.5689	3.6253	1507.7295
908	28.5949	3.6221	369.7567	908	28.5949	3.6221	1205.9774	908	28.5949	3.6221	423.6245	908	28.5949	3.6221	1481.9865
909	28.6209	3.6189	324.1461	909	28.6209	3.6189	1159.4438	909	28.6209	3.6189	397.8367	909	28.6209	3.6189	1454.2644
910	28.6469	3.6157	395.2312	910	28.6469	3.6157	1229.6058	910	28.6469	3.6157	358.3199	910	28.6469	3.6157	1412.8133
911	28.6729	3.6125	449.967	911	28.6729	3.6125	1283.4185	911	28.6729	3.6125	413.801	911	28.6729	3.6125	1466.36
912	28.6989	3.6093	379.4513	912	28.6989	3.6093	1211.9798	912	28.6989	3.6093	308.8059	912	28.6989	3.6093	1359.4306
913	28.7249	3.6061	352.6719	913	28.7249	3.6061	1184.2774	913	28.7249	3.6061	394.7405	913	28.7249	3.6061	1443.4308
914	28.7509	3.6029	412.5382	914	28.7509	3.6029	1243.2206	914	28.7509	3.6029	472.756	914	28.7509	3.6029	1519.512
915	28.7769	3.5997	358.5861	915	28.7769	3.5997	1188.3455	915	28.7769	3.5997	432.6272	915	28.7769	3.5997	1477.4488
916	28.8029	3.5965	309.1086	916	28.8029	3.5965	1137.9449	916	28.8029	3.5965	401.6375	916	28.8029	3.5965	1444.5247
917	28.8289	3.5933	386.2706	917	28.8289	3.5933	1214.1838	917	28.8289	3.5933	464.8297	917	28.8289	3.5933	1505.7826
918	28.8549	3.5902	379.6884	918	28.8549	3.5902	1206.6786	918	28.8549	3.5902	361.2255	918	28.8549	3.5902	1400.244
919	28.8809	3.587	397.6509	919	28.8809	3.587	1223.718	919	28.8809	3.587	427.5706	919	28.8809	3.587	1464.6548
920	28.9069	3.5838	318.8542	920	28.9069	3.5838	1143.1472	920	28.9069	3.5838	437.9687	920	28.9069	3.5838	1473.1186
921	28.9329	3.5807	409.7027	921	28.9329	3.5807	1232.2214	921	28.9329	3.5807	509.5038	921	28.9329	3.5807	1542.7193
922	28.9589	3.5775	380.5924	922	28.9589	3.5775	1201.3369	922	28.9589	3.5775	423.5	922	28.9589	3.5775	1454.7812
923	28.9849	3.5744	374.1781	923	28.9849	3.5744	1193.1484	923	28.9849	3.5744	360.2577	923	28.9849	3.5744	1389.6045
924	29.0109	3.5713	360.653	924	29.0109	3.5713	1177.849	924	29.0109	3.5713	431.0261	924	29.0109	3.5713	1458.4386
925	29.0369	3.5681	401.1683	925	29.0369	3.5681	1216.5901	925	29.0369	3.5681	435.0449	925	29.0369	3.5681	1460.523
926	29.0629	3.565	376.0116	926	29.0629	3.565	1189.6592	926	29.0629	3.565	395.8279	926	29.0629	3.565	1419.3717
927	29.0889	3.5619	342.5201	927	29.0889	3.5619	1154.3935	927	29.0889	3.5619	429.9884	927	29.0889	3.5619	1451.5979
928	29.1149	3.5588	418.9064	928	29.1149	3.5588	1229.0055	928	29.1149	3.5588	410.8476	928	29.1149	3.5588	1430.5227
929	29.1409	3.5557	393.1484	929	29.1409	3.5557	1201.4732	929	29.1409	3.5557	424.27	929	29.1409	3.5557	1442.0107
930	29.1669	3.5526	414.5191	930	29.1669	3.5526	1221.0698	930	29.1669	3.5526	464.8278	930	29.1669	3.5526	1480.6342
931	29.1929	3.5495	334.8682	931	29.1929	3.5495	1139.6447	931	29.1929	3.5495	387.3172	931	29.1929	3.5495	1401.1892

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
932	29.2189	3.5464	304.6614	932	29.2189	3.5464	1107.6636	932	29.2189	3.5464	440.8216	932	29.2189	3.5464	1452.7593
933	29.2449	3.5433	346.1553	933	29.2449	3.5433	1147.3833	933	29.2449	3.5433	454.9579	933	29.2449	3.5433	1464.9612
934	29.2709	3.5402	368.9713	934	29.2709	3.5402	1168.425	934	29.2709	3.5402	403.1835	934	29.2709	3.5402	1411.2524
935	29.2969	3.5372	376.2508	935	29.2969	3.5372	1173.9303	935	29.2969	3.5372	477.9726	935	29.2969	3.5372	1484.1072
936	29.3229	3.5341	351.6338	936	29.3229	3.5341	1147.5391	936	29.3229	3.5341	452.0966	936	29.3229	3.5341	1456.2969
937	29.3489	3.531	388.4839	937	29.3489	3.531	1182.615	937	29.3489	3.531	438.5742	937	29.3489	3.531	1440.8401
938	29.3749	3.528	359.4463	938	29.3749	3.528	1151.8032	938	29.3749	3.528	436.6403	938	29.3749	3.528	1436.9719
939	29.4009	3.5249	397.9272	939	29.4009	3.5249	1188.5098	939	29.4009	3.5249	427.981	939	29.4009	3.5249	1426.3782
940	29.4269	3.5219	386.9455	940	29.4269	3.5219	1175.7538	940	29.4269	3.5219	405.3651	940	29.4269	3.5219	1401.828
941	29.4529	3.5188	387.792	941	29.4529	3.5188	1174.8261	941	29.4529	3.5188	487.6595	941	29.4529	3.5188	1482.188
942	29.4789	3.5158	384.4776	942	29.4789	3.5158	1169.7375	942	29.4789	3.5158	488.3135	942	29.4789	3.5158	1480.9077
943	29.5049	3.5128	365.7971	943	29.5049	3.5128	1149.2828	943	29.5049	3.5128	436.6398	943	29.5049	3.5128	1427.2996
944	29.5309	3.5097	367.3646	944	29.5309	3.5097	1149.0761	944	29.5309	3.5097	467.304	944	29.5309	3.5097	1456.0295
945	29.5569	3.5067	428.1647	945	29.5569	3.5067	1208.102	945	29.5569	3.5067	452.4074	945	29.5569	3.5067	1439.1985
946	29.5829	3.5037	439.3934	946	29.5829	3.5037	1217.5564	946	29.5829	3.5037	451.9634	946	29.5829	3.5037	1436.8202
947	29.6089	3.5007	430.0653	947	29.6089	3.5007	1206.454	947	29.6089	3.5007	430.2669	947	29.6089	3.5007	1413.1893
948	29.6349	3.4977	408.0347	948	29.6349	3.4977	1182.6493	948	29.6349	3.4977	397.5437	948	29.6349	3.4977	1378.5318
949	29.6609	3.4947	447.777	949	29.6609	3.4947	1220.6173	949	29.6609	3.4947	428.7536	949	29.6609	3.4947	1407.8073
950	29.6869	3.4917	440.8181	950	29.6869	3.4917	1211.8842	950	29.6869	3.4917	435.4496	950	29.6869	3.4917	1412.5689
951	29.7129	3.4887	417.7416	951	29.7129	3.4887	1187.0335	951	29.7129	3.4887	436.5867	951	29.7129	3.4887	1411.7717
952	29.7389	3.4857	415.8961	952	29.7389	3.4857	1183.4137	952	29.7389	3.4857	470.7414	952	29.7389	3.4857	1443.9921
953	29.7649	3.4828	410.2566	953	29.7649	3.4828	1176	953	29.7649	3.4828	460.8768	953	29.7649	3.4828	1432.1932
954	29.7909	3.4798	415.2951	954	29.7909	3.4798	1179.2643	954	29.7909	3.4798	421.1202	954	29.7909	3.4798	1390.5021
955	29.8169	3.4768	409.6565	955	29.8169	3.4768	1171.8515	955	29.8169	3.4768	425.1788	955	29.8169	3.4768	1392.6264
956	29.8429	3.4739	407.2972	956	29.8429	3.4739	1167.7179	956	29.8429	3.4739	436.7204	956	29.8429	3.4739	1402.2337
957	29.8689	3.4709	415.9249	957	29.8689	3.4709	1174.5714	957	29.8689	3.4709	448.3354	957	29.8689	3.4709	1411.9144
958	29.8949	3.468	421.6408	958	29.8949	3.468	1178.5131	958	29.8949	3.468	451.2419	958	29.8949	3.468	1412.8865
959	29.9209	3.465	422.9242	959	29.9209	3.465	1178.0222	959	29.9209	3.465	419.5231	959	29.9209	3.465	1379.2334
960	29.9469	3.4621	405.2334	960	29.9469	3.4621	1158.5572	960	29.9469	3.4621	393.4408	960	29.9469	3.4621	1351.2167
961	29.9729	3.4592	436.8595	961	29.9729	3.4592	1188.4091	961	29.9729	3.4592	420.4312	961	29.9729	3.4592	1376.2727
962	29.9989	3.4562	456.9092	962	29.9989	3.4562	1206.6846	962	29.9989	3.4562	444.1525	962	29.9989	3.4562	1398.0597
963	30.0249	3.4533	435.7343	963	30.0249	3.4533	1183.7354	963	30.0249	3.4533	444.1246	963	30.0249	3.4533	1396.0974
964	30.0509	3.4504	461.8869	964	30.0509	3.4504	1208.1138	964	30.0509	3.4504	450.9511	964	30.0509	3.4504	1400.9895
965	30.0769	3.4475	418.8374	965	30.0769	3.4475	1163.2901	965	30.0769	3.4475	445.2893	965	30.0769	3.4475	1393.3935
966	30.1029	3.4446	361.1464	966	30.1029	3.4446	1103.8249	966	30.1029	3.4446	467.4549	966	30.1029	3.4446	1413.6247
967	30.1289	3.4417	409.6023	967	30.1289	3.4417	1150.5065	967	30.1289	3.4417	465.0866	967	30.1289	3.4417	1409.3221

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
968	30.1549	3.4388	439.4843	968	30.1549	3.4388	1178.6143	968	30.1549	3.4388	461.7664	968	30.1549	3.4388	1404.0674
969	30.1809	3.4359	382.021	969	30.1809	3.4359	1119.3768	969	30.1809	3.4359	487.5193	969	30.1809	3.4359	1427.886
970	30.2069	3.433	388.3893	970	30.2069	3.433	1123.9709	970	30.2069	3.433	495.5208	970	30.2069	3.433	1433.9531
971	30.2329	3.4301	430.1897	971	30.2329	3.4301	1163.997	971	30.2329	3.4301	478.7061	971	30.2329	3.4301	1415.2041
972	30.2589	3.4272	408.3287	972	30.2589	3.4272	1140.3618	972	30.2589	3.4272	396.7618	972	30.2589	3.4272	1331.3255
973	30.2849	3.4243	397.6509	973	30.2849	3.4243	1127.9098	973	30.2849	3.4243	402.0807	973	30.2849	3.4243	1334.71
974	30.3109	3.4215	454.6658	974	30.3109	3.4215	1184.0453	974	30.3109	3.4215	432.7101	974	30.3109	3.4215	1364.3088
975	30.3369	3.4186	472.3516	975	30.3369	3.4186	1200.8517	975	30.3369	3.4186	447.2022	975	30.3369	3.4186	1377.7702
976	30.3629	3.4157	409.553	976	30.3629	3.4157	1137.1738	976	30.3629	3.4157	468.3412	976	30.3629	3.4157	1397.8786
977	30.3889	3.4129	391.4736	977	30.3889	3.4129	1118.2149	977	30.3889	3.4129	435.3329	977	30.3889	3.4129	1363.8396
978	30.4149	3.41	443.6315	978	30.4149	3.41	1169.4934	978	30.4149	3.41	410.866	978	30.4149	3.41	1338.3421
979	30.4409	3.4072	447.4093	979	30.4409	3.4072	1172.3919	979	30.4409	3.4072	430.9226	979	30.4409	3.4072	1357.368
980	30.4669	3.4044	481.4639	980	30.4669	3.4044	1205.5671	980	30.4669	3.4044	427.0005	980	30.4669	3.4044	1352.4152
981	30.4929	3.4015	468.2531	981	30.4929	3.4015	1191.4769	981	30.4929	3.4015	413.4905	981	30.4929	3.4015	1337.8746
982	30.5189	3.3987	450.3959	982	30.5189	3.3987	1172.7403	982	30.5189	3.3987	453.6335	982	30.5189	3.3987	1376.9869
983	30.5449	3.3959	436.9719	983	30.5449	3.3959	1158.4369	983	30.5449	3.3959	469.5006	983	30.5449	3.3959	1391.8234
984	30.5709	3.3931	437.3131	984	30.5709	3.3931	1157.8988	984	30.5709	3.3931	436.1566	984	30.5709	3.3931	1357.4487
985	30.5969	3.3902	449.1257	985	30.5969	3.3902	1168.832	985	30.5969	3.3902	416.0744	985	30.5969	3.3902	1336.3359
986	30.6229	3.3874	417.3996	986	30.6229	3.3874	1136.2265	986	30.6229	3.3874	466.2316	986	30.6229	3.3874	1385.4624
987	30.6489	3.3846	421.6519	987	30.6489	3.3846	1139.5994	987	30.6489	3.3846	402.3517	987	30.6489	3.3846	1320.5518
988	30.6749	3.3818	432.5519	988	30.6749	3.3818	1149.6201	988	30.6749	3.3818	386.6792	988	30.6749	3.3818	1303.8487
989	30.7009	3.379	446.2403	989	30.7009	3.379	1162.4291	989	30.7009	3.379	450.8967	989	30.7009	3.379	1367.0355
990	30.7269	3.3762	480.9085	990	30.7269	3.3762	1196.2179	990	30.7269	3.3762	502.795	990	30.7269	3.3762	1417.9032
991	30.7529	3.3735	437.3774	991	30.7529	3.3735	1151.8074	991	30.7529	3.3735	542.1453	991	30.7529	3.3735	1456.2229
992	30.7789	3.3707	411.4535	992	30.7789	3.3707	1125.0041	992	30.7789	3.3707	512.7697	992	30.7789	3.3707	1425.8166
993	30.8049	3.3679	430.3401	993	30.8049	3.3679	1143.0114	993	30.8049	3.3679	466.3862	993	30.8049	3.3679	1378.4024
994	30.8309	3.3651	461.1106	994	30.8309	3.3651	1172.9024	994	30.8309	3.3651	444.3761	994	30.8309	3.3651	1355.3617
995	30.8569	3.3624	394.0475	995	30.8569	3.3624	1104.96	995	30.8569	3.3624	520.7506	995	30.8569	3.3624	1430.7055
996	30.8829	3.3596	437.3278	996	30.8829	3.3596	1147.3609	996	30.8829	3.3596	556.6617	996	30.8829	3.3596	1465.586
997	30.9089	3.3568	389.9552	997	30.9089	3.3568	1099.1089	997	30.9089	3.3568	643.5632	997	30.9089	3.3568	1551.4568
998	30.9349	3.3541	424.52	998	30.9349	3.3541	1132.7943	998	30.9349	3.3541	689.6979	998	30.9349	3.3541	1596.5608
999	30.9609	3.3513	447.4344	999	30.9609	3.3513	1154.8294	999	30.9609	3.3513	664.9967	999	30.9609	3.3513	1570.829
1000	30.9869	3.3486	433.1906	1000	30.9869	3.3486	1139.7061	1000	30.9869	3.3486	690.4457	1000	30.9869	3.3486	1595.2474
1001	31.0129	3.3459	391.2288	1001	31.0129	3.3459	1096.865	1001	31.0129	3.3459	666.7793	1001	31.0129	3.3459	1570.5503
1002	31.0389	3.3431	410.2439	1002	31.0389	3.3431	1115.0007	1002	31.0389	3.3431	586.5147	1002	31.0389	3.3431	1489.255
1003	31.0649	3.3404	359.305	1003	31.0649	3.3404	1063.1825	1003	31.0649	3.3404	517.6034	1003	31.0649	3.3404	1419.3131

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1004	31.0909	3.3377	410.324	1004	31.0909	3.3377	1113.3221	1004	31.0909	3.3377	443.8551	1004	31.0909	3.3377	1344.5341
1005	31.1169	3.3349	375.8283	1005	31.1169	3.3349	1077.947	1005	31.1169	3.3349	475.2756	1005	31.1169	3.3349	1374.924
1006	31.1429	3.3322	326.5027	1006	31.1429	3.3322	1027.742	1006	31.1429	3.3322	473.8203	1006	31.1429	3.3322	1372.4381
1007	31.1689	3.3295	388.258	1007	31.1689	3.3295	1088.6179	1007	31.1689	3.3295	454.9041	1007	31.1689	3.3295	1352.4911
1008	31.1949	3.3268	422.5195	1008	31.1949	3.3268	1122	1008	31.1949	3.3268	428.5261	1008	31.1949	3.3268	1325.0825
1009	31.2209	3.3241	423.3989	1009	31.2209	3.3241	1122	1009	31.2209	3.3241	439.4575	1009	31.2209	3.3241	1334.9833
1010	31.2469	3.3214	450.9652	1010	31.2469	3.3214	1148.687	1010	31.2469	3.3214	495.8557	1010	31.2469	3.3214	1390.3508
1011	31.2729	3.3187	406.1689	1011	31.2729	3.3187	1103.0112	1011	31.2729	3.3187	406.5365	1011	31.2729	3.3187	1300.0009
1012	31.2989	3.316	443.8109	1012	31.2989	3.316	1139.7739	1012	31.2989	3.316	439.4659	1012	31.2989	3.316	1331.8997
1013	31.3249	3.3134	445.9164	1013	31.3249	3.3134	1141	1013	31.3249	3.3134	413.7963	1013	31.3249	3.3134	1305.1994
1014	31.3509	3.3107	424.0265	1014	31.3509	3.3107	1118.2308	1014	31.3509	3.3107	402.2429	1014	31.3509	3.3107	1292.6154
1015	31.3769	3.308	427.4303	1015	31.3769	3.308	1120.7552	1015	31.3769	3.308	448.6591	1015	31.3769	3.308	1338.001
1016	31.4029	3.3053	339.3827	1016	31.4029	3.3053	1031.8282	1016	31.4029	3.3053	393.2409	1016	31.4029	3.3053	1281.5521
1017	31.4289	3.3027	415.2205	1017	31.4289	3.3027	1106.7866	1017	31.4289	3.3027	408.0985	1017	31.4289	3.3027	1295.379
1018	31.4549	3.3	405.1327	1018	31.4549	3.3	1095.8194	1018	31.4549	3.3	457.1106	1018	31.4549	3.3	1343.3605
1019	31.4809	3.2973	501.2961	1019	31.4809	3.2973	1191.1035	1019	31.4809	3.2973	391.7514	1019	31.4809	3.2973	1276.9706
1020	31.5069	3.2947	489.0641	1020	31.5069	3.2947	1177.992	1020	31.5069	3.2947	450.611	1020	31.5069	3.2947	1334.7996
1021	31.5329	3.292	396.3875	1021	31.5329	3.292	1084.4361	1021	31.5329	3.292	488.8577	1021	31.5329	3.292	1372.0156
1022	31.5589	3.2894	383.0921	1022	31.5589	3.2894	1070.2613	1022	31.5589	3.2894	419.9789	1022	31.5589	3.2894	1302.1062
1023	31.5849	3.2868	453.323	1023	31.5849	3.2868	1139.6128	1023	31.5849	3.2868	432.2482	1023	31.5849	3.2868	1313.3448
1024	31.6109	3.2841	415.4694	1024	31.6109	3.2841	1100.8798	1024	31.6109	3.2841	448.827	1024	31.6109	3.2841	1328.8929
1025	31.6369	3.2815	415.8647	1025	31.6369	3.2815	1100.3957	1025	31.6369	3.2815	466.2374	1025	31.6369	3.2815	1345.2727
1026	31.6629	3.2789	345.3391	1026	31.6629	3.2789	1028.9908	1026	31.6629	3.2789	428.5128	1026	31.6629	3.2789	1306.5175
1027	31.6889	3.2763	436.9726	1027	31.6889	3.2763	1119.7449	1027	31.6889	3.2763	443.9784	1027	31.6889	3.2763	1320.9524
1028	31.7149	3.2736	440.5587	1028	31.7149	3.2736	1121.1353	1028	31.7149	3.2736	413.6154	1028	31.7149	3.2736	1289.5588
1029	31.7409	3.271	408.0234	1029	31.7409	3.271	1086.4043	1029	31.7409	3.271	459.6795	1029	31.7409	3.271	1334.5922
1030	31.7669	3.2684	400.4448	1030	31.7669	3.2684	1076.6301	1030	31.7669	3.2684	459.1087	1030	31.7669	3.2684	1332.9907
1031	31.7929	3.2658	386.4096	1031	31.7929	3.2658	1060.3992	1031	31.7929	3.2658	429.6273	1031	31.7929	3.2658	1302.4787
1032	31.8189	3.2632	433.4935	1032	31.8189	3.2632	1105.2874	1032	31.8189	3.2632	428.5701	1032	31.8189	3.2632	1300.3908
1033	31.8449	3.2606	447.361	1033	31.8449	3.2606	1116.9592	1033	31.8449	3.2606	421.3274	1033	31.8449	3.2606	1292.1175
1034	31.8709	3.258	441.0947	1034	31.8709	3.258	1108.4973	1034	31.8709	3.258	420.7411	1034	31.8709	3.258	1290.5005
1035	31.8969	3.2554	416.3615	1035	31.8969	3.2554	1081.5685	1035	31.8969	3.2554	462.9905	1035	31.8969	3.2554	1331.7192
1036	31.9229	3.2529	401.954	1036	31.9229	3.2529	1064.9653	1036	31.9229	3.2529	455.6587	1036	31.9229	3.2529	1323.3568
1037	31.9489	3.2503	453.7813	1037	31.9489	3.2503	1114.5969	1037	31.9489	3.2503	428.8789	1037	31.9489	3.2503	1295.5464
1038	31.9749	3.2477	461.4578	1038	31.9749	3.2477	1120.0778	1038	31.9749	3.2477	401.0457	1038	31.9749	3.2477	1266.6825
1039	32.0009	3.2451	427.4473	1039	32.0009	3.2451	1083.8716	1039	32.0009	3.2451	394.0945	1039	32.0009	3.2451	1258.7007

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1040	32.0269	3.2426	428.5139	1040	32.0269	3.2426	1082.7425	1040	32.0269	3.2426	430.6522	1040	32.0269	3.2426	1294.2276
1041	32.0529	3.24	431.2014	1041	32.0529	3.24	1083.2343	1041	32.0529	3.24	418.8609	1041	32.0529	3.24	1281.4057
1042	32.0789	3.2374	426.4665	1042	32.0789	3.2374	1076.3037	1042	32.0789	3.2374	378.3083	1042	32.0789	3.2374	1239.8225
1043	32.1049	3.2349	427.0194	1043	32.1049	3.2349	1074.661	1043	32.1049	3.2349	421.699	1043	32.1049	3.2349	1282.1825
1044	32.1309	3.2323	398.9548	1044	32.1309	3.2323	1044.4007	1044	32.1309	3.2323	396.859	1044	32.1309	3.2323	1256.3119
1045	32.1569	3.2298	403.3424	1045	32.1569	3.2298	1046.5927	1045	32.1569	3.2298	444.2307	1045	32.1569	3.2298	1302.6529
1046	32.1829	3.2273	402.6901	1046	32.1829	3.2273	1043.7447	1046	32.1829	3.2273	427.0128	1046	32.1829	3.2273	1284.4044
1047	32.2089	3.2247	417.0221	1047	32.2089	3.2247	1055.881	1047	32.2089	3.2247	400.0945	1047	32.2089	3.2247	1256.4554
1048	32.2349	3.2222	431.9481	1048	32.2349	3.2222	1068.6114	1048	32.2349	3.2222	387.9403	1048	32.2349	3.2222	1243.2706
1049	32.2609	3.2197	404.4605	1049	32.2609	3.2197	1038.9281	1049	32.2609	3.2197	427.6197	1049	32.2609	3.2197	1281.9193
1050	32.2869	3.2171	381.4044	1050	32.2869	3.2171	1013.6764	1050	32.2869	3.2171	434.5214	1050	32.2869	3.2171	1287.7903
1051	32.3129	3.2146	421.2168	1051	32.3129	3.2146	1051.2931	1051	32.3129	3.2146	416.7617	1051	32.3129	3.2146	1269
1052	32.3389	3.2121	447.4027	1052	32.3389	3.2121	1075.2833	1052	32.3389	3.2121	430.9408	1052	32.3389	3.2121	1282.1484
1053	32.3649	3.2096	410.4867	1053	32.3649	3.2096	1036.1716	1053	32.3649	3.2096	445.1935	1053	32.3649	3.2096	1295.3705
1054	32.3909	3.2071	397.6509	1054	32.3909	3.2071	1021.1402	1054	32.3909	3.2071	469.2712	1054	32.3909	3.2071	1318.4176
1055	32.4169	3.2046	411.2868	1055	32.4169	3.2046	1036.9609	1055	32.4169	3.2046	452.2025	1055	32.4169	3.2046	1300.3182
1056	32.4429	3.2021	429.0365	1056	32.4429	3.2021	1056.8955	1056	32.4429	3.2021	430.2988	1056	32.4429	3.2021	1277.3838
1057	32.4689	3.1996	415.4195	1057	32.4689	3.1996	1045.4632	1057	32.4689	3.1996	435.9015	1057	32.4689	3.1996	1281.9559
1058	32.4949	3.1971	466.0555	1058	32.4949	3.1971	1098.2841	1058	32.4949	3.1971	419.0758	1058	32.4949	3.1971	1264.0995
1059	32.5209	3.1946	503.9471	1059	32.5209	3.1946	1138.3605	1059	32.5209	3.1946	453.224	1059	32.5209	3.1946	1297.217
1060	32.5469	3.1921	496.4932	1060	32.5469	3.1921	1133.0915	1060	32.5469	3.1921	477.9307	1060	32.5469	3.1921	1320.8931
1061	32.5729	3.1896	490.3452	1061	32.5729	3.1896	1129.1283	1061	32.5729	3.1896	481.0457	1061	32.5729	3.1896	1322.9775
1062	32.5989	3.1872	423.3781	1062	32.5989	3.1872	1064.346	1062	32.5989	3.1872	508.3193	1062	32.5989	3.1872	1349.2204
1063	32.6249	3.1847	403.4232	1063	32.6249	3.1847	1046.576	1063	32.6249	3.1847	474.1404	1063	32.6249	3.1847	1314.0108
1064	32.6509	3.1822	423.9254	1064	32.6509	3.1822	1069.263	1064	32.6509	3.1822	449.5701	1064	32.6509	3.1822	1288.4099
1065	32.6769	3.1798	441.7421	1065	32.6769	3.1798	1089.2645	1065	32.6769	3.1798	455.2226	1065	32.6769	3.1798	1293.0317
1066	32.7029	3.1773	459.9945	1066	32.7029	3.1773	1109.7017	1066	32.7029	3.1773	424.5836	1066	32.7029	3.1773	1261.3621
1067	32.7289	3.1749	451.0339	1067	32.7289	3.1749	1102.926	1067	32.7289	3.1749	431.9247	1067	32.7289	3.1749	1267.6726
1068	32.7549	3.1724	412.1933	1068	32.7549	3.1724	1066.2702	1068	32.7549	3.1724	488.5411	1068	32.7549	3.1724	1323.2583
1069	32.7809	3.17	361.2904	1069	32.7809	3.17	1017.5521	1069	32.7809	3.17	475.925	1069	32.7809	3.17	1309.6115
1070	32.8069	3.1675	386.895	1070	32.8069	3.1675	1045.3416	1070	32.8069	3.1675	424.0144	1070	32.8069	3.1675	1256.6703
1071	32.8329	3.1651	455.7788	1071	32.8329	3.1651	1116.4101	1071	32.8329	3.1651	426.2794	1071	32.8329	3.1651	1257.9046
1072	32.8589	3.1626	456.1493	1072	32.8589	3.1626	1118.9655	1072	32.8589	3.1626	444.2655	1072	32.8589	3.1626	1274.8601
1073	32.8849	3.1602	423.4522	1073	32.8849	3.1602	1088.4532	1073	32.8849	3.1602	431.8673	1073	32.8849	3.1602	1261.4312
1074	32.9109	3.1578	428.7615	1074	32.9109	3.1578	1095.9473	1074	32.9109	3.1578	457.6775	1074	32.9109	3.1578	1286.2107
1075	32.9369	3.1554	419.1433	1075	32.9369	3.1554	1088.514	1075	32.9369	3.1554	406.3549	1075	32.9369	3.1554	1233.8575

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1076	32.9629	3.1529	406.1237	1076	32.9629	3.1529	1077.6792	1076	32.9629	3.1529	410.2152	1076	32.9629	3.1529	1236.6871
1077	32.9889	3.1505	432.6387	1077	32.9889	3.1505	1106.3791	1077	32.9889	3.1505	484.7074	1077	32.9889	3.1505	1310.1487
1078	33.0149	3.1481	447.6779	1078	33.0149	3.1481	1123.603	1078	33.0149	3.1481	485.7281	1078	33.0149	3.1481	1310.1387
1079	33.0409	3.1457	522.3601	1079	33.0409	3.1457	1200.4701	1079	33.0409	3.1457	473.5047	1079	33.0409	3.1457	1296.8847
1080	33.0669	3.1433	476.8236	1080	33.0669	3.1433	1157.1185	1080	33.0669	3.1433	527.7507	1080	33.0669	3.1433	1350.1
1081	33.0929	3.1409	468.5454	1081	33.0929	3.1409	1151.0251	1081	33.0929	3.1409	560.2012	1081	33.0929	3.1409	1381.5199
1082	33.1189	3.1385	466.7463	1082	33.1189	3.1385	1150.0421	1082	33.1189	3.1385	511.8339	1082	33.1189	3.1385	1332.1219
1083	33.1449	3.1361	505.997	1083	33.1449	3.1361	1190.1088	1083	33.1449	3.1361	486.1369	1083	33.1449	3.1361	1305.3942
1084	33.1709	3.1337	509.9153	1084	33.1709	3.1337	1194.8432	1084	33.1709	3.1337	510.569	1084	33.1709	3.1337	1328.7957
1085	33.1969	3.1313	411.039	1085	33.1969	3.1313	1096.783	1085	33.1969	3.1313	526.6425	1085	33.1969	3.1313	1343.8386
1086	33.2229	3.129	482.9212	1086	33.2229	3.129	1169.4813	1086	33.2229	3.129	533.1357	1086	33.2229	3.129	1349.3011
1087	33.2489	3.1266	520.5214	1087	33.2489	3.1266	1207.8976	1087	33.2489	3.1266	496.7775	1087	33.2489	3.1266	1311.9122
1088	33.2749	3.1242	515.5159	1088	33.2749	3.1242	1203.7081	1088	33.2749	3.1242	526.5938	1088	33.2749	3.1242	1340.6979
1089	33.3009	3.1218	489.219	1089	33.3009	3.1218	1178.2273	1089	33.3009	3.1218	481.8812	1089	33.3009	3.1218	1294.9546
1090	33.3269	3.1195	495.5111	1090	33.3269	3.1195	1185.3355	1090	33.3269	3.1195	584.6282	1090	33.3269	3.1195	1396.671
1091	33.3529	3.1171	508.9771	1091	33.3529	3.1171	1199.6175	1091	33.3529	3.1171	596.1222	1091	33.3529	3.1171	1407.1343
1092	33.3789	3.1147	539.2049	1092	33.3789	3.1147	1230.6615	1092	33.3789	3.1147	580.7398	1092	33.3789	3.1147	1390.7212
1093	33.4049	3.1124	584.7708	1093	33.4049	3.1124	1277.0434	1093	33.4049	3.1124	697.292	1093	33.4049	3.1124	1506.2428
1094	33.4309	3.11	565.9254	1094	33.4309	3.11	1259.0141	1094	33.4309	3.11	712.9664	1094	33.4309	3.11	1520.8865
1095	33.4569	3.1077	586.8261	1095	33.4569	3.1077	1280.7309	1095	33.4569	3.1077	578.7265	1095	33.4569	3.1077	1385.616
1096	33.4829	3.1053	656.9792	1096	33.4829	3.1053	1351.7001	1096	33.4829	3.1053	650.899	1096	33.4829	3.1053	1456.7578
1097	33.5089	3.103	714.8506	1097	33.5089	3.103	1410.3876	1097	33.5089	3.103	651.1986	1097	33.5089	3.103	1456.0268
1098	33.5349	3.1007	781.7214	1098	33.5349	3.1007	1478.0744	1098	33.5349	3.1007	782.1762	1098	33.5349	3.1007	1585.9737
1099	33.5609	3.0983	803.2556	1099	33.5609	3.0983	1500.4247	1099	33.5609	3.0983	708.2343	1099	33.5609	3.0983	1511.0011
1100	33.5869	3.096	876.6673	1100	33.5869	3.096	1574.6525	1100	33.5869	3.096	724.2604	1100	33.5869	3.096	1525.9966
1101	33.6129	3.0937	1074.935	1101	33.6129	3.0937	1773.7362	1101	33.6129	3.0937	703.2172	1101	33.6129	3.0937	1503.9228
1102	33.6389	3.0914	1221.4893	1102	33.6389	3.0914	1921.1067	1102	33.6389	3.0914	679.1073	1102	33.6389	3.0914	1478.7823
1103	33.6649	3.089	1374.7471	1103	33.6649	3.089	2075.1805	1103	33.6649	3.089	778.9656	1103	33.6649	3.089	1577.6098
1104	33.6909	3.0867	1648.7396	1104	33.6909	3.0867	2349.9891	1104	33.6909	3.0867	828.768	1104	33.6909	3.0867	1626.3816
1105	33.7169	3.0844	1947.4152	1105	33.7169	3.0844	2649.4808	1105	33.7169	3.0844	788.3933	1105	33.7169	3.0844	1584.9763
1106	33.7429	3.0821	2561.6025	1106	33.7429	3.0821	3264.4842	1106	33.7429	3.0821	855.0702	1106	33.7429	3.0821	1650.6225
1107	33.7689	3.0798	3161.756	1107	33.7689	3.0798	3865.4538	1107	33.7689	3.0798	952.8298	1107	33.7689	3.0798	1747.3514
1108	33.7949	3.0775	4052.8458	1108	33.7949	3.0775	4757.3597	1108	33.7949	3.0775	929.6372	1108	33.7949	3.0775	1723.1282
1109	33.8209	3.0752	4751.0791	1109	33.8209	3.0752	5456.4091	1109	33.8209	3.0752	939.7535	1109	33.8209	3.0752	1732.2139
1110	33.8469	3.0729	4978.971	1110	33.8469	3.0729	5685.117	1110	33.8469	3.0729	1137.8097	1110	33.8469	3.0729	1929.2393
1111	33.8729	3.0706	4551.9894	1111	33.8729	3.0706	5258.9515	1111	33.8729	3.0706	1105.082	1111	33.8729	3.0706	1895.4811

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1112	33.8989	3.0683	4265.0143	1112	33.8989	3.0683	4972.7924	1112	33.8989	3.0683	1193.5016	1112	33.8989	3.0683	1982.87
1113	33.9249	3.066	3606.0449	1113	33.9249	3.066	4314.6392	1113	33.9249	3.066	1330.027	1113	33.9249	3.066	2118.3647
1114	33.9509	3.0638	3056.521	1114	33.9509	3.0638	3765.9314	1114	33.9509	3.0638	1544.2074	1114	33.9509	3.0638	2331.5145
1115	33.9769	3.0615	2567.0096	1115	33.9769	3.0615	3277.236	1115	33.9769	3.0615	1782.846	1115	33.9769	3.0615	2569.1224
1116	34.0029	3.0592	2370.425	1116	34.0029	3.0592	3081.4675	1116	34.0029	3.0592	2161.1087	1116	34.0029	3.0592	2946.3544
1117	34.0289	3.057	2109.78	1117	34.0289	3.057	2821.6386	1117	34.0289	3.057	2459.241	1117	34.0289	3.057	3243.4561
1118	34.0549	3.0547	2013.231	1118	34.0549	3.0547	2725.9057	1118	34.0549	3.0547	2961.3015	1118	34.0549	3.0547	3744.486
1119	34.0809	3.0524	1810.5307	1119	34.0809	3.0524	2524.0215	1119	34.0809	3.0524	3595.3162	1119	34.0809	3.0524	4377.47
1120	34.1069	3.0502	1739.4637	1120	34.1069	3.0502	2453.7705	1120	34.1069	3.0502	4639.0422	1120	34.1069	3.0502	5420.1653
1121	34.1329	3.0479	1733.7641	1121	34.1329	3.0479	2448.887	1121	34.1329	3.0479	5824.4426	1121	34.1329	3.0479	6604.5351
1122	34.1589	3.0457	1739.2008	1122	34.1589	3.0457	2455.1398	1122	34.1589	3.0457	7860.0043	1122	34.1589	3.0457	8639.0661
1123	34.1849	3.0434	1962.9794	1123	34.1849	3.0434	2679.7344	1123	34.1849	3.0434	11273.9932	1123	34.1849	3.0434	12052.0243
1124	34.2109	3.0412	2304.1871	1124	34.2109	3.0412	3021.7583	1124	34.2109	3.0412	16435.9544	1124	34.2109	3.0412	17212.9549
1125	34.2369	3.0389	2507.1345	1125	34.2369	3.0389	3225.5218	1125	34.2369	3.0389	22920.3443	1125	34.2369	3.0389	23696.3142
1126	34.2629	3.0367	2361.288	1126	34.2629	3.0367	3080.4913	1126	34.2629	3.0367	29028.0184	1126	34.2629	3.0367	29802.9576
1127	34.2889	3.0345	2110.176	1127	34.2889	3.0345	2830.1954	1127	34.2889	3.0345	32097.9054	1127	34.2889	3.0345	32871.8139
1128	34.3149	3.0322	1995.4881	1128	34.3149	3.0322	2716.3236	1128	34.3149	3.0322	30880.8004	1128	34.3149	3.0322	31653.6783
1129	34.3409	3.03	1779.0502	1129	34.3409	3.03	2500.7018	1129	34.3409	3.03	27712.2087	1129	34.3409	3.03	28484.0559
1130	34.3669	3.0278	1729.7346	1130	34.3669	3.0278	2452.2023	1130	34.3669	3.0278	22537.4038	1130	34.3669	3.0278	23308.2204
1131	34.3929	3.0256	1729.5041	1131	34.3929	3.0256	2452.7878	1131	34.3929	3.0256	17285.2124	1131	34.3929	3.0256	18054.9983
1132	34.4189	3.0233	1900.0354	1132	34.4189	3.0233	2624.1352	1132	34.4189	3.0233	12786.1011	1132	34.4189	3.0233	13554.8564
1133	34.4449	3.0211	2209.9601	1133	34.4449	3.0211	2934.876	1133	34.4449	3.0211	8954.5345	1133	34.4449	3.0211	9722.2592
1134	34.4709	3.0189	2552.0668	1134	34.4709	3.0189	3277.7988	1134	34.4709	3.0189	6518.1258	1134	34.4709	3.0189	7284.8198
1135	34.4969	3.0167	2826.2226	1135	34.4969	3.0167	3552.7707	1135	34.4969	3.0167	4845.7804	1135	34.4969	3.0167	5611.4437
1136	34.5229	3.0145	2961.8716	1136	34.5229	3.0145	3687.867	1136	34.5229	3.0145	3850.736	1136	34.5229	3.0145	4615.3687
1137	34.5489	3.0123	3079.32	1137	34.5489	3.0123	3804.7627	1137	34.5489	3.0123	3173.7581	1137	34.5489	3.0123	3937.3601
1138	34.5749	3.0101	2897.1672	1138	34.5749	3.0101	3622.0573	1138	34.5749	3.0101	2583.347	1138	34.5749	3.0101	3345.9183
1139	34.6009	3.0079	2755.2797	1139	34.6009	3.0079	3479.6171	1139	34.6009	3.0079	2194.4698	1139	34.6009	3.0079	2956.0105
1140	34.6269	3.0057	2462.5909	1140	34.6269	3.0057	3186.3756	1140	34.6269	3.0057	1773.4923	1140	34.6269	3.0057	2534.0024
1141	34.6529	3.0036	2211.1164	1141	34.6529	3.0036	2934.3485	1141	34.6529	3.0036	1582.2538	1141	34.6529	3.0036	2341.7332
1142	34.6789	3.0014	1871.3896	1142	34.6789	3.0014	2594.069	1142	34.6789	3.0014	1501.5075	1142	34.6789	3.0014	2259.9562
1143	34.7049	2.9992	1527.2134	1143	34.7049	2.9992	2249.3401	1143	34.7049	2.9992	1360.8958	1143	34.7049	2.9992	2118.3139
1144	34.7309	2.997	1330.85	1144	34.7309	2.997	2052.4241	1144	34.7309	2.997	1233.1424	1144	34.7309	2.997	1989.5298
1145	34.7569	2.9948	1199.622	1145	34.7569	2.9948	1920.6433	1145	34.7569	2.9948	1112.9355	1145	34.7569	2.9948	1868.2922
1146	34.7829	2.9927	1052.9343	1146	34.7829	2.9927	1773.403	1146	34.7829	2.9927	1022.0287	1146	34.7829	2.9927	1776.3548
1147	34.8089	2.9905	970.9218	1147	34.8089	2.9905	1690.8379	1147	34.8089	2.9905	923.7344	1147	34.8089	2.9905	1677.0299

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1148	34.8349	2.9883	887.9131	1148	34.8349	2.9883	1607.2765	1148	34.8349	2.9883	917.6448	1148	34.8349	2.9883	1669.9096
1149	34.8609	2.9862	746.2791	1149	34.8609	2.9862	1465.0899	1149	34.8609	2.9862	904.8226	1149	34.8609	2.9862	1656.0567
1150	34.8869	2.984	684.5398	1150	34.8869	2.984	1402.7979	1150	34.8869	2.984	836.6515	1150	34.8869	2.984	1586.855
1151	34.9129	2.9819	673.3286	1151	34.9129	2.9819	1391.034	1151	34.9129	2.9819	827.4549	1151	34.9129	2.9819	1576.6277
1152	34.9389	2.9797	628.9219	1152	34.9389	2.9797	1346.0746	1152	34.9389	2.9797	820.839	1152	34.9389	2.9797	1568.9812
1153	34.9649	2.9776	574.924	1153	34.9649	2.9776	1291.5241	1153	34.9649	2.9776	801.3323	1153	34.9649	2.9776	1548.4438
1154	34.9909	2.9754	555.0718	1154	34.9909	2.9754	1271.1192	1154	34.9909	2.9754	737.3635	1154	34.9909	2.9754	1483.4444
1155	35.0169	2.9733	543.8628	1155	35.0169	2.9733	1259.3575	1155	35.0169	2.9733	682.2543	1155	35.0169	2.9733	1427.3046
1156	35.0429	2.9712	498.9741	1156	35.0429	2.9712	1213.9161	1156	35.0429	2.9712	678.0599	1156	35.0429	2.9712	1422.0795
1157	35.0689	2.969	466.4316	1157	35.0689	2.969	1180.821	1157	35.0689	2.969	711.271	1157	35.0689	2.969	1454.26
1158	35.0949	2.9669	461.0438	1158	35.0949	2.9669	1174.8806	1158	35.0949	2.9669	691.6903	1158	35.0949	2.9669	1433.6486
1159	35.1209	2.9648	454.1261	1159	35.1209	2.9648	1167.4101	1159	35.1209	2.9648	637.8727	1159	35.1209	2.9648	1378.8003
1160	35.1469	2.9626	443.2677	1160	35.1469	2.9626	1155.9991	1160	35.1469	2.9626	666.6078	1160	35.1469	2.9626	1406.5047
1161	35.1729	2.9605	420.6466	1161	35.1729	2.9605	1132.8254	1161	35.1729	2.9605	689.4492	1161	35.1729	2.9605	1428.3155
1162	35.1989	2.9584	397.6509	1162	35.1989	2.9584	1109.2769	1162	35.1989	2.9584	654.9556	1162	35.1989	2.9584	1392.7913
1163	35.2249	2.9563	377.6898	1163	35.2249	2.9563	1089.302	1163	35.2249	2.9563	632.8435	1163	35.2249	2.9563	1369.6485
1164	35.2509	2.9542	382.7372	1164	35.2509	2.9542	1094.3357	1164	35.2509	2.9542	638.1313	1164	35.2509	2.9542	1373.9056
1165	35.2769	2.9521	415.3253	1165	35.2769	2.9521	1126.9099	1165	35.2769	2.9521	645.905	1165	35.2769	2.9521	1380.6486
1166	35.3029	2.95	426.1076	1166	35.3029	2.95	1137.6784	1166	35.3029	2.95	643.0843	1166	35.3029	2.95	1376.7974
1167	35.3289	2.9479	391.7168	1167	35.3289	2.9479	1103.2739	1167	35.3289	2.9479	628.83	1167	35.3289	2.9479	1361.5124
1168	35.3549	2.9458	364.4427	1168	35.3549	2.9458	1075.986	1168	35.3549	2.9458	604.0932	1168	35.3549	2.9458	1335.7449
1169	35.3809	2.9437	391.8104	1169	35.3809	2.9437	1103.3399	1169	35.3809	2.9437	589.9144	1169	35.3809	2.9437	1320.5354
1170	35.4069	2.9416	401.0877	1170	35.4069	2.9416	1112.6034	1170	35.4069	2.9416	599.8356	1170	35.4069	2.9416	1329.426
1171	35.4329	2.9395	385.125	1171	35.4329	2.9395	1096.6269	1171	35.4329	2.9395	611.6219	1171	35.4329	2.9395	1340.1816
1172	35.4589	2.9374	369.0848	1172	35.4589	2.9374	1080.5728	1172	35.4589	2.9374	597.8039	1172	35.4589	2.9374	1325.333
1173	35.4849	2.9353	375.0539	1173	35.4849	2.9353	1086.5281	1173	35.4849	2.9353	578.5454	1173	35.4849	2.9353	1305.0439
1174	35.5109	2.9332	362.8186	1174	35.5109	2.9332	1074.2791	1174	35.5109	2.9332	572.7567	1174	35.5109	2.9332	1298.2244
1175	35.5369	2.9312	372.2603	1175	35.5369	2.9312	1083.707	1175	35.5369	2.9312	613.7776	1175	35.5369	2.9312	1338.2147
1176	35.5629	2.9291	341.7171	1176	35.5629	2.9291	1053.15	1176	35.5629	2.9291	604.163	1176	35.5629	2.9291	1327.5695
1177	35.5889	2.927	354.0858	1177	35.5889	2.927	1065.5049	1177	35.5889	2.927	577.5774	1177	35.5889	2.927	1299.9532
1178	35.6149	2.9249	381.949	1178	35.6149	2.9249	1093.3543	1178	35.6149	2.9249	576.01	1178	35.6149	2.9249	1297.3552
1179	35.6409	2.9229	337.9393	1179	35.6409	2.9229	1049.3308	1179	35.6409	2.9229	554.1971	1179	35.6409	2.9229	1274.5116
1180	35.6669	2.9208	346.3978	1180	35.6669	2.9208	1057.7755	1180	35.6669	2.9208	593.8275	1180	35.6669	2.9208	1313.1113
1181	35.6929	2.9188	322.6807	1181	35.6929	2.9188	1034.0446	1181	35.6929	2.9188	592.4544	1181	35.6929	2.9188	1310.7076
1182	35.7189	2.9167	368.8815	1182	35.7189	2.9167	1080.2316	1182	35.7189	2.9167	573.5233	1182	35.7189	2.9167	1290.7458
1183	35.7449	2.9147	303.6541	1183	35.7449	2.9147	1014.9904	1183	35.7449	2.9147	574.5169	1183	35.7449	2.9147	1290.7089

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1184	35.7709	2.9126	328.4409	1184	35.7709	2.9126	1039.7634	1184	35.7709	2.9126	568.3129	1184	35.7709	2.9126	1283.4742
1185	35.7969	2.9106	355.5308	1185	35.7969	2.9106	1066.8396	1185	35.7969	2.9106	503.3493	1185	35.7969	2.9106	1217.4799
1186	35.8229	2.9085	298.1259	1186	35.8229	2.9085	1009.4208	1186	35.8229	2.9085	506.5834	1186	35.8229	2.9085	1219.6833
1187	35.8489	2.9065	317.3269	1187	35.8489	2.9065	1028.6081	1187	35.8489	2.9065	528.8764	1187	35.8489	2.9065	1240.9457
1188	35.8749	2.9044	366.1779	1188	35.8749	2.9044	1077.4452	1188	35.8749	2.9044	503.2949	1188	35.8749	2.9044	1214.3336
1189	35.9009	2.9024	397.6509	1189	35.9009	2.9024	1108.9044	1189	35.9009	2.9024	530.8542	1189	35.9009	2.9024	1240.8622
1190	35.9269	2.9004	373.8542	1190	35.9269	2.9004	1083.7258	1190	35.9269	2.9004	578.7245	1190	35.9269	2.9004	1287.7018
1191	35.9529	2.8983	358.7867	1191	35.9529	2.8983	1067.2763	1191	35.9529	2.8983	538.3921	1191	35.9529	2.8983	1246.3388
1192	35.9789	2.8963	381.5662	1192	35.9789	2.8963	1088.6739	1192	35.9789	2.8963	502.5363	1192	35.9789	2.8963	1209.4524
1193	36.0049	2.8943	328.971	1193	36.0049	2.8943	1034.6967	1193	36.0049	2.8943	489.8939	1193	36.0049	2.8943	1195.7792
1194	36.0309	2.8923	375.0657	1194	36.0309	2.8923	1079.4094	1194	36.0309	2.8923	451.4633	1194	36.0309	2.8923	1156.318
1195	36.0569	2.8903	449.5377	1195	36.0569	2.8903	1152.4995	1195	36.0569	2.8903	519.1479	1195	36.0569	2.8903	1222.972
1196	36.0829	2.8882	357.2773	1196	36.0829	2.8882	1058.8571	1196	36.0829	2.8882	478.0637	1196	36.0829	2.8882	1180.8571
1197	36.1089	2.8862	348.9927	1197	36.1089	2.8862	1049.1905	1197	36.1089	2.8862	463.5607	1197	36.1089	2.8862	1165.3235
1198	36.1349	2.8842	373.6444	1198	36.1349	2.8842	1072.4603	1198	36.1349	2.8842	487.252	1198	36.1349	2.8842	1187.9841
1199	36.1609	2.8822	391.7744	1199	36.1609	2.8822	1089.2083	1199	36.1609	2.8822	496.7688	1199	36.1609	2.8822	1196.4702
1200	36.1869	2.8802	387.8766	1200	36.1869	2.8802	1083.9285	1200	36.1869	2.8802	511.1863	1200	36.1869	2.8802	1209.8571
1201	36.2129	2.8782	398.1692	1201	36.2129	2.8782	1092.8392	1201	36.2129	2.8782	526.4949	1201	36.2129	2.8782	1224.135
1202	36.2389	2.8762	406.8787	1202	36.2389	2.8762	1100.1667	1202	36.2389	2.8762	508.6406	1202	36.2389	2.8762	1205.2501
1203	36.2649	2.8742	399.6811	1203	36.2649	2.8742	1091.5872	1203	36.2649	2.8742	497.5308	1203	36.2649	2.8742	1193.1096
1204	36.2909	2.8722	412.9196	1204	36.2909	2.8722	1103.4437	1204	36.2909	2.8722	449.1344	1204	36.2909	2.8722	1143.6826
1205	36.3169	2.8703	474.7696	1205	36.3169	2.8703	1163.9118	1205	36.3169	2.8703	451.0527	1205	36.3169	2.8703	1144.5702
1206	36.3429	2.8683	388.2471	1206	36.3429	2.8683	1076.0073	1206	36.3429	2.8683	546.1058	1206	36.3429	2.8683	1238.5926
1207	36.3689	2.8663	433.6892	1207	36.3689	2.8663	1120.0674	1207	36.3689	2.8663	451.9936	1207	36.3689	2.8663	1143.4498
1208	36.3949	2.8643	436.9323	1208	36.3949	2.8643	1121.9286	1208	36.3949	2.8643	495.0503	1208	36.3949	2.8643	1185.4759
1209	36.4209	2.8623	435.8434	1209	36.4209	2.8623	1119.4577	1209	36.4209	2.8623	515.8825	1209	36.4209	2.8623	1205.2774
1210	36.4469	2.8604	470.0716	1210	36.4469	2.8604	1152.304	1210	36.4469	2.8604	536.466	1210	36.4469	2.8604	1224.8302
1211	36.4729	2.8584	547.6896	1211	36.4729	2.8584	1228.54	1211	36.4729	2.8584	494.9233	1211	36.4729	2.8584	1182.2569
1212	36.4989	2.8564	525.913	1212	36.4989	2.8564	1205.3815	1212	36.4989	2.8564	523.252	1212	36.4989	2.8564	1209.5549
1213	36.5249	2.8545	636.0218	1213	36.5249	2.8545	1314.1083	1213	36.5249	2.8545	484.7863	1213	36.5249	2.8545	1170.0586
1214	36.5509	2.8525	657.6521	1214	36.5509	2.8525	1334.3567	1214	36.5509	2.8525	570.5774	1214	36.5509	2.8525	1254.8191
1215	36.5769	2.8505	760.8371	1215	36.5769	2.8505	1436.1597	1215	36.5769	2.8505	581.4694	1215	36.5769	2.8505	1264.6804
1216	36.6029	2.8486	831.2795	1216	36.6029	2.8486	1505.2202	1216	36.6029	2.8486	681.9832	1216	36.6029	2.8486	1364.1635
1217	36.6289	2.8466	932.694	1217	36.6289	2.8466	1605.2527	1217	36.6289	2.8466	855.19	1217	36.6289	2.8466	1536.3396
1218	36.6549	2.8447	1078.5842	1218	36.6549	2.8447	1749.7609	1218	36.6549	2.8447	1080.5321	1218	36.6549	2.8447	1760.6511
1219	36.6809	2.8427	1168.9503	1219	36.6809	2.8427	1838.7451	1219	36.6809	2.8427	1248.9139	1219	36.6809	2.8427	1928.0022

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1220	36.7069	2.8408	1394.7213	1220	36.7069	2.8408	2063.1341	1220	36.7069	2.8408	1389.6991	1220	36.7069	2.8408	2067.7568
1221	36.7329	2.8389	1722.3074	1221	36.7329	2.8389	2389.3382	1221	36.7329	2.8389	1369.9704	1221	36.7329	2.8389	2046.9975
1222	36.7589	2.8369	2135.4254	1222	36.7589	2.8369	2801.0743	1222	36.7589	2.8369	1204.1856	1222	36.7589	2.8369	1880.1819
1223	36.7849	2.835	2490.2186	1223	36.7849	2.835	3154.4856	1223	36.7849	2.835	1192.7839	1223	36.7849	2.835	1867.7496
1224	36.8109	2.833	2628.5389	1224	36.8109	2.833	3291.4239	1224	36.8109	2.833	985.7262	1224	36.8109	2.833	1659.6612
1225	36.8369	2.8311	2556.4202	1225	36.8369	2.8311	3217.9233	1225	36.8369	2.8311	813.8569	1225	36.8369	2.8311	1486.7613
1226	36.8629	2.8292	2394.9704	1226	36.8629	2.8292	3055.0915	1226	36.8629	2.8292	680.4061	1226	36.8629	2.8292	1352.2799
1227	36.8889	2.8273	2163.7846	1227	36.8889	2.8273	2822.5237	1227	36.8889	2.8273	658.6511	1227	36.8889	2.8273	1329.4942
1228	36.9149	2.8253	1860.5318	1228	36.9149	2.8253	2517.8889	1228	36.9149	2.8253	589.8584	1228	36.9149	2.8253	1259.6708
1229	36.9409	2.8234	1527.1495	1229	36.9409	2.8234	2183.1247	1229	36.9409	2.8234	531.3698	1229	36.9409	2.8234	1200.1516
1230	36.9669	2.8215	1218.923	1230	36.9669	2.8215	1873.5163	1230	36.9669	2.8215	541.5809	1230	36.9669	2.8215	1209.3321
1231	36.9929	2.8196	1049.4075	1231	36.9929	2.8196	1702.6188	1231	36.9929	2.8196	528.9812	1231	36.9929	2.8196	1195.7017
1232	37.0189	2.8177	939.6766	1232	37.0189	2.8177	1591.5059	1232	37.0189	2.8177	515.8823	1232	37.0189	2.8177	1181.5721
1233	37.0449	2.8158	837.1004	1233	37.0449	2.8158	1487.5478	1233	37.0449	2.8158	437.543	1233	37.0449	2.8158	1102.2022
1234	37.0709	2.8139	723.8028	1234	37.0709	2.8139	1372.8682	1234	37.0709	2.8139	468.4468	1234	37.0709	2.8139	1132.0753
1235	37.0969	2.812	625.5069	1235	37.0969	2.812	1273.1904	1235	37.0969	2.812	461.2136	1235	37.0969	2.812	1123.8115
1236	37.1229	2.8101	653.6784	1236	37.1229	2.8101	1299.9799	1236	37.1229	2.8101	480.5417	1236	37.1229	2.8101	1142.1089
1237	37.1489	2.8082	643.3746	1237	37.1489	2.8082	1288.2942	1237	37.1489	2.8082	440.4123	1237	37.1489	2.8082	1100.9488
1238	37.1749	2.8063	553.1365	1238	37.1749	2.8063	1196.6741	1238	37.1749	2.8063	473.5967	1238	37.1749	2.8063	1133.1026
1239	37.2009	2.8044	549.6276	1239	37.2009	2.8044	1191.7833	1239	37.2009	2.8044	489.2275	1239	37.2009	2.8044	1147.7028
1240	37.2269	2.8025	501.8988	1240	37.2269	2.8025	1142.6725	1240	37.2269	2.8025	493.4994	1240	37.2269	2.8025	1150.944
1241	37.2529	2.8006	465.3775	1241	37.2529	2.8006	1104.7692	1241	37.2529	2.8006	463.1609	1241	37.2529	2.8006	1119.5749
1242	37.2789	2.7987	435.5922	1242	37.2789	2.7987	1073.6019	1242	37.2789	2.7987	455.1082	1242	37.2789	2.7987	1110.4915
1243	37.3049	2.7968	460.5509	1243	37.3049	2.7968	1097.1787	1243	37.3049	2.7968	477.5897	1243	37.3049	2.7968	1131.9424
1244	37.3309	2.795	450.589	1244	37.3309	2.795	1084.67	1244	37.3309	2.795	489.0112	1244	37.3309	2.795	1142.3332
1245	37.3569	2.7931	452.2558	1245	37.3569	2.7931	1083.79	1245	37.3569	2.7931	424.3852	1245	37.3569	2.7931	1076.6765
1246	37.3829	2.7912	412.8598	1246	37.3829	2.7912	1041.8473	1246	37.3829	2.7912	446.3595	1246	37.3829	2.7912	1097.6201
1247	37.4089	2.7893	408.3008	1247	37.4089	2.7893	1034.7415	1247	37.4089	2.7893	455.4812	1247	37.4089	2.7893	1105.7112
1248	37.4349	2.7875	447.809	1248	37.4349	2.7875	1071.7029	1248	37.4349	2.7875	449.4427	1248	37.4349	2.7875	1098.6421
1249	37.4609	2.7856	424.9322	1249	37.4609	2.7856	1046.2794	1249	37.4609	2.7856	428.5352	1249	37.4609	2.7856	1076.7039
1250	37.4869	2.7837	388.8444	1250	37.4869	2.7837	1007.6448	1250	37.4869	2.7837	454.5347	1250	37.4869	2.7837	1101.6728
1251	37.5129	2.7819	432.3085	1251	37.5129	2.7819	1048.5621	1251	37.5129	2.7819	478.3098	1251	37.5129	2.7819	1124.4172
1252	37.5389	2.78	444.2175	1252	37.5389	2.78	1057.9243	1252	37.5389	2.78	439.3417	1252	37.5389	2.78	1084.4184
1253	37.5649	2.7782	398.6663	1253	37.5649	2.7782	1009.8264	1253	37.5649	2.7782	413.3766	1253	37.5649	2.7782	1057.4227
1254	37.5909	2.7763	380.0888	1254	37.5909	2.7763	988.7021	1254	37.5909	2.7763	413.4172	1254	37.5909	2.7763	1056.4326
1255	37.6169	2.7745	416.8227	1255	37.6169	2.7745	1022.8893	1255	37.6169	2.7745	412.3429	1255	37.6169	2.7745	1054.3277

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1256	37.6429	2.7726	390.728	1256	37.6429	2.7726	994.2477	1256	37.6429	2.7726	456.3952	1256	37.6429	2.7726	1097.3494
1257	37.6689	2.7708	364.6926	1257	37.6689	2.7708	965.6656	1257	37.6689	2.7708	469.8845	1257	37.6689	2.7708	1109.808
1258	37.6949	2.7689	382.6291	1258	37.6949	2.7689	981.0554	1258	37.6949	2.7689	455.9116	1258	37.6949	2.7689	1094.8045
1259	37.7209	2.7671	389.2271	1259	37.7209	2.7671	985.1065	1259	37.7209	2.7671	454.3715	1259	37.7209	2.7671	1092.2337
1260	37.7469	2.7653	380.9558	1260	37.7469	2.7653	974.2885	1260	37.7469	2.7653	459.3408	1260	37.7469	2.7653	1096.1723
1261	37.7729	2.7634	355.7747	1261	37.7729	2.7634	946.5606	1261	37.7729	2.7634	455.7639	1261	37.7729	2.7634	1091.5647
1262	37.7989	2.7616	369.1363	1262	37.7989	2.7616	957.3754	1262	37.7989	2.7616	437.3259	1262	37.7989	2.7616	1072.0961
1263	37.8249	2.7598	406.9128	1263	37.8249	2.7598	992.6052	1263	37.8249	2.7598	481.111	1263	37.8249	2.7598	1114.8505
1264	37.8509	2.7579	379.0621	1264	37.8509	2.7579	962.2077	1264	37.8509	2.7579	480.8589	1264	37.8509	2.7579	1113.5678
1265	37.8769	2.7561	373.5172	1265	37.8769	2.7561	954.116	1265	37.8769	2.7561	464.9364	1265	37.8769	2.7561	1096.6147
1266	37.9029	2.7543	419.948	1266	37.9029	2.7543	998	1266	37.9029	2.7543	507.3864	1266	37.9029	2.7543	1138.034
1267	37.9289	2.7525	439.5915	1267	37.9289	2.7525	1015.0967	1267	37.9289	2.7525	507.0274	1267	37.9289	2.7525	1136.6443
1268	37.9549	2.7507	417.3399	1268	37.9549	2.7507	990.2984	1268	37.9549	2.7507	505.8462	1268	37.9549	2.7507	1134.4325
1269	37.9809	2.7488	378.9335	1269	37.9809	2.7488	949.3452	1269	37.9809	2.7488	490.3741	1269	37.9809	2.7488	1117.9297
1270	38.0069	2.747	397.6509	1270	38.0069	2.747	965.5158	1270	38.0069	2.747	484.8511	1270	38.0069	2.747	1111.3761
1271	38.0329	2.7452	382.9901	1271	38.0329	2.7452	947.9934	1271	38.0329	2.7452	485.6558	1271	38.0329	2.7452	1111.1502
1272	38.0589	2.7434	381.4718	1272	38.0589	2.7434	943.6134	1272	38.0589	2.7434	501.761	1272	38.0589	2.7434	1126.2247
1273	38.0849	2.7416	373.8565	1273	38.0849	2.7416	933.1365	1273	38.0849	2.7416	494.3554	1273	38.0849	2.7416	1117.7884
1274	38.1109	2.7398	364.1937	1274	38.1109	2.7398	920.6121	1274	38.1109	2.7398	506.7625	1274	38.1109	2.7398	1129.1649
1275	38.1369	2.738	361.4702	1275	38.1369	2.738	915.027	1275	38.1369	2.738	507.2943	1275	38.1369	2.738	1128.666
1276	38.1629	2.7362	382.9455	1276	38.1629	2.7362	933.6406	1276	38.1629	2.7362	489.9136	1276	38.1629	2.7362	1110.2546
1277	38.1889	2.7344	368.0195	1277	38.1889	2.7344	915.853	1277	38.1889	2.7344	478.8716	1277	38.1889	2.7344	1098.182
1278	38.2149	2.7326	395.6498	1278	38.2149	2.7326	940.6216	1278	38.2149	2.7326	433.7478	1278	38.2149	2.7326	1052.0275
1279	38.2409	2.7309	421.2168	1279	38.2409	2.7309	963.3269	1279	38.2409	2.7309	408.6399	1279	38.2409	2.7309	1025.8889
1280	38.2669	2.7291	428.9066	1280	38.2669	2.7291	968.1551	1280	38.2669	2.7291	468.953	1280	38.2669	2.7291	1085.1714
1281	38.2929	2.7273	391.7736	1281	38.2929	2.7273	928.1604	1281	38.2929	2.7273	429.0422	1281	38.2929	2.7273	1044.2299
1282	38.3189	2.7255	427.6545	1282	38.3189	2.7255	961.1797	1282	38.3189	2.7255	394.0279	1282	38.3189	2.7255	1008.185
1283	38.3449	2.7237	409.2227	1283	38.3449	2.7237	939.8863	1283	38.3449	2.7237	404.8309	1283	38.3449	2.7237	1017.9573
1284	38.3709	2.7219	463.5223	1284	38.3709	2.7219	991.3242	1284	38.3709	2.7219	432.7498	1284	38.3709	2.7219	1044.8456
1285	38.3969	2.7202	432.3195	1285	38.3969	2.7202	957.2598	1285	38.3969	2.7202	467.7365	1285	38.3969	2.7202	1078.8017
1286	38.4229	2.7184	429.9249	1286	38.4229	2.7184	952.0035	1286	38.4229	2.7184	416.704	1286	38.4229	2.7184	1026.7385
1287	38.4489	2.7166	410.2244	1287	38.4489	2.7166	929.4413	1287	38.4489	2.7166	459.4811	1287	38.4489	2.7166	1068.485
1288	38.4749	2.7149	398.1847	1288	38.4749	2.7149	914.54	1288	38.4749	2.7149	407.7869	1288	38.4749	2.7149	1015.7601
1289	38.5009	2.7131	407.8697	1289	38.5009	2.7131	921.3633	1289	38.5009	2.7131	422.019	1289	38.5009	2.7131	1028.9616
1290	38.5269	2.7113	428.5988	1290	38.5269	2.7113	939.2308	1290	38.5269	2.7113	429.5222	1290	38.5269	2.7113	1035.4341
1291	38.5529	2.7096	392.6362	1291	38.5529	2.7096	900.4066	1291	38.5529	2.7096	417.5375	1291	38.5529	2.7096	1022.4187

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1292	38.5789	2.7078	411.7623	1292	38.5789	2.7078	916.671	1292	38.5789	2.7078	473.6785	1292	38.5789	2.7078	1077.5291
1293	38.6049	2.7061	398.6277	1293	38.6049	2.7061	900.6747	1293	38.6049	2.7061	459.8079	1293	38.6049	2.7061	1062.6279
1294	38.6309	2.7043	432.8375	1294	38.6309	2.7043	932.0229	1294	38.6309	2.7043	509.5165	1294	38.6309	2.7043	1111.3057
1295	38.6569	2.7026	434.5752	1295	38.6569	2.7026	930.899	1295	38.6569	2.7026	468.8836	1295	38.6569	2.7026	1069.6422
1296	38.6829	2.7008	403.5797	1296	38.6829	2.7008	897.0418	1296	38.6829	2.7008	469.205	1296	38.6829	2.7008	1068.933
1297	38.7089	2.6991	397.6509	1297	38.7089	2.6991	888.2513	1297	38.7089	2.6991	439.5637	1297	38.7089	2.6991	1038.261
1298	38.7349	2.6973	420.0266	1298	38.7349	2.6973	911.1551	1298	38.7349	2.6973	396.9954	1298	38.7349	2.6973	994.662
1299	38.7609	2.6956	471.5204	1299	38.7609	2.6956	963.1769	1299	38.7609	2.6956	424.2978	1299	38.7609	2.6956	1020.9338
1300	38.7869	2.6939	408.1467	1300	38.7869	2.6939	900.3313	1300	38.7869	2.6939	445.3855	1300	38.7869	2.6939	1040.9909
1301	38.8129	2.6921	423.9444	1301	38.8129	2.6921	916.6571	1301	38.8129	2.6921	487.1519	1301	38.8129	2.6921	1081.7266
1302	38.8389	2.6904	468.3845	1302	38.8389	2.6904	961.6253	1302	38.8389	2.6904	428.6485	1302	38.8389	2.6904	1022.1926
1303	38.8649	2.6887	416.91	1303	38.8649	2.6887	910.6788	1303	38.8649	2.6887	482.136	1303	38.8649	2.6887	1074.6494
1304	38.8909	2.6869	444.2093	1304	38.8909	2.6869	938.5062	1304	38.8909	2.6869	485.4583	1304	38.8909	2.6869	1076.9411
1305	38.9169	2.6852	413.3217	1305	38.9169	2.6852	908.1466	1305	38.9169	2.6852	422.6945	1305	38.9169	2.6852	1013.1466
1306	38.9429	2.6835	444.5161	1306	38.9429	2.6835	939.869	1306	38.9429	2.6835	456.1159	1306	38.9429	2.6835	1045.5373
1307	38.9689	2.6818	421.9574	1307	38.9689	2.6818	917.8384	1307	38.9689	2.6818	446.9083	1307	38.9689	2.6818	1035.2991
1308	38.9949	2.68	395.2222	1308	38.9949	2.68	891.6313	1308	38.9949	2.68	410.1234	1308	38.9949	2.68	997.4835
1309	39.0209	2.6783	414.2577	1309	39.0209	2.6783	911.1948	1309	39.0209	2.6783	456.3026	1309	39.0209	2.6783	1042.6321
1310	39.0469	2.6766	422.2419	1310	39.0469	2.6766	919.707	1310	39.0469	2.6766	440.877	1310	39.0469	2.6766	1026.1758
1311	39.0729	2.6749	396.9637	1311	39.0729	2.6749	894.9569	1311	39.0729	2.6749	456.6869	1311	39.0729	2.6749	1040.9551
1312	39.0989	2.6732	372.6738	1312	39.0989	2.6732	871.195	1312	39.0989	2.6732	432.9657	1312	39.0989	2.6732	1016.2031
1313	39.1249	2.6715	385.698	1313	39.1249	2.6715	884.7473	1313	39.1249	2.6715	484.8547	1313	39.1249	2.6715	1067.0615
1314	39.1509	2.6698	402.9192	1314	39.1509	2.6698	902.4965	1314	39.1509	2.6698	503.3483	1314	39.1509	2.6698	1084.5245
1315	39.1769	2.6681	436.5684	1315	39.1769	2.6681	936.6738	1315	39.1769	2.6681	516.3998	1315	39.1769	2.6681	1096.5453
1316	39.2029	2.6664	386.9007	1316	39.2029	2.6664	887.5342	1316	39.2029	2.6664	485.5108	1316	39.2029	2.6664	1064.6257
1317	39.2289	2.6647	448.8546	1317	39.2289	2.6647	950.0161	1317	39.2289	2.6647	509.4146	1317	39.2289	2.6647	1087.4988
1318	39.2549	2.663	455.1075	1318	39.2549	2.663	956.797	1318	39.2549	2.663	442.0209	1318	39.2549	2.663	1019.0744
1319	39.2809	2.6613	410.5063	1319	39.2809	2.6613	912.7239	1319	39.2809	2.6613	433.365	1319	39.2809	2.6613	1009.3879
1320	39.3069	2.6596	410.8168	1320	39.3069	2.6596	913.5625	1320	39.3069	2.6596	458.6451	1320	39.3069	2.6596	1033.6374
1321	39.3329	2.6579	378.2336	1321	39.3329	2.6579	881.5073	1321	39.3329	2.6579	467.4538	1321	39.3329	2.6579	1041.4154
1322	39.3589	2.6562	417.0455	1322	39.3589	2.6562	920.8473	1322	39.3589	2.6562	443.1822	1322	39.3589	2.6562	1016.1131
1323	39.3849	2.6545	404.0156	1323	39.3849	2.6545	908.3454	1323	39.3849	2.6545	449.0443	1323	39.3849	2.6545	1020.9446
1324	39.4109	2.6529	397.6509	1324	39.4109	2.6529	902.5088	1324	39.4109	2.6529	459.8584	1324	39.4109	2.6529	1030.7281
1325	39.4369	2.6512	390.5226	1325	39.4369	2.6512	895.0969	1325	39.4369	2.6512	404.3477	1325	39.4369	2.6512	974.1867
1326	39.4629	2.6495	371.797	1326	39.4629	2.6495	876.0878	1326	39.4629	2.6495	419.2217	1326	39.4629	2.6495	988.03
1327	39.4889	2.6478	391.7548	1327	39.4889	2.6478	895.7621	1327	39.4889	2.6478	451.1996	1327	39.4889	2.6478	1018.9773

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1328	39.5149	2.6462	419.6035	1328	39.5149	2.6462	923.3273	1328	39.5149	2.6462	372.275	1328	39.5149	2.6462	939.022
1329	39.5409	2.6445	451.7252	1329	39.5409	2.6445	955.1655	1329	39.5409	2.6445	451.7743	1329	39.5409	2.6445	1017.4907
1330	39.5669	2.6428	423.6858	1330	39.5669	2.6428	926.8425	1330	39.5669	2.6428	469.2479	1330	39.5669	2.6428	1033.9336
1331	39.5929	2.6412	379.1727	1331	39.5929	2.6412	882.0459	1331	39.5929	2.6412	449.2612	1331	39.5929	2.6412	1012.9162
1332	39.6189	2.6395	389.4526	1332	39.6189	2.6395	892.0423	1332	39.6189	2.6395	481.8733	1332	39.6189	2.6395	1044.4977
1333	39.6449	2.6378	408.797	1333	39.6449	2.6378	911.1031	1333	39.6449	2.6378	426.5917	1333	39.6449	2.6378	988.1855
1334	39.6709	2.6362	433.8642	1334	39.6709	2.6362	935.8868	1334	39.6709	2.6362	408.6633	1334	39.6709	2.6362	969.2264
1335	39.6969	2.6345	459.3525	1335	39.6969	2.6345	961.0915	1335	39.6969	2.6345	435.4321	1335	39.6969	2.6345	994.9645
1336	39.7229	2.6329	421.0738	1336	39.7229	2.6329	922.5294	1336	39.7229	2.6329	436.2071	1336	39.7229	2.6329	994.7089
1337	39.7489	2.6312	362.199	1337	39.7489	2.6312	863.371	1337	39.7489	2.6312	412.9582	1337	39.7489	2.6312	970.4293
1338	39.7749	2.6296	419.0332	1338	39.7749	2.6296	919.9217	1338	39.7749	2.6296	449.1254	1338	39.7749	2.6296	1005.5659
1339	39.8009	2.6279	432.3636	1339	39.8009	2.6279	932.9685	1339	39.8009	2.6279	425.7717	1339	39.8009	2.6279	981.1815
1340	39.8269	2.6263	423.3943	1340	39.8269	2.6263	923.7157	1340	39.8269	2.6263	516.5862	1340	39.8269	2.6263	1070.9654
1341	39.8529	2.6246	434.6364	1341	39.8529	2.6246	934.6743	1341	39.8529	2.6246	488.5346	1341	39.8529	2.6246	1041.8831
1342	39.8789	2.623	412.4774	1342	39.8789	2.623	912.2318	1342	39.8789	2.623	477.0373	1342	39.8789	2.623	1029.3551
1343	39.9049	2.6213	427.2162	1343	39.9049	2.6213	926.6871	1343	39.9049	2.6213	521.2955	1343	39.9049	2.6213	1072.5827
1344	39.9309	2.6197	453.2999	1344	39.9309	2.6197	952.4872	1344	39.9309	2.6197	497.6074	1344	39.9309	2.6197	1047.864
1345	39.9569	2.6181	416.2433	1345	39.9569	2.6181	915.147	1345	39.9569	2.6181	432.9278	1345	39.9569	2.6181	982.1537
1346	39.9829	2.6164	421.8695	1346	39.9829	2.6164	920.4897	1346	39.9829	2.6164	505.0551	1346	39.9829	2.6164	1053.2504
1347	40.0089	2.6148	410.2349	1347	40.0089	2.6148	908.5716	1347	40.0089	2.6148	466.8814	1347	40.0089	2.6148	1014.046
1348	40.0349	2.6132	388.3308	1348	40.0349	2.6132	886.3839	1348	40.0349	2.6132	401.7299	1348	40.0349	2.6132	947.8639
1349	40.0609	2.6115	418.5916	1349	40.0609	2.6115	916.3612	1349	40.0609	2.6115	421.6352	1349	40.0609	2.6115	966.7385
1350	40.0869	2.6099	438.8991	1350	40.0869	2.6099	936.3852	1350	40.0869	2.6099	406.7267	1350	40.0869	2.6099	950.7993
1351	40.1129	2.6083	433.3533	1351	40.1129	2.6083	930.5559	1351	40.1129	2.6083	402.0807	1351	40.1129	2.6083	945.1226
1352	40.1389	2.6067	409.2566	1352	40.1389	2.6067	906.1756	1352	40.1389	2.6067	400.0029	1352	40.1389	2.6067	942.5054
1353	40.1649	2.6051	404.1404	1353	40.1649	2.6051	900.7759	1353	40.1649	2.6051	404.9084	1353	40.1649	2.6051	946.8713
1354	40.1909	2.6034	387.6425	1354	40.1909	2.6034	883.9945	1354	40.1909	2.6034	428.955	1354	40.1909	2.6034	970.3785
1355	40.2169	2.6018	373.1924	1355	40.2169	2.6018	869.2609	1355	40.2169	2.6018	464.9855	1355	40.2169	2.6018	1005.8695
1356	40.2429	2.6002	390.208	1356	40.2429	2.6002	885.9929	1356	40.2429	2.6002	470.2179	1356	40.2429	2.6002	1010.5624
1357	40.2689	2.5986	411.7699	1357	40.2689	2.5986	907.2713	1357	40.2689	2.5986	453.7413	1357	40.2689	2.5986	993.5463
1358	40.2949	2.597	419.7821	1358	40.2949	2.597	915	1358	40.2949	2.597	449.7345	1358	40.2949	2.597	989
1359	40.3209	2.5954	418.4891	1359	40.3209	2.5954	913.4234	1359	40.3209	2.5954	409.8085	1359	40.3209	2.5954	948.5344
1360	40.3469	2.5938	430.2393	1360	40.3469	2.5938	924.8901	1360	40.3469	2.5938	422.2803	1360	40.3469	2.5938	960.4668
1361	40.3729	2.5922	379.4225	1361	40.3729	2.5922	873.7897	1361	40.3729	2.5922	472.9041	1361	40.3729	2.5922	1010.5511
1362	40.3989	2.5906	379.8862	1362	40.3989	2.5906	873.97	1362	40.3989	2.5906	495.7399	1362	40.3989	2.5906	1032.8474
1363	40.4249	2.589	436.3981	1363	40.4249	2.589	930.1983	1363	40.4249	2.589	486.7393	1363	40.4249	2.589	1023.3073

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1364	40.4509	2.5874	423.2964	1364	40.4509	2.5874	916.8131	1364	40.4509	2.5874	482.2432	1364	40.4509	2.5874	1018.2717
1365	40.4769	2.5858	377.6234	1365	40.4769	2.5858	870.8566	1365	40.4769	2.5858	508.579	1365	40.4769	2.5858	1044.068
1366	40.5029	2.5842	366.3435	1366	40.5029	2.5842	859.2932	1366	40.5029	2.5842	517.628	1366	40.5029	2.5842	1052.5775
1367	40.5289	2.5826	412.58	1367	40.5289	2.5826	905.2461	1367	40.5289	2.5826	515.7594	1367	40.5289	2.5826	1050.1694
1368	40.5549	2.581	419.3087	1368	40.5549	2.581	911.6913	1368	40.5549	2.581	497.8208	1368	40.5549	2.581	1031.6913
1369	40.5809	2.5795	409.3749	1369	40.5809	2.5795	901.4739	1369	40.5809	2.5795	487.7166	1369	40.5809	2.5795	1021.0476
1370	40.6069	2.5779	423.5838	1370	40.6069	2.5779	915.3993	1370	40.6069	2.5779	467.8808	1370	40.6069	2.5779	1000.6724
1371	40.6329	2.5763	434.2675	1371	40.6329	2.5763	925.7995	1371	40.6329	2.5763	471.787	1371	40.6329	2.5763	1004.039
1372	40.6589	2.5747	388.6312	1372	40.6589	2.5747	879.8797	1372	40.6589	2.5747	489.529	1372	40.6589	2.5747	1021.2416
1373	40.6849	2.5731	373.4886	1373	40.6849	2.5731	864.4535	1373	40.6849	2.5731	473.5482	1373	40.6849	2.5731	1004.7212
1374	40.7109	2.5716	376.5923	1374	40.7109	2.5716	867.2737	1374	40.7109	2.5716	471.4206	1374	40.7109	2.5716	1002.0542
1375	40.7369	2.57	378.2667	1375	40.7369	2.57	868.6646	1375	40.7369	2.57	496.674	1375	40.7369	2.57	1026.768
1376	40.7629	2.5684	366.2425	1376	40.7629	2.5684	856.3568	1376	40.7629	2.5684	475.4702	1376	40.7629	2.5684	1005.0248
1377	40.7889	2.5669	371.3323	1377	40.7889	2.5669	861.1631	1377	40.7889	2.5669	412.271	1377	40.7889	2.5669	941.2861
1378	40.8149	2.5653	397.6509	1378	40.8149	2.5653	887.1982	1378	40.8149	2.5653	403.9605	1378	40.8149	2.5653	932.4361
1379	40.8409	2.5637	415.5143	1379	40.8409	2.5637	906.3189	1379	40.8409	2.5637	396.5704	1379	40.8409	2.5637	924.5065
1380	40.8669	2.5622	380.2553	1380	40.8669	2.5622	872.3172	1380	40.8669	2.5622	377.4909	1380	40.8669	2.5622	904.8874
1381	40.8929	2.5606	378.4519	1381	40.8929	2.5606	871.7711	1381	40.8929	2.5606	441.468	1381	40.8929	2.5606	968.325
1382	40.9189	2.5591	380.9645	1382	40.9189	2.5591	875.5409	1382	40.9189	2.5591	411.8174	1382	40.9189	2.5591	938.1349
1383	40.9449	2.5575	393.7293	1383	40.9449	2.5575	889.563	1383	40.9449	2.5575	414.4302	1383	40.9449	2.5575	940.2083
1384	40.9709	2.5559	385.3019	1384	40.9709	2.5559	882.3929	1384	40.9709	2.5559	442.7614	1384	40.9709	2.5559	968
1385	40.9969	2.5544	365.5551	1385	40.9969	2.5544	863.9034	1385	40.9969	2.5544	443.3009	1385	40.9969	2.5544	968
1386	41.0229	2.5528	338.8792	1386	41.0229	2.5528	838.4848	1386	41.0229	2.5528	452.342	1386	41.0229	2.5528	976.5016
1387	41.0489	2.5513	357.9349	1387	41.0489	2.5513	858.7978	1387	41.0489	2.5513	467.2241	1387	41.0489	2.5513	990.8442
1388	41.0749	2.5498	419.3131	1388	41.0749	2.5498	921.4333	1388	41.0749	2.5498	438.8217	1388	41.0749	2.5498	961.9022
1389	41.1009	2.5482	397.5082	1389	41.1009	2.5482	900.8857	1389	41.1009	2.5482	462.0925	1389	41.1009	2.5482	984.6336
1390	41.1269	2.5467	372.3392	1390	41.1269	2.5467	876.9739	1390	41.1269	2.5467	507.2299	1390	41.1269	2.5467	1029.2315
1391	41.1529	2.5451	395.6919	1391	41.1529	2.5451	901.584	1391	41.1529	2.5451	462.4177	1391	41.1529	2.5451	983.8798
1392	41.1789	2.5436	395.624	1392	41.1789	2.5436	902.7733	1392	41.1789	2.5436	445.5309	1392	41.1789	2.5436	966.4535
1393	41.2049	2.5421	399.0075	1393	41.2049	2.5421	907.4141	1393	41.2049	2.5421	434.907	1393	41.2049	2.5421	955.2901
1394	41.2309	2.5405	369.6926	1394	41.2309	2.5405	879.3565	1394	41.2309	2.5405	471.5009	1394	41.2309	2.5405	991.3445
1395	41.2569	2.539	379.505	1395	41.2569	2.539	890.4262	1395	41.2569	2.539	419.9239	1395	41.2569	2.539	939.228
1396	41.2829	2.5375	424.0295	1396	41.2829	2.5375	936.208	1396	41.2829	2.5375	456.1459	1396	41.2829	2.5375	974.9105
1397	41.3089	2.5359	418.1188	1397	41.3089	2.5359	931.5546	1397	41.3089	2.5359	479.2114	1397	41.3089	2.5359	997.4365
1398	41.3349	2.5344	408.0719	1398	41.3349	2.5344	922.7649	1398	41.3349	2.5344	456.6818	1398	41.3349	2.5344	974.3674
1399	41.3609	2.5329	370.4937	1399	41.3609	2.5329	886.4441	1399	41.3609	2.5329	453.4601	1399	41.3609	2.5329	970.6062

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1400	41.3869	2.5314	395.1707	1400	41.3869	2.5314	912.3783	1400	41.3869	2.5314	535.9507	1400	41.3869	2.5314	1052.5573
1401	41.4129	2.5298	458.4219	1401	41.4129	2.5298	976.8869	1401	41.4129	2.5298	507.234	1401	41.4129	2.5298	1023.3011
1402	41.4389	2.5283	417.6506	1402	41.4389	2.5283	937.3728	1402	41.4389	2.5283	484.492	1402	41.4389	2.5283	1000.0196
1403	41.4649	2.5268	436.6863	1403	41.4649	2.5268	957.6658	1403	41.4649	2.5268	546.2545	1403	41.4649	2.5268	1061.2427
1404	41.4909	2.5253	425.6354	1404	41.4909	2.5253	947.8722	1404	41.4909	2.5253	516.4177	1404	41.4909	2.5253	1030.8664
1405	41.5169	2.5238	465.2217	1405	41.5169	2.5238	988.7157	1405	41.5169	2.5238	496.306	1405	41.5169	2.5238	1010.2152
1406	41.5429	2.5223	416.9094	1406	41.5429	2.5223	940.4095	1406	41.5429	2.5223	552.3876	1406	41.5429	2.5223	1065.7572
1407	41.5689	2.5208	571.1734	1407	41.5689	2.5208	1094.6794	1407	41.5689	2.5208	533.3176	1407	41.5689	2.5208	1046.1478
1408	41.5949	2.5193	663.5334	1408	41.5949	2.5193	1187.0454	1408	41.5949	2.5193	538.0074	1408	41.5949	2.5193	1050.298
1409	41.6209	2.5178	713.7761	1409	41.6209	2.5178	1237.2941	1409	41.6209	2.5178	571.0724	1409	41.6209	2.5178	1082.8235
1410	41.6469	2.5163	725.6979	1410	41.6469	2.5163	1249.2218	1410	41.6469	2.5163	598.4765	1410	41.6469	2.5163	1109.6882
1411	41.6729	2.5148	836.9534	1411	41.6729	2.5148	1360.4834	1411	41.6729	2.5148	583.5383	1411	41.6729	2.5148	1094.2105
1412	41.6989	2.5133	783.4832	1412	41.6989	2.5133	1307.0192	1412	41.6989	2.5133	605.8595	1412	41.6989	2.5133	1115.9922
1413	41.7249	2.5118	771.5814	1413	41.7249	2.5118	1295.1233	1413	41.7249	2.5118	695.4819	1413	41.7249	2.5118	1205.0751
1414	41.7509	2.5103	728.3409	1414	41.7509	2.5103	1251.8888	1414	41.7509	2.5103	756.7142	1414	41.7509	2.5103	1265.7678
1415	41.7769	2.5088	724.5365	1415	41.7769	2.5088	1248.0904	1415	41.7769	2.5088	765.275	1415	41.7769	2.5088	1273.7891
1416	41.8029	2.5073	735.9596	1416	41.8029	2.5073	1259.5195	1416	41.8029	2.5073	718.9875	1416	41.8029	2.5073	1226.9622
1417	41.8289	2.5058	690.8326	1417	41.8289	2.5058	1214.3984	1417	41.8289	2.5058	885.7208	1417	41.8289	2.5058	1393.156
1418	41.8549	2.5043	774.9185	1418	41.8549	2.5043	1298.4903	1418	41.8549	2.5043	1014.4985	1418	41.8549	2.5043	1521.3942
1419	41.8809	2.5028	894.8355	1419	41.8809	2.5028	1418.4133	1419	41.8809	2.5028	1278.4458	1419	41.8809	2.5028	1784.802
1420	41.9069	2.5013	1015.6888	1420	41.9069	2.5013	1539.2726	1420	41.9069	2.5013	1511.6852	1420	41.9069	2.5013	2017.5019
1421	41.9329	2.4999	1128.2792	1421	41.9329	2.4999	1651.8689	1421	41.9329	2.4999	1978.6123	1421	41.9329	2.4999	2483.8895
1422	41.9589	2.4984	1348.2027	1422	41.9589	2.4984	1871.7984	1422	41.9589	2.4984	2567.1174	1422	41.9589	2.4984	3071.8551
1423	41.9849	2.4969	1447.0908	1423	41.9849	2.4969	1970.6925	1423	41.9849	2.4969	3172.7878	1423	41.9849	2.4969	3676.986
1424	42.0109	2.4954	1304.0524	1424	42.0109	2.4954	1827.6601	1424	42.0109	2.4954	3497.47	1424	42.0109	2.4954	4001.1287
1425	42.0369	2.494	1191.9676	1425	42.0369	2.494	1715.5812	1425	42.0369	2.494	3599.9213	1425	42.0369	2.494	4103.0405
1426	42.0629	2.4925	1217.1134	1426	42.0629	2.4925	1740.733	1426	42.0629	2.4925	3262.6841	1426	42.0629	2.4925	3765.2638
1427	42.0889	2.491	1074.4825	1427	42.0889	2.491	1598.1081	1427	42.0889	2.491	2906.6236	1427	42.0889	2.491	3408.6638
1428	42.1149	2.4895	901.2129	1428	42.1149	2.4895	1424.8445	1428	42.1149	2.4895	2677.0718	1428	42.1149	2.4895	3178.5725
1429	42.1409	2.4881	822.6735	1429	42.1409	2.4881	1346.3111	1429	42.1409	2.4881	2217.7531	1429	42.1409	2.4881	2718.7143
1430	42.1669	2.4866	722.8627	1430	42.1669	2.4866	1246.5062	1430	42.1669	2.4866	1771.961	1430	42.1669	2.4866	2272.3828
1431	42.1929	2.4852	730.1175	1431	42.1929	2.4852	1253.767	1431	42.1929	2.4852	1417.5253	1431	42.1929	2.4852	1917.4075
1432	42.2189	2.4837	720.3205	1432	42.2189	2.4837	1243.976	1432	42.2189	2.4837	1164.5742	1432	42.2189	2.4837	1663.917
1433	42.2449	2.4822	713.1734	1433	42.2449	2.4822	1236.8349	1433	42.2449	2.4822	1004.2529	1433	42.2449	2.4822	1503.0561
1434	42.2709	2.4808	740.4613	1434	42.2709	2.4808	1264.1288	1434	42.2709	2.4808	895.8194	1434	42.2709	2.4808	1394.0832
1435	42.2969	2.4793	756.0409	1435	42.2969	2.4793	1279.7143	1435	42.2969	2.4793	775.5324	1435	42.2969	2.4793	1273.2566

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1436	42.3229	2.4779	682.9311	1436	42.3229	2.4779	1206.6105	1436	42.3229	2.4779	730.062	1436	42.3229	2.4779	1227.2468
1437	42.3489	2.4764	645.0345	1437	42.3489	2.4764	1168.7198	1437	42.3489	2.4764	633.661	1437	42.3489	2.4764	1130.3063
1438	42.3749	2.475	638.8253	1438	42.3749	2.475	1162.5167	1438	42.3749	2.475	610.5693	1438	42.3749	2.475	1106.675
1439	42.4009	2.4735	543.9078	1439	42.4009	2.4735	1067.6051	1439	42.4009	2.4735	594.4084	1439	42.4009	2.4735	1089.9747
1440	42.4269	2.4721	544.6659	1440	42.4269	2.4721	1068.3692	1440	42.4269	2.4721	553.3258	1440	42.4269	2.4721	1048.3526
1441	42.4529	2.4706	517.7125	1441	42.4529	2.4706	1041.4218	1441	42.4529	2.4706	568.9887	1441	42.4529	2.4706	1063.4759
1442	42.4789	2.4692	506.1986	1442	42.4789	2.4692	1029.9138	1442	42.4789	2.4692	508.7487	1442	42.4789	2.4692	1002.6964
1443	42.5049	2.4677	444.6098	1443	42.5049	2.4677	968.331	1443	42.5049	2.4677	496.5852	1443	42.5049	2.4677	989.9934
1444	42.5309	2.4663	425.8226	1444	42.5309	2.4663	949.5498	1444	42.5309	2.4663	498.9921	1444	42.5309	2.4663	991.8608
1445	42.5569	2.4649	431.6112	1445	42.5569	2.4649	955.3444	1445	42.5569	2.4649	487.932	1445	42.5569	2.4649	980.2613
1446	42.5829	2.4634	439.546	1446	42.5829	2.4634	963.2852	1446	42.5829	2.4634	512.0263	1446	42.5829	2.4634	1003.8161
1447	42.6089	2.462	420.4221	1447	42.6089	2.462	944.1672	1447	42.6089	2.462	529.3592	1447	42.6089	2.462	1020.6095
1448	42.6349	2.4606	409.5338	1448	42.6349	2.4606	933.2849	1448	42.6349	2.4606	479.8938	1448	42.6349	2.4606	970.6046
1449	42.6609	2.4591	390.0022	1449	42.6609	2.4591	913.7593	1449	42.6609	2.4591	453.0938	1449	42.6609	2.4591	943.265
1450	42.6869	2.4577	388.8211	1450	42.6869	2.4577	912.5842	1450	42.6869	2.4577	481.7625	1450	42.6869	2.4577	971.3943
1451	42.7129	2.4563	407.4845	1451	42.7129	2.4563	931.2535	1451	42.7129	2.4563	505.0345	1451	42.7129	2.4563	994.1268
1452	42.7389	2.4549	415.8277	1452	42.7389	2.4549	939.6028	1452	42.7389	2.4549	474.4875	1452	42.7389	2.4549	963.0403
1453	42.7649	2.4534	393.6914	1453	42.7649	2.4534	917.4724	1453	42.7649	2.4534	461.472	1453	42.7649	2.4534	949.4853
1454	42.7909	2.452	377.6301	1454	42.7909	2.452	901.4171	1454	42.7909	2.452	511.0786	1454	42.7909	2.452	998.5524
1455	42.8169	2.4506	377.78	1455	42.8169	2.4506	901.573	1455	42.8169	2.4506	464.7125	1455	42.8169	2.4506	951.6468
1456	42.8429	2.4492	360.183	1456	42.8429	2.4492	883.9819	1456	42.8429	2.4492	413.7989	1456	42.8429	2.4492	900.1937
1457	42.8689	2.4478	361.683	1457	42.8689	2.4478	885.488	1457	42.8689	2.4478	405.3162	1457	42.8689	2.4478	891.1714
1458	42.8949	2.4464	395.9179	1458	42.8949	2.4464	919.7288	1458	42.8949	2.4464	403.3757	1458	42.8949	2.4464	888.6915
1459	42.9209	2.4449	397.6509	1459	42.9209	2.4449	921.4678	1459	42.9209	2.4449	418.1566	1459	42.9209	2.4449	902.9329
1460	42.9469	2.4435	392.5361	1460	42.9469	2.4435	915.8974	1460	42.9469	2.4435	430.5203	1460	42.9469	2.4435	914.7571
1461	42.9729	2.4421	381.0697	1461	42.9729	2.4421	903.9753	1461	42.9729	2.4421	423.9798	1461	42.9729	2.4421	907.6771
1462	42.9989	2.4407	343.4159	1462	42.9989	2.4407	865.8658	1462	42.9989	2.4407	434.494	1462	42.9989	2.4407	917.6518
1463	43.0249	2.4393	353.6349	1463	43.0249	2.4393	875.6293	1463	43.0249	2.4393	434.1693	1463	43.0249	2.4393	916.7876
1464	43.0509	2.4379	396.5208	1464	43.0509	2.4379	918.0595	1464	43.0509	2.4379	409.0191	1464	43.0509	2.4379	891.0979
1465	43.0769	2.4365	418.4971	1465	43.0769	2.4365	939.5802	1465	43.0769	2.4365	448.6256	1465	43.0769	2.4365	930.165
1466	43.1029	2.4351	389.8014	1466	43.1029	2.4351	910.4288	1466	43.1029	2.4351	475.5912	1466	43.1029	2.4351	956.591
1467	43.1289	2.4337	381.7799	1467	43.1289	2.4337	901.9518	1467	43.1289	2.4337	433.0211	1467	43.1289	2.4337	913.4815
1468	43.1549	2.4323	417.1799	1468	43.1549	2.4323	936.8961	1468	43.1549	2.4323	367.8995	1468	43.1549	2.4323	847.8203
1469	43.1809	2.4309	422.1958	1469	43.1809	2.4309	941.4563	1469	43.1809	2.4309	364.235	1469	43.1809	2.4309	843.6163
1470	43.2069	2.4295	440.1951	1470	43.2069	2.4295	959	1470	43.2069	2.4295	395.9226	1470	43.2069	2.4295	874.7644
1471	43.2329	2.4281	406.6839	1471	43.2329	2.4281	925.0331	1471	43.2329	2.4281	380.8653	1471	43.2329	2.4281	859.1676

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1472	43.2589	2.4267	396.707	1472	43.2589	2.4267	914.6006	1472	43.2589	2.4267	432.1535	1472	43.2589	2.4267	909.9163
1473	43.2849	2.4254	435.209	1473	43.2849	2.4254	952.647	1473	43.2849	2.4254	412.0988	1473	43.2849	2.4254	889.3222
1474	43.3109	2.424	413.2467	1474	43.3109	2.424	930.2291	1474	43.3109	2.424	368.2345	1474	43.3109	2.424	844.9184
1475	43.3369	2.4226	400.6226	1475	43.3369	2.4226	917.1493	1475	43.3369	2.4226	406.2081	1475	43.3369	2.4226	882.3525
1476	43.3629	2.4212	402.5676	1476	43.3629	2.4212	918.6388	1476	43.3629	2.4212	432.2905	1476	43.3629	2.4212	907.8953
1477	43.3889	2.4198	442.1027	1477	43.3889	2.4198	957.7182	1477	43.3889	2.4198	442.0241	1477	43.3889	2.4198	917.0895
1478	43.4149	2.4184	394.876	1478	43.4149	2.4184	910.0359	1478	43.4149	2.4184	456.5116	1478	43.4149	2.4184	931.0374
1479	43.4409	2.4171	381.3094	1479	43.4409	2.4171	896.0137	1479	43.4409	2.4171	432.7334	1479	43.4409	2.4171	906.7198
1480	43.4669	2.4157	357.8579	1480	43.4669	2.4157	872.1065	1480	43.4669	2.4157	420.8109	1480	43.4669	2.4157	894.2578
1481	43.4929	2.4143	323.9277	1481	43.4929	2.4143	837.7206	1481	43.4929	2.4143	368.5131	1481	43.4929	2.4143	841.4205
1482	43.5189	2.4129	398.3915	1482	43.5189	2.4129	911.7288	1482	43.5189	2.4129	393.666	1482	43.5189	2.4129	866.0339
1483	43.5449	2.4116	423.3296	1483	43.5449	2.4116	936.2113	1483	43.5449	2.4116	367.1943	1483	43.5449	2.4116	839.0227
1484	43.5709	2.4102	393.3119	1484	43.5709	2.4102	905.738	1484	43.5709	2.4102	420.7144	1484	43.5709	2.4102	892.0033
1485	43.5969	2.4088	366.8397	1485	43.5969	2.4088	878.8102	1485	43.5969	2.4088	399.1809	1485	43.5969	2.4088	869.9303
1486	43.6229	2.4075	397.6509	1486	43.6229	2.4075	909.1657	1486	43.6229	2.4075	373.8986	1486	43.6229	2.4075	844.1085
1487	43.6489	2.4061	410.7419	1487	43.6489	2.4061	920.5694	1487	43.6489	2.4061	423.4975	1487	43.6489	2.4061	893.1679
1488	43.6749	2.4047	398.173	1488	43.6749	2.4047	906.3131	1488	43.6749	2.4047	407.7125	1488	43.6749	2.4047	876.8434
1489	43.7009	2.4034	435.0816	1489	43.7009	2.4034	941.5344	1489	43.7009	2.4034	388.1673	1489	43.7009	2.4034	856.7587
1490	43.7269	2.402	444.8488	1490	43.7269	2.402	949.6144	1490	43.7269	2.402	381.0422	1490	43.7269	2.402	849.0941
1491	43.7529	2.4007	424.3483	1491	43.7529	2.4007	927.4266	1491	43.7529	2.4007	403.3507	1491	43.7529	2.4007	870.8631
1492	43.7789	2.3993	407.1659	1492	43.7789	2.3993	908.5569	1492	43.7789	2.3993	409.2916	1492	43.7789	2.3993	876.2645
1493	43.8049	2.398	470.5806	1493	43.8049	2.398	970.2842	1493	43.8049	2.398	407.7899	1493	43.8049	2.398	874.2233
1494	43.8309	2.3966	424.1684	1494	43.8309	2.3966	922.1848	1494	43.8309	2.3966	370.8027	1494	43.8309	2.3966	836.6966
1495	43.8569	2.3953	463.7841	1495	43.8569	2.3953	960.1131	1495	43.8569	2.3953	397.1237	1495	43.8569	2.3953	862.4781
1496	43.8829	2.3939	474.8598	1496	43.8829	2.3939	969.5015	1496	43.8829	2.3939	387.9982	1496	43.8829	2.3939	852.8131
1497	43.9089	2.3926	482.7956	1497	43.9089	2.3926	975.75	1497	43.9089	2.3926	417.4121	1497	43.9089	2.3926	881.6875
1498	43.9349	2.3912	527.0504	1498	43.9349	2.3912	1018.3175	1498	43.9349	2.3912	386.3375	1498	43.9349	2.3912	850.0734
1499	43.9609	2.3899	512.4691	1499	43.9609	2.3899	1002.0489	1499	43.9609	2.3899	374.305	1499	43.9609	2.3899	837.5014
1500	43.9869	2.3885	582.3368	1500	43.9869	2.3885	1070.2292	1500	43.9869	2.3885	400.3075	1500	43.9869	2.3885	862.9644
1501	44.0129	2.3872	572.4942	1501	44.0129	2.3872	1058.6994	1501	44.0129	2.3872	378.6004	1501	44.0129	2.3872	840.7178
1502	44.0389	2.3858	586.7336	1502	44.0389	2.3858	1071.2514	1502	44.0389	2.3858	376.3536	1502	44.0389	2.3858	837.9315
1503	44.0649	2.3845	654.3922	1503	44.0649	2.3845	1137.2227	1503	44.0649	2.3845	436.7992	1503	44.0649	2.3845	897.8376
1504	44.0909	2.3832	709.3701	1504	44.0909	2.3832	1190.5133	1504	44.0909	2.3832	447.1235	1504	44.0909	2.3832	907.6225
1505	44.1169	2.3818	772.996	1505	44.1169	2.3818	1252.4519	1505	44.1169	2.3818	374.1148	1505	44.1169	2.3818	834.0742
1506	44.1429	2.3805	958.073	1506	44.1429	2.3805	1435.8416	1506	44.1429	2.3805	419.8978	1506	44.1429	2.3805	879.3178
1507	44.1689	2.3792	1107.982	1507	44.1689	2.3792	1584.0633	1507	44.1689	2.3792	369.8039	1507	44.1689	2.3792	828.6843

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1508	44.1949	2.3778	1310.3646	1508	44.1949	2.3778	1784.7586	1508	44.1949	2.3778	382.554	1508	44.1949	2.3778	840.895
1509	44.2209	2.3765	1677.8747	1509	44.2209	2.3765	2150.5814	1509	44.2209	2.3765	401.0498	1509	44.2209	2.3765	858.8513
1510	44.2469	2.3752	1849.9806	1510	44.2469	2.3752	2321	1510	44.2469	2.3752	398.1197	1510	44.2469	2.3752	855.3816
1511	44.2729	2.3739	1848.8591	1511	44.2729	2.3739	2318.1912	1511	44.2729	2.3739	412.711	1511	44.2729	2.3739	869.4335
1512	44.2989	2.3725	1691.066	1512	44.2989	2.3725	2158.7108	1512	44.2989	2.3725	437.7206	1512	44.2989	2.3725	893.9036
1513	44.3249	2.3712	1654.1403	1513	44.3249	2.3712	2120.0977	1513	44.3249	2.3712	425.3891	1513	44.3249	2.3712	881.0326
1514	44.3509	2.3699	1409.8246	1514	44.3509	2.3699	1874.0947	1514	44.3509	2.3699	403.1819	1514	44.3509	2.3699	858.2859
1515	44.3769	2.3686	1289.144	1515	44.3769	2.3686	1751.7268	1515	44.3769	2.3686	470.8933	1515	44.3769	2.3686	925.4578
1516	44.4029	2.3673	1049.076	1516	44.4029	2.3673	1509.9715	1516	44.4029	2.3673	392.6537	1516	44.4029	2.3673	846.6787
1517	44.4289	2.3659	946.0535	1517	44.4289	2.3659	1405.2617	1517	44.4289	2.3659	424.0377	1517	44.4289	2.3659	877.5232
1518	44.4549	2.3646	846.7951	1518	44.4549	2.3646	1304.316	1518	44.4549	2.3646	463.9693	1518	44.4549	2.3646	916.9153
1519	44.4809	2.3633	767.1916	1519	44.4809	2.3633	1223.0252	1519	44.4809	2.3633	379.3632	1519	44.4809	2.3633	831.7697
1520	44.5069	2.362	673.8341	1520	44.5069	2.362	1127.9804	1520	44.5069	2.362	358.3564	1520	44.5069	2.362	810.2234
1521	44.5329	2.3607	663.9504	1521	44.5329	2.3607	1116.4094	1521	44.5329	2.3607	389.8065	1521	44.5329	2.3607	841.134
1522	44.5589	2.3594	593.4811	1522	44.5589	2.3594	1044.2528	1522	44.5589	2.3594	424.0906	1522	44.5589	2.3594	874.8786
1523	44.5849	2.3581	527.7315	1523	44.5849	2.3581	976.8159	1523	44.5849	2.3581	451.1065	1523	44.5849	2.3581	901.355
1524	44.6109	2.3568	463.0836	1524	44.6109	2.3568	910.4807	1524	44.6109	2.3568	384.9998	1524	44.6109	2.3568	834.7088
1525	44.6369	2.3555	462.5608	1525	44.6369	2.3555	908.2706	1525	44.6369	2.3555	389.1285	1525	44.6369	2.3555	838.298
1526	44.6629	2.3542	464.9776	1526	44.6629	2.3542	909	1526	44.6629	2.3542	395.7125	1526	44.6629	2.3542	844.3425
1527	44.6889	2.3529	496.7152	1527	44.6889	2.3529	939.0504	1527	44.6889	2.3529	417.5154	1527	44.6889	2.3529	865.606
1528	44.7149	2.3516	470.2545	1528	44.7149	2.3516	910.9023	1528	44.7149	2.3516	446.0601	1528	44.7149	2.3516	893.6111
1529	44.7409	2.3503	466.0395	1529	44.7409	2.3503	905	1529	44.7409	2.3503	442.6011	1529	44.7409	2.3503	889.6126
1530	44.7669	2.349	439.5471	1530	44.7669	2.349	876.8203	1530	44.7669	2.349	395.1144	1530	44.7669	2.349	841.5864
1531	44.7929	2.3477	425.5874	1531	44.7929	2.3477	861.1733	1531	44.7929	2.3477	404.0831	1531	44.7929	2.3477	850.0156
1532	44.8189	2.3464	391.9336	1532	44.8189	2.3464	825.8322	1532	44.8189	2.3464	471.7066	1532	44.8189	2.3464	917.0997
1533	44.8449	2.3451	394.5782	1533	44.8449	2.3451	826.7895	1533	44.8449	2.3451	460.7779	1533	44.8449	2.3451	905.6314
1534	44.8709	2.3438	418.2042	1534	44.8709	2.3438	848.7281	1534	44.8709	2.3438	440.4817	1534	44.8709	2.3438	884.7957
1535	44.8969	2.3425	399.4496	1535	44.8969	2.3425	828.2863	1535	44.8969	2.3425	459.8224	1535	44.8969	2.3425	903.5969
1536	44.9229	2.3413	421.5448	1536	44.9229	2.3413	848.6941	1536	44.9229	2.3413	478.3042	1536	44.9229	2.3413	921.5392
1537	44.9489	2.34	486.2118	1537	44.9489	2.34	911.6738	1537	44.9489	2.34	506.6039	1537	44.9489	2.34	949.2995
1538	44.9749	2.3387	407.0491	1538	44.9749	2.3387	830.8238	1538	44.9749	2.3387	458.6362	1538	44.9749	2.3387	900.7923
1539	45.0009	2.3374	378.8706	1539	45.0009	2.3374	800.9581	1539	45.0009	2.3374	449.2576	1539	45.0009	2.3374	890.8742
1540	45.0269	2.3361	397.6509	1540	45.0269	2.3361	818.051	1540	45.0269	2.3361	437.6015	1540	45.0269	2.3361	878.6786
1541	45.0529	2.3349	416.5907	1541	45.0529	2.3349	837.6737	1541	45.0529	2.3349	460.5295	1541	45.0529	2.3349	901.0671
1542	45.0789	2.3336	396.3929	1542	45.0789	2.3336	818.1588	1542	45.0789	2.3336	425.8684	1542	45.0789	2.3336	865.8664
1543	45.1049	2.3323	382.052	1543	45.1049	2.3323	804.5009	1543	45.1049	2.3323	437.6339	1543	45.1049	2.3323	877.0925

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1544	45.1309	2.331	402.635	1544	45.1309	2.331	825.7668	1544	45.1309	2.331	431.7637	1544	45.1309	2.331	870.6827
1545	45.1569	2.3298	406.0654	1545	45.1569	2.3298	829.8802	1545	45.1569	2.3298	450.8196	1545	45.1569	2.3298	889.1992
1546	45.1829	2.3285	362.9689	1546	45.1829	2.3285	787.4666	1546	45.1829	2.3285	462.8198	1546	45.1829	2.3285	900.6599
1547	45.2089	2.3272	364.6039	1547	45.2089	2.3272	789.7845	1547	45.2089	2.3272	471.9413	1547	45.2089	2.3272	909.2419
1548	45.2349	2.3259	371.8854	1548	45.2349	2.3259	797.7489	1548	45.2349	2.3259	459.6832	1548	45.2349	2.3259	896.4442
1549	45.2609	2.3247	372.0147	1549	45.2609	2.3247	798.5612	1549	45.2609	2.3247	473.1886	1549	45.2609	2.3247	909.4102
1550	45.2869	2.3234	355.1203	1550	45.2869	2.3234	782.3497	1550	45.2869	2.3234	509.0112	1550	45.2869	2.3234	944.6933
1551	45.3129	2.3222	361.4602	1551	45.3129	2.3222	789.3725	1551	45.3129	2.3222	496.1782	1551	45.3129	2.3222	931.3208
1552	45.3389	2.3209	396.4363	1552	45.3389	2.3209	825.0315	1552	45.3389	2.3209	479.1759	1552	45.3389	2.3209	913.779
1553	45.3649	2.3196	373.2834	1553	45.3649	2.3196	802.5615	1553	45.3649	2.3196	487.3448	1553	45.3649	2.3196	921.4084
1554	45.3909	2.3184	387.7959	1554	45.3909	2.3184	817.7569	1554	45.3909	2.3184	467.486	1554	45.3909	2.3184	901.0101
1555	45.4169	2.3171	379.3491	1555	45.4169	2.3171	809.993	1555	45.4169	2.3171	467.4381	1555	45.4169	2.3171	900.4227
1556	45.4429	2.3159	360.6648	1556	45.4429	2.3159	791.9917	1556	45.4429	2.3159	505.1008	1556	45.4429	2.3159	937.5459
1557	45.4689	2.3146	381.1348	1557	45.4689	2.3146	813.1446	1557	45.4689	2.3146	503.3406	1557	45.4689	2.3146	935.2462
1558	45.4949	2.3134	381.8384	1558	45.4949	2.3134	814.5312	1558	45.4949	2.3134	538.876	1558	45.4949	2.3134	970.2421
1559	45.5209	2.3121	380.1993	1559	45.5209	2.3121	813.575	1559	45.5209	2.3121	551.9557	1559	45.5209	2.3121	982.7823
1560	45.5469	2.3109	401.8758	1560	45.5469	2.3109	835.9344	1560	45.5469	2.3109	539.9292	1560	45.5469	2.3109	970.2164
1561	45.5729	2.3096	365.221	1561	45.5729	2.3096	799.9625	1561	45.5729	2.3096	554.9009	1561	45.5729	2.3096	984.6486
1562	45.5989	2.3084	331.3581	1562	45.5989	2.3084	766.7825	1562	45.5989	2.3084	570.5518	1562	45.5989	2.3084	999.7599
1563	45.6249	2.3071	358.9368	1563	45.6249	2.3071	795.0441	1563	45.6249	2.3071	566.2872	1563	45.6249	2.3071	994.9559
1564	45.6509	2.3059	388.9534	1564	45.6509	2.3059	825.7437	1564	45.6509	2.3059	553.3282	1564	45.6509	2.3059	981.4573
1565	45.6769	2.3046	403.0453	1565	45.6769	2.3046	840.5185	1565	45.6769	2.3046	538.1121	1565	45.6769	2.3046	965.7017
1566	45.7029	2.3034	422.1232	1566	45.7029	2.3034	860.2793	1566	45.7029	2.3034	545.3601	1566	45.7029	2.3034	972.4103
1567	45.7289	2.3021	434.4655	1567	45.7289	2.3021	873.3045	1567	45.7289	2.3021	595.342	1567	45.7289	2.3021	1021.8527
1568	45.7549	2.3009	430.1581	1568	45.7549	2.3009	869.68	1568	45.7549	2.3009	673.6927	1568	45.7549	2.3009	1099.6639
1569	45.7809	2.2997	421.5632	1569	45.7809	2.2997	861.768	1569	45.7809	2.2997	763.5443	1569	45.7809	2.2997	1188.976
1570	45.8069	2.2984	372.7649	1570	45.8069	2.2984	813.6527	1570	45.8069	2.2984	784.0375	1570	45.8069	2.2984	1208.9296
1571	45.8329	2.2972	349.6673	1571	45.8329	2.2972	791.238	1571	45.8329	2.2972	828.3514	1571	45.8329	2.2972	1252.7041
1572	45.8589	2.296	391.2952	1572	45.8589	2.296	833.5489	1572	45.8589	2.296	916.313	1572	45.8589	2.296	1340.1261
1573	45.8849	2.2947	443.5518	1573	45.8849	2.2947	886.4884	1573	45.8849	2.2947	995.0605	1573	45.8849	2.2947	1418.3342
1574	45.9109	2.2935	464.2426	1574	45.9109	2.2935	907.8621	1574	45.9109	2.2935	1119.2523	1574	45.9109	2.2935	1541.9865
1575	45.9369	2.2923	432.3181	1575	45.9369	2.2923	876.6205	1575	45.9369	2.2923	1267.2063	1575	45.9369	2.2923	1689.401
1576	45.9629	2.2911	412.4752	1576	45.9629	2.2911	857.4605	1576	45.9629	2.2911	1567.6184	1576	45.9629	2.2911	1989.2736
1577	45.9889	2.2898	476.342	1577	45.9889	2.2898	922.0102	1577	45.9889	2.2898	1983.0304	1577	45.9889	2.2898	2404.1461
1578	46.0149	2.2886	562.3067	1578	46.0149	2.2886	1008.6579	1578	46.0149	2.2886	2642.7447	1578	46.0149	2.2886	3063.3208
1579	46.0409	2.2874	635.8544	1579	46.0409	2.2874	1082.8885	1579	46.0409	2.2874	3631.3742	1579	46.0409	2.2874	4051.4108

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1580	46.0669	2.2862	617.6347	1580	46.0669	2.2862	1065.3517	1580	46.0669	2.2862	4590.6572	1580	46.0669	2.2862	5010.1543
1581	46.0929	2.2849	596.9545	1581	46.0929	2.2849	1045.3544	1581	46.0929	2.2849	5212.3823	1581	46.0929	2.2849	5631.34
1582	46.1189	2.2837	605.5542	1582	46.1189	2.2837	1054.6371	1582	46.1189	2.2837	5266.5739	1582	46.1189	2.2837	5684.9921
1583	46.1449	2.2825	624.9019	1583	46.1449	2.2825	1074.6677	1583	46.1449	2.2825	4865.6222	1583	46.1449	2.2825	5283.5009
1584	46.1709	2.2813	633.8389	1584	46.1709	2.2813	1084.2876	1584	46.1709	2.2813	4458.943	1584	46.1709	2.2813	4876.2822
1585	46.1969	2.2801	650.2396	1585	46.1969	2.2801	1101.3713	1585	46.1969	2.2801	4127.1817	1585	46.1969	2.2801	4543.9814
1586	46.2229	2.2789	606.5802	1586	46.2229	2.2789	1058.3948	1586	46.2229	2.2789	3583.2107	1586	46.2229	2.2789	3999.4709
1587	46.2489	2.2777	674.6134	1587	46.2489	2.2777	1127.1109	1587	46.2489	2.2777	2973.6923	1587	46.2489	2.2777	3389.413
1588	46.2749	2.2765	746.8984	1588	46.2749	2.2765	1200.0788	1588	46.2749	2.2765	2325.6247	1588	46.2749	2.2765	2740.8059
1589	46.3009	2.2752	836.9312	1589	46.3009	2.2752	1290.7946	1589	46.3009	2.2752	1843.6173	1589	46.3009	2.2752	2258.259
1590	46.3269	2.274	903.3963	1590	46.3269	2.274	1357.9425	1590	46.3269	2.274	1472.0968	1590	46.3269	2.274	1886.199
1591	46.3529	2.2728	983.7392	1591	46.3529	2.2728	1438.9683	1591	46.3529	2.2728	1252.9978	1591	46.3529	2.2728	1666.5606
1592	46.3789	2.2716	1085.5426	1592	46.3789	2.2716	1541.4547	1592	46.3789	2.2716	1094.7183	1592	46.3789	2.2716	1507.7415
1593	46.4049	2.2704	1055.8495	1593	46.4049	2.2704	1512.4445	1593	46.4049	2.2704	962.0528	1593	46.4049	2.2704	1374.5366
1594	46.4309	2.2692	1060.2649	1594	46.4309	2.2692	1517.5429	1594	46.4309	2.2692	894.4285	1594	46.4309	2.2692	1306.3727
1595	46.4569	2.268	1033.3932	1595	46.4569	2.268	1489.9906	1595	46.4569	2.268	827.2894	1595	46.4569	2.268	1238.6941
1596	46.4829	2.2668	983.8206	1596	46.4829	2.2668	1439.7373	1596	46.4829	2.2668	738.482	1596	46.4829	2.2668	1149.3472
1597	46.5089	2.2656	930.1871	1597	46.5089	2.2656	1385.4233	1597	46.5089	2.2656	709.2087	1597	46.5089	2.2656	1119.5344
1598	46.5349	2.2644	881.7951	1598	46.5349	2.2644	1336.3508	1598	46.5349	2.2644	650.8367	1598	46.5349	2.2644	1060.623
1599	46.5609	2.2632	751.1029	1599	46.5609	2.2632	1204.9779	1599	46.5609	2.2632	666.5167	1599	46.5609	2.2632	1075.7635
1600	46.5869	2.262	646.6851	1600	46.5869	2.262	1099.8796	1600	46.5869	2.262	604.1447	1600	46.5869	2.262	1012.8519
1601	46.6129	2.2609	646.5556	1601	46.6129	2.2609	1099.0695	1601	46.6129	2.2609	592.9459	1601	46.6129	2.2609	1001.1136
1602	46.6389	2.2597	556.1667	1602	46.6389	2.2597	1008	1602	46.6389	2.2597	600.7063	1602	46.6389	2.2597	1008.3346
1603	46.6649	2.2585	553.0857	1603	46.6649	2.2585	1004.2385	1603	46.6649	2.2585	539.8215	1603	46.6649	2.2585	946.9103
1604	46.6909	2.2573	519.2583	1604	46.6909	2.2573	969.7304	1604	46.6909	2.2573	526.517	1604	46.6909	2.2573	933.0663
1605	46.7169	2.2561	498.2931	1605	46.7169	2.2561	948.0846	1605	46.7169	2.2561	565.4824	1605	46.7169	2.2561	971.4921
1606	46.7429	2.2549	501.4581	1606	46.7429	2.2549	950.5691	1606	46.7429	2.2549	556.0465	1606	46.7429	2.2549	961.5168
1607	46.7689	2.2537	516.7745	1607	46.7689	2.2537	965.2049	1607	46.7689	2.2537	499.6437	1607	46.7689	2.2537	904.5744
1608	46.7949	2.2526	447.4819	1608	46.7949	2.2526	895.2317	1608	46.7949	2.2526	476.2613	1608	46.7949	2.2526	880.6526
1609	46.8209	2.2514	433.4023	1609	46.8209	2.2514	880.4716	1609	46.8209	2.2514	423.8684	1609	46.8209	2.2514	827.7201
1610	46.8469	2.2502	399.8598	1610	46.8469	2.2502	846.2484	1610	46.8469	2.2502	523.9521	1610	46.8469	2.2502	927.2643
1611	46.8729	2.249	352.769	1611	46.8729	2.249	798.4771	1611	46.8729	2.249	503.1726	1611	46.8729	2.249	905.9454
1612	46.8989	2.2478	372.0181	1612	46.8989	2.2478	817.0456	1612	46.8989	2.2478	463.5261	1612	46.8989	2.2478	865.7593
1613	46.9249	2.2467	375.5689	1613	46.9249	2.2467	819.9158	1613	46.9249	2.2467	512.9061	1613	46.9249	2.2467	914.5999
1614	46.9509	2.2455	360.4082	1614	46.9509	2.2455	804.0745	1614	46.9509	2.2455	438.1997	1614	46.9509	2.2455	839.354
1615	46.9769	2.2443	353.1309	1615	46.9769	2.2443	796.1166	1615	46.9769	2.2443	472.8749	1615	46.9769	2.2443	873.4897

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1616	47.0029	2.2431	395.6412	1616	47.0029	2.2431	837.9464	1616	47.0029	2.2431	445.6353	1616	47.0029	2.2431	845.7106
1617	47.0289	2.242	346.1999	1617	47.0289	2.242	787.8245	1617	47.0289	2.242	451.2577	1617	47.0289	2.242	850.7935
1618	47.0549	2.2408	328.8099	1618	47.0549	2.2408	769.7539	1618	47.0549	2.2408	491.1855	1618	47.0549	2.2408	890.1818
1619	47.0809	2.2396	372.2402	1619	47.0809	2.2396	812.5036	1619	47.0809	2.2396	461.3884	1619	47.0809	2.2396	859.8452
1620	47.1069	2.2385	343.5997	1620	47.1069	2.2385	783.1825	1620	47.1069	2.2385	459.1469	1620	47.1069	2.2385	857.0642
1621	47.1329	2.2373	397.6509	1621	47.1329	2.2373	836.5532	1621	47.1329	2.2373	411.4761	1621	47.1329	2.2373	808.8539
1622	47.1589	2.2361	400.5026	1622	47.1589	2.2361	839.1681	1622	47.1589	2.2361	441.1364	1622	47.1589	2.2361	837.9747
1623	47.1849	2.235	362.5176	1623	47.1849	2.235	800.9463	1623	47.1849	2.235	444.7012	1623	47.1849	2.235	841
1624	47.2109	2.2338	323.8595	1624	47.2109	2.2338	762.0514	1624	47.2109	2.2338	450.6174	1624	47.2109	2.2338	846.3767
1625	47.2369	2.2327	369.6719	1625	47.2369	2.2327	807.627	1625	47.2369	2.2327	450.894	1625	47.2369	2.2327	846.1138
1626	47.2629	2.2315	342.107	1626	47.2629	2.2315	779.8253	1626	47.2629	2.2315	437.2993	1626	47.2629	2.2315	831.9796
1627	47.2889	2.2304	375.638	1627	47.2889	2.2304	813.1195	1627	47.2889	2.2304	467.0479	1627	47.2889	2.2304	861.1887
1628	47.3149	2.2292	373.191	1628	47.3149	2.2292	810.4357	1628	47.3149	2.2292	450.1315	1628	47.3149	2.2292	843.7328
1629	47.3409	2.228	364.3735	1629	47.3409	2.228	801.3814	1629	47.3409	2.228	366.5199	1629	47.3409	2.228	759.5818
1630	47.3669	2.2269	298.8118	1630	47.3669	2.2269	735.5829	1630	47.3669	2.2269	432.7899	1630	47.3669	2.2269	825.3122
1631	47.3929	2.2257	307.1323	1631	47.3929	2.2257	743.6666	1631	47.3929	2.2257	422.5639	1631	47.3929	2.2257	814.5468
1632	47.4189	2.2246	332.121	1632	47.4189	2.2246	768.4185	1632	47.4189	2.2246	408.5725	1632	47.4189	2.2246	800.0159
1633	47.4449	2.2234	324.837	1633	47.4449	2.2234	760.8977	1633	47.4449	2.2234	420.0052	1633	47.4449	2.2234	810.9091
1634	47.4709	2.2223	326.1606	1634	47.4709	2.2223	761.9845	1634	47.4709	2.2223	477.0277	1634	47.4709	2.2223	867.392
1635	47.4969	2.2211	357.3179	1635	47.4969	2.2211	792.905	1635	47.4969	2.2211	474.6487	1635	47.4969	2.2211	864.4735
1636	47.5229	2.22	358.6562	1636	47.5229	2.22	794.0065	1636	47.5229	2.22	461.39	1636	47.5229	2.22	850.6754
1637	47.5489	2.2189	376.8318	1637	47.5489	2.2189	811.9454	1637	47.5489	2.2189	446.9801	1637	47.5489	2.2189	835.7259
1638	47.5749	2.2177	354.3494	1638	47.5749	2.2177	789.2261	1638	47.5749	2.2177	439.2504	1638	47.5749	2.2177	827.4568
1639	47.6009	2.2166	354.3275	1639	47.6009	2.2166	788.9674	1639	47.6009	2.2166	459.2571	1639	47.6009	2.2166	846.924
1640	47.6269	2.2154	319.9914	1640	47.6269	2.2154	754.3945	1640	47.6269	2.2154	460.9737	1640	47.6269	2.2154	848.1011
1641	47.6529	2.2143	359.2093	1641	47.6529	2.2143	793.3757	1641	47.6529	2.2143	441.2261	1641	47.6529	2.2143	827.814
1642	47.6789	2.2132	392.7033	1642	47.6789	2.2132	826.6328	1642	47.6789	2.2132	416.2962	1642	47.6789	2.2132	802.3445
1643	47.7049	2.212	406.0908	1643	47.7049	2.212	839.7836	1643	47.7049	2.212	388.2633	1643	47.7049	2.212	773.7721
1644	47.7309	2.2109	379.5441	1644	47.7309	2.2109	813	1644	47.7309	2.2109	390.4957	1644	47.7309	2.2109	775.4651
1645	47.7569	2.2098	340.6463	1645	47.7569	2.2098	773.8655	1645	47.7569	2.2098	426.5189	1645	47.7569	2.2098	810.9488
1646	47.7829	2.2086	390.7	1646	47.7829	2.2086	823.6824	1646	47.7829	2.2086	426.1974	1646	47.7829	2.2086	810.0878
1647	47.8089	2.2075	396.2098	1647	47.8089	2.2075	828.9554	1647	47.8089	2.2075	473.7495	1647	47.8089	2.2075	857.1004
1648	47.8349	2.2064	397.6509	1648	47.8349	2.2064	830.1597	1648	47.8349	2.2064	426.8364	1648	47.8349	2.2064	809.6478
1649	47.8609	2.2052	394.2934	1649	47.8609	2.2052	826.631	1649	47.8609	2.2052	407.5219	1649	47.8609	2.2052	789.7938
1650	47.8869	2.2041	386.9191	1650	47.8869	2.2041	819.0856	1650	47.8869	2.2041	436.1355	1650	47.8869	2.2041	817.8679
1651	47.9129	2.203	397.3125	1651	47.9129	2.203	829.3079	1651	47.9129	2.203	423.5631	1651	47.9129	2.203	804.756

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1652	47.9389	2.2019	415.3051	1652	47.9389	2.2019	847.1293	1652	47.9389	2.2019	443.7345	1652	47.9389	2.2019	824.3879
1653	47.9649	2.2007	404.0957	1653	47.9649	2.2007	835.7488	1653	47.9649	2.2007	393.0981	1653	47.9649	2.2007	773.212
1654	47.9909	2.1996	373.3676	1654	47.9909	2.1996	804.8496	1654	47.9909	2.1996	352.2132	1654	47.9909	2.1996	731.7876
1655	48.0169	2.1985	348.3301	1655	48.0169	2.1985	779.6409	1655	48.0169	2.1985	388.3341	1655	48.0169	2.1985	767.369
1656	48.0429	2.1974	379.2055	1656	48.0429	2.1974	810.3452	1656	48.0429	2.1974	414.3976	1656	48.0429	2.1974	792.893
1657	48.0689	2.1963	396.6578	1657	48.0689	2.1963	827.6263	1657	48.0689	2.1963	407.3765	1657	48.0689	2.1963	785.3324
1658	48.0949	2.1951	393.2314	1658	48.0949	2.1951	824.0289	1658	48.0949	2.1951	417.3464	1658	48.0949	2.1951	794.7628
1659	48.1209	2.194	368.8341	1659	48.1209	2.194	799.4604	1659	48.1209	2.194	392.1555	1659	48.1209	2.194	769.0324
1660	48.1469	2.1929	388.1193	1660	48.1469	2.1929	818.5744	1660	48.1469	2.1929	388.6862	1660	48.1469	2.1929	765.0237
1661	48.1729	2.1918	397.2083	1661	48.1729	2.1918	827.4923	1661	48.1729	2.1918	417.434	1661	48.1729	2.1918	793.232
1662	48.1989	2.1907	393.1309	1662	48.1989	2.1907	823.2438	1662	48.1989	2.1907	416.5508	1662	48.1989	2.1907	791.8093
1663	48.2249	2.1896	428.8602	1663	48.2249	2.1896	858.8019	1663	48.2249	2.1896	414.8268	1663	48.2249	2.1896	789.5457
1664	48.2509	2.1885	420.7672	1664	48.2509	2.1885	850.5379	1664	48.2509	2.1885	393.3584	1664	48.2509	2.1885	767.5379
1665	48.2769	2.1874	404.7187	1665	48.2769	2.1874	834.3182	1665	48.2769	2.1874	405.0793	1665	48.2769	2.1874	778.7193
1666	48.3029	2.1863	411.6541	1666	48.3029	2.1863	841.0825	1666	48.3029	2.1863	423.7242	1666	48.3029	2.1863	796.8247
1667	48.3289	2.1851	436.9715	1667	48.3289	2.1851	866.2287	1667	48.3289	2.1851	402.5001	1667	48.3289	2.1851	775.0611
1668	48.3549	2.184	464.6972	1668	48.3549	2.184	893.7832	1668	48.3549	2.184	425.8745	1668	48.3549	2.184	797.896
1669	48.3809	2.1829	519.5351	1669	48.3809	2.1829	948.4501	1669	48.3809	2.1829	466.2081	1669	48.3809	2.1829	837.69
1670	48.4069	2.1818	570.1509	1670	48.4069	2.1818	998.8947	1670	48.4069	2.1818	463.4698	1670	48.4069	2.1818	834.4123
1671	48.4329	2.1807	544.2869	1671	48.4329	2.1807	972.8595	1671	48.4329	2.1807	446.3245	1671	48.4329	2.1807	816.7275
1672	48.4589	2.1796	588.8429	1672	48.4589	2.1796	1017.2445	1672	48.4589	2.1796	439.7014	1672	48.4589	2.1796	809.5648
1673	48.4849	2.1785	676.2347	1673	48.4849	2.1785	1104.4651	1673	48.4849	2.1785	412.6576	1673	48.4849	2.1785	781.9816
1674	48.5109	2.1774	711.5407	1674	48.5109	2.1774	1139.5999	1674	48.5109	2.1774	409.0156	1674	48.5109	2.1774	777.8001
1675	48.5369	2.1763	730.8573	1675	48.5369	2.1763	1158.7454	1675	48.5369	2.1763	402.0807	1675	48.5369	2.1763	770.3256
1676	48.5629	2.1752	814.6212	1676	48.5629	2.1752	1242.3382	1676	48.5629	2.1752	395.9894	1676	48.5629	2.1752	763.8509
1677	48.5889	2.1742	899.8934	1677	48.5889	2.1742	1327.4393	1677	48.5889	2.1742	429.6363	1677	48.5889	2.1742	797.1143
1678	48.6149	2.1731	995.6074	1678	48.6149	2.1731	1422.9821	1678	48.6149	2.1731	413.4643	1678	48.6149	2.1731	780.5587
1679	48.6409	2.172	1163.8436	1679	48.6409	2.172	1591.0472	1679	48.6409	2.172	414.4426	1679	48.6409	2.172	781.1535
1680	48.6669	2.1709	1313.4664	1680	48.6669	2.1709	1740.4989	1680	48.6669	2.1709	414.2036	1680	48.6669	2.1709	780.5311
1681	48.6929	2.1698	1596.5884	1681	48.6929	2.1698	2023.4497	1681	48.6929	2.1698	407.3448	1681	48.6929	2.1698	773.2888
1682	48.7189	2.1687	2015.6366	1682	48.7189	2.1687	2442.3267	1682	48.7189	2.1687	424.852	1682	48.7189	2.1687	790.4125
1683	48.7449	2.1676	2377.0028	1683	48.7449	2.1676	2803.5219	1683	48.7449	2.1676	430.434	1683	48.7449	2.1676	795.611
1684	48.7709	2.1665	2651.4256	1684	48.7709	2.1665	3077.7735	1684	48.7709	2.1665	426.3433	1684	48.7709	2.1665	791.1367
1685	48.7969	2.1655	2739.6347	1685	48.7969	2.1655	3165.8115	1685	48.7969	2.1655	443.011	1685	48.7969	2.1655	807.421
1686	48.8229	2.1644	2501.2651	1686	48.8229	2.1644	2927.2707	1686	48.8229	2.1644	396.512	1686	48.8229	2.1644	760.5384
1687	48.8489	2.1633	2296.8858	1687	48.8489	2.1633	2722.7203	1687	48.8489	2.1633	399.8701	1687	48.8489	2.1633	763.5131

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1688	48.8749	2.1622	2196.3246	1688	48.8749	2.1622	2621.988	1688	48.8749	2.1622	432.8975	1688	48.8749	2.1622	796.157
1689	48.9009	2.1611	1961.7714	1689	48.9009	2.1611	2387.2636	1689	48.9009	2.1611	390.436	1689	48.9009	2.1611	753.312
1690	48.9269	2.1601	1716.8335	1690	48.9269	2.1601	2142.1546	1690	48.9269	2.1601	426.4063	1690	48.9269	2.1601	788.8988
1691	48.9529	2.159	1359.6235	1691	48.9529	2.159	1784.7734	1691	48.9529	2.159	417.3609	1691	48.9529	2.159	779.4699
1692	48.9789	2.1579	1126.8956	1692	48.9789	2.1579	1551.8744	1692	48.9789	2.1579	428.8317	1692	48.9789	2.1579	790.5572
1693	49.0049	2.1568	1007.2768	1693	49.0049	2.1568	1432.0845	1693	49.0049	2.1568	418.7758	1693	49.0049	2.1568	780.1178
1694	49.0309	2.1558	891.2699	1694	49.0309	2.1558	1315.9065	1694	49.0309	2.1558	393.0961	1694	49.0309	2.1558	754.0546
1695	49.0569	2.1547	818.8135	1695	49.0569	2.1547	1243.2789	1695	49.0569	2.1547	428.8988	1695	49.0569	2.1547	789.4738
1696	49.0829	2.1536	708.8909	1696	49.0829	2.1536	1133.1851	1696	49.0829	2.1536	457.9011	1696	49.0829	2.1536	818.0926
1697	49.1089	2.1525	664.3234	1697	49.1089	2.1525	1088.4465	1697	49.1089	2.1525	444.5049	1697	49.1089	2.1525	804.3128
1698	49.1349	2.1515	572.4581	1698	49.1349	2.1515	996.4101	1698	49.1349	2.1515	440.6043	1698	49.1349	2.1515	800.0288
1699	49.1609	2.1504	559.675	1699	49.1609	2.1504	983.4558	1699	49.1609	2.1504	432.6162	1699	49.1609	2.1504	791.6572
1700	49.1869	2.1493	559.1237	1700	49.1869	2.1493	982.7334	1700	49.1869	2.1493	425.5625	1700	49.1869	2.1493	784.22
1701	49.2129	2.1483	530.5784	1701	49.2129	2.1483	954.017	1701	49.2129	2.1483	481.8368	1701	49.2129	2.1483	840.1108
1702	49.2389	2.1472	476.4976	1702	49.2389	2.1472	899.765	1702	49.2389	2.1472	398.1227	1702	49.2389	2.1472	756.0132
1703	49.2649	2.1461	506.9754	1703	49.2649	2.1461	928.6116	1703	49.2649	2.1461	360.9937	1703	49.2649	2.1461	718.5006
1704	49.2909	2.1451	462.5157	1704	49.2909	2.1451	882.5206	1704	49.2909	2.1451	405.0812	1704	49.2909	2.1451	762.2047
1705	49.3169	2.144	439.1711	1705	49.3169	2.144	857.5448	1705	49.3169	2.144	411.5111	1705	49.3169	2.144	768.251
1706	49.3429	2.143	486.8435	1706	49.3429	2.143	903.5859	1706	49.3429	2.143	451.7462	1706	49.3429	2.143	808.1027
1707	49.3689	2.1419	399.6058	1707	49.3689	2.1419	814.717	1707	49.3689	2.1419	431.3899	1707	49.3689	2.1419	787.3628
1708	49.3949	2.1409	458.2625	1708	49.3949	2.1409	871.7424	1708	49.3949	2.1409	436.3479	1708	49.3949	2.1409	791.9374
1709	49.4209	2.1398	408.726	1709	49.4209	2.1398	820.5747	1709	49.4209	2.1398	436.1104	1709	49.4209	2.1398	791.3163
1710	49.4469	2.1387	370.3352	1710	49.4469	2.1387	780.5526	1710	49.4469	2.1387	440.9791	1710	49.4469	2.1387	795.8015
1711	49.4729	2.1377	449.0137	1711	49.4729	2.1377	857.5998	1711	49.4729	2.1377	416.3365	1711	49.4729	2.1377	770.7755
1712	49.4989	2.1366	380.8027	1712	49.4989	2.1366	787.7576	1712	49.4989	2.1366	469.1971	1712	49.4989	2.1366	823.2525
1713	49.5249	2.1356	414.3375	1713	49.5249	2.1356	819.6611	1713	49.5249	2.1356	479.7415	1713	49.5249	2.1356	833.4134
1714	49.5509	2.1345	390.2859	1714	49.5509	2.1345	793.9782	1714	49.5509	2.1345	435.7115	1714	49.5509	2.1345	789
1715	49.5769	2.1335	384.9866	1715	49.5769	2.1335	787.0477	1715	49.5769	2.1335	436.095	1715	49.5769	2.1335	789
1716	49.6029	2.1324	437.7001	1716	49.6029	2.1324	838.1299	1716	49.6029	2.1324	420.7462	1716	49.6029	2.1324	773.2677
1717	49.6289	2.1314	387.6408	1717	49.6289	2.1314	786.4393	1717	49.6289	2.1314	463.6893	1717	49.6289	2.1314	815.8272
1718	49.6549	2.1303	410.9549	1718	49.6549	2.1303	808.1222	1718	49.6549	2.1303	444.0502	1718	49.6549	2.1303	795.8047
1719	49.6809	2.1293	354.3469	1719	49.6809	2.1293	749.8829	1719	49.6809	2.1293	494.1646	1719	49.6809	2.1293	845.5356
1720	49.7069	2.1283	388.0076	1720	49.7069	2.1283	781.9124	1720	49.7069	2.1283	468.7052	1720	49.7069	2.1283	819.6926
1721	49.7329	2.1272	396.3948	1721	49.7329	2.1272	788.6683	1721	49.7329	2.1272	458.0595	1721	49.7329	2.1272	808.6634
1722	49.7589	2.1262	390.9679	1722	49.7589	2.1262	781.6101	1722	49.7589	2.1262	475.3305	1722	49.7589	2.1262	825.551
1723	49.7849	2.1251	383.7647	1723	49.7849	2.1251	772.7757	1723	49.7849	2.1251	511.8879	1723	49.7849	2.1251	861.7249

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1724	49.8109	2.1241	326.7713	1724	49.8109	2.1241	714.151	1724	49.8109	2.1241	500.1804	1724	49.8109	2.1241	849.6339
1725	49.8369	2.1231	357.1163	1725	49.8369	2.1231	742.8647	1725	49.8369	2.1231	459.5955	1725	49.8369	2.1231	808.6654
1726	49.8629	2.122	372.6073	1726	49.8629	2.122	756.7245	1726	49.8629	2.122	486.2551	1726	49.8629	2.122	834.9416
1727	49.8889	2.121	388.6259	1727	49.8889	2.121	771.1118	1727	49.8889	2.121	506.4313	1727	49.8889	2.121	854.7342
1728	49.9149	2.12	399.9231	1728	49.9149	2.12	780.7778	1728	49.9149	2.12	511.6731	1728	49.9149	2.12	859.5926
1729	49.9409	2.1189	397.6509	1729	49.9409	2.1189	776.8743	1729	49.9409	2.1189	500.5041	1729	49.9409	2.1189	848.0401
1730	49.9669	2.1179	356.9833	1730	49.9669	2.1179	735.4709	1730	49.9669	2.1179	545.2871	1730	49.9669	2.1179	892.4396
1731	49.9929	2.1169	392.8044	1731	49.9929	2.1169	770.5561	1731	49.9929	2.1169	525.8603	1731	49.9929	2.1169	872.6292
1732	50.0189	2.1158	350.0399	1732	50.0189	2.1158	727.0558	1732	50.0189	2.1158	490.9322	1732	50.0189	2.1158	837.3176
1733	50.0449	2.1148	400.8142	1733	50.0449	2.1148	777.0942	1733	50.0449	2.1148	491.5148	1733	50.0449	2.1148	837.5167
1734	50.0709	2.1138	380.0505	1734	50.0709	2.1138	755.5947	1734	50.0709	2.1138	517.5216	1734	50.0709	2.1138	863.14
1735	50.0969	2.1127	355.502	1735	50.0969	2.1127	730.3104	1735	50.0969	2.1127	529.3283	1735	50.0969	2.1127	874.5632
1736	50.1229	2.1117	409.2196	1736	50.1229	2.1117	783.292	1736	50.1229	2.1117	560.9719	1736	50.1229	2.1117	905.8233
1737	50.1489	2.1107	368.3208	1737	50.1489	2.1107	741.6574	1737	50.1489	2.1107	586.58	1737	50.1489	2.1107	931.0478
1738	50.1749	2.1097	382.9984	1738	50.1749	2.1097	755.5991	1738	50.1749	2.1097	617.1599	1738	50.1749	2.1097	961.2443
1739	50.2009	2.1087	359.9127	1739	50.2009	2.1087	731.7776	1739	50.2009	2.1087	637.3801	1739	50.2009	2.1087	981.0809
1740	50.2269	2.1076	384.1471	1740	50.2269	2.1076	755.2761	1740	50.2269	2.1076	649.8792	1740	50.2269	2.1076	993.1965
1741	50.2529	2.1066	362.0519	1741	50.2529	2.1066	732.4451	1741	50.2529	2.1066	681.7394	1741	50.2529	2.1066	1024.6732
1742	50.2789	2.1056	398.937	1742	50.2789	2.1056	768.5943	1742	50.2789	2.1056	740.3188	1742	50.2789	2.1056	1082.8691
1743	50.3049	2.1046	376.5873	1743	50.3049	2.1046	745.5088	1743	50.3049	2.1046	750.9642	1743	50.3049	2.1046	1093.131
1744	50.3309	2.1036	429.9479	1744	50.3309	2.1036	798.1335	1744	50.3309	2.1036	852.6225	1744	50.3309	2.1036	1194.4057
1745	50.3569	2.1025	429.6428	1745	50.3569	2.1025	797.0926	1745	50.3569	2.1025	920.9435	1745	50.3569	2.1025	1262.3433
1746	50.3829	2.1015	413.8581	1746	50.3829	2.1015	780.572	1746	50.3829	2.1015	988.8885	1746	50.3829	2.1015	1329.9048
1747	50.4089	2.1005	415.7246	1747	50.4089	2.1005	781.7027	1747	50.4089	2.1005	1102.5297	1747	50.4089	2.1005	1443.1624
1748	50.4349	2.0995	430.4071	1748	50.4349	2.0995	795.6493	1748	50.4349	2.0995	1377.0993	1748	50.4349	2.0995	1717.3485
1749	50.4609	2.0985	505.0444	1749	50.4609	2.0985	869.5508	1749	50.4609	2.0985	1803.0315	1749	50.4609	2.0985	2142.8972
1750	50.4869	2.0975	560.6068	1750	50.4869	2.0975	924.3773	1750	50.4869	2.0975	2473.8493	1750	50.4869	2.0975	2813.3314
1751	50.5129	2.0965	582.1412	1751	50.5129	2.0965	945.1758	1751	50.5129	2.0965	3165.0216	1751	50.5129	2.0965	3504.1202
1752	50.5389	2.0955	627.5173	1752	50.5389	2.0955	989.8161	1752	50.5389	2.0955	3872.0863	1752	50.5389	2.0955	4210.8014
1753	50.5649	2.0945	612.62	1753	50.5649	2.0945	974.183	1753	50.5649	2.0945	4215.2827	1753	50.5649	2.0945	4553.6143
1754	50.5909	2.0935	581.8983	1754	50.5909	2.0935	942.7253	1754	50.5909	2.0935	4154.0254	1754	50.5909	2.0935	4491.9735
1755	50.6169	2.0925	619.0534	1755	50.6169	2.0925	979.1446	1755	50.6169	2.0925	3920.6828	1755	50.6169	2.0925	4258.2474
1756	50.6429	2.0914	620.0849	1756	50.6429	2.0914	979.4403	1756	50.6429	2.0914	3623.2831	1756	50.6429	2.0914	3960.4641
1757	50.6689	2.0904	582.9339	1757	50.6689	2.0904	941.5535	1757	50.6689	2.0904	3338.5598	1757	50.6689	2.0904	3675.3573
1758	50.6949	2.0894	532.1587	1758	50.6949	2.0894	890.0424	1758	50.6949	2.0894	2950.3845	1758	50.6949	2.0894	3286.7985
1759	50.7209	2.0884	514.4278	1759	50.7209	2.0884	871.5756	1759	50.7209	2.0884	2493.8348	1759	50.7209	2.0884	2829.8653

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1760	50.7469	2.0874	545.4555	1760	50.7469	2.0874	901.8675	1760	50.7469	2.0874	2046.9702	1760	50.7469	2.0874	2382.6172
1761	50.7729	2.0864	576.6695	1761	50.7729	2.0864	932.3456	1761	50.7729	2.0864	1657.7731	1761	50.7729	2.0864	1993.0366
1762	50.7989	2.0854	586.4792	1762	50.7989	2.0854	941.4195	1762	50.7989	2.0854	1410.5031	1762	50.7989	2.0854	1745.383
1763	50.8249	2.0845	622.497	1763	50.8249	2.0845	976.7014	1763	50.8249	2.0845	1249.8978	1763	50.8249	2.0845	1584.3942
1764	50.8509	2.0835	649.9265	1764	50.8509	2.0835	1003.395	1764	50.8509	2.0835	1049.1375	1764	50.8509	2.0835	1383.2504
1765	50.8769	2.0825	621.396	1765	50.8769	2.0825	974.1287	1765	50.8769	2.0825	891.4752	1765	50.8769	2.0825	1225.2047
1766	50.9029	2.0815	642.8727	1766	50.9029	2.0815	994.8695	1766	50.9029	2.0815	809.4002	1766	50.9029	2.0815	1142.7461
1767	50.9289	2.0805	705.9193	1767	50.9289	2.0805	1057.1803	1767	50.9289	2.0805	737.1305	1767	50.9289	2.0805	1070.0929
1768	50.9549	2.0795	725.0076	1768	50.9549	2.0795	1075.5327	1768	50.9549	2.0795	733.45	1768	50.9549	2.0795	1066.0289
1769	50.9809	2.0785	722.4664	1769	50.9809	2.0785	1072.2557	1769	50.9809	2.0785	736.7648	1769	50.9809	2.0785	1068.9602
1770	51.0069	2.0775	692.6513	1770	51.0069	2.0775	1041.7047	1770	51.0069	2.0775	691.1573	1770	51.0069	2.0775	1022.9692
1771	51.0329	2.0765	626.8668	1771	51.0329	2.0765	975.1843	1771	51.0329	2.0765	644.5696	1771	51.0329	2.0765	975.998
1772	51.0589	2.0755	586.7012	1772	51.0589	2.0755	934.2829	1772	51.0589	2.0755	606.4094	1772	51.0589	2.0755	937.4543
1773	51.0849	2.0746	585.8126	1773	51.0849	2.0746	932.6584	1773	51.0849	2.0746	567.1122	1773	51.0849	2.0746	897.7735
1774	51.1109	2.0736	571.2878	1774	51.1109	2.0736	917.3978	1774	51.1109	2.0736	532.9066	1774	51.1109	2.0736	863.1844
1775	51.1369	2.0726	550.2602	1775	51.1369	2.0726	895.6344	1775	51.1369	2.0726	561.9447	1775	51.1369	2.0726	891.839
1776	51.1629	2.0716	488.9911	1776	51.1629	2.0716	833.6294	1776	51.1629	2.0716	606.7134	1776	51.1629	2.0716	936.2241
1777	51.1889	2.0706	433.5582	1777	51.1889	2.0706	777.4606	1777	51.1889	2.0706	581.3022	1777	51.1889	2.0706	910.4295
1778	51.2149	2.0696	474.5206	1778	51.2149	2.0696	817.6872	1778	51.2149	2.0696	543.0967	1778	51.2149	2.0696	871.8404
1779	51.2409	2.0687	476.0162	1779	51.2409	2.0687	818.4469	1779	51.2409	2.0687	530.5224	1779	51.2409	2.0687	858.8826
1780	51.2669	2.0677	479.9473	1780	51.2669	2.0677	821.6422	1780	51.2669	2.0677	517.6942	1780	51.2669	2.0677	845.6709
1781	51.2929	2.0667	441.3586	1781	51.2929	2.0667	782.3177	1781	51.2929	2.0667	534.2123	1781	51.2929	2.0667	861.8055
1782	51.3189	2.0657	414.1671	1782	51.3189	2.0657	754.3902	1782	51.3189	2.0657	504.8495	1782	51.3189	2.0657	832.0592
1783	51.3449	2.0648	453.7866	1783	51.3449	2.0648	793.2739	1783	51.3449	2.0648	522.0148	1783	51.3449	2.0648	848.841
1784	51.3709	2.0638	421.8789	1784	51.3709	2.0638	759.5908	1784	51.3709	2.0638	540.3824	1784	51.3709	2.0638	866.825
1785	51.3969	2.0628	360.5786	1785	51.3969	2.0628	696.5151	1785	51.3969	2.0628	471.7957	1785	51.3969	2.0628	797.8548
1786	51.4229	2.0618	406.4163	1786	51.4229	2.0618	740.5774	1786	51.4229	2.0618	501.676	1786	51.4229	2.0618	827.3516
1787	51.4489	2.0609	394.0023	1787	51.4489	2.0609	726.388	1787	51.4489	2.0609	500.9808	1787	51.4489	2.0609	826.2729
1788	51.4749	2.0599	365.8754	1788	51.4749	2.0599	696.4857	1788	51.4749	2.0599	480.4071	1788	51.4749	2.0599	805.3156
1789	51.5009	2.0589	400.0492	1789	51.5009	2.0589	728.8841	1789	51.5009	2.0589	525.9386	1789	51.5009	2.0589	850.4635
1790	51.5269	2.058	414.6836	1790	51.5269	2.058	741.7431	1790	51.5269	2.058	473.89	1790	51.5269	2.058	798.0314
1791	51.5529	2.057	421.955	1791	51.5529	2.057	747.2391	1791	51.5529	2.057	445.2211	1791	51.5529	2.057	768.979
1792	51.5789	2.056	415.0952	1792	51.5789	2.056	738.6039	1792	51.5789	2.056	436.9592	1792	51.5789	2.056	760.3336
1793	51.6049	2.0551	389.6518	1793	51.6049	2.0551	711.385	1793	51.6049	2.0551	468.1482	1793	51.6049	2.0551	791.139
1794	51.6309	2.0541	408.0888	1794	51.6309	2.0541	728.0466	1794	51.6309	2.0541	495.6259	1794	51.6309	2.0541	818.2332
1795	51.6569	2.0531	406.8383	1795	51.6569	2.0531	725.0207	1795	51.6569	2.0531	504.0112	1795	51.6569	2.0531	826.235

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1796	51.6829	2.0522	377.5612	1796	51.6829	2.0522	693.9682	1796	51.6829	2.0522	463.7917	1796	51.6829	2.0522	785.632
1797	51.7089	2.0512	378.2195	1797	51.7089	2.0512	692.8511	1797	51.7089	2.0512	481.9491	1797	51.7089	2.0512	803.4058
1798	51.7349	2.0502	433.6348	1798	51.7349	2.0502	746.4911	1798	51.7349	2.0502	430.534	1798	51.7349	2.0502	751.6072
1799	51.7609	2.0493	423.3361	1799	51.7609	2.0493	734.4169	1799	51.7609	2.0493	422.456	1799	51.7609	2.0493	743.1456
1800	51.7869	2.0483	377.6905	1800	51.7869	2.0483	686.9959	1800	51.7869	2.0483	465.9935	1800	51.7869	2.0483	786.2996
1801	51.8129	2.0474	400.9459	1801	51.8129	2.0474	708.4759	1801	51.8129	2.0474	462.6224	1801	51.8129	2.0474	782.5449
1802	51.8389	2.0464	428.0362	1802	51.8389	2.0464	733.7908	1802	51.8389	2.0464	435.9585	1802	51.8389	2.0464	755.4976
1803	51.8649	2.0455	417.4213	1803	51.8649	2.0455	721.4006	1803	51.8649	2.0455	479.7245	1803	51.8649	2.0455	798.88
1804	51.8909	2.0445	433.6031	1804	51.8909	2.0445	735.8069	1804	51.8909	2.0445	477.136	1804	51.8909	2.0445	795.908
1805	51.9169	2.0436	411.976	1805	51.9169	2.0436	712.4044	1805	51.9169	2.0436	456.1033	1805	51.9169	2.0436	774.4917
1806	51.9429	2.0426	430.2923	1806	51.9429	2.0426	728.9453	1806	51.9429	2.0426	421.4108	1806	51.9429	2.0426	739.4157
1807	51.9689	2.0417	383.2916	1807	51.9689	2.0417	680.1692	1807	51.9689	2.0417	472.1206	1807	51.9689	2.0417	789.742
1808	51.9949	2.0407	410.2499	1808	51.9949	2.0407	705.3521	1808	51.9949	2.0407	423.6917	1808	51.9949	2.0407	740.9296
1809	52.0209	2.0398	415.4028	1809	52.0209	2.0398	708.7296	1809	52.0209	2.0398	426.2309	1809	52.0209	2.0398	743.0852
1810	52.0469	2.0388	397.6509	1810	52.0469	2.0388	689.2023	1810	52.0469	2.0388	477.6142	1810	52.0469	2.0388	794.0849
1811	52.0729	2.0379	400.253	1811	52.0729	2.0379	693.4878	1811	52.0729	2.0379	530.9941	1811	52.0729	2.0379	847.0813
1812	52.0989	2.0369	411.1265	1812	52.0989	2.0369	706.0448	1812	52.0989	2.0369	415.4499	1812	52.0989	2.0369	731.1536
1813	52.1249	2.036	441.6909	1813	52.1249	2.036	738.2926	1813	52.1249	2.036	420.5134	1813	52.1249	2.036	735.8336
1814	52.1509	2.035	406.7693	1814	52.1509	2.035	705.0544	1814	52.1509	2.035	413.4769	1814	52.1509	2.035	728.4136
1815	52.1769	2.0341	410.0142	1815	52.1769	2.0341	709.9827	1815	52.1769	2.0341	451.445	1815	52.1769	2.0341	765.9981
1816	52.2029	2.0331	390.5093	1816	52.2029	2.0331	692.1613	1816	52.2029	2.0331	449.8483	1816	52.2029	2.0331	764.0179
1817	52.2289	2.0322	423.0037	1817	52.2289	2.0322	726.3391	1817	52.2289	2.0322	521.8355	1817	52.2289	2.0322	835.6215
1818	52.2549	2.0313	380.2198	1818	52.2549	2.0313	685.2386	1818	52.2549	2.0313	364.3216	1818	52.2549	2.0313	677.7241
1819	52.2809	2.0303	371.5301	1819	52.2809	2.0303	678.2324	1819	52.2809	2.0303	411.8897	1819	52.2809	2.0303	724.9087
1820	52.3069	2.0294	415.2791	1820	52.3069	2.0294	723.6648	1820	52.3069	2.0294	407.7051	1820	52.3069	2.0294	720.3406
1821	52.3329	2.0284	367.9181	1821	52.3329	2.0284	677.9872	1821	52.3329	2.0284	463.2923	1821	52.3329	2.0284	775.5442
1822	52.3589	2.0275	366.042	1822	52.3589	2.0275	677.7945	1822	52.3589	2.0275	451.296	1822	52.3589	2.0275	763.1644
1823	52.3849	2.0266	396.8194	1823	52.3849	2.0266	710.2554	1823	52.3849	2.0266	429.3188	1823	52.3849	2.0266	740.8036
1824	52.4109	2.0256	393.3223	1824	52.4109	2.0256	708.4417	1824	52.4109	2.0256	441.5736	1824	52.4109	2.0256	752.6749
1825	52.4369	2.0247	362.3416	1825	52.4369	2.0247	679.1444	1825	52.4369	2.0247	388.2762	1825	52.4369	2.0247	698.994
1826	52.4629	2.0238	406.5636	1826	52.4629	2.0238	725.0499	1826	52.4629	2.0238	441.5256	1826	52.4629	2.0238	751.8599
1827	52.4889	2.0228	388.783	1827	52.4889	2.0228	708.9527	1827	52.4889	2.0228	434.939	1827	52.4889	2.0228	744.8897
1828	52.5149	2.0219	424.2576	1828	52.5149	2.0219	746.1107	1828	52.5149	2.0219	456.9761	1828	52.5149	2.0219	766.5432
1829	52.5409	2.021	417.2568	1829	52.5409	2.021	740.7934	1829	52.5409	2.021	417.7139	1829	52.5409	2.021	726.8975
1830	52.5669	2.0201	424.0056	1830	52.5669	2.0201	749.2255	1830	52.5669	2.0201	411.1999	1830	52.5669	2.0201	720
1831	52.5929	2.0191	439.2563	1831	52.5929	2.0191	766.1597	1831	52.5929	2.0191	489.9085	1831	52.5929	2.0191	798.325

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1832	52.6189	2.0182	399.6313	1832	52.6189	2.0182	728.2182	1832	52.6189	2.0182	444.2104	1832	52.6189	2.0182	752.2434
1833	52.6449	2.0173	398.7757	1833	52.6449	2.0173	729.046	1833	52.6449	2.0173	482.5145	1833	52.6449	2.0173	790.164
1834	52.6709	2.0163	449.4175	1834	52.6709	2.0163	781.3711	1834	52.6709	2.0163	473.4231	1834	52.6709	2.0163	780.6891
1835	52.6969	2.0154	433.6824	1835	52.6969	2.0154	767.3195	1835	52.6969	2.0154	451.4622	1835	52.6969	2.0154	758.3447
1836	52.7229	2.0145	378.1239	1836	52.7229	2.0145	713.4444	1836	52.7229	2.0145	369.0344	1836	52.7229	2.0145	675.5333
1837	52.7489	2.0136	397.6509	1837	52.7489	2.0136	734.6548	1837	52.7489	2.0136	443.5878	1837	52.7489	2.0136	749.7032
1838	52.7749	2.0127	410.7352	1838	52.7749	2.0127	747.8637	1838	52.7749	2.0127	479.5412	1838	52.7749	2.0127	785.273
1839	52.8009	2.0117	392.6763	1839	52.8009	2.0117	729.9293	1839	52.8009	2.0117	494.0941	1839	52.8009	2.0117	799.4424
1840	52.8269	2.0108	412.974	1840	52.8269	2.0108	750.3516	1840	52.8269	2.0108	472.4366	1840	52.8269	2.0108	777.4013
1841	52.8529	2.0099	448.2452	1841	52.8529	2.0099	785.7473	1841	52.8529	2.0099	444.3583	1841	52.8529	2.0099	748.9395
1842	52.8789	2.009	441.2459	1842	52.8789	2.009	778.8727	1842	52.8789	2.009	469.324	1842	52.8789	2.009	773.5216
1843	52.9049	2.0081	446.0958	1843	52.9049	2.0081	783.8471	1843	52.9049	2.0081	470.3389	1843	52.9049	2.0081	774.1529
1844	52.9309	2.0072	504.3285	1844	52.9309	2.0072	842.2043	1844	52.9309	2.0072	450.1656	1844	52.9309	2.0072	753.5961
1845	52.9569	2.0062	540.0654	1845	52.9569	2.0062	878.0659	1845	52.9569	2.0062	434.8103	1845	52.9569	2.0062	737.8572
1846	52.9829	2.0053	558.3557	1846	52.9829	2.0053	896.4807	1846	52.9829	2.0053	432.7234	1846	52.9829	2.0053	735.3867
1847	53.0089	2.0044	578.1029	1847	53.0089	2.0044	916.3524	1847	53.0089	2.0044	425.5188	1847	53.0089	2.0044	727.7986
1848	53.0349	2.0035	632.4462	1848	53.0349	2.0035	970.8203	1848	53.0349	2.0035	411.3273	1848	53.0349	2.0035	713.2236
1849	53.0609	2.0026	710.5804	1849	53.0609	2.0026	1049.0791	1849	53.0609	2.0026	413.7869	1849	53.0609	2.0026	715.2996
1850	53.0869	2.0017	814.2038	1850	53.0869	2.0017	1152.827	1850	53.0869	2.0017	427.6761	1850	53.0869	2.0017	728.8052
1851	53.1129	2.0008	910.903	1851	53.1129	2.0008	1249.6508	1851	53.1129	2.0008	440.9795	1851	53.1129	2.0008	741.7251
1852	53.1389	1.9999	961.7766	1852	53.1389	1.9999	1300.6489	1852	53.1389	1.9999	431.0597	1852	53.1389	1.9999	731.4218
1853	53.1649	1.999	974.8749	1853	53.1649	1.999	1313.8717	1853	53.1649	1.999	414.2867	1853	53.1649	1.999	714.2652
1854	53.1909	1.9981	934.7411	1854	53.1909	1.9981	1273.8625	1854	53.1909	1.9981	403.8791	1854	53.1909	1.9981	703.4741
1855	53.2169	1.9971	892.4441	1855	53.2169	1.9971	1231.6901	1855	53.2169	1.9971	374.2096	1855	53.2169	1.9971	673.4209
1856	53.2429	1.9962	894.1065	1856	53.2429	1.9962	1233.4771	1856	53.2429	1.9962	393.4152	1856	53.2429	1.9962	692.243
1857	53.2689	1.9953	803.1866	1857	53.2689	1.9953	1142.6817	1857	53.2689	1.9953	401.6132	1857	53.2689	1.9953	700.0575
1858	53.2949	1.9944	678.3959	1858	53.2949	1.9944	1018.0155	1858	53.2949	1.9944	473.7875	1858	53.2949	1.9944	771.8482
1859	53.3209	1.9935	645.0283	1859	53.3209	1.9935	984.7726	1859	53.3209	1.9935	527.8571	1859	53.3209	1.9935	825.5343
1860	53.3469	1.9926	616.3093	1860	53.3469	1.9926	956.1781	1860	53.3469	1.9926	483.4488	1860	53.3469	1.9926	780.7424
1861	53.3729	1.9917	566.1362	1861	53.3729	1.9917	906.1295	1861	53.3729	1.9917	440.5656	1861	53.3729	1.9917	737.4757
1862	53.3989	1.9908	556.5052	1862	53.3989	1.9908	896.623	1862	53.3989	1.9908	438.4927	1862	53.3989	1.9908	735.0192
1863	53.4249	1.9899	515.9613	1863	53.4249	1.9899	856.2037	1863	53.4249	1.9899	446.9064	1863	53.4249	1.9899	743.0494
1864	53.4509	1.989	480.3841	1864	53.4509	1.989	820.7511	1864	53.4509	1.989	447.7258	1864	53.4509	1.989	743.4852
1865	53.4769	1.9881	434.9947	1865	53.4769	1.9881	775.4863	1865	53.4769	1.9881	466.3035	1865	53.4769	1.9881	761.6793
1866	53.5029	1.9873	413.0692	1866	53.5029	1.9873	753.6853	1866	53.5029	1.9873	473.6245	1866	53.5029	1.9873	768.6167
1867	53.5289	1.9864	424.8592	1867	53.5289	1.9864	765.5999	1867	53.5289	1.9864	462.8763	1867	53.5289	1.9864	757.485

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1868	53.5549	1.9855	428.8389	1868	53.5549	1.9855	769.7041	1868	53.5549	1.9855	451.4228	1868	53.5549	1.9855	745.6479
1869	53.5809	1.9846	429.4962	1869	53.5809	1.9846	770.486	1869	53.5809	1.9846	432.5765	1869	53.5809	1.9846	726.4181
1870	53.6069	1.9837	391.6019	1870	53.6069	1.9837	732.7162	1870	53.6069	1.9837	433.3705	1870	53.6069	1.9837	726.8285
1871	53.6329	1.9828	385.8783	1871	53.6329	1.9828	727.1172	1871	53.6329	1.9828	444.1521	1871	53.6329	1.9828	737.2266
1872	53.6589	1.9819	409.2291	1872	53.6589	1.9819	750.5926	1872	53.6589	1.9819	453.8399	1872	53.6589	1.9819	746.5309
1873	53.6849	1.981	415.7914	1873	53.6849	1.981	757.2794	1873	53.6849	1.981	476.3076	1873	53.6849	1.981	768.615
1874	53.7109	1.9801	399.5294	1874	53.7109	1.9801	741.142	1874	53.7109	1.9801	472.2211	1874	53.7109	1.9801	764.145
1875	53.7369	1.9792	402.9335	1875	53.7369	1.9792	744.6707	1875	53.7369	1.9792	451.0059	1875	53.7369	1.9792	742.5462
1876	53.7629	1.9784	367.7704	1876	53.7629	1.9784	709.6321	1876	53.7629	1.9784	464.4691	1876	53.7629	1.9784	755.6258
1877	53.7889	1.9775	377.4495	1877	53.7889	1.9775	719.4357	1877	53.7889	1.9775	455.8259	1877	53.7889	1.9775	746.5991
1878	53.8149	1.9766	413.6931	1878	53.8149	1.9766	755.8039	1878	53.8149	1.9766	450.2414	1878	53.8149	1.9766	740.631
1879	53.8409	1.9757	375.3042	1879	53.8409	1.9757	717.5396	1879	53.8409	1.9757	451.7005	1879	53.8409	1.9757	741.7066
1880	53.8669	1.9748	380.1274	1880	53.8669	1.9748	722.4874	1880	53.8669	1.9748	436.4092	1880	53.8669	1.9748	726.0317
1881	53.8929	1.9739	356.8982	1881	53.8929	1.9739	699.3827	1881	53.8929	1.9739	422.9141	1881	53.8929	1.9739	712.1531
1882	53.9189	1.9731	398.2419	1882	53.9189	1.9731	740.8509	1882	53.9189	1.9731	446.9445	1882	53.9189	1.9731	735.7999
1883	53.9449	1.9722	430.8265	1883	53.9449	1.9722	773.5601	1883	53.9449	1.9722	472.3295	1883	53.9449	1.9722	760.8013
1884	53.9709	1.9713	401.8664	1884	53.9709	1.9713	744.7246	1884	53.9709	1.9713	449.4731	1884	53.9709	1.9713	737.5613
1885	53.9969	1.9704	389.6941	1885	53.9969	1.9704	732.6768	1885	53.9969	1.9704	442.0025	1885	53.9969	1.9704	729.7072
1886	54.0229	1.9695	375.3604	1886	54.0229	1.9695	718.4676	1886	54.0229	1.9695	474.1964	1886	54.0229	1.9695	761.5176
1887	54.0489	1.9687	348.991	1887	54.0489	1.9687	692.2228	1887	54.0489	1.9687	471.3489	1887	54.0489	1.9687	758.2866
1888	54.0749	1.9678	409.1745	1888	54.0749	1.9678	752.5309	1888	54.0749	1.9678	462.2105	1888	54.0749	1.9678	748.7645
1889	54.1009	1.9669	392.4529	1889	54.1009	1.9669	735.9338	1889	54.1009	1.9669	433.4291	1889	54.1009	1.9669	719.5996
1890	54.1269	1.966	397.313	1890	54.1269	1.966	740.9185	1890	54.1269	1.966	437.9982	1890	54.1269	1.966	723.7852
1891	54.1529	1.9652	397.6509	1891	54.1529	1.9652	741.3809	1891	54.1529	1.9652	470.3372	1891	54.1529	1.9652	755.7406
1892	54.1789	1.9643	425.2174	1892	54.1789	1.9643	771.4217	1892	54.1789	1.9643	487.6708	1892	54.1789	1.9643	772.6906
1893	54.2049	1.9634	413.7001	1893	54.2049	1.9634	762.3787	1893	54.2049	1.9634	508.8021	1893	54.2049	1.9634	793.4384
1894	54.2309	1.9626	376.3536	1894	54.2309	1.9626	727.5063	1894	54.2309	1.9626	430.0366	1894	54.2309	1.9626	714.2892
1895	54.2569	1.9617	407.9146	1895	54.2569	1.9617	761.5416	1895	54.2569	1.9617	468.2304	1895	54.2569	1.9617	752.0995
1896	54.2829	1.9608	392.482	1896	54.2829	1.9608	748.5832	1896	54.2829	1.9608	443.5094	1896	54.2829	1.9608	726.9949
1897	54.3089	1.96	454.3613	1897	54.3089	1.96	812.9367	1897	54.3089	1.96	409.3781	1897	54.3089	1.96	692.48
1898	54.3349	1.9591	456.1278	1898	54.3349	1.9591	817.1774	1898	54.3349	1.9591	506.3946	1898	54.3349	1.9591	789.1129
1899	54.3609	1.9582	452.9688	1899	54.3609	1.9582	816.4926	1899	54.3609	1.9582	499.4829	1899	54.3609	1.9582	781.8177
1900	54.3869	1.9574	448.2016	1900	54.3869	1.9574	814.1997	1900	54.3869	1.9574	480.5823	1900	54.3869	1.9574	762.5335
1901	54.4129	1.9565	473.3801	1901	54.4129	1.9565	841.8524	1901	54.4129	1.9565	453.869	1901	54.4129	1.9565	735.4366
1902	54.4389	1.9556	468.2631	1902	54.4389	1.9556	839.2096	1902	54.4389	1.9556	423.133	1902	54.4389	1.9556	704.317
1903	54.4649	1.9548	460.5858	1903	54.4649	1.9548	834.0066	1903	54.4649	1.9548	526.1864	1903	54.4649	1.9548	806.9868

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1904	54.4909	1.9539	500.9911	1904	54.4909	1.9539	876.886	1904	54.4909	1.9539	448.1194	1904	54.4909	1.9539	728.5363
1905	54.5169	1.953	510.7956	1905	54.5169	1.953	889.1648	1905	54.5169	1.953	474.8587	1905	54.5169	1.953	754.892
1906	54.5429	1.9522	505.0185	1906	54.5429	1.9522	885.862	1906	54.5429	1.9522	473.9581	1906	54.5429	1.9522	753.6079
1907	54.5689	1.9513	610.1845	1907	54.5689	1.9513	993.5021	1907	54.5689	1.9513	472.7604	1907	54.5689	1.9513	752.0265
1908	54.5949	1.9505	591.9736	1908	54.5949	1.9505	977.7654	1908	54.5949	1.9505	493.5701	1908	54.5949	1.9505	772.4527
1909	54.6209	1.9496	590.9664	1909	54.6209	1.9496	979.2325	1909	54.6209	1.9496	489.2759	1909	54.6209	1.9496	767.7749
1910	54.6469	1.9488	651.1022	1910	54.6469	1.9488	1041.8425	1910	54.6469	1.9488	515.1098	1910	54.6469	1.9488	793.2252
1911	54.6729	1.9479	729.0128	1911	54.6729	1.9479	1122.2274	1911	54.6729	1.9479	536.3334	1911	54.6729	1.9479	814.0653
1912	54.6989	1.947	772.3517	1912	54.6989	1.947	1168.0404	1912	54.6989	1.947	553.1089	1912	54.6989	1.947	830.4571
1913	54.7249	1.9462	823.9519	1913	54.7249	1.9462	1222.1149	1913	54.7249	1.9462	440.8926	1913	54.7249	1.9462	717.8573
1914	54.7509	1.9453	931.2802	1914	54.7509	1.9453	1331.9174	1914	54.7509	1.9453	470.7733	1914	54.7509	1.9453	747.3544
1915	54.7769	1.9445	1136.4341	1915	54.7769	1.9445	1539.5456	1915	54.7769	1.9445	489.6715	1915	54.7769	1.9445	765.869
1916	54.8029	1.9436	1309.2037	1916	54.8029	1.9436	1714.7893	1916	54.8029	1.9436	475.2039	1916	54.8029	1.9436	751.0179
1917	54.8289	1.9428	1657.9952	1917	54.8289	1.9428	2066.055	1917	54.8289	1.9428	483.4807	1917	54.8289	1.9428	758.9111
1918	54.8549	1.9419	1892.4596	1918	54.8549	1.9419	2302.9937	1918	54.8549	1.9419	544.6491	1918	54.8549	1.9419	819.6958
1919	54.8809	1.9411	1931.0585	1919	54.8809	1.9411	2342.8855	1919	54.8809	1.9411	514.3584	1919	54.8809	1.9411	789.0216
1920	54.9069	1.9402	1847.4365	1920	54.9069	1.9402	2260.5565	1920	54.9069	1.9402	546.3305	1920	54.9069	1.9402	820.6101
1921	54.9329	1.9394	1711.5976	1921	54.9329	1.9394	2126.0106	1921	54.9329	1.9394	591.7671	1921	54.9329	1.9394	865.6631
1922	54.9589	1.9385	1834.7927	1922	54.9589	1.9385	2250.4986	1922	54.9589	1.9385	582.2769	1922	54.9589	1.9385	855.7894
1923	54.9849	1.9377	2021.3663	1923	54.9849	1.9377	2438.3653	1923	54.9849	1.9377	599.5288	1923	54.9849	1.9377	872.6577
1924	55.0109	1.9369	2013.4806	1924	55.0109	1.9369	2431.7725	1924	55.0109	1.9369	623.321	1924	55.0109	1.9369	896.0664
1925	55.0369	1.936	2122.2847	1925	55.0369	1.936	2541.8696	1925	55.0369	1.936	633.8238	1925	55.0369	1.936	906.1856
1926	55.0629	1.9352	2388.5044	1926	55.0629	1.9352	2809.3822	1926	55.0629	1.9352	578.3479	1926	55.0629	1.9352	850.326
1927	55.0889	1.9343	2736.9981	1927	55.0889	1.9343	3159.1689	1927	55.0889	1.9343	636.4613	1927	55.0889	1.9343	908.0558
1928	55.1149	1.9335	2983.1554	1928	55.1149	1.9335	3406.6192	1928	55.1149	1.9335	738.0417	1928	55.1149	1.9335	1009.2527
1929	55.1409	1.9326	3077.2194	1929	55.1409	1.9326	3501.9761	1929	55.1409	1.9326	746.8235	1929	55.1409	1.9326	1017.6509
1930	55.1669	1.9318	2845.1789	1930	55.1669	1.9318	3271.2287	1930	55.1669	1.9318	821.3672	1930	55.1669	1.9318	1091.8111
1931	55.1929	1.931	2722.2097	1931	55.1929	1.931	3149.5524	1931	55.1929	1.931	1003.9348	1931	55.1929	1.931	1273.9951
1932	55.2189	1.9301	2419.0662	1932	55.2189	1.9301	2847.7018	1932	55.2189	1.9301	1170.4119	1932	55.2189	1.9301	1440.0886
1933	55.2449	1.9293	2343.9784	1933	55.2449	1.9293	2773.907	1933	55.2449	1.9293	1356.092	1933	55.2449	1.9293	1625.3851
1934	55.2709	1.9285	2092.7159	1934	55.2709	1.9285	2523.9375	1934	55.2709	1.9285	1710.6122	1934	55.2709	1.9285	1979.5217
1935	55.2969	1.9276	1935.3894	1935	55.2969	1.9276	2367.9039	1935	55.2969	1.9276	1898.1553	1935	55.2969	1.9276	2166.6812
1936	55.3229	1.9268	1566.8363	1936	55.3229	1.9268	2000.6439	1936	55.3229	1.9268	1869.8321	1936	55.3229	1.9268	2137.9745
1937	55.3489	1.926	1325.7634	1937	55.3489	1.926	1760.8639	1937	55.3489	1.926	1875.2118	1937	55.3489	1.926	2142.9706
1938	55.3749	1.9251	1126.7221	1938	55.3749	1.9251	1563.1156	1938	55.3749	1.9251	1769.0105	1938	55.3749	1.9251	2036.3857
1939	55.4009	1.9243	1002.7127	1939	55.4009	1.9243	1440.3991	1939	55.4009	1.9243	1773.4558	1939	55.4009	1.9243	2040.4475

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1940	55.4269	1.9235	850.9879	1940	55.4269	1.9235	1289.9673	1940	55.4269	1.9235	1675.6154	1940	55.4269	1.9235	1942.2235
1941	55.4529	1.9226	782.7005	1941	55.4529	1.9226	1222.9729	1941	55.4529	1.9226	1625.259	1941	55.4529	1.9226	1891.4834
1942	55.4789	1.9218	707.9824	1942	55.4789	1.9218	1149.5478	1942	55.4789	1.9218	1531.2595	1942	55.4789	1.9218	1797.1004
1943	55.5049	1.921	573.7746	1943	55.5049	1.921	1016.6329	1943	55.5049	1.921	1362.4011	1943	55.5049	1.921	1627.8584
1944	55.5309	1.9201	588.8066	1944	55.5309	1.9201	1032.9579	1944	55.5309	1.9201	1264.3412	1944	55.5309	1.9201	1529.415
1945	55.5569	1.9193	576.1358	1945	55.5569	1.9193	1021.58	1945	55.5569	1.9193	1221.4226	1945	55.5569	1.9193	1486.1128
1946	55.5829	1.9185	508.1799	1946	55.5829	1.9185	953.311	1946	55.5829	1.9185	1167.5215	1946	55.5829	1.9185	1431.8281
1947	55.6089	1.9177	537.0234	1947	55.6089	1.9177	981.8414	1947	55.6089	1.9177	1173.2697	1947	55.6089	1.9177	1437.1927
1948	55.6349	1.9168	559.1326	1948	55.6349	1.9168	1003.6374	1948	55.6349	1.9168	1258.7219	1948	55.6349	1.9168	1522.2613
1949	55.6609	1.916	568.2076	1949	55.6609	1.916	1012.3992	1949	55.6609	1.916	1370.3809	1949	55.6609	1.916	1633.5366
1950	55.6869	1.9152	600.241	1950	55.6869	1.9152	1044.1195	1950	55.6869	1.9152	1717.1258	1950	55.6869	1.9152	1979.898
1951	55.7129	1.9144	604.0102	1951	55.7129	1.9144	1047.5755	1951	55.7129	1.9144	2192.9063	1951	55.7129	1.9144	2455.2949
1952	55.7389	1.9135	584.6325	1952	55.7389	1.9135	1027.8846	1952	55.7389	1.9135	3033.4746	1952	55.7389	1.9135	3295.4795
1953	55.7649	1.9127	627.5958	1953	55.7649	1.9127	1070.5348	1953	55.7649	1.9127	4007.2159	1953	55.7649	1.9127	4268.8373
1954	55.7909	1.9119	618.8248	1954	55.7909	1.9119	1061.4507	1954	55.7909	1.9119	4778.3173	1954	55.7909	1.9119	5039.5551
1955	55.8169	1.9111	540.0098	1955	55.8169	1.9111	982.3225	1955	55.8169	1.9111	5184.4349	1955	55.8169	1.9111	5445.289
1956	55.8429	1.9103	486.9429	1956	55.8429	1.9103	928.9425	1956	55.8429	1.9103	5106.177	1956	55.8429	1.9103	5366.6476
1957	55.8689	1.9095	533.9212	1957	55.8689	1.9095	975.6076	1957	55.8689	1.9095	4951.6573	1957	55.8689	1.9095	5211.7443
1958	55.8949	1.9086	523.4043	1958	55.8949	1.9086	964.7775	1958	55.8949	1.9086	4792.748	1958	55.8949	1.9086	5052.4514
1959	55.9209	1.9078	478.3576	1959	55.9209	1.9078	919.4177	1959	55.9209	1.9078	4583.6778	1959	55.9209	1.9078	4842.9976
1960	55.9469	1.907	448.6394	1960	55.9469	1.907	889.3864	1960	55.9469	1.907	4281.0435	1960	55.9469	1.907	4539.9797
1961	55.9729	1.9062	418.4154	1961	55.9729	1.9062	858.8493	1961	55.9729	1.9062	3735.7743	1961	55.9729	1.9062	3994.3269
1962	55.9989	1.9054	395.8621	1962	55.9989	1.9054	835.9828	1962	55.9989	1.9054	3119.5024	1962	55.9989	1.9054	3377.6714
1963	56.0249	1.9046	424.5947	1963	56.0249	1.9046	864.4022	1963	56.0249	1.9046	2587.2564	1963	56.0249	1.9046	2845.0418
1964	56.0509	1.9038	426.5856	1964	56.0509	1.9038	866.08	1964	56.0509	1.9038	2150.4655	1964	56.0509	1.9038	2407.8673
1965	56.0769	1.9029	401.4323	1965	56.0769	1.9029	840.6136	1965	56.0769	1.9029	1814.1966	1965	56.0769	1.9029	2071.2148
1966	56.1029	1.9021	411.6616	1966	56.1029	1.9021	850.5296	1966	56.1029	1.9021	1512.5299	1966	56.1029	1.9021	1769.1645
1967	56.1289	1.9013	388.8643	1967	56.1289	1.9013	827.4192	1967	56.1289	1.9013	1327.7043	1967	56.1289	1.9013	1583.9553
1968	56.1549	1.9005	402.7319	1968	56.1549	1.9005	840.9737	1968	56.1549	1.9005	1192.3198	1968	56.1549	1.9005	1448.1871
1969	56.1809	1.8997	434.8836	1969	56.1809	1.8997	872.8122	1969	56.1809	1.8997	1001.1184	1969	56.1809	1.8997	1256.6022
1970	56.2069	1.8989	445.7759	1970	56.2069	1.8989	883.3913	1970	56.2069	1.8989	868.8403	1970	56.2069	1.8989	1123.9404
1971	56.2329	1.8981	491.6495	1971	56.2329	1.8981	928.9518	1971	56.2329	1.8981	825.6266	1971	56.2329	1.8981	1080.3432
1972	56.2589	1.8973	536.6005	1972	56.2589	1.8973	973.5897	1972	56.2589	1.8973	815.4974	1972	56.2589	1.8973	1069.8304
1973	56.2849	1.8965	575.9672	1973	56.2849	1.8965	1011.3324	1973	56.2849	1.8965	768.7892	1973	56.2849	1.8965	1022.7386
1974	56.3109	1.8957	590.8785	1974	56.3109	1.8957	1024.6197	1974	56.3109	1.8957	741.2441	1974	56.3109	1.8957	994.8099
1975	56.3369	1.8949	623.9659	1975	56.3369	1.8949	1056.0831	1975	56.3369	1.8949	717.4668	1975	56.3369	1.8949	970.649

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1976	56.3629	1.8941	638.5609	1976	56.3629	1.8941	1069.0542	1976	56.3629	1.8941	693.1472	1976	56.3629	1.8941	945.9458
1977	56.3889	1.8933	616.7049	1977	56.3889	1.8933	1045.5742	1977	56.3889	1.8933	718.585	1977	56.3889	1.8933	971
1978	56.4149	1.8925	610.3967	1978	56.4149	1.8925	1037.6421	1978	56.4149	1.8925	699.02	1978	56.4149	1.8925	951.0514
1979	56.4409	1.8917	584.9148	1979	56.4409	1.8917	1010.5363	1979	56.4409	1.8917	665.4837	1979	56.4409	1.8917	917.1315
1980	56.4669	1.8909	546.448	1980	56.4669	1.8909	970.4455	1980	56.4669	1.8909	662.372	1980	56.4669	1.8909	913.6362
1981	56.4929	1.8901	505.7956	1981	56.4929	1.8901	928.1691	1981	56.4929	1.8901	666.0119	1981	56.4929	1.8901	916.8925
1982	56.5189	1.8893	509.8171	1982	56.5189	1.8893	930.5666	1982	56.5189	1.8893	661.4652	1982	56.5189	1.8893	911.9622
1983	56.5449	1.8885	511.1777	1983	56.5449	1.8885	930.3033	1983	56.5449	1.8885	652.5813	1983	56.5449	1.8885	902.6947
1984	56.5709	1.8877	462.7564	1984	56.5709	1.8877	880.258	1984	56.5709	1.8877	678.6497	1984	56.5709	1.8877	928.3795
1985	56.5969	1.8869	408.5555	1985	56.5969	1.8869	824.4331	1985	56.5969	1.8869	673.7688	1985	56.5969	1.8869	923.115
1986	56.6229	1.8861	380.6166	1986	56.6229	1.8861	794.8703	1986	56.6229	1.8861	688.9009	1986	56.6229	1.8861	937.8635
1987	56.6489	1.8853	374.427	1987	56.6489	1.8853	787.0567	1987	56.6489	1.8853	749.7863	1987	56.6489	1.8853	998.3653
1988	56.6749	1.8845	384.0677	1988	56.6749	1.8845	795.0734	1988	56.6749	1.8845	783.5569	1988	56.6749	1.8845	1031.7523
1989	56.7009	1.8837	412.9134	1989	56.7009	1.8837	822.2952	1989	56.7009	1.8837	788.7151	1989	56.7009	1.8837	1036.5269
1990	56.7269	1.8829	383.332	1990	56.7269	1.8829	791.0898	1990	56.7269	1.8829	887.5253	1990	56.7269	1.8829	1134.9535
1991	56.7529	1.8821	374.829	1991	56.7529	1.8821	780.9629	1991	56.7529	1.8821	961.2235	1991	56.7529	1.8821	1208.2681
1992	56.7789	1.8813	368.5323	1992	56.7789	1.8813	773.0423	1992	56.7789	1.8813	968.1431	1992	56.7789	1.8813	1214.8041
1993	56.8049	1.8805	362.4705	1993	56.8049	1.8805	765.3564	1993	56.8049	1.8805	1125.7932	1993	56.8049	1.8805	1372.0706
1994	56.8309	1.8798	356.2644	1994	56.8309	1.8798	757.5264	1994	56.8309	1.8798	1257.697	1994	56.8309	1.8798	1503.5908
1995	56.8569	1.879	368.0625	1995	56.8569	1.879	767.7005	1995	56.8569	1.879	1539.1517	1995	56.8569	1.879	1784.6619
1996	56.8829	1.8782	437.5758	1996	56.8829	1.8782	835.5899	1996	56.8829	1.8782	1969.6432	1996	56.8829	1.8782	2214.7698
1997	56.9089	1.8774	444.0483	1997	56.9089	1.8774	840.4384	1997	56.9089	1.8774	2698.5376	1997	56.9089	1.8774	2943.2805
1998	56.9349	1.8766	481.4929	1998	56.9349	1.8766	876.2591	1998	56.9349	1.8766	3435.0075	1998	56.9349	1.8766	3679.3669
1999	56.9609	1.8758	510.3628	1999	56.9609	1.8758	903.505	1999	56.9609	1.8758	4398.3347	1999	56.9609	1.8758	4642.3105
2000	56.9869	1.875	451.7885	2000	56.9869	1.875	843.3067	2000	56.9869	1.875	4994.856	2000	56.9869	1.875	5238.4481
2001	57.0129	1.8743	463.4229	2001	57.0129	1.8743	853.3172	2001	57.0129	1.8743	4999.3505	2001	57.0129	1.8743	5242.5591
2002	57.0389	1.8735	432.8034	2002	57.0389	1.8735	821.0738	2002	57.0389	1.8735	4815.2036	2002	57.0389	1.8735	5058.0285
2003	57.0649	1.8727	456.4556	2003	57.0649	1.8727	843.102	2003	57.0649	1.8727	4607.293	2003	57.0649	1.8727	4849.7343
2004	57.0909	1.8719	450.124	2004	57.0909	1.8719	835.1464	2004	57.0909	1.8719	4363.3684	2004	57.0909	1.8719	4605.4261
2005	57.1169	1.8711	476.3197	2005	57.1169	1.8711	859.7181	2005	57.1169	1.8711	4063.1542	2005	57.1169	1.8711	4304.8283
2006	57.1429	1.8704	442.5804	2006	57.1429	1.8704	824.3549	2006	57.1429	1.8704	3764.173	2006	57.1429	1.8704	4005.4635
2007	57.1689	1.8696	416.7678	2007	57.1689	1.8696	796.9183	2007	57.1689	1.8696	3258.6874	2007	57.1689	1.8696	3499.5942
2008	57.1949	1.8688	374.0837	2008	57.1949	1.8688	752.6103	2008	57.1949	1.8688	2708.6292	2008	57.1949	1.8688	2949.1524
2009	57.2209	1.868	417.0628	2009	57.2209	1.868	793.9654	2009	57.2209	1.868	2186.6047	2009	57.2209	1.868	2426.7443
2010	57.2469	1.8672	451.085	2010	57.2469	1.8672	826.3637	2010	57.2469	1.8672	1865.7983	2010	57.2469	1.8672	2105.5543
2011	57.2729	1.8665	403.2558	2011	57.2729	1.8665	776.9105	2011	57.2729	1.8665	1481.895	2011	57.2729	1.8665	1721.2673

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2012	57.2989	1.8657	439.4678	2012	57.2989	1.8657	811.4986	2012	57.2989	1.8657	1294.8395	2012	57.2989	1.8657	1533.8282
2013	57.3249	1.8649	494.5196	2013	57.3249	1.8649	864.9264	2013	57.3249	1.8649	1142.3789	2013	57.3249	1.8649	1380.9841
2014	57.3509	1.8641	547.8778	2014	57.3509	1.8641	916.6606	2014	57.3509	1.8641	1007.2417	2014	57.3509	1.8641	1245.4632
2015	57.3769	1.8634	573.9236	2015	57.3769	1.8634	941.0825	2015	57.3769	1.8634	912.4788	2015	57.3769	1.8634	1150.3167
2016	57.4029	1.8626	580.702	2016	57.4029	1.8626	946.2369	2016	57.4029	1.8626	812.5786	2016	57.4029	1.8626	1050.0329
2017	57.4289	1.8618	617.9687	2017	57.4289	1.8618	981.8797	2017	57.4289	1.8618	817.9126	2017	57.4289	1.8618	1054.9833
2018	57.4549	1.8611	562.4823	2018	57.4549	1.8611	924.7693	2018	57.4549	1.8611	803.5119	2018	57.4549	1.8611	1040.199
2019	57.4809	1.8603	629.7603	2019	57.4809	1.8603	990.4233	2019	57.4809	1.8603	680.6181	2019	57.4809	1.8603	916.9215
2020	57.5069	1.8595	692.9082	2020	57.5069	1.8595	1051.9473	2020	57.5069	1.8595	649.0735	2020	57.5069	1.8595	884.9933
2021	57.5329	1.8587	592.2753	2021	57.5329	1.8587	949.6904	2021	57.5329	1.8587	636.9802	2021	57.5329	1.8587	872.5164
2022	57.5589	1.858	628.0378	2022	57.5589	1.858	983.8289	2022	57.5589	1.858	595.1774	2022	57.5589	1.858	830.3299
2023	57.5849	1.8572	584.9766	2023	57.5849	1.8572	939.1438	2023	57.5849	1.8572	573.5515	2023	57.5849	1.8572	808.3204
2024	57.6109	1.8564	549.1503	2024	57.6109	1.8564	901.6935	2024	57.6109	1.8564	543.8714	2024	57.6109	1.8564	778.2567
2025	57.6369	1.8557	576.5164	2025	57.6369	1.8557	927.4357	2025	57.6369	1.8557	536.4946	2025	57.6369	1.8557	770.4963
2026	57.6629	1.8549	497.2278	2026	57.6629	1.8549	846.5231	2026	57.6629	1.8549	513.698	2026	57.6629	1.8549	747.3161
2027	57.6889	1.8542	543.6907	2027	57.6889	1.8542	890.0512	2027	57.6889	1.8542	535.9963	2027	57.6889	1.8542	769.2308
2028	57.7149	1.8534	513.5237	2028	57.7149	1.8534	856.9494	2028	57.7149	1.8534	493.886	2028	57.7149	1.8534	726.7368
2029	57.7409	1.8526	462.3639	2029	57.7409	1.8526	802.8549	2029	57.7409	1.8526	500.8191	2029	57.7409	1.8526	733.2863
2030	57.7669	1.8519	454.1054	2030	57.7669	1.8519	791.6617	2030	57.7669	1.8519	532.4171	2030	57.7669	1.8519	764.5007
2031	57.7929	1.8511	380.8969	2031	57.7929	1.8511	715.5183	2031	57.7929	1.8511	550.1662	2031	57.7929	1.8511	781.8662
2032	57.8189	1.8503	395.9002	2032	57.8189	1.8503	727.5869	2032	57.8189	1.8503	540.8141	2032	57.8189	1.8503	772.1305
2033	57.8449	1.8496	389.0037	2033	57.8449	1.8496	717.7557	2033	57.8449	1.8496	504.7133	2033	57.8449	1.8496	735.646
2034	57.8709	1.8488	375.9352	2034	57.8709	1.8488	701.7523	2034	57.8709	1.8488	489.3431	2034	57.8709	1.8488	719.8922
2035	57.8969	1.8481	381.0259	2035	57.8969	1.8481	703.9083	2035	57.8969	1.8481	491.9248	2035	57.8969	1.8481	722.0903
2036	57.9229	1.8473	410.9127	2036	57.9229	1.8473	730.8603	2036	57.9229	1.8473	530.3923	2036	57.9229	1.8473	760.1742
2037	57.9489	1.8465	355.3319	2037	57.9489	1.8465	672.3448	2037	57.9489	1.8465	522.8393	2037	57.9489	1.8465	752.2375
2038	57.9749	1.8458	348.2282	2038	57.9749	1.8458	662.3063	2038	57.9749	1.8458	463.0168	2038	57.9749	1.8458	692.0314
2039	58.0009	1.845	391.7751	2039	58.0009	1.845	702.9184	2039	58.0009	1.845	453.8176	2039	58.0009	1.845	682.4486
2040	58.0269	1.8443	375.0536	2040	58.0269	1.8443	683.2622	2040	58.0269	1.8443	493.4064	2040	58.0269	1.8443	721.6538
2041	58.0529	1.8435	412.7205	2041	58.0529	1.8435	717.9943	2041	58.0529	1.8435	500.5851	2041	58.0529	1.8435	728.4489
2042	58.0789	1.8428	389.9851	2042	58.0789	1.8428	692.3242	2042	58.0789	1.8428	524.9723	2042	58.0789	1.8428	752.4524
2043	58.1049	1.842	380.3344	2043	58.1049	1.842	679.7387	2043	58.1049	1.842	506.5723	2043	58.1049	1.842	733.6689
2044	58.1309	1.8413	417.7821	2044	58.1309	1.8413	714.2515	2044	58.1309	1.8413	449.9179	2044	58.1309	1.8413	676.6308
2045	58.1569	1.8405	406.8684	2045	58.1569	1.8405	700.4031	2045	58.1569	1.8405	463.5806	2045	58.1569	1.8405	689.9099
2046	58.1829	1.8398	393.0198	2046	58.1829	1.8398	683.6198	2046	58.1829	1.8398	451.9513	2046	58.1829	1.8398	677.897
2047	58.2089	1.839	395.4318	2047	58.2089	1.839	683.097	2047	58.2089	1.839	440.341	2047	58.2089	1.839	665.903

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2048	58.2349	1.8383	393.068	2048	58.2349	1.8383	677.7984	2048	58.2349	1.8383	460.4936	2048	58.2349	1.8383	685.672
2049	58.2609	1.8375	386.4129	2049	58.2609	1.8375	668.2086	2049	58.2609	1.8375	483.7881	2049	58.2609	1.8375	708.5829
2050	58.2869	1.8368	423.6156	2050	58.2869	1.8368	702.4765	2050	58.2869	1.8368	435.0433	2050	58.2869	1.8368	659.4545
2051	58.3129	1.836	425.9542	2051	58.3129	1.836	701.8803	2051	58.3129	1.836	440.2781	2051	58.3129	1.836	664.3057
2052	58.3389	1.8353	393.6829	2052	58.3389	1.8353	666.6743	2052	58.3389	1.8353	436.5759	2052	58.3389	1.8353	660.2199
2053	58.3649	1.8345	397.6509	2053	58.3649	1.8345	667.7075	2053	58.3649	1.8345	485.209	2053	58.3649	1.8345	708.4694
2054	58.3909	1.8338	416.9192	2054	58.3909	1.8338	686.7021	2054	58.3909	1.8338	442.3202	2054	58.3909	1.8338	665.1969
2055	58.4169	1.833	419.1536	2055	58.4169	1.833	688.6627	2055	58.4169	1.833	459.468	2055	58.4169	1.833	681.9611
2056	58.4429	1.8323	424.0808	2056	58.4429	1.8323	693.3163	2056	58.4429	1.8323	470.4546	2056	58.4429	1.8323	692.564
2057	58.4689	1.8316	429.638	2057	58.4689	1.8316	698.5998	2057	58.4689	1.8316	462.8704	2057	58.4689	1.8316	684.5963
2058	58.4949	1.8308	424.4135	2058	58.4949	1.8308	693.1016	2058	58.4949	1.8308	472.607	2058	58.4949	1.8308	693.9492
2059	58.5209	1.8301	424.6451	2059	58.5209	1.8301	693.0595	2059	58.5209	1.8301	450.1048	2059	58.5209	1.8301	671.0634
2060	58.5469	1.8293	402.2094	2060	58.5469	1.8293	670.35	2060	58.5469	1.8293	451.8051	2060	58.5469	1.8293	672.38
2061	58.5729	1.8286	417.8579	2061	58.5729	1.8286	685.7248	2061	58.5729	1.8286	461.768	2061	58.5729	1.8286	681.9593
2062	58.5989	1.8279	442.6561	2062	58.5989	1.8279	710.2492	2062	58.5989	1.8279	449.3899	2062	58.5989	1.8279	669.1975
2063	58.6249	1.8271	484.4394	2063	58.6249	1.8271	751.7589	2063	58.6249	1.8271	432.8518	2063	58.6249	1.8271	652.2758
2064	58.6509	1.8264	520.8936	2064	58.6509	1.8264	787.9394	2064	58.6509	1.8264	439.8083	2064	58.6509	1.8264	658.8487
2065	58.6769	1.8256	542.6047	2065	58.6769	1.8256	809.3767	2065	58.6769	1.8256	445.0171	2065	58.6769	1.8256	663.6738
2066	58.7029	1.8249	598.7238	2066	58.7029	1.8249	865.2221	2066	58.7029	1.8249	435.685	2066	58.7029	1.8249	653.9581
2067	58.7289	1.8242	657.8026	2067	58.7289	1.8242	924.0272	2067	58.7289	1.8242	449.1268	2067	58.7289	1.8242	667.0163
2068	58.7549	1.8234	747.8111	2068	58.7549	1.8234	1013.762	2068	58.7549	1.8234	480.6847	2068	58.7549	1.8234	698.1905
2069	58.7809	1.8227	800.9019	2069	58.7809	1.8227	1066.579	2069	58.7809	1.8227	484.8989	2069	58.7809	1.8227	702.0211
2070	58.8069	1.822	784.1842	2070	58.8069	1.822	1049.5877	2070	58.8069	1.822	459.9628	2070	58.8069	1.822	676.7014
2071	58.8329	1.8212	765.3578	2071	58.8329	1.8212	1030.4875	2071	58.8329	1.8212	455.4796	2071	58.8329	1.8212	671.8345
2072	58.8589	1.8205	718.088	2072	58.8589	1.8205	982.9441	2072	58.8589	1.8205	459.6175	2072	58.8589	1.8205	675.5888
2073	58.8849	1.8198	667.7773	2073	58.8849	1.8198	932.3596	2073	58.8849	1.8198	429.5978	2073	58.8849	1.8198	645.1855
2074	58.9109	1.819	671.1256	2074	58.9109	1.819	935.4342	2074	58.9109	1.819	402.8136	2074	58.9109	1.819	618.0176
2075	58.9369	1.8183	664.9544	2075	58.9369	1.8183	928.9893	2075	58.9369	1.8183	424.4474	2075	58.9369	1.8183	639.2678
2076	58.9629	1.8176	603.6589	2076	58.9629	1.8176	867.4201	2076	58.9629	1.8176	460.4893	2076	58.9629	1.8176	674.926
2077	58.9889	1.8168	592.5059	2077	58.9889	1.8168	855.9934	2077	58.9889	1.8168	462.2954	2077	58.9889	1.8168	676.3485
2078	59.0149	1.8161	537.3389	2078	59.0149	1.8161	800.5526	2078	59.0149	1.8161	431.1111	2078	59.0149	1.8161	644.7806
2079	59.0409	1.8154	448.4304	2079	59.0409	1.8154	711.3705	2079	59.0409	1.8154	440.0768	2079	59.0409	1.8154	653.3627
2080	59.0669	1.8147	430.0173	2080	59.0669	1.8147	692.6836	2080	59.0669	1.8147	455.0339	2080	59.0669	1.8147	667.9361
2081	59.0929	1.8139	431.9029	2081	59.0929	1.8139	694.2955	2081	59.0929	1.8139	435.585	2081	59.0929	1.8139	648.1036
2082	59.1189	1.8132	448.2537	2082	59.1189	1.8132	710.3727	2082	59.1189	1.8132	447.1484	2082	59.1189	1.8132	659.2833
2083	59.1449	1.8125	415.5969	2083	59.1449	1.8125	677.4421	2083	59.1449	1.8125	422.5905	2083	59.1449	1.8125	634.3418

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2084	59.1709	1.8118	374.7516	2084	59.1709	1.8118	636.3231	2084	59.1709	1.8118	423.6323	2084	59.1709	1.8118	635
2085	59.1969	1.811	385.4972	2085	59.1969	1.811	646.795	2085	59.1969	1.811	438.5034	2085	59.1969	1.811	649.4874
2086	59.2229	1.8103	409.2087	2086	59.2229	1.8103	670.2327	2086	59.2229	1.8103	468.4635	2086	59.2229	1.8103	679.0639
2087	59.2489	1.8096	429.114	2087	59.2489	1.8096	689.8643	2087	59.2489	1.8096	444.428	2087	59.2489	1.8096	654.6448
2088	59.2749	1.8089	403.7911	2088	59.2749	1.8089	664.2678	2088	59.2749	1.8089	413.0348	2088	59.2749	1.8089	622.8679
2089	59.3009	1.8081	369.3858	2089	59.3009	1.8081	629.5887	2089	59.3009	1.8081	450.2604	2089	59.3009	1.8081	659.7099
2090	59.3269	1.8074	385.4063	2090	59.3269	1.8074	645.3355	2090	59.3269	1.8074	445.8992	2090	59.3269	1.8074	654.9651
2091	59.3529	1.8067	424.2241	2091	59.3529	1.8067	683.8796	2091	59.3529	1.8067	484.0769	2091	59.3529	1.8067	692.7591
2092	59.3789	1.806	387.3657	2092	59.3789	1.806	646.7475	2092	59.3789	1.806	410.1964	2092	59.3789	1.806	618.495
2093	59.4049	1.8053	386.1643	2093	59.4049	1.8053	645.2723	2093	59.4049	1.8053	407.3871	2093	59.4049	1.8053	615.3021
2094	59.4309	1.8046	381.374	2094	59.4309	1.8046	640.2083	2094	59.4309	1.8046	409.9132	2094	59.4309	1.8046	617.4445
2095	59.4569	1.8038	381.7936	2095	59.4569	1.8038	640.3542	2095	59.4569	1.8038	439.084	2095	59.4569	1.8038	646.2317
2096	59.4829	1.8031	397.0509	2096	59.4829	1.8031	655.3378	2096	59.4829	1.8031	448.2776	2096	59.4829	1.8031	655.0417
2097	59.5089	1.8024	345.7823	2097	59.5089	1.8024	603.7955	2097	59.5089	1.8024	429.0541	2097	59.5089	1.8024	635.4345
2098	59.5349	1.8017	401.2253	2098	59.5349	1.8017	658.9648	2098	59.5349	1.8017	431.864	2098	59.5349	1.8017	637.8608
2099	59.5609	1.801	409.9269	2099	59.5609	1.801	667.3927	2099	59.5609	1.801	409.525	2099	59.5609	1.801	615.1382
2100	59.5869	1.8003	424.9609	2100	59.5869	1.8003	682.153	2100	59.5869	1.8003	441.5974	2100	59.5869	1.8003	646.8269
2101	59.6129	1.7995	401.9185	2101	59.6129	1.7995	658.8368	2101	59.6129	1.7995	439.3591	2101	59.6129	1.7995	644.205
2102	59.6389	1.7988	399.2097	2102	59.6389	1.7988	655.8543	2102	59.6389	1.7988	434.3693	2102	59.6389	1.7988	638.8316
2103	59.6649	1.7981	384.9056	2103	59.6649	1.7981	641.2765	2103	59.6649	1.7981	450.4744	2103	59.6649	1.7981	654.553
2104	59.6909	1.7974	371.0375	2104	59.6909	1.7974	627.1347	2104	59.6909	1.7974	422.0407	2104	59.6909	1.7974	625.7357
2105	59.7169	1.7967	384.065	2105	59.7169	1.7967	639.8885	2105	59.7169	1.7967	444.7127	2105	59.7169	1.7967	648.0241
2106	59.7429	1.796	379.0624	2106	59.7429	1.796	634.6122	2106	59.7429	1.796	429.1415	2106	59.7429	1.796	632.0692
2107	59.7689	1.7953	397.6509	2107	59.7689	1.7953	652.927	2107	59.7689	1.7953	412.5902	2107	59.7689	1.7953	615.1343
2108	59.7949	1.7946	379.7779	2108	59.7949	1.7946	635.1875	2108	59.7949	1.7946	398.5267	2108	59.7949	1.7946	600.6871
2109	59.8209	1.7939	382.3789	2109	59.8209	1.7939	637.9219	2109	59.8209	1.7939	413.8823	2109	59.8209	1.7939	615.6591
2110	59.8469	1.7932	388.4816	2110	59.8469	1.7932	644.158	2110	59.8469	1.7932	399.6068	2110	59.8469	1.7932	601
2111	59.8729	1.7925	340.3181	2111	59.8729	1.7925	596.1279	2111	59.8729	1.7925	403.2526	2111	59.8729	1.7925	604.2621
2112	59.8989	1.7917	343.2996	2112	59.8989	1.7917	599.2429	2112	59.8989	1.7917	448.456	2112	59.8989	1.7917	649.0818
2113	59.9249	1.791	367.4821	2113	59.9249	1.791	623.5589	2113	59.9249	1.791	398.8607	2113	59.9249	1.791	599.103
2114	59.9509	1.7903	422.4479	2114	59.9509	1.7903	678.658	2114	59.9509	1.7903	423.3466	2114	59.9509	1.7903	623.2052
2115	59.9769	1.7896	412.0495	2115	59.9769	1.7896	668.3932	2115	59.9769	1.7896	430.4717	2115	59.9769	1.7896	629.9467
2116	60.0029	1.7889	388.0539	2116	60.0029	1.7889	644.531	2116	60.0029	1.7889	469.0809	2116	60.0029	1.7889	668.1722
2117	60.0289	1.7882	424.2123	2117	60.0289	1.7882	680.8228	2117	60.0289	1.7882	481.2126	2117	60.0289	1.7882	679.9203
2118	60.0549	1.7875	384.4758	2118	60.0549	1.7875	641.2197	2118	60.0549	1.7875	463.7749	2118	60.0549	1.7875	662.0989
2119	60.0809	1.7868	408.7372	2119	60.0809	1.7868	665.6146	2119	60.0809	1.7868	452.2446	2119	60.0809	1.7868	650.185

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2120	60.1069	1.7861	396.3185	2120	60.1069	1.7861	653.3294	2120	60.1069	1.7861	433.9247	2120	60.1069	1.7861	631.4814
2121	60.1329	1.7854	411.2915	2121	60.1329	1.7854	668.4358	2121	60.1329	1.7854	467.5928	2121	60.1329	1.7854	664.7659
2122	60.1589	1.7847	421.2704	2122	60.1589	1.7847	678.5482	2122	60.1589	1.7847	426.2438	2122	60.1589	1.7847	623.0332
2123	60.1849	1.784	451.8254	2123	60.1849	1.784	709.2366	2123	60.1849	1.784	447.2717	2123	60.1849	1.784	643.6775
2124	60.2109	1.7833	471.2198	2124	60.2109	1.7833	728.7645	2124	60.2109	1.7833	490.1167	2124	60.2109	1.7833	686.1388
2125	60.2369	1.7826	506.5488	2125	60.2369	1.7826	764.2269	2125	60.2369	1.7826	430.4581	2125	60.2369	1.7826	626.0966
2126	60.2629	1.7819	449.7051	2126	60.2629	1.7819	707.5167	2126	60.2629	1.7819	431.2359	2126	60.2629	1.7819	626.4908
2127	60.2889	1.7812	495.6518	2127	60.2889	1.7812	753.5967	2127	60.2889	1.7812	452.9485	2127	60.2889	1.7812	647.8197
2128	60.3149	1.7805	581.4971	2128	60.3149	1.7805	839.5755	2128	60.3149	1.7805	405.3766	2128	60.3149	1.7805	599.8641
2129	60.3409	1.7798	589.0174	2129	60.3409	1.7798	847.2293	2129	60.3409	1.7798	410.5204	2129	60.3409	1.7798	604.6243
2130	60.3669	1.7792	691.9565	2130	60.3669	1.7792	950.3018	2130	60.3669	1.7792	422.785	2130	60.3669	1.7792	616.5053
2131	60.3929	1.7785	754.9902	2131	60.3929	1.7785	1013.4689	2131	60.3929	1.7785	455.822	2131	60.3929	1.7785	649.1586
2132	60.4189	1.7778	909.5501	2132	60.4189	1.7778	1168.1623	2132	60.4189	1.7778	431.9568	2132	60.4189	1.7778	624.9098
2133	60.4449	1.7771	1106.7715	2133	60.4449	1.7771	1365.5171	2133	60.4449	1.7771	422.3566	2133	60.4449	1.7771	614.926
2134	60.4709	1.7764	1146.4784	2134	60.4709	1.7764	1405.3575	2134	60.4709	1.7764	434.3506	2134	60.4709	1.7764	626.5362
2135	60.4969	1.7757	1186.4337	2135	60.4969	1.7757	1444.1622	2135	60.4969	1.7757	447.1079	2135	60.4969	1.7757	638.9099
2136	60.5229	1.775	1117.0952	2136	60.5229	1.775	1373.6731	2136	60.5229	1.775	449.5816	2136	60.5229	1.775	641
2137	60.5489	1.7743	1085.259	2137	60.5489	1.7743	1340.6863	2137	60.5489	1.7743	383.0687	2137	60.5489	1.7743	574.1034
2138	60.5749	1.7736	1067.5981	2138	60.5749	1.7736	1321.8748	2138	60.5749	1.7736	393.6189	2138	60.5749	1.7736	584.27
2139	60.6009	1.7729	1011.4164	2139	60.6009	1.7729	1264.5426	2139	60.6009	1.7729	415.6692	2139	60.6009	1.7729	605.9366
2140	60.6269	1.7722	961.5422	2140	60.6269	1.7722	1213.5178	2140	60.6269	1.7722	443.4027	2140	60.6269	1.7722	633.2865
2141	60.6529	1.7716	932.2513	2141	60.6529	1.7716	1183.0764	2141	60.6529	1.7716	425.9784	2141	60.6529	1.7716	615.4786
2142	60.6789	1.7709	884.2124	2142	60.6789	1.7709	1133.8868	2142	60.6789	1.7709	458.9712	2142	60.6789	1.7709	648.0877
2143	60.7049	1.7702	828.1821	2143	60.7049	1.7702	1076.7059	2143	60.7049	1.7702	452.113	2143	60.7049	1.7702	640.8459
2144	60.7309	1.7695	847.7705	2144	60.7309	1.7695	1095.1437	2144	60.7309	1.7695	447.1238	2144	60.7309	1.7695	635.4731
2145	60.7569	1.7688	870.2232	2145	60.7569	1.7688	1116.4459	2145	60.7569	1.7688	453.1207	2145	60.7569	1.7688	641.0862
2146	60.7829	1.7681	922.9456	2146	60.7829	1.7681	1168.0177	2146	60.7829	1.7681	476.9185	2146	60.7829	1.7681	664.5005
2147	60.8089	1.7674	1013.7545	2147	60.8089	1.7674	1257.676	2147	60.8089	1.7674	444.8096	2147	60.8089	1.7674	632.0079
2148	60.8349	1.7668	1028.2018	2148	60.8349	1.7668	1270.9727	2148	60.8349	1.7668	401.0087	2148	60.8349	1.7668	587.8233
2149	60.8609	1.7661	1027.875	2149	60.8609	1.7661	1269.4953	2149	60.8609	1.7661	428.0363	2149	60.8609	1.7661	614.4673
2150	60.8869	1.7654	992.9416	2150	60.8869	1.7654	1233.4114	2150	60.8869	1.7654	387.7312	2150	60.8869	1.7654	573.7786
2151	60.9129	1.7647	987.6881	2151	60.9129	1.7647	1227.0073	2151	60.9129	1.7647	404.363	2151	60.9129	1.7647	590.0267
2152	60.9389	1.764	1015.203	2152	60.9389	1.764	1253.3716	2152	60.9389	1.764	432.6343	2152	60.9389	1.764	617.9143
2153	60.9649	1.7634	982.3234	2153	60.9649	1.7634	1219.3414	2153	60.9649	1.7634	415.3923	2153	60.9649	1.7634	600.2888
2154	60.9909	1.7627	913.2467	2154	60.9909	1.7627	1149.1141	2154	60.9909	1.7627	399.3888	2154	60.9909	1.7627	583.9016
2155	61.0169	1.762	829.3093	2155	61.0169	1.762	1064.0261	2155	61.0169	1.762	425.1031	2155	61.0169	1.762	609.2322

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2156	61.0429	1.7613	799.756	2156	61.0429	1.7613	1033.3222	2156	61.0429	1.7613	422.4958	2156	61.0429	1.7613	606.2413
2157	61.0689	1.7606	731.8949	2157	61.0689	1.7606	964.3106	2157	61.0689	1.7606	427.0417	2157	61.0689	1.7606	610.4035
2158	61.0949	1.76	647.8899	2158	61.0949	1.76	879.155	2158	61.0949	1.76	413.5196	2158	61.0949	1.76	596.4978
2159	61.1209	1.7593	628.1747	2159	61.1209	1.7593	858.2892	2159	61.1209	1.7593	405.6331	2159	61.1209	1.7593	588.2277
2160	61.1469	1.7586	631.3028	2160	61.1469	1.7586	860.2667	2160	61.1469	1.7586	418.7223	2160	61.1469	1.7586	600.9332
2161	61.1729	1.7579	570.9948	2161	61.1729	1.7579	798.8081	2161	61.1729	1.7579	412.2479	2161	61.1729	1.7579	594.0752
2162	61.1989	1.7573	486.1666	2162	61.1989	1.7573	712.8293	2162	61.1989	1.7573	399.6509	2162	61.1989	1.7573	581.0945
2163	61.2249	1.7566	475.7639	2163	61.2249	1.7566	701.2761	2163	61.2249	1.7566	387.076	2163	61.2249	1.7566	568.1359
2164	61.2509	1.7559	471.5771	2164	61.2509	1.7559	695.9387	2164	61.2509	1.7559	397.6185	2164	61.2509	1.7559	578.2948
2165	61.2769	1.7552	424.2121	2165	61.2769	1.7552	647.4231	2165	61.2769	1.7552	418.4608	2165	61.2769	1.7552	598.7534
2166	61.3029	1.7546	434.1797	2166	61.3029	1.7546	656.2401	2166	61.3029	1.7546	414.7992	2166	61.3029	1.7546	594.7082
2167	61.3289	1.7539	461.9904	2167	61.3289	1.7539	682.9002	2167	61.3289	1.7539	417.6409	2167	61.3289	1.7539	597.1663
2168	61.3549	1.7532	438.3018	2168	61.3549	1.7532	658.0611	2168	61.3549	1.7532	441.3149	2168	61.3549	1.7532	620.4566
2169	61.3809	1.7526	406.2257	2169	61.3809	1.7526	624.8344	2169	61.3809	1.7526	430.33	2169	61.3809	1.7526	609.088
2170	61.4069	1.7519	405.9412	2170	61.4069	1.7519	623.3993	2170	61.4069	1.7519	407.4969	2170	61.4069	1.7519	585.8713
2171	61.4329	1.7512	416.069	2171	61.4329	1.7512	632.3765	2171	61.4329	1.7512	421.7876	2171	61.4329	1.7512	599.7784
2172	61.4589	1.7506	397.9994	2172	61.4589	1.7506	613.1563	2172	61.4589	1.7506	419.2557	2172	61.4589	1.7506	596.8628
2173	61.4849	1.7499	405.0863	2173	61.4849	1.7499	619.0927	2173	61.4849	1.7499	407.1619	2173	61.4849	1.7499	584.3854
2174	61.5109	1.7492	418.9785	2174	61.5109	1.7492	631.8343	2174	61.5109	1.7492	423.8151	2174	61.5109	1.7492	600.6549
2175	61.5369	1.7485	401.1501	2175	61.5369	1.7485	612.8553	2175	61.5369	1.7485	436.9728	2175	61.5369	1.7485	613.4289
2176	61.5629	1.7479	393.5792	2176	61.5629	1.7479	604.1338	2176	61.5629	1.7479	437.9275	2176	61.5629	1.7479	614
2177	61.5889	1.7472	385.7778	2177	61.5889	1.7472	595.1818	2177	61.5889	1.7472	438.3111	2177	61.5889	1.7472	614
2178	61.6149	1.7466	400.915	2178	61.6149	1.7466	609.1684	2178	61.6149	1.7466	436.2998	2178	61.6149	1.7466	611.605
2179	61.6409	1.7459	404.6563	2179	61.6409	1.7459	611.7592	2179	61.6409	1.7459	424.515	2179	61.6409	1.7459	599.4366
2180	61.6669	1.7452	378.5996	2180	61.6669	1.7452	584.5519	2180	61.6669	1.7452	401.979	2180	61.6669	1.7452	576.5169
2181	61.6929	1.7446	375.3774	2181	61.6929	1.7446	580.1791	2181	61.6929	1.7446	395.7114	2181	61.6929	1.7446	569.8657
2182	61.7189	1.7439	357.4273	2182	61.7189	1.7439	561.0784	2182	61.7189	1.7439	405.4777	2182	61.7189	1.7439	579.2483
2183	61.7449	1.7432	364.3446	2183	61.7449	1.7432	566.8451	2183	61.7449	1.7432	403.3033	2183	61.7449	1.7432	576.6903
2184	61.7709	1.7426	376.3861	2184	61.7709	1.7426	577.736	2184	61.7709	1.7426	419.6949	2184	61.7709	1.7426	592.6982
2185	61.7969	1.7419	402.6052	2185	61.7969	1.7419	602.8045	2185	61.7969	1.7419	416.4564	2185	61.7969	1.7419	589.076
2186	61.8229	1.7413	428.119	2186	61.8229	1.7413	627.1677	2186	61.8229	1.7413	438.5806	2186	61.8229	1.7413	610.8166
2187	61.8489	1.7406	399.1439	2187	61.8489	1.7406	597.0421	2187	61.8489	1.7406	493.7667	2187	61.8489	1.7406	665.6191
2188	61.8749	1.7399	397.6509	2188	61.8749	1.7399	594.3985	2188	61.8749	1.7399	446.2314	2188	61.8749	1.7399	617.7001
2189	61.9009	1.7393	419.3867	2189	61.9009	1.7393	615.7401	2189	61.9009	1.7393	431.1237	2189	61.9009	1.7393	602.2088
2190	61.9269	1.7386	415.6377	2190	61.9269	1.7386	611.597	2190	61.9269	1.7386	395.8588	2190	61.9269	1.7386	566.5602
2191	61.9529	1.738	400.3789	2191	61.9529	1.738	595.9439	2191	61.9529	1.738	399.8437	2191	61.9529	1.738	570.1614

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2192	61.9789	1.7373	425.9381	2192	61.9789	1.7373	621.109	2192	61.9789	1.7373	408.9287	2192	61.9789	1.7373	578.8628
2193	62.0049	1.7367	440.2072	2193	62.0049	1.7367	634.9839	2193	62.0049	1.7367	419.9529	2193	62.0049	1.7367	589.5033
2194	62.0309	1.736	404.1366	2194	62.0309	1.736	598.5192	2194	62.0309	1.736	423.2654	2194	62.0309	1.736	592.4322
2195	62.0569	1.7353	397.4798	2195	62.0569	1.7353	591.4682	2195	62.0569	1.7353	421.2023	2195	62.0569	1.7353	589.9855
2196	62.0829	1.7347	380.0675	2196	62.0829	1.7347	573.6617	2196	62.0829	1.7347	459.836	2196	62.0829	1.7347	628.2355
2197	62.1089	1.734	379.8509	2197	62.1089	1.734	573.051	2197	62.1089	1.734	447.4541	2197	62.1089	1.734	615.47
2198	62.1349	1.7334	378.026	2198	62.1349	1.7334	570.8318	2198	62.1349	1.7334	422.1635	2198	62.1349	1.7334	589.7957
2199	62.1609	1.7327	407.2919	2199	62.1609	1.7327	599.7036	2199	62.1609	1.7327	424.0479	2199	62.1609	1.7327	591.2964
2200	62.1869	1.7321	380.259	2200	62.1869	1.7321	572.2765	2200	62.1869	1.7321	447.6984	2200	62.1869	1.7321	614.5633
2201	62.2129	1.7314	377.5476	2201	62.2129	1.7314	569.171	2201	62.2129	1.7314	434.0574	2201	62.2129	1.7314	600.5386
2202	62.2389	1.7308	382.9577	2202	62.2389	1.7308	574.1869	2202	62.2389	1.7308	434.8169	2202	62.2389	1.7308	600.9145
2203	62.2649	1.7301	393.5294	2203	62.2649	1.7301	584.3644	2203	62.2649	1.7301	404.4816	2203	62.2649	1.7301	570.1956
2204	62.2909	1.7295	335.0539	2204	62.2909	1.7295	525.4947	2204	62.2909	1.7295	433.4574	2204	62.2909	1.7295	598.7877
2205	62.3169	1.7288	382.6981	2205	62.3169	1.7288	572.7448	2205	62.3169	1.7288	390.9339	2205	62.3169	1.7288	555.8806
2206	62.3429	1.7282	430.7072	2206	62.3429	1.7282	620.3597	2206	62.3429	1.7282	369.2075	2206	62.3429	1.7282	533.7705
2207	62.3689	1.7275	399.5048	2207	62.3689	1.7275	588.7631	2207	62.3689	1.7275	453.8179	2207	62.3689	1.7275	617.9972
2208	62.3949	1.7269	365.5454	2208	62.3949	1.7269	554.4095	2208	62.3949	1.7269	444.9863	2208	62.3949	1.7269	608.782
2209	62.4209	1.7262	435.4679	2209	62.4209	1.7262	623.9379	2209	62.4209	1.7262	431.3827	2209	62.4209	1.7262	594.7948
2210	62.4469	1.7256	465.9421	2210	62.4469	1.7256	654.0179	2210	62.4469	1.7256	400.7065	2210	62.4469	1.7256	563.7349
2211	62.4729	1.7249	365.8922	2211	62.4729	1.7249	553.5739	2211	62.4729	1.7249	408.0641	2211	62.4729	1.7249	570.7088
2212	62.4989	1.7243	374.4543	2212	62.4989	1.7243	561.7417	2212	62.4989	1.7243	393.5932	2212	62.4989	1.7243	555.8543
2213	62.5249	1.7237	385.1727	2213	62.5249	1.7237	572.066	2213	62.5249	1.7237	419.1649	2213	62.5249	1.7237	581.0423
2214	62.5509	1.723	371.0609	2214	62.5509	1.723	557.56	2214	62.5509	1.723	368.5278	2214	62.5509	1.723	530.0216
2215	62.5769	1.7224	427.3956	2215	62.5769	1.7224	613.5005	2215	62.5769	1.7224	437.249	2215	62.5769	1.7224	598.3591
2216	62.6029	1.7217	353.152	2216	62.6029	1.7217	538.8628	2216	62.6029	1.7217	418.9814	2216	62.6029	1.7217	579.7079
2217	62.6289	1.7211	391.7078	2217	62.6289	1.7211	577.0244	2217	62.6289	1.7211	449.364	2217	62.6289	1.7211	609.7068
2218	62.6549	1.7204	394.0525	2218	62.6549	1.7204	578.9749	2218	62.6549	1.7204	345.2617	2218	62.6549	1.7204	505.2209
2219	62.6809	1.7198	383.5559	2219	62.6809	1.7198	568.0841	2219	62.6809	1.7198	441.6829	2219	62.6809	1.7198	601.2584
2220	62.7069	1.7192	404.497	2220	62.7069	1.7192	588.6311	2220	62.7069	1.7192	407.4405	2220	62.7069	1.7192	566.6324
2221	62.7329	1.7185	422.7653	2221	62.7329	1.7185	606.5052	2221	62.7329	1.7185	429.5595	2221	62.7329	1.7185	588.3677
2222	62.7589	1.7179	435.2053	2222	62.7589	1.7179	618.5511	2222	62.7589	1.7179	439.2387	2222	62.7589	1.7179	597.6633
2223	62.7849	1.7172	432.2378	2223	62.7849	1.7172	615.1893	2223	62.7849	1.7172	428.5271	2223	62.7849	1.7172	586.568
2224	62.8109	1.7166	411.7023	2224	62.8109	1.7166	594.2596	2224	62.8109	1.7166	425.5145	2224	62.8109	1.7166	583.1718
2225	62.8369	1.716	415.5009	2225	62.8369	1.716	597.6641	2225	62.8369	1.716	400.5402	2225	62.8369	1.716	557.8138
2226	62.8629	1.7153	386.6982	2226	62.8629	1.7153	568.4672	2226	62.8629	1.7153	411.1077	2226	62.8629	1.7153	567.9977
2227	62.8889	1.7147	416.5793	2227	62.8889	1.7147	597.9542	2227	62.8889	1.7147	441.7089	2227	62.8889	1.7147	598.2153

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2228	62.9149	1.7141	391.1216	2228	62.9149	1.7141	572.1023	2228	62.9149	1.7141	426.8162	2228	62.9149	1.7141	582.9389
2229	62.9409	1.7134	416.1006	2229	62.9409	1.7134	596.6871	2229	62.9409	1.7134	444.0167	2229	62.9409	1.7134	599.7558
2230	62.9669	1.7128	404.7931	2230	62.9669	1.7128	584.9854	2230	62.9669	1.7128	365.3893	2230	62.9669	1.7128	520.7447
2231	62.9929	1.7121	377.0032	2231	62.9929	1.7121	556.8014	2231	62.9929	1.7121	384.72	2231	62.9929	1.7121	539.6918
2232	63.0189	1.7115	419.3544	2232	63.0189	1.7115	598.7584	2232	63.0189	1.7115	338.4734	2232	63.0189	1.7115	493.0614
2233	63.0449	1.7109	373.2233	2233	63.0449	1.7109	552.2331	2233	63.0449	1.7109	405.0451	2233	63.0449	1.7109	559.2495
2234	63.0709	1.7102	400.6558	2234	63.0709	1.7102	579.2714	2234	63.0709	1.7102	425.7709	2234	63.0709	1.7102	579.5917
2235	63.0969	1.7096	405.2777	2235	63.0969	1.7096	583.4992	2235	63.0969	1.7096	413.3917	2235	63.0969	1.7096	566.8288
2236	63.1229	1.709	385.4045	2236	63.1229	1.709	563.2318	2236	63.1229	1.709	379.6468	2236	63.1229	1.709	532.7003
2237	63.1489	1.7084	385.6357	2237	63.1489	1.7084	563.0688	2237	63.1489	1.7084	364.3789	2237	63.1489	1.7084	517.0487
2238	63.1749	1.7077	372.4921	2238	63.1749	1.7077	549.531	2238	63.1749	1.7077	357.087	2238	63.1749	1.7077	509.3732
2239	63.2009	1.7071	369.3552	2239	63.2009	1.7071	546	2239	63.2009	1.7071	425.1676	2239	63.2009	1.7071	577.0701
2240	63.2269	1.7065	376.8053	2240	63.2269	1.7065	553.0559	2240	63.2269	1.7065	406.6337	2240	63.2269	1.7065	558.1526
2241	63.2529	1.7058	388.4324	2241	63.2529	1.7058	564.2888	2241	63.2529	1.7058	447.953	2241	63.2529	1.7058	599.0883
2242	63.2789	1.7052	397.6509	2242	63.2789	1.7052	573.1131	2242	63.2789	1.7052	425.0413	2242	63.2789	1.7052	575.7929
2243	63.3049	1.7046	357.4594	2243	63.3049	1.7046	531.2552	2243	63.3049	1.7046	400.8103	2243	63.3049	1.7046	551.1783
2244	63.3309	1.704	375.3868	2244	63.3309	1.704	547.5162	2244	63.3309	1.704	421.5775	2244	63.3309	1.704	571.5618
2245	63.3569	1.7033	391.2088	2245	63.3569	1.7033	561.6719	2245	63.3569	1.7033	406.165	2245	63.3569	1.7033	555.7656
2246	63.3829	1.7027	383.3366	2246	63.3829	1.7027	552.1332	2246	63.3829	1.7027	428.9345	2246	63.3829	1.7027	578.1515
2247	63.4089	1.7021	361.5774	2247	63.4089	1.7021	528.7077	2247	63.4089	1.7021	434.0214	2247	63.4089	1.7021	582.8547
2248	63.4349	1.7015	360.4684	2248	63.4349	1.7015	525.9323	2248	63.4349	1.7015	401.9568	2248	63.4349	1.7015	550.4064
2249	63.4609	1.7008	385.7378	2249	63.4609	1.7008	549.5353	2249	63.4609	1.7008	385.0712	2249	63.4609	1.7008	533.1372
2250	63.4869	1.7002	361.2612	2250	63.4869	1.7002	523.3923	2250	63.4869	1.7002	423.0339	2250	63.4869	1.7002	570.7163
2251	63.5129	1.6996	384.3265	2251	63.5129	1.6996	544.7911	2251	63.5129	1.6996	447.7748	2251	63.5129	1.6996	595.0736
2252	63.5389	1.699	399.5473	2252	63.5389	1.699	558.3456	2252	63.5389	1.699	423.1583	2252	63.5389	1.699	570.0734
2253	63.5649	1.6983	393.6282	2253	63.5649	1.6983	550.76	2253	63.5649	1.6983	455.3184	2253	63.5649	1.6983	601.8498
2254	63.5909	1.6977	418.9826	2254	63.5909	1.6977	574.4481	2254	63.5909	1.6977	444.3731	2254	63.5909	1.6977	590.5209
2255	63.6169	1.6971	446.6337	2255	63.6169	1.6971	600.4327	2255	63.6169	1.6971	423.9656	2255	63.6169	1.6971	569.7297
2256	63.6429	1.6965	410.476	2256	63.6429	1.6965	562.6087	2256	63.6429	1.6965	426.7457	2256	63.6429	1.6965	572.1262
2257	63.6689	1.6959	376.3042	2257	63.6689	1.6959	526.7704	2257	63.6689	1.6959	414.2358	2257	63.6689	1.6959	559.2326
2258	63.6949	1.6952	381.8863	2258	63.6949	1.6952	530.6862	2258	63.6949	1.6952	387.8306	2258	63.6949	1.6952	532.4438
2259	63.7209	1.6946	382.721	2259	63.7209	1.6946	529.8544	2259	63.7209	1.6946	382.7251	2259	63.7209	1.6946	526.9546
2260	63.7469	1.694	393.0004	2260	63.7469	1.694	538.4674	2260	63.7469	1.694	389.4963	2260	63.7469	1.694	533.3422
2261	63.7729	1.6934	408.8043	2261	63.7729	1.6934	552.605	2261	63.7729	1.6934	396.7183	2261	63.7729	1.6934	540.1806
2262	63.7989	1.6928	417.8257	2262	63.7989	1.6928	559.9599	2262	63.7989	1.6928	429.2063	2262	63.7989	1.6928	572.2848
2263	63.8249	1.6921	433.0919	2263	63.8249	1.6921	573.5597	2263	63.8249	1.6921	412.9567	2263	63.8249	1.6921	555.6516

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2264	63.8509	1.6915	438.2859	2264	63.8509	1.6915	577.0873	2264	63.8509	1.6915	399.0643	2264	63.8509	1.6915	541.3756
2265	63.8769	1.6909	418.7152	2265	63.8769	1.6909	555.8503	2265	63.8769	1.6909	437.7251	2265	63.8769	1.6909	579.6528
2266	63.9029	1.6903	408.6874	2266	63.9029	1.6903	544.156	2266	63.9029	1.6903	406.8553	2266	63.9029	1.6903	548.3993
2267	63.9289	1.6897	393.0705	2267	63.9289	1.6897	526.8727	2267	63.9289	1.6897	403.7069	2267	63.9289	1.6897	544.8672
2268	63.9549	1.6891	394.086	2268	63.9549	1.6891	526.2219	2268	63.9549	1.6891	421.4337	2268	63.9549	1.6891	562.2103
2269	63.9809	1.6885	397.6509	2269	63.9809	1.6885	528.1203	2269	63.9809	1.6885	402.0807	2269	63.9809	1.6885	542.4737
2270	64.0069	1.6878	384.6786	2270	64.0069	1.6878	513.9453	2270	64.0069	1.6878	415.575	2270	64.0069	1.6878	555.7264
2271	64.0329	1.6872	396.9877	2271	64.0329	1.6872	525.0515	2271	64.0329	1.6872	416.0861	2271	64.0329	1.6872	555.9957
2272	64.0589	1.6866	425.3984	2272	64.0589	1.6866	552.2595	2272	64.0589	1.6866	434.2535	2272	64.0589	1.6866	573.9214
2273	64.0849	1.686	457.7555	2273	64.0849	1.686	583.4138	2273	64.0849	1.686	469.8566	2273	64.0849	1.686	609.2828
2274	64.1109	1.6854	474.331	2274	64.1109	1.6854	598.7865	2274	64.1109	1.6854	483.088	2274	64.1109	1.6854	622.2725
2275	64.1369	1.6848	462.4625	2275	64.1369	1.6848	585.7153	2275	64.1369	1.6848	473.3485	2275	64.1369	1.6848	612.2913
2276	64.1629	1.6842	461.875	2276	64.1629	1.6842	583.9249	2276	64.1629	1.6842	442.5918	2276	64.1629	1.6842	581.2929
2277	64.1889	1.6836	467.1434	2277	64.1889	1.6836	587.9906	2277	64.1889	1.6836	440.1238	2277	64.1889	1.6836	578.5831
2278	64.2149	1.683	432.2168	2278	64.2149	1.683	551.8612	2278	64.2149	1.683	444.6656	2278	64.2149	1.683	582.8833
2279	64.2409	1.6823	442.9973	2279	64.2409	1.6823	561.4389	2279	64.2409	1.6823	487.7556	2279	64.2409	1.6823	625.7316
2280	64.2669	1.6817	493.0192	2280	64.2669	1.6817	610.258	2280	64.2669	1.6817	535.6852	2280	64.2669	1.6817	673.4194
2281	64.2929	1.6811	500.7281	2281	64.2929	1.6811	616.7642	2281	64.2929	1.6811	503.6314	2281	64.2929	1.6811	641.124
2282	64.3189	1.6805	476.41	2282	64.3189	1.6805	591.2433	2282	64.3189	1.6805	485.01	2282	64.3189	1.6805	622.2608
2283	64.3449	1.6799	471.9324	2283	64.3449	1.6799	585.5629	2283	64.3449	1.6799	480.6874	2283	64.3449	1.6799	617.6965
2284	64.3709	1.6793	438.3612	2284	64.3709	1.6793	550.7889	2284	64.3709	1.6793	429.3074	2284	64.3709	1.6793	566.0748
2285	64.3969	1.6787	434.1623	2285	64.3969	1.6787	545.3873	2285	64.3969	1.6787	444.762	2285	64.3969	1.6787	581.2877
2286	64.4229	1.6781	448.2361	2286	64.4229	1.6781	558.2583	2286	64.4229	1.6781	433.7853	2286	64.4229	1.6781	570.0693
2287	64.4489	1.6775	454.6866	2287	64.4489	1.6775	563.506	2287	64.4489	1.6775	431.6752	2287	64.4489	1.6775	567.7175
2288	64.4749	1.6769	444.9985	2288	64.4749	1.6769	552.6151	2288	64.4749	1.6769	429.429	2288	64.4749	1.6769	565.2296
2289	64.5009	1.6763	450.498	2289	64.5009	1.6763	556.9118	2289	64.5009	1.6763	409.5441	2289	64.5009	1.6763	545.103
2290	64.5269	1.6757	481.8041	2290	64.5269	1.6757	587.0151	2290	64.5269	1.6757	441.5465	2290	64.5269	1.6757	576.8636
2291	64.5529	1.6751	476.0399	2291	64.5529	1.6751	580.0481	2291	64.5529	1.6751	433.6404	2291	64.5529	1.6751	568.7158
2292	64.5789	1.6745	446.9986	2292	64.5789	1.6745	549.8041	2292	64.5789	1.6745	414.403	2292	64.5789	1.6745	549.2367
2293	64.6049	1.6739	448.8487	2293	64.6049	1.6739	550.4514	2293	64.6049	1.6739	435.9566	2293	64.6049	1.6739	570.5486
2294	64.6309	1.6733	451.8046	2294	64.6309	1.6733	552.2046	2294	64.6309	1.6733	443.6279	2294	64.6309	1.6733	577.9782
2295	64.6569	1.6727	451.0741	2295	64.6569	1.6727	550.2713	2295	64.6569	1.6727	448.841	2295	64.6569	1.6727	582.9496
2296	64.6829	1.6721	397.6509	2296	64.6829	1.6721	495.6453	2296	64.6829	1.6721	436.5898	2296	64.6829	1.6721	570.4567
2297	64.7089	1.6715	425.5933	2297	64.7089	1.6715	523.8608	2297	64.7089	1.6715	438.3748	2297	64.7089	1.6715	572
2298	64.7349	1.6709	411.1042	2298	64.7349	1.6709	509.6448	2298	64.7349	1.6709	441.7439	2298	64.7349	1.6709	575.1274
2299	64.7609	1.6703	491.1093	2299	64.7609	1.6703	589.9228	2299	64.7609	1.6703	453.4611	2299	64.7609	1.6703	586.6029

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2300	64.7869	1.6697	432.2891	2300	64.7869	1.6697	531.3757	2300	64.7869	1.6697	449.2702	2300	64.7869	1.6697	582.1703
2301	64.8129	1.6691	480.9297	2301	64.8129	1.6691	580.2895	2301	64.8129	1.6691	434.1246	2301	64.8129	1.6691	566.7829
2302	64.8389	1.6685	502.7305	2302	64.8389	1.6685	602.3633	2302	64.8389	1.6685	426.1668	2302	64.8389	1.6685	558.5834
2303	64.8649	1.6679	494.2338	2303	64.8649	1.6679	594.1397	2303	64.8649	1.6679	454.3764	2303	64.8649	1.6679	586.5513
2304	64.8909	1.6673	393.2899	2304	64.8909	1.6673	493.4688	2304	64.8909	1.6673	429.4282	2304	64.8909	1.6673	561.3614
2305	64.9169	1.6667	422.7191	2305	64.9169	1.6667	523.1711	2305	64.9169	1.6667	421.1427	2305	64.9169	1.6667	552.8342
2306	64.9429	1.6661	447.1129	2306	64.9429	1.6661	547.838	2306	64.9429	1.6661	431.4566	2306	64.9429	1.6661	562.9064
2307	64.9689	1.6655	441.9817	2307	64.9689	1.6655	542.9798	2307	64.9689	1.6655	464.3151	2307	64.9689	1.6655	595.5232
2308	64.9949	1.6649	460.2321	2308	64.9949	1.6649	561.5033	2308	64.9949	1.6649	456.772	2308	64.9949	1.6649	587.7384
2309	65.0209	1.6643	434.1381	2309	65.0209	1.6643	535.6824	2309	65.0209	1.6643	418.3014	2309	65.0209	1.6643	549.026
2310	65.0469	1.6637	455.1422	2310	65.0469	1.6637	556.9595	2310	65.0469	1.6637	386.2729	2310	65.0469	1.6637	516.7559
2311	65.0729	1.6632	426.2152	2311	65.0729	1.6632	528.3056	2311	65.0729	1.6632	423.4072	2311	65.0729	1.6632	553.6484
2312	65.0989	1.6626	448.7399	2312	65.0989	1.6626	551.1034	2312	65.0989	1.6626	408.4179	2312	65.0989	1.6626	538.4175
2313	65.1249	1.662	397.8549	2313	65.1249	1.662	500.4915	2313	65.1249	1.662	412.8103	2313	65.1249	1.662	542.5682
2314	65.1509	1.6614	419.5983	2314	65.1509	1.6614	522.5079	2314	65.1509	1.6614	393.2692	2314	65.1509	1.6614	522.7853
2315	65.1769	1.6608	392.5294	2315	65.1769	1.6608	495.712	2315	65.1769	1.6608	448.0395	2315	65.1769	1.6608	577.3139
2316	65.2029	1.6602	432.9165	2316	65.2029	1.6602	536.3723	2316	65.2029	1.6602	477.3666	2316	65.2029	1.6602	606.3993
2317	65.2289	1.6596	412.9102	2317	65.2289	1.6596	516.6391	2317	65.2289	1.6596	393.8281	2317	65.2289	1.6596	522.6191
2318	65.2549	1.659	443.6665	2318	65.2549	1.659	547.6684	2318	65.2549	1.659	424.4808	2318	65.2549	1.659	553.0301
2319	65.2809	1.6584	410.7254	2319	65.2809	1.6584	515.0004	2319	65.2809	1.6584	427.6883	2319	65.2809	1.6584	555.9958
2320	65.3069	1.6579	413.4226	2320	65.3069	1.6579	517.9706	2320	65.3069	1.6579	395.2574	2320	65.3069	1.6579	523.3233
2321	65.3329	1.6573	406.3169	2321	65.3329	1.6573	511.138	2321	65.3329	1.6573	404.9786	2321	65.3329	1.6573	532.8028
2322	65.3589	1.6567	449.572	2322	65.3589	1.6567	554.6662	2322	65.3589	1.6567	416.0915	2322	65.3589	1.6567	543.6739
2323	65.3849	1.6561	466.9602	2323	65.3849	1.6561	572.3274	2323	65.3849	1.6561	454.1163	2323	65.3849	1.6561	581.457
2324	65.4109	1.6555	396.0711	2324	65.4109	1.6555	501.7114	2324	65.4109	1.6555	415.9794	2324	65.4109	1.6555	543.0784
2325	65.4369	1.6549	420.3044	2325	65.4369	1.6549	526.2178	2325	65.4369	1.6549	422.608	2325	65.4369	1.6549	549.4653
2326	65.4629	1.6543	454.387	2326	65.4629	1.6543	560.5734	2326	65.4629	1.6543	410.355	2326	65.4629	1.6543	536.9706
2327	65.4889	1.6538	463.9065	2327	65.4889	1.6538	570.366	2327	65.4889	1.6538	457.505	2327	65.4889	1.6538	583.8789
2328	65.5149	1.6532	446.0509	2328	65.5149	1.6532	552.7835	2328	65.5149	1.6532	393.5559	2328	65.5149	1.6532	519.6881
2329	65.5409	1.6526	411.5619	2329	65.5409	1.6526	518.5675	2329	65.5409	1.6526	443.8664	2329	65.5409	1.6526	569.7569
2330	65.5669	1.652	456.7252	2330	65.5669	1.652	564.0039	2330	65.5669	1.652	470.8438	2330	65.5669	1.652	596.4926
2331	65.5929	1.6514	408.7037	2331	65.5929	1.6514	516.2554	2331	65.5929	1.6514	448.9233	2331	65.5929	1.6514	574.3304
2332	65.6189	1.6508	456.0567	2332	65.6189	1.6508	563.8816	2332	65.6189	1.6508	404.8913	2332	65.6189	1.6508	530.0566
2333	65.6449	1.6503	389.8377	2333	65.6449	1.6503	497.9356	2333	65.6449	1.6503	372.3787	2333	65.6449	1.6503	497.3024
2334	65.6709	1.6497	409.1268	2334	65.6709	1.6497	517.4978	2334	65.6709	1.6497	374.2771	2334	65.6709	1.6497	498.959
2335	65.6969	1.6491	400.894	2335	65.6969	1.6491	509.5381	2335	65.6969	1.6491	389.8631	2335	65.6969	1.6491	514.3033

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2336	65.7229	1.6485	398.0829	2336	65.7229	1.6485	507	2336	65.7229	1.6485	385.3185	2336	65.7229	1.6485	509.517
2337	65.7489	1.6479	395.3452	2337	65.7489	1.6479	504.5354	2337	65.7489	1.6479	427.584	2337	65.7489	1.6479	551.5408
2338	65.7749	1.6474	398.5948	2338	65.7749	1.6474	508.058	2338	65.7749	1.6474	421.8645	2338	65.7749	1.6474	545.5796
2339	65.8009	1.6468	440.951	2339	65.8009	1.6468	550.6874	2339	65.8009	1.6468	435.3619	2339	65.8009	1.6468	558.8353
2340	65.8269	1.6462	404.2769	2340	65.8269	1.6462	514.2863	2340	65.8269	1.6462	453.2282	2340	65.8269	1.6462	576.4599
2341	65.8529	1.6456	394.063	2341	65.8529	1.6456	504.3455	2341	65.8529	1.6456	436.6824	2341	65.8529	1.6456	559.6723
2342	65.8789	1.6451	416.8299	2342	65.8789	1.6451	527.3855	2342	65.8789	1.6451	425.0765	2342	65.8789	1.6451	547.8247
2343	65.9049	1.6445	393.4538	2343	65.9049	1.6445	504.2824	2343	65.9049	1.6445	481.4048	2343	65.9049	1.6445	603.9113
2344	65.9309	1.6439	412.4769	2344	65.9309	1.6439	523.5786	2344	65.9309	1.6439	417.7597	2344	65.9309	1.6439	540.0245
2345	65.9569	1.6433	403.8138	2345	65.9569	1.6433	515.1885	2345	65.9569	1.6433	404.3356	2345	65.9569	1.6433	526.3586
2346	65.9829	1.6428	413.4611	2346	65.9829	1.6428	525.1089	2346	65.9829	1.6428	434.8465	2346	65.9829	1.6428	556.6278
2347	66.0089	1.6422	404.6331	2347	66.0089	1.6422	516.554	2347	66.0089	1.6422	453.128	2347	66.0089	1.6422	574.6676
2348	66.0349	1.6416	399.5184	2348	66.0349	1.6416	511.7124	2348	66.0349	1.6416	415.3841	2348	66.0349	1.6416	536.682
2349	66.0609	1.641	384.7814	2349	66.0609	1.641	497.2484	2349	66.0609	1.641	392.6217	2349	66.0609	1.641	513.6779
2350	66.0869	1.6405	397.6509	2350	66.0869	1.6405	510.391	2350	66.0869	1.6405	425.5048	2350	66.0869	1.6405	546.3193
2351	66.1129	1.6399	437.9307	2351	66.1129	1.6399	551.7654	2351	66.1129	1.6399	453.7142	2351	66.1129	1.6399	574.287
2352	66.1389	1.6393	398.9282	2352	66.1389	1.6393	513.8575	2352	66.1389	1.6393	445.5424	2352	66.1389	1.6393	565.8735
2353	66.1649	1.6388	397.1613	2353	66.1649	1.6388	513.1852	2353	66.1649	1.6388	423.667	2353	66.1649	1.6388	543.7563
2354	66.1909	1.6382	391.2547	2354	66.1909	1.6382	508.3732	2354	66.1909	1.6382	457.9345	2354	66.1909	1.6382	577.7821
2355	66.2169	1.6376	401.3605	2355	66.2169	1.6376	519.5735	2355	66.2169	1.6376	488.1091	2355	66.2169	1.6376	607.7151
2356	66.2429	1.637	422.4534	2356	66.2429	1.637	541.761	2356	66.2429	1.637	446.4267	2356	66.2429	1.637	565.7909
2357	66.2689	1.6365	391.4592	2357	66.2689	1.6365	511.8614	2357	66.2689	1.6365	438.5698	2357	66.2689	1.6365	557.6924
2358	66.2949	1.6359	394.2558	2358	66.2949	1.6359	515.7526	2358	66.2949	1.6359	446.4402	2358	66.2949	1.6359	565.3211
2359	66.3209	1.6353	377.4372	2359	66.3209	1.6353	500.0286	2359	66.3209	1.6353	443.1544	2359	66.3209	1.6353	561.7935
2360	66.3469	1.6348	342.8545	2360	66.3469	1.6348	466.5405	2360	66.3469	1.6348	427.7698	2360	66.3469	1.6348	546.1672
2361	66.3729	1.6342	382.8076	2361	66.3729	1.6342	507.5881	2361	66.3729	1.6342	448.1806	2361	66.3729	1.6342	566.3363
2362	66.3989	1.6336	418.8453	2362	66.3989	1.6336	544.7204	2362	66.3989	1.6336	462.0575	2362	66.3989	1.6336	579.9715
2363	66.4249	1.6331	402.1239	2363	66.4249	1.6331	529.0937	2363	66.4249	1.6331	465.3445	2363	66.4249	1.6331	583.0167
2364	66.4509	1.6325	384.6139	2364	66.4509	1.6325	512.6783	2364	66.4509	1.6325	475.3376	2364	66.4509	1.6325	592.7681
2365	66.4769	1.6319	371.0545	2365	66.4769	1.6319	500.2134	2365	66.4769	1.6319	481.0734	2365	66.4769	1.6319	598.2622
2366	66.5029	1.6314	399.6447	2366	66.5029	1.6314	529.8982	2366	66.5029	1.6314	488.3231	2366	66.5029	1.6314	605.2702
2367	66.5289	1.6308	420.6509	2367	66.5289	1.6308	551.999	2367	66.5289	1.6308	530.5361	2367	66.5289	1.6308	647.2415
2368	66.5549	1.6302	400.3065	2368	66.5549	1.6302	532.7492	2368	66.5549	1.6302	518.2544	2368	66.5549	1.6302	634.7181
2369	66.5809	1.6297	407.5991	2369	66.5809	1.6297	541.1364	2369	66.5809	1.6297	504.5227	2369	66.5809	1.6297	620.7447
2370	66.6069	1.6291	406.5691	2370	66.6069	1.6291	541.201	2370	66.6069	1.6291	574.0528	2370	66.6069	1.6291	690.033
2371	66.6329	1.6286	372.7802	2371	66.6329	1.6286	508.5067	2371	66.6329	1.6286	621.0398	2371	66.6329	1.6286	736.7783

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2372	66.6589	1.628	359.9214	2372	66.6589	1.628	496.7424	2372	66.6589	1.628	709.5989	2372	66.6589	1.628	825.0958
2373	66.6849	1.6274	391.0151	2373	66.6849	1.6274	528.9307	2373	66.6849	1.6274	847.57	2373	66.6849	1.6274	962.8252
2374	66.7109	1.6269	416.4458	2374	66.7109	1.6269	555.456	2374	66.7109	1.6269	947.5178	2374	66.7109	1.6269	1062.5312
2375	66.7369	1.6263	417.8958	2375	66.7369	1.6263	558.0006	2375	66.7369	1.6263	1028.3414	2375	66.7369	1.6263	1143.1131
2376	66.7629	1.6258	412.0257	2376	66.7629	1.6258	553.2251	2376	66.7629	1.6258	1042.0459	2376	66.7629	1.6258	1156.5759
2377	66.7889	1.6252	397.6509	2377	66.7889	1.6252	539.9449	2377	66.7889	1.6252	1024.2044	2377	66.7889	1.6252	1138.4927
2378	66.8149	1.6246	391.3939	2378	66.8149	1.6246	533.4851	2378	66.8149	1.6246	988.2617	2378	66.8149	1.6246	1102.3083
2379	66.8409	1.6241	388.9222	2379	66.8409	1.6241	530.8107	2379	66.8409	1.6241	954.7926	2379	66.8409	1.6241	1068.5974
2380	66.8669	1.6235	415.7091	2380	66.8669	1.6235	557.3949	2380	66.8669	1.6235	997.3293	2380	66.8669	1.6235	1110.8924
2381	66.8929	1.623	404.5838	2381	66.8929	1.623	546.0667	2381	66.8929	1.623	953.5734	2381	66.8929	1.623	1066.8948
2382	66.9189	1.6224	397.3454	2382	66.9189	1.6224	538.6257	2382	66.9189	1.6224	894.1699	2382	66.9189	1.6224	1007.2496
2383	66.9449	1.6218	424.5896	2383	66.9449	1.6218	565.6671	2383	66.9449	1.6218	851.7635	2383	66.9449	1.6218	964.6015
2384	66.9709	1.6213	426.4044	2384	66.9709	1.6213	567.2792	2384	66.9709	1.6213	774.3173	2384	66.9709	1.6213	886.9135
2385	66.9969	1.6207	384.958	2385	66.9969	1.6207	525.63	2385	66.9969	1.6207	716.7638	2385	66.9969	1.6207	829.1183
2386	67.0229	1.6202	355.5847	2386	67.0229	1.6202	496.054	2386	67.0229	1.6202	664.0846	2386	67.0229	1.6202	776.1974
2387	67.0489	1.6196	398.4647	2387	67.0489	1.6196	538.7312	2387	67.0489	1.6196	603.5092	2387	67.0489	1.6196	715.3803
2388	67.0749	1.6191	432.2689	2388	67.0749	1.6191	572.3327	2388	67.0749	1.6191	564.7454	2388	67.0749	1.6191	676.3748
2389	67.1009	1.6185	397.1946	2389	67.1009	1.6185	537.0557	2389	67.1009	1.6185	537.1675	2389	67.1009	1.6185	648.5551
2390	67.1269	1.618	388.9683	2390	67.1269	1.618	528.6266	2390	67.1269	1.618	513.6538	2390	67.1269	1.618	624.7998
2391	67.1529	1.6174	368.5448	2391	67.1529	1.6174	508.0004	2391	67.1529	1.6174	530.3815	2391	67.1529	1.6174	641.2857
2392	67.1789	1.6169	405.1618	2392	67.1789	1.6169	544.4146	2392	67.1789	1.6169	529.6827	2392	67.1789	1.6169	640.3452
2393	67.2049	1.6163	411.6367	2393	67.2049	1.6163	550.6867	2393	67.2049	1.6163	530.365	2393	67.2049	1.6163	640.7858
2394	67.2309	1.6157	452.8491	2394	67.2309	1.6157	591.6964	2394	67.2309	1.6157	531.7911	2394	67.2309	1.6157	641.9702
2395	67.2569	1.6152	442.911	2395	67.2569	1.6152	581.5556	2395	67.2569	1.6152	495.8325	2395	67.2569	1.6152	605.7698
2396	67.2829	1.6146	426.6555	2396	67.2829	1.6146	565.0973	2396	67.2829	1.6146	496.7904	2396	67.2829	1.6146	606.4861
2397	67.3089	1.6141	410.7014	2397	67.3089	1.6141	548.9404	2397	67.3089	1.6141	509.058	2397	67.3089	1.6141	618.5119
2398	67.3349	1.6135	422.4776	2398	67.3349	1.6135	560.5139	2398	67.3349	1.6135	497.3276	2398	67.3349	1.6135	606.5398
2399	67.3609	1.613	431.4679	2399	67.3609	1.613	569.3015	2399	67.3609	1.613	489.9817	2399	67.3609	1.613	598.9522
2400	67.3869	1.6124	442.2086	2400	67.3869	1.6124	579.8394	2400	67.3869	1.6124	524.592	2400	67.3869	1.6124	633.3208
2401	67.4129	1.6119	432.453	2401	67.4129	1.6119	569.881	2401	67.4129	1.6119	577.2556	2401	67.4129	1.6119	685.7426
2402	67.4389	1.6114	426.7152	2402	67.4389	1.6114	563.9405	2402	67.4389	1.6114	538.2285	2402	67.4389	1.6114	646.4738
2403	67.4649	1.6108	423.144	2403	67.4649	1.6108	560.1666	2403	67.4649	1.6108	565.163	2403	67.4649	1.6108	673.1666
2404	67.4909	1.6103	429.1802	2404	67.4909	1.6103	566	2404	67.4909	1.6103	575.7833	2404	67.4909	1.6103	683.5452
2405	67.5169	1.6097	430.117	2405	67.5169	1.6097	566.734	2405	67.5169	1.6097	604.4436	2405	67.5169	1.6097	711.9638
2406	67.5429	1.6092	433.9012	2406	67.5429	1.6092	570.3156	2406	67.5429	1.6092	626.2158	2406	67.5429	1.6092	733.4942
2407	67.5689	1.6086	435.3748	2407	67.5689	1.6086	571.5864	2407	67.5689	1.6086	637.4045	2407	67.5689	1.6086	744.4412

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2408	67.5949	1.6081	472.5867	2408	67.5949	1.6081	608.5955	2408	67.5949	1.6081	778.6731	2408	67.5949	1.6081	885.4682
2409	67.6209	1.6075	460.3729	2409	67.6209	1.6075	596.179	2409	67.6209	1.6075	791.8732	2409	67.6209	1.6075	898.4265
2410	67.6469	1.607	449.8677	2410	67.6469	1.607	585.4711	2410	67.6469	1.607	893.7241	2410	67.6469	1.607	1000.0357
2411	67.6729	1.6064	492.3849	2411	67.6729	1.6064	627.7855	2411	67.6729	1.6064	1120.1486	2411	67.6729	1.6064	1226.2185
2412	67.6989	1.6059	505.6754	2412	67.6989	1.6059	640.8732	2412	67.6989	1.6059	1274.7038	2412	67.6989	1.6059	1380.532
2413	67.7249	1.6054	561.6448	2413	67.7249	1.6054	696.6399	2413	67.7249	1.6054	1607.1248	2413	67.7249	1.6054	1712.7113
2414	67.7509	1.6048	526.1022	2414	67.7509	1.6048	660.8946	2414	67.7509	1.6048	1831.4987	2414	67.7509	1.6048	1936.8435
2415	67.7769	1.6043	481.0255	2415	67.7769	1.6043	615.6151	2415	67.7769	1.6043	1952.8907	2415	67.7769	1.6043	2057.9937
2416	67.8029	1.6037	591.391	2416	67.8029	1.6037	725.7779	2416	67.8029	1.6037	2126.6983	2416	67.8029	1.6037	2231.5595
2417	67.8289	1.6032	534.6494	2417	67.8289	1.6032	668.8336	2417	67.8289	1.6032	1960.3831	2417	67.8289	1.6032	2065.0026
2418	67.8549	1.6026	528.3415	2418	67.8549	1.6026	662.3229	2418	67.8549	1.6026	1889.357	2418	67.8549	1.6026	1993.7349
2419	67.8809	1.6021	491.8768	2419	67.8809	1.6021	625.6554	2419	67.8809	1.6021	1819.469	2419	67.8809	1.6021	1923.6052
2420	67.9069	1.6016	574.256	2420	67.9069	1.6016	707.8319	2420	67.9069	1.6016	1770.2069	2420	67.9069	1.6016	1874.1013
2421	67.9329	1.601	553.8778	2421	67.9329	1.601	687.2509	2421	67.9329	1.601	1655.7333	2421	67.9329	1.601	1759.386
2422	67.9589	1.6005	555.7859	2422	67.9589	1.6005	688.9563	2422	67.9589	1.6005	1540.1478	2422	67.9589	1.6005	1643.5588
2423	67.9849	1.5999	526.9861	2423	67.9849	1.5999	659.9538	2423	67.9849	1.5999	1418.7412	2423	67.9849	1.5999	1521.9105
2424	68.0109	1.5994	498.4448	2424	68.0109	1.5994	631.2097	2424	68.0109	1.5994	1288.5788	2424	68.0109	1.5994	1391.5064
2425	68.0369	1.5989	572.3585	2425	68.0369	1.5989	704.9207	2425	68.0369	1.5989	1136.3179	2425	68.0369	1.5989	1239.0038
2426	68.0629	1.5983	563.5024	2426	68.0629	1.5983	695.8618	2426	68.0629	1.5983	964.3288	2426	68.0629	1.5983	1066.7729
2427	68.0889	1.5978	594.413	2427	68.0889	1.5978	726.5696	2427	68.0889	1.5978	885.0872	2427	68.0889	1.5978	987.2896
2428	68.1149	1.5973	587.8601	2428	68.1149	1.5973	719.814	2428	68.1149	1.5973	837.7839	2428	68.1149	1.5973	939.7446
2429	68.1409	1.5967	594.5182	2429	68.1409	1.5967	726.2694	2429	68.1409	1.5967	765.2218	2429	68.1409	1.5967	866.9408
2430	68.1669	1.5962	557.704	2430	68.1669	1.5962	689.2524	2430	68.1669	1.5962	705.4964	2430	68.1669	1.5962	806.9737
2431	68.1929	1.5957	569.6533	2431	68.1929	1.5957	700.9989	2431	68.1929	1.5957	621.5475	2431	68.1929	1.5957	722.783
2432	68.2189	1.5951	582.6928	2432	68.2189	1.5951	712.668	2432	68.2189	1.5951	600.5804	2432	68.2189	1.5951	701.5742
2433	68.2449	1.5946	570.6226	2433	68.2449	1.5946	699.2273	2433	68.2449	1.5946	580.1303	2433	68.2449	1.5946	680.8823
2434	68.2709	1.5941	583.5108	2434	68.2709	1.5941	710.745	2434	68.2709	1.5941	562.0265	2434	68.2709	1.5941	662.5369
2435	68.2969	1.5935	582.8906	2435	68.2969	1.5935	708.7543	2435	68.2969	1.5935	571.6193	2435	68.2969	1.5935	671.888
2436	68.3229	1.593	548.2597	2436	68.3229	1.593	672.7529	2436	68.3229	1.593	576.4907	2436	68.3229	1.593	676.5177
2437	68.3489	1.5925	540.3894	2437	68.3489	1.5925	663.5121	2437	68.3489	1.5925	607.0694	2437	68.3489	1.5925	706.8546
2438	68.3749	1.5919	560.0934	2438	68.3749	1.5919	681.8456	2438	68.3749	1.5919	525.7836	2438	68.3749	1.5919	625.3271
2439	68.4009	1.5914	524.3363	2439	68.4009	1.5914	644.718	2439	68.4009	1.5914	518.0306	2439	68.4009	1.5914	617.3323
2440	68.4269	1.5909	482.4086	2440	68.4269	1.5909	601.4198	2440	68.4269	1.5909	529.7348	2440	68.4269	1.5909	628.7948
2441	68.4529	1.5903	533.7902	2441	68.4529	1.5903	651.4309	2441	68.4529	1.5903	547.9738	2441	68.4529	1.5903	646.7921
2442	68.4789	1.5898	546.8314	2442	68.4789	1.5898	663.1016	2442	68.4789	1.5898	525.9142	2442	68.4789	1.5898	624.4907
2443	68.5049	1.5893	554.0282	2443	68.5049	1.5893	668.9279	2443	68.5049	1.5893	511.7373	2443	68.5049	1.5893	610.0721

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2444	68.5309	1.5887	483.7664	2444	68.5309	1.5887	597.2956	2444	68.5309	1.5887	521.3045	2444	68.5309	1.5887	619.3976
2445	68.5569	1.5882	447.5929	2445	68.5569	1.5882	559.7516	2445	68.5569	1.5882	564.1443	2445	68.5569	1.5882	661.9957
2446	68.5829	1.5877	458.2717	2446	68.5829	1.5877	569.0599	2446	68.5829	1.5877	573.6903	2446	68.5829	1.5877	671.3
2447	68.6089	1.5872	438.2997	2447	68.6089	1.5872	547.7174	2447	68.6089	1.5872	578.4726	2447	68.6089	1.5872	675.8406
2448	68.6349	1.5866	463.7999	2448	68.6349	1.5866	571.8471	2448	68.6349	1.5866	614.0007	2448	68.6349	1.5866	711.1269
2449	68.6609	1.5861	448.4937	2449	68.6609	1.5861	555.1704	2449	68.6609	1.5861	672.5701	2449	68.6609	1.5861	769.4546
2450	68.6869	1.5856	453.1005	2450	68.6869	1.5856	558.4067	2450	68.6869	1.5856	678.7517	2450	68.6869	1.5856	775.3945
2451	68.7129	1.585	461.7547	2451	68.7129	1.585	565.6904	2451	68.7129	1.585	657.0297	2451	68.7129	1.585	753.4308
2452	68.7389	1.5845	449.8256	2452	68.7389	1.5845	552.3908	2452	68.7389	1.5845	643.7165	2452	68.7389	1.5845	739.8759
2453	68.7649	1.584	454.1928	2453	68.7649	1.584	555.3875	2453	68.7649	1.584	656.5048	2453	68.7649	1.584	752.4224
2454	68.7909	1.5835	433.7511	2454	68.7909	1.5835	533.5753	2454	68.7909	1.5835	659.6998	2454	68.7909	1.5835	755.3757
2455	68.8169	1.5829	416.3407	2455	68.8169	1.5829	514.7944	2455	68.8169	1.5829	621.7776	2455	68.8169	1.5829	717.2118
2456	68.8429	1.5824	416.8391	2456	68.8429	1.5824	513.9223	2456	68.8429	1.5824	602.8075	2456	68.8429	1.5824	698
2457	68.8689	1.5819	416.133	2457	68.8689	1.5819	511.8458	2457	68.8689	1.5819	601.7876	2457	68.8689	1.5819	696.7383
2458	68.8949	1.5814	397.6509	2458	68.8949	1.5814	491.9931	2458	68.8949	1.5814	570.2446	2458	68.8949	1.5814	664.9536
2459	68.9209	1.5809	408.4005	2459	68.9209	1.5809	502.9962	2459	68.9209	1.5809	588.804	2459	68.9209	1.5809	683.2713
2460	68.9469	1.5803	445.5931	2460	68.9469	1.5803	540.4422	2460	68.9469	1.5803	571.2997	2460	68.9469	1.5803	665.5253
2461	68.9729	1.5798	435.4775	2461	68.9729	1.5798	530.5801	2461	68.9729	1.5798	544.0162	2461	68.9729	1.5798	638
2462	68.9989	1.5793	411.2503	2462	68.9989	1.5793	506.6064	2462	68.9989	1.5793	486.7153	2462	68.9989	1.5793	580.4574
2463	69.0249	1.5788	426.9578	2463	69.0249	1.5788	522.5674	2463	69.0249	1.5788	446.6422	2463	69.0249	1.5788	540.1426
2464	69.0509	1.5782	440.4528	2464	69.0509	1.5782	536.3158	2464	69.0509	1.5782	453.3553	2464	69.0509	1.5782	546.6139
2465	69.0769	1.5777	428.4056	2465	69.0769	1.5777	524.522	2465	69.0769	1.5777	460.1889	2465	69.0769	1.5777	553.2059
2466	69.1029	1.5772	419.6301	2466	69.1029	1.5772	516	2466	69.1029	1.5772	443.2706	2466	69.1029	1.5772	536.0458
2467	69.1289	1.5767	416.7185	2467	69.1289	1.5767	513.3419	2467	69.1289	1.5767	438.099	2467	69.1289	1.5767	530.6325
2468	69.1549	1.5762	434.9913	2468	69.1549	1.5762	531.8682	2468	69.1549	1.5762	440.9261	2468	69.1549	1.5762	533.2178
2469	69.1809	1.5756	419.0685	2469	69.1809	1.5756	516.1988	2469	69.1809	1.5756	444.6738	2469	69.1809	1.5756	536.7239
2470	69.2069	1.5751	386.1181	2470	69.2069	1.5751	483.5019	2470	69.2069	1.5751	455.1954	2470	69.2069	1.5751	547.0037
2471	69.2329	1.5746	425.2258	2471	69.2329	1.5746	522.8631	2471	69.2329	1.5746	452.9898	2471	69.2329	1.5746	544.5564
2472	69.2589	1.5741	453.0589	2472	69.2589	1.5741	550.9496	2472	69.2589	1.5741	456.4233	2472	69.2589	1.5741	547.7482
2473	69.2849	1.5736	434.1907	2473	69.2849	1.5736	532.3349	2473	69.2849	1.5736	454.475	2473	69.2849	1.5736	545.5581
2474	69.3109	1.5731	410.9642	2474	69.3109	1.5731	509.3619	2474	69.3109	1.5731	427.9826	2474	69.3109	1.5731	518.824
2475	69.3369	1.5725	390.8966	2475	69.3369	1.5725	489.5478	2475	69.3369	1.5725	424.3245	2475	69.3369	1.5725	514.9242
2476	69.3629	1.572	408.6731	2476	69.3629	1.572	507.5777	2476	69.3629	1.572	450.1615	2476	69.3629	1.572	540.5195
2477	69.3889	1.5715	419.3023	2477	69.3889	1.5715	518.4603	2477	69.3889	1.5715	454.6949	2477	69.3889	1.5715	544.8112
2478	69.4149	1.571	411.8831	2478	69.4149	1.571	511.2946	2478	69.4149	1.571	463.7573	2478	69.4149	1.571	553.6318
2479	69.4409	1.5705	432.5862	2479	69.4409	1.5705	532.2512	2479	69.4409	1.5705	461.8513	2479	69.4409	1.5705	551.4841

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2480	69.4669	1.57	441.2631	2480	69.4669	1.57	541.1815	2480	69.4669	1.57	430.6221	2480	69.4669	1.57	520.0132
2481	69.4929	1.5695	411.6944	2481	69.4929	1.5695	511.8663	2481	69.4929	1.5695	428.3526	2481	69.4929	1.5695	517.502
2482	69.5189	1.5689	384.4412	2482	69.5189	1.5689	484.8666	2482	69.5189	1.5689	415.8816	2482	69.5189	1.5689	504.7893
2483	69.5449	1.5684	419.7274	2483	69.5449	1.5684	520.4063	2483	69.5449	1.5684	427.2318	2483	69.5449	1.5684	515.8978
2484	69.5709	1.5679	459.045	2484	69.5709	1.5679	559.9773	2484	69.5709	1.5679	456.8499	2484	69.5709	1.5679	545.2741
2485	69.5969	1.5674	478.0491	2485	69.5969	1.5674	579.2349	2485	69.5969	1.5674	439.9314	2485	69.5969	1.5674	528.1139
2486	69.6229	1.5669	472.8453	2486	69.6229	1.5669	574.2845	2486	69.6229	1.5669	411.7454	2486	69.6229	1.5669	499.6862
2487	69.6489	1.5664	468.3078	2487	69.6489	1.5664	570.0005	2487	69.6489	1.5664	400.3069	2487	69.6489	1.5664	488.006
2488	69.6749	1.5659	487.7122	2488	69.6749	1.5659	589.6583	2488	69.6749	1.5659	378.7451	2488	69.6749	1.5659	466.2024
2489	69.7009	1.5654	531.547	2489	69.7009	1.5654	633.7467	2489	69.7009	1.5654	407.5246	2489	69.7009	1.5654	494.7402
2490	69.7269	1.5649	527.3333	2490	69.7269	1.5649	629.7863	2490	69.7269	1.5649	456.791	2490	69.7269	1.5649	543.7649
2491	69.7529	1.5643	519.8911	2491	69.7529	1.5643	622.5976	2491	69.7529	1.5643	461.4631	2491	69.7529	1.5643	548.1953
2492	69.7789	1.5638	503.3686	2492	69.7789	1.5638	606.3286	2492	69.7789	1.5638	430.0175	2492	69.7789	1.5638	516.5079
2493	69.8049	1.5633	485.7764	2493	69.8049	1.5633	588.9899	2493	69.8049	1.5633	412.7817	2493	69.8049	1.5633	499.0303
2494	69.8309	1.5628	490.7193	2494	69.8309	1.5628	594.1862	2494	69.8309	1.5628	439.1029	2494	69.8309	1.5628	525.1098
2495	69.8569	1.5623	518.9041	2495	69.8569	1.5623	622.6245	2495	69.8569	1.5623	444.7272	2495	69.8569	1.5623	530.4924
2496	69.8829	1.5618	493.5384	2496	69.8829	1.5618	597.5122	2496	69.8829	1.5618	436.6479	2496	69.8829	1.5618	522.1714
2497	69.9089	1.5613	489.901	2497	69.9089	1.5613	594.1283	2497	69.9089	1.5613	412.4428	2497	69.9089	1.5613	497.7246
2498	69.9349	1.5608	479.4866	2498	69.9349	1.5608	583.9674	2498	69.9349	1.5608	414.0579	2498	69.9349	1.5608	499.0979
2499	69.9609	1.5603	470.4045	2499	69.9609	1.5603	575.1387	2499	69.9609	1.5603	454.917	2499	69.9609	1.5603	539.7153
2500	69.9869	1.5598	479.2111	2500	69.9869	1.5598	584.1988	2500	69.9869	1.5598	450.2392	2500	69.9869	1.5598	534.7958
2501	70.0129	1.5593	430.4626	2501	70.0129	1.5593	535.7038	2501	70.0129	1.5593	444.0514	2501	70.0129	1.5593	528.3662
2502	70.0389	1.5588	391.561	2502	70.0389	1.5588	497.0556	2502	70.0389	1.5588	420.3739	2502	70.0389	1.5588	504.447
2503	70.0649	1.5583	405.2401	2503	70.0649	1.5583	510.9882	2503	70.0649	1.5583	417.8198	2503	70.0649	1.5583	501.6512
2504	70.0909	1.5578	395.2105	2504	70.0909	1.5578	501.2121	2504	70.0909	1.5578	425.6224	2504	70.0909	1.5578	509.2121
2505	70.1169	1.5573	438.4988	2505	70.1169	1.5573	544.7538	2505	70.1169	1.5573	467.8601	2505	70.1169	1.5573	551.208
2506	70.1429	1.5567	415.8625	2506	70.1429	1.5567	522.371	2506	70.1429	1.5567	434.6609	2506	70.1429	1.5567	517.7671
2507	70.1689	1.5562	387.6991	2507	70.1689	1.5562	494.4611	2507	70.1689	1.5562	397.1207	2507	70.1689	1.5562	479.9852
2508	70.1949	1.5557	382.8612	2508	70.1949	1.5557	489.8767	2508	70.1949	1.5557	423.3863	2508	70.1949	1.5557	506.009
2509	70.2209	1.5552	376.914	2509	70.2209	1.5552	484.1829	2509	70.2209	1.5552	382.5381	2509	70.2209	1.5552	464.9191
2510	70.2469	1.5547	395.0522	2510	70.2469	1.5547	502.5745	2510	70.2469	1.5547	395.8439	2510	70.2469	1.5547	477.9832
2511	70.2729	1.5542	407.5588	2511	70.2729	1.5542	515.3347	2511	70.2729	1.5542	443.7758	2511	70.2729	1.5542	525.6734
2512	70.2989	1.5537	397.6509	2512	70.2989	1.5537	505.6802	2512	70.2989	1.5537	417.1962	2512	70.2989	1.5537	498.852
2513	70.3249	1.5532	362.4279	2513	70.3249	1.5532	470.0752	2513	70.3249	1.5532	465.149	2513	70.3249	1.5532	546.5631
2514	70.3509	1.5527	364.3223	2514	70.3509	1.5527	471.5875	2514	70.3509	1.5527	412.1985	2514	70.3509	1.5527	493.3709
2515	70.3769	1.5522	375.3864	2515	70.3769	1.5522	482.2696	2515	70.3769	1.5522	432.1801	2515	70.3769	1.5522	513.1107

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2516	70.4029	1.5517	411.5001	2516	70.4029	1.5517	518.0013	2516	70.4029	1.5517	436.4011	2516	70.4029	1.5517	517.09
2517	70.4289	1.5512	350.5499	2517	70.4289	1.5512	456.6691	2517	70.4289	1.5512	479.3809	2517	70.4289	1.5512	559.8281
2518	70.4549	1.5507	395.8022	2518	70.4549	1.5507	501.5394	2518	70.4549	1.5507	447.078	2518	70.4549	1.5507	527.2835
2519	70.4809	1.5502	378.3159	2519	70.4809	1.5502	483.671	2519	70.4809	1.5502	420.24	2519	70.4809	1.5502	500.2037
2520	70.5069	1.5497	357.889	2520	70.5069	1.5497	462.8621	2520	70.5069	1.5497	433.3699	2520	70.5069	1.5497	513.0919
2521	70.5329	1.5492	334.5092	2521	70.5329	1.5492	439.1003	2521	70.5329	1.5492	449.4529	2521	70.5329	1.5492	528.9332
2522	70.5589	1.5488	384.086	2522	70.5589	1.5488	488.295	2522	70.5589	1.5488	425.114	2522	70.5589	1.5488	504.3525
2523	70.5849	1.5483	404.6925	2523	70.5849	1.5483	508.5196	2523	70.5849	1.5483	457.2105	2523	70.5849	1.5483	536.2073
2524	70.6109	1.5478	363.0485	2524	70.6109	1.5478	466.4935	2524	70.6109	1.5478	450.5165	2524	70.6109	1.5478	529.2716
2525	70.6369	1.5473	334.2091	2525	70.6369	1.5473	437.2721	2525	70.6369	1.5473	409.3729	2525	70.6369	1.5473	487.8863
2526	70.6629	1.5468	408.0697	2526	70.6629	1.5468	510.7507	2526	70.6629	1.5468	433.2761	2526	70.6629	1.5468	511.5477
2527	70.6889	1.5463	323.7536	2527	70.6889	1.5463	426.0525	2527	70.6889	1.5463	391.9008	2527	70.6889	1.5463	469.9307
2528	70.7149	1.5458	419.9834	2528	70.7149	1.5458	521.9003	2528	70.7149	1.5458	417.9292	2528	70.7149	1.5458	495.7174
2529	70.7409	1.5453	363.3975	2529	70.7409	1.5453	464.9324	2529	70.7409	1.5453	433.2838	2529	70.7409	1.5453	510.8302
2530	70.7669	1.5448	336.0906	2530	70.7669	1.5448	437.2435	2530	70.7669	1.5448	466.4236	2530	70.7669	1.5448	543.7283
2531	70.7929	1.5443	375.4727	2531	70.7929	1.5443	476.2436	2531	70.7929	1.5443	456.488	2531	70.7929	1.5443	533.551
2532	70.8189	1.5438	390.3646	2532	70.8189	1.5438	490.7535	2532	70.8189	1.5438	443.6519	2532	70.8189	1.5438	520.4732
2533	70.8449	1.5433	368.3208	2533	70.8449	1.5433	468.3276	2533	70.8449	1.5433	416.1178	2533	70.8449	1.5433	492.6973
2534	70.8709	1.5428	361.9079	2534	70.8709	1.5428	461.5327	2534	70.8709	1.5428	458.6044	2534	70.8709	1.5428	534.9421
2535	70.8969	1.5423	376.3247	2535	70.8969	1.5423	475.5675	2535	70.8969	1.5423	476.1869	2535	70.8969	1.5423	552.2829
2536	70.9229	1.5418	383.3742	2536	70.9229	1.5418	482.2349	2536	70.9229	1.5418	434.9493	2536	70.9229	1.5418	510.8036
2537	70.9489	1.5413	396.2402	2537	70.9489	1.5413	494.7189	2537	70.9489	1.5413	427.3874	2537	70.9489	1.5413	503
2538	70.9749	1.5409	398.9033	2538	70.9749	1.5409	497	2538	70.9749	1.5409	432.592	2538	70.9749	1.5409	507.9629
2539	71.0009	1.5404	397.6509	2539	71.0009	1.5404	495.3656	2539	71.0009	1.5404	435.5053	2539	71.0009	1.5404	510.6344
2540	71.0269	1.5399	420.6779	2540	71.0269	1.5399	519.219	2540	71.0269	1.5399	446.6075	2540	71.0269	1.5399	521.4949
2541	71.0529	1.5394	400.1164	2541	71.0529	1.5394	499.4839	2541	71.0529	1.5394	438.191	2541	71.0529	1.5394	512.8367
2542	71.0789	1.5389	379.4194	2542	71.0789	1.5389	479.6133	2542	71.0789	1.5389	450.5577	2542	71.0789	1.5389	524.9616
2543	71.1049	1.5384	392.0854	2543	71.1049	1.5384	493.1057	2543	71.1049	1.5384	461.8356	2543	71.1049	1.5384	535.9978
2544	71.1309	1.5379	432.9986	2544	71.1309	1.5379	534.8453	2544	71.1309	1.5379	481.7345	2544	71.1309	1.5379	555.655
2545	71.1569	1.5374	436.5077	2545	71.1569	1.5374	539.1808	2545	71.1569	1.5374	469.8944	2545	71.1569	1.5374	543.5732
2546	71.1829	1.5369	462.6633	2546	71.1829	1.5369	566.1629	2546	71.1829	1.5369	441.3823	2546	71.1829	1.5369	514.8193
2547	71.2089	1.5365	453.228	2547	71.2089	1.5365	557.5539	2547	71.2089	1.5365	452.2508	2547	71.2089	1.5365	525.4461
2548	71.2349	1.536	478.6041	2548	71.2349	1.536	583.7564	2548	71.2349	1.536	472.8769	2548	71.2349	1.536	545.8305
2549	71.2609	1.5355	449.0953	2549	71.2609	1.5355	555.0741	2549	71.2609	1.5355	466.0822	2549	71.2609	1.5355	538.794
2550	71.2869	1.535	451.3129	2550	71.2869	1.535	558.1181	2550	71.2869	1.535	477.8157	2550	71.2869	1.535	550.2858
2551	71.3129	1.5345	467.4444	2551	71.3129	1.5345	575.076	2551	71.3129	1.5345	454.751	2551	71.3129	1.5345	526.9794

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2552	71.3389	1.534	460.2185	2552	71.3389	1.534	568.6765	2552	71.3389	1.534	455.0898	2552	71.3389	1.534	527.0764
2553	71.3649	1.5335	449.2891	2553	71.3649	1.5335	558.5735	2553	71.3649	1.5335	472.7864	2553	71.3649	1.5335	544.5313
2554	71.3909	1.5331	449.2311	2554	71.3909	1.5331	559.3419	2554	71.3909	1.5331	473.8181	2554	71.3909	1.5331	545.3213
2555	71.4169	1.5326	427.0165	2555	71.4169	1.5326	537.9537	2555	71.4169	1.5326	481.6156	2555	71.4169	1.5326	552.877
2556	71.4429	1.5321	446.0149	2556	71.4429	1.5321	557.7786	2556	71.4429	1.5321	498.6541	2556	71.4429	1.5321	569.6738
2557	71.4689	1.5316	480.2913	2557	71.4689	1.5316	592.8814	2557	71.4689	1.5316	490.5338	2557	71.4689	1.5316	561.3117
2558	71.4949	1.5311	468.2078	2558	71.4949	1.5311	581.6243	2558	71.4949	1.5311	486.236	2558	71.4949	1.5311	556.7722
2559	71.5209	1.5306	415.7742	2559	71.5209	1.5306	530.0171	2559	71.5209	1.5306	516.5504	2559	71.5209	1.5306	586.8449
2560	71.5469	1.5302	400.6723	2560	71.5469	1.5302	515.7417	2560	71.5469	1.5302	544.9066	2560	71.5469	1.5302	614.9594
2561	71.5729	1.5297	413.2914	2561	71.5729	1.5297	529.1872	2561	71.5729	1.5297	540.2104	2561	71.5729	1.5297	610.0214
2562	71.5989	1.5292	466.1656	2562	71.5989	1.5292	582.8877	2562	71.5989	1.5292	553.635	2562	71.5989	1.5292	623.2043
2563	71.6249	1.5287	484.9743	2563	71.6249	1.5287	602.5228	2563	71.6249	1.5287	586.6241	2563	71.6249	1.5287	655.9517
2564	71.6509	1.5282	434.3527	2564	71.6509	1.5282	552.7277	2564	71.6509	1.5282	624.9574	2564	71.6509	1.5282	694.0432
2565	71.6769	1.5278	449.6564	2565	71.6769	1.5278	568.8578	2565	71.6769	1.5278	676.0327	2565	71.6769	1.5278	744.8768
2566	71.7029	1.5273	495.4093	2566	71.7029	1.5273	615.4371	2566	71.7029	1.5273	777.7531	2566	71.7029	1.5273	846.3554
2567	71.7289	1.5268	483.7275	2567	71.7289	1.5268	604.5817	2567	71.7289	1.5268	950.137	2567	71.7289	1.5268	1018.4977
2568	71.7549	1.5263	488.0278	2568	71.7549	1.5263	609.7085	2568	71.7549	1.5263	1107.9476	2568	71.7549	1.5263	1176.0665
2569	71.7809	1.5258	483.1131	2569	71.7809	1.5258	605.6201	2569	71.7809	1.5258	1298.6479	2569	71.7809	1.5258	1366.525
2570	71.8069	1.5254	470.3495	2570	71.8069	1.5254	593.683	2570	71.8069	1.5254	1407.0757	2570	71.8069	1.5254	1474.7111
2571	71.8329	1.5249	478.3404	2571	71.8329	1.5249	602.5003	2571	71.8329	1.5249	1368.6203	2571	71.8329	1.5249	1436.014
2572	71.8589	1.5244	469.6669	2572	71.8589	1.5244	594.6532	2572	71.8589	1.5244	1359.5416	2572	71.8589	1.5244	1426.6936
2573	71.8849	1.5239	467.4255	2573	71.8849	1.5239	593.2382	2573	71.8849	1.5239	1348.6973	2573	71.8849	1.5239	1415.6075
2574	71.9109	1.5235	445.1644	2574	71.9109	1.5235	571.8035	2574	71.9109	1.5235	1307.1732	2574	71.9109	1.5235	1373.8416
2575	71.9369	1.523	431.3952	2575	71.9369	1.523	558.8608	2575	71.9369	1.523	1227.7106	2575	71.9369	1.523	1294.1373
2576	71.9629	1.5225	425.2522	2576	71.9629	1.5225	553.5441	2576	71.9629	1.5225	1184.672	2576	71.9629	1.5225	1250.8571
2577	71.9889	1.522	397.9244	2577	71.9889	1.522	527.0428	2577	71.9889	1.522	1202.6078	2577	71.9889	1.522	1268.5511
2578	72.0149	1.5215	399.6014	2578	72.0149	1.5215	529.5462	2578	72.0149	1.5215	1144.6111	2578	72.0149	1.5215	1210.3126
2579	72.0409	1.5211	389.8085	2579	72.0409	1.5211	520.5797	2579	72.0409	1.5211	1079.9001	2579	72.0409	1.5211	1145.3599
2580	72.0669	1.5206	386.7608	2580	72.0669	1.5206	518.3584	2580	72.0669	1.5206	1010.7181	2580	72.0669	1.5206	1075.9362
2581	72.0929	1.5201	367.1561	2581	72.0929	1.5201	499.5801	2581	72.0929	1.5201	941.1984	2581	72.0929	1.5201	1006.1748
2582	72.1189	1.5197	354.2476	2582	72.1189	1.5197	487.498	2582	72.1189	1.5197	877.0675	2582	72.1189	1.5197	941.8022
2583	72.1449	1.5192	382.4392	2583	72.1449	1.5192	516.516	2583	72.1449	1.5192	847.2036	2583	72.1449	1.5192	911.6965
2584	72.1709	1.5187	409.7012	2584	72.1709	1.5187	544.6044	2584	72.1709	1.5187	893.129	2584	72.1709	1.5187	957.3801
2585	72.1969	1.5182	429.5487	2585	72.1969	1.5182	565.2784	2585	72.1969	1.5182	932.9991	2585	72.1969	1.5182	997.0086
2586	72.2229	1.5178	421.4791	2586	72.2229	1.5178	558.0351	2586	72.2229	1.5178	990.1269	2586	72.2229	1.5178	1053.8946
2587	72.2489	1.5173	397.3433	2587	72.2489	1.5173	534.7257	2587	72.2489	1.5173	1005.0627	2587	72.2489	1.5173	1068.5886

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2588	72.2749	1.5168	373.1221	2588	72.2749	1.5168	511.331	2588	72.2749	1.5168	957.4677	2588	72.2749	1.5168	1020.7519
2589	72.3009	1.5163	384.5245	2589	72.3009	1.5163	523.5598	2589	72.3009	1.5163	935.8475	2589	72.3009	1.5163	998.89
2590	72.3269	1.5159	406.2712	2590	72.3269	1.5159	546.1329	2590	72.3269	1.5159	908.9025	2590	72.3269	1.5159	971.7033
2591	72.3529	1.5154	401.0106	2591	72.3529	1.5154	541.6987	2591	72.3529	1.5154	838.1523	2591	72.3529	1.5154	900.7114
2592	72.3789	1.5149	417.2572	2592	72.3789	1.5149	558.7717	2592	72.3789	1.5149	842.9347	2592	72.3789	1.5149	905.252
2593	72.4049	1.5145	447.5581	2593	72.4049	1.5145	589.899	2593	72.4049	1.5145	826.5421	2593	72.4049	1.5145	888.6176
2594	72.4309	1.514	417.8428	2594	72.4309	1.514	560.086	2594	72.4309	1.514	790.0078	2594	72.4309	1.514	851.8416
2595	72.4569	1.5135	425.8245	2595	72.4569	1.5135	567.9699	2595	72.4569	1.5135	784.2551	2595	72.4569	1.5135	845.8472
2596	72.4829	1.5131	422.5885	2596	72.4829	1.5131	564.6361	2596	72.4829	1.5131	788.7825	2596	72.4829	1.5131	850.1328
2597	72.5089	1.5126	392.5641	2597	72.5089	1.5126	534.5138	2597	72.5089	1.5126	730.3316	2597	72.5089	1.5126	791.4402
2598	72.5349	1.5121	455.5119	2598	72.5349	1.5121	597.3639	2598	72.5349	1.5121	705.0199	2598	72.5349	1.5121	765.8868
2599	72.5609	1.5117	428.0422	2599	72.5609	1.5117	569.7964	2599	72.5609	1.5117	675.2685	2599	72.5609	1.5117	735.8936
2600	72.5869	1.5112	388.523	2600	72.5869	1.5112	530.1794	2600	72.5869	1.5112	675.0027	2600	72.5869	1.5112	735.3861
2601	72.6129	1.5107	397.4108	2601	72.6129	1.5107	538.9694	2601	72.6129	1.5107	715.2726	2601	72.6129	1.5107	775.4143
2602	72.6389	1.5103	379.1993	2602	72.6389	1.5103	520.6601	2602	72.6389	1.5103	737.6222	2602	72.6389	1.5103	797.5221
2603	72.6649	1.5098	359.9248	2603	72.6649	1.5098	501.2878	2603	72.6649	1.5098	823.0106	2603	72.6649	1.5098	882.6687
2604	72.6909	1.5093	392.3902	2604	72.6909	1.5093	533.6555	2604	72.6909	1.5093	893.4113	2604	72.6909	1.5093	952.8277
2605	72.7169	1.5089	395.5407	2605	72.7169	1.5089	536.7082	2605	72.7169	1.5089	901.1052	2605	72.7169	1.5089	960.2799
2606	72.7429	1.5084	419.0158	2606	72.7429	1.5084	560.0854	2606	72.7429	1.5084	943	2606	72.7429	1.5084	1001.933
2607	72.7689	1.5079	414.3132	2607	72.7689	1.5079	555.285	2607	72.7689	1.5079	933.6036	2607	72.7689	1.5079	992.2949
2608	72.7949	1.5075	419.9709	2608	72.7949	1.5075	560.8449	2608	72.7949	1.5075	899.7506	2608	72.7949	1.5075	958.2001
2609	72.8209	1.507	438.968	2609	72.8209	1.507	579.7443	2609	72.8209	1.507	821.5656	2609	72.8209	1.507	879.7734
2610	72.8469	1.5065	394.4343	2610	72.8469	1.5065	535.1127	2610	72.8469	1.5065	814.1614	2610	72.8469	1.5065	872.1274
2611	72.8729	1.5061	394.6996	2611	72.8729	1.5061	535.2803	2611	72.8729	1.5061	823.687	2611	72.8729	1.5061	881.4113
2612	72.8989	1.5056	384.6156	2612	72.8989	1.5056	525.0984	2612	72.8989	1.5056	823.8946	2612	72.8989	1.5056	881.3771
2613	72.9249	1.5052	351.0124	2613	72.9249	1.5052	491.3975	2613	72.9249	1.5052	785.0255	2613	72.9249	1.5052	842.2663
2614	72.9509	1.5047	398.9092	2614	72.9509	1.5047	539.1965	2614	72.9509	1.5047	741.079	2614	72.9509	1.5047	798.078
2615	72.9769	1.5042	388.2424	2615	72.9769	1.5042	528.4319	2615	72.9769	1.5042	703.8639	2615	72.9769	1.5042	760.6212
2616	73.0029	1.5038	380.6532	2616	73.0029	1.5038	520.7449	2616	73.0029	1.5038	696.4094	2616	73.0029	1.5038	752.925
2617	73.0289	1.5033	394.0494	2617	73.0289	1.5033	534.0433	2617	73.0289	1.5033	657.1725	2617	73.0289	1.5033	713.4463
2618	73.0549	1.5028	394.837	2618	73.0549	1.5028	534.7331	2618	73.0549	1.5028	600.701	2618	73.0549	1.5028	656.7331
2619	73.0809	1.5024	387.4361	2619	73.0809	1.5024	527.2344	2619	73.0809	1.5024	591.7096	2619	73.0809	1.5024	647.5
2620	73.1069	1.5019	397.6509	2620	73.1069	1.5019	537.3514	2620	73.1069	1.5019	529.3162	2620	73.1069	1.5019	584.8648
2621	73.1329	1.5015	424.846	2621	73.1329	1.5015	562.8886	2621	73.1329	1.5015	519.6895	2621	73.1329	1.5015	574.9964
2622	73.1589	1.501	395.8115	2622	73.1589	1.501	532.1962	2622	73.1589	1.501	518.9412	2622	73.1589	1.501	574.0063
2623	73.1849	1.5005	413.0132	2623	73.1849	1.5005	547.74	2623	73.1849	1.5005	499.5016	2623	73.1849	1.5005	554.325

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2624	73.2109	1.5001	381.821	2624	73.2109	1.5001	514.8899	2624	73.2109	1.5001	562.717	2624	73.2109	1.5001	617.2987
2625	73.2369	1.4996	393.192	2625	73.2369	1.4996	524.6029	2625	73.2369	1.4996	491.4033	2625	73.2369	1.4996	545.7433
2626	73.2629	1.4992	416.2346	2626	73.2629	1.4992	545.9876	2626	73.2629	1.4992	495.5797	2626	73.2629	1.4992	549.6779
2627	73.2889	1.4987	444.3945	2627	73.2889	1.4987	572.4896	2627	73.2889	1.4987	481.9826	2627	73.2889	1.4987	535.8391
2628	73.3149	1.4983	420.4728	2628	73.3149	1.4983	546.91	2628	73.3149	1.4983	449.6246	2628	73.3149	1.4983	503.2393
2629	73.3409	1.4978	453.4925	2629	73.3409	1.4978	578.2717	2629	73.3409	1.4978	494.762	2629	73.3409	1.4978	548.135
2630	73.3669	1.4973	484.3931	2630	73.3669	1.4973	607.5145	2630	73.3669	1.4973	469.6114	2630	73.3669	1.4973	522.7426
2631	73.3929	1.4969	540.0857	2631	73.3929	1.4969	661.5491	2631	73.3929	1.4969	484.2935	2631	73.3929	1.4969	537.183
2632	73.4189	1.4964	530.1999	2632	73.4189	1.4964	650.0055	2632	73.4189	1.4964	506.0301	2632	73.4189	1.4964	558.6779
2633	73.4449	1.496	555.5036	2633	73.4449	1.496	673.6513	2633	73.4449	1.496	462.5986	2633	73.4449	1.496	515.0046
2634	73.4709	1.4955	510.6579	2634	73.4709	1.4955	627.1476	2634	73.4709	1.4955	453.3373	2634	73.4709	1.4955	505.5016
2635	73.4969	1.4951	492.198	2635	73.4969	1.4951	607.0298	2635	73.4969	1.4951	446.16	2635	73.4969	1.4951	498.0825
2636	73.5229	1.4946	508.0665	2636	73.5229	1.4946	621.2404	2636	73.5229	1.4946	480.3643	2636	73.5229	1.4946	532.0451
2637	73.5489	1.4942	487.9838	2637	73.5489	1.4942	599.4997	2637	73.5489	1.4942	469.6642	2637	73.5489	1.4942	521.1033
2638	73.5749	1.4937	464.2691	2638	73.5749	1.4937	574.1271	2638	73.5749	1.4937	461.7932	2638	73.5749	1.4937	512.9905
2639	73.6009	1.4933	458.4999	2639	73.6009	1.4933	566.7	2639	73.6009	1.4933	444.5445	2639	73.6009	1.4933	495.5002
2640	73.6269	1.4928	457.0126	2640	73.6269	1.4928	563.5548	2640	73.6269	1.4928	446.1765	2640	73.6269	1.4928	496.8904
2641	73.6529	1.4924	472.6083	2641	73.6529	1.4924	577.4927	2641	73.6529	1.4924	436.2558	2641	73.6529	1.4924	486.7279
2642	73.6789	1.4919	456.3025	2642	73.6789	1.4919	559.5289	2642	73.6789	1.4919	472.7356	2642	73.6789	1.4919	522.966
2643	73.7049	1.4914	443.7932	2643	73.7049	1.4914	545.3617	2643	73.7049	1.4914	457.0963	2643	73.7049	1.4914	507.085
2644	73.7309	1.491	415.1757	2644	73.7309	1.491	515.0863	2644	73.7309	1.491	439.3977	2644	73.7309	1.491	489.1447
2645	73.7569	1.4905	355.1653	2645	73.7569	1.4905	453.4179	2645	73.7569	1.4905	420.4202	2645	73.7569	1.4905	469.9254
2646	73.7829	1.4901	361.5603	2646	73.7829	1.4901	458.155	2646	73.7829	1.4901	446.7135	2646	73.7829	1.4901	495.977
2647	73.8089	1.4896	397.6509	2647	73.8089	1.4896	492.5877	2647	73.8089	1.4896	468.1625	2647	73.8089	1.4896	517.1842
2648	73.8349	1.4892	393.5137	2648	73.8349	1.4892	486.5505	2648	73.8349	1.4892	460.449	2648	73.8349	1.4892	509.2289
2649	73.8609	1.4887	376.0736	2649	73.8609	1.4887	467.2104	2649	73.8609	1.4887	389.691	2649	73.8609	1.4887	438.2292
2650	73.8869	1.4883	376.3425	2650	73.8869	1.4883	465.5792	2650	73.8869	1.4883	416.9603	2650	73.8869	1.4883	465.2568
2651	73.9129	1.4878	366.9567	2651	73.9129	1.4878	454.2934	2651	73.9129	1.4878	436.5334	2651	73.9129	1.4878	484.5882
2652	73.9389	1.4874	383.7474	2652	73.9389	1.4874	469.1841	2652	73.9389	1.4874	435.491	2652	73.9389	1.4874	483.304
2653	73.9649	1.4869	385.5443	2653	73.9649	1.4869	469.081	2653	73.9649	1.4869	462.8719	2653	73.9649	1.4869	510.4432
2654	73.9909	1.4865	373.8972	2654	73.9909	1.4865	455.5338	2654	73.9909	1.4865	452.6811	2654	73.9909	1.4865	500.0106
2655	74.0169	1.4861	391.9168	2655	74.0169	1.4861	471.6533	2655	74.0169	1.4861	436.5823	2655	74.0169	1.4861	483.6701
2656	74.0429	1.4856	406.1324	2656	74.0429	1.4856	483.9689	2656	74.0429	1.4856	453.187	2656	74.0429	1.4856	500.0331
2657	74.0689	1.4852	414.2346	2657	74.0689	1.4852	490.1711	2657	74.0689	1.4852	442.0648	2657	74.0689	1.4852	488.6691
2658	74.0949	1.4847	388.4131	2658	74.0949	1.4847	462.4495	2658	74.0949	1.4847	429.3645	2658	74.0949	1.4847	475.7271
2659	74.1209	1.4843	395.4193	2659	74.1209	1.4843	467.5557	2659	74.1209	1.4843	433.265	2659	74.1209	1.4843	479.3858

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2660	74.1469	1.4838	408.9138	2660	74.1469	1.4838	479.1501	2660	74.1469	1.4838	442.9038	2660	74.1469	1.4838	488.7829
2661	74.1729	1.4834	399.9564	2661	74.1729	1.4834	468.2928	2661	74.1729	1.4834	459.4967	2661	74.1729	1.4834	505.134
2662	74.1989	1.4829	380.0474	2662	74.1989	1.4829	446.4837	2662	74.1989	1.4829	440.1525	2662	74.1989	1.4829	485.5481
2663	74.2249	1.4825	389.0694	2663	74.2249	1.4825	453.6057	2663	74.2249	1.4825	458.2313	2663	74.2249	1.4825	503.3851
2664	74.2509	1.482	398.1713	2664	74.2509	1.482	460.8076	2664	74.2509	1.482	456.395	2664	74.2509	1.482	501.3071
2665	74.2769	1.4816	408.1711	2665	74.2769	1.4816	468.9073	2665	74.2769	1.4816	451.6389	2665	74.2769	1.4816	496.3093
2666	74.3029	1.4812	415.8213	2666	74.3029	1.4812	474.6575	2666	74.3029	1.4812	446.3015	2666	74.3029	1.4812	490.7302
2667	74.3289	1.4807	398.1017	2667	74.3289	1.4807	455.0378	2667	74.3289	1.4807	451.4168	2667	74.3289	1.4807	495.6037
2668	74.3549	1.4803	396.7088	2668	74.3549	1.4803	451.7449	2668	74.3549	1.4803	457.9216	2668	74.3549	1.4803	501.8668
2669	74.3809	1.4798	405.7546	2669	74.3809	1.4798	458.8907	2669	74.3809	1.4798	440.2774	2669	74.3809	1.4798	483.9809
2670	74.4069	1.4794	401.1074	2670	74.4069	1.4794	452.3434	2670	74.4069	1.4794	440.3341	2670	74.4069	1.4794	483.7958
2671	74.4329	1.4789	388.5144	2671	74.4329	1.4789	437.8504	2671	74.4329	1.4789	449.795	2671	74.4329	1.4789	493.015
2672	74.4589	1.4785	376.086	2672	74.4589	1.4785	423.522	2672	74.4589	1.4785	443.5584	2672	74.4589	1.4785	486.5367
2673	74.4849	1.4781	376.8775	2673	74.4849	1.4781	422.4134	2673	74.4849	1.4781	448.4544	2673	74.4849	1.4781	491.1909
2674	74.5109	1.4776	397.6509	2674	74.5109	1.4776	441.2868	2674	74.5109	1.4776	440.0082	2674	74.5109	1.4776	482.503
2675	74.5369	1.4772	440.5345	2675	74.5369	1.4772	485.1318	2675	74.5369	1.4772	447.1533	2675	74.5369	1.4772	489.4063
2676	74.5629	1.4767	451.2108	2676	74.5629	1.4767	496.7696	2676	74.5629	1.4767	487.4832	2676	74.5629	1.4767	529.4944
2677	74.5889	1.4763	429.2716	2677	74.5889	1.4763	475.7918	2677	74.5889	1.4763	510.8045	2677	74.5889	1.4763	552.574
2678	74.6149	1.4759	427.0142	2678	74.6149	1.4759	474.4958	2678	74.6149	1.4759	523.5878	2678	74.6149	1.4759	565.1156
2679	74.6409	1.4754	433.1157	2679	74.6409	1.4754	481.5587	2679	74.6409	1.4754	525.2727	2679	74.6409	1.4754	566.5587
2680	74.6669	1.475	417.4867	2680	74.6669	1.475	466.8912	2680	74.6669	1.475	549.7375	2680	74.6669	1.475	590.7817
2681	74.6929	1.4745	410.9689	2681	74.6929	1.4745	461.3348	2681	74.6929	1.4745	606.6973	2681	74.6929	1.4745	647.4999
2682	74.7189	1.4741	447.1377	2682	74.7189	1.4741	498.465	2682	74.7189	1.4741	678.6092	2682	74.7189	1.4741	719.17
2683	74.7449	1.4737	442.5203	2683	74.7449	1.4737	494.809	2683	74.7449	1.4737	749.8847	2683	74.7449	1.4737	790.2038
2684	74.7709	1.4732	446.6341	2684	74.7709	1.4732	499.8843	2684	74.7709	1.4732	824.4843	2684	74.7709	1.4732	864.5616
2685	74.7969	1.4728	406.8427	2685	74.7969	1.4728	461.0542	2685	74.7969	1.4728	798.9043	2685	74.7969	1.4728	838.7399
2686	74.8229	1.4724	423.5863	2686	74.8229	1.4724	478.7593	2686	74.8229	1.4724	794.1153	2686	74.8229	1.4724	833.7091
2687	74.8489	1.4719	424.4295	2687	74.8489	1.4719	480.5639	2687	74.8489	1.4719	748.3964	2687	74.8489	1.4719	787.7486
2688	74.8749	1.4715	388.1938	2688	74.8749	1.4715	445.2896	2688	74.8749	1.4715	724.2284	2688	74.8749	1.4715	763.3388
2689	74.9009	1.471	398.7155	2689	74.9009	1.471	456.7728	2689	74.9009	1.471	731.7089	2689	74.9009	1.471	770.5776
2690	74.9269	1.4706	439.3173	2690	74.9269	1.4706	498.336	2690	74.9269	1.4706	746.9679	2690	74.9269	1.4706	785.5948
2691	74.9529	1.4702	454.0199	2691	74.9529	1.4702	514	2691	74.9529	1.4702	736.0903	2691	74.9529	1.4702	774.4754
2692	74.9789	1.4697	434.2145	2692	74.9789	1.4697	495.156	2692	74.9789	1.4697	694.285	2692	74.9789	1.4697	732.4285
2693	75.0049	1.4693	393.7241	2693	75.0049	1.4693	455.627	2693	75.0049	1.4693	667.1821	2693	75.0049	1.4693	705.0838
2694	75.0309	1.4689	405.2527	2694	75.0309	1.4689	468.1171	2694	75.0309	1.4689	626.8549	2694	75.0309	1.4689	664.5149
2695	75.0569	1.4684	407.7129	2695	75.0569	1.4684	471.5387	2695	75.0569	1.4684	564.6249	2695	75.0569	1.4684	602.0431

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2696	75.0829	1.468	402.5055	2696	75.0829	1.468	467.2927	2696	75.0829	1.468	583.409	2696	75.0829	1.468	620.5855
2697	75.1089	1.4676	403.2153	2697	75.1089	1.4676	468.9639	2697	75.1089	1.4676	550.0673	2697	75.1089	1.4676	587.002
2698	75.1349	1.4671	448.6234	2698	75.1349	1.4671	515.3335	2698	75.1349	1.4671	543.7134	2698	75.1349	1.4671	580.4063
2699	75.1609	1.4667	422.4099	2699	75.1609	1.4667	490.0814	2699	75.1609	1.4667	534.6157	2699	75.1609	1.4667	571.0669
2700	75.1869	1.4663	412.8738	2700	75.1869	1.4663	481.5067	2700	75.1869	1.4663	530.8039	2700	75.1869	1.4663	567.0134
2701	75.2129	1.4658	397.6509	2701	75.2129	1.4658	467.2453	2701	75.2129	1.4658	491.4028	2701	75.2129	1.4658	527.3706
2702	75.2389	1.4654	415.017	2702	75.2389	1.4654	485.0011	2702	75.2389	1.4654	488.2746	2702	75.2389	1.4654	524.0006
2703	75.2649	1.465	404.5366	2703	75.2649	1.465	474.9104	2703	75.2649	1.465	488.695	2703	75.2649	1.465	524.1792
2704	75.2909	1.4645	400.6378	2704	75.2909	1.4645	471.4013	2704	75.2909	1.4645	494.8746	2704	75.2909	1.4645	530.1171
2705	75.3169	1.4641	424.3364	2705	75.3169	1.4641	495.4896	2705	75.3169	1.4641	440.3187	2705	75.3169	1.4641	475.3195
2706	75.3429	1.4637	423.2192	2706	75.3429	1.4637	494.7622	2706	75.3429	1.4637	437.5614	2706	75.3429	1.4637	472.3204
2707	75.3689	1.4633	428.1601	2707	75.3689	1.4633	500.0928	2707	75.3689	1.4633	442.4882	2707	75.3689	1.4633	477.0055
2708	75.3949	1.4628	405.9583	2708	75.3949	1.4628	478.2807	2708	75.3949	1.4628	456.0752	2708	75.3949	1.4628	490.3508
2709	75.4209	1.4624	411.5921	2709	75.4209	1.4624	484.3042	2709	75.4209	1.4624	438.0096	2709	75.4209	1.4624	472.0434
2710	75.4469	1.462	434.2342	2710	75.4469	1.462	507.3361	2710	75.4469	1.462	464.0028	2710	75.4469	1.462	497.7949
2711	75.4729	1.4615	391.4026	2711	75.4729	1.4615	464.8941	2711	75.4729	1.4615	457.9932	2711	75.4729	1.4615	491.5435
2712	75.4989	1.4611	383.2261	2712	75.4989	1.4611	457.1073	2712	75.4989	1.4611	473.2555	2712	75.4989	1.4611	506.5641
2713	75.5249	1.4607	394.5439	2713	75.5249	1.4607	468.8149	2713	75.5249	1.4607	426.6573	2713	75.5249	1.4607	459.7241
2714	75.5509	1.4603	410.7229	2714	75.5509	1.4603	485.3836	2714	75.5509	1.4603	443.69	2714	75.5509	1.4603	476.5151
2715	75.5769	1.4598	392.5877	2715	75.5769	1.4598	467.6381	2715	75.5769	1.4598	439.2674	2715	75.5769	1.4598	471.8508
2716	75.6029	1.4594	398.1818	2716	75.6029	1.4594	473.6219	2716	75.6029	1.4594	453.0974	2716	75.6029	1.4594	485.439
2717	75.6289	1.459	361.4765	2717	75.6289	1.459	437.3063	2717	75.6289	1.459	489.1133	2717	75.6289	1.459	521.2131
2718	75.6549	1.4585	368.7136	2718	75.6549	1.4585	444.9332	2718	75.6549	1.4585	457.0056	2718	75.6549	1.4585	488.8638
2719	75.6809	1.4581	413.2035	2719	75.6809	1.4581	489.8127	2719	75.6809	1.4581	476.104	2719	75.6809	1.4581	507.7204
2720	75.7069	1.4577	406.9371	2720	75.7069	1.4577	483.9361	2720	75.7069	1.4577	436.3912	2720	75.7069	1.4577	467.7658
2721	75.7329	1.4573	404.0431	2721	75.7329	1.4573	481.4318	2721	75.7329	1.4573	426.5717	2721	75.7329	1.4573	457.7046
2722	75.7589	1.4568	441.2057	2722	75.7589	1.4568	518.9841	2722	75.7589	1.4568	488.0497	2722	75.7589	1.4568	518.9409
2723	75.7849	1.4564	429.9251	2723	75.7849	1.4564	508.0933	2723	75.7849	1.4564	447.6983	2723	75.7849	1.4564	478.3477
2724	75.8109	1.456	378.3991	2724	75.8109	1.456	456.9569	2724	75.8109	1.456	407.3468	2724	75.8109	1.456	437.7545
2725	75.8369	1.4556	417.8628	2725	75.8369	1.4556	496.8104	2725	75.8369	1.4556	477.7663	2725	75.8369	1.4556	507.9323
2726	75.8629	1.4551	402.3129	2726	75.8629	1.4551	481.6502	2726	75.8629	1.4551	435.8352	2726	75.8629	1.4551	465.7594
2727	75.8889	1.4547	394.6102	2727	75.8889	1.4547	474.3372	2727	75.8889	1.4547	494.2829	2727	75.8889	1.4547	523.9653
2728	75.9149	1.4543	397.6509	2728	75.9149	1.4543	477.7676	2728	75.9149	1.4543	482.4887	2728	75.9149	1.4543	511.9295
2729	75.9409	1.4539	430.0807	2729	75.9409	1.4539	510.6195	2729	75.9409	1.4539	482.733	2729	75.9409	1.4539	511.932
2730	75.9669	1.4535	432.9612	2730	75.9669	1.4535	513.9221	2730	75.9669	1.4535	476.5883	2730	75.9669	1.4535	505.5456
2731	75.9929	1.453	416.1986	2731	75.9929	1.453	497.5815	2731	75.9929	1.453	479.0209	2731	75.9929	1.453	507.7364

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2732	76.0189	1.4526	434.0439	2732	76.0189	1.4526	515.8488	2732	76.0189	1.4526	462.3841	2732	76.0189	1.4526	490.8578
2733	76.0449	1.4522	444.696	2733	76.0449	1.4522	526.923	2733	76.0449	1.4522	483.0754	2733	76.0449	1.4522	511.3074
2734	76.0709	1.4518	437.4096	2734	76.0709	1.4518	520.0586	2734	76.0709	1.4518	415.4198	2734	76.0709	1.4518	443.41
2735	76.0969	1.4513	462.1025	2735	76.0969	1.4513	545.1736	2735	76.0969	1.4513	440.2771	2735	76.0969	1.4513	468.0256
2736	76.1229	1.4509	506.0458	2736	76.1229	1.4509	589.5389	2736	76.1229	1.4509	474.8192	2736	76.1229	1.4509	502.326
2737	76.1489	1.4505	518.9057	2737	76.1489	1.4505	602.8209	2737	76.1489	1.4505	487.4084	2737	76.1489	1.4505	514.6735
2738	76.1749	1.4501	524.7189	2738	76.1749	1.4501	609.0561	2738	76.1749	1.4501	488.9767	2738	76.1749	1.4501	516
2739	76.2009	1.4497	527.739	2739	76.2009	1.4497	612.4983	2739	76.2009	1.4497	457.5734	2739	76.2009	1.4497	484.355
2740	76.2269	1.4492	525.3502	2740	76.2269	1.4492	610.5315	2740	76.2269	1.4492	487.6652	2740	76.2269	1.4492	514.205
2741	76.2529	1.4488	547.1584	2741	76.2529	1.4488	632.7617	2741	76.2529	1.4488	454.2431	2741	76.2529	1.4488	480.5412
2742	76.2789	1.4484	522.2638	2742	76.2789	1.4484	608.2891	2742	76.2789	1.4484	507.5774	2742	76.2789	1.4484	533.6337
2743	76.3049	1.448	473.3127	2743	76.3049	1.448	559.7602	2743	76.3049	1.448	513.6685	2743	76.3049	1.448	539.4831
2744	76.3309	1.4476	493.4566	2744	76.3309	1.4476	580.3261	2744	76.3309	1.4476	515.3429	2744	76.3309	1.4476	540.9158
2745	76.3569	1.4472	519.4927	2745	76.3569	1.4472	606.7843	2745	76.3569	1.4472	518.9886	2745	76.3569	1.4472	544.3197
2746	76.3829	1.4467	495.2808	2746	76.3829	1.4467	582.9943	2746	76.3829	1.4467	509.9876	2746	76.3829	1.4467	535.077
2747	76.4089	1.4463	506.2058	2747	76.4089	1.4463	594.3414	2747	76.4089	1.4463	503.3854	2747	76.4089	1.4463	528.2331
2748	76.4349	1.4459	482.7038	2748	76.4349	1.4459	571.2615	2748	76.4349	1.4459	506.8549	2748	76.4349	1.4459	531.4608
2749	76.4609	1.4455	506.4967	2749	76.4609	1.4455	595.4764	2749	76.4609	1.4455	521.8396	2749	76.4609	1.4455	546.2037
2750	76.4869	1.4451	522.9399	2750	76.4869	1.4451	612.3417	2750	76.4869	1.4451	577.5308	2750	76.4869	1.4451	601.6532
2751	76.5129	1.4447	533.4542	2751	76.5129	1.4447	623.278	2751	76.5129	1.4447	563.5756	2751	76.5129	1.4447	587.4563
2752	76.5389	1.4442	526.1975	2752	76.5389	1.4442	616.4434	2752	76.5389	1.4442	567.2516	2752	76.5389	1.4442	590.8906
2753	76.5649	1.4438	567.1263	2753	76.5649	1.4438	657.7942	2753	76.5649	1.4438	626.6416	2753	76.5649	1.4438	650.0388
2754	76.5909	1.4434	565.7083	2754	76.5909	1.4434	656.7982	2754	76.5909	1.4434	626.591	2754	76.5909	1.4434	649.7464
2755	76.6169	1.443	583.7963	2755	76.6169	1.443	675.3083	2755	76.6169	1.443	663.9408	2755	76.6169	1.443	686.8544
2756	76.6429	1.4426	612.6645	2756	76.6429	1.4426	703.6098	2756	76.6429	1.4426	735.6656	2756	76.6429	1.4426	758.4781
2757	76.6689	1.4422	625.2004	2757	76.6689	1.4422	715.5791	2757	76.6689	1.4422	861.0296	2757	76.6689	1.4422	883.7409
2758	76.6949	1.4418	650.7362	2758	76.6949	1.4418	740.5484	2758	76.6949	1.4418	1032.2857	2758	76.6949	1.4418	1054.8958
2759	76.7209	1.4413	613.6434	2759	76.7209	1.4413	702.8889	2759	76.7209	1.4413	1179.318	2759	76.7209	1.4413	1201.8269
2760	76.7469	1.4409	636.5215	2760	76.7469	1.4409	725.2004	2760	76.7469	1.4409	1314.6319	2760	76.7469	1.4409	1337.0397
2761	76.7729	1.4405	681.4061	2761	76.7729	1.4405	769.5184	2761	76.7729	1.4405	1422.3815	2761	76.7729	1.4405	1444.6881
2762	76.7989	1.4401	694.0816	2762	76.7989	1.4401	781.6273	2762	76.7989	1.4401	1464.6538	2762	76.7989	1.4401	1486.8592
2763	76.8249	1.4397	696.4263	2763	76.8249	1.4397	783.4054	2763	76.8249	1.4397	1399.1351	2763	76.8249	1.4397	1421.2393
2764	76.8509	1.4393	677.2923	2764	76.8509	1.4393	763.7047	2764	76.8509	1.4393	1312.4065	2764	76.8509	1.4393	1334.4094
2765	76.8769	1.4389	660.7055	2765	76.8769	1.4389	746.5513	2765	76.8769	1.4389	1275.3269	2765	76.8769	1.4389	1297.2287
2766	76.9029	1.4385	646.8587	2766	76.9029	1.4385	732.1379	2766	76.9029	1.4385	1250.1239	2766	76.9029	1.4385	1271.9244
2767	76.9289	1.438	601.6614	2767	76.9289	1.438	686.374	2767	76.9289	1.438	1205.2241	2767	76.9289	1.438	1226.9234

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2768	76.9549	1.4376	595.1997	2768	76.9549	1.4376	679.3457	2768	76.9549	1.4376	1200.5674	2768	76.9549	1.4376	1222.1656
2769	76.9809	1.4372	587.6659	2769	76.9809	1.4372	671.2453	2769	76.9809	1.4372	1170.4147	2769	76.9809	1.4372	1191.9117
2770	77.0069	1.4368	579.6921	2770	77.0069	1.4368	662.7048	2770	77.0069	1.4368	1073.4108	2770	77.0069	1.4368	1094.8066
2771	77.0329	1.4364	580.6726	2771	77.0329	1.4364	663.1188	2771	77.0329	1.4364	963.967	2771	77.0329	1.4364	985.2615
2772	77.0589	1.436	570.1311	2772	77.0589	1.436	652.0107	2772	77.0589	1.436	918.4078	2772	77.0589	1.436	939.6012
2773	77.0849	1.4356	545.926	2773	77.0849	1.4356	627.2389	2773	77.0849	1.4356	889.7616	2773	77.0849	1.4356	910.8538
2774	77.1109	1.4352	508.6021	2774	77.1109	1.4352	589.3484	2774	77.1109	1.4352	785.4688	2774	77.1109	1.4352	806.4598
2775	77.1369	1.4348	499.1981	2775	77.1369	1.4348	579.3778	2775	77.1369	1.4348	722.768	2775	77.1369	1.4348	743.6578
2776	77.1629	1.4344	487.0209	2776	77.1629	1.4344	566.6339	2776	77.1629	1.4344	687.3727	2776	77.1629	1.4344	708.1613
2777	77.1889	1.434	470.4093	2777	77.1889	1.434	549.4557	2777	77.1889	1.434	628.7425	2777	77.1889	1.434	649.43
2778	77.2149	1.4335	467.508	2778	77.2149	1.4335	545.9879	2778	77.2149	1.4335	622.3175	2778	77.2149	1.4335	642.9037
2779	77.2409	1.4331	472.2401	2779	77.2409	1.4331	550.1533	2779	77.2409	1.4331	624.5921	2779	77.2409	1.4331	645.0772
2780	77.2669	1.4327	466.3376	2780	77.2669	1.4327	543.6842	2780	77.2669	1.4327	604.7079	2780	77.2669	1.4327	625.0918
2781	77.2929	1.4323	463.8534	2781	77.2929	1.4323	540.6334	2781	77.2929	1.4323	577.6449	2781	77.2929	1.4323	597.9275
2782	77.3189	1.4319	477.7302	2782	77.3189	1.4319	553.9436	2782	77.3189	1.4319	550.7622	2782	77.3189	1.4319	570.9436
2783	77.3449	1.4315	452.5609	2783	77.3449	1.4315	528.2076	2783	77.3449	1.4315	544.5403	2783	77.3449	1.4315	564.6206
2784	77.3709	1.4311	455.0099	2784	77.3709	1.4311	530.0901	2784	77.3709	1.4311	564.137	2784	77.3709	1.4311	584.116
2785	77.3969	1.4307	441.6696	2785	77.3969	1.4307	516.1831	2785	77.3969	1.4307	541.09	2785	77.3969	1.4307	560.9679
2786	77.4229	1.4303	416.5493	2786	77.4229	1.4303	490.4962	2786	77.4229	1.4303	507.9026	2786	77.4229	1.4303	527.6792
2787	77.4489	1.4299	427.3327	2787	77.4489	1.4299	500.713	2787	77.4489	1.4299	486.3063	2787	77.4489	1.4299	505.9818
2788	77.4749	1.4295	428.1466	2788	77.4749	1.4295	500.9603	2788	77.4749	1.4295	492.9889	2788	77.4749	1.4295	512.5632
2789	77.5009	1.4291	431.1294	2789	77.5009	1.4291	503.3764	2789	77.5009	1.4291	478.9332	2789	77.5009	1.4291	498.4063
2790	77.5269	1.4287	440.973	2790	77.5269	1.4287	512.6535	2790	77.5269	1.4287	494.935	2790	77.5269	1.4287	514.3069
2791	77.5529	1.4283	439.0845	2791	77.5529	1.4283	510.1984	2791	77.5529	1.4283	493.6108	2791	77.5529	1.4283	512.8816
2792	77.5789	1.4279	431.4528	2792	77.5789	1.4279	502	2792	77.5789	1.4279	494.9576	2792	77.5789	1.4279	514.1271
2793	77.6049	1.4275	442.116	2793	77.6049	1.4275	512.0966	2793	77.6049	1.4275	509.3199	2793	77.6049	1.4275	528.3882
2794	77.6309	1.4271	464.5768	2794	77.6309	1.4271	533.9907	2794	77.6309	1.4271	480.1347	2794	77.6309	1.4271	499.1019
2795	77.6569	1.4267	437.1521	2795	77.6569	1.4267	505.9995	2795	77.6569	1.4267	474.4838	2795	77.6569	1.4267	493.3498
2796	77.6829	1.4263	385.2006	2796	77.6829	1.4263	453.4814	2796	77.6829	1.4263	526.587	2796	77.6829	1.4263	545.3517
2797	77.7089	1.4259	410.4022	2797	77.7089	1.4259	478.1163	2797	77.7089	1.4259	541.7884	2797	77.7089	1.4259	560.4519
2798	77.7349	1.4255	421.8631	2798	77.7349	1.4255	489.0106	2798	77.7349	1.4255	516.1373	2798	77.7349	1.4255	534.6996
2799	77.7609	1.4251	417.2823	2799	77.7609	1.4251	483.8632	2799	77.7609	1.4251	527.9272	2799	77.7609	1.4251	546.3883
2800	77.7869	1.4247	410.0757	2800	77.7869	1.4247	476.09	2800	77.7869	1.4247	523.7351	2800	77.7869	1.4247	542.0951
2801	77.8129	1.4243	406.2469	2801	77.8129	1.4243	471.6945	2801	77.8129	1.4243	523.1633	2801	77.8129	1.4243	541.4221
2802	77.8389	1.4239	407.7257	2802	77.8389	1.4239	472.6068	2802	77.8389	1.4239	485.3785	2802	77.8389	1.4239	503.5361
2803	77.8649	1.4235	424.9399	2803	77.8649	1.4235	489.2543	2803	77.8649	1.4235	545.2938	2803	77.8649	1.4235	563.3502

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2804	77.8909	1.4231	408.3181	2804	77.8909	1.4231	472.066	2804	77.8909	1.4231	572.0599	2804	77.8909	1.4231	590.0151
2805	77.9169	1.4227	412.8378	2805	77.9169	1.4227	476.019	2805	77.9169	1.4227	617.5501	2805	77.9169	1.4227	635.4041
2806	77.9429	1.4223	394.2487	2806	77.9429	1.4223	456.8633	2806	77.9429	1.4223	663.7082	2806	77.9429	1.4223	681.461
2807	77.9689	1.4219	417.271	2807	77.9689	1.4219	479.319	2807	77.9689	1.4219	768.5813	2807	77.9689	1.4219	786.2329
2808	77.9949	1.4215	434.9261	2808	77.9949	1.4215	496.4075	2808	77.9949	1.4215	901.3371	2808	77.9949	1.4215	918.8875
2809	78.0209	1.4211	424.3459	2809	78.0209	1.4211	485.2607	2809	78.0209	1.4211	962.5014	2809	78.0209	1.4211	979.9506
2810	78.0469	1.4207	379.0825	2810	78.0469	1.4207	439.4373	2810	78.0469	1.4207	1022.4712	2810	78.0469	1.4207	1039.8192
2811	78.0729	1.4203	398.8089	2811	78.0729	1.4203	458.6039	2811	78.0729	1.4203	1010.5938	2811	78.0729	1.4203	1027.8406
2812	78.0989	1.4199	414.4275	2812	78.0989	1.4199	473.6626	2812	78.0989	1.4199	1028.4929	2812	78.0989	1.4199	1045.6385
2813	78.1249	1.4195	383.5609	2813	78.1249	1.4195	442.2361	2813	78.1249	1.4195	1004.502	2813	78.1249	1.4195	1021.5465
2814	78.1509	1.4191	416.8606	2814	78.1509	1.4191	474.9758	2814	78.1509	1.4191	1029.9695	2814	78.1509	1.4191	1046.9127
2815	78.1769	1.4187	355.5233	2815	78.1769	1.4187	413.0787	2815	78.1769	1.4187	959.4393	2815	78.1769	1.4187	976.2814
2816	78.2029	1.4183	363.3292	2816	78.2029	1.4183	420.3247	2816	78.2029	1.4183	988.1153	2816	78.2029	1.4183	1004.8562
2817	78.2289	1.4179	446.9174	2817	78.2289	1.4179	503.3529	2817	78.2289	1.4179	1006.0073	2817	78.2289	1.4179	1022.647
2818	78.2549	1.4175	404.9777	2818	78.2549	1.4175	460.8533	2818	78.2549	1.4175	891.0044	2818	78.2549	1.4175	907.5429
2819	78.2809	1.4171	401.9047	2819	78.2809	1.4171	457.2204	2819	78.2809	1.4171	936.8597	2819	78.2809	1.4171	953.2969
2820	78.3069	1.4167	383.8253	2820	78.3069	1.4167	438.5811	2820	78.3069	1.4167	844.9084	2820	78.3069	1.4167	861.2445
2821	78.3329	1.4163	404.0146	2821	78.3329	1.4163	458.2105	2821	78.3329	1.4163	818.2917	2821	78.3329	1.4163	834.5266
2822	78.3589	1.4159	415.2995	2822	78.3589	1.4159	468.9355	2822	78.3589	1.4159	742.2859	2822	78.3589	1.4159	758.4196
2823	78.3849	1.4155	408.9288	2823	78.3849	1.4155	462.005	2823	78.3849	1.4155	680.0122	2823	78.3849	1.4155	696.0447
2824	78.4109	1.4151	398.6007	2824	78.4109	1.4151	451.117	2824	78.4109	1.4151	677.1006	2824	78.4109	1.4151	693.0319
2825	78.4369	1.4147	437.2421	2825	78.4369	1.4147	489.1984	2825	78.4369	1.4147	631.1359	2825	78.4369	1.4147	646.966
2826	78.4629	1.4143	446.3598	2826	78.4629	1.4143	497.7562	2826	78.4629	1.4143	593.4292	2826	78.4629	1.4143	609.1581
2827	78.4889	1.4139	393.4258	2827	78.4889	1.4139	444.2623	2827	78.4889	1.4139	553.0286	2827	78.4889	1.4139	568.6563
2828	78.5149	1.4136	412.6163	2828	78.5149	1.4136	462.8929	2828	78.5149	1.4136	531.5302	2828	78.5149	1.4136	547.0567
2829	78.5409	1.4132	387.9701	2829	78.5409	1.4132	437.6868	2829	78.5409	1.4132	507.0808	2829	78.5409	1.4132	522.5061
2830	78.5669	1.4128	424.0365	2830	78.5669	1.4128	473.1934	2830	78.5669	1.4128	485.2195	2830	78.5669	1.4128	500.5436
2831	78.5929	1.4124	443.9615	2831	78.5929	1.4124	492.5584	2831	78.5929	1.4124	458.9394	2831	78.5929	1.4124	474.1624
2832	78.6189	1.412	420.4833	2832	78.6189	1.412	468.5203	2832	78.6189	1.412	519.6676	2832	78.6189	1.412	534.7893
2833	78.6449	1.4116	418.5229	2833	78.6449	1.4116	466	2833	78.6449	1.4116	524.1793	2833	78.6449	1.4116	539.1999
2834	78.6709	1.4112	427.9842	2834	78.6709	1.4112	474.9015	2834	78.6709	1.4112	467.1114	2834	78.6709	1.4112	482.0307
2835	78.6969	1.4108	466.612	2835	78.6969	1.4108	512.9694	2835	78.6969	1.4108	483.9479	2835	78.6969	1.4108	498.766
2836	78.7229	1.4104	447.8342	2836	78.7229	1.4104	493.6316	2836	78.7229	1.4104	442.8977	2836	78.7229	1.4104	457.6147
2837	78.7489	1.41	396.5813	2837	78.7489	1.41	441.8188	2837	78.7489	1.41	469.939	2837	78.7489	1.41	484.5548
2838	78.7749	1.4096	391.8737	2838	78.7749	1.4096	436.5514	2838	78.7749	1.4096	506.9523	2838	78.7749	1.4096	521.4669
2839	78.8009	1.4093	435.7495	2839	78.8009	1.4093	479.8672	2839	78.8009	1.4093	436.9386	2839	78.8009	1.4093	451.352

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2840	78.8269	1.4089	379.6545	2840	78.8269	1.4089	423.2123	2840	78.8269	1.4089	413.5511	2840	78.8269	1.4089	427.8633
2841	78.8529	1.4085	390.8021	2841	78.8529	1.4085	433.8	2841	78.8529	1.4085	446.2579	2841	78.8529	1.4085	460.4689
2842	78.8789	1.4081	355.2129	2842	78.8789	1.4081	397.6509	2842	78.8789	1.4081	463.6194	2842	78.8789	1.4081	477.7292
2843	78.9049	1.4077	410.9903	2843	78.9049	1.4077	452.8684	2843	78.9049	1.4077	477.2032	2843	78.9049	1.4077	491.2118
2844	78.9309	1.4073	403.1632	2844	78.9309	1.4073	444.4814	2844	78.9309	1.4073	492.7473	2844	78.9309	1.4073	506.6548
2845	78.9569	1.4069	432.3867	2845	78.9569	1.4069	473.145	2845	78.9569	1.4069	482.1358	2845	78.9569	1.4069	495.942
2846	78.9829	1.4065	433.5486	2846	78.9829	1.4065	473.7471	2846	78.9829	1.4065	485.2347	2846	78.9829	1.4065	498.9397
2847	79.0089	1.4061	406.2433	2847	79.0089	1.4061	445.8819	2847	79.0089	1.4061	492.7243	2847	79.0089	1.4061	506.3281
2848	79.0349	1.4058	427.4682	2848	79.0349	1.4058	466.5469	2848	79.0349	1.4058	447.9209	2848	79.0349	1.4058	461.4235
2849	79.0609	1.4054	437.4813	2849	79.0609	1.4054	476	2849	79.0609	1.4054	455.5792	2849	79.0609	1.4054	468.9806
2850	79.0869	1.405	425.6076	2850	79.0869	1.405	463.5664	2850	79.0869	1.405	441.0267	2850	79.0869	1.405	454.327
2851	79.1129	1.4046	415.1079	2851	79.1129	1.4046	452.5068	2851	79.1129	1.4046	440.0156	2851	79.1129	1.4046	453.2147
2852	79.1389	1.4042	430.9496	2852	79.1389	1.4042	467.7886	2852	79.1389	1.4042	428.6713	2852	79.1389	1.4042	441.7691
2853	79.1649	1.4038	413.4625	2853	79.1649	1.4038	449.7416	2853	79.1649	1.4038	453.1731	2853	79.1649	1.4038	466.1697
2854	79.1909	1.4034	387.3717	2854	79.1909	1.4034	423.0909	2854	79.1909	1.4034	439.1283	2854	79.1909	1.4034	452.0237
2855	79.2169	1.4031	429.9286	2855	79.2169	1.4031	465.0879	2855	79.2169	1.4031	434.0235	2855	79.2169	1.4031	446.8178
2856	79.2429	1.4027	432.5731	2856	79.2429	1.4027	467.1725	2856	79.2429	1.4027	429.9165	2856	79.2429	1.4027	442.6096
2857	79.2689	1.4023	423.6224	2857	79.2689	1.4023	457.6619	2857	79.2689	1.4023	468.7718	2857	79.2689	1.4023	481.3637
2858	79.2949	1.4019	398.44	2858	79.2949	1.4019	431.9196	2858	79.2949	1.4019	457.9088	2858	79.2949	1.4019	470.3995
2859	79.3209	1.4015	409.4796	2859	79.3209	1.4015	442.3993	2859	79.3209	1.4015	434.1896	2859	79.3209	1.4015	446.5791
2860	79.3469	1.4011	416.6864	2860	79.3469	1.4011	449.0462	2860	79.3469	1.4011	422.4935	2860	79.3469	1.4011	434.7818
2861	79.3729	1.4008	396.3995	2861	79.3729	1.4008	428.1994	2861	79.3729	1.4008	449.5473	2861	79.3729	1.4008	461.7344
2862	79.3989	1.4004	398.3941	2862	79.3989	1.4004	429.6341	2862	79.3989	1.4004	445.6459	2862	79.3989	1.4004	457.7318
2863	79.4249	1.4	412.3439	2863	79.4249	1.4	443.024	2863	79.4249	1.4	433.4249	2863	79.4249	1.4	445.4096
2864	79.4509	1.3996	414.5099	2864	79.4509	1.3996	444.6301	2864	79.4509	1.3996	440.4488	2864	79.4509	1.3996	452.3323
2865	79.4769	1.3992	411.1095	2865	79.4769	1.3992	440.6698	2865	79.4769	1.3992	432.5666	2865	79.4769	1.3992	444.3489
2866	79.5029	1.3988	435.768	2866	79.5029	1.3988	464.7684	2866	79.5029	1.3988	416.8746	2866	79.5029	1.3988	428.5558
2867	79.5289	1.3985	421.2342	2867	79.5289	1.3985	449.6747	2867	79.5289	1.3985	396.2269	2867	79.5289	1.3985	407.8068
2868	79.5549	1.3981	411.1502	2868	79.5549	1.3981	439.0308	2868	79.5549	1.3981	390.6019	2868	79.5549	1.3981	402.0807
2869	79.5809	1.3977	417.622	2869	79.5809	1.3977	444.9428	2869	79.5809	1.3977	423.8514	2869	79.5809	1.3977	435.229
2870	79.6069	1.3973	393.5862	2870	79.6069	1.3973	420.347	2870	79.6069	1.3973	441.8613	2870	79.6069	1.3973	453.1376
2871	79.6329	1.3969	385.1214	2871	79.6329	1.3969	411.3223	2871	79.6329	1.3969	421.1342	2871	79.6329	1.3969	432.3094
2872	79.6589	1.3966	404.1602	2872	79.6589	1.3966	429.8013	2872	79.6589	1.3966	411.5439	2872	79.6589	1.3966	422.6179
2873	79.6849	1.3962	406.3585	2873	79.6849	1.3962	431.4397	2873	79.6849	1.3962	450.7463	2873	79.6849	1.3962	461.7191
2874	79.7109	1.3958	422.6347	2874	79.7109	1.3958	447.1559	2874	79.7109	1.3958	472.7971	2874	79.7109	1.3958	483.6687
2875	79.7369	1.3954	410.3722	2875	79.7369	1.3954	434.3335	2875	79.7369	1.3954	459.2629	2875	79.7369	1.3954	470.0333

Table I. part 3: *Continued*

E027_vial2_ConstCompExp_BackgrndRmvod_MHC				E027_vial2_ConstCompExp_raw_MHC				E017_first_v2_ConstCompExp_BackgrdRmovd				E017_first_v2_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2876	79.7629	1.395	391.8488	2876	79.7629	1.395	415.2502	2876	79.7629	1.395	448.8626	2876	79.7629	1.395	459.5318
2877	79.7889	1.3947	410.6697	2877	79.7889	1.3947	433.5112	2877	79.7889	1.3947	425.9179	2877	79.7889	1.3947	436.4859
2878	79.8149	1.3943	410.5218	2878	79.8149	1.3943	432.8035	2878	79.8149	1.3943	398.8334	2878	79.8149	1.3943	409.3002
2879	79.8409	1.3939	411.7364	2879	79.8409	1.3939	433.4581	2879	79.8409	1.3939	407.5911	2879	79.8409	1.3939	417.9567
2880	79.8669	1.3935	395.8987	2880	79.8669	1.3935	417.0605	2880	79.8669	1.3935	441.6391	2880	79.8669	1.3935	451.9035
2881	79.8929	1.3932	392.9074	2881	79.8929	1.3932	413.5094	2881	79.8929	1.3932	438.7846	2881	79.8929	1.3932	448.9478
2882	79.9189	1.3928	393.5082	2882	79.9189	1.3928	413.5502	2882	79.9189	1.3928	433.7322	2882	79.9189	1.3928	443.7943
2883	79.9449	1.3924	393.6167	2883	79.9449	1.3924	413.0988	2883	79.9449	1.3924	424.2652	2883	79.9449	1.3924	434.2261
2884	79.9709	1.392	397.091	2884	79.9709	1.392	416.5731	2884	79.9709	1.392	401.9795	2884	79.9709	1.392	411.9403

APPENDIX I

Table I. part 4: Raw and processed X-ray diffraction data from synthetic samples produced in constant composition experiments shown in Chapter 5.

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1	5.0129	20.4542	273.625	1	5.0129	20.4542	5686	1	5.0129	20.4542	380.8498	1	5.0129	20.4542	5923
2	5.0389	20.3487	427.417	2	5.0389	20.3487	5815.7002	2	5.0389	20.3487	325.6558	2	5.0389	20.3487	5838.8434
3	5.0649	20.2443	439.0864	3	5.0649	20.2443	5803.2778	3	5.0649	20.2443	310.6481	3	5.0649	20.2443	5794.8732
4	5.0909	20.141	389.1626	4	5.0909	20.141	5729.2623	4	5.0909	20.141	281.4937	4	5.0909	20.141	5736.7562
5	5.1169	20.0387	283.2708	5	5.1169	20.0387	5599.2787	5	5.1169	20.0387	290.4541	5	5.1169	20.0387	5716.7541
6	5.1429	19.9375	393.3212	6	5.1429	19.9375	5685.2373	6	5.1429	19.9375	252.1354	6	5.1429	19.9375	5649.4728
7	5.1689	19.8373	393.0212	7	5.1689	19.8373	5660.8455	7	5.1689	19.8373	297.3749	7	5.1689	19.8373	5665.7498
8	5.1949	19.7381	355.7126	8	5.1949	19.7381	5599.4452	8	5.1949	19.7381	316.4212	8	5.1949	19.7381	5655.8335
9	5.2209	19.6398	233.5834	9	5.2209	19.6398	5453.2243	9	5.2209	19.6398	274.583	9	5.2209	19.6398	5585.0328
10	5.2469	19.5426	267.3077	10	5.2469	19.5426	5462.8568	10	5.2469	19.5426	210.0857	10	5.2469	19.5426	5491.5729
11	5.2729	19.4463	255.7101	11	5.2729	19.4463	5427.1674	11	5.2729	19.4463	267.4072	11	5.2729	19.4463	5519.9319
12	5.2989	19.3509	299.6876	12	5.2989	19.3509	5447.0531	12	5.2989	19.3509	191.7536	12	5.2989	19.3509	5415.3157
13	5.3249	19.2565	297.6555	13	5.3249	19.2565	5420.9292	13	5.3249	19.2565	213.567	13	5.3249	19.2565	5408.1665
14	5.3509	19.163	208.0707	14	5.3509	19.163	5307.2527	14	5.3509	19.163	104.0014	14	5.3509	19.163	5269.6384
15	5.3769	19.0704	326.9901	15	5.3769	19.0704	5402.0803	15	5.3769	19.0704	255.2662	15	5.3769	19.0704	5391.9406
16	5.4029	18.9787	123.8658	16	5.4029	18.9787	5174.8643	16	5.4029	18.9787	286.8602	16	5.4029	18.9787	5394.572
17	5.4289	18.8879	312.0392	17	5.4289	18.8879	5338.9459	17	5.4289	18.8879	173.4455	17	5.4289	18.8879	5252.1949
18	5.4549	18.7979	178.9933	18	5.4549	18.7979	5181.8082	18	5.4549	18.7979	261.008	18	5.4549	18.7979	5310.7947
19	5.4809	18.7088	215.025	19	5.4809	18.7088	5193.7481	19	5.4809	18.7088	260.3561	19	5.4809	18.7088	5281.1803
20	5.5069	18.6206	217.9096	20	5.5069	18.6206	5172.5409	20	5.5069	18.6206	309.9745	20	5.5069	18.6206	5301.8361
21	5.5329	18.5331	222.4371	21	5.5329	18.5331	5152.9767	21	5.5329	18.5331	373.3537	21	5.5329	18.5331	5336.2528
22	5.5589	18.4465	159.6392	22	5.5589	18.4465	5066.087	22	5.5589	18.4465	253.9036	22	5.5589	18.4465	5187.8402
23	5.5849	18.3607	160.0805	23	5.5849	18.3607	5042.4366	23	5.5849	18.3607	188.8698	23	5.5849	18.3607	5093.8437
24	5.6109	18.2757	115.0466	24	5.6109	18.2757	4973.3109	24	5.6109	18.2757	243.1215	24	5.6109	18.2757	5119.1329
25	5.6369	18.1915	300.9132	25	5.6369	18.1915	5135.0857	25	5.6369	18.1915	259.5714	25	5.6369	18.1915	5106.6203
26	5.6629	18.108	293.9419	26	5.6629	18.108	5104.0227	26	5.6629	18.108	349.3405	26	5.6629	18.108	5167.4268
27	5.6889	18.0253	313.4977	27	5.6889	18.0253	5099.4867	27	5.6889	18.0253	281.411	27	5.6889	18.0253	5070.5347
28	5.7149	17.9434	273.625	28	5.7149	17.9434	5035.5223	28	5.7149	17.9434	380.8498	28	5.7149	17.9434	5141.011
29	5.7409	17.8622	320.1409	29	5.7409	17.8622	5068.2184	29	5.7409	17.8622	370.7321	29	5.7409	17.8622	5116.282
30	5.7669	17.7817	306.8844	30	5.7669	17.7817	5041.1423	30	5.7669	17.7817	288.836	30	5.7669	17.7817	5019.7746
31	5.7929	17.702	251.3987	31	5.7929	17.702	4971.8368	31	5.7929	17.702	318.9195	31	5.7929	17.702	5035.2469

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
32	5.8189	17.623	272.7704	32	5.8189	17.623	4979.3888	32	5.8189	17.623	420.8324	32	5.8189	17.623	5122.5485
33	5.8449	17.5446	340.833	33	5.8449	17.5446	5033.6317	33	5.8449	17.5446	396.2816	33	5.8449	17.5446	5083.3864
34	5.8709	17.467	335.0123	34	5.8709	17.467	5013.9913	34	5.8709	17.467	353.6216	34	5.8709	17.467	5026.1151
35	5.8969	17.3901	287.4316	35	5.8969	17.3901	4952.5909	35	5.8969	17.3901	318.3472	35	5.8969	17.3901	4976.2294
36	5.9229	17.3138	205.9031	36	5.9229	17.3138	4857.2427	36	5.9229	17.3138	287.6203	36	5.9229	17.3138	4930.8912
37	5.9489	17.2382	222.262	37	5.9489	17.2382	4859.7818	37	5.9489	17.2382	350.0489	37	5.9489	17.2382	4978.7086
38	5.9749	17.1632	232.0862	38	5.9749	17.1632	4855.7864	38	5.9749	17.1632	352.7518	38	5.9749	17.1632	4966.8001
39	6.0009	17.0889	281.2017	39	6.0009	17.0889	4891.0821	39	6.0009	17.0889	315.6448	39	6.0009	17.0889	4915.0819
40	6.0269	17.0153	320.422	40	6.0269	17.0153	4916.4827	40	6.0269	17.0153	308.4309	40	6.0269	17.0153	4893.2567
41	6.0529	16.9423	298.1911	41	6.0529	16.9423	4880.4322	41	6.0529	16.9423	262.6965	41	6.0529	16.9423	4832.9109
42	6.0789	16.8699	262.1058	42	6.0789	16.8699	4830.5271	42	6.0789	16.8699	281.9198	42	6.0789	16.8699	4837.523
43	6.1049	16.7981	240.6503	43	6.1049	16.7981	4795.2519	43	6.1049	16.7981	368.7529	43	6.1049	16.7981	4909.7448
44	6.1309	16.7269	234.0447	44	6.1309	16.7269	4774.8265	44	6.1309	16.7269	337.7916	44	6.1309	16.7269	4864.1722
45	6.1569	16.6564	318.2263	45	6.1569	16.6564	4845.1884	45	6.1569	16.6564	336.9237	45	6.1569	16.6564	4848.693
46	6.1829	16.5864	292.2281	46	6.1829	16.5864	4805.3706	46	6.1829	16.5864	405.9818	46	6.1829	16.5864	4903.1399
47	6.2089	16.517	226.2208	47	6.2089	16.517	4725.5436	47	6.2089	16.517	395.5109	47	6.2089	16.517	4878.0576
48	6.2349	16.4482	292.7949	48	6.2349	16.4482	4778.2979	48	6.2349	16.4482	345.781	48	6.2349	16.4482	4813.7164
49	6.2609	16.38	299.42	49	6.2609	16.38	4771.1033	49	6.2609	16.38	299.5385	49	6.2609	16.38	4752.8626
50	6.2869	16.3123	256.9155	50	6.2869	16.3123	4714.7791	50	6.2869	16.3123	298.2428	50	6.2869	16.3123	4736.9557
51	6.3129	16.2452	264.9716	51	6.3129	16.2452	4709.0155	51	6.3129	16.2452	368.2014	51	6.3129	16.2452	4792.3031
52	6.3389	16.1786	325.2325	52	6.3389	16.1786	4755.4567	52	6.3389	16.1786	385.9443	52	6.3389	16.1786	4795.4347
53	6.3649	16.1126	398.6327	53	6.3649	16.1126	4815.0372	53	6.3649	16.1126	396.0677	53	6.3649	16.1126	4790.9467
54	6.3909	16.0471	341.1257	54	6.3909	16.0471	4743.7104	54	6.3909	16.0471	422.9228	54	6.3909	16.0471	4803.1905
55	6.4169	15.9821	273.625	55	6.4169	15.9821	4662.3901	55	6.4169	15.9821	380.8498	55	6.4169	15.9821	4746.5063
56	6.4429	15.9177	315.7757	56	6.4429	15.9177	4697.6252	56	6.4429	15.9177	328.14	56	6.4429	15.9177	4687.1949
57	6.4689	15.8538	260.6392	57	6.4689	15.8538	4635.5732	57	6.4689	15.8538	351.2045	57	6.4689	15.8538	4703.6578
58	6.4949	15.7904	189.3506	58	6.4949	15.7904	4557.369	58	6.4949	15.7904	340.3364	58	6.4949	15.7904	4686.188
59	6.5209	15.7275	262.0371	59	6.5209	15.7275	4623.14	59	6.5209	15.7275	327.3407	59	6.5209	15.7275	4666.5907
60	6.5469	15.6651	285.7667	60	6.5469	15.6651	4639.9541	60	6.5469	15.6651	434.4245	60	6.5469	15.6651	4767.0729
61	6.5729	15.6032	261.9655	61	6.5729	15.6032	4609.2373	61	6.5729	15.6032	450.8324	61	6.5729	15.6032	4776.8793
62	6.5989	15.5418	277.1964	62	6.5989	15.5418	4617.5527	62	6.5989	15.5418	399.6595	62	6.5989	15.5418	4719.1047
63	6.6249	15.4809	311.8787	63	6.6249	15.4809	4645.3194	63	6.6249	15.4809	338.7141	63	6.6249	15.4809	4651.5577
64	6.6509	15.4204	293.3668	64	6.6509	15.4204	4619.892	64	6.6509	15.4204	373.0166	64	6.6509	15.4204	4679.2586
65	6.6769	15.3605	219.1938	65	6.6769	15.3605	4538.8035	65	6.6769	15.3605	339.3088	65	6.6769	15.3605	4638.9492
66	6.7029	15.3009	254.4948	66	6.7029	15.3009	4567.1889	66	6.7029	15.3009	330.8763	66	6.7029	15.3009	4623.9151
67	6.7289	15.2419	255.8496	67	6.7289	15.2419	4561.6282	67	6.7289	15.2419	325.9516	67	6.7289	15.2419	4612.3888

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
68	6.7549	15.1833	230.8672	68	6.7549	15.1833	4529.7303	68	6.7549	15.1833	390.9565	68	6.7549	15.1833	4670.7921
69	6.7809	15.1251	145.3053	69	6.7809	15.1251	4437.2528	69	6.7809	15.1251	369.3058	69	6.7809	15.1251	4642.5398
70	6.8069	15.0674	193.3425	70	6.8069	15.0674	4478.3744	70	6.8069	15.0674	418.6483	70	6.8069	15.0674	4685.2807
71	6.8329	15.0102	266.6367	71	6.8329	15.0102	4544.7531	71	6.8329	15.0102	322.4379	71	6.8329	15.0102	4582.4686
72	6.8589	14.9533	217.564	72	6.8589	14.9533	4488.7648	72	6.8589	14.9533	325.4519	72	6.8589	14.9533	4578.881
73	6.8849	14.8969	175.1268	73	6.8849	14.8969	4439.4121	73	6.8849	14.8969	295.5912	73	6.8849	14.8969	4542.4188
74	6.9109	14.841	274.2897	74	6.9109	14.841	4531.6595	74	6.9109	14.841	356.0876	74	6.9109	14.841	4596.3136
75	6.9369	14.7854	279.9593	75	6.9369	14.7854	4530.4135	75	6.9369	14.7854	360.2084	75	6.9369	14.7854	4593.8328
76	6.9629	14.7303	334.0662	76	6.9629	14.7303	4577.6049	76	6.9629	14.7303	396.0239	76	6.9629	14.7303	4623.0466
77	6.9889	14.6755	326.5895	77	6.9889	14.6755	4563.2126	77	6.9889	14.6755	400.9558	77	6.9889	14.6755	4621.3769
78	7.0149	14.6212	270.4748	78	7.0149	14.6212	4500.1824	78	7.0149	14.6212	337.6917	78	7.0149	14.6212	4551.5113
79	7.0409	14.5673	345.1388	79	7.0409	14.5673	4567.9309	79	7.0409	14.5673	219.1009	79	7.0409	14.5673	4426.3189
80	7.0669	14.5138	335.962	80	7.0669	14.5138	4551.8386	80	7.0669	14.5138	310.0062	80	7.0669	14.5138	4510.6225
81	7.0929	14.4606	323.9033	81	7.0929	14.4606	4532.8643	81	7.0929	14.4606	320.1521	81	7.0929	14.4606	4514.1668
82	7.1189	14.4079	273.625	82	7.1189	14.4079	4475.6705	82	7.1189	14.4079	380.8498	82	7.1189	14.4079	4568.2629
83	7.1449	14.3555	245.0993	83	7.1449	14.3555	4440.4829	83	7.1449	14.3555	391.8343	83	7.1449	14.3555	4573.3989
84	7.1709	14.3035	344.0442	84	7.1709	14.3035	4532.7659	84	7.1709	14.3035	295.401	84	7.1709	14.3035	4471.117
85	7.1969	14.2519	302.9401	85	7.1969	14.2519	4485	85	7.1969	14.2519	311.9768	85	7.1969	14.2519	4481.8443
86	7.2229	14.2007	326.2021	86	7.2229	14.2007	4501.6001	86	7.2229	14.2007	269.0509	86	7.2229	14.2007	4433.07
87	7.2489	14.1498	407.5955	87	7.2489	14.1498	4576.3317	87	7.2489	14.1498	381.6444	87	7.2489	14.1498	4539.815
88	7.2749	14.0993	323.592	88	7.2749	14.0993	4485.6663	88	7.2749	14.0993	458.9079	88	7.2749	14.0993	4611.2299
89	7.3009	14.0492	280.4791	89	7.3009	14.0492	4435.8915	89	7.3009	14.0492	367.4677	89	7.3009	14.0492	4513.9412
90	7.3269	13.9994	199.048	90	7.3269	13.9994	4347.7986	90	7.3269	13.9994	350.4024	90	7.3269	13.9994	4491.0274
91	7.3529	13.95	378.1253	91	7.3529	13.95	4520.214	91	7.3529	13.95	377.2115	91	7.3529	13.95	4511.988
92	7.3789	13.9009	382.7874	92	7.3789	13.9009	4518.2142	92	7.3789	13.9009	250.7792	92	7.3789	13.9009	4379.7071
93	7.4049	13.8521	333.4064	93	7.4049	13.8521	4462.1714	93	7.4049	13.8521	326.0919	93	7.4049	13.8521	4449.1714
94	7.4309	13.8037	139.659	94	7.4309	13.8037	4261.7622	94	7.4309	13.8037	138.25	94	7.4309	13.8037	4255.4809
95	7.4569	13.7557	358.3568	95	7.4569	13.7557	4473.7981	95	7.4569	13.7557	432.0409	95	7.4569	13.7557	4543.4233
96	7.4829	13.7079	348.7932	96	7.4829	13.7079	4457.5726	96	7.4829	13.7079	371.7691	96	7.4829	13.7079	4477.303
97	7.5089	13.6605	143.093	97	7.5089	13.6605	4245.2106	97	7.5089	13.6605	332.223	97	7.5089	13.6605	4431.9084
98	7.5349	13.6135	312.8551	98	7.5349	13.6135	4408.3108	98	7.5349	13.6135	318.6782	98	7.5349	13.6135	4412.515
99	7.5609	13.5667	277.725	99	7.5609	13.5667	4366.5188	99	7.5609	13.5667	385.3112	99	7.5609	13.5667	4473.2995
100	7.5869	13.5203	337.4611	100	7.5869	13.5203	4419.5931	100	7.5869	13.5203	261.2494	100	7.5869	13.5203	4343.3892
101	7.6129	13.4742	321.732	101	7.6129	13.4742	4397.202	101	7.6129	13.4742	289.3614	101	7.6129	13.4742	4365.6527
102	7.6389	13.4284	354.1358	102	7.6389	13.4284	4422.9441	102	7.6389	13.4284	378.3765	102	7.6389	13.4284	4448.8193
103	7.6649	13.3829	207.7251	103	7.6649	13.3829	4269.8714	103	7.6649	13.3829	405.1521	103	7.6649	13.3829	4469.7464

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
104	7.6909	13.3378	305.4259	104	7.6909	13.3378	4360.9104	104	7.6909	13.3378	361.376	104	7.6909	13.3378	4420.1218
105	7.7169	13.2929	300.6242	105	7.7169	13.2929	4349.4469	105	7.7169	13.2929	213.1458	105	7.7169	13.2929	4266.0431
106	7.7429	13.2483	365.2869	106	7.7429	13.2483	4407.4477	106	7.7429	13.2483	327.014	106	7.7429	13.2483	4374.0628
107	7.7689	13.204	333.7269	107	7.7689	13.204	4369.2258	107	7.7689	13.204	207.8913	107	7.7689	13.204	4249.0915
108	7.7949	13.1601	341.9162	108	7.7949	13.1601	4370.7533	108	7.7949	13.1601	344.5805	108	7.7949	13.1601	4379.9323
109	7.8209	13.1164	273.625	109	7.8209	13.1164	4295.8002	109	7.8209	13.1164	380.8498	109	7.8209	13.1164	4410.353
110	7.8469	13.073	340.0688	110	7.8469	13.073	4356.1298	110	7.8469	13.073	277.5805	110	7.8469	13.073	4298.1097
111	7.8729	13.0299	300.2659	111	7.8729	13.0299	4310.2128	111	7.8729	13.0299	334.5918	111	7.8729	13.0299	4346.1471
112	7.8989	12.9871	258.9319	112	7.8989	12.9871	4262.7646	112	7.8989	12.9871	311.6765	112	7.8989	12.9871	4314.2577
113	7.9249	12.9445	227.3994	113	7.9249	12.9445	4225.118	113	7.9249	12.9445	318.1702	113	7.9249	12.9445	4311.7774
114	7.9509	12.9023	297.9405	114	7.9509	12.9023	4289.5449	114	7.9509	12.9023	351.0939	114	7.9509	12.9023	4335.7271
115	7.9769	12.8603	312.6409	115	7.9769	12.8603	4298.1311	115	7.9769	12.8603	352.0456	115	7.9769	12.8603	4327.7048
116	8.0029	12.8186	332.3669	116	8.0029	12.8186	4311.743	116	8.0029	12.8186	399.6848	116	8.0029	12.8186	4366.37
117	8.0289	12.7771	401.8671	117	8.0289	12.7771	4375.129	117	8.0289	12.7771	327.8403	117	8.0289	12.7771	4285.5516
118	8.0549	12.7359	440.6686	118	8.0549	12.7359	4407.8164	118	8.0549	12.7359	351.4701	118	8.0549	12.7359	4300.2073
119	8.0809	12.695	437.6997	119	8.0809	12.695	4398.7333	119	8.0809	12.695	313.1699	119	8.0809	12.695	4252.9332
120	8.1069	12.6544	396.8412	120	8.1069	12.6544	4351.7607	120	8.1069	12.6544	321.861	120	8.1069	12.6544	4252.6502
121	8.1329	12.614	325.2114	121	8.1329	12.614	4274.0167	121	8.1329	12.614	358.2738	121	8.1329	12.614	4280.0891
122	8.1589	12.5739	340.0903	122	8.1589	12.5739	4282.7815	122	8.1589	12.5739	348.3773	122	8.1589	12.5739	4261.2185
123	8.1849	12.534	402.1603	123	8.1849	12.534	4338.7373	123	8.1849	12.534	336.1326	123	8.1849	12.534	4239.9999
124	8.2109	12.4944	255.4913	124	8.2109	12.4944	4185.9541	124	8.2109	12.4944	377.746	124	8.2109	12.4944	4272.6392
125	8.2369	12.455	325.4789	125	8.2369	12.455	4249.8275	125	8.2369	12.455	486.3585	125	8.2369	12.455	4372.2777
126	8.2629	12.4159	347.2921	126	8.2629	12.4159	4265.5266	126	8.2629	12.4159	317.6919	126	8.2629	12.4159	4194.6371
127	8.2889	12.377	500.837	127	8.2889	12.377	4412.9574	127	8.2889	12.377	390.9928	127	8.2889	12.377	4258.9641
128	8.3149	12.3384	359.709	128	8.3149	12.3384	4265.7151	128	8.3149	12.3384	320.9244	128	8.3149	12.3384	4179.9216
129	8.3409	12.3	361.8032	129	8.3409	12.3	4261.6952	129	8.3409	12.3	359.9714	129	8.3409	12.3	4209.9947
130	8.3669	12.2618	369.9014	130	8.3669	12.2618	4263.6792	130	8.3669	12.2618	298.0275	130	8.3669	12.2618	4139.0767
131	8.3929	12.2239	285.6746	131	8.3929	12.2239	4173.3383	131	8.3929	12.2239	334.2541	131	8.3929	12.2239	4166.3294
132	8.4189	12.1862	263.3517	132	8.4189	12.1862	4144.9013	132	8.4189	12.1862	403.5074	132	8.4189	12.1862	4226.6086
133	8.4449	12.1488	287.4405	133	8.4449	12.1488	4162.8759	133	8.4449	12.1488	382.006	133	8.4449	12.1488	4196.1333
134	8.4709	12.1116	395.9257	134	8.4709	12.1116	4265.2469	134	8.4709	12.1116	352.4777	134	8.4709	12.1116	4157.631
135	8.4969	12.0746	396.512	135	8.4969	12.0746	4259.719	135	8.4969	12.0746	297.8469	135	8.4969	12.0746	4094.0262
136	8.5229	12.0378	416.2155	136	8.5229	12.0378	4273.3084	136	8.5229	12.0378	380.8498	136	8.5229	12.0378	4168.055
137	8.5489	12.0013	306.1564	137	8.5489	12.0013	4156.3807	137	8.5489	12.0013	446.3906	137	8.5489	12.0013	4225.2045
138	8.5749	11.9649	281.2863	138	8.5749	11.9649	4124.642	138	8.5749	11.9649	410.8103	138	8.5749	11.9649	4181.2328
139	8.6009	11.9288	353.7715	139	8.6009	11.9288	4190.2585	139	8.6009	11.9288	447.211	139	8.6009	11.9288	4209.2422

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
140	8.6269	11.8929	384.7608	140	8.6269	11.8929	4214.3792	140	8.6269	11.8929	443.904	140	8.6269	11.8929	4197.5439
141	8.6529	11.8573	347.8778	141	8.6529	11.8573	4170.6276	141	8.6529	11.8573	431.2494	141	8.6529	11.8573	4176.4979
142	8.6789	11.8218	306.6864	142	8.6789	11.8218	4122.5675	142	8.6789	11.8218	523.0701	142	8.6789	11.8218	4259.9272
143	8.7049	11.7866	384.5055	143	8.7049	11.7866	4193.5179	143	8.7049	11.7866	487.0135	143	8.7049	11.7866	4215.4793
144	8.7309	11.7516	433.0039	144	8.7309	11.7516	4235.1477	144	8.7309	11.7516	368.6521	144	8.7309	11.7516	4088.7266
145	8.7569	11.7167	368.3211	145	8.7569	11.7167	4163.5963	145	8.7569	11.7167	423.4225	145	8.7569	11.7167	4135.1056
146	8.7829	11.6821	327.7871	146	8.7829	11.6821	4116.1937	146	8.7829	11.6821	491.4117	146	8.7829	11.6821	4194.7035
147	8.8089	11.6477	318.6784	147	8.8089	11.6477	4100.2164	147	8.8089	11.6477	429.5922	147	8.8089	11.6477	4124.4926
148	8.8349	11.6135	376.5944	148	8.8349	11.6135	4151.2636	148	8.8349	11.6135	411.4792	148	8.8349	11.6135	4097.9883
149	8.8609	11.5795	435.6679	149	8.8609	11.5795	4203.4685	149	8.8609	11.5795	429.6577	149	8.8609	11.5795	4107.7755
150	8.8869	11.5457	450.4132	150	8.8869	11.5457	4211.3453	150	8.8869	11.5457	443.4425	150	8.8869	11.5457	4113.1689
151	8.9129	11.5121	401.4913	151	8.9129	11.5121	4155.5546	151	8.9129	11.5121	463.595	151	8.9129	11.5121	4124.9301
152	8.9389	11.4786	343.7914	152	8.9389	11.4786	4090.9861	152	8.9389	11.4786	426.9106	152	8.9389	11.4786	4079.8544
153	8.9649	11.4454	346.1821	153	8.9649	11.4454	4086.5082	153	8.9649	11.4454	426.399	153	8.9649	11.4454	4070.9514
154	8.9909	11.4124	353.0244	154	8.9909	11.4124	4086.4819	154	8.9909	11.4124	445.2264	154	8.9909	11.4124	4081.3874
155	9.0169	11.3795	376.458	155	9.0169	11.3795	4103.0469	155	9.0169	11.3795	441.9174	155	9.0169	11.3795	4069.687
156	9.0429	11.3469	411.9068	156	9.0429	11.3469	4131.627	156	9.0429	11.3469	456.3808	156	9.0429	11.3469	4075.7591
157	9.0689	11.3144	401.7605	157	9.0689	11.3144	4114.612	157	9.0689	11.3144	463.5076	157	9.0689	11.3144	4074.4946
158	9.0949	11.2822	366.3841	158	9.0949	11.2822	4072.367	158	9.0949	11.2822	491.364	158	9.0949	11.2822	4093.9596
159	9.1209	11.2501	358.8338	159	9.1209	11.2501	4057.9481	159	9.1209	11.2501	485.5881	159	9.1209	11.2501	4079.7924
160	9.1469	11.2182	320.5871	160	9.1469	11.2182	4012.8327	160	9.1469	11.2182	513.2921	160	9.1469	11.2182	4099.105
161	9.1729	11.1864	321.5782	161	9.1729	11.1864	4006.9552	161	9.1729	11.1864	557.3464	161	9.1729	11.1864	4134.768
162	9.1989	11.1549	357.4732	162	9.1989	11.1549	4035.9816	162	9.1989	11.1549	452.1655	162	9.1989	11.1549	4021.1957
163	9.2249	11.1235	334.7378	163	9.2249	11.1235	4006.3776	163	9.2249	11.1235	380.8498	163	9.2249	11.1235	3941.4887
164	9.2509	11.0923	383.4996	164	9.2509	11.0923	4048.2707	164	9.2509	11.0923	445.9085	164	9.2509	11.0923	3999.144
165	9.2769	11.0613	371.5325	165	9.2769	11.0613	4029.435	165	9.2769	11.0613	512.9956	165	9.2769	11.0613	4058.8276
166	9.3029	11.0304	357.4432	166	9.3029	11.0304	4008.477	166	9.3029	11.0304	519.7842	166	9.3029	11.0304	4058.2128
167	9.3289	10.9998	398.0724	167	9.3289	10.9998	4042.2376	167	9.3289	10.9998	489.9176	167	9.3289	10.9998	4020.9427
168	9.3549	10.9693	390.997	168	9.3549	10.9693	4028.2935	168	9.3549	10.9693	462.06	168	9.3549	10.9693	3985.6818
169	9.3809	10.9389	444.5687	169	9.3809	10.9389	4074.9967	169	9.3809	10.9389	433.1273	169	9.3809	10.9389	3949.3456
170	9.4069	10.9088	441.0222	170	9.4069	10.9088	4064.5814	170	9.4069	10.9088	456.7469	170	9.4069	10.9088	3965.5617
171	9.4329	10.8788	462.5551	171	9.4329	10.8788	4079.2457	171	9.4329	10.8788	478.1539	171	9.4329	10.8788	3979.5653
172	9.4589	10.8489	500.9541	172	9.4589	10.8489	4110.7761	172	9.4589	10.8489	396.1587	172	9.4589	10.8489	3890.1667
173	9.4849	10.8193	339.0363	173	9.4849	10.8193	3941.9896	173	9.4849	10.8193	543.855	173	9.4849	10.8193	4030.4596
174	9.5109	10.7897	378.3193	174	9.5109	10.7897	3974.404	174	9.5109	10.7897	401.7512	174	9.5109	10.7897	3880.9523
175	9.5369	10.7604	342.4445	175	9.5369	10.7604	3931.6606	175	9.5369	10.7604	409.7058	175	9.5369	10.7604	3881.5034

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
176	9.5629	10.7312	433.0374	176	9.5629	10.7312	4015.3849	176	9.5629	10.7312	407.3381	176	9.5629	10.7312	3871.7323
177	9.5889	10.7022	376.2234	177	9.5889	10.7022	3951.7022	177	9.5889	10.7022	461.0166	177	9.5889	10.7022	3918.0073
178	9.6149	10.6733	388.0151	178	9.6149	10.6733	3956.6253	178	9.6149	10.6733	399.1257	178	9.6149	10.6733	3848.713
179	9.6409	10.6446	434.4127	179	9.6409	10.6446	3996.1542	179	9.6409	10.6446	523.0948	179	9.6409	10.6446	3965.2787
180	9.6669	10.616	424.814	180	9.6669	10.616	3979.6869	180	9.6669	10.616	578.5003	180	9.6669	10.616	4013.2808
181	9.6929	10.5876	444.4195	181	9.6929	10.5876	3992.4238	181	9.6929	10.5876	518.5405	181	9.6929	10.5876	3945.9175
182	9.7189	10.5594	446.3148	182	9.7189	10.5594	3987.4504	182	9.7189	10.5594	528.7021	182	9.7189	10.5594	3948.6756
183	9.7449	10.5313	394.4401	183	9.7449	10.5313	3928.7071	183	9.7449	10.5313	458.086	183	9.7449	10.5313	3870.6561
184	9.7709	10.5033	433.3117	184	9.7709	10.5033	3960.7101	184	9.7709	10.5033	550.8851	184	9.7709	10.5033	3956.0517
185	9.7969	10.4755	424.5603	185	9.7969	10.4755	3945.0901	185	9.7969	10.4755	472.7789	185	9.7969	10.4755	3870.5421
186	9.8229	10.4478	516.3807	186	9.8229	10.4478	4030.0418	186	9.8229	10.4478	431.9552	186	9.8229	10.4478	3822.315
187	9.8489	10.4203	454.7758	187	9.8489	10.4203	3961.5682	187	9.8489	10.4203	447.4337	187	9.8489	10.4203	3830.3901
188	9.8749	10.393	517.6738	188	9.8749	10.393	4017.5977	188	9.8749	10.393	468.951	188	9.8749	10.393	3844.5039
189	9.9009	10.3657	600.8491	189	9.9009	10.3657	4093.9043	189	9.9009	10.3657	514.8505	189	9.9009	10.3657	3883
190	9.9269	10.3386	531.0929	190	9.9269	10.3386	4017.2794	190	9.9269	10.3386	516.6431	190	9.9269	10.3386	3877.3891
191	9.9529	10.3117	457.699	191	9.9529	10.3117	3936.2624	191	9.9529	10.3117	479.493	191	9.9529	10.3117	3832.8356
192	9.9789	10.2849	468.874	192	9.9789	10.2849	3939.8143	192	9.9789	10.2849	443.7059	192	9.9789	10.2849	3789.6451
193	10.0049	10.2582	428.3339	193	10.0049	10.2582	3891.6511	193	10.0049	10.2582	426.9255	193	10.0049	10.2582	3765.4612
194	10.0309	10.2317	470.9562	194	10.0309	10.2317	3926.6503	194	10.0309	10.2317	478.2277	194	10.0309	10.2317	3809.36
195	10.0569	10.2053	382.2834	195	10.0569	10.2053	3830.3544	195	10.0569	10.2053	497.4183	195	10.0569	10.2053	3821.1471
196	10.0829	10.1791	450.0674	196	10.0829	10.1791	3890.5153	196	10.0829	10.1791	467.5897	196	10.0829	10.1791	3783.9151
197	10.1089	10.153	545.6522	197	10.1089	10.153	3978.4769	197	10.1089	10.153	444.7467	197	10.1089	10.153	3753.6686
198	10.1349	10.127	458.889	198	10.1349	10.127	3884.0906	198	10.1349	10.127	450.1062	198	10.1349	10.127	3751.6247
199	10.1609	10.1012	469.8723	199	10.1609	10.1012	3887.4508	199	10.1609	10.1012	531.0187	199	10.1609	10.1012	3825.1337
200	10.1869	10.0754	514.0908	200	10.1869	10.0754	3924.0462	200	10.1869	10.0754	459.2189	200	10.1869	10.0754	3745.9305
201	10.2129	10.0499	408.5434	201	10.2129	10.0499	3810.8757	201	10.2129	10.0499	427.1683	201	10.2129	10.0499	3706.4764
202	10.2389	10.0244	408.8078	202	10.2389	10.0244	3803.517	202	10.2389	10.0244	527.6795	202	10.2389	10.0244	3799.5842
203	10.2649	9.9991	507.5181	203	10.2649	9.9991	3894.6041	203	10.2649	9.9991	461.8171	203	10.2649	9.9991	3726.3184
204	10.2909	9.9739	500.7504	204	10.2909	9.9739	3880.2134	204	10.2909	9.9739	448.2009	204	10.2909	9.9739	3705.2987
205	10.3169	9.9488	457.4159	205	10.3169	9.9488	3829.2557	205	10.3169	9.9488	462.1366	205	10.3169	9.9488	3711.831
206	10.3429	9.9239	314.0641	206	10.3429	9.9239	3678.2808	206	10.3429	9.9239	462.9475	206	10.3429	9.9239	3705.2385
207	10.3689	9.8991	383.327	207	10.3689	9.8991	3739.9205	207	10.3689	9.8991	470.1125	207	10.3689	9.8991	3705
208	10.3949	9.8744	354.2939	208	10.3949	9.8744	3703.2644	208	10.3949	9.8744	472.7855	208	10.3949	9.8744	3700.2696
209	10.4209	9.8498	427.0564	209	10.4209	9.8498	3768.4037	209	10.4209	9.8498	515.4936	209	10.4209	9.8498	3735.5742
210	10.4469	9.8254	379.9963	210	10.4469	9.8254	3713.7206	210	10.4469	9.8254	554.0363	210	10.4469	9.8254	3766.7135
211	10.4729	9.801	424.1332	211	10.4729	9.801	3750.2343	211	10.4729	9.801	517.9103	211	10.4729	9.801	3723.1841

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
212	10.4989	9.7768	322.2225	212	10.4989	9.7768	3640.7005	212	10.4989	9.7768	452.2436	212	10.4989	9.7768	3650.1139
213	10.5249	9.7527	262.5637	213	10.5249	9.7527	3573.4186	213	10.5249	9.7527	369.161	213	10.5249	9.7527	3559.6279
214	10.5509	9.7288	289.4782	214	10.5509	9.7288	3592.71	214	10.5509	9.7288	420.1297	214	10.5509	9.7288	3603.1931
215	10.5769	9.7049	307.4044	215	10.5769	9.7049	3603.013	215	10.5769	9.7049	464.1454	215	10.5769	9.7049	3639.8054
216	10.6029	9.6812	246.6779	216	10.6029	9.6812	3534.6634	216	10.6029	9.6812	431.5414	216	10.6029	9.6812	3599.7979
217	10.6289	9.6576	273.625	217	10.6289	9.6576	3553.9875	217	10.6289	9.6576	510.1143	217	10.6289	9.6576	3670.9674
218	10.6549	9.6341	231.0619	218	10.6549	9.6341	3503.1071	218	10.6549	9.6341	434.7081	218	10.6549	9.6341	3585.7639
219	10.6809	9.6107	187.4251	219	10.6809	9.6107	3451.153	219	10.6809	9.6107	356.4384	219	10.6809	9.6107	3497.697
220	10.7069	9.5874	254.5778	220	10.7069	9.5874	3509.9885	220	10.7069	9.5874	267.3557	220	10.7069	9.5874	3398.8172
221	10.7329	9.5643	239.3202	221	10.7329	9.5643	3486.4136	221	10.7329	9.5643	387.6198	221	10.7329	9.5643	3509.284
222	10.7589	9.5412	332.8559	222	10.7589	9.5412	3571.6321	222	10.7589	9.5412	462.4558	222	10.7589	9.5412	3574.3228
223	10.7849	9.5183	302.1528	223	10.7849	9.5183	3532.6117	223	10.7849	9.5183	429.9062	223	10.7849	9.5183	3531.9759
224	10.8109	9.4955	255.4919	224	10.8109	9.4955	3477.6336	224	10.8109	9.4955	359.8045	224	10.8109	9.4955	3452.0771
225	10.8369	9.4728	333.2485	225	10.8369	9.4728	3547.0729	225	10.8369	9.4728	488.3482	225	10.8369	9.4728	3570.8235
226	10.8629	9.4502	237.858	226	10.8629	9.4502	3443.3651	226	10.8629	9.4502	403.7797	226	10.8629	9.4502	3476.4578
227	10.8889	9.4277	265.3848	227	10.8889	9.4277	3462.5747	227	10.8889	9.4277	398.1187	227	10.8889	9.4277	3460.9995
228	10.9149	9.4053	343.7145	228	10.9149	9.4053	3532.5871	228	10.9149	9.4053	448.8125	228	10.9149	9.4053	3501.8961
229	10.9409	9.383	272.8037	229	10.9409	9.383	3453.359	229	10.9409	9.383	447.5821	229	10.9409	9.383	3490.8685
230	10.9669	9.3608	345.0142	230	10.9669	9.3608	3517.2523	230	10.9669	9.3608	396.3818	230	10.9669	9.3608	3429.871
231	10.9929	9.3387	315.4204	231	10.9929	9.3387	3479.3412	231	10.9929	9.3387	365.4898	231	10.9929	9.3387	3389.1817
232	11.0189	9.3168	382.1822	232	11.0189	9.3168	3537.7859	232	11.0189	9.3168	402.5028	232	11.0189	9.3168	3416.3975
233	11.0449	9.2949	338.7621	233	11.0449	9.2949	3486.0485	233	11.0449	9.2949	462.502	233	11.0449	9.2949	3466.5994
234	11.0709	9.2731	289.0758	234	11.0709	9.2731	3428.0449	234	11.0709	9.2731	524.8575	234	11.0709	9.2731	3519.1577
235	11.0969	9.2515	283.6009	235	11.0969	9.2515	3414.2527	235	11.0969	9.2515	449.7695	235	11.0969	9.2515	3434.2725
236	11.1229	9.2299	260.2619	236	11.1229	9.2299	3382.5965	236	11.1229	9.2299	428.0007	236	11.1229	9.2299	3402.7065
237	11.1489	9.2085	214.4823	237	11.1489	9.2085	3328.4997	237	11.1489	9.2085	499.4169	237	11.1489	9.2085	3464.3255
238	11.1749	9.1871	263.8995	238	11.1749	9.1871	3369.5996	238	11.1749	9.1871	458.4303	238	11.1749	9.1871	3413.5416
239	11.2009	9.1659	261.5611	239	11.2009	9.1659	3358.9439	239	11.2009	9.1659	404.6156	239	11.2009	9.1659	3349.9297
240	11.2269	9.1447	213.5058	240	11.2269	9.1447	3302.5714	240	11.2269	9.1447	428.2546	240	11.2269	9.1447	3363.7715
241	11.2529	9.1236	192.116	241	11.2529	9.1236	3272.8643	241	11.2529	9.1236	410.5935	241	11.2529	9.1236	3336.3132
242	11.2789	9.1027	256.8766	242	11.2789	9.1027	3329.3077	242	11.2789	9.1027	409.9045	242	11.2789	9.1027	3325.8269
243	11.3049	9.0818	244.2093	243	11.3049	9.0818	3308.3231	243	11.3049	9.0818	393.9465	243	11.3049	9.0818	3300.0717
244	11.3309	9.061	273.625	244	11.3309	9.061	3329.4216	244	11.3309	9.061	380.8498	244	11.3309	9.061	3277.1778
245	11.3569	9.0404	272.5244	245	11.3569	9.0404	3319.1567	245	11.3569	9.0404	433.7639	245	11.3569	9.0404	3324.8958
246	11.3829	9.0198	259.6031	246	11.3829	9.0198	3297.0711	246	11.3829	9.0198	451.4406	246	11.3829	9.0198	3337.3765
247	11.4089	8.9993	225.2255	247	11.4089	8.9993	3253.5293	247	11.4089	8.9993	463.1839	247	11.4089	8.9993	3343.9238

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
248	11.4349	8.9789	234.8943	248	11.4349	8.9789	3254.0339	248	11.4349	8.9789	488.6529	248	11.4349	8.9789	3364.1968
249	11.4609	8.9586	248.6684	249	11.4609	8.9586	3258.6437	249	11.4609	8.9586	488.6416	249	11.4609	8.9586	3358.9895
250	11.4869	8.9384	231.2476	250	11.4869	8.9384	3232.0587	250	11.4869	8.9384	439.1481	250	11.4869	8.9384	3304.2999
251	11.5129	8.9183	207.5904	251	11.5129	8.9183	3199.2373	251	11.5129	8.9183	391.6945	251	11.5129	8.9183	3251.6503
252	11.5389	8.8982	178.8939	252	11.5389	8.8982	3161.3764	252	11.5389	8.8982	440.2097	252	11.5389	8.8982	3294.9695
253	11.5649	8.8783	235.137	253	11.5649	8.8783	3208.4553	253	11.5649	8.8783	452.9718	253	11.5649	8.8783	3302.5355
254	11.5909	8.8585	257.2041	254	11.5909	8.8585	3221.3582	254	11.5909	8.8585	461.6603	254	11.5909	8.8585	3306.028
255	11.6169	8.8387	209.1383	255	11.6169	8.8387	3164.1281	255	11.6169	8.8387	502.3551	255	11.6169	8.8387	3341.5268
256	11.6429	8.819	182.912	256	11.6429	8.819	3128.7376	256	11.6429	8.819	482.7488	256	11.6429	8.819	3316.7244
257	11.6689	8.7994	222.7665	257	11.6689	8.7994	3159.4278	257	11.6689	8.7994	460.9637	257	11.6689	8.7994	3289.7433
258	11.6949	8.7799	313.3016	258	11.6949	8.7799	3240.7987	258	11.6949	8.7799	424.218	258	11.6949	8.7799	3247.8016
259	11.7209	8.7605	286.3805	259	11.7209	8.7605	3204.7134	259	11.7209	8.7605	418.8547	259	11.7209	8.7605	3237.2422
260	11.7469	8.7412	183.1309	260	11.7469	8.7412	3092.2995	260	11.7469	8.7412	454.1097	260	11.7469	8.7412	3267.3013
261	11.7729	8.722	168.9473	261	11.7729	8.722	3068.9516	261	11.7729	8.722	462.9035	261	11.7729	8.722	3270.899
262	11.7989	8.7028	228.802	262	11.7989	8.7028	3119.6421	262	11.7989	8.7028	466.8416	262	11.7989	8.7028	3269.6411
263	11.8249	8.6838	274.1338	263	11.8249	8.6838	3155.8097	263	11.8249	8.6838	461.1847	263	11.8249	8.6838	3258.7881
264	11.8509	8.6648	253.4168	264	11.8509	8.6648	3125.9284	264	11.8509	8.6648	470.7997	264	11.8509	8.6648	3263.2071
265	11.8769	8.6459	194.0773	265	11.8769	8.6459	3057.4246	265	11.8769	8.6459	471.5514	265	11.8769	8.6459	3258.7629
266	11.9029	8.6271	181.7636	266	11.9029	8.6271	3035.9467	266	11.9029	8.6271	417.62	266	11.9029	8.6271	3199.6354
267	11.9289	8.6083	128.0296	267	11.9289	8.6083	2973.0485	267	11.9289	8.6083	399.8676	267	11.9289	8.6083	3176.687
268	11.9549	8.5897	174.489	268	11.9549	8.5897	3010.3436	268	11.9549	8.5897	352.5633	268	11.9549	8.5897	3124.1866
269	11.9809	8.5711	297.0624	269	11.9809	8.5711	3123.7528	269	11.9809	8.5711	402.8649	269	11.9809	8.5711	3169.2922
270	12.0069	8.5526	266.2742	270	12.0069	8.5526	3083.8003	270	12.0069	8.5526	452.6302	270	12.0069	8.5526	3213.8615
271	12.0329	8.5342	273.625	271	12.0329	8.5342	3081.9869	271	12.0329	8.5342	469.9653	271	12.0329	8.5342	3226.0005
272	12.0589	8.5159	342.6276	272	12.0589	8.5159	3143.2466	272	12.0589	8.5159	421.405	272	12.0589	8.5159	3172.2442
273	12.0849	8.4976	320.0159	273	12.0849	8.4976	3112.892	273	12.0849	8.4976	416.1068	273	12.0849	8.4976	3161.75
274	12.1109	8.4794	291.1244	274	12.1109	8.4794	3076.2577	274	12.1109	8.4794	414.1412	274	12.1109	8.4794	3154.5883
275	12.1369	8.4613	268.0228	275	12.1369	8.4613	3045.4132	275	12.1369	8.4613	445.2442	275	12.1369	8.4613	3180.4953
276	12.1629	8.4433	345.2346	276	12.1629	8.4433	3114.8821	276	12.1629	8.4433	395.9963	276	12.1629	8.4433	3126.0515
277	12.1889	8.4254	218.4809	277	12.1889	8.4254	2980.3855	277	12.1889	8.4254	436.8913	277	12.1889	8.4254	3161.7504
278	12.2149	8.4075	225.1264	278	12.2149	8.4075	2979.2881	278	12.2149	8.4075	381.0535	278	12.2149	8.4075	3100.7165
279	12.2409	8.3897	216.5487	279	12.2409	8.3897	2962.9676	279	12.2409	8.3897	465.4734	279	12.2409	8.3897	3179.9405
280	12.2669	8.372	135.1752	280	12.2669	8.372	2873.8512	280	12.2669	8.372	385.9606	280	12.2669	8.372	3095.2317
281	12.2929	8.3544	237.3473	281	12.2929	8.3544	2968.2804	281	12.2929	8.3544	372.1885	281	12.2929	8.3544	3076.2635
282	12.3189	8.3368	327.4547	282	12.3189	8.3368	3050.6449	282	12.3189	8.3368	321.4667	282	12.3189	8.3368	3020.3457
283	12.3449	8.3193	300.8512	283	12.3449	8.3193	3016.2986	283	12.3449	8.3193	374.096	283	12.3449	8.3193	3067.779

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
284	12.3709	8.3019	264.9516	284	12.3709	8.3019	2972.6561	284	12.3709	8.3019	361.1055	284	12.3709	8.3019	3049.5924
285	12.3969	8.2845	270.4977	285	12.3969	8.2845	2970.4593	285	12.3969	8.2845	345.2801	285	12.3969	8.2845	3028.571
286	12.4229	8.2673	273.6401	286	12.4229	8.2673	2965.8588	286	12.4229	8.2673	417.8955	286	12.4229	8.2673	3095.9904
287	12.4489	8.2501	189.2286	287	12.4489	8.2501	2873.7045	287	12.4489	8.2501	341.2344	287	12.4489	8.2501	3014.1333
288	12.4749	8.2329	231.319	288	12.4749	8.2329	2908.0519	288	12.4749	8.2329	323.5817	288	12.4749	8.2329	2991.2845
289	12.5009	8.2159	283.1924	289	12.5009	8.2159	2952.1825	289	12.5009	8.2159	348.185	289	12.5009	8.2159	3010.6918
290	12.5269	8.1989	229.0248	290	12.5269	8.1989	2890.272	290	12.5269	8.1989	395.6761	290	12.5269	8.1989	3052.9869
291	12.5529	8.182	280.4633	291	12.5529	8.182	2933.9676	291	12.5529	8.182	396.2402	291	12.5529	8.182	3048.3549
292	12.5789	8.1652	171.4187	292	12.5789	8.1652	2817.1802	292	12.5789	8.1652	297.4912	292	12.5789	8.1652	2944.41
293	12.6049	8.1484	215.1549	293	12.6049	8.1484	2853.1735	293	12.6049	8.1484	461.7172	293	12.6049	8.1484	3103.4399
294	12.6309	8.1317	183.7856	294	12.6309	8.1317	2814.0614	294	12.6309	8.1317	322.7502	294	12.6309	8.1317	2959.2768
295	12.6569	8.115	227.4321	295	12.6569	8.115	2849.9649	295	12.6569	8.115	407.568	295	12.6569	8.115	3038.8986
296	12.6829	8.0985	290.3444	296	12.6829	8.0985	2905.1344	296	12.6829	8.0985	296.7931	296	12.6829	8.0985	2922.9278
297	12.7089	8.082	168.2691	297	12.7089	8.082	2775.3162	297	12.7089	8.082	389.0534	297	12.7089	8.082	3009.992
298	12.7349	8.0655	292.1586	298	12.7349	8.0655	2891.4628	298	12.7349	8.0655	380.8498	298	12.7349	8.0655	2996.5924
299	12.7609	8.0492	164.5324	299	12.7609	8.0492	2756.0937	299	12.7609	8.0492	415.3806	299	12.7609	8.0492	3024.8705
300	12.7869	8.0329	155.7709	300	12.7869	8.0329	2739.5893	300	12.7869	8.0329	412.98	300	12.7869	8.0329	3016.2172
301	12.8129	8.0166	264.2178	301	12.8129	8.0166	2840.2934	301	12.8129	8.0166	254.6755	301	12.8129	8.0166	2851.66
302	12.8389	8.0005	117.2698	302	12.8389	8.0005	2685.6025	302	12.8389	8.0005	414.3217	302	12.8389	8.0005	3005.0536
303	12.8649	7.9844	169.4899	303	12.8649	7.9844	2730.0798	303	12.8649	7.9844	424.3093	303	12.8649	7.9844	3008.7885
304	12.8909	7.9683	200.0046	304	12.8909	7.9683	2752.8515	304	12.8909	7.9683	370.1672	304	12.8909	7.9683	2948.3937
305	12.9169	7.9524	163.6329	305	12.9169	7.9524	2708.737	305	12.9169	7.9524	417.3383	305	12.9169	7.9524	2989.3122
306	12.9429	7.9365	157.007	306	12.9429	7.9365	2694.3682	306	12.9429	7.9365	393.1204	306	12.9429	7.9365	2958.8416
307	12.9689	7.9206	183.6573	307	12.9689	7.9206	2713.2756	307	12.9689	7.9206	371.5457	307	12.9689	7.9206	2931.0142
308	12.9949	7.9048	136.8009	308	12.9949	7.9048	2658.6763	308	12.9949	7.9048	259.4599	308	12.9949	7.9048	2812.6757
309	13.0209	7.8891	216.4382	309	13.0209	7.8891	2730.5708	309	13.0209	7.8891	393.1315	309	13.0209	7.8891	2940.0947
310	13.0469	7.8735	301.4632	310	13.0469	7.8735	2807.8529	310	13.0469	7.8735	405.4215	310	13.0469	7.8735	2946.132
311	13.0729	7.8579	149.8653	311	13.0729	7.8579	2648.5121	311	13.0729	7.8579	373.6545	311	13.0729	7.8579	2908.1123
312	13.0989	7.8423	227.2853	312	13.0989	7.8423	2718.1892	312	13.0989	7.8423	285.3782	312	13.0989	7.8423	2813.5833
313	13.1249	7.8269	243.7432	313	13.1249	7.8269	2726.9042	313	13.1249	7.8269	398.7909	313	13.1249	7.8269	2920.7433
314	13.1509	7.8115	290.932	314	13.1509	7.8115	2766.3502	314	13.1509	7.8115	331.4453	314	13.1509	7.8115	2847.145
315	13.1769	7.7961	126.4447	315	13.1769	7.7961	2594.12	315	13.1769	7.7961	383.2701	315	13.1769	7.7961	2892.7172
316	13.2029	7.7808	131.1806	316	13.2029	7.7808	2591.113	316	13.2029	7.7808	444.9019	316	13.2029	7.7808	2948.0963
317	13.2289	7.7656	188.4965	317	13.2289	7.7656	2640.686	317	13.2289	7.7656	334.4268	317	13.2289	7.7656	2831.3686
318	13.2549	7.7504	167.6587	318	13.2549	7.7504	2612.1054	318	13.2549	7.7504	338.4036	318	13.2549	7.7504	2829.0927
319	13.2809	7.7353	248.699	319	13.2809	7.7353	2685.4028	319	13.2809	7.7353	347.5636	319	13.2809	7.7353	2832

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
320	13.3069	7.7203	149.1599	320	13.3069	7.7203	2578.1209	320	13.3069	7.7203	428.1125	320	13.3069	7.7203	2906.2962
321	13.3329	7.7053	212.794	321	13.3329	7.7053	2634.012	321	13.3329	7.7053	342.6612	321	13.3329	7.7053	2814.5922
322	13.3589	7.6904	200.8524	322	13.3589	7.6904	2614.3275	322	13.3589	7.6904	308.3929	322	13.3589	7.6904	2774.0712
323	13.3849	7.6755	252.5941	323	13.3849	7.6755	2658.3264	323	13.3849	7.6755	406.3719	323	13.3849	7.6755	2865.7976
324	13.4109	7.6607	258.6988	324	13.4109	7.6607	2656.6882	324	13.4109	7.6607	369.0386	324	13.4109	7.6607	2822.2116
325	13.4369	7.6459	319.2862	325	13.4369	7.6459	2709.5328	325	13.4369	7.6459	380.8498	325	13.4369	7.6459	2827.7701
326	13.4629	7.6312	193.5586	326	13.4629	7.6312	2575.3758	326	13.4629	7.6312	289.8407	326	13.4629	7.6312	2730.1158
327	13.4889	7.6166	249.6867	327	13.4889	7.6166	2623.0746	327	13.4889	7.6166	330.658	327	13.4889	7.6166	2764.2879
328	13.5149	7.602	255.0696	328	13.5149	7.602	2620.0282	328	13.5149	7.602	397.8075	328	13.5149	7.602	2824.7922
329	13.5409	7.5875	280.3083	329	13.5409	7.5875	2636.8376	329	13.5409	7.5875	358.767	329	13.5409	7.5875	2779.1064
330	13.5669	7.573	228.0213	330	13.5669	7.573	2576.1213	330	13.5669	7.573	366.6371	330	13.5669	7.573	2780.3314
331	13.5929	7.5586	173.5958	331	13.5929	7.5586	2513.2665	331	13.5929	7.5586	364.9868	331	13.5929	7.5586	2772.0358
332	13.6189	7.5442	208.5547	332	13.6189	7.5442	2539.7961	332	13.6189	7.5442	412.118	332	13.6189	7.5442	2812.5219
333	13.6449	7.5299	269.1837	333	13.6449	7.5299	2591.9957	333	13.6449	7.5299	370.1905	333	13.6449	7.5299	2763.9491
334	13.6709	7.5157	279.3956	334	13.6709	7.5157	2593.7783	334	13.6709	7.5157	397.5979	334	13.6709	7.5157	2784.7114
335	13.6969	7.5015	203.8477	335	13.6969	7.5015	2509.8012	335	13.6969	7.5015	383.0026	335	13.6969	7.5015	2763.4708
336	13.7229	7.4873	280.5848	336	13.7229	7.4873	2578.1089	336	13.7229	7.4873	377.6133	336	13.7229	7.4873	2751.4364
337	13.7489	7.4732	280.2875	337	13.7489	7.4732	2569.3823	337	13.7489	7.4732	345.8573	337	13.7489	7.4732	2713.0351
338	13.7749	7.4592	273.1144	338	13.7749	7.4592	2553.7799	338	13.7749	7.4592	360.3397	338	13.7749	7.4592	2720.8722
339	13.8009	7.4452	237.0625	339	13.8009	7.4452	2509.2988	339	13.8009	7.4452	341.3979	339	13.8009	7.4452	2695.2853
340	13.8269	7.4313	222.9201	340	13.8269	7.4313	2486.7271	340	13.8269	7.4313	333.3939	340	13.8269	7.4313	2680.6361
341	13.8529	7.4174	235.8752	341	13.8529	7.4174	2491.2528	341	13.8529	7.4174	343.1502	341	13.8529	7.4174	2683.7472
342	13.8789	7.4036	215.4597	342	13.8789	7.4036	2462.4081	342	13.8789	7.4036	435.358	342	13.8789	7.4036	2769.3098
343	13.9049	7.3898	233.99	343	13.9049	7.3898	2472.5091	343	13.9049	7.3898	411.3794	343	13.9049	7.3898	2738.6859
344	13.9309	7.3761	195.2784	344	13.9309	7.3761	2425.3681	344	13.9309	7.3761	381.8349	344	13.9309	7.3761	2702.4963
345	13.9569	7.3624	223.2933	345	13.9569	7.3624	2444.9537	345	13.9569	7.3624	376.3412	345	13.9569	7.3624	2690.3573
346	13.9829	7.3488	279.6529	346	13.9829	7.3488	2492.884	346	13.9829	7.3488	399.084	346	13.9829	7.3488	2706.4549
347	14.0089	7.3352	290.7651	347	14.0089	7.3352	2495.5669	347	14.0089	7.3352	363.3817	347	14.0089	7.3352	2664.1074
348	14.0349	7.3217	341.3998	348	14.0349	7.3217	2537.7723	348	14.0349	7.3217	394.1097	348	14.0349	7.3217	2688.1902
349	14.0609	7.3082	326.7114	349	14.0609	7.3082	2514.6547	349	14.0609	7.3082	399.296	349	14.0609	7.3082	2686.7313
350	14.0869	7.2948	312.6565	350	14.0869	7.2948	2492.1704	350	14.0869	7.2948	346.616	350	14.0869	7.2948	2627.4061
351	14.1129	7.2814	265.4717	351	14.1129	7.2814	2436.5563	351	14.1129	7.2814	323.7129	351	14.1129	7.2814	2597.8577
352	14.1389	7.2681	273.625	352	14.1389	7.2681	2436.2803	352	14.1389	7.2681	380.8498	352	14.1389	7.2681	2648.3494
353	14.1649	7.2548	296.8902	353	14.1649	7.2548	2454.3382	353	14.1649	7.2548	483.4709	353	14.1649	7.2548	2744.4412
354	14.1909	7.2416	223.4366	354	14.1909	7.2416	2375.6773	354	14.1909	7.2416	436.4881	354	14.1909	7.2416	2690.9291
355	14.2169	7.2284	229.5547	355	14.2169	7.2284	2376.5881	355	14.2169	7.2284	374.2011	355	14.2169	7.2284	2622.1128

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
356	14.2429	7.2153	223.9377	356	14.2429	7.2153	2365.7638	356	14.2429	7.2153	338.3522	356	14.2429	7.2153	2579.7345
357	14.2689	7.2022	225.0183	357	14.2689	7.2022	2361.637	357	14.2689	7.2022	325.1074	357	14.2689	7.2022	2559.9604
358	14.2949	7.1892	275.5182	358	14.2949	7.1892	2406.9297	358	14.2949	7.1892	390.3734	358	14.2949	7.1892	2618.6971
359	14.3209	7.1762	314.4734	359	14.3209	7.1762	2440.6776	359	14.3209	7.1762	447.5094	359	14.3209	7.1762	2669.3037
360	14.3469	7.1633	318.6387	360	14.3469	7.1633	2439.6355	360	14.3469	7.1633	481.4022	360	14.3469	7.1633	2696.6673
361	14.3729	7.1504	277.6009	361	14.3729	7.1504	2393.3904	361	14.3729	7.1504	441.2894	361	14.3729	7.1504	2650.0251
362	14.3989	7.1375	298.5152	362	14.3989	7.1375	2409.0974	362	14.3989	7.1375	420.0311	362	14.3989	7.1375	2622.2375
363	14.4249	7.1247	275.0332	363	14.4249	7.1247	2380.4081	363	14.4249	7.1247	392.7538	363	14.4249	7.1247	2588.4309
364	14.4509	7.112	294.3715	364	14.4509	7.112	2394.5391	364	14.4509	7.112	400.4605	364	14.4509	7.112	2589.6082
365	14.4769	7.0993	325.0874	365	14.4769	7.0993	2420.0477	365	14.4769	7.0993	457.4033	365	14.4769	7.0993	2640.0217
366	14.5029	7.0866	339.3821	366	14.5029	7.0866	2429.1351	366	14.5029	7.0866	418.074	366	14.5029	7.0866	2594.1631
367	14.5289	7.074	334.6642	367	14.5289	7.074	2419.2099	367	14.5289	7.074	386.1771	367	14.5289	7.074	2555.7369
368	14.5549	7.0614	347.2676	368	14.5549	7.0614	2426.6059	368	14.5549	7.0614	411.8955	368	14.5549	7.0614	2574.9259
369	14.5809	7.0489	362.4776	369	14.5809	7.0489	2436.6086	369	14.5809	7.0489	441.0868	369	14.5809	7.0489	2597.5879
370	14.6069	7.0364	299.4951	370	14.6069	7.0364	2368.4188	370	14.6069	7.0364	406.321	370	14.6069	7.0364	2556.2928
371	14.6329	7.024	315.2836	371	14.6329	7.024	2379	371	14.6329	7.024	389.8989	371	14.6329	7.024	2533.3414
372	14.6589	7.0116	342.4901	372	14.6589	7.0116	2400.9992	372	14.6589	7.0116	422.4065	372	14.6589	7.0116	2559.3196
373	14.6849	6.9993	362.263	373	14.6849	6.9993	2415.5647	373	14.6849	6.9993	402.6952	373	14.6849	6.9993	2533.079
374	14.7109	6.987	294.3076	374	14.7109	6.987	2342.402	374	14.7109	6.987	461.0222	374	14.7109	6.987	2584.8767
375	14.7369	6.9747	272.6753	375	14.7369	6.9747	2315.5625	375	14.7369	6.9747	469.2217	375	14.7369	6.9747	2586.5469
376	14.7629	6.9625	216.995	376	14.7629	6.9625	2254.6748	376	14.7629	6.9625	453.0446	376	14.7629	6.9625	2563.8405
377	14.7889	6.9503	236.2193	377	14.7889	6.9503	2268.6918	377	14.7889	6.9503	465.2733	377	14.7889	6.9503	2569.5398
378	14.8149	6.9382	260.9931	378	14.8149	6.9382	2288.2583	378	14.8149	6.9382	397.2628	378	14.8149	6.9382	2495
379	14.8409	6.9261	273.625	379	14.8409	6.9261	2295.683	379	14.8409	6.9261	380.8498	379	14.8409	6.9261	2472.0576
380	14.8669	6.9141	331.1095	380	14.8669	6.9141	2348.4631	380	14.8669	6.9141	321.5839	380	14.8669	6.9141	2409.4652
381	14.8929	6.9021	247.8917	381	14.8929	6.9021	2260.5409	381	14.8929	6.9021	352.7903	381	14.8929	6.9021	2437.3449
382	14.9189	6.8901	266.8667	382	14.9189	6.8901	2274.8117	382	14.9189	6.8901	372.2073	382	14.9189	6.8901	2453.4353
383	14.9449	6.8782	320.4205	383	14.9449	6.8782	2323.6611	383	14.9449	6.8782	361.4539	383	14.9449	6.8782	2439.3554
384	14.9709	6.8663	298.063	384	14.9709	6.8663	2296.5993	384	14.9709	6.8663	409.6451	384	14.9709	6.8663	2484.22
385	14.9969	6.8545	278.2108	385	14.9969	6.8545	2272.0428	385	14.9969	6.8545	355.6233	385	14.9969	6.8545	2426.8717
386	15.0229	6.8427	168.2322	386	15.0229	6.8427	2157.3598	386	15.0229	6.8427	407.0155	386	15.0229	6.8427	2474.9373
387	15.0489	6.8309	185.7964	387	15.0489	6.8309	2170.2197	387	15.0489	6.8309	438.0848	387	15.0489	6.8309	2502.68
388	15.0749	6.8192	255.0455	388	15.0749	6.8192	2234.7644	388	15.0749	6.8192	450.4941	388	15.0749	6.8192	2511.7626
389	15.1009	6.8075	307.3818	389	15.1009	6.8075	2282.3964	389	15.1009	6.8075	473.2472	389	15.1009	6.8075	2531.1892
390	15.1269	6.7959	284.3979	390	15.1269	6.7959	2254.7081	390	15.1269	6.7959	412.0191	390	15.1269	6.7959	2466.6345
391	15.1529	6.7843	249.3457	391	15.1529	6.7843	2214.9516	391	15.1529	6.7843	404.2235	391	15.1529	6.7843	2455.5123

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
392	15.1789	6.7727	292.2749	392	15.1789	6.7727	2253.1765	392	15.1789	6.7727	460.2033	392	15.1789	6.7727	2508.1655
393	15.2049	6.7612	327.1809	393	15.2049	6.7612	2283.3782	393	15.2049	6.7612	396.1837	393	15.2049	6.7612	2440.8194
394	15.2309	6.7498	260.8553	394	15.2309	6.7498	2212.3483	394	15.2309	6.7498	491.6748	394	15.2309	6.7498	2532.9838
395	15.2569	6.7383	182.4736	395	15.2569	6.7383	2129.2622	395	15.2569	6.7383	462.6712	395	15.2569	6.7383	2500.6536
396	15.2829	6.7269	213.4602	396	15.2829	6.7269	2155.5444	396	15.2829	6.7269	402.6608	396	15.2829	6.7269	2437.3167
397	15.3089	6.7156	145.7524	397	15.3089	6.7156	2083.1324	397	15.3089	6.7156	298.7847	397	15.3089	6.7156	2330.114
398	15.3349	6.7043	172.5655	398	15.3349	6.7043	2105.2411	398	15.3349	6.7043	345.4313	398	15.3349	6.7043	2373.434
399	15.3609	6.693	286.5842	399	15.3609	6.693	2214.5555	399	15.3609	6.693	388.9212	399	15.3609	6.693	2413.5973
400	15.3869	6.6817	246.5122	400	15.3869	6.6817	2169.7791	400	15.3869	6.6817	438.8463	400	15.3869	6.6817	2460.1958
401	15.4129	6.6705	266.9819	401	15.4129	6.6705	2185.5444	401	15.4129	6.6705	399.5108	401	15.4129	6.6705	2417.5338
402	15.4389	6.6594	194.6551	402	15.4389	6.6594	2108.5133	402	15.4389	6.6594	390.2293	402	15.4389	6.6594	2404.9256
403	15.4649	6.6482	175.8122	403	15.4649	6.6482	2084.9661	403	15.4649	6.6482	481.158	403	15.4649	6.6482	2492.5278
404	15.4909	6.6371	89.6873	404	15.4909	6.6371	1994.1369	404	15.4909	6.6371	354.8594	404	15.4909	6.6371	2362.9026
405	15.5169	6.6261	197.3597	405	15.5169	6.6261	2097.105	405	15.5169	6.6261	284.9203	405	15.5169	6.6261	2289.6369
406	15.5429	6.6151	273.625	406	15.5429	6.6151	2168.6659	406	15.5429	6.6151	380.8498	406	15.5429	6.6151	2382.2398
407	15.5689	6.6041	252.4204	407	15.5689	6.6041	2142.7966	407	15.5689	6.6041	427.9341	407	15.5689	6.6041	2425.7766
408	15.5949	6.5932	324.564	408	15.5949	6.5932	2210.2755	408	15.5949	6.5932	400.9713	408	15.5949	6.5932	2395.2663
409	15.6209	6.5823	260.5754	409	15.6209	6.5823	2141.6222	409	15.6209	6.5823	402.3008	409	15.6209	6.5823	2393.0483
410	15.6469	6.5714	254.0837	410	15.6469	6.5714	2130.4657	410	15.6469	6.5714	378.4883	410	15.6469	6.5714	2365.6883
411	15.6729	6.5605	165.0967	411	15.6729	6.5605	2036.814	411	15.6729	6.5605	464.2149	411	15.6729	6.5605	2447.8674
412	15.6989	6.5497	288.3309	412	15.6989	6.5497	2155.3835	412	15.6989	6.5497	307.0243	412	15.6989	6.5497	2287.1293
413	15.7249	6.539	256.1873	413	15.7249	6.539	2118.5752	413	15.7249	6.539	374.8759	413	15.7249	6.539	2351.4333
414	15.7509	6.5283	282.4375	414	15.7509	6.5283	2140.1607	414	15.7509	6.5283	389.5984	414	15.7509	6.5283	2362.6084
415	15.7769	6.5176	265.8529	415	15.7769	6.5176	2118.9114	415	15.7769	6.5176	423.8713	415	15.7769	6.5176	2393.3338
416	15.8029	6.5069	239.3743	416	15.8029	6.5069	2087.768	416	15.8029	6.5069	437.2608	416	15.8029	6.5069	2403.1757
417	15.8289	6.4963	230.6754	417	15.8289	6.4963	2074.4044	417	15.8289	6.4963	445.9942	417	15.8289	6.4963	2408.3616
418	15.8549	6.4857	155.4569	418	15.8549	6.4857	1994.5212	418	15.8549	6.4857	390.6742	418	15.8549	6.4857	2349.4941
419	15.8809	6.4752	267.8003	419	15.8809	6.4752	2102.1999	419	15.8809	6.4752	429.9091	419	15.8809	6.4752	2385.1815
420	15.9069	6.4646	285.6821	420	15.9069	6.4646	2115.417	420	15.9069	6.4646	436.2197	420	15.9069	6.4646	2387.9446
421	15.9329	6.4542	234.8084	421	15.9329	6.4542	2059.8786	421	15.9329	6.4542	373.8769	421	15.9329	6.4542	2322.0543
422	15.9589	6.4437	203.0904	422	15.9589	6.4437	2023.4958	422	15.9589	6.4437	341.334	422	15.9589	6.4437	2285.964
423	15.9849	6.4333	225.0175	423	15.9849	6.4333	2040.7582	423	15.9849	6.4333	328.5385	423	15.9849	6.4333	2269.6209
424	16.0109	6.4229	246.967	424	16.0109	6.4229	2058.0431	424	16.0109	6.4229	360.777	424	16.0109	6.4229	2298.3119
425	16.0369	6.4126	235.558	425	16.0369	6.4126	2041.9692	425	16.0369	6.4126	438.6202	425	16.0369	6.4126	2372.6076
426	16.0629	6.4023	218.0269	426	16.0629	6.4023	2019.7734	426	16.0629	6.4023	361.6819	426	16.0629	6.4023	2292.1218
427	16.0889	6.392	282.0857	427	16.0889	6.392	2079.1676	427	16.0889	6.392	317.2338	427	16.0889	6.392	2244.1262

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
428	16.1149	6.3817	230.7911	428	16.1149	6.3817	2023.2083	428	16.1149	6.3817	372.6568	428	16.1149	6.3817	2296.0018
429	16.1409	6.3715	310.9245	429	16.1409	6.3715	2098.6769	429	16.1409	6.3715	394.9558	429	16.1409	6.3715	2314.7533
430	16.1669	6.3614	260.9419	430	16.1669	6.3614	2044.0296	430	16.1669	6.3614	339.2832	430	16.1669	6.3614	2255.5331
431	16.1929	6.3512	197.4395	431	16.1929	6.3512	1975.8625	431	16.1929	6.3512	327.4315	431	16.1929	6.3512	2240.1339
432	16.2189	6.3411	249.7385	432	16.2189	6.3411	2023.4968	432	16.2189	6.3411	385.66	432	16.2189	6.3411	2294.8149
433	16.2449	6.331	273.625	433	16.2449	6.331	2042.7186	433	16.2449	6.331	380.8498	433	16.2449	6.331	2286.4572
434	16.2709	6.321	298.7413	434	16.2709	6.321	2062.1094	434	16.2709	6.321	339.3729	434	16.2709	6.321	2241.2249
435	16.2969	6.3109	323.0696	435	16.2969	6.3109	2080.7122	435	16.2969	6.3109	354.5711	435	16.2969	6.3109	2252.6678
436	16.3229	6.301	272.2244	436	16.3229	6.301	2024.1416	436	16.3229	6.301	301.2783	436	16.3229	6.301	2195.6197
437	16.3489	6.291	224.2009	437	16.3489	6.291	1970.3925	437	16.3489	6.291	318.5639	437	16.3489	6.291	2209.15
438	16.3749	6.2811	209.5663	438	16.3749	6.2811	1950.0325	438	16.3749	6.2811	370.0636	438	16.3749	6.2811	2256.8944
439	16.4009	6.2712	219.7618	439	16.4009	6.2712	1954.5025	439	16.4009	6.2712	320.2129	439	16.4009	6.2712	2203.2883
440	16.4269	6.2613	267.9875	440	16.4269	6.2613	1997.0027	440	16.4269	6.2613	353.7354	440	16.4269	6.2613	2233.0555
441	16.4529	6.2515	285.1974	441	16.4529	6.2515	2008.4871	441	16.4529	6.2515	346.5051	441	16.4529	6.2515	2222.0698
442	16.4789	6.2417	306.6609	442	16.4789	6.2417	2024.2251	442	16.4789	6.2417	394.3573	442	16.4789	6.2417	2266.1667
443	16.5049	6.232	240.9957	443	16.5049	6.232	1952.8345	443	16.5049	6.232	391.1838	443	16.5049	6.232	2259.2379
444	16.5309	6.2222	262.7911	444	16.5309	6.2222	1968.9044	444	16.5309	6.2222	412.6596	444	16.5309	6.2222	2276.9584
445	16.5569	6.2125	283.2926	445	16.5569	6.2125	1983.6804	445	16.5569	6.2125	406.8414	445	16.5569	6.2125	2267.3849
446	16.5829	6.2028	276.5218	446	16.5829	6.2028	1971.1841	446	16.5829	6.2028	305.0474	446	16.5829	6.2028	2161.8355
447	16.6089	6.1932	273.6967	447	16.6089	6.1932	1962.6336	447	16.6089	6.1932	276.3789	447	16.6089	6.1932	2129.4116
448	16.6349	6.1836	258.6234	448	16.6349	6.1836	1941.8348	448	16.6349	6.1836	322.1357	448	16.6349	6.1836	2171.4131
449	16.6609	6.174	263.1718	449	16.6609	6.174	1940.6578	449	16.6609	6.174	363.7868	449	16.6609	6.174	2209.3088
450	16.6869	6.1645	252.9888	450	16.6869	6.1645	1924.7493	450	16.6869	6.1645	374.0599	450	16.6869	6.1645	2215.8266
451	16.7129	6.1549	253.8043	451	16.7129	6.1549	1919.8392	451	16.7129	6.1549	381.153	451	16.7129	6.1549	2219.1644
452	16.7389	6.1454	212.4104	452	16.7389	6.1454	1872.7199	452	16.7389	6.1454	381.6679	452	16.7389	6.1454	2215.9239
453	16.7649	6.136	246.2904	453	16.7649	6.136	1900.8744	453	16.7649	6.136	344.107	453	16.7649	6.136	2174.6077
454	16.7909	6.1265	322.5843	454	16.7909	6.1265	1971.4428	454	16.7909	6.1265	414.7377	454	16.7909	6.1265	2241.4831
455	16.8169	6.1171	320.8858	455	16.8169	6.1171	1964.0189	455	16.8169	6.1171	432.27	455	16.8169	6.1171	2255.2601
456	16.8429	6.1078	344.0067	456	16.8429	6.1078	1981.4143	456	16.8429	6.1078	403.301	456	16.8429	6.1078	2222.5357
457	16.8689	6.0984	343.6936	457	16.8689	6.0984	1975.3757	457	16.8689	6.0984	421.4367	457	16.8689	6.0984	2236.9161
458	16.8949	6.0891	307.009	458	16.8949	6.0891	1932.9657	458	16.8949	6.0891	400.1034	458	16.8949	6.0891	2211.8274
459	16.9209	6.0798	280.912	459	16.9209	6.0798	1901.1432	459	16.9209	6.0798	427.9539	459	16.9209	6.0798	2235.9227
460	16.9469	6.0706	273.625	460	16.9469	6.0706	1888.1307	460	16.9469	6.0706	380.8498	460	16.9469	6.0706	2185.0632
461	16.9729	6.0613	296.6855	461	16.9729	6.0613	1907.4579	461	16.9729	6.0613	337.4465	461	16.9729	6.0613	2138.2732
462	16.9989	6.0521	264.5654	462	16.9989	6.0521	1871.6045	462	16.9989	6.0521	365.8951	462	16.9989	6.0521	2163.3352
463	17.0249	6.0429	242.0365	463	17.0249	6.0429	1845.3424	463	17.0249	6.0429	359.3625	463	17.0249	6.0429	2153.4159

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
464	17.0509	6.0338	289.842	464	17.0509	6.0338	1889.4147	464	17.0509	6.0338	376.3246	464	17.0509	6.0338	2166.9913
465	17.0769	6.0247	299.7161	465	17.0769	6.0247	1895.5555	465	17.0769	6.0247	405.849	465	17.0769	6.0247	2193.129
466	17.1029	6.0156	357.8837	466	17.1029	6.0156	1949.9899	466	17.1029	6.0156	394.6218	466	17.1029	6.0156	2178.5152
467	17.1289	6.0065	355.1443	467	17.1289	6.0065	1943.5172	467	17.1289	6.0065	351.8502	467	17.1289	6.0065	2132.3568
468	17.1549	5.9975	306.6569	468	17.1549	5.9975	1891.2966	468	17.1549	5.9975	334.525	468	17.1549	5.9975	2111.645
469	17.1809	5.9885	305.4026	469	17.1809	5.9885	1886.309	469	17.1809	5.9885	358.5362	469	17.1809	5.9885	2132.2695
470	17.2069	5.9795	289.8268	470	17.2069	5.9795	1867	470	17.2069	5.9795	429.4567	470	17.2069	5.9795	2199.8033
471	17.2329	5.9706	301.9731	471	17.2329	5.9706	1875.4131	471	17.2329	5.9706	427.0783	471	17.2329	5.9706	2194.0383
472	17.2589	5.9616	311.5155	472	17.2589	5.9616	1881.2222	472	17.2589	5.9616	412.2987	472	17.2589	5.9616	2175.872
473	17.2849	5.9527	280.9928	473	17.2849	5.9527	1846.9662	473	17.2849	5.9527	355.7965	473	17.2849	5.9527	2115.9831
474	17.3109	5.9439	269.1895	474	17.3109	5.9439	1831.4297	474	17.3109	5.9439	355.4027	474	17.3109	5.9439	2112.2027
475	17.3369	5.935	295.3057	475	17.3369	5.935	1853.8127	475	17.3369	5.935	371.5722	475	17.3369	5.935	2124.9855
476	17.3629	5.9262	307.4159	476	17.3629	5.9262	1862.1895	476	17.3629	5.9262	368.3106	476	17.3629	5.9262	2118.3372
477	17.3889	5.9174	330.0959	477	17.3889	5.9174	1881.1364	477	17.3889	5.9174	377.9851	477	17.3889	5.9174	2124.625
478	17.4149	5.9086	301.3455	478	17.4149	5.9086	1848.6527	478	17.4149	5.9086	348.4594	478	17.4149	5.9086	2091.7126
479	17.4409	5.8999	275.5689	479	17.4409	5.8999	1819.1428	479	17.4409	5.8999	418.1333	479	17.4409	5.8999	2157.9999
480	17.4669	5.8912	272.1149	480	17.4669	5.8912	1811.9555	480	17.4669	5.8912	349.9896	480	17.4669	5.8912	2086.4695
481	17.4929	5.8825	305.2154	481	17.4929	5.8825	1841.3229	481	17.4929	5.8825	309.8058	481	17.4929	5.8825	2042.8991
482	17.5189	5.8738	350.7558	482	17.5189	5.8738	1883.13	482	17.5189	5.8738	362.9292	482	17.5189	5.8738	2092.6357
483	17.5449	5.8652	304.5322	483	17.5449	5.8652	1833.1731	483	17.5449	5.8652	361.2452	483	17.5449	5.8652	2087.5651
484	17.5709	5.8566	296.6396	484	17.5709	5.8566	1821.5473	484	17.5709	5.8566	360.5764	484	17.5709	5.8566	2083.5096
485	17.5969	5.848	312.8081	485	17.5969	5.848	1833.9825	485	17.5969	5.848	362.1603	485	17.5969	5.848	2081.7068
486	17.6229	5.8394	366.0978	486	17.6229	5.8394	1883.539	486	17.6229	5.8394	395.3386	486	17.6229	5.8394	2111.4985
487	17.6489	5.8309	273.625	487	17.6489	5.8309	1787.333	487	17.6489	5.8309	380.8498	487	17.6489	5.8309	2093.623
488	17.6749	5.8224	301.0409	488	17.6749	5.8224	1810.9929	488	17.6749	5.8224	339.2636	488	17.6749	5.8224	2045.3639
489	17.7009	5.8139	294.2766	489	17.7009	5.8139	1800.4728	489	17.7009	5.8139	359.0448	489	17.7009	5.8139	2058.4723
490	17.7269	5.8054	280.3997	490	17.7269	5.8054	1782.8399	490	17.7269	5.8054	332.6773	490	17.7269	5.8054	2025.4319
491	17.7529	5.797	337.9557	491	17.7529	5.797	1836.64	491	17.7529	5.797	411.0563	491	17.7529	5.797	2097.1381
492	17.7789	5.7886	254.5065	492	17.7789	5.7886	1749.4349	492	17.7789	5.7886	414.7465	492	17.7789	5.7886	2094.1554
493	17.8049	5.7802	280.9756	493	17.8049	5.7802	1772.1481	493	17.8049	5.7802	377.4109	493	17.8049	5.7802	2050.147
494	17.8309	5.7719	335.674	494	17.8309	5.7719	1823.0906	494	17.8309	5.7719	262.7426	494	17.8309	5.7719	1928.8058
495	17.8569	5.7635	369.828	495	17.8569	5.7635	1853.4887	495	17.8569	5.7635	368.7742	495	17.8569	5.7635	2028.1645
496	17.8829	5.7552	270.6607	496	17.8829	5.7552	1750.5655	496	17.8829	5.7552	395.9018	496	17.8829	5.7552	2048.6193
497	17.9089	5.7469	302.8147	497	17.9089	5.7469	1778.9636	497	17.9089	5.7469	406.6777	497	17.9089	5.7469	2052.7223
498	17.9349	5.7387	330.0188	498	17.9349	5.7387	1802.4117	498	17.9349	5.7387	386.7655	498	17.9349	5.7387	2026.1372
499	17.9609	5.7304	341.2413	499	17.9609	5.7304	1809.8783	499	17.9609	5.7304	395.0663	499	17.9609	5.7304	2027.7652

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
500	17.9869	5.7222	369.8023	500	17.9869	5.7222	1834.6834	500	17.9869	5.7222	398.6081	500	17.9869	5.7222	2024.6341
501	18.0129	5.714	268.2041	501	18.0129	5.714	1729.3293	501	18.0129	5.714	414.7328	501	18.0129	5.714	2034.086
502	18.0389	5.7058	232.2798	502	18.0389	5.7058	1689.6491	502	18.0389	5.7058	351.6053	502	18.0389	5.7058	1964.2856
503	18.0649	5.6977	290.8733	503	18.0649	5.6977	1744.4868	503	18.0649	5.6977	435.7719	503	18.0649	5.6977	2041.7794
504	18.0909	5.6896	267.9789	504	18.0909	5.6896	1717.8364	504	18.0909	5.6896	481.784	504	18.0909	5.6896	2081.1186
505	18.1169	5.6815	253.9134	505	18.1169	5.6815	1700.015	505	18.1169	5.6815	392.4193	505	18.1169	5.6815	1985.081
506	18.1429	5.6734	265.5682	506	18.1429	5.6734	1707.9139	506	18.1429	5.6734	331.7427	506	18.1429	5.6734	1917.7315
507	18.1689	5.6654	307.6037	507	18.1689	5.6654	1746.1935	507	18.1689	5.6654	306.3458	507	18.1689	5.6654	1885.6618
508	18.1949	5.6573	286.9618	508	18.1949	5.6573	1721.7957	508	18.1949	5.6573	426.7458	508	18.1949	5.6573	1999.3889
509	18.2209	5.6493	338.8553	509	18.2209	5.6493	1769.9332	509	18.2209	5.6493	342.0417	509	18.2209	5.6493	1908.0119
510	18.2469	5.6413	265.865	510	18.2469	5.6413	1693.1871	510	18.2469	5.6413	428.2633	510	18.2469	5.6413	1987.5607
511	18.2729	5.6334	305.838	511	18.2729	5.6334	1729.4041	511	18.2729	5.6334	457.2284	511	18.2729	5.6334	2009.853
512	18.2989	5.6254	352.1672	512	18.2989	5.6254	1771.9775	512	18.2989	5.6254	463.1889	512	18.2989	5.6254	2009.1406
513	18.3249	5.6175	359.8654	513	18.3249	5.6175	1775.9198	513	18.3249	5.6175	478.919	513	18.3249	5.6175	2018.1979
514	18.3509	5.6096	273.625	514	18.3509	5.6096	1685.9235	514	18.3509	5.6096	380.8498	514	18.3509	5.6096	1913.4558
515	18.3769	5.6018	306.0598	515	18.3769	5.6018	1716.5974	515	18.3769	5.6018	338.2488	515	18.3769	5.6018	1869.7022
516	18.4029	5.5939	354.9441	516	18.4029	5.5939	1763.7209	516	18.4029	5.5939	384.6504	516	18.4029	5.5939	1914.9511
517	18.4289	5.5861	341.7417	517	18.4289	5.5861	1748.7578	517	18.4289	5.5861	487.7826	517	18.4289	5.5861	2016.9306
518	18.4549	5.5783	338.1342	518	18.4549	5.5783	1743.3895	518	18.4549	5.5783	389.7521	518	18.4549	5.5783	1917.7475
519	18.4809	5.5705	298.2134	519	18.4809	5.5705	1701.7079	519	18.4809	5.5705	317.3806	519	18.4809	5.5705	1844.2233
520	18.5069	5.5628	337.4835	520	18.5069	5.5628	1739.2172	520	18.5069	5.5628	408.7986	520	18.5069	5.5628	1934.4886
521	18.5329	5.555	405.0153	521	18.5329	5.555	1804.9881	521	18.5329	5.555	407.2928	521	18.5329	5.555	1931.8302
522	18.5589	5.5473	319.7907	522	18.5589	5.5473	1718.0027	522	18.5589	5.5473	360.5995	522	18.5589	5.5473	1883.9843
523	18.5849	5.5396	358.9882	523	18.5849	5.5396	1755.4394	523	18.5849	5.5396	402.0017	523	18.5849	5.5396	1924.2338
524	18.6109	5.532	324.6711	524	18.6109	5.532	1719.3615	524	18.6109	5.532	413.1099	524	18.6109	5.532	1934.1894
525	18.6369	5.5243	315.0704	525	18.6369	5.5243	1708	525	18.6369	5.5243	407.6675	525	18.6369	5.5243	1927.5943
526	18.6629	5.5167	297.8521	526	18.6629	5.5167	1689.0209	526	18.6629	5.5167	449.1381	526	18.6629	5.5167	1967.9122
527	18.6889	5.5091	286.0024	527	18.6889	5.5091	1675.4104	527	18.6889	5.5091	391.0999	527	18.6889	5.5091	1908.7213
528	18.7149	5.5015	326.9842	528	18.7149	5.5015	1714.6314	528	18.7149	5.5015	428.0397	528	18.7149	5.5015	1944.5085
529	18.7409	5.4939	290.1246	529	18.7409	5.4939	1676.011	529	18.7409	5.4939	400.7831	529	18.7409	5.4939	1916.0993
530	18.7669	5.4864	335.2118	530	18.7669	5.4864	1719.3375	530	18.7669	5.4864	427.6452	530	18.7669	5.4864	1941.8087
531	18.7929	5.4789	303.2699	531	18.7929	5.4789	1685.6347	531	18.7929	5.4789	447.1775	531	18.7929	5.4789	1960.1883
532	18.8189	5.4713	306.8713	532	18.8189	5.4713	1687.4754	532	18.8189	5.4713	374.0905	532	18.8189	5.4713	1885.9487
533	18.8449	5.4639	268.5483	533	18.8449	5.4639	1647.3915	533	18.8449	5.4639	409.3298	533	18.8449	5.4639	1920.0353
534	18.8709	5.4564	278.9515	534	18.8709	5.4564	1656.0339	534	18.8709	5.4564	441.5613	534	18.8709	5.4564	1951.1142
535	18.8969	5.449	324.6487	535	18.8969	5.449	1699.9703	535	18.8969	5.449	384.5697	535	18.8969	5.449	1892.9699

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
536	18.9229	5.4415	325.9161	536	18.9229	5.4415	1699.477	536	18.9229	5.4415	331.398	536	18.9229	5.4415	1838.6455
537	18.9489	5.4342	303.4771	537	18.9489	5.4342	1675.2771	537	18.9489	5.4342	371.7106	537	18.9489	5.4342	1877.8055
538	18.9749	5.4268	348.6839	538	18.9749	5.4268	1718.7231	538	18.9749	5.4268	386.3101	538	18.9749	5.4268	1891.2523
539	19.0009	5.4194	373.0744	539	19.0009	5.4194	1741.3528	539	19.0009	5.4194	349.1201	539	19.0009	5.4194	1852.9097
540	19.0269	5.4121	351.3183	540	19.0269	5.4121	1717.8359	540	19.0269	5.4121	386.1657	540	19.0269	5.4121	1888.8026
541	19.0529	5.4048	385.5386	541	19.0529	5.4048	1750.2954	541	19.0529	5.4048	380.8498	541	19.0529	5.4048	1882.3341
542	19.0789	5.3975	377.2418	542	19.0789	5.3975	1740.2378	542	19.0789	5.3975	413.4749	542	19.0789	5.3975	1911.035
543	19.1049	5.3902	336.9907	543	19.1049	5.3902	1698.2259	543	19.1049	5.3902	422.3457	543	19.1049	5.3902	1915.9817
544	19.1309	5.3829	360.4207	544	19.1309	5.3829	1719.8951	544	19.1309	5.3829	438.6126	544	19.1309	5.3829	1928.3244
545	19.1569	5.3757	349.9568	545	19.1569	5.3757	1707.6704	545	19.1569	5.3757	414.6442	545	19.1569	5.3757	1900.4318
546	19.1829	5.3685	375.2505	546	19.1829	5.3685	1731.2033	546	19.1829	5.3685	454.8875	546	19.1829	5.3685	1936.7509
547	19.2089	5.3613	430.3578	547	19.2089	5.3613	1784.5498	547	19.2089	5.3613	497.0716	547	19.2089	5.3613	1975.0109
548	19.2349	5.3541	528.2921	548	19.2349	5.3541	1880.7233	548	19.2349	5.3541	494.8399	548	19.2349	5.3541	1968.855
549	19.2609	5.3469	543.6351	549	19.2609	5.3469	1894.3056	549	19.2609	5.3469	490.0329	549	19.2609	5.3469	1960.1238
550	19.2869	5.3398	568.7778	550	19.2869	5.3398	1917.6874	550	19.2869	5.3398	482.3066	550	19.2869	5.3398	1948.4734
551	19.3129	5.3327	625.9068	551	19.3129	5.3327	1973.0556	551	19.3129	5.3327	485.0138	551	19.3129	5.3327	1947.2564
552	19.3389	5.3256	646.3996	552	19.3389	5.3256	1991.7876	552	19.3389	5.3256	524.7162	552	19.3389	5.3256	1983.0346
553	19.3649	5.3185	676.1054	553	19.3649	5.3185	2019.7326	553	19.3649	5.3185	570.6781	553	19.3649	5.3185	2025.0724
554	19.3909	5.3114	715.7044	554	19.3909	5.3114	2057.5708	554	19.3909	5.3114	633.7233	554	19.3909	5.3114	2084.1934
555	19.4169	5.3044	776.1201	555	19.4169	5.3044	2116.2257	555	19.4169	5.3044	645.7314	555	19.4169	5.3044	2092.2774
556	19.4429	5.2974	777.6706	556	19.4429	5.2974	2116.0154	556	19.4429	5.2974	568.9968	556	19.4429	5.2974	2011.6185
557	19.4689	5.2904	732.2351	557	19.4689	5.2904	2068.8191	557	19.4689	5.2904	490.5788	557	19.4689	5.2904	1929.2764
558	19.4949	5.2834	735.5356	558	19.4949	5.2834	2070.3588	558	19.4949	5.2834	457.1197	558	19.4949	5.2834	1891.8931
559	19.5209	5.2764	696.6511	559	19.5209	5.2764	2029.7135	559	19.5209	5.2764	454.8102	559	19.5209	5.2764	1885.6595
560	19.5469	5.2694	590.4477	560	19.5469	5.2694	1921.7493	560	19.5469	5.2694	438.1924	560	19.5469	5.2694	1865.1175
561	19.5729	5.2625	523.1537	561	19.5729	5.2625	1852.6945	561	19.5729	5.2625	435.2083	561	19.5729	5.2625	1858.2092
562	19.5989	5.2556	497.3802	562	19.5989	5.2556	1825.1602	562	19.5989	5.2556	408.3334	562	19.5989	5.2556	1827.4101
563	19.6249	5.2487	446.8504	563	19.6249	5.2487	1772.8696	563	19.6249	5.2487	403.3672	563	19.6249	5.2487	1818.5198
564	19.6509	5.2418	396.3279	564	19.6509	5.2418	1720.5863	564	19.6509	5.2418	453.0141	564	19.6509	5.2418	1864.2425
565	19.6769	5.235	409.6172	565	19.6769	5.235	1732.1148	565	19.6769	5.235	426.7541	565	19.6769	5.235	1834.0584
566	19.7029	5.2281	403.6594	566	19.7029	5.2281	1724.3962	566	19.7029	5.2281	410.1955	566	19.7029	5.2281	1813.5756
567	19.7289	5.2213	324.5539	567	19.7289	5.2213	1643.5299	567	19.7289	5.2213	402.3367	567	19.7289	5.2213	1801.7927
568	19.7549	5.2145	273.625	568	19.7549	5.2145	1590.8402	568	19.7549	5.2145	380.8498	568	19.7549	5.2145	1776.3816
569	19.7809	5.2077	310.619	569	19.7809	5.2077	1626.7448	569	19.7809	5.2077	375.7608	569	19.7809	5.2077	1769.0869
570	19.8069	5.201	348.4863	570	19.8069	5.201	1663.5228	570	19.8069	5.201	389.8819	570	19.8069	5.201	1781.0023
571	19.8329	5.1942	334.049	571	19.8329	5.1942	1647.9962	571	19.8329	5.1942	424.4624	571	19.8329	5.1942	1813.3772

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
572	19.8589	5.1875	247.4516	572	19.8589	5.1875	1560.3095	572	19.8589	5.1875	453.3657	572	19.8589	5.1875	1840.0747
573	19.8849	5.1808	261.7829	573	19.8849	5.1808	1573.5515	573	19.8849	5.1808	471.0518	573	19.8849	5.1808	1855.5551
574	19.9109	5.1741	325.466	574	19.9109	5.1741	1636.1453	574	19.9109	5.1741	406.9604	574	19.9109	5.1741	1789.2581
575	19.9369	5.1674	342.5482	575	19.9369	5.1674	1652.1381	575	19.9369	5.1674	418.6093	575	19.9369	5.1674	1798.7013
576	19.9629	5.1607	348.8812	576	19.9629	5.1607	1657.3819	576	19.9629	5.1607	417.8434	576	19.9629	5.1607	1795.7297
577	19.9889	5.1541	294.6488	577	19.9889	5.1541	1602.0602	577	19.9889	5.1541	377.7432	577	19.9889	5.1541	1753.4238
578	20.0149	5.1474	245.7309	578	20.0149	5.1474	1552.0529	578	20.0149	5.1474	410.1843	578	20.0149	5.1474	1783.6592
579	20.0409	5.1408	244.099	579	20.0409	5.1408	1549.3317	579	20.0409	5.1408	470.0148	579	20.0409	5.1408	1841.2841
580	20.0669	5.1342	279.7215	580	20.0669	5.1342	1583.8648	580	20.0669	5.1342	456.3159	580	20.0669	5.1342	1825.3794
581	20.0929	5.1277	290.3488	581	20.0929	5.1277	1593.4028	581	20.0929	5.1277	477.4013	581	20.0929	5.1277	1844.2592
582	20.1189	5.1211	258.3942	582	20.1189	5.1211	1560.3589	582	20.1189	5.1211	374.3997	582	20.1189	5.1211	1739.052
583	20.1449	5.1146	254.9265	583	20.1449	5.1146	1555.8019	583	20.1449	5.1146	421.5625	583	20.1449	5.1146	1784.009
584	20.1709	5.108	349.2905	584	20.1709	5.108	1649.0765	584	20.1709	5.108	456.2663	584	20.1709	5.108	1816.5071
585	20.1969	5.1015	348.9633	585	20.1969	5.1015	1647.6601	585	20.1969	5.1015	449.3828	585	20.1969	5.1015	1807.4179
586	20.2229	5.095	319.2287	586	20.2229	5.095	1616.8361	586	20.2229	5.095	408.4617	586	20.2229	5.095	1764.2912
587	20.2489	5.0886	280.5228	587	20.2489	5.0886	1577.0409	587	20.2489	5.0886	454.244	587	20.2489	5.0886	1807.8678
588	20.2749	5.0821	270.9024	588	20.2749	5.0821	1566.3312	588	20.2749	5.0821	400.2061	588	20.2749	5.0821	1751.6242
589	20.3009	5.0757	205.8399	589	20.3009	5.0757	1500.1793	589	20.3009	5.0757	377.7291	589	20.3009	5.0757	1726.9415
590	20.3269	5.0692	326.9114	590	20.3269	5.0692	1620.1615	590	20.3269	5.0692	422.8278	590	20.3269	5.0692	1769.8346
591	20.3529	5.0628	258.4428	591	20.3529	5.0628	1550.6036	591	20.3529	5.0628	388.2408	591	20.3529	5.0628	1733.0419
592	20.3789	5.0564	219.0934	592	20.3789	5.0564	1510.1649	592	20.3789	5.0564	402.8124	592	20.3789	5.0564	1745.4078
593	20.4049	5.0501	182.7922	593	20.4049	5.0501	1472.7744	593	20.4049	5.0501	404.9642	593	20.4049	5.0501	1745.3539
594	20.4309	5.0437	312.9463	594	20.4309	5.0437	1601.8392	594	20.4309	5.0437	386.3783	594	20.4309	5.0437	1724.5623
595	20.4569	5.0374	298.4023	595	20.4569	5.0374	1586.2059	595	20.4569	5.0374	380.8498	595	20.4569	5.0374	1716.8281
596	20.4829	5.031	245.1984	596	20.4829	5.031	1530.8285	596	20.4829	5.031	476.7887	596	20.4829	5.031	1810.7908
597	20.5089	5.0247	262.9035	597	20.5089	5.0247	1546.36	597	20.5089	5.0247	496.2565	597	20.5089	5.0247	1828.2823
598	20.5349	5.0184	241.3001	598	20.5349	5.0184	1522.5831	598	20.5349	5.0184	408.3949	598	20.5349	5.0184	1738.4445
599	20.5609	5.0122	172.4709	599	20.5609	5.0122	1451.5804	599	20.5609	5.0122	440.3254	599	20.5609	5.0122	1768.3988
600	20.5869	5.0059	264.18	600	20.5869	5.0059	1541.1161	600	20.5869	5.0059	447.3939	600	20.5869	5.0059	1773.4911
601	20.6129	4.9997	224.2986	601	20.6129	4.9997	1499.0612	601	20.6129	4.9997	441.5785	601	20.6129	4.9997	1765.6994
602	20.6389	4.9934	349.3465	602	20.6389	4.9934	1621.9356	602	20.6389	4.9934	453.4511	602	20.6389	4.9934	1775.5957
603	20.6649	4.9872	322.9149	603	20.6649	4.9872	1593.3305	603	20.6649	4.9872	340.7956	603	20.6649	4.9872	1660.9641
604	20.6909	4.981	299.2238	604	20.6909	4.981	1567.466	604	20.6909	4.981	378.0775	604	20.6909	4.981	1696.2697
605	20.7169	4.9748	212.4307	605	20.7169	4.9748	1478.4993	605	20.7169	4.9748	396.3597	605	20.7169	4.9748	1712.5756
606	20.7429	4.9687	285.8898	606	20.7429	4.9687	1549.7849	606	20.7429	4.9687	480.5123	606	20.7429	4.9687	1794.7521
607	20.7689	4.9625	230.04	607	20.7689	4.9625	1491.7616	607	20.7689	4.9625	459.0463	607	20.7689	4.9625	1771.3098

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
608	20.7949	4.9564	269.5614	608	20.7949	4.9564	1529.1096	608	20.7949	4.9564	425.5347	608	20.7949	4.9564	1735.8219
609	20.8209	4.9503	252.3131	609	20.8209	4.9503	1509.6878	609	20.8209	4.9503	387.0319	609	20.8209	4.9503	1695.3429
610	20.8469	4.9441	247.0975	610	20.8469	4.9441	1502.2987	610	20.8469	4.9441	409.6837	610	20.8469	4.9441	1716.0184
611	20.8729	4.9381	194.023	611	20.8729	4.9381	1447.0507	611	20.8729	4.9381	378.535	611	20.8729	4.9381	1682.8935
612	20.8989	4.932	210.9579	612	20.8989	4.932	1461.8121	612	20.8989	4.932	441.4288	612	20.8989	4.932	1743.8111
613	20.9249	4.9259	243.0735	613	20.9249	4.9259	1491.7543	613	20.9249	4.9259	359.476	613	20.9249	4.9259	1659.8821
614	20.9509	4.9199	308.9743	614	20.9509	4.9199	1555.4815	614	20.9509	4.9199	436.2396	614	20.9509	4.9199	1734.6695
615	20.9769	4.9138	254.0341	615	20.9769	4.9138	1498.3678	615	20.9769	4.9138	450.9927	615	20.9769	4.9138	1747.4463
616	21.0029	4.9078	134.0248	616	21.0029	4.9078	1376.1851	616	21.0029	4.9078	429.2823	616	21.0029	4.9078	1723.7597
617	21.0289	4.9018	286.3809	617	21.0289	4.9018	1526.3677	617	21.0289	4.9018	404.5264	617	21.0289	4.9018	1697.0276
618	21.0549	4.8958	231.0496	618	21.0549	4.8958	1468.8629	618	21.0549	4.8958	467.5651	618	21.0549	4.8958	1758.09
619	21.0809	4.8899	211.0759	619	21.0809	4.8899	1446.7157	619	21.0809	4.8899	467.167	619	21.0809	4.8899	1755.7157
620	21.1069	4.8839	283.6142	620	21.1069	4.8839	1517.0805	620	21.1069	4.8839	423.6644	620	21.1069	4.8839	1710.2369
621	21.1329	4.878	225.612	621	21.1329	4.878	1456.9048	621	21.1329	4.878	413.3147	621	21.1329	4.878	1697.9109
622	21.1589	4.8721	302.8976	622	21.1589	4.8721	1532.0169	622	21.1589	4.8721	380.8498	622	21.1589	4.8721	1663.4697
623	21.1849	4.8661	277.4111	623	21.1849	4.8661	1503.4416	623	21.1849	4.8661	419.759	623	21.1849	4.8661	1700.9017
624	21.2109	4.8602	209.6773	624	21.2109	4.8602	1432.6191	624	21.2109	4.8602	418.0583	624	21.2109	4.8602	1697.7238
625	21.2369	4.8544	258.1667	625	21.2369	4.8544	1478.0197	625	21.2369	4.8544	460.4701	625	21.2369	4.8544	1738.6584
626	21.2629	4.8485	261.6601	626	21.2629	4.8485	1478.4244	626	21.2629	4.8485	416.3891	626	21.2629	4.8485	1693.1003
627	21.2889	4.8426	273.9428	627	21.2889	4.8426	1487.6183	627	21.2889	4.8426	434.5232	627	21.2889	4.8426	1709.7571
628	21.3149	4.8368	219.6729	628	21.3149	4.8368	1430.2596	628	21.3149	4.8368	433.3411	628	21.3149	4.8368	1707.0979
629	21.3409	4.831	212.4212	629	21.3409	4.831	1419.9192	629	21.3409	4.831	433.258	629	21.3409	4.831	1705.5376
630	21.3669	4.8252	225.1796	630	21.3669	4.8252	1429.5888	630	21.3669	4.8252	341.8557	630	21.3669	4.8252	1612.658
631	21.3929	4.8194	217.1984	631	21.3929	4.8194	1418.5188	631	21.3929	4.8194	402.8006	631	21.3929	4.8194	1672.1257
632	21.4189	4.8136	196.5535	632	21.4189	4.8136	1394.7851	632	21.4189	4.8136	324.0361	632	21.4189	4.8136	1591.884
633	21.4449	4.8078	252.6442	633	21.4449	4.8078	1447.7871	633	21.4449	4.8078	379.9555	633	21.4449	4.8078	1646.3262
634	21.4709	4.8021	274.3499	634	21.4709	4.8021	1466.4041	634	21.4709	4.8021	398.8459	634	21.4709	4.8021	1663.7395
635	21.4969	4.7963	264.6864	635	21.4969	4.7963	1453.6517	635	21.4969	4.7963	387.2002	635	21.4969	4.7963	1650.6166
636	21.5229	4.7906	291.0972	636	21.5229	4.7906	1476.9738	636	21.5229	4.7906	388.1589	636	21.5229	4.7906	1650.098
637	21.5489	4.7849	261.3998	637	21.5489	4.7849	1444.1876	637	21.5489	4.7849	358.8246	637	21.5489	4.7849	1619.2866
638	21.5749	4.7792	259.9294	638	21.5749	4.7792	1439.6285	638	21.5749	4.7792	374.5542	638	21.5749	4.7792	1633.539
639	21.6009	4.7735	228.2063	639	21.6009	4.7735	1404.8166	639	21.6009	4.7735	399.5361	639	21.6009	4.7735	1657.0437
640	21.6269	4.7678	257.314	640	21.6269	4.7678	1430.8355	640	21.6269	4.7678	395.4151	640	21.6269	4.7678	1651.4455
641	21.6529	4.7622	274.1715	641	21.6529	4.7622	1444.6043	641	21.6529	4.7622	408.9896	641	21.6529	4.7622	1663.5428
642	21.6789	4.7565	256.9404	642	21.6789	4.7565	1424.2844	642	21.6789	4.7565	403.289	642	21.6789	4.7565	1656.3649
643	21.7049	4.7509	258.6735	643	21.7049	4.7509	1422.9288	643	21.7049	4.7509	363.2769	643	21.7049	4.7509	1614.8757

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
644	21.7309	4.7453	282.5726	644	21.7309	4.7453	1443.7391	644	21.7309	4.7453	393.6158	644	21.7309	4.7453	1643.7374
645	21.7569	4.7397	244.6786	645	21.7569	4.7397	1402.7563	645	21.7569	4.7397	438.9967	645	21.7569	4.7397	1687.641
646	21.7829	4.7341	194.607	646	21.7829	4.7341	1349.5959	646	21.7829	4.7341	411.4251	646	21.7829	4.7341	1658.5922
647	21.8089	4.7285	235.4472	647	21.8089	4.7285	1387.3473	647	21.8089	4.7285	420.3612	647	21.8089	4.7285	1666.0511
648	21.8349	4.723	304.9433	648	21.8349	4.723	1453.7547	648	21.8349	4.723	411.1312	648	21.8349	4.723	1655.344
649	21.8609	4.7174	298.3375	649	21.8609	4.7174	1444.0602	649	21.8609	4.7174	380.8498	649	21.8609	4.7174	1623.5854
650	21.8869	4.7119	246.5424	650	21.8869	4.7119	1389.1762	650	21.8869	4.7119	389.2873	650	21.8869	4.7119	1629.7691
651	21.9129	4.7064	244.7228	651	21.9129	4.7064	1384.2678	651	21.9129	4.7064	384.8072	651	21.9129	4.7064	1623.0352
652	21.9389	4.7008	252.7319	652	21.9389	4.7008	1389.1882	652	21.9389	4.7008	333.4817	652	21.9389	4.7008	1569.4559
653	21.9649	4.6954	248.2244	653	21.9649	4.6954	1381.592	653	21.9649	4.6954	333.6502	653	21.9649	4.6954	1567.3706
654	21.9909	4.6899	235.016	654	21.9909	4.6899	1365.2947	654	21.9909	4.6899	350.4733	654	21.9909	4.6899	1581.9399
655	22.0169	4.6844	249.9051	655	22.0169	4.6844	1377.0951	655	22.0169	4.6844	334.1681	655	22.0169	4.6844	1563.381
656	22.0429	4.6789	244.8359	656	22.0429	4.6789	1368.9371	656	22.0429	4.6789	349.0733	656	22.0429	4.6789	1576.0323
657	22.0689	4.6735	232.6266	657	22.0689	4.6735	1353.639	657	22.0689	4.6735	364.876	657	22.0689	4.6735	1589.5812
658	22.0949	4.6681	238.2773	658	22.0949	4.6681	1356.201	658	22.0949	4.6681	344.2685	658	22.0949	4.6681	1566.72
659	22.1209	4.6626	212.2713	659	22.1209	4.6626	1327.1062	659	22.1209	4.6626	312.6684	659	22.1209	4.6626	1532.8661
660	22.1469	4.6572	216.7065	660	22.1469	4.6572	1328.4526	660	22.1469	4.6572	309.2027	660	22.1469	4.6572	1527.1466
661	22.1729	4.6519	243.8196	661	22.1729	4.6519	1352.477	661	22.1729	4.6519	363.4745	661	22.1729	4.6519	1579.1645
662	22.1989	4.6465	255.7832	662	22.1989	4.6465	1361.3518	662	22.1989	4.6465	374.8409	662	22.1989	4.6465	1588.2772
663	22.2249	4.6411	275.3665	663	22.2249	4.6411	1377.8463	663	22.2249	4.6411	360.0386	663	22.2249	4.6411	1571.2211
664	22.2509	4.6357	317.2545	664	22.2509	4.6357	1416.6456	664	22.2509	4.6357	412.3941	664	22.2509	4.6357	1621.3228
665	22.2769	4.6304	306.8278	665	22.2769	4.6304	1403.1302	665	22.2769	4.6304	398.6292	665	22.2769	4.6304	1605.3041
666	22.3029	4.6251	278.64	666	22.3029	4.6251	1371.8536	666	22.3029	4.6251	343.0851	666	22.3029	4.6251	1547.5062
667	22.3289	4.6198	271.4937	667	22.3289	4.6198	1361.6185	667	22.3289	4.6198	351.3997	667	22.3289	4.6198	1553.5671
668	22.3549	4.6145	227.4366	668	22.3549	4.6145	1314.4727	668	22.3549	4.6145	405.1589	668	22.3549	4.6145	1605.0724
669	22.3809	4.6092	245.1605	669	22.3809	4.6092	1329.1078	669	22.3809	4.6092	396.9189	669	22.3809	4.6092	1594.5786
670	22.4069	4.6039	271.3497	670	22.4069	4.6039	1352.2082	670	22.4069	4.6039	388.3228	670	22.4069	4.6039	1583.7288
671	22.4329	4.5986	256.8369	671	22.4329	4.5986	1334.6067	671	22.4329	4.5986	350.9751	671	22.4329	4.5986	1544.1273
672	22.4589	4.5934	242.2133	672	22.4589	4.5934	1316.8943	672	22.4589	4.5934	352.9445	672	22.4589	4.5934	1543.8428
673	22.4849	4.5881	245.381	673	22.4849	4.5881	1316.9733	673	22.4849	4.5881	348.7545	673	22.4849	4.5881	1537.3991
674	22.5109	4.5829	267.0749	674	22.5109	4.5829	1335.5784	674	22.5109	4.5829	325.1457	674	22.5109	4.5829	1511.5365
675	22.5369	4.5777	275.8977	675	22.5369	4.5777	1341.3124	675	22.5369	4.5777	353.9888	675	22.5369	4.5777	1538.1258
676	22.5629	4.5725	273.625	676	22.5629	4.5725	1335.9509	676	22.5629	4.5725	380.8498	676	22.5629	4.5725	1562.733
677	22.5889	4.5673	259.9447	677	22.5889	4.5673	1321.4149	677	22.5889	4.5673	439.132	677	22.5889	4.5673	1620.5166
678	22.6149	4.5621	277.4723	678	22.6149	4.5621	1338.0869	678	22.6149	4.5621	410.9183	678	22.6149	4.5621	1591.8044
679	22.6409	4.5569	298.3359	679	22.6409	4.5569	1358.0949	679	22.6409	4.5569	389.249	679	22.6409	4.5569	1569.6366

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
680	22.6669	4.5518	239.5562	680	22.6669	4.5518	1298.4595	680	22.6669	4.5518	382.9578	680	22.6669	4.5518	1562.8468
681	22.6929	4.5466	270.745	681	22.6929	4.5466	1328.7926	681	22.6929	4.5466	374.6095	681	22.6929	4.5466	1554
682	22.7189	4.5415	280.136	682	22.7189	4.5415	1337.3279	682	22.7189	4.5415	366.6059	682	22.7189	4.5415	1545.4978
683	22.7449	4.5363	280.3526	683	22.7449	4.5363	1336.6889	683	22.7449	4.5363	344.8005	683	22.7449	4.5363	1523.1939
684	22.7709	4.5312	298.0426	684	22.7709	4.5312	1353.5232	684	22.7709	4.5312	345.4976	684	22.7709	4.5312	1523.3925
685	22.7969	4.5261	234.8445	685	22.7969	4.5261	1289.4694	685	22.7969	4.5261	326.3134	685	22.7969	4.5261	1503.7097
686	22.8229	4.521	129.1634	686	22.8229	4.521	1182.9326	686	22.8229	4.521	435.8088	686	22.8229	4.521	1612.7066
687	22.8489	4.516	225.8112	687	22.8489	4.516	1278.7248	687	22.8489	4.516	434.7645	687	22.8489	4.516	1611.1637
688	22.8749	4.5109	286.1427	688	22.8749	4.5109	1338.2006	688	22.8749	4.5109	324.9676	688	22.8749	4.5109	1500.8683
689	22.9009	4.5059	299.2262	689	22.9009	4.5059	1350.4285	689	22.9009	4.5059	360.2709	689	22.9009	4.5059	1535.6731
690	22.9269	4.5008	309.6909	690	22.9269	4.5008	1360.0375	690	22.9269	4.5008	408.965	690	22.9269	4.5008	1583.8687
691	22.9529	4.4958	299.5873	691	22.9529	4.4958	1349.0783	691	22.9529	4.4958	434.1488	691	22.9529	4.4958	1608.554
692	22.9789	4.4908	293.2093	692	22.9789	4.4908	1341.8446	692	22.9789	4.4908	377.6682	692	22.9789	4.4908	1551.5748
693	23.0049	4.4858	283.8958	693	23.0049	4.4858	1331.6755	693	23.0049	4.4858	372.2278	693	23.0049	4.4858	1545.6359
694	23.0309	4.4808	293.9019	694	23.0309	4.4808	1340.8258	694	23.0309	4.4808	318.4069	694	23.0309	4.4808	1491.3164
695	23.0569	4.4758	242.2864	695	23.0569	4.4758	1288.3547	695	23.0569	4.4758	360.1712	695	23.0569	4.4758	1532.5821
696	23.0829	4.4708	277.4029	696	23.0829	4.4708	1322.6155	696	23.0829	4.4708	332.3195	696	23.0829	4.4708	1504.2319
697	23.1089	4.4658	217.4656	697	23.1089	4.4658	1261.8225	697	23.1089	4.4658	312.3174	697	23.1089	4.4658	1483.7313
698	23.1349	4.4609	251.39	698	23.1349	4.4609	1294.8913	698	23.1349	4.4609	268.8176	698	23.1349	4.4609	1439.733
699	23.1609	4.456	314.6468	699	23.1609	4.456	1357.2925	699	23.1609	4.456	344.2907	699	23.1609	4.456	1514.7075
700	23.1869	4.451	295.2391	700	23.1869	4.451	1337.0291	700	23.1869	4.451	363.7663	700	23.1869	4.451	1533.6846
701	23.2129	4.4461	312.0448	701	23.2129	4.4461	1352.9791	701	23.2129	4.4461	333.7352	701	23.2129	4.4461	1503.1549
702	23.2389	4.4412	328.943	702	23.2389	4.4412	1369.0216	702	23.2389	4.4412	388.7675	702	23.2389	4.4412	1557.6887
703	23.2649	4.4363	310.2972	703	23.2649	4.4363	1349.5202	703	23.2649	4.4363	380.8498	703	23.2649	4.4363	1549.2725
704	23.2909	4.4314	353.573	704	23.2909	4.4314	1391.2612	704	23.2909	4.4314	335.093	704	23.2909	4.4314	1502.1822
705	23.3169	4.4265	326.3907	705	23.3169	4.4265	1362.5441	705	23.3169	4.4265	383.0678	705	23.3169	4.4265	1548.8235
706	23.3429	4.4217	364.4388	706	23.3429	4.4217	1399.0574	706	23.3429	4.4217	372.5778	706	23.3429	4.4217	1537
707	23.3689	4.4168	377.8545	707	23.3689	4.4168	1410.9383	707	23.3689	4.4168	373.9113	707	23.3689	4.4168	1537
708	23.3949	4.412	496.6587	708	23.3949	4.412	1528.2078	708	23.3949	4.412	403.808	708	23.3949	4.412	1565.5632
709	23.4209	4.4072	395.6589	709	23.4209	4.4072	1425.6732	709	23.4209	4.4072	337.327	709	23.4209	4.4072	1497.7488
710	23.4469	4.4023	438.9148	710	23.4469	4.4023	1467.3944	710	23.4469	4.4023	415.0843	710	23.4469	4.4023	1574.1727
711	23.4729	4.3975	486.9484	711	23.4729	4.3975	1513.8931	711	23.4729	4.3975	370.5314	711	23.4729	4.3975	1528.2862
712	23.4989	4.3927	473.5755	712	23.4989	4.3927	1498.9855	712	23.4989	4.3927	431.0199	712	23.4989	4.3927	1587.4412
713	23.5249	4.388	568.5929	713	23.5249	4.388	1592.4681	713	23.5249	4.388	429.3648	713	23.5249	4.388	1584.4527
714	23.5509	4.3832	689.5591	714	23.5509	4.3832	1711.8995	714	23.5509	4.3832	456.157	714	23.5509	4.3832	1609.9114
715	23.5769	4.3784	698.3634	715	23.5769	4.3784	1719.169	715	23.5769	4.3784	438.523	715	23.5769	4.3784	1590.9439

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
716	23.6029	4.3737	777.6074	716	23.6029	4.3737	1796.8782	716	23.6029	4.3737	521.2242	716	23.6029	4.3737	1672.3116
717	23.6289	4.3689	887.5754	717	23.6289	4.3689	1905.3115	717	23.6289	4.3689	544.6806	717	23.6289	4.3689	1694.4346
718	23.6549	4.3642	961.0274	718	23.6549	4.3642	1977.2287	718	23.6549	4.3642	552.0081	718	23.6549	4.3642	1700.4286
719	23.6809	4.3595	1163.0082	719	23.6809	4.3595	2177.6747	719	23.6809	4.3595	604.709	719	23.6809	4.3595	1751.796
720	23.7069	4.3547	1299.2364	720	23.7069	4.3547	2312.3681	720	23.7069	4.3547	782.9573	720	23.7069	4.3547	1928.7108
721	23.7329	4.35	1439.8038	721	23.7329	4.35	2451.4008	721	23.7329	4.35	979.202	721	23.7329	4.35	2123.622
722	23.7589	4.3453	1616.7608	722	23.7589	4.3453	2626.823	722	23.7589	4.3453	1132.4334	722	23.7589	4.3453	2275.52
723	23.7849	4.3407	1728.4109	723	23.7849	4.3407	2736.9383	723	23.7849	4.3407	1119.4583	723	23.7849	4.3407	2261.2114
724	23.8109	4.336	1823.6685	724	23.8109	4.336	2830.6612	724	23.8109	4.336	963.2152	724	23.8109	4.336	2103.6348
725	23.8369	4.3313	1817.8706	725	23.8369	4.3313	2823.3285	725	23.8369	4.3313	776.1919	725	23.8369	4.3313	1915.278
726	23.8629	4.3267	1668.1298	726	23.8629	4.3267	2672.0528	726	23.8629	4.3267	593.8812	726	23.8629	4.3267	1731.6338
727	23.8889	4.322	1416.3939	727	23.8889	4.322	2418.7821	727	23.8889	4.322	578.6948	727	23.8889	4.322	1715.114
728	23.9149	4.3174	1291.3621	728	23.9149	4.3174	2292.2156	728	23.9149	4.3174	403.2344	728	23.9149	4.3174	1538.32
729	23.9409	4.3128	1161.8551	729	23.9409	4.3128	2161.1738	729	23.9409	4.3128	436.0112	729	23.9409	4.3128	1569.7634
730	23.9669	4.3082	944.9204	730	23.9669	4.3082	1942.7044	730	23.9669	4.3082	380.8498	730	23.9669	4.3082	1513.2685
731	23.9929	4.3036	849.0922	731	23.9929	4.3036	1844.38	731	23.9929	4.3036	359.1506	731	23.9929	4.3036	1487.4865
732	24.0189	4.299	730.6685	732	24.0189	4.299	1723.4602	732	24.0189	4.299	347.8108	732	24.0189	4.299	1472.0639
733	24.0449	4.2944	620.8055	733	24.0449	4.2944	1611.1012	733	24.0449	4.2944	379.2525	733	24.0449	4.2944	1499.4228
734	24.0709	4.2898	602.7431	734	24.0709	4.2898	1590.5426	734	24.0709	4.2898	391.2777	734	24.0709	4.2898	1507.3652
735	24.0969	4.2853	485.8002	735	24.0969	4.2853	1471.1037	735	24.0969	4.2853	405.4679	735	24.0969	4.2853	1517.4726
736	24.1229	4.2807	469.1843	736	24.1229	4.2807	1451.9917	736	24.1229	4.2807	426.8062	736	24.1229	4.2807	1534.7281
737	24.1489	4.2762	418.8498	737	24.1489	4.2762	1399.1611	737	24.1489	4.2762	362.9557	737	24.1489	4.2762	1466.7948
738	24.1749	4.2717	435.1083	738	24.1749	4.2717	1412.9235	738	24.1749	4.2717	401.909	738	24.1749	4.2717	1501.6652
739	24.2009	4.2671	417.3947	739	24.2009	4.2671	1392.7138	739	24.2009	4.2671	436.3266	739	24.2009	4.2671	1532
740	24.2269	4.2626	403.1793	740	24.2269	4.2626	1376.0023	740	24.2269	4.2626	459.0973	740	24.2269	4.2626	1550.6879
741	24.2529	4.2581	395.4955	741	24.2529	4.2581	1365.8224	741	24.2529	4.2581	459.3421	741	24.2529	4.2581	1546.8499
742	24.2789	4.2536	385.6934	742	24.2789	4.2536	1353.5242	742	24.2789	4.2536	476.0025	742	24.2789	4.2536	1559.4274
743	24.3049	4.2492	396.1432	743	24.3049	4.2492	1361.4779	743	24.3049	4.2492	507.8746	743	24.3049	4.2492	1587.2168
744	24.3309	4.2447	386.3293	744	24.3309	4.2447	1349.1679	744	24.3309	4.2447	529.9012	744	24.3309	4.2447	1605.1606
745	24.3569	4.2402	338.1174	745	24.3569	4.2402	1298.4599	745	24.3569	4.2402	510.404	745	24.3569	4.2402	1581.5805
746	24.3829	4.2358	293.6616	746	24.3829	4.2358	1251.508	746	24.3829	4.2358	529.7324	746	24.3829	4.2358	1596.8262
747	24.4089	4.2313	307.3624	747	24.4089	4.2313	1262.7127	747	24.4089	4.2313	445.5606	747	24.4089	4.2313	1508.5715
748	24.4349	4.2269	353.6079	748	24.4349	4.2269	1306.4621	748	24.4349	4.2269	383.7165	748	24.4349	4.2269	1442.6446
749	24.4609	4.2225	335.3294	749	24.4609	4.2225	1285.6875	749	24.4609	4.2225	431.311	749	24.4609	4.2225	1486.1563
750	24.4869	4.218	255.7269	750	24.4869	4.218	1203.5889	750	24.4869	4.218	455.2827	750	24.4869	4.218	1506.0452
751	24.5129	4.2136	236.6156	751	24.5129	4.2136	1181.9815	751	24.5129	4.2136	417.0321	751	24.5129	4.2136	1463.7118

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
752	24.5389	4.2092	270.5809	752	24.5389	4.2092	1213.4507	752	24.5389	4.2092	405.5638	752	24.5389	4.2092	1448.1606
753	24.5649	4.2049	279.0881	753	24.5649	4.2049	1219.4619	753	24.5649	4.2049	416.7169	753	24.5649	4.2049	1455.2309
754	24.5909	4.2005	262.438	754	24.5909	4.2005	1200.3157	754	24.5909	4.2005	420.2114	754	24.5909	4.2005	1454.6426
755	24.6169	4.1961	260.8787	755	24.6169	4.1961	1196.2603	755	24.6169	4.1961	413.1682	755	24.6169	4.1961	1443.5166
756	24.6429	4.1918	277.7446	756	24.6429	4.1918	1210.63	756	24.6429	4.1918	397.1044	756	24.6429	4.1918	1423.37
757	24.6689	4.1874	299.5805	757	24.6689	4.1874	1229.9699	757	24.6689	4.1874	380.8498	757	24.6689	4.1874	1403.0326
758	24.6949	4.1831	303.3526	758	24.6949	4.1831	1231.2459	758	24.6949	4.1831	382.3296	758	24.6949	4.1831	1402.2206
759	24.7209	4.1787	310.4066	759	24.7209	4.1787	1235.8038	759	24.7209	4.1787	351.9051	759	24.7209	4.1787	1369.5043
760	24.7469	4.1744	336.1956	760	24.7469	4.1744	1259.0967	760	24.7469	4.1744	341.273	760	24.7469	4.1744	1356.5804
761	24.7729	4.1701	322.1831	761	24.7729	4.1701	1242.5881	761	24.7729	4.1701	382.23	761	24.7729	4.1701	1395.2457
762	24.7989	4.1658	280.4731	762	24.7989	4.1658	1198.382	762	24.7989	4.1658	395.6485	762	24.7989	4.1658	1406.3723
763	24.8249	4.1615	272.2499	763	24.8249	4.1615	1187.6627	763	24.8249	4.1615	437.0894	763	24.8249	4.1615	1445.5214
764	24.8509	4.1572	311.1236	764	24.8509	4.1572	1224.0403	764	24.8509	4.1572	433.3751	764	24.8509	4.1572	1439.5153
765	24.8769	4.1529	309.0943	765	24.8769	4.1529	1219.5149	765	24.8769	4.1529	410.4425	765	24.8769	4.1529	1414.291
766	24.9029	4.1487	263.9416	766	24.9029	4.1487	1171.8661	766	24.9029	4.1487	408.3254	766	24.9029	4.1487	1409.8821
767	24.9289	4.1444	243.0044	767	24.9289	4.1444	1148.4329	767	24.9289	4.1444	392.5032	767	24.9289	4.1444	1391.7681
768	24.9549	4.1402	255.1055	768	24.9549	4.1402	1158.0378	768	24.9549	4.1402	412.8196	768	24.9549	4.1402	1409.7927
769	24.9809	4.1359	342.1199	769	24.9809	4.1359	1242.5562	769	24.9809	4.1359	375.7626	769	24.9809	4.1359	1370.4438
770	25.0069	4.1317	313.2354	770	25.0069	4.1317	1211.1755	770	25.0069	4.1317	352.1227	770	25.0069	4.1317	1344.5121
771	25.0329	4.1275	271.5059	771	25.0329	4.1275	1166.9499	771	25.0329	4.1275	336.9359	771	25.0329	4.1275	1327.0336
772	25.0589	4.1233	305.354	772	25.0589	4.1233	1198.3019	772	25.0589	4.1233	363.1443	772	25.0589	4.1233	1350.9503
773	25.0849	4.119	303.4079	773	25.0849	4.119	1193.8597	773	25.0849	4.119	376.4055	773	25.0849	4.119	1361.9196
774	25.1109	4.1148	310.8513	774	25.1109	4.1148	1198.8071	774	25.1109	4.1148	426.2223	774	25.1109	4.1148	1409.4446
775	25.1369	4.1107	296.3857	775	25.1369	4.1107	1181.8454	775	25.1369	4.1107	443.6556	775	25.1369	4.1107	1424.5862
776	25.1629	4.1065	327.1387	776	25.1629	4.1065	1210.1022	776	25.1629	4.1065	369.5728	776	25.1629	4.1065	1348.2115
777	25.1889	4.1023	327.2232	777	25.1889	4.1023	1207.6907	777	25.1889	4.1023	345.3527	777	25.1889	4.1023	1321.6997
778	25.2149	4.0982	308.0286	778	25.2149	4.0982	1186	778	25.2149	4.0982	375.1116	778	25.2149	4.0982	1349.1667
779	25.2409	4.094	316.4143	779	25.2409	4.094	1191.8896	779	25.2409	4.094	424.0806	779	25.2409	4.094	1395.8439
780	25.2669	4.0899	344.0306	780	25.2669	4.0899	1217.0098	780	25.2669	4.0899	382.5141	780	25.2669	4.0899	1351.9856
781	25.2929	4.0857	346.6739	781	25.2929	4.0857	1217.157	781	25.2929	4.0857	409.917	781	25.2929	4.0857	1377.0968
782	25.3189	4.0816	272.5116	782	25.3189	4.0816	1140.4986	782	25.3189	4.0816	395.393	782	25.3189	4.0816	1360.281
783	25.3449	4.0775	269.6568	783	25.3449	4.0775	1135.1477	783	25.3449	4.0775	418.4024	783	25.3449	4.0775	1380.9986
784	25.3709	4.0734	273.625	784	25.3709	4.0734	1136.6199	784	25.3709	4.0734	380.8498	784	25.3709	4.0734	1341.1542
785	25.3969	4.0693	313.435	785	25.3969	4.0693	1176.0351	785	25.3969	4.0693	389.1772	785	25.3969	4.0693	1348.7557
786	25.4229	4.0652	295.3265	786	25.4229	4.0652	1157.532	786	25.4229	4.0652	384.7904	786	25.4229	4.0652	1343.643
787	25.4489	4.0611	302.1731	787	25.4489	4.0611	1163.9838	787	25.4489	4.0611	325.7207	787	25.4489	4.0611	1283.8474

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
788	25.4749	4.057	278.7322	788	25.4749	4.057	1140.1483	788	25.4749	4.057	374.7889	788	25.4749	4.057	1332.1897
789	25.5009	4.0529	241.8462	789	25.5009	4.0529	1102.8676	789	25.5009	4.0529	413.0205	789	25.5009	4.0529	1369.6954
790	25.5269	4.0489	301.4011	790	25.5269	4.0489	1162.0279	790	25.5269	4.0489	344.7559	790	25.5269	4.0489	1300.7049
791	25.5529	4.0448	302.8946	791	25.5529	4.0448	1163.1267	791	25.5529	4.0448	397.2519	791	25.5529	4.0448	1352.475
792	25.5789	4.0408	278.6186	792	25.5789	4.0408	1138.456	792	25.5789	4.0408	329.0159	792	25.5789	4.0408	1283.5131
793	25.6049	4.0367	254.1235	793	25.6049	4.0367	1113.5662	793	25.6049	4.0367	365.2379	793	25.6049	4.0367	1319.0092
794	25.6309	4.0327	257.8204	794	25.6309	4.0327	1116.8684	794	25.6309	4.0327	371.8006	794	25.6309	4.0327	1324.846
795	25.6569	4.0287	267.8128	795	25.6569	4.0287	1126.4662	795	25.6569	4.0287	434.2511	795	25.6569	4.0287	1386.5705
796	25.6829	4.0247	331.8929	796	25.6829	4.0247	1190.1516	796	25.6829	4.0247	322.5542	796	25.6829	4.0247	1274.1478
797	25.7089	4.0207	243.2288	797	25.7089	4.0207	1101.0928	797	25.7089	4.0207	366.4285	797	25.7089	4.0207	1317.2961
798	25.7349	4.0167	288.7146	798	25.7349	4.0167	1146.1839	798	25.7349	4.0167	321.1791	798	25.7349	4.0167	1271.3208
799	25.7609	4.0127	290.7614	799	25.7609	4.0127	1147.836	799	25.7609	4.0127	364.9122	799	25.7609	4.0127	1314.328
800	25.7869	4.0087	292.4199	800	25.7869	4.0087	1149.0998	800	25.7869	4.0087	371.1844	800	25.7869	4.0087	1319.8743
801	25.8129	4.0048	327.928	801	25.8129	4.0048	1184.2132	801	25.8129	4.0048	390.441	801	25.8129	4.0048	1338.4051
802	25.8389	4.0008	254.4899	802	25.8389	4.0008	1110.3804	802	25.8389	4.0008	310.001	802	25.8389	4.0008	1257.2391
803	25.8649	3.9969	226.6045	803	25.8649	3.9969	1082.1004	803	25.8649	3.9969	364.2399	803	25.8649	3.9969	1310.7522
804	25.8909	3.9929	251.348	804	25.8909	3.9929	1106.4492	804	25.8909	3.9929	250.5876	804	25.8909	3.9929	1196.3739
805	25.9169	3.989	237.3164	805	25.9169	3.989	1092.0229	805	25.9169	3.989	380.0515	805	25.9169	3.989	1325.112
806	25.9429	3.985	325.8639	806	25.9429	3.985	1180.1758	806	25.9429	3.985	299.6447	806	25.9429	3.985	1243.9793
807	25.9689	3.9811	339.9038	807	25.9689	3.9811	1193.821	807	25.9689	3.9811	377.3861	807	25.9689	3.9811	1320.9947
808	25.9949	3.9772	272.9732	808	25.9949	3.9772	1126.4957	808	25.9949	3.9772	376.1319	808	25.9949	3.9772	1319.0146
809	26.0209	3.9733	243.3886	809	26.0209	3.9733	1096.5164	809	26.0209	3.9733	378.8088	809	26.0209	3.9733	1320.9656
810	26.0469	3.9694	296.7745	810	26.0469	3.9694	1149.5076	810	26.0469	3.9694	343.5731	810	26.0469	3.9694	1285.004
811	26.0729	3.9655	273.625	811	26.0729	3.9655	1125.9635	811	26.0729	3.9655	380.8498	811	26.0729	3.9655	1321.5548
812	26.0989	3.9616	253.5054	812	26.0989	3.9616	1104.9866	812	26.0989	3.9616	415.7971	812	26.0989	3.9616	1355.4027
813	26.1249	3.9578	252.4331	813	26.1249	3.9578	1103.0569	813	26.1249	3.9578	426.0385	813	26.1249	3.9578	1364.5448
814	26.1509	3.9539	286.8278	814	26.1509	3.9539	1136.5943	814	26.1509	3.9539	350.1394	814	26.1509	3.9539	1287.5464
815	26.1769	3.95	321.4814	815	26.1769	3.95	1170.3906	815	26.1769	3.95	354.0016	815	26.1769	3.95	1290.3093
816	26.2029	3.9462	292.9815	816	26.2029	3.9462	1141.0334	816	26.2029	3.9462	366.7516	816	26.2029	3.9462	1301.96
817	26.2289	3.9423	230.277	817	26.2289	3.9423	1077.4716	817	26.2289	3.9423	402.3171	817	26.2289	3.9423	1336.4261
818	26.2549	3.9385	275.5915	818	26.2549	3.9385	1121.9288	818	26.2549	3.9385	406.0968	818	26.2549	3.9385	1339.1065
819	26.2809	3.9347	255.1296	819	26.2809	3.9347	1100.6095	819	26.2809	3.9347	438.0144	819	26.2809	3.9347	1369.9248
820	26.3069	3.9309	296.9332	820	26.3069	3.9309	1141.5558	820	26.3069	3.9309	401.2541	820	26.3069	3.9309	1332.0652
821	26.3329	3.927	281.778	821	26.3329	3.927	1125.5433	821	26.3329	3.927	378.1502	821	26.3329	3.927	1307.8619
822	26.3589	3.9232	297.8756	822	26.3589	3.9232	1140.7836	822	26.3589	3.9232	400.2939	822	26.3589	3.9232	1328.9063
823	26.3849	3.9194	274.1014	823	26.3849	3.9194	1116.1521	823	26.3849	3.9194	420.6767	823	26.3849	3.9194	1348.1898

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
824	26.4109	3.9156	242.2862	824	26.4109	3.9156	1083.4795	824	26.4109	3.9156	418.7486	824	26.4109	3.9156	1345.1623
825	26.4369	3.9119	297.8182	825	26.4369	3.9119	1138.1543	825	26.4369	3.9119	414.5654	825	26.4369	3.9119	1339.8798
826	26.4629	3.9081	238.2515	826	26.4629	3.9081	1077.7302	826	26.4629	3.9081	450.6057	826	26.4629	3.9081	1374.8208
827	26.4889	3.9043	199.8614	827	26.4889	3.9043	1038.4828	827	26.4889	3.9043	414.0456	827	26.4889	3.9043	1337.1614
828	26.5149	3.9006	249.2459	828	26.5149	3.9006	1087.01	828	26.5149	3.9006	462.7591	828	26.5149	3.9006	1384.7755
829	26.5409	3.8968	279.7801	829	26.5409	3.8968	1116.6868	829	26.5409	3.8968	497.9071	829	26.5409	3.8968	1418.8242
830	26.5669	3.8931	301.2134	830	26.5669	3.8931	1137.2628	830	26.5669	3.8931	503.4078	830	26.5669	3.8931	1423.2256
831	26.5929	3.8893	275.4635	831	26.5929	3.8893	1110.6556	831	26.5929	3.8893	607.4887	831	26.5929	3.8893	1526.2071
832	26.6189	3.8856	226.6727	832	26.6189	3.8856	1061.0075	832	26.6189	3.8856	632.8351	832	26.6189	3.8856	1550.4543
833	26.6449	3.8819	247.2872	833	26.6449	3.8819	1080.7647	833	26.6449	3.8819	665.7342	833	26.6449	3.8819	1582.254
834	26.6709	3.8782	271.1355	834	26.6709	3.8782	1103.7557	834	26.6709	3.8782	857.8537	834	26.6709	3.8782	1773.2742
835	26.6969	3.8744	259.5665	835	26.6969	3.8744	1091.3294	835	26.6969	3.8744	1245.4936	835	26.6969	3.8744	2159.8148
836	26.7229	3.8707	249.8051	836	26.7229	3.8707	1080.7107	836	26.7229	3.8707	1741.2336	836	26.7229	3.8707	2654.4555
837	26.7489	3.8671	247.5418	837	26.7489	3.8671	1077.5901	837	26.7489	3.8671	2194.7167	837	26.7489	3.8671	3106.8392
838	26.7749	3.8634	314.533	838	26.7749	3.8634	1143.7239	838	26.7749	3.8634	2415.4173	838	26.7749	3.8634	3326.4405
839	26.8009	3.8597	369.3307	839	26.8009	3.8597	1197.6643	839	26.8009	3.8597	2393.3601	839	26.8009	3.8597	3303.2839
840	26.8269	3.856	334.2599	840	26.8269	3.856	1161.7362	840	26.8269	3.856	2072.1402	840	26.8269	3.856	2980.9647
841	26.8529	3.8524	293.7533	841	26.8529	3.8524	1120.3723	841	26.8529	3.8524	1623.5875	841	26.8529	3.8524	2531.3127
842	26.8789	3.8487	308.1756	842	26.8789	3.8487	1133.9373	842	26.8789	3.8487	1207.8887	842	26.8789	3.8487	2114.5146
843	26.9049	3.845	299.151	843	26.9049	3.845	1124.0554	843	26.9049	3.845	893.3349	843	26.9049	3.845	1798.8614
844	26.9309	3.8414	266.9812	844	26.9309	3.8414	1091.0283	844	26.9309	3.8414	808.6474	844	26.9309	3.8414	1713.0746
845	26.9569	3.8378	257.687	845	26.9569	3.8378	1080.8768	845	26.9569	3.8378	762.8718	845	26.9569	3.8378	1666.1997
846	26.9829	3.8341	252.8953	846	26.9829	3.8341	1075.2277	846	26.9829	3.8341	670.2051	846	26.9829	3.8341	1572.4337
847	27.0089	3.8305	279.2062	847	27.0089	3.8305	1100.6813	847	27.0089	3.8305	638.3224	847	27.0089	3.8305	1539.4517
848	27.0349	3.8269	311.2986	848	27.0349	3.8269	1131.9164	848	27.0349	3.8269	582.1966	848	27.0349	3.8269	1482.2265
849	27.0609	3.8233	268.6807	849	27.0609	3.8233	1088.4412	849	27.0609	3.8233	518.6336	849	27.0609	3.8233	1417.5642
850	27.0869	3.8197	245.7683	850	27.0869	3.8197	1064.6714	850	27.0869	3.8197	486.4655	850	27.0869	3.8197	1384.2968
851	27.1129	3.8161	248.5955	851	27.1129	3.8161	1066.6413	851	27.1129	3.8161	448.6636	851	27.1129	3.8161	1345.3956
852	27.1389	3.8125	259.3831	852	27.1389	3.8125	1076.5716	852	27.1389	3.8125	406.5661	852	27.1389	3.8125	1302.1987
853	27.1649	3.8089	263.3833	853	27.1649	3.8089	1079.7145	853	27.1649	3.8089	345.224	853	27.1649	3.8089	1239.7573
854	27.1909	3.8053	259.2075	854	27.1909	3.8053	1074.6814	854	27.1909	3.8053	343.352	854	27.1909	3.8053	1236.7859
855	27.2169	3.8018	243.9607	855	27.2169	3.8018	1058.5773	855	27.2169	3.8018	405.7734	855	27.2169	3.8018	1298.1081
856	27.2429	3.7982	251.997	856	27.2429	3.7982	1065.7562	856	27.2429	3.7982	411.492	856	27.2429	3.7982	1302.7273
857	27.2689	3.7947	273.5785	857	27.2689	3.7947	1086.4804	857	27.2689	3.7947	397.9683	857	27.2689	3.7947	1288.1043
858	27.2949	3.7911	283.8805	858	27.2949	3.7911	1095.9251	858	27.2949	3.7911	404.4804	858	27.2949	3.7911	1293.517
859	27.3209	3.7876	241.792	859	27.3209	3.7876	1052.9793	859	27.3209	3.7876	375.809	859	27.3209	3.7876	1263.7463

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
860	27.3469	3.7841	194.7283	860	27.3469	3.7841	1005.0583	860	27.3469	3.7841	362.9413	860	27.3469	3.7841	1249.7793
861	27.3729	3.7805	223.2668	861	27.3729	3.7805	1032.7395	861	27.3729	3.7805	362.9887	861	27.3729	3.7805	1248.7273
862	27.3989	3.777	272.7128	862	27.3989	3.777	1081.3282	862	27.3989	3.777	349.8435	862	27.3989	3.777	1234.4829
863	27.4249	3.7735	286.2337	863	27.4249	3.7735	1093.9918	863	27.4249	3.7735	392.7717	863	27.4249	3.7735	1276.3117
864	27.4509	3.77	260.2251	864	27.4509	3.77	1067.1259	864	27.4509	3.77	399.972	864	27.4509	3.77	1282.4127
865	27.4769	3.7665	273.625	865	27.4769	3.7665	1079.6685	865	27.4769	3.7665	380.8498	865	27.4769	3.7665	1262.1912
866	27.5029	3.763	264.8217	866	27.5029	3.763	1068.7948	866	27.5029	3.763	392.7054	866	27.5029	3.763	1272.8809
867	27.5289	3.7595	241.9816	867	27.5289	3.7595	1043.8845	867	27.5289	3.7595	354.7684	867	27.5289	3.7595	1233.7781
868	27.5549	3.756	262.0016	868	27.5549	3.756	1061.8342	868	27.5549	3.756	340.6455	868	27.5549	3.756	1218.4893
869	27.5809	3.7526	236.0903	869	27.5809	3.7526	1033.8526	869	27.5809	3.7526	346.8937	869	27.5809	3.7526	1223.5717
870	27.6069	3.7491	230.4698	870	27.6069	3.7491	1026.1618	870	27.6069	3.7491	376.407	870	27.6069	3.7491	1251.9191
871	27.6329	3.7456	261.3501	871	27.6329	3.7456	1054.9718	871	27.6329	3.7456	378.6072	871	27.6329	3.7456	1252.9535
872	27.6589	3.7422	258.3982	872	27.6589	3.7422	1049.9496	872	27.6589	3.7422	402.2276	872	27.6589	3.7422	1275.408
873	27.6849	3.7387	272.304	873	27.6849	3.7387	1061.7851	873	27.6849	3.7387	378.9854	873	27.6849	3.7387	1251
874	27.7109	3.7353	251.954	874	27.7109	3.7353	1039.3649	874	27.7109	3.7353	388.5972	874	27.7109	3.7353	1259.446
875	27.7369	3.7319	253.4128	875	27.7369	3.7319	1038.7533	875	27.7369	3.7319	389.2655	875	27.7369	3.7319	1258.9484
876	27.7629	3.7284	249.1817	876	27.7629	3.7284	1032.4519	876	27.7629	3.7284	366.9308	876	27.7629	3.7284	1235.4478
877	27.7889	3.725	269.118	877	27.7889	3.725	1050.3179	877	27.7889	3.725	376.013	877	27.7889	3.725	1243.3641
878	27.8149	3.7216	277.9443	878	27.8149	3.7216	1057.074	878	27.8149	3.7216	333.8517	878	27.8149	3.7216	1200.037
879	27.8409	3.7182	265.7755	879	27.8409	3.7182	1042.8349	879	27.8409	3.7182	347.2092	879	27.8409	3.7182	1212.2287
880	27.8669	3.7148	303.4024	880	27.8669	3.7148	1078.3915	880	27.8669	3.7148	397.8396	880	27.8669	3.7148	1261.6932
881	27.8929	3.7114	296.7356	881	27.8929	3.7114	1069.6544	881	27.8929	3.7114	351.2608	881	27.8929	3.7114	1213.9485
882	27.9189	3.708	273.1637	882	27.9189	3.708	1044.0123	882	27.9189	3.708	327.635	882	27.9189	3.708	1189.1569
883	27.9449	3.7046	299.9615	883	27.9449	3.7046	1068.7398	883	27.9449	3.7046	331.5796	883	27.9449	3.7046	1191.9357
884	27.9709	3.7013	302.2811	884	27.9709	3.7013	1068.9891	884	27.9709	3.7013	364.8553	884	27.9709	3.7013	1224.0455
885	27.9969	3.6979	297.9675	885	27.9969	3.6979	1062.6051	885	27.9969	3.6979	368.4643	885	27.9969	3.6979	1226.4886
886	28.0229	3.6945	313.8371	886	28.0229	3.6945	1076.4045	886	28.0229	3.6945	393.6108	886	28.0229	3.6945	1250.4693
887	28.0489	3.6912	249.2941	887	28.0489	3.6912	1009.7912	887	28.0489	3.6912	420.7816	887	28.0489	3.6912	1276.4743
888	28.0749	3.6878	252.1646	888	28.0749	3.6878	1010.5914	888	28.0749	3.6878	425.5859	888	28.0749	3.6878	1280.1127
889	28.1009	3.6845	261.0215	889	28.1009	3.6845	1017.378	889	28.1009	3.6845	347.3641	889	28.1009	3.6845	1200.7251
890	28.1269	3.6811	265.4301	890	28.1269	3.6811	1019.7163	890	28.1269	3.6811	371.133	890	28.1269	3.6811	1223.3281
891	28.1529	3.6778	271.2915	891	28.1529	3.6778	1023.5075	891	28.1529	3.6778	385.0007	891	28.1529	3.6778	1236.0299
892	28.1789	3.6745	273.625	892	28.1789	3.6745	1023.7707	892	28.1789	3.6745	380.8498	892	28.1789	3.6745	1230.7132
893	28.2049	3.6712	269.9569	893	28.2049	3.6712	1019.6151	893	28.2049	3.6712	310.5965	893	28.2049	3.6712	1157.4658
894	28.2309	3.6679	316.6171	894	28.2309	3.6679	1065.7879	894	28.2309	3.6679	353.3371	894	28.2309	3.6679	1197.2121
895	28.2569	3.6645	318.6508	895	28.2569	3.6645	1067.3341	895	28.2569	3.6645	344.039	895	28.2569	3.6645	1184.9199

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
896	28.2829	3.6612	223.368	896	28.2829	3.6612	971.5639	896	28.2829	3.6612	379.9937	896	28.2829	3.6612	1217.8805
897	28.3089	3.658	292.7569	897	28.3089	3.658	1040.4652	897	28.3089	3.658	380.0245	897	28.3089	3.658	1214.9171
898	28.3349	3.6547	282.5738	898	28.3349	3.6547	1029.7947	898	28.3349	3.6547	364.3069	898	28.3349	3.6547	1196.2053
899	28.3609	3.6514	301.8702	899	28.3609	3.6514	1048.6037	899	28.3609	3.6514	360.0739	899	28.3609	3.6514	1188.9781
900	28.3869	3.6481	326.9172	900	28.3869	3.6481	1073.1632	900	28.3869	3.6481	447.4616	900	28.3869	3.6481	1273.3717
901	28.4129	3.6448	300.7165	901	28.4129	3.6448	1046.475	901	28.4129	3.6448	373.8043	901	28.4129	3.6448	1196.7203
902	28.4389	3.6416	231.3298	902	28.4389	3.6416	976.6009	902	28.4389	3.6416	369.8375	902	28.4389	3.6416	1189.7592
903	28.4649	3.6383	290.0197	903	28.4649	3.6383	1034.8033	903	28.4649	3.6383	322.924	903	28.4649	3.6383	1139.8516
904	28.4909	3.6351	321.2894	904	28.4909	3.6351	1065.5856	904	28.4909	3.6351	345.1195	904	28.4909	3.6351	1159.0529
905	28.5169	3.6318	241.5222	905	28.5169	3.6318	985.3309	905	28.5169	3.6318	419.4879	905	28.5169	3.6318	1230.4271
906	28.5429	3.6286	285.0446	906	28.5429	3.6286	1028.3659	906	28.5429	3.6286	371.2825	906	28.5429	3.6286	1179.2276
907	28.5689	3.6253	302.8541	907	28.5689	3.6253	1045.6879	907	28.5689	3.6253	337.9853	907	28.5689	3.6253	1142.9363
908	28.5949	3.6221	273.6474	908	28.5949	3.6221	1015.9938	908	28.5949	3.6221	430.0264	908	28.5949	3.6221	1231.9832
909	28.6209	3.6189	261.2638	909	28.6209	3.6189	1003.1227	909	28.6209	3.6189	398.3679	909	28.6209	3.6189	1197.3305
910	28.6469	3.6157	252.8028	910	28.6469	3.6157	994.1743	910	28.6469	3.6157	376.5157	910	28.6469	3.6157	1172.4841
911	28.6729	3.6125	209.4339	911	28.6729	3.6125	950.3179	911	28.6729	3.6125	354.7579	911	28.6729	3.6125	1147.7322
912	28.6989	3.6093	321.0161	912	28.6989	3.6093	1061.4126	912	28.6989	3.6093	354.1375	912	28.6989	3.6093	1144.1176
913	28.7249	3.6061	250.0214	913	28.7249	3.6061	989.9305	913	28.7249	3.6061	441.6414	913	28.7249	3.6061	1228.6274
914	28.7509	3.6029	277.6296	914	28.7509	3.6029	1017.0512	914	28.7509	3.6029	436.7759	914	28.7509	3.6029	1220.7677
915	28.7769	3.5997	240.0318	915	28.7769	3.5997	978.9659	915	28.7769	3.5997	377.5548	915	28.7769	3.5997	1158.5524
916	28.8029	3.5965	298.346	916	28.8029	3.5965	1036.7928	916	28.8029	3.5965	426.6572	916	28.8029	3.5965	1204.6606
917	28.8289	3.5933	224.7681	917	28.8289	3.5933	962.7273	917	28.8289	3.5933	405.7441	917	28.8289	3.5933	1180.7534
918	28.8549	3.5902	249.9735	918	28.8549	3.5902	987.4453	918	28.8549	3.5902	350.1069	918	28.8549	3.5902	1122.122
919	28.8809	3.587	273.625	919	28.8809	3.587	1010.6094	919	28.8809	3.587	380.8498	919	28.8809	3.587	1149.8707
920	28.9069	3.5838	238.5176	920	28.9069	3.5838	974.2178	920	28.9069	3.5838	414.9466	920	28.9069	3.5838	1184.8495
921	28.9329	3.5807	272.9295	921	28.9329	3.5807	1007.3456	921	28.9329	3.5807	452.2034	921	28.9329	3.5807	1222.9881
922	28.9589	3.5775	254.8826	922	28.9589	3.5775	988.0145	922	28.9589	3.5775	348.6373	922	28.9589	3.5775	1120.3039
923	28.9849	3.5744	265.7785	923	28.9849	3.5744	997.6263	923	28.9849	3.5744	335.5613	923	28.9849	3.5744	1108.1099
924	29.0109	3.5713	299.7384	924	29.0109	3.5713	1030.3021	924	29.0109	3.5713	336.4112	924	29.0109	3.5713	1109.8417
925	29.0369	3.5681	300.066	925	29.0369	3.5681	1029.3456	925	29.0369	3.5681	373.1187	925	29.0369	3.5681	1147.4311
926	29.0629	3.565	267.1294	926	29.0629	3.565	995.1248	926	29.0629	3.565	342.8211	926	29.0629	3.565	1118.0154
927	29.0889	3.5619	322.1855	927	29.0889	3.5619	1048.8968	927	29.0889	3.5619	406.188	927	29.0889	3.5619	1182.2642
928	29.1149	3.5588	264.5877	928	29.1149	3.5588	990.0148	928	29.1149	3.5588	385.9503	928	29.1149	3.5588	1162.9084
929	29.1409	3.5557	247.0648	929	29.1409	3.5557	971.2079	929	29.1409	3.5557	372.9915	929	29.1409	3.5557	1150.8315
930	29.1669	3.5526	283.3396	930	29.1669	3.5526	1006.1986	930	29.1669	3.5526	383.0109	930	29.1669	3.5526	1161.7329
931	29.1929	3.5495	323.7714	931	29.1929	3.5495	1045.3462	931	29.1929	3.5495	365.3172	931	29.1929	3.5495	1144.921

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
932	29.2189	3.5464	302.4532	932	29.2189	3.5464	1022.7438	932	29.2189	3.5464	325.7334	932	29.2189	3.5464	1106.2191
933	29.2449	3.5433	287.2217	933	29.2449	3.5433	1006.2282	933	29.2449	3.5433	375.5786	933	29.2449	3.5433	1156.9463
934	29.2709	3.5402	313.0076	934	29.2709	3.5402	1030.73	934	29.2709	3.5402	402.1754	934	29.2709	3.5402	1184.425
935	29.2969	3.5372	310.3753	935	29.2969	3.5372	1026.8136	935	29.2969	3.5372	407.5314	935	29.2969	3.5372	1190.6629
936	29.3229	3.5341	314.0724	936	29.3229	3.5341	1029.2266	936	29.3229	3.5341	361.0139	936	29.3229	3.5341	1145.0273
937	29.3489	3.531	333.8101	937	29.3489	3.531	1047.6802	937	29.3489	3.531	400.5489	937	29.3489	3.531	1185.4442
938	29.3749	3.528	294.3257	938	29.3749	3.528	1006.9116	938	29.3749	3.528	383.8653	938	29.3749	3.528	1169.6425
939	29.4009	3.5249	294.4063	939	29.4009	3.5249	1005.708	939	29.4009	3.5249	348.3257	939	29.4009	3.5249	1134.9849
940	29.4269	3.5219	309.4461	940	29.4269	3.5219	1019.4637	940	29.4269	3.5219	355.8502	940	29.4269	3.5219	1143.3912
941	29.4529	3.5188	324.0352	941	29.4529	3.5188	1032.7687	941	29.4529	3.5188	378.7301	941	29.4529	3.5188	1167.1531
942	29.4789	3.5158	329.2244	942	29.4789	3.5158	1036.6738	942	29.4789	3.5158	392.9895	942	29.4789	3.5158	1182.2943
943	29.5049	3.5128	311.5452	943	29.5049	3.5128	1017.7104	943	29.5049	3.5128	344.8636	943	29.5049	3.5128	1135.0504
944	29.5309	3.5097	288.3235	944	29.5309	3.5097	993.2046	944	29.5309	3.5097	308.5687	944	29.5309	3.5097	1099.6374
945	29.5569	3.5067	272.536	945	29.5569	3.5067	976.133	945	29.5569	3.5067	304.3161	945	29.5569	3.5067	1096.2667
946	29.5829	3.5037	297.9885	946	29.5829	3.5037	1000.3014	946	29.5829	3.5037	380.8498	946	29.5829	3.5037	1173.6823
947	29.6089	3.5007	296.7254	947	29.6089	3.5007	997.7541	947	29.6089	3.5007	375.8617	947	29.6089	3.5007	1166.6245
948	29.6349	3.4977	274.9944	948	29.6349	3.4977	974.739	948	29.6349	3.4977	353.9643	948	29.6349	3.4977	1142.6574
949	29.6609	3.4947	255.2915	949	29.6609	3.4947	953.752	949	29.6609	3.4947	354.6589	949	29.6609	3.4947	1141.2823
950	29.6869	3.4917	320.3755	950	29.6869	3.4917	1017.5518	950	29.6869	3.4917	317.0054	950	29.6869	3.4917	1101.5591
951	29.7129	3.4887	345.4167	951	29.7129	3.4887	1041.3089	951	29.7129	3.4887	322.0595	951	29.7129	3.4887	1104.5435
952	29.7389	3.4857	311.8583	952	29.7389	3.4857	1006.4664	952	29.7389	3.4857	386.8782	952	29.7389	3.4857	1167.2925
953	29.7649	3.4828	326.4971	953	29.7649	3.4828	1019.821	953	29.7649	3.4828	369.0276	953	29.7649	3.4828	1147.3721
954	29.7909	3.4798	351.8567	954	29.7909	3.4798	1043.8965	954	29.7909	3.4798	343.4146	954	29.7909	3.4798	1119.6895
955	29.8169	3.4768	292.6142	955	29.8169	3.4768	983.3699	955	29.8169	3.4768	371.1482	955	29.8169	3.4768	1145.3533
956	29.8429	3.4739	248.5369	956	29.8429	3.4739	938.0084	956	29.8429	3.4739	371.7593	956	29.8429	3.4739	1143.8947
957	29.8689	3.4709	275.2412	957	29.8689	3.4709	963.4286	957	29.8689	3.4709	341.877	957	29.8689	3.4709	1111.9428
958	29.8949	3.468	268.4002	958	29.8949	3.468	955.3035	958	29.8949	3.468	343.1611	958	29.8949	3.468	1111.1572
959	29.9209	3.465	242.9308	959	29.9209	3.465	928.55	959	29.9209	3.465	369.9959	959	29.9209	3.465	1135.9222
960	29.9469	3.4621	272.6124	960	29.9469	3.4621	956.9475	960	29.9469	3.4621	356.8554	960	29.9469	3.4621	1120.712
961	29.9729	3.4592	313.2205	961	29.9729	3.4592	996.2714	961	29.9729	3.4592	300.0928	961	29.9729	3.4592	1061.8797
962	29.9989	3.4562	317.3745	962	29.9989	3.4562	999.1413	962	29.9989	3.4562	299.5276	962	29.9989	3.4562	1059.2448
963	30.0249	3.4533	296.9629	963	30.0249	3.4533	977.4456	963	30.0249	3.4533	345.1715	963	30.0249	3.4533	1102.819
964	30.0509	3.4504	268.129	964	30.0509	3.4504	947.3275	964	30.0509	3.4504	344.0842	964	30.0509	3.4504	1099.662
965	30.0769	3.4475	267.1744	965	30.0769	3.4475	945.0887	965	30.0769	3.4475	332.9683	965	30.0769	3.4475	1086.4764
966	30.1029	3.4446	286.1445	966	30.1029	3.4446	962.7747	966	30.1029	3.4446	317.2119	966	30.1029	3.4446	1068.6503
967	30.1289	3.4417	287.7868	967	30.1289	3.4417	963.133	967	30.1289	3.4417	362.6652	967	30.1289	3.4417	1112.0338

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
968	30.1549	3.4388	261.6197	968	30.1549	3.4388	935.6817	968	30.1549	3.4388	413.7205	968	30.1549	3.4388	1161.0194
969	30.1809	3.4359	274.9115	969	30.1809	3.4359	947.6894	969	30.1809	3.4359	366.2377	969	30.1809	3.4359	1111.4669
970	30.2069	3.433	296.6266	970	30.2069	3.433	968.1204	970	30.2069	3.433	374.8671	970	30.2069	3.433	1118.0266
971	30.2329	3.4301	281.6793	971	30.2329	3.4301	951.8889	971	30.2329	3.4301	378.3876	971	30.2329	3.4301	1119.4774
972	30.2589	3.4272	292.1873	972	30.2589	3.4272	961.1128	972	30.2589	3.4272	357.2326	972	30.2589	3.4272	1096.2527
973	30.2849	3.4243	273.625	973	30.2849	3.4243	941.2664	973	30.2849	3.4243	380.8498	973	30.2849	3.4243	1117.8002
974	30.3109	3.4215	305.748	974	30.3109	3.4215	972.847	974	30.3109	3.4215	379.3639	974	30.3109	3.4215	1114.4193
975	30.3369	3.4186	317.8745	975	30.3369	3.4186	984.4313	975	30.3369	3.4186	364.6913	975	30.3369	3.4186	1097.8517
976	30.3629	3.4157	275.4406	976	30.3629	3.4157	941.4551	976	30.3629	3.4157	328.9696	976	30.3629	3.4157	1060.2349
977	30.3889	3.4129	322.3169	977	30.3889	3.4129	987.7891	977	30.3889	3.4129	351.9475	977	30.3889	3.4129	1081.3179
978	30.4149	3.41	336.4253	978	30.4149	3.41	1001.3552	978	30.4149	3.41	374.1003	978	30.4149	3.41	1101.5757
979	30.4409	3.4072	361.7405	979	30.4409	3.4072	1026.1281	979	30.4409	3.4072	363.4917	979	30.4409	3.4072	1089.072
980	30.4669	3.4044	315.5749	980	30.4669	3.4044	979.4203	980	30.4669	3.4044	379.7552	980	30.4669	3.4044	1103.4405
981	30.4929	3.4015	290.86	981	30.4929	3.4015	954.1631	981	30.4929	3.4015	387.8121	981	30.4929	3.4015	1109.6023
982	30.5189	3.3987	263.9795	982	30.5189	3.3987	926.7403	982	30.5189	3.3987	377.9161	982	30.5189	3.3987	1097.8113
983	30.5449	3.3959	261.2397	983	30.5449	3.3959	923.4582	983	30.5449	3.3959	448.6504	983	30.5449	3.3959	1166.6507
984	30.5709	3.3931	282.1352	984	30.5709	3.3931	943.8114	984	30.5709	3.3931	384.5761	984	30.5709	3.3931	1100.6813
985	30.5969	3.3902	277.6694	985	30.5969	3.3902	938.8033	985	30.5969	3.3902	396.0605	985	30.5969	3.3902	1110.2707
986	30.6229	3.3874	289.8158	986	30.6229	3.3874	950.4075	986	30.6229	3.3874	374.0762	986	30.6229	3.3874	1086.3914
987	30.6489	3.3846	259.5472	987	30.6489	3.3846	919.5966	987	30.6489	3.3846	327.7339	987	30.6489	3.3846	1038.1541
988	30.6749	3.3818	320.2135	988	30.6749	3.3818	979.7206	988	30.6749	3.3818	293.0995	988	30.6749	3.3818	1001.6247
989	30.7009	3.379	338.5772	989	30.7009	3.379	997.5419	989	30.7009	3.379	409.8763	989	30.7009	3.379	1116.5064
990	30.7269	3.3762	355.0723	990	30.7269	3.3762	1013.4948	990	30.7269	3.3762	377.417	990	30.7269	3.3762	1082.1522
991	30.7529	3.3735	361.589	991	30.7529	3.3735	1019.4692	991	30.7529	3.3735	361.7913	991	30.7529	3.3735	1064.6315
992	30.7789	3.3707	348.3055	992	30.7789	3.3707	1005.6435	992	30.7789	3.3707	447.4012	992	30.7789	3.3707	1148.3463
993	30.8049	3.3679	285.4497	993	30.8049	3.3679	942.2453	993	30.8049	3.3679	475.1377	993	30.8049	3.3679	1174.1878
994	30.8309	3.3651	262.1084	994	30.8309	3.3651	918.3617	994	30.8309	3.3651	453.2031	994	30.8309	3.3651	1150.3582
995	30.8569	3.3624	328.1131	995	30.8569	3.3624	983.8241	995	30.8569	3.3624	506.5234	995	30.8569	3.3624	1201.7834
996	30.8829	3.3596	301.6719	996	30.8829	3.3596	956.8407	996	30.8829	3.3596	570.0009	996	30.8829	3.3596	1263.3659
997	30.9089	3.3568	378.4428	997	30.9089	3.3568	1033.0693	997	30.9089	3.3568	607.547	997	30.9089	3.3568	1299.017
998	30.9349	3.3541	346.8596	998	30.9349	3.3541	1000.9438	998	30.9349	3.3541	543.5139	998	30.9349	3.3541	1233.0889
999	30.9609	3.3513	385.3364	999	30.9609	3.3513	1038.8783	999	30.9609	3.3513	503.1486	999	30.9609	3.3513	1190.8286
1000	30.9869	3.3486	356.124	1000	30.9869	3.3486	1009.1237	1000	30.9869	3.3486	560.0654	1000	30.9869	3.3486	1245.8504
1001	31.0129	3.3459	342.0254	1001	31.0129	3.3459	994.4828	1001	31.0129	3.3459	473.1469	1001	31.0129	3.3459	1157.0369
1002	31.0389	3.3431	283.05	1002	31.0389	3.3431	934.9651	1002	31.0389	3.3431	431.2587	1002	31.0389	3.3431	1113.2537
1003	31.0649	3.3404	364.007	1003	31.0649	3.3404	1015.3798	1003	31.0649	3.3404	475.6434	1003	31.0649	3.3404	1155.7433

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1004	31.0909	3.3377	338.5051	1004	31.0909	3.3377	989.3356	1004	31.0909	3.3377	439.0213	1004	31.0909	3.3377	1117.2262
1005	31.1169	3.3349	346.4721	1005	31.1169	3.3349	996.7604	1005	31.1169	3.3349	405.0818	1005	31.1169	3.3349	1081.3917
1006	31.1429	3.3322	365.355	1006	31.1429	3.3322	1015.1009	1006	31.1429	3.3322	392.7932	1006	31.1429	3.3322	1067.2081
1007	31.1689	3.3295	335.5596	1007	31.1689	3.3295	984.7633	1007	31.1689	3.3295	436.1166	1007	31.1689	3.3295	1108.6365
1008	31.1949	3.3268	377.1653	1008	31.1949	3.3268	1025.8267	1008	31.1949	3.3268	418.5897	1008	31.1949	3.3268	1089.2145
1009	31.2209	3.3241	356.916	1009	31.2209	3.3241	1005.0351	1009	31.2209	3.3241	446.2267	1009	31.2209	3.3241	1114.9566
1010	31.2469	3.3214	367.3073	1010	31.2469	3.3214	1014.8841	1010	31.2469	3.3214	451.1304	1010	31.2469	3.3214	1117.9652
1011	31.2729	3.3187	313.1703	1011	31.2729	3.3187	960.2049	1011	31.2729	3.3187	375.7599	1011	31.2729	3.3187	1040.6997
1012	31.2989	3.316	399.6784	1012	31.2989	3.316	1046.1706	1012	31.2989	3.316	416.6348	1012	31.2989	3.316	1079.6796
1013	31.3249	3.3134	358.9526	1013	31.3249	3.3134	1004.9026	1013	31.3249	3.3134	500.376	1013	31.3249	3.3134	1161.5258
1014	31.3509	3.3107	302.5667	1014	31.3509	3.3107	947.9744	1014	31.3509	3.3107	387.1555	1014	31.3509	3.3107	1046.4103
1015	31.3769	3.308	371.4831	1015	31.3769	3.308	1016.3484	1015	31.3769	3.308	388.273	1015	31.3769	3.308	1045.6328
1016	31.4029	3.3053	397.1121	1016	31.4029	3.3053	1041.4352	1016	31.4029	3.3053	428.619	1016	31.4029	3.3053	1084.0838
1017	31.4289	3.3027	310.081	1017	31.4289	3.3027	953.8618	1017	31.4289	3.3027	449.9714	1017	31.4289	3.3027	1103.5411
1018	31.4549	3.3	270.0365	1018	31.4549	3.3	913.275	1018	31.4549	3.3	426.0544	1018	31.4549	3.3	1077.7291
1019	31.4809	3.2973	288.8823	1019	31.4809	3.2973	931.5785	1019	31.4809	3.2973	392.8525	1019	31.4809	3.2973	1042.6322
1020	31.5069	3.2947	279.3975	1020	31.5069	3.2947	921.5514	1020	31.5069	3.2947	422.2367	1020	31.5069	3.2947	1070.1214
1021	31.5329	3.292	345.2122	1021	31.5329	3.292	986.8239	1021	31.5329	3.292	401.6325	1021	31.5329	3.292	1047.6222
1022	31.5589	3.2894	303.6396	1022	31.5589	3.2894	944.709	1022	31.5589	3.2894	377.3025	1022	31.5589	3.2894	1021.3972
1023	31.5849	3.2868	329.9902	1023	31.5849	3.2868	970.5173	1023	31.5849	3.2868	411.8959	1023	31.5849	3.2868	1054.0955
1024	31.6109	3.2841	247.6677	1024	31.6109	3.2841	887.6525	1024	31.6109	3.2841	412.8994	1024	31.6109	3.2841	1053.204
1025	31.6369	3.2815	313.996	1025	31.6369	3.2815	953.4385	1025	31.6369	3.2815	495.0289	1025	31.6369	3.2815	1133.4385
1026	31.6629	3.2789	290.2765	1026	31.6629	3.2789	929.1768	1026	31.6629	3.2789	475.1511	1026	31.6629	3.2789	1111.6657
1027	31.6889	3.2763	273.625	1027	31.6889	3.2763	911.983	1027	31.6889	3.2763	380.8498	1027	31.6889	3.2763	1015.4694
1028	31.7149	3.2736	315.1815	1028	31.7149	3.2736	952.1099	1028	31.7149	3.2736	443.4619	1028	31.7149	3.2736	1081.0296
1029	31.7409	3.271	304.9044	1029	31.7409	3.271	940.4032	1029	31.7409	3.271	409.2918	1029	31.7409	3.271	1049.8075
1030	31.7669	3.2684	342.7987	1030	31.7669	3.2684	976.8679	1030	31.7669	3.2684	433.8242	1030	31.7669	3.2684	1077.288
1031	31.7929	3.2658	288.2771	1031	31.7929	3.2658	920.9167	1031	31.7929	3.2658	362.8042	1031	31.7929	3.2658	1009.2161
1032	31.8189	3.2632	293.8935	1032	31.8189	3.2632	925.1035	1032	31.8189	3.2632	409.2609	1032	31.8189	3.2632	1058.6208
1033	31.8449	3.2606	343.2701	1033	31.8449	3.2606	973.0505	1033	31.8449	3.2606	425.4114	1033	31.8449	3.2606	1077.7194
1034	31.8709	3.258	278.1204	1034	31.8709	3.258	906.4712	1034	31.8709	3.258	460.0078	1034	31.8709	3.258	1115.2639
1035	31.8969	3.2554	267.8858	1035	31.8969	3.2554	894.807	1035	31.8969	3.2554	372.8101	1035	31.8969	3.2554	1031.0142
1036	31.9229	3.2529	283.2735	1036	31.9229	3.2529	908.7651	1036	31.9229	3.2529	370.1779	1036	31.9229	3.2529	1031.3301
1037	31.9489	3.2503	251.9127	1037	31.9489	3.2503	875.9748	1037	31.9489	3.2503	397.9124	1037	31.9489	3.2503	1062.0126
1038	31.9749	3.2477	282.7131	1038	31.9749	3.2477	905.3455	1038	31.9749	3.2477	387.0295	1038	31.9749	3.2477	1054.0778
1039	32.0009	3.2451	257.6556	1039	32.0009	3.2451	878.8584	1039	32.0009	3.2451	350.6779	1039	32.0009	3.2451	1020.6742

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1040	32.0269	3.2426	253.3508	1040	32.0269	3.2426	873.124	1040	32.0269	3.2426	380.9535	1040	32.0269	3.2426	1053.898
1041	32.0529	3.24	259.9755	1041	32.0529	3.24	878.3192	1041	32.0529	3.24	362.7051	1041	32.0529	3.24	1038.5976
1042	32.0789	3.2374	293.9597	1042	32.0789	3.2374	910.8738	1042	32.0789	3.2374	365.2989	1042	32.0789	3.2374	1044.1395
1043	32.1049	3.2349	279.7889	1043	32.1049	3.2349	895.2734	1043	32.1049	3.2349	336.197	1043	32.1049	3.2349	1017.9856
1044	32.1309	3.2323	219.3717	1044	32.1309	3.2323	833.4266	1044	32.1309	3.2323	321.4249	1044	32.1309	3.2323	1006.1615
1045	32.1569	3.2298	248.306	1045	32.1569	3.2298	860.9313	1045	32.1569	3.2298	337.0612	1045	32.1569	3.2298	1024.7459
1046	32.1829	3.2273	291.4284	1046	32.1829	3.2273	902.6241	1046	32.1829	3.2273	364.4593	1046	32.1829	3.2273	1055.0921
1047	32.2089	3.2247	302.719	1047	32.2089	3.2247	912.4851	1047	32.2089	3.2247	338.3848	1047	32.2089	3.2247	1031.9656
1048	32.2349	3.2222	325.8384	1048	32.2349	3.2222	934.1749	1048	32.2349	3.2222	326.921	1048	32.2349	3.2222	1023.4499
1049	32.2609	3.2197	317.2385	1049	32.2609	3.2197	924.1454	1049	32.2609	3.2197	362.5949	1049	32.2609	3.2197	1062.0719
1050	32.2869	3.2171	296.4245	1050	32.2869	3.2171	901.9018	1050	32.2869	3.2171	336.3943	1050	32.2869	3.2171	1038.8194
1051	32.3129	3.2146	284.2284	1051	32.3129	3.2146	888.2761	1051	32.3129	3.2146	330.9617	1051	32.3129	3.2146	1036.3349
1052	32.3389	3.2121	316.5404	1052	32.3389	3.2121	919.1586	1052	32.3389	3.2121	329.3853	1052	32.3389	3.2121	1037.7065
1053	32.3649	3.2096	290.1984	1053	32.3649	3.2096	891.3869	1053	32.3649	3.2096	358.2323	1053	32.3649	3.2096	1069.5016
1054	32.3909	3.2071	273.625	1054	32.3909	3.2071	873.384	1054	32.3909	3.2071	380.8498	1054	32.3909	3.2071	1095.0671
1055	32.4169	3.2046	306.3877	1055	32.4169	3.2046	906.4638	1055	32.4169	3.2046	339.7386	1055	32.4169	3.2046	1053.9439
1056	32.4429	3.2021	303.3072	1056	32.4429	3.2021	903.7005	1056	32.4429	3.2021	329.8942	1056	32.4429	3.2021	1044.0874
1057	32.4689	3.1996	264.6645	1057	32.4689	3.1996	865.375	1057	32.4689	3.1996	362.0027	1057	32.4689	3.1996	1076.1838
1058	32.4949	3.1971	252.7758	1058	32.4949	3.1971	853.8034	1058	32.4949	3.1971	343.0299	1058	32.4949	3.1971	1057.199
1059	32.5209	3.1946	279.2194	1059	32.5209	3.1946	880.5642	1059	32.5209	3.1946	323.9006	1059	32.5209	3.1946	1038.0576
1060	32.5469	3.1921	296.784	1060	32.5469	3.1921	898.446	1060	32.5469	3.1921	326.0247	1060	32.5469	3.1921	1040.1696
1061	32.5729	3.1896	321.7275	1061	32.5729	3.1896	923.7066	1061	32.5729	3.1896	311.4906	1061	32.5729	3.1896	1025.6234
1062	32.5989	3.1872	331.9476	1062	32.5989	3.1872	934.2439	1062	32.5989	3.1872	304.5721	1062	32.5989	3.1872	1018.6929
1063	32.6249	3.1847	312.2987	1063	32.6249	3.1847	914.9122	1063	32.6249	3.1847	295.341	1063	32.6249	3.1847	1009.4497
1064	32.6509	3.1822	296.5646	1064	32.6509	3.1822	899.4953	1064	32.6509	3.1822	302.4815	1064	32.6509	3.1822	1016.5781
1065	32.6769	3.1798	305.5581	1065	32.6769	3.1798	908.806	1065	32.6769	3.1798	306.0777	1065	32.6769	3.1798	1020.1623
1066	32.7029	3.1773	314.9901	1066	32.7029	3.1773	918.5552	1066	32.7029	3.1773	306.3724	1066	32.7029	3.1773	1020.4448
1067	32.7289	3.1749	282.1241	1067	32.7289	3.1749	886.0063	1067	32.7289	3.1749	326.2483	1067	32.7289	3.1749	1040.3087
1068	32.7549	3.1724	270.1039	1068	32.7549	3.1724	874.3033	1068	32.7549	3.1724	302.0673	1068	32.7549	3.1724	1016.1156
1069	32.7809	3.17	278.5134	1069	32.7809	3.17	883.0299	1069	32.7809	3.17	312.8749	1069	32.7809	3.17	1026.9111
1070	32.8069	3.1675	286.9178	1070	32.8069	3.1675	891.7515	1070	32.8069	3.1675	365.1491	1070	32.8069	3.1675	1079.1733
1071	32.8329	3.1651	291.6154	1071	32.8329	3.1651	896.7663	1071	32.8329	3.1651	334.662	1071	32.8329	3.1651	1048.6741
1072	32.8589	3.1626	288.0532	1072	32.8589	3.1626	893.5213	1072	32.8589	3.1626	316.3448	1072	32.8589	3.1626	1030.3448
1073	32.8849	3.1602	274.7652	1073	32.8849	3.1602	880.5505	1073	32.8849	3.1602	319.3827	1073	32.8849	3.1602	1033.3707
1074	32.9109	3.1578	261.7172	1074	32.9109	3.1578	867.8196	1074	32.9109	3.1578	312.0316	1074	32.9109	3.1578	1026.0075
1075	32.9369	3.1554	283.744	1075	32.9369	3.1554	890.1635	1075	32.9369	3.1554	333.6834	1075	32.9369	3.1554	1047.6472

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1076	32.9629	3.1529	314.2493	1076	32.9629	3.1529	920.9861	1076	32.9629	3.1529	326.0313	1076	32.9629	3.1529	1039.983
1077	32.9889	3.1505	279.2725	1077	32.9889	3.1505	886.3265	1077	32.9889	3.1505	294.9786	1077	32.9889	3.1505	1008.9182
1078	33.0149	3.1481	311.7259	1078	33.0149	3.1481	919.097	1078	33.0149	3.1481	339.8576	1078	33.0149	3.1481	1053.7851
1079	33.0409	3.1457	309.4404	1079	33.0409	3.1457	917.1287	1079	33.0409	3.1457	316.7941	1079	33.0409	3.1457	1030.7096
1080	33.0669	3.1433	270.4546	1080	33.0669	3.1433	878.46	1080	33.0669	3.1433	325.0735	1080	33.0669	3.1433	1038.9769
1081	33.0929	3.1409	291.431	1081	33.0929	3.1409	899.7537	1081	33.0929	3.1409	380.8498	1081	33.0929	3.1409	1094.7411
1082	33.1189	3.1385	283.7456	1082	33.1189	3.1385	891.672	1082	33.1189	3.1385	355.8268	1082	33.1189	3.1385	1070.8479
1083	33.1449	3.1361	300.7727	1083	33.1449	3.1361	908.3029	1083	33.1449	3.1361	319.8491	1083	33.1449	3.1361	1036
1084	33.1709	3.1337	304.5905	1084	33.1709	3.1337	911.7245	1084	33.1709	3.1337	298.8951	1084	33.1709	3.1337	1016.1757
1085	33.1969	3.1313	332.0735	1085	33.1969	3.1313	938.8113	1085	33.1969	3.1313	261.815	1085	33.1969	3.1313	980.2254
1086	33.2229	3.129	301.2652	1086	33.2229	3.129	907.6068	1086	33.2229	3.129	318.6815	1086	33.2229	3.129	1038.2216
1087	33.2489	3.1266	332.6058	1087	33.2489	3.1266	938.5512	1087	33.2489	3.1266	298.935	1087	33.2489	3.1266	1019.6049
1088	33.2749	3.1242	311.7198	1088	33.2749	3.1242	917.2689	1088	33.2749	3.1242	342.1178	1088	33.2749	3.1242	1063.9175
1089	33.3009	3.1218	252.1198	1089	33.3009	3.1218	857.2727	1089	33.3009	3.1218	306.1615	1089	33.3009	3.1218	1029.0909
1090	33.3269	3.1195	296.1562	1090	33.3269	3.1195	900.9129	1090	33.3269	3.1195	363.1418	1090	33.3269	3.1195	1087.2011
1091	33.3529	3.1171	286.8428	1091	33.3529	3.1171	891.2033	1091	33.3529	3.1171	375.3726	1091	33.3529	3.1171	1100.5616
1092	33.3789	3.1147	316.5888	1092	33.3789	3.1147	920.5531	1092	33.3789	3.1147	311.4689	1092	33.3789	3.1147	1037.7876
1093	33.4049	3.1124	310.2127	1093	33.4049	3.1124	913.7808	1093	33.4049	3.1124	352.1004	1093	33.4049	3.1124	1079.5489
1094	33.4309	3.11	327.0814	1094	33.4309	3.11	930.2533	1094	33.4309	3.11	333.0697	1094	33.4309	3.11	1061.648
1095	33.4569	3.1077	286.8194	1095	33.4569	3.1077	889.5951	1095	33.4569	3.1077	354.8268	1095	33.4569	3.1077	1084.5348
1096	33.4829	3.1053	301.2136	1096	33.4829	3.1053	903.593	1096	33.4829	3.1053	341.1885	1096	33.4829	3.1053	1072.0263
1097	33.5089	3.103	333.2697	1097	33.5089	3.103	935.253	1097	33.5089	3.103	351.9059	1097	33.5089	3.103	1083.8735
1098	33.5349	3.1007	355.0599	1098	33.5349	3.1007	956.647	1098	33.5349	3.1007	358.576	1098	33.5349	3.1007	1091.6733
1099	33.5609	3.0983	400.9156	1099	33.5609	3.0983	1002.1065	1099	33.5609	3.0983	460.5	1099	33.5609	3.0983	1194.7271
1100	33.5869	3.096	425.0248	1100	33.5869	3.096	1025.8194	1100	33.5869	3.096	318.6534	1100	33.5869	3.096	1054.0102
1101	33.6129	3.0937	475.9002	1101	33.6129	3.0937	1076.2987	1101	33.6129	3.0937	374.4279	1101	33.6129	3.0937	1110.9145
1102	33.6389	3.0914	433.3267	1102	33.6389	3.0914	1033.3289	1102	33.6389	3.0914	380.4681	1102	33.6389	3.0914	1118.0845
1103	33.6649	3.089	526.6756	1103	33.6649	3.089	1126.2817	1103	33.6649	3.089	478.582	1103	33.6649	3.089	1217.3282
1104	33.6909	3.0867	579.9741	1104	33.6909	3.0867	1179.184	1104	33.6909	3.0867	488.3637	1104	33.6909	3.0867	1228.2397
1105	33.7169	3.0844	687.4758	1105	33.7169	3.0844	1286.2895	1105	33.7169	3.0844	596.108	1105	33.7169	3.0844	1337.1137
1106	33.7429	3.0821	741.5365	1106	33.7429	3.0821	1339.9539	1106	33.7429	3.0821	660.3308	1106	33.7429	3.0821	1402.4663
1107	33.7689	3.0798	903.9246	1107	33.7689	3.0798	1501.9458	1107	33.7689	3.0798	676.6642	1107	33.7689	3.0798	1419.9294
1108	33.7949	3.0775	980.291	1108	33.7949	3.0775	1577.916	1108	33.7949	3.0775	862.3354	1108	33.7949	3.0775	1606.7304
1109	33.8209	3.0752	1159.9237	1109	33.8209	3.0752	1757.1525	1109	33.8209	3.0752	967.5972	1109	33.8209	3.0752	1713.122
1110	33.8469	3.0729	1185.0719	1110	33.8469	3.0729	1781.9044	1110	33.8469	3.0729	986.269	1110	33.8469	3.0729	1732.9236
1111	33.8729	3.0706	1165.8385	1111	33.8729	3.0706	1762.2749	1111	33.8729	3.0706	940.8342	1111	33.8729	3.0706	1688.6185

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1112	33.8989	3.0683	1252.8535	1112	33.8989	3.0683	1848.8936	1112	33.8989	3.0683	920.5356	1112	33.8989	3.0683	1669.4497
1113	33.9249	3.066	1140.3532	1113	33.9249	3.066	1735.9971	1113	33.9249	3.066	971.1424	1113	33.9249	3.066	1721.1862
1114	33.9509	3.0638	1045.8859	1114	33.9509	3.0638	1641.1336	1114	33.9509	3.0638	1094.2569	1114	33.9509	3.0638	1845.4305
1115	33.9769	3.0615	981.5682	1115	33.9769	3.0615	1576.4198	1115	33.9769	3.0615	1184.8342	1115	33.9769	3.0615	1937.1375
1116	34.0029	3.0592	881.1337	1116	34.0029	3.0592	1475.589	1116	34.0029	3.0592	1351.5429	1116	34.0029	3.0592	2104.976
1117	34.0289	3.057	871.234	1117	34.0289	3.057	1465.2931	1117	34.0289	3.057	1638.5269	1117	34.0289	3.057	2393.0897
1118	34.0549	3.0547	686.1437	1118	34.0549	3.0547	1279.8066	1118	34.0549	3.0547	1988.4383	1118	34.0549	3.0547	2744.1309
1119	34.0809	3.0524	727.7734	1119	34.0809	3.0524	1321.0401	1119	34.0809	3.0524	2684.639	1119	34.0809	3.0524	3441.4614
1120	34.1069	3.0502	672.2396	1120	34.1069	3.0502	1265.1101	1120	34.1069	3.0502	3851.7142	1120	34.1069	3.0502	4609.6664
1121	34.1329	3.0479	686.8145	1121	34.1329	3.0479	1279.2888	1121	34.1329	3.0479	5817.5102	1121	34.1329	3.0479	6576.5921
1122	34.1589	3.0457	732.0232	1122	34.1589	3.0457	1324.1013	1122	34.1589	3.0457	9343.4594	1122	34.1589	3.0457	10103.6711
1123	34.1849	3.0434	807.6932	1123	34.1849	3.0434	1399.375	1123	34.1849	3.0434	14569.7224	1123	34.1849	3.0434	15331.0639
1124	34.2109	3.0412	973.0221	1124	34.2109	3.0412	1564.3078	1124	34.2109	3.0412	17920.9038	1124	34.2109	3.0412	18683.375
1125	34.2369	3.0389	1060.1193	1125	34.2369	3.0389	1651.0087	1125	34.2369	3.0389	18175.0676	1125	34.2369	3.0389	18938.6686
1126	34.2629	3.0367	1133.4759	1126	34.2629	3.0367	1723.9691	1126	34.2629	3.0367	17586.8966	1126	34.2629	3.0367	18351.6274
1127	34.2889	3.0345	961.3708	1127	34.2889	3.0345	1551.4678	1127	34.2889	3.0345	15999.3995	1127	34.2889	3.0345	16765.26
1128	34.3149	3.0322	835.8185	1128	34.3149	3.0322	1425.5193	1128	34.3149	3.0322	12727.9308	1128	34.3149	3.0322	13494.9211
1129	34.3409	3.03	655.9722	1129	34.3409	3.03	1245.2769	1129	34.3409	3.03	9619.496	1129	34.3409	3.03	10387.6161
1130	34.3669	3.0278	503.2182	1130	34.3669	3.0278	1092.1266	1130	34.3669	3.0278	7278.3472	1130	34.3669	3.0278	8047.5971
1131	34.3929	3.0256	459.5194	1131	34.3929	3.0256	1048.0316	1131	34.3929	3.0256	5721.597	1131	34.3929	3.0256	6491.9765
1132	34.4189	3.0233	387.43	1132	34.4189	3.0233	975.5459	1132	34.4189	3.0233	4544.8119	1132	34.4189	3.0233	5316.3212
1133	34.4449	3.0211	357.5287	1133	34.4449	3.0211	945.2485	1133	34.4449	3.0211	3993.8546	1133	34.4449	3.0211	4766.4937
1134	34.4709	3.0189	412.2877	1134	34.4709	3.0189	999.6112	1134	34.4709	3.0189	3672.5442	1134	34.4709	3.0189	4446.3131
1135	34.4969	3.0167	377.208	1135	34.4969	3.0167	964.1353	1135	34.4969	3.0167	3392.3683	1135	34.4969	3.0167	4167.2669
1136	34.5229	3.0145	329.1779	1136	34.5229	3.0145	914.9957	1136	34.5229	3.0145	3242.1218	1136	34.5229	3.0145	4014.5836
1137	34.5489	3.0123	336.7704	1137	34.5489	3.0123	921.4786	1137	34.5489	3.0123	2884.3378	1137	34.5489	3.0123	3654.3629
1138	34.5749	3.0101	376.009	1138	34.5749	3.0101	959.6075	1138	34.5749	3.0101	2519.89	1138	34.5749	3.0101	3287.4782
1139	34.6009	3.0079	383.8436	1139	34.6009	3.0079	966.3326	1139	34.6009	3.0079	2075.4667	1139	34.6009	3.0079	2840.6182
1140	34.6269	3.0057	461.5521	1140	34.6269	3.0057	1042.9315	1140	34.6269	3.0057	1748.879	1140	34.6269	3.0057	2511.5937
1141	34.6529	3.0036	422.3628	1141	34.6529	3.0036	1002.6327	1141	34.6529	3.0036	1463.769	1141	34.6529	3.0036	2224.0469
1142	34.6789	3.0014	340.976	1142	34.6789	3.0014	920.1362	1142	34.6789	3.0014	1125.8038	1142	34.6789	3.0014	1883.6449
1143	34.7049	2.9992	379.1361	1143	34.7049	2.9992	957.1868	1143	34.7049	2.9992	918.6406	1143	34.7049	2.9992	1674.0449
1144	34.7309	2.997	377.118	1144	34.7309	2.997	954.059	1144	34.7309	2.997	801.2447	1144	34.7309	2.997	1554.2122
1145	34.7569	2.9948	384.5289	1145	34.7569	2.9948	960.3603	1145	34.7569	2.9948	692.7928	1145	34.7569	2.9948	1443.3235
1146	34.7829	2.9927	356.1058	1146	34.7829	2.9927	930.8276	1146	34.7829	2.9927	606.705	1146	34.7829	2.9927	1354.7989
1147	34.8089	2.9905	305.7094	1147	34.8089	2.9905	879.3217	1147	34.8089	2.9905	537.3092	1147	34.8089	2.9905	1282.9663

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1148	34.8349	2.9883	327.026	1148	34.8349	2.9883	899.5287	1148	34.8349	2.9883	500.778	1148	34.8349	2.9883	1243.9983
1149	34.8609	2.9862	343.2964	1149	34.8609	2.9862	914.6895	1149	34.8609	2.9862	455.0088	1149	34.8609	2.9862	1195.7923
1150	34.8869	2.984	346.9079	1150	34.8869	2.984	917.1914	1150	34.8869	2.984	440.0433	1150	34.8869	2.984	1178.39
1151	34.9129	2.9819	327.4835	1151	34.9129	2.9819	896.6574	1151	34.9129	2.9819	388.5644	1151	34.9129	2.9819	1124.4743
1152	34.9389	2.9797	320.2067	1152	34.9389	2.9797	888.2711	1152	34.9389	2.9797	375.6017	1152	34.9389	2.9797	1109.0749
1153	34.9649	2.9776	314.3768	1153	34.9649	2.9776	881.3315	1153	34.9649	2.9776	400.9503	1153	34.9649	2.9776	1131.9866
1154	34.9909	2.9754	280.5326	1154	34.9909	2.9754	846.3777	1154	34.9909	2.9754	375.6226	1154	34.9909	2.9754	1104.2222
1155	35.0169	2.9733	297.4436	1155	35.0169	2.9733	862.1792	1155	35.0169	2.9733	374.1752	1155	35.0169	2.9733	1100.338
1156	35.0429	2.9712	319.2778	1156	35.0429	2.9712	882.9037	1156	35.0429	2.9712	402.9896	1156	35.0429	2.9712	1126.7155
1157	35.0689	2.969	347.9226	1157	35.0689	2.969	910.4389	1157	35.0689	2.969	403.6441	1157	35.0689	2.969	1124.9332
1158	35.0949	2.9669	330.202	1158	35.0949	2.9669	891.6088	1158	35.0949	2.9669	384.15	1158	35.0949	2.9669	1103.0023
1159	35.1209	2.9648	278.563	1159	35.1209	2.9648	838.8602	1159	35.1209	2.9648	345.0053	1159	35.1209	2.9648	1061.4209
1160	35.1469	2.9626	254.3101	1160	35.1469	2.9626	813.4977	1160	35.1469	2.9626	302.5192	1160	35.1469	2.9626	1016.4979
1161	35.1729	2.9605	261.429	1161	35.1729	2.9605	819.507	1161	35.1729	2.9605	337.9622	1161	35.1729	2.9605	1049.5042
1162	35.1989	2.9584	273.625	1162	35.1989	2.9584	830.5934	1162	35.1989	2.9584	380.8498	1162	35.1989	2.9584	1089.955
1163	35.2249	2.9563	284.3866	1163	35.2249	2.9563	840.8663	1163	35.2249	2.9563	362.7093	1163	35.2249	2.9563	1066.7129
1164	35.2509	2.9542	316.311	1164	35.2509	2.9542	872.3019	1164	35.2509	2.9542	366.147	1164	35.2509	2.9542	1065.049
1165	35.2769	2.9521	322.2006	1165	35.2769	2.9521	877.7027	1165	35.2769	2.9521	399.5149	1165	35.2769	2.9521	1093.3153
1166	35.3029	2.95	311.8897	1166	35.3029	2.95	866.9031	1166	35.3029	2.95	396.4289	1166	35.3029	2.95	1085.1277
1167	35.3289	2.9479	296.1978	1167	35.3289	2.9479	850.7224	1167	35.3289	2.9479	377.7373	1167	35.3289	2.9479	1061.3346
1168	35.3549	2.9458	286.3436	1168	35.3549	2.9458	840.3795	1168	35.3549	2.9458	393.5595	1168	35.3549	2.9458	1072.0552
1169	35.3809	2.9437	274.382	1169	35.3809	2.9437	827.9291	1169	35.3809	2.9437	388.4445	1169	35.3809	2.9437	1061.8386
1170	35.4069	2.9416	295.971	1170	35.4069	2.9416	849.0294	1170	35.4069	2.9416	365.0663	1170	35.4069	2.9416	1033.3588
1171	35.4329	2.9395	307.6574	1171	35.4329	2.9395	860.2271	1171	35.4329	2.9395	371.6915	1171	35.4329	2.9395	1034.8825
1172	35.4589	2.9374	281.8703	1172	35.4589	2.9374	833.9511	1172	35.4589	2.9374	400.1459	1172	35.4589	2.9374	1058.2353
1173	35.4849	2.9353	256.6154	1173	35.4849	2.9353	808.2075	1173	35.4849	2.9353	357.9618	1173	35.4849	2.9353	1010.9496
1174	35.5109	2.9332	239.924	1174	35.5109	2.9332	791.0273	1174	35.5109	2.9332	353.2807	1174	35.5109	2.9332	1001.1669
1175	35.5369	2.9312	255.1616	1175	35.5369	2.9312	805.7762	1175	35.5369	2.9312	383.2891	1175	35.5369	2.9312	1026.0737
1176	35.5629	2.9291	286.3176	1176	35.5629	2.9291	836.4434	1176	35.5629	2.9291	416.0538	1176	35.5629	2.9291	1053.7369
1177	35.5889	2.927	278.3044	1177	35.5889	2.927	827.9415	1177	35.5889	2.927	401.7382	1177	35.5889	2.927	1034.3197
1178	35.6149	2.9249	288.2434	1178	35.6149	2.9249	837.3918	1178	35.6149	2.9249	407.0196	1178	35.6149	2.9249	1034.4995
1179	35.6409	2.9229	266.0289	1179	35.6409	2.9229	814.6885	1179	35.6409	2.9229	387.0447	1179	35.6409	2.9229	1009.423
1180	35.6669	2.9208	265.8292	1180	35.6669	2.9208	814	1180	35.6669	2.9208	352.2942	1180	35.6669	2.9208	969.5709
1181	35.6929	2.9188	273.3186	1181	35.6929	2.9188	821.0007	1181	35.6929	2.9188	352.9923	1181	35.6929	2.9188	965.1675
1182	35.7189	2.9167	285.453	1182	35.7189	2.9167	832.6463	1182	35.7189	2.9167	375.3905	1182	35.7189	2.9167	982.464
1183	35.7449	2.9147	279.3635	1183	35.7449	2.9147	826.0681	1183	35.7449	2.9147	368.3192	1183	35.7449	2.9147	970.2911

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1184	35.7709	2.9126	293.8076	1184	35.7709	2.9126	840.0234	1184	35.7709	2.9126	372.7975	1184	35.7709	2.9126	969.668
1185	35.7969	2.9106	280.0209	1185	35.7969	2.9106	825.748	1185	35.7969	2.9106	412.931	1185	35.7969	2.9106	1004.6999
1186	35.8229	2.9085	295.7392	1186	35.8229	2.9085	840.9775	1186	35.8229	2.9085	402.7219	1186	35.8229	2.9085	989.3892
1187	35.8489	2.9065	320.0163	1187	35.8489	2.9065	864.7658	1187	35.8489	2.9065	412.6303	1187	35.8489	2.9065	994.196
1188	35.8749	2.9044	241.7398	1188	35.8749	2.9044	786.0006	1188	35.8749	2.9044	393.4244	1188	35.8749	2.9044	969.8885
1189	35.9009	2.9024	273.625	1189	35.9009	2.9024	817.3971	1189	35.9009	2.9024	380.8498	1189	35.9009	2.9024	952.2123
1190	35.9269	2.9004	285.2138	1190	35.9269	2.9004	828.1785	1190	35.9269	2.9004	372.2219	1190	35.9269	2.9004	943.0827
1191	35.9529	2.8983	284.8094	1191	35.9529	2.8983	826.9666	1191	35.9529	2.8983	356.5452	1191	35.9529	2.8983	926.9042
1192	35.9789	2.8963	308.2771	1192	35.9789	2.8963	849.6269	1192	35.9789	2.8963	448.214	1192	35.9789	2.8963	1018.0712
1193	36.0049	2.8943	298.9756	1193	36.0049	2.8943	839.5179	1193	36.0049	2.8943	409.3818	1193	36.0049	2.8943	978.7373
1194	36.0309	2.8923	308.2852	1194	36.0309	2.8923	848.0201	1194	36.0309	2.8923	340.1627	1194	36.0309	2.8923	909.0164
1195	36.0569	2.8903	331.0583	1195	36.0569	2.8903	869.9858	1195	36.0569	2.8903	402.1479	1195	36.0569	2.8903	970.4998
1196	36.0829	2.8882	284.4514	1196	36.0829	2.8882	822.5715	1196	36.0829	2.8882	383.7216	1196	36.0829	2.8882	951.5717
1197	36.1089	2.8862	298.1615	1197	36.1089	2.8862	835.4742	1197	36.1089	2.8862	445.6754	1197	36.1089	2.8862	1013.0237
1198	36.1349	2.8842	278.0662	1198	36.1349	2.8842	814.5714	1198	36.1349	2.8842	395.2606	1198	36.1349	2.8842	962.1071
1199	36.1609	2.8822	257.7068	1199	36.1609	2.8822	793.4046	1199	36.1609	2.8822	396.7565	1199	36.1609	2.8822	963.1013
1200	36.1869	2.8802	338.2526	1200	36.1869	2.8802	873.1429	1200	36.1869	2.8802	351.8233	1200	36.1869	2.8802	917.6664
1201	36.2129	2.8782	317.3221	1201	36.2129	2.8782	851.4051	1201	36.2129	2.8782	427.9385	1201	36.2129	2.8782	993.2797
1202	36.2389	2.8762	266.391	1202	36.2389	2.8762	799.6665	1202	36.2389	2.8762	429.7439	1202	36.2389	2.8762	994.5834
1203	36.2649	2.8742	297.4862	1203	36.2649	2.8742	829.9543	1203	36.2649	2.8742	411.2123	1203	36.2649	2.8742	975.55
1204	36.2909	2.8722	309.5776	1204	36.2909	2.8722	841.2382	1204	36.2909	2.8722	368.2275	1204	36.2909	2.8722	932.0635
1205	36.3169	2.8703	296.683	1205	36.3169	2.8703	827.5363	1205	36.3169	2.8703	370.8977	1205	36.3169	2.8703	934.2319
1206	36.3429	2.8683	261.0235	1206	36.3429	2.8683	791.0693	1206	36.3429	2.8683	393.0367	1206	36.3429	2.8683	955.8691
1207	36.3689	2.8663	415.649	1207	36.3689	2.8663	944.8874	1207	36.3689	2.8663	389.2196	1207	36.3689	2.8663	951.5502
1208	36.3949	2.8643	383.9266	1208	36.3949	2.8643	912.3576	1208	36.3949	2.8643	350.5028	1208	36.3949	2.8643	912.3317
1209	36.4209	2.8623	357.7246	1209	36.4209	2.8623	885.3481	1209	36.4209	2.8623	447.0335	1209	36.4209	2.8623	1008.3606
1210	36.4469	2.8604	312.4208	1210	36.4469	2.8604	839.2369	1210	36.4469	2.8604	473.0996	1210	36.4469	2.8604	1033.925
1211	36.4729	2.8584	372.6329	1211	36.4729	2.8584	898.6416	1211	36.4729	2.8584	454.7899	1211	36.4729	2.8584	1015.1135
1212	36.4989	2.8564	362.9736	1212	36.4989	2.8564	888.1749	1212	36.4989	2.8564	433.5279	1212	36.4989	2.8564	993.3497
1213	36.5249	2.8545	363.6062	1213	36.5249	2.8545	888	1213	36.5249	2.8545	440.4992	1213	36.5249	2.8545	999.8193
1214	36.5509	2.8525	374.0562	1214	36.5509	2.8525	897.6426	1214	36.5509	2.8525	537.6077	1214	36.5509	2.8525	1096.4259
1215	36.5769	2.8505	375.221	1215	36.5769	2.8505	898	1215	36.5769	2.8505	618.9848	1215	36.5769	2.8505	1177.3013
1216	36.6029	2.8486	399.6388	1216	36.6029	2.8486	921.6104	1216	36.6029	2.8486	713.8491	1216	36.6029	2.8486	1271.6638
1217	36.6289	2.8466	449.495	1217	36.6289	2.8466	970.6591	1217	36.6289	2.8466	669.2245	1217	36.6289	2.8466	1226.5374
1218	36.6549	2.8447	475.833	1218	36.6549	2.8447	996.1897	1218	36.6549	2.8447	635.678	1218	36.6549	2.8447	1192.4892
1219	36.6809	2.8427	493.0851	1219	36.6809	2.8427	1012.6344	1219	36.6809	2.8427	748.9362	1219	36.6809	2.8427	1305.2456

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1220	36.7069	2.8408	575.7787	1220	36.7069	2.8408	1094.5206	1220	36.7069	2.8408	760.1924	1220	36.7069	2.8408	1316
1221	36.7329	2.8389	522.4294	1221	36.7329	2.8389	1040.3638	1221	36.7329	2.8389	777.6954	1221	36.7329	2.8389	1333.0013
1222	36.7589	2.8369	538.8799	1222	36.7589	2.8369	1056.0069	1222	36.7589	2.8369	823.5551	1222	36.7589	2.8369	1378.3592
1223	36.7849	2.835	568.0542	1223	36.7849	2.835	1084.3738	1223	36.7849	2.835	905.8191	1223	36.7849	2.835	1460.1214
1224	36.8109	2.833	662.4516	1224	36.8109	2.833	1177.9638	1224	36.8109	2.833	838.4812	1224	36.8109	2.833	1392.2817
1225	36.8369	2.8311	699.5282	1225	36.8369	2.8311	1214.233	1225	36.8369	2.8311	695.0137	1225	36.8369	2.8311	1248.3125
1226	36.8629	2.8292	654.2364	1226	36.8629	2.8292	1168.1337	1226	36.8629	2.8292	648.6924	1226	36.8629	2.8292	1201.4894
1227	36.8889	2.8273	647.5807	1227	36.8889	2.8273	1160.6705	1227	36.8889	2.8273	655.5633	1227	36.8889	2.8273	1207.8585
1228	36.9149	2.8253	609.1009	1228	36.9149	2.8253	1121.3833	1228	36.9149	2.8253	570.7197	1228	36.9149	2.8253	1122.5132
1229	36.9409	2.8234	608.8638	1229	36.9409	2.8234	1120.3388	1229	36.9409	2.8234	501.3365	1229	36.9409	2.8234	1052.6282
1230	36.9669	2.8215	572.6683	1230	36.9669	2.8215	1083.3359	1230	36.9669	2.8215	415.2983	1230	36.9669	2.8215	966.0883
1231	36.9929	2.8196	533.1122	1231	36.9929	2.8196	1042.9724	1231	36.9929	2.8196	468.5185	1231	36.9929	2.8196	1018.8066
1232	37.0189	2.8177	472.5225	1232	37.0189	2.8177	981.5753	1232	37.0189	2.8177	502.1411	1232	37.0189	2.8177	1051.9275
1233	37.0449	2.8158	395.9201	1233	37.0449	2.8158	904.1654	1233	37.0449	2.8158	488.0977	1233	37.0449	2.8158	1037.3823
1234	37.0709	2.8139	370.1382	1234	37.0709	2.8139	877.5761	1234	37.0709	2.8139	428.8444	1234	37.0709	2.8139	977.6273
1235	37.0969	2.812	390.2904	1235	37.0969	2.812	896.9208	1235	37.0969	2.812	425.5691	1235	37.0969	2.812	973.8501
1236	37.1229	2.8101	338.4995	1236	37.1229	2.8101	844.3225	1236	37.1229	2.8101	396.6521	1236	37.1229	2.8101	944.4314
1237	37.1489	2.8082	349.8983	1237	37.1489	2.8082	854.9139	1237	37.1489	2.8082	410.012	1237	37.1489	2.8082	957.2895
1238	37.1749	2.8063	324.7595	1238	37.1749	2.8063	828.9677	1238	37.1749	2.8063	390.9054	1238	37.1749	2.8063	937.6812
1239	37.2009	2.8044	334.5177	1239	37.2009	2.8044	837.9185	1239	37.2009	2.8044	379.2936	1239	37.2009	2.8044	925.5676
1240	37.2269	2.8025	345.8192	1240	37.2269	2.8025	848.4126	1240	37.2269	2.8025	425.8422	1240	37.2269	2.8025	971.6144
1241	37.2529	2.8006	306.129	1241	37.2529	2.8006	807.9149	1241	37.2529	2.8006	447.1223	1241	37.2529	2.8006	992.3927
1242	37.2789	2.7987	256.0726	1242	37.2789	2.7987	757.0511	1242	37.2789	2.7987	411.8503	1242	37.2789	2.7987	956.6189
1243	37.3049	2.7968	273.625	1243	37.3049	2.7968	773.7961	1243	37.3049	2.7968	380.8498	1243	37.3049	2.7968	925.1167
1244	37.3309	2.795	286.3924	1244	37.3309	2.795	785.0005	1244	37.3309	2.795	366.3479	1244	37.3309	2.795	908.0011
1245	37.3569	2.7931	302.3717	1245	37.3569	2.7931	799.4167	1245	37.3569	2.7931	325.217	1245	37.3569	2.7931	864.2566
1246	37.3829	2.7912	320.279	1246	37.3829	2.7912	815.7609	1246	37.3829	2.7912	357.3734	1246	37.3829	2.7912	893.7994
1247	37.4089	2.7893	285.3244	1247	37.4089	2.7893	779.2433	1247	37.4089	2.7893	423.4866	1247	37.4089	2.7893	957.2989
1248	37.4349	2.7875	273.6745	1248	37.4349	2.7875	766.0304	1248	37.4349	2.7875	421.7253	1248	37.4349	2.7875	952.924
1249	37.4609	2.7856	271.3355	1249	37.4609	2.7856	762.1283	1249	37.4609	2.7856	382.8849	1249	37.4609	2.7856	911.4699
1250	37.4869	2.7837	266.1631	1250	37.4869	2.7837	755.3929	1250	37.4869	2.7837	387.2403	1250	37.4869	2.7837	913.2117
1251	37.5129	2.7819	267.3332	1251	37.5129	2.7819	755	1251	37.5129	2.7819	392.6852	1251	37.5129	2.7819	916.043
1252	37.5389	2.78	298.2569	1252	37.5389	2.78	784.3606	1252	37.5389	2.78	410.9827	1252	37.5389	2.78	931.7268
1253	37.5649	2.7782	287.5538	1253	37.5649	2.7782	772.0945	1253	37.5649	2.7782	415.0146	1253	37.5649	2.7782	933.145
1254	37.5909	2.7763	257.0792	1254	37.5909	2.7763	740.0569	1254	37.5909	2.7763	402.9442	1254	37.5909	2.7763	918.4611
1255	37.6169	2.7745	261.5045	1255	37.6169	2.7745	742.9191	1255	37.6169	2.7745	417.1478	1255	37.6169	2.7745	930.051

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1256	37.6429	2.7726	276.1712	1256	37.6429	2.7726	756.0228	1256	37.6429	2.7726	422.4026	1256	37.6429	2.7726	932.6921
1257	37.6689	2.7708	325.7195	1257	37.6689	2.7708	804.008	1257	37.6689	2.7708	400.6585	1257	37.6689	2.7708	908.3344
1258	37.6949	2.7689	328.9201	1258	37.6949	2.7689	805.6456	1258	37.6949	2.7689	384.1886	1258	37.6949	2.7689	889.2509
1259	37.7209	2.7671	272.9497	1259	37.7209	2.7671	748.1122	1259	37.7209	2.7671	412.5812	1259	37.7209	2.7671	915.0298
1260	37.7469	2.7653	289.5038	1260	37.7469	2.7653	763.1032	1260	37.7469	2.7653	441.6415	1260	37.7469	2.7653	941.4765
1261	37.7729	2.7634	320.4991	1261	37.7729	2.7634	792.5355	1261	37.7729	2.7634	423.858	1261	37.7729	2.7634	921.0794
1262	37.7989	2.7616	306.2068	1262	37.7989	2.7616	776.6802	1262	37.7989	2.7616	391.7767	1262	37.7989	2.7616	886.3843
1263	37.8249	2.7598	288.6161	1263	37.8249	2.7598	757.5264	1263	37.8249	2.7598	417.6855	1263	37.8249	2.7598	909.6795
1264	37.8509	2.7579	268.2898	1264	37.8509	2.7579	735.6371	1264	37.8509	2.7579	457.5337	1264	37.8509	2.7579	946.9141
1265	37.8769	2.7561	251.8842	1265	37.8769	2.7561	717.6684	1265	37.8769	2.7561	446.8181	1265	37.8769	2.7561	933.5849
1266	37.9029	2.7543	275.2632	1266	37.9029	2.7543	739.4844	1266	37.9029	2.7543	438.7088	1266	37.9029	2.7543	922.8619
1267	37.9289	2.7525	310.3964	1267	37.9289	2.7525	773.0546	1267	37.9289	2.7525	399.3217	1267	37.9289	2.7525	880.8611
1268	37.9549	2.7507	276.0561	1268	37.9549	2.7507	737.1512	1268	37.9549	2.7507	364.6425	1268	37.9549	2.7507	843.5683
1269	37.9809	2.7488	262.8355	1269	37.9809	2.7488	722.3676	1269	37.9809	2.7488	381.8508	1269	37.9809	2.7488	858.1629
1270	38.0069	2.747	303.4826	1270	38.0069	2.747	761.4517	1270	38.0069	2.747	380.8498	1270	38.0069	2.747	854.5483
1271	38.0329	2.7452	334.1101	1271	38.0329	2.7452	790.5161	1271	38.0329	2.7452	399.5142	1271	38.0329	2.7452	872.9279
1272	38.0589	2.7434	354.7187	1272	38.0589	2.7434	809.5617	1272	38.0589	2.7434	444.5341	1272	38.0589	2.7434	917.663
1273	38.0849	2.7416	310.5663	1273	38.0849	2.7416	763.8462	1273	38.0849	2.7416	430.1966	1273	38.0849	2.7416	903.0406
1274	38.1109	2.7398	303.1467	1274	38.1109	2.7398	754.8636	1274	38.1109	2.7398	375.703	1274	38.1109	2.7398	848.2622
1275	38.1369	2.738	328.6152	1275	38.1369	2.738	778.769	1275	38.1369	2.738	388.3677	1275	38.1369	2.738	860.642
1276	38.1629	2.7362	307.3044	1276	38.1629	2.7362	755.8952	1276	38.1629	2.7362	411.2652	1276	38.1629	2.7362	883.2546
1277	38.1889	2.7344	288.8426	1277	38.1889	2.7344	735.8704	1277	38.1889	2.7344	404.5647	1277	38.1889	2.7344	876.2693
1278	38.2149	2.7326	313.5353	1278	38.2149	2.7326	759	1278	38.2149	2.7326	399.5556	1278	38.2149	2.7326	870.9754
1279	38.2409	2.7309	319.5686	1279	38.2409	2.7309	763.4703	1279	38.2409	2.7309	402.5878	1279	38.2409	2.7309	873.7228
1280	38.2669	2.7291	315.1919	1280	38.2669	2.7291	757.5306	1280	38.2669	2.7291	406.3377	1280	38.2669	2.7291	877.1878
1281	38.2929	2.7273	281.326	1281	38.2929	2.7273	722.1016	1281	38.2929	2.7273	395.2797	1281	38.2929	2.7273	865.8449
1282	38.3189	2.7255	283.3933	1282	38.3189	2.7255	722.6059	1282	38.3189	2.7255	352.6445	1282	38.3189	2.7255	822.9249
1283	38.3449	2.7237	295.8244	1283	38.3449	2.7237	733.4739	1283	38.3449	2.7237	398.4357	1283	38.3449	2.7237	868.4313
1284	38.3709	2.7219	298.6649	1284	38.3709	2.7219	734.7515	1284	38.3709	2.7219	413.1317	1284	38.3709	2.7219	882.8424
1285	38.3969	2.7202	276.3732	1285	38.3969	2.7202	710.8966	1285	38.3969	2.7202	403.6775	1285	38.3969	2.7202	873.1034
1286	38.4229	2.7184	278.5457	1286	38.4229	2.7184	711.5061	1286	38.4229	2.7184	399.1054	1286	38.4229	2.7184	868.2464
1287	38.4489	2.7166	264.1982	1287	38.4489	2.7166	695.5956	1287	38.4489	2.7166	420.7831	1287	38.4489	2.7166	889.6392
1288	38.4749	2.7149	307.5753	1288	38.4749	2.7149	737.4097	1288	38.4749	2.7149	431.7288	1288	38.4749	2.7149	900.3001
1289	38.5009	2.7131	285.7095	1289	38.5009	2.7131	713.9808	1289	38.5009	2.7131	430.69	1289	38.5009	2.7131	898.9764
1290	38.5269	2.7113	303.9593	1290	38.5269	2.7113	730.6676	1290	38.5269	2.7113	403.4118	1290	38.5269	2.7113	871.4135
1291	38.5529	2.7096	338.6509	1291	38.5529	2.7096	763.7961	1291	38.5529	2.7096	411.6728	1291	38.5529	2.7096	879.3896

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1292	38.5789	2.7078	323.0404	1292	38.5789	2.7078	746.6226	1292	38.5789	2.7078	377.5681	1292	38.5789	2.7078	845
1293	38.6049	2.7061	307.6044	1293	38.6049	2.7061	729.6236	1293	38.6049	2.7061	383.8061	1293	38.6049	2.7061	850.9531
1294	38.6309	2.7043	316.7143	1294	38.6309	2.7043	737.1705	1294	38.6309	2.7043	411.1378	1294	38.6309	2.7043	878
1295	38.6569	2.7026	318.9464	1295	38.6569	2.7026	737.8394	1295	38.6569	2.7026	410.7804	1295	38.6569	2.7026	877.3578
1296	38.6829	2.7008	312.1384	1296	38.6829	2.7008	729.4684	1296	38.6829	2.7008	416.7453	1296	38.6829	2.7008	883.0379
1297	38.7089	2.6991	273.625	1297	38.7089	2.6991	689.3921	1297	38.7089	2.6991	462.6454	1297	38.7089	2.6991	928.6531
1298	38.7349	2.6973	294.1703	1298	38.7349	2.6973	710.0162	1298	38.7349	2.6973	437.732	1298	38.7349	2.6973	903.4548
1299	38.7609	2.6956	333.9543	1299	38.7609	2.6956	749.8791	1299	38.7609	2.6956	478.8598	1299	38.7609	2.6956	944.2978
1300	38.7869	2.6939	329.89	1300	38.7869	2.6939	745.8936	1300	38.7869	2.6939	418.0657	1300	38.7869	2.6939	883.2188
1301	38.8129	2.6921	305.6246	1301	38.8129	2.6921	721.7071	1301	38.8129	2.6921	434.5154	1301	38.8129	2.6921	899.3837
1302	38.8389	2.6904	309.6522	1302	38.8389	2.6904	725.8137	1302	38.8389	2.6904	419.3234	1302	38.8389	2.6904	883.9068
1303	38.8649	2.6887	290.5196	1303	38.8649	2.6887	706.76	1303	38.8649	2.6887	413.7342	1303	38.8649	2.6887	878.0329
1304	38.8909	2.6869	318.6169	1304	38.8909	2.6869	734.9361	1304	38.8909	2.6869	462.2934	1304	38.8909	2.6869	926.3072
1305	38.9169	2.6852	282.6497	1305	38.9169	2.6852	699.0478	1305	38.9169	2.6852	351.7856	1305	38.9169	2.6852	815.5146
1306	38.9429	2.6835	343.6491	1306	38.9429	2.6835	760.1261	1306	38.9429	2.6835	392.9207	1306	38.9429	2.6835	856.3648
1307	38.9689	2.6818	325.6188	1307	38.9689	2.6818	742.1746	1307	38.9689	2.6818	437.1726	1307	38.9689	2.6818	900.3319
1308	38.9949	2.68	284.0281	1308	38.9949	2.68	700.6628	1308	38.9949	2.68	444.3365	1308	38.9949	2.68	907.2109
1309	39.0209	2.6783	305.2819	1309	39.0209	2.6783	721.9955	1309	39.0209	2.6783	420.3672	1309	39.0209	2.6783	882.9567
1310	39.0469	2.6766	350.5122	1310	39.0469	2.6766	767.3047	1310	39.0469	2.6766	419	1310	39.0469	2.6766	881.3047
1311	39.0729	2.6749	376.0495	1311	39.0729	2.6749	792.9209	1311	39.0729	2.6749	444.9909	1311	39.0729	2.6749	907.0108
1312	39.0989	2.6732	332.4072	1312	39.0989	2.6732	749.3575	1312	39.0989	2.6732	451.2162	1312	39.0989	2.6732	912.9512
1313	39.1249	2.6715	254.3966	1313	39.1249	2.6715	671.4258	1313	39.1249	2.6715	372.9937	1313	39.1249	2.6715	834.4438
1314	39.1509	2.6698	301.4934	1314	39.1509	2.6698	718.6015	1314	39.1509	2.6698	398.0795	1314	39.1509	2.6698	859.2448
1315	39.1769	2.6681	281.6467	1315	39.1769	2.6681	698.8336	1315	39.1769	2.6681	383.7258	1315	39.1769	2.6681	844.6063
1316	39.2029	2.6664	318.8216	1316	39.2029	2.6664	736.0874	1316	39.2029	2.6664	423.3962	1316	39.2029	2.6664	883.9918
1317	39.2289	2.6647	281.0802	1317	39.2289	2.6647	698.425	1317	39.2289	2.6647	443.5922	1317	39.2289	2.6647	903.903
1318	39.2549	2.663	262.7266	1318	39.2549	2.663	680.1502	1318	39.2549	2.663	432.8536	1318	39.2549	2.663	892.8796
1319	39.2809	2.6613	288.2477	1319	39.2809	2.6613	705.7501	1319	39.2809	2.6613	435.9486	1319	39.2809	2.6613	895.6897
1320	39.3069	2.6596	271.2562	1320	39.3069	2.6596	688.8376	1320	39.3069	2.6596	410.9939	1320	39.3069	2.6596	870.4501
1321	39.3329	2.6579	327.1045	1321	39.3329	2.6579	744.7647	1321	39.3329	2.6579	395.29	1321	39.3329	2.6579	854.4614
1322	39.3589	2.6562	303.8034	1322	39.3589	2.6562	721.5425	1322	39.3589	2.6562	389.6502	1322	39.3589	2.6562	848.5367
1323	39.3849	2.6545	328.4293	1323	39.3849	2.6545	746.2473	1323	39.3849	2.6545	352.3237	1323	39.3849	2.6545	810.9254
1324	39.4109	2.6529	273.625	1324	39.4109	2.6529	691.5219	1324	39.4109	2.6529	380.8498	1324	39.4109	2.6529	839.1667
1325	39.4369	2.6512	319.2895	1325	39.4369	2.6512	736.4988	1325	39.4369	2.6512	372.3267	1325	39.4369	2.6512	829.331
1326	39.4629	2.6495	319.0957	1326	39.4629	2.6495	735.6174	1326	39.4629	2.6495	414.8093	1326	39.4629	2.6495	870.5011
1327	39.4889	2.6478	284.4443	1327	39.4889	2.6478	700.2784	1327	39.4889	2.6478	401.7018	1327	39.4889	2.6478	856.081

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1328	39.5149	2.6462	265.5236	1328	39.5149	2.6462	680.6701	1328	39.5149	2.6462	416.4289	1328	39.5149	2.6462	869.4955
1329	39.5409	2.6445	285.7673	1329	39.5409	2.6445	700.2263	1329	39.5409	2.6445	393.2573	1329	39.5409	2.6445	845.0114
1330	39.5669	2.6428	304.241	1330	39.5669	2.6428	718.0124	1330	39.5669	2.6428	395.0647	1330	39.5669	2.6428	845.5062
1331	39.5929	2.6412	303.0961	1331	39.5929	2.6412	716.1799	1331	39.5929	2.6412	428.3984	1331	39.5929	2.6412	877.5273
1332	39.6189	2.6395	282.7681	1332	39.6189	2.6395	695.1643	1332	39.6189	2.6395	411.0005	1332	39.6189	2.6395	858.8169
1333	39.6449	2.6378	251.6522	1333	39.6449	2.6378	663.3608	1333	39.6449	2.6378	410.1972	1333	39.6449	2.6378	856.701
1334	39.6709	2.6362	328.5261	1334	39.6709	2.6362	739.5471	1334	39.6709	2.6362	449.9408	1334	39.6709	2.6362	895.132
1335	39.6969	2.6345	313.1925	1335	39.6969	2.6345	723.5259	1335	39.6969	2.6345	420.8836	1335	39.6969	2.6345	864.7623
1336	39.7229	2.6329	305.8766	1336	39.7229	2.6329	715.5224	1336	39.7229	2.6329	351.3959	1336	39.7229	2.6329	793.9621
1337	39.7489	2.6312	299.116	1337	39.7489	2.6312	708.0742	1337	39.7489	2.6312	362.0115	1337	39.7489	2.6312	803.2651
1338	39.7749	2.6296	314.3428	1338	39.7749	2.6296	722.6135	1338	39.7749	2.6296	370.8573	1338	39.7749	2.6296	810.7983
1339	39.8009	2.6279	315.6252	1339	39.8009	2.6279	723.2082	1339	39.8009	2.6279	428.5654	1339	39.8009	2.6279	867.1938
1340	39.8269	2.6263	307.6781	1340	39.8269	2.6263	714.5735	1340	39.8269	2.6263	425.9783	1340	39.8269	2.6263	863.2942
1341	39.8529	2.6246	284.6683	1341	39.8529	2.6246	690.8762	1341	39.8529	2.6246	419.1091	1341	39.8529	2.6246	855.1124
1342	39.8789	2.623	288.9754	1342	39.8789	2.623	694.4957	1342	39.8789	2.623	464.35	1342	39.8789	2.623	899.0408
1343	39.9049	2.6213	276.0074	1343	39.9049	2.6213	680.8401	1343	39.9049	2.6213	455.8819	1343	39.9049	2.6213	889.2601
1344	39.9309	2.6197	300.2242	1344	39.9309	2.6197	704.3693	1344	39.9309	2.6197	437.1907	1344	39.9309	2.6197	869.2564
1345	39.9569	2.6181	290.6294	1345	39.9569	2.6181	694.0869	1345	39.9569	2.6181	418.6359	1345	39.9569	2.6181	849.389
1346	39.9829	2.6164	269.0669	1346	39.9829	2.6164	671.8368	1346	39.9829	2.6164	402.3962	1346	39.9829	2.6164	831.8368
1347	40.0089	2.6148	248.8028	1347	40.0089	2.6148	650.8851	1347	40.0089	2.6148	414.9869	1347	40.0089	2.6148	843.1149
1348	40.0349	2.6132	268.5308	1348	40.0349	2.6132	669.9256	1348	40.0349	2.6132	418.2032	1348	40.0349	2.6132	845.0186
1349	40.0609	2.6115	312.1571	1349	40.0609	2.6115	712.8642	1349	40.0609	2.6115	427.9921	1349	40.0609	2.6115	853.495
1350	40.0869	2.6099	340.6622	1350	40.0869	2.6099	740.6817	1350	40.0869	2.6099	391.9273	1350	40.0869	2.6099	816.1176
1351	40.1129	2.6083	314.7934	1351	40.1129	2.6083	714.1253	1351	40.1129	2.6083	380.8498	1351	40.1129	2.6083	803.7275
1352	40.1389	2.6067	297.5205	1352	40.1389	2.6067	696.1649	1352	40.1389	2.6067	428.6562	1352	40.1389	2.6067	852.0789
1353	40.1649	2.6051	278.8109	1353	40.1649	2.6051	676.7677	1353	40.1649	2.6051	438.2356	1353	40.1649	2.6051	862.2034
1354	40.1909	2.6034	263.7308	1354	40.1909	2.6034	661	1354	40.1909	2.6034	422.4613	1354	40.1909	2.6034	846.974
1355	40.2169	2.6018	261.5923	1355	40.2169	2.6018	658.1739	1355	40.2169	2.6018	398.5945	1355	40.2169	2.6018	823.6522
1356	40.2429	2.6002	283.4283	1356	40.2429	2.6002	679.3223	1356	40.2429	2.6002	389.616	1356	40.2429	2.6002	815.2188
1357	40.2689	2.5986	301.1575	1357	40.2689	2.5986	696.3639	1357	40.2689	2.5986	374.1281	1357	40.2689	2.5986	800.2759
1358	40.2949	2.597	304.7648	1358	40.2949	2.597	699.2836	1358	40.2949	2.597	390.5759	1358	40.2949	2.597	817.2687
1359	40.3209	2.5954	296.5561	1359	40.3209	2.5954	690.3874	1359	40.3209	2.5954	402.4198	1359	40.3209	2.5954	829.6576
1360	40.3469	2.5938	282.2471	1360	40.3469	2.5938	675.3908	1360	40.3469	2.5938	420.2471	1360	40.3469	2.5938	848.0299
1361	40.3729	2.5922	270.9473	1361	40.3729	2.5922	663.4034	1361	40.3729	2.5922	420.8256	1361	40.3729	2.5922	849.1534
1362	40.3989	2.5906	285.045	1362	40.3989	2.5906	676.8134	1362	40.3989	2.5906	375.7501	1362	40.3989	2.5906	804.623
1363	40.4249	2.589	317.6359	1363	40.4249	2.589	708.7168	1363	40.4249	2.589	399.935	1363	40.4249	2.589	829.3528

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1364	40.4509	2.5874	320.5162	1364	40.4509	2.5874	710.9094	1364	40.4509	2.5874	439.6094	1364	40.4509	2.5874	869.5723
1365	40.4769	2.5858	318.3522	1365	40.4769	2.5858	708.0579	1365	40.4769	2.5858	436.5601	1365	40.4769	2.5858	867.068
1366	40.5029	2.5842	312.2998	1366	40.5029	2.5842	701.3179	1366	40.5029	2.5842	423.0893	1366	40.5029	2.5842	854.1422
1367	40.5289	2.5826	291.3157	1367	40.5289	2.5826	679.6462	1367	40.5289	2.5826	418.2174	1367	40.5289	2.5826	849.8153
1368	40.5549	2.581	267.0356	1368	40.5549	2.581	654.6785	1368	40.5549	2.581	420.2601	1368	40.5549	2.581	852.403
1369	40.5809	2.5795	274.3122	1369	40.5809	2.5795	661.2676	1369	40.5809	2.5795	385.5706	1369	40.5809	2.5795	818.2585
1370	40.6069	2.5779	308.2374	1370	40.6069	2.5779	694.5051	1370	40.6069	2.5779	375.337	1370	40.6069	2.5779	808.5699
1371	40.6329	2.5763	292.7294	1371	40.6329	2.5763	678.3096	1371	40.6329	2.5763	398.9704	1371	40.6329	2.5763	832.7483
1372	40.6589	2.5747	300.5724	1372	40.6589	2.5747	685.4649	1372	40.6589	2.5747	374.6433	1372	40.6589	2.5747	808.9662
1373	40.6849	2.5731	323.6352	1373	40.6849	2.5731	707.8402	1373	40.6849	2.5731	360.5966	1373	40.6849	2.5731	795.4646
1374	40.7109	2.5716	310.0518	1374	40.7109	2.5716	693.5692	1374	40.7109	2.5716	400.4081	1374	40.7109	2.5716	835.8211
1375	40.7369	2.57	283.5684	1375	40.7369	2.57	666.3981	1375	40.7369	2.57	406.6032	1375	40.7369	2.57	842.5612
1376	40.7629	2.5684	284.6338	1376	40.7629	2.5684	666.776	1376	40.7629	2.5684	372.497	1376	40.7629	2.5684	809
1377	40.7889	2.5669	293.0153	1377	40.7889	2.5669	674.4699	1377	40.7889	2.5669	382.3598	1377	40.7889	2.5669	819.4078
1378	40.8149	2.5653	273.625	1378	40.8149	2.5653	654.3921	1378	40.8149	2.5653	380.8498	1378	40.8149	2.5653	818.4428
1379	40.8409	2.5637	270.8282	1379	40.8409	2.5637	651.9168	1379	40.8409	2.5637	368.3253	1379	40.8409	2.5637	806.7831
1380	40.8669	2.5622	249.2988	1380	40.8669	2.5622	630.7089	1380	40.8669	2.5622	427.3117	1380	40.8669	2.5622	866.6343
1381	40.8929	2.5606	263.1118	1381	40.8929	2.5606	644.8434	1381	40.8929	2.5606	430.2705	1381	40.8929	2.5606	870.4579
1382	40.9189	2.5591	263.6764	1382	40.9189	2.5591	645.7295	1382	40.9189	2.5591	425.731	1382	40.9189	2.5591	866.7833
1383	40.9449	2.5575	274.3058	1383	40.9449	2.5575	656.6805	1383	40.9449	2.5575	384.6899	1383	40.9449	2.5575	826.6069
1384	40.9709	2.5559	320.5813	1384	40.9709	2.5559	703.2775	1384	40.9709	2.5559	343.4901	1384	40.9709	2.5559	786.2719
1385	40.9969	2.5544	319.6445	1385	40.9969	2.5544	702.6623	1385	40.9969	2.5544	349.9322	1385	40.9969	2.5544	793.5789
1386	41.0229	2.5528	307.1591	1386	41.0229	2.5528	690.4984	1386	41.0229	2.5528	345.6579	1386	41.0229	2.5528	790.1694
1387	41.0489	2.5513	287.2933	1387	41.0489	2.5513	670.9541	1387	41.0489	2.5513	391.8163	1387	41.0489	2.5513	837.1926
1388	41.0749	2.5498	302.2554	1388	41.0749	2.5498	686.2378	1388	41.0749	2.5498	407.6189	1388	41.0749	2.5498	853.86
1389	41.1009	2.5482	285.8347	1389	41.1009	2.5482	670.1385	1389	41.1009	2.5482	398.5269	1389	41.1009	2.5482	845.6329
1390	41.1269	2.5467	244.7198	1390	41.1269	2.5467	629.3452	1390	41.1269	2.5467	404.5799	1390	41.1269	2.5467	852.5506
1391	41.1529	2.5451	303.2611	1391	41.1529	2.5451	688.208	1391	41.1529	2.5451	435.3878	1391	41.1529	2.5451	884.2234
1392	41.1789	2.5436	299.1754	1392	41.1789	2.5436	684.4439	1392	41.1789	2.5436	397.4977	1392	41.1789	2.5436	847.1981
1393	41.2049	2.5421	283.0444	1393	41.2049	2.5421	668.6344	1393	41.2049	2.5421	387.4619	1393	41.2049	2.5421	838.0271
1394	41.2309	2.5405	293.732	1394	41.2309	2.5405	679.6435	1394	41.2309	2.5405	352.3041	1394	41.2309	2.5405	803.7341
1395	41.2569	2.539	290.4204	1395	41.2569	2.539	676.6534	1395	41.2569	2.539	397.4282	1395	41.2569	2.539	849.723
1396	41.2829	2.5375	281.8614	1396	41.2829	2.5375	668.416	1396	41.2829	2.5375	409.7922	1396	41.2829	2.5375	862.9518
1397	41.3089	2.5359	276.242	1397	41.3089	2.5359	663.1181	1397	41.3089	2.5359	345.6053	1397	41.3089	2.5359	799.6297
1398	41.3349	2.5344	297.9591	1398	41.3349	2.5344	685.1567	1398	41.3349	2.5344	430.2732	1398	41.3349	2.5344	885.1624
1399	41.3609	2.5329	321.0368	1399	41.3609	2.5329	708.5559	1399	41.3609	2.5329	373.2627	1399	41.3609	2.5329	829.0168

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1400	41.3869	2.5314	300.2418	1400	41.3869	2.5314	688.0825	1400	41.3869	2.5314	404.1256	1400	41.3869	2.5314	860.7445
1401	41.4129	2.5298	276.6037	1401	41.4129	2.5298	664.7659	1401	41.4129	2.5298	390.2152	1401	41.4129	2.5298	847.6989
1402	41.4389	2.5283	324.0106	1402	41.4389	2.5283	712.4943	1402	41.4389	2.5283	427.2644	1402	41.4389	2.5283	885.6128
1403	41.4649	2.5268	328.4615	1403	41.4649	2.5268	717.2668	1403	41.4649	2.5268	488.6711	1403	41.4649	2.5268	947.8843
1404	41.4909	2.5253	329.2137	1404	41.4909	2.5253	718.3405	1404	41.4909	2.5253	412.3141	1404	41.4909	2.5253	872.3922
1405	41.5169	2.5238	305.0601	1405	41.5169	2.5238	694.5084	1405	41.5169	2.5238	380.8498	1405	41.5169	2.5238	841.7927
1406	41.5429	2.5223	249.3787	1406	41.5429	2.5223	639.1486	1406	41.5429	2.5223	379.3472	1406	41.5429	2.5223	838.8816
1407	41.5689	2.5208	331.9922	1407	41.5689	2.5208	722.0836	1407	41.5689	2.5208	380.9921	1407	41.5689	2.5208	839.118
1408	41.5949	2.5193	352.8624	1408	41.5949	2.5193	743.2753	1408	41.5949	2.5193	422.2992	1408	41.5949	2.5193	879.0166
1409	41.6209	2.5178	359.5008	1409	41.6209	2.5178	750.2353	1409	41.6209	2.5178	399.3675	1409	41.6209	2.5178	854.6765
1410	41.6469	2.5163	366.866	1410	41.6469	2.5163	757.922	1410	41.6469	2.5163	391.5028	1410	41.6469	2.5163	845.4033
1411	41.6729	2.5148	362.7947	1411	41.6729	2.5148	754.1722	1411	41.6729	2.5148	463.7951	1411	41.6729	2.5148	916.287
1412	41.6989	2.5133	380.2945	1412	41.6989	2.5133	771.9936	1412	41.6989	2.5133	494.9059	1412	41.6989	2.5133	945.9894
1413	41.7249	2.5118	403.7327	1413	41.7249	2.5118	795.7533	1413	41.7249	2.5118	483.4586	1413	41.7249	2.5118	933.1336
1414	41.7509	2.5103	368.385	1414	41.7509	2.5103	760.7272	1414	41.7509	2.5103	511.1881	1414	41.7509	2.5103	959.4546
1415	41.7769	2.5088	394.4929	1415	41.7769	2.5088	787.1566	1415	41.7769	2.5088	585.8829	1415	41.7769	2.5088	1032.7409
1416	41.8029	2.5073	428.6132	1416	41.8029	2.5073	821.5985	1416	41.8029	2.5073	616.4293	1416	41.8029	2.5073	1061.8788
1417	41.8289	2.5058	389.7918	1417	41.8289	2.5058	783.0986	1417	41.8289	2.5058	707.3121	1417	41.8289	2.5058	1151.3531
1418	41.8549	2.5043	366.6893	1418	41.8549	2.5043	760.3175	1418	41.8549	2.5043	814.8995	1418	41.8549	2.5043	1257.532
1419	41.8809	2.5028	335.2841	1419	41.8809	2.5028	729.2339	1419	41.8809	2.5028	1165.0856	1419	41.8809	2.5028	1606.3096
1420	41.9069	2.5013	381.5028	1420	41.9069	2.5013	775.7741	1420	41.9069	2.5013	1762.7499	1420	41.9069	2.5013	2202.5655
1421	41.9329	2.4999	417.2692	1421	41.9329	2.4999	811.8621	1421	41.9329	2.4999	2689.3444	1421	41.9329	2.4999	3127.7515
1422	41.9589	2.4984	415.5835	1422	41.9589	2.4984	810.4979	1422	41.9589	2.4984	3176.789	1422	41.9589	2.4984	3613.7875
1423	41.9849	2.4969	485.1136	1423	41.9849	2.4969	880.3495	1423	41.9849	2.4969	3042.529	1423	41.9849	2.4969	3478.119
1424	42.0109	2.4954	484.6368	1424	42.0109	2.4954	880.1942	1424	42.0109	2.4954	2801.674	1424	42.0109	2.4954	3235.8556
1425	42.0369	2.494	485.733	1425	42.0369	2.494	881.612	1425	42.0369	2.494	2718.3756	1425	42.0369	2.494	3151.1487
1426	42.0629	2.4925	455.6738	1426	42.0629	2.4925	851.8743	1426	42.0629	2.4925	2389.7212	1426	42.0629	2.4925	2821.0858
1427	42.0889	2.491	402.8325	1427	42.0889	2.491	799.3546	1427	42.0889	2.491	1957.0299	1427	42.0889	2.491	2386.9859
1428	42.1149	2.4895	384.0657	1428	42.1149	2.4895	780.9093	1428	42.1149	2.4895	1496.2348	1428	42.1149	2.4895	1924.7824
1429	42.1409	2.4881	399.2852	1429	42.1409	2.4881	796.4503	1429	42.1409	2.4881	1267.4702	1429	42.1409	2.4881	1694.6093
1430	42.1669	2.4866	403.3344	1430	42.1669	2.4866	800.821	1430	42.1669	2.4866	1040.2188	1430	42.1669	2.4866	1465.9495
1431	42.1929	2.4852	332.6242	1431	42.1929	2.4852	730.4324	1431	42.1929	2.4852	902.9655	1431	42.1929	2.4852	1327.2876
1432	42.2189	2.4837	315.8703	1432	42.2189	2.4837	714	1432	42.2189	2.4837	780.3341	1432	42.2189	2.4837	1203.2477
1433	42.2449	2.4822	285.0619	1433	42.2449	2.4822	682.3489	1433	42.2449	2.4822	710.6008	1433	42.2449	2.4822	1132.1059
1434	42.2709	2.4808	295.5269	1434	42.2709	2.4808	691.9712	1434	42.2709	2.4808	682.7136	1434	42.2709	2.4808	1102.8102
1435	42.2969	2.4793	292.1413	1435	42.2969	2.4793	687.7428	1435	42.2969	2.4793	680.8547	1435	42.2969	2.4793	1099.5429

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1436	42.3229	2.4779	316.8941	1436	42.3229	2.4779	711.6529	1436	42.3229	2.4779	616.469	1436	42.3229	2.4779	1033.7486
1437	42.3489	2.4764	299.7784	1437	42.3489	2.4764	693.6944	1437	42.3489	2.4764	602.3899	1437	42.3489	2.4764	1018.2611
1438	42.3749	2.475	300.085	1438	42.3749	2.475	693.1583	1438	42.3749	2.475	617.404	1438	42.3749	2.475	1031.8666
1439	42.4009	2.4735	263.5235	1439	42.4009	2.4735	655.7541	1439	42.4009	2.4735	587.8221	1439	42.4009	2.4735	1000.8763
1440	42.4269	2.4721	272.7104	1440	42.4269	2.4721	664.0983	1440	42.4269	2.4721	528.7141	1440	42.4269	2.4721	940.3598
1441	42.4529	2.4706	342.9662	1441	42.4529	2.4706	733.5114	1441	42.4529	2.4706	476.1679	1441	42.4529	2.4706	886.4051
1442	42.4789	2.4692	317.0533	1442	42.4789	2.4692	706.7557	1442	42.4789	2.4692	467.3831	1442	42.4789	2.4692	876.2119
1443	42.5049	2.4677	265.6899	1443	42.5049	2.4677	654.5496	1443	42.5049	2.4677	424.2122	1443	42.5049	2.4677	831.6324
1444	42.5309	2.4663	270.0363	1444	42.5309	2.4663	658.0533	1444	42.5309	2.4663	434.3199	1444	42.5309	2.4663	840.3317
1445	42.5569	2.4649	286.2201	1445	42.5569	2.4649	673.3943	1445	42.5569	2.4649	464.8576	1445	42.5569	2.4649	869.4608
1446	42.5829	2.4634	309.2125	1446	42.5829	2.4634	695.544	1446	42.5829	2.4634	428.7697	1446	42.5829	2.4634	831.9645
1447	42.6089	2.462	299.2879	1447	42.6089	2.462	684.7767	1447	42.6089	2.462	402.6472	1447	42.6089	2.462	804.4334
1448	42.6349	2.4606	260.444	1448	42.6349	2.4606	645.0901	1448	42.6349	2.4606	430.5322	1448	42.6349	2.4606	830.9099
1449	42.6609	2.4591	286.3105	1449	42.6609	2.4591	670.1138	1449	42.6609	2.4591	438.5429	1449	42.6609	2.4591	837.5122
1450	42.6869	2.4577	276.1739	1450	42.6869	2.4577	659.1345	1450	42.6869	2.4577	405.7997	1450	42.6869	2.4577	803.3605
1451	42.7129	2.4563	279.1638	1451	42.7129	2.4563	661.2817	1451	42.7129	2.4563	411.904	1451	42.7129	2.4563	808.0563
1452	42.7389	2.4549	266.3954	1452	42.7389	2.4549	647.6706	1452	42.7389	2.4549	391.6937	1452	42.7389	2.4549	786.4375
1453	42.7649	2.4534	277.6163	1453	42.7649	2.4534	658.0487	1453	42.7649	2.4534	384.4855	1453	42.7649	2.4534	777.8208
1454	42.7909	2.452	285.5863	1454	42.7909	2.452	665.176	1454	42.7909	2.452	382.6663	1454	42.7909	2.452	774.5931
1455	42.8169	2.4506	265.2203	1455	42.8169	2.4506	643.9673	1455	42.8169	2.4506	451.8349	1455	42.8169	2.4506	842.3532
1456	42.8429	2.4492	249.2129	1456	42.8429	2.4492	627.1171	1456	42.8429	2.4492	432.6242	1456	42.8429	2.4492	821.7341
1457	42.8689	2.4478	242.8322	1457	42.8689	2.4478	619.8937	1457	42.8689	2.4478	404.2746	1457	42.8689	2.4478	791.976
1458	42.8949	2.4464	267.7693	1458	42.8949	2.4464	643.9881	1458	42.8949	2.4464	409.5216	1458	42.8949	2.4464	795.8144
1459	42.9209	2.4449	273.625	1459	42.9209	2.4449	649.0011	1459	42.9209	2.4449	380.8498	1459	42.9209	2.4449	765.7342
1460	42.9469	2.4435	273.474	1460	42.9469	2.4435	648.6078	1460	42.9469	2.4435	387.9791	1460	42.9469	2.4435	771.748
1461	42.9729	2.4421	287.1355	1461	42.9729	2.4421	662.0269	1461	42.9729	2.4421	384.322	1461	42.9729	2.4421	766.9753
1462	42.9989	2.4407	267.2027	1462	42.9989	2.4407	641.8517	1462	42.9989	2.4407	387.6104	1462	42.9989	2.4407	769.1483
1463	43.0249	2.4393	281.6395	1463	43.0249	2.4393	656.0462	1463	43.0249	2.4393	441.1686	1463	43.0249	2.4393	821.5909
1464	43.0509	2.4379	300.9066	1464	43.0509	2.4379	675.071	1464	43.0509	2.4379	441.8025	1464	43.0509	2.4379	821.1094
1465	43.0769	2.4365	272.1814	1465	43.0769	2.4365	646.1034	1465	43.0769	2.4365	383.6467	1465	43.0769	2.4365	761.8381
1466	43.1029	2.4351	260.7842	1466	43.1029	2.4351	634.4638	1466	43.1029	2.4351	365.3456	1466	43.1029	2.4351	742.4215
1467	43.1289	2.4337	258.3852	1467	43.1289	2.4337	631.8226	1467	43.1289	2.4337	380.9405	1467	43.1289	2.4337	756.9009
1468	43.1549	2.4323	259.245	1468	43.1549	2.4323	632.44	1468	43.1549	2.4323	374.9472	1468	43.1549	2.4323	749.7921
1469	43.1809	2.4309	278.0696	1469	43.1809	2.4309	651.0222	1469	43.1809	2.4309	376.5017	1469	43.1809	2.4309	750.2311
1470	43.2069	2.4295	291.4723	1470	43.2069	2.4295	664.1826	1470	43.2069	2.4295	393.7513	1470	43.2069	2.4295	766.3653
1471	43.2329	2.4281	289.4316	1471	43.2329	2.4281	661.8996	1471	43.2329	2.4281	381.602	1471	43.2329	2.4281	753.1004

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1472	43.2589	2.4267	278.4106	1472	43.2589	2.4267	650.6363	1472	43.2589	2.4267	386.2989	1472	43.2589	2.4267	756.6818
1473	43.2849	2.4254	262.7212	1473	43.2849	2.4254	634.7046	1473	43.2849	2.4254	394.7887	1473	43.2849	2.4254	764.0561
1474	43.3109	2.424	252.8825	1474	43.3109	2.424	624.6235	1474	43.3109	2.424	389.0791	1474	43.3109	2.424	757.2311
1475	43.3369	2.4226	240.7265	1475	43.3369	2.4226	612.2252	1475	43.3369	2.4226	407.316	1475	43.3369	2.4226	774.3525
1476	43.3629	2.4212	268.9098	1476	43.3629	2.4212	640.1661	1476	43.3629	2.4212	427.4113	1476	43.3629	2.4212	793.3322
1477	43.3889	2.4198	265.0158	1477	43.3889	2.4198	636.0298	1477	43.3889	2.4198	398.263	1477	43.3889	2.4198	763.0685
1478	43.4149	2.4184	277.9522	1478	43.4149	2.4184	648.7239	1478	43.4149	2.4184	382.6891	1478	43.4149	2.4184	746.3791
1479	43.4409	2.4171	271.76	1479	43.4409	2.4171	642.2893	1479	43.4409	2.4171	388.0998	1479	43.4409	2.4171	750.6743
1480	43.4669	2.4157	264.7354	1480	43.4669	2.4157	635.0224	1480	43.4669	2.4157	412.6866	1480	43.4669	2.4157	774.1456
1481	43.4929	2.4143	282.3952	1481	43.4929	2.4143	652.4398	1481	43.4929	2.4143	457.8616	1481	43.4929	2.4143	818.205
1482	43.5189	2.4129	270.774	1482	43.5189	2.4129	640.5763	1482	43.5189	2.4129	455.8398	1482	43.5189	2.4129	815.0678
1483	43.5449	2.4116	278.7836	1483	43.5449	2.4116	648.3435	1483	43.5449	2.4116	432.0988	1483	43.5449	2.4116	790.2113
1484	43.5709	2.4102	268.689	1484	43.5709	2.4102	638.0066	1484	43.5709	2.4102	405.3081	1484	43.5709	2.4102	762.3052
1485	43.5969	2.4088	269.9374	1485	43.5969	2.4088	639.0127	1485	43.5969	2.4088	374.9159	1485	43.5969	2.4088	730.7975
1486	43.6229	2.4075	293.8591	1486	43.6229	2.4075	662.6921	1486	43.6229	2.4075	380.8498	1486	43.6229	2.4075	735.6158
1487	43.6489	2.4061	283.7524	1487	43.6489	2.4061	652.343	1487	43.6489	2.4061	404.9282	1487	43.6489	2.4061	760.146
1488	43.6749	2.4047	293.7051	1488	43.6749	2.4047	662.0534	1488	43.6749	2.4047	382.4729	1488	43.6749	2.4047	738.1424
1489	43.7009	2.4034	285.1297	1489	43.7009	2.4034	653.2356	1489	43.7009	2.4034	352.4593	1489	43.7009	2.4034	708.5805
1490	43.7269	2.402	278.4624	1490	43.7269	2.402	646.326	1490	43.7269	2.402	348.4208	1490	43.7269	2.402	704.9938
1491	43.7529	2.4007	251.5156	1491	43.7529	2.4007	619.1369	1491	43.7529	2.4007	402.0172	1491	43.7529	2.4007	759.042
1492	43.7789	2.3993	245.3273	1492	43.7789	2.3993	612.7062	1492	43.7789	2.3993	428.67	1492	43.7789	2.3993	786.1465
1493	43.8049	2.398	238.5456	1493	43.8049	2.398	605.6822	1493	43.8049	2.398	446.3083	1493	43.8049	2.398	804.2365
1494	43.8309	2.3966	272.7087	1494	43.8309	2.3966	639.603	1494	43.8309	2.3966	432.8535	1494	43.8309	2.3966	791.2335
1495	43.8569	2.3953	312.1282	1495	43.8569	2.3953	678.7801	1495	43.8569	2.3953	410.338	1495	43.8569	2.3953	769.1697
1496	43.8829	2.3939	285.5696	1496	43.8829	2.3939	651.9793	1496	43.8829	2.3939	418.9005	1496	43.8829	2.3939	778.184
1497	43.9089	2.3926	317.239	1497	43.9089	2.3926	683.4062	1497	43.9089	2.3926	385.3585	1497	43.9089	2.3926	745.0937
1498	43.9349	2.3912	291.1976	1498	43.9349	2.3912	657.1226	1498	43.9349	2.3912	372.8853	1498	43.9349	2.3912	733.0723
1499	43.9609	2.3899	265.0944	1499	43.9609	2.3899	630.777	1499	43.9609	2.3899	421.2691	1499	43.9609	2.3899	781.9078
1500	43.9869	2.3885	346.1091	1500	43.9869	2.3885	711.5493	1500	43.9869	2.3885	403.3839	1500	43.9869	2.3885	764.4744
1501	44.0129	2.3872	300.1702	1501	44.0129	2.3872	665.3681	1501	44.0129	2.3872	459.3597	1501	44.0129	2.3872	820.9019
1502	44.0389	2.3858	298.0685	1502	44.0389	2.3858	663.0241	1502	44.0389	2.3858	439.167	1502	44.0389	2.3858	801.161
1503	44.0649	2.3845	380.3524	1503	44.0649	2.3845	745.0657	1503	44.0649	2.3845	411.2934	1503	44.0649	2.3845	773.7391
1504	44.0909	2.3832	357.6686	1504	44.0909	2.3832	722.1395	1504	44.0909	2.3832	451.7175	1504	44.0909	2.3832	814.615
1505	44.1169	2.3818	309.5388	1505	44.1169	2.3818	673.7674	1505	44.1169	2.3818	417.4188	1505	44.1169	2.3818	780.7681
1506	44.1429	2.3805	346.8968	1506	44.1429	2.3805	710.8831	1506	44.1429	2.3805	440.1406	1506	44.1429	2.3805	803.9415
1507	44.1689	2.3792	405.6472	1507	44.1689	2.3792	769.3911	1507	44.1689	2.3792	469.1424	1507	44.1689	2.3792	833.3952

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1508	44.1949	2.3778	476.7084	1508	44.1949	2.3778	840.21	1508	44.1949	2.3778	510.0855	1508	44.1949	2.3778	874.79
1509	44.2209	2.3765	440.6664	1509	44.2209	2.3765	803.9256	1509	44.2209	2.3765	545.1745	1509	44.2209	2.3765	910.3307
1510	44.2469	2.3752	440.9731	1510	44.2469	2.3752	803.99	1510	44.2469	2.3752	528.5915	1510	44.2469	2.3752	894.1995
1511	44.2729	2.3739	511.8093	1511	44.2729	2.3739	874.5839	1511	44.2729	2.3739	569.9347	1511	44.2729	2.3739	935.9944
1512	44.2989	2.3725	487.9412	1512	44.2989	2.3725	850.4735	1512	44.2989	2.3725	512.3773	1512	44.2989	2.3725	878.8888
1513	44.3249	2.3712	417.8881	1513	44.3249	2.3712	780.178	1513	44.3249	2.3712	497.0744	1513	44.3249	2.3712	864.0376
1514	44.3509	2.3699	467.0929	1514	44.3509	2.3699	828.391	1514	44.3509	2.3699	476.8336	1514	44.3509	2.3699	844.2486
1515	44.3769	2.3686	476.5148	1515	44.3769	2.3686	836.8212	1515	44.3769	2.3686	475.1556	1515	44.3769	2.3686	843.0224
1516	44.4029	2.3673	405.1058	1516	44.4029	2.3673	764.4205	1516	44.4029	2.3673	473.7138	1516	44.4029	2.3673	842.0323
1517	44.4289	2.3659	383.5632	1517	44.4289	2.3659	741.8861	1517	44.4289	2.3659	415.7615	1517	44.4289	2.3659	784.5317
1518	44.4549	2.3646	391.2519	1518	44.4549	2.3646	748.5831	1518	44.4549	2.3646	420.3611	1518	44.4549	2.3646	789.5831
1519	44.4809	2.3633	343.8867	1519	44.4809	2.3633	700.2261	1519	44.4809	2.3633	426.892	1519	44.4809	2.3633	796.5657
1520	44.5069	2.362	332.372	1520	44.5069	2.362	687.7196	1520	44.5069	2.362	416.6661	1520	44.5069	2.362	786.7916
1521	44.5329	2.3607	317.0361	1521	44.5329	2.3607	671.392	1521	44.5329	2.3607	393.388	1521	44.5329	2.3607	763.9652
1522	44.5589	2.3594	344.7898	1522	44.5589	2.3594	698.154	1522	44.5589	2.3594	412.7677	1522	44.5589	2.3594	783.7966
1523	44.5849	2.3581	322.5777	1523	44.5849	2.3581	674.9501	1523	44.5849	2.3581	424.4003	1523	44.5849	2.3581	795.881
1524	44.6109	2.3568	321.5077	1524	44.6109	2.3568	672.8883	1524	44.6109	2.3568	411.7423	1524	44.6109	2.3568	783.6748
1525	44.6369	2.3555	338.4227	1525	44.6369	2.3555	688.8117	1525	44.6369	2.3555	396.4394	1525	44.6369	2.3555	768.8236
1526	44.6629	2.3542	308.5997	1526	44.6629	2.3542	657.9969	1526	44.6629	2.3542	344.6593	1526	44.6629	2.3542	717.4953
1527	44.6889	2.3529	329.4934	1527	44.6889	2.3529	677.8989	1527	44.6889	2.3529	371.0556	1527	44.6889	2.3529	744.3433
1528	44.7149	2.3516	283.6668	1528	44.7149	2.3516	631.0804	1528	44.7149	2.3516	409.3583	1528	44.7149	2.3516	783.0977
1529	44.7409	2.3503	294.869	1529	44.7409	2.3503	641.291	1529	44.7409	2.3503	330.0964	1529	44.7409	2.3503	704.2876
1530	44.7669	2.349	310.3444	1530	44.7669	2.349	655.7746	1530	44.7669	2.349	388.7792	1530	44.7669	2.349	763.4221
1531	44.7929	2.3477	311.1049	1531	44.7929	2.3477	655.5433	1531	44.7929	2.3477	337.575	1531	44.7929	2.3477	712.6697
1532	44.8189	2.3464	286.4752	1532	44.8189	2.3464	629.9219	1532	44.8189	2.3464	345.1047	1532	44.8189	2.3464	720.6512
1533	44.8449	2.3451	276.7508	1533	44.8449	2.3451	619.2057	1533	44.8449	2.3451	359.5904	1533	44.8449	2.3451	735.5886
1534	44.8709	2.3438	257.5978	1534	44.8709	2.3438	599.061	1534	44.8709	2.3438	386.8021	1534	44.8709	2.3438	763.252
1535	44.8969	2.3425	251.9701	1535	44.8969	2.3425	592.4416	1535	44.8969	2.3425	374.3975	1535	44.8969	2.3425	751.2991
1536	44.9229	2.3413	257.9053	1536	44.9229	2.3413	597.385	1536	44.9229	2.3413	360.9538	1536	44.9229	2.3413	738.3072
1537	44.9489	2.34	277.2179	1537	44.9489	2.34	615.7059	1537	44.9489	2.34	412.1093	1537	44.9489	2.34	789.9145
1538	44.9749	2.3387	252.7769	1538	44.9749	2.3387	590.2731	1538	44.9749	2.3387	398.7656	1538	44.9749	2.3387	777.0225
1539	45.0009	2.3374	275.2946	1539	45.0009	2.3374	611.7991	1539	45.0009	2.3374	423.0485	1539	45.0009	2.3374	801.7572
1540	45.0269	2.3361	273.625	1540	45.0269	2.3361	609.1378	1540	45.0269	2.3361	380.8498	1540	45.0269	2.3361	760.0102
1541	45.0529	2.3349	259.8847	1541	45.0529	2.3349	595.364	1541	45.0529	2.3349	331.0514	1541	45.0529	2.3349	710.4936
1542	45.0789	2.3336	262.9418	1542	45.0789	2.3336	598.3877	1542	45.0789	2.3336	348.3758	1542	45.0789	2.3336	728.0996
1543	45.1049	2.3323	241.0936	1543	45.1049	2.3323	576.5061	1543	45.1049	2.3323	344.5983	1543	45.1049	2.3323	724.6039

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1544	45.1309	2.331	252.6978	1544	45.1309	2.331	588.0769	1544	45.1309	2.331	362.5492	1544	45.1309	2.331	742.8365
1545	45.1569	2.3298	245.6548	1545	45.1569	2.3298	581.0005	1545	45.1569	2.3298	378.8708	1545	45.1569	2.3298	759.4398
1546	45.1829	2.3285	252.429	1546	45.1829	2.3285	587.7413	1546	45.1829	2.3285	366.4079	1546	45.1829	2.3285	747.2587
1547	45.2089	2.3272	231.3353	1547	45.2089	2.3272	566.6142	1547	45.2089	2.3272	372.7303	1547	45.2089	2.3272	753.8628
1548	45.2349	2.3259	238.8618	1548	45.2349	2.3259	574.1073	1548	45.2349	2.3259	379.5858	1548	45.2349	2.3259	761
1549	45.2609	2.3247	248.8671	1549	45.2609	2.3247	584.0791	1549	45.2609	2.3247	385.0666	1549	45.2609	2.3247	766.7626
1550	45.2869	2.3234	264.8413	1550	45.2869	2.3234	600.02	1550	45.2869	2.3234	383.6097	1550	45.2869	2.3234	765.5874
1551	45.3129	2.3222	258.1027	1551	45.3129	2.3222	593.2479	1551	45.3129	2.3222	383.8428	1551	45.3129	2.3222	766.1022
1552	45.3389	2.3209	263.7618	1552	45.3389	2.3209	598.8736	1552	45.3389	2.3209	375.6905	1552	45.3389	2.3209	758.2316
1553	45.3649	2.3196	261.9095	1553	45.3649	2.3196	596.988	1553	45.3649	2.3196	393.8018	1553	45.3649	2.3196	776.6247
1554	45.3909	2.3184	278.7635	1554	45.3909	2.3184	613.8085	1554	45.3909	2.3184	405.1699	1554	45.3909	2.3184	788.2746
1555	45.4169	2.3171	283.7925	1555	45.4169	2.3171	618.8041	1555	45.4169	2.3171	406.8405	1555	45.4169	2.3171	790.2268
1556	45.4429	2.3159	232.78	1556	45.4429	2.3159	567.7582	1556	45.4429	2.3159	441.157	1556	45.4429	2.3159	824.8251
1557	45.4689	2.3146	230.2227	1557	45.4689	2.3146	565.1675	1557	45.4689	2.3146	427.03	1557	45.4689	2.3146	810.9798
1558	45.4949	2.3134	243.7218	1558	45.4949	2.3134	578.6332	1558	45.4949	2.3134	390.0546	1558	45.4949	2.3134	774.2861
1559	45.5209	2.3121	228.006	1559	45.5209	2.3121	562.884	1559	45.5209	2.3121	417.574	1559	45.5209	2.3121	802.0873
1560	45.5469	2.3109	241.8701	1560	45.5469	2.3109	576.7147	1560	45.5469	2.3109	414.8674	1560	45.5469	2.3109	799.6624
1561	45.5729	2.3096	272.6982	1561	45.5729	2.3096	607.5094	1561	45.5729	2.3096	390.0506	1561	45.5729	2.3096	775.1273
1562	45.5989	2.3084	270.4171	1562	45.5989	2.3084	605.1949	1562	45.5989	2.3084	396.2207	1562	45.5989	2.3084	781.5791
1563	45.6249	2.3071	239.7074	1563	45.6249	2.3071	574.4517	1563	45.6249	2.3071	402.3681	1563	45.6249	2.3071	788.0083
1564	45.6509	2.3059	241.4559	1564	45.6509	2.3059	576.1668	1564	45.6509	2.3059	409.0097	1564	45.6509	2.3059	794.9317
1565	45.6769	2.3046	276.25	1565	45.6769	2.3046	610.9276	1565	45.6769	2.3046	435.4285	1565	45.6769	2.3046	821.6321
1566	45.7029	2.3034	276.321	1566	45.7029	2.3034	610.9652	1566	45.7029	2.3034	461.8727	1566	45.7029	2.3034	848.3581
1567	45.7289	2.3021	273.625	1567	45.7289	2.3021	608.2358	1567	45.7289	2.3021	463.3095	1567	45.7289	2.3021	850.0766
1568	45.7549	2.3009	263.5455	1568	45.7549	2.3009	597.5386	1568	45.7549	2.3009	476.8595	1568	45.7549	2.3009	863.9083
1569	45.7809	2.2997	248.6237	1569	45.7809	2.2997	581.9993	1569	45.7809	2.2997	492.9021	1569	45.7809	2.2997	880.2326
1570	45.8069	2.2984	257.2608	1570	45.8069	2.2984	590.0188	1570	45.8069	2.2984	502.4816	1570	45.8069	2.2984	890.0938
1571	45.8329	2.2972	232.6394	1571	45.8329	2.2972	564.78	1571	45.8329	2.2972	548.49	1571	45.8329	2.2972	936.384
1572	45.8589	2.296	235.7186	1572	45.8589	2.296	567.2416	1572	45.8589	2.296	611.6644	1572	45.8589	2.296	999.8402
1573	45.8849	2.2947	244.8773	1573	45.8849	2.2947	575.7828	1573	45.8849	2.2947	672.7042	1573	45.8849	2.2947	1061.1617
1574	45.9109	2.2935	235.613	1574	45.9109	2.2935	565.901	1574	45.9109	2.2935	776.8803	1574	45.9109	2.2935	1165.6195
1575	45.9369	2.2923	246.2983	1575	45.9369	2.2923	575.9686	1575	45.9369	2.2923	993.6126	1575	45.9369	2.2923	1382.6336
1576	45.9629	2.2911	267.3822	1576	45.9629	2.2911	596.435	1576	45.9629	2.2911	1397.2771	1576	45.9629	2.2911	1786.5797
1577	45.9889	2.2898	267.3385	1577	45.9889	2.2898	595.7737	1577	45.9889	2.2898	2106.3195	1577	45.9889	2.2898	2495.9039
1578	46.0149	2.2886	284.0737	1578	46.0149	2.2886	611.8915	1578	46.0149	2.2886	3061.6104	1578	46.0149	2.2886	3451.4766
1579	46.0409	2.2874	294.4686	1579	46.0409	2.2874	621.6688	1579	46.0409	2.2874	3603.526	1579	46.0409	2.2874	3993.6738

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1580	46.0669	2.2862	348.406	1580	46.0669	2.2862	674.9886	1580	46.0669	2.2862	3514.9829	1580	46.0669	2.2862	3905.4125
1581	46.0929	2.2849	360.7121	1581	46.0929	2.2849	686.6772	1581	46.0929	2.2849	3360.6004	1581	46.0929	2.2849	3751.3117
1582	46.1189	2.2837	355.3339	1582	46.1189	2.2837	680.6815	1582	46.1189	2.2837	3211.0684	1582	46.1189	2.2837	3602.0614
1583	46.1449	2.2825	344.8759	1583	46.1449	2.2825	669.6059	1583	46.1449	2.2825	3077.8581	1583	46.1449	2.2825	3469.1329
1584	46.1709	2.2813	356.8499	1584	46.1709	2.2813	680.9624	1584	46.1709	2.2813	2629.352	1584	46.1709	2.2813	3020.9085
1585	46.1969	2.2801	371.3139	1585	46.1969	2.2801	694.8088	1585	46.1969	2.2801	2156.1138	1585	46.1969	2.2801	2547.9521
1586	46.2229	2.2789	335.196	1586	46.2229	2.2789	658.0733	1586	46.2229	2.2789	1753.35	1586	46.2229	2.2789	2145.47
1587	46.2489	2.2777	306.7402	1587	46.2489	2.2777	629	1587	46.2489	2.2777	1414.683	1587	46.2489	2.2777	1807.0847
1588	46.2749	2.2765	306.0911	1588	46.2749	2.2765	627.7334	1588	46.2749	2.2765	1197.2785	1588	46.2749	2.2765	1589.9619
1589	46.3009	2.2752	303.2187	1589	46.3009	2.2752	624.2434	1589	46.3009	2.2752	1061.4309	1589	46.3009	2.2752	1454.396
1590	46.3269	2.274	307.3945	1590	46.3269	2.274	627.8017	1590	46.3269	2.274	1012.0175	1590	46.3269	2.274	1405.2644
1591	46.3529	2.2728	326.8232	1591	46.3529	2.2728	646.6129	1591	46.3529	2.2728	981.8106	1591	46.3529	2.2728	1375.3392
1592	46.3789	2.2716	355.0598	1592	46.3789	2.2716	674.2319	1592	46.3789	2.2716	896.4765	1592	46.3789	2.2716	1290.2868
1593	46.4049	2.2704	339.5382	1593	46.4049	2.2704	658.0928	1593	46.4049	2.2704	809.7228	1593	46.4049	2.2704	1203.8148
1594	46.4309	2.2692	358.7065	1594	46.4309	2.2692	676.6435	1594	46.4309	2.2692	810.4945	1594	46.4309	2.2692	1204.8683
1595	46.4569	2.268	350.1871	1595	46.4569	2.268	667.5066	1595	46.4569	2.268	774.6123	1595	46.4569	2.268	1166.2138
1596	46.4829	2.2668	329.9059	1596	46.4829	2.2668	646.6078	1596	46.4829	2.2668	643.6054	1596	46.4829	2.2668	1032.4345
1597	46.5089	2.2656	308.1961	1597	46.5089	2.2656	624.2804	1597	46.5089	2.2656	638.1231	1597	46.5089	2.2656	1024.1799
1598	46.5349	2.2644	327.6906	1598	46.5349	2.2644	643.1574	1598	46.5349	2.2644	622.2303	1598	46.5349	2.2644	1005.5147
1599	46.5609	2.2632	336.4021	1599	46.5609	2.2632	651.2514	1599	46.5609	2.2632	533.3771	1599	46.5609	2.2632	913.8892
1600	46.5869	2.262	312.486	1600	46.5869	2.262	626.7177	1600	46.5869	2.262	471.6442	1600	46.5869	2.262	849.384
1601	46.6129	2.2609	303.8564	1601	46.6129	2.2609	617.4706	1601	46.6129	2.2609	520.7892	1601	46.6129	2.2609	895.7567
1602	46.6389	2.2597	338.3126	1602	46.6389	2.2597	651.3092	1602	46.6389	2.2597	508.5124	1602	46.6389	2.2597	880.7075
1603	46.6649	2.2585	301.3671	1603	46.6649	2.2585	613.7462	1603	46.6649	2.2585	463.6221	1603	46.6649	2.2585	833.0449
1604	46.6909	2.2573	292.9406	1604	46.6909	2.2573	604.7022	1604	46.6909	2.2573	474.9713	1604	46.6909	2.2573	841.6217
1605	46.7169	2.2561	307.9939	1605	46.7169	2.2561	619.1379	1605	46.7169	2.2561	469.2972	1605	46.7169	2.2561	833.1754
1606	46.7429	2.2549	284.7375	1606	46.7429	2.2549	595.264	1606	46.7429	2.2549	417.1296	1606	46.7429	2.2549	778.2353
1607	46.7689	2.2537	243.2382	1607	46.7689	2.2537	553.1471	1607	46.7689	2.2537	386.4441	1607	46.7689	2.2537	744.7776
1608	46.7949	2.2526	301.1844	1608	46.7949	2.2526	610.4757	1608	46.7949	2.2526	402.1949	1608	46.7949	2.2526	757.756
1609	46.8209	2.2514	258.4161	1609	46.8209	2.2514	567.0899	1609	46.8209	2.2514	434.8516	1609	46.8209	2.2514	787.6404
1610	46.8469	2.2502	262.0297	1610	46.8469	2.2502	570.086	1610	46.8469	2.2502	429.388	1610	46.8469	2.2502	779.4045
1611	46.8729	2.249	291.4816	1611	46.8729	2.249	598.9203	1611	46.8729	2.249	417.0113	1611	46.8729	2.249	764.2554
1612	46.8989	2.2478	250.8167	1612	46.8989	2.2478	557.6378	1612	46.8989	2.2478	467.7385	1612	46.8989	2.2478	812.2103
1613	46.9249	2.2467	292.5858	1613	46.9249	2.2467	598.7894	1613	46.9249	2.2467	418.9531	1613	46.9249	2.2467	760.6525
1614	46.9509	2.2455	253.6002	1614	46.9509	2.2455	559.1863	1614	46.9509	2.2455	356.3803	1614	46.9509	2.2455	695.3074
1615	46.9769	2.2443	255.0169	1615	46.9769	2.2443	559.9854	1615	46.9769	2.2443	418.9558	1615	46.9769	2.2443	755.1106

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1616	47.0029	2.2431	295.6444	1616	47.0029	2.2431	599.9954	1616	47.0029	2.2431	406.0341	1616	47.0029	2.2431	739.4165
1617	47.0289	2.242	242.2288	1617	47.0289	2.242	545.9622	1617	47.0289	2.242	458.5998	1617	47.0289	2.242	789.2099
1618	47.0549	2.2408	244.7067	1618	47.0549	2.2408	547.8226	1618	47.0549	2.2408	409.6457	1618	47.0549	2.2408	737.4834
1619	47.0809	2.2396	240.773	1619	47.0809	2.2396	543.2713	1619	47.0809	2.2396	412.7718	1619	47.0809	2.2396	737.8372
1620	47.1069	2.2385	257.9637	1620	47.1069	2.2385	559.8446	1620	47.1069	2.2385	384.8252	1620	47.1069	2.2385	707.1183
1621	47.1329	2.2373	273.625	1621	47.1329	2.2373	574.8883	1621	47.1329	2.2373	380.8498	1621	47.1329	2.2373	700.3706
1622	47.1589	2.2361	256.3882	1622	47.1589	2.2361	556.7648	1622	47.1589	2.2361	383.2606	1622	47.1589	2.2361	704.5798
1623	47.1849	2.235	295.3759	1623	47.1849	2.235	594.8658	1623	47.1849	2.235	381.8823	1623	47.1849	2.235	705
1624	47.2109	2.2338	218.8499	1624	47.2109	2.2338	517.4532	1624	47.2109	2.2338	375.6033	1624	47.2109	2.2338	700.5194
1625	47.2369	2.2327	242.1866	1625	47.2369	2.2327	539.9031	1625	47.2369	2.2327	406.9609	1625	47.2369	2.2327	733.6755
1626	47.2629	2.2315	281.3449	1626	47.2629	2.2315	578.1747	1626	47.2629	2.2315	397.2192	1626	47.2629	2.2315	725.7322
1627	47.2889	2.2304	264.5317	1627	47.2889	2.2304	560.4748	1627	47.2889	2.2304	368.5643	1627	47.2889	2.2304	698.8758
1628	47.3149	2.2292	282.4978	1628	47.3149	2.2292	577.5543	1628	47.3149	2.2292	397.1473	1628	47.3149	2.2292	729.2572
1629	47.3409	2.228	285.9837	1629	47.3409	2.228	580.1535	1629	47.3409	2.228	387.5475	1629	47.3409	2.228	721.4559
1630	47.3669	2.2269	305.1218	1630	47.3669	2.2269	598.4049	1630	47.3669	2.2269	395.842	1630	47.3669	2.2269	731.5488
1631	47.3929	2.2257	274.8837	1631	47.3929	2.2257	567.2801	1631	47.3929	2.2257	394.8414	1631	47.3929	2.2257	732.3467
1632	47.4189	2.2246	242.3545	1632	47.4189	2.2246	533.8643	1632	47.4189	2.2246	418.832	1632	47.4189	2.2246	758.1357
1633	47.4449	2.2234	279.3315	1633	47.4449	2.2234	569.9546	1633	47.4449	2.2234	420.4774	1633	47.4449	2.2234	761.5795
1634	47.4709	2.2223	277.5133	1634	47.4709	2.2223	567.2497	1634	47.4709	2.2223	361.5198	1634	47.4709	2.2223	704.4204
1635	47.4969	2.2211	279.0851	1635	47.4969	2.2211	567.9349	1635	47.4969	2.2211	350.8098	1635	47.4969	2.2211	695.5088
1636	47.5229	2.22	263.1648	1636	47.5229	2.22	551.1278	1636	47.5229	2.22	366.8206	1636	47.5229	2.22	713.3181
1637	47.5489	2.2189	271.1977	1637	47.5489	2.2189	558.2741	1637	47.5489	2.2189	372.0055	1637	47.5489	2.2189	720.3014
1638	47.5749	2.2177	286.4112	1638	47.5749	2.2177	572.6009	1638	47.5749	2.2177	388.3214	1638	47.5749	2.2177	738.4158
1639	47.6009	2.2166	298.9171	1639	47.6009	2.2166	584.2201	1639	47.6009	2.2166	375.6669	1639	47.6009	2.2166	727.5597
1640	47.6269	2.2154	305.5331	1640	47.6269	2.2154	589.9494	1640	47.6269	2.2154	367.5714	1640	47.6269	2.2154	721.2626
1641	47.6529	2.2143	311.1076	1641	47.6529	2.2143	594.6372	1641	47.6529	2.2143	340.7773	1641	47.6529	2.2143	696.267
1642	47.6789	2.2132	270.306	1642	47.6789	2.2132	552.9489	1642	47.6789	2.2132	371.3279	1642	47.6789	2.2132	728.616
1643	47.7049	2.212	257.0741	1643	47.7049	2.212	538.8304	1643	47.7049	2.212	376.007	1643	47.7049	2.212	735.0937
1644	47.7309	2.2109	266.1071	1644	47.7309	2.2109	546.9767	1644	47.7309	2.2109	365.2312	1644	47.7309	2.2109	726.1163
1645	47.7569	2.2098	276.2068	1645	47.7569	2.2098	556.1898	1645	47.7569	2.2098	347.5615	1645	47.7569	2.2098	710.245
1646	47.7829	2.2086	287.3599	1646	47.7829	2.2086	566.4561	1646	47.7829	2.2086	338.8402	1646	47.7829	2.2086	703.3222
1647	47.8089	2.2075	276.4286	1647	47.8089	2.2075	554.6382	1647	47.8089	2.2075	330.0405	1647	47.8089	2.2075	696.3209
1648	47.8349	2.2064	273.625	1648	47.8349	2.2064	550.9479	1648	47.8349	2.2064	380.8498	1648	47.8349	2.2064	748.9287
1649	47.8609	2.2052	258.3576	1649	47.8609	2.2052	535.5023	1649	47.8609	2.2052	377.0735	1649	47.8609	2.2052	744.3008
1650	47.8869	2.2041	279.6641	1650	47.8869	2.2041	556.6307	1650	47.8869	2.2041	357.7099	1650	47.8869	2.2041	724.0856
1651	47.9129	2.203	321.0838	1651	47.9129	2.203	597.8723	1651	47.9129	2.203	337.373	1651	47.9129	2.203	702.897

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1652	47.9389	2.2019	352.7019	1652	47.9389	2.2019	629.3123	1652	47.9389	2.2019	338.6934	1652	47.9389	2.2019	703.3659
1653	47.9649	2.2007	346.5334	1653	47.9649	2.2007	622.9656	1653	47.9649	2.2007	355.6963	1653	47.9649	2.2007	719.5172
1654	47.9909	2.1996	310.0126	1654	47.9909	2.1996	586.2666	1654	47.9909	2.1996	323.1315	1654	47.9909	2.1996	686.1007
1655	48.0169	2.1985	315.8766	1655	48.0169	2.1985	591.9526	1655	48.0169	2.1985	322.6005	1655	48.0169	2.1985	684.7182
1656	48.0429	2.1974	277.1346	1656	48.0429	2.1974	553.0324	1656	48.0429	2.1974	332.6334	1656	48.0429	2.1974	693.8995
1657	48.0689	2.1963	262.3024	1657	48.0689	2.1963	538.0221	1657	48.0689	2.1963	338.9592	1657	48.0689	2.1963	699.3737
1658	48.0949	2.1951	276.9884	1658	48.0949	2.1951	552.5299	1658	48.0949	2.1951	332.7918	1658	48.0949	2.1951	692.3547
1659	48.1209	2.194	303.8227	1659	48.1209	2.194	579.1861	1659	48.1209	2.194	347.633	1659	48.1209	2.194	706.3443
1660	48.1469	2.1929	308.8748	1660	48.1469	2.1929	584.0601	1660	48.1469	2.1929	357.2063	1660	48.1469	2.1929	715.066
1661	48.1729	2.1918	284.0579	1661	48.1729	2.1918	559.0651	1661	48.1729	2.1918	350.6949	1661	48.1729	2.1918	707.703
1662	48.1989	2.1907	270.9421	1662	48.1989	2.1907	545.7711	1662	48.1989	2.1907	361.0724	1662	48.1989	2.1907	717.2289
1663	48.2249	2.1896	296.9164	1663	48.2249	2.1896	571.5673	1663	48.2249	2.1896	353.948	1663	48.2249	2.1896	709.253
1664	48.2509	2.1885	329.0249	1664	48.2509	2.1885	603.4977	1664	48.2509	2.1885	340.5482	1664	48.2509	2.1885	695.0015
1665	48.2769	2.1874	322.3872	1665	48.2769	2.1874	596.6818	1665	48.2769	2.1874	336.9731	1665	48.2769	2.1874	690.5749
1666	48.3029	2.1863	315.801	1666	48.3029	2.1863	589.9175	1666	48.3029	2.1863	349.5901	1666	48.3029	2.1863	702.3403
1667	48.3289	2.1851	308.6724	1667	48.3289	2.1851	582.6108	1667	48.3289	2.1851	364.2847	1667	48.3289	2.1851	716.1832
1668	48.3549	2.184	290.4276	1668	48.3549	2.184	564.1878	1668	48.3549	2.184	363.7912	1668	48.3549	2.184	714.8382
1669	48.3809	2.1829	311.0926	1669	48.3809	2.1829	584.6747	1669	48.3809	2.1829	364.5566	1669	48.3809	2.1829	714.7519
1670	48.4069	2.1818	343.6388	1670	48.4069	2.1818	617.0428	1670	48.4069	2.1818	356.5006	1670	48.4069	2.1818	705.8443
1671	48.4329	2.1807	333.1871	1671	48.4329	2.1807	606.413	1671	48.4329	2.1807	365.8392	1671	48.4329	2.1807	714.3313
1672	48.4589	2.1796	323.0134	1672	48.4589	2.1796	596.0611	1672	48.4589	2.1796	399.2755	1672	48.4589	2.1796	746.9161
1673	48.4849	2.1785	317.4907	1673	48.4849	2.1785	590.3603	1673	48.4849	2.1785	407.4224	1673	48.4849	2.1785	754.2114
1674	48.5109	2.1774	338.9088	1674	48.5109	2.1774	611.6003	1674	48.5109	2.1774	398.6627	1674	48.5109	2.1774	744.6
1675	48.5369	2.1763	385.0189	1675	48.5369	2.1763	657.5322	1675	48.5369	2.1763	380.8498	1675	48.5369	2.1763	725.9356
1676	48.5629	2.1752	382.6568	1676	48.5629	2.1752	654.992	1676	48.5629	2.1752	366.9447	1676	48.5629	2.1752	711.2477
1677	48.5889	2.1742	379.6108	1677	48.5889	2.1742	651.7678	1677	48.5889	2.1742	406.3655	1677	48.5889	2.1742	749.8857
1678	48.6149	2.1731	419.0942	1678	48.6149	2.1731	691.0731	1678	48.6149	2.1731	409.2912	1678	48.6149	2.1731	752.0286
1679	48.6409	2.172	420.6165	1679	48.6409	2.172	692.4173	1679	48.6409	2.172	388.4469	1679	48.6409	2.172	730.4016
1680	48.6669	2.1709	457.2082	1680	48.6669	2.1709	728.8308	1680	48.6669	2.1709	412.9373	1680	48.6669	2.1709	754.1092
1681	48.6929	2.1698	477.5137	1681	48.6929	2.1698	748.9582	1681	48.6929	2.1698	465.1884	1681	48.6929	2.1698	805.5776
1682	48.7189	2.1687	494.4668	1682	48.7189	2.1687	765.7332	1682	48.7189	2.1687	517.2119	1682	48.7189	2.1687	856.8182
1683	48.7449	2.1676	535.6323	1683	48.7449	2.1676	806.7205	1683	48.7449	2.1676	604.4792	1683	48.7449	2.1676	943.3028
1684	48.7709	2.1665	574.9375	1684	48.7709	2.1665	845.8476	1684	48.7709	2.1665	647.3342	1684	48.7709	2.1665	985.375
1685	48.7969	2.1655	571.8969	1685	48.7969	2.1655	842.6289	1685	48.7969	2.1655	601.3098	1685	48.7969	2.1655	938.5678
1686	48.8229	2.1644	651.7571	1686	48.8229	2.1644	922.311	1686	48.8229	2.1644	531.8491	1686	48.8229	2.1644	868.3244
1687	48.8489	2.1633	586.0634	1687	48.8489	2.1633	856.4391	1687	48.8489	2.1633	515.064	1687	48.8489	2.1633	850.7565

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1688	48.8749	2.1622	591.758	1688	48.8749	2.1622	861.9556	1688	48.8749	2.1622	530.3411	1688	48.8749	2.1622	865.2508
1689	48.9009	2.1611	586.4688	1689	48.9009	2.1611	856.4883	1689	48.9009	2.1611	483.3052	1689	48.9009	2.1611	817.4321
1690	48.9269	2.1601	561.7888	1690	48.9269	2.1601	831.6302	1690	48.9269	2.1601	443.792	1690	48.9269	2.1601	777.1362
1691	48.9529	2.159	495.0766	1691	48.9529	2.159	764.7397	1691	48.9529	2.159	446.1109	1691	48.9529	2.159	778.6723
1692	48.9789	2.1579	452.3009	1692	48.9789	2.1579	721.786	1692	48.9789	2.1579	409.0368	1692	48.9789	2.1579	740.8154
1693	49.0049	2.1568	442.7897	1693	49.0049	2.1568	712.0967	1693	49.0049	2.1568	373.7926	1693	49.0049	2.1568	704.7885
1694	49.0309	2.1558	434.0572	1694	49.0309	2.1558	703.186	1694	49.0309	2.1558	369.9573	1694	49.0309	2.1558	700.1704
1695	49.0569	2.1547	415.3595	1695	49.0569	2.1547	684.3102	1695	49.0569	2.1547	361.702	1695	49.0569	2.1547	691.1324
1696	49.0829	2.1536	366.2275	1696	49.0829	2.1536	635	1696	49.0829	2.1536	373.0884	1696	49.0829	2.1536	701.736
1697	49.1089	2.1525	364.0005	1697	49.1089	2.1525	632.5949	1697	49.1089	2.1525	318.3632	1697	49.1089	2.1525	646.228
1698	49.1349	2.1515	355.4974	1698	49.1349	2.1515	623.9137	1698	49.1349	2.1515	382.918	1698	49.1349	2.1515	710
1699	49.1609	2.1504	368.6346	1699	49.1609	2.1504	636.8727	1699	49.1609	2.1504	383.5488	1699	49.1609	2.1504	709.8481
1700	49.1869	2.1493	352.5372	1700	49.1869	2.1493	620.5972	1700	49.1869	2.1493	385.8979	1700	49.1869	2.1493	711.4144
1701	49.2129	2.1483	327.9676	1701	49.2129	2.1483	595.8494	1701	49.2129	2.1483	398.7563	1701	49.2129	2.1483	723.49
1702	49.2389	2.1472	336.1421	1702	49.2389	2.1472	603.8459	1702	49.2389	2.1472	380.8498	1702	49.2389	2.1472	704.8008
1703	49.2649	2.1461	303.8153	1703	49.2649	2.1461	570.1832	1703	49.2649	2.1461	364.8423	1703	49.2649	2.1461	689.6735
1704	49.2909	2.1451	278.2427	1704	49.2909	2.1451	543.2747	1704	49.2909	2.1451	368.0605	1704	49.2909	2.1451	693.772
1705	49.3169	2.144	306.2707	1705	49.3169	2.144	569.9669	1705	49.3169	2.144	356.8703	1705	49.3169	2.144	683.4621
1706	49.3429	2.143	287.9696	1706	49.3429	2.143	550.33	1706	49.3429	2.143	360.4455	1706	49.3429	2.143	687.9175
1707	49.3689	2.1419	295.1526	1707	49.3689	2.1419	556.1771	1707	49.3689	2.1419	358.6477	1707	49.3689	2.1419	687
1708	49.3949	2.1409	322.432	1708	49.3949	2.1409	582.1206	1708	49.3949	2.1409	355.9506	1708	49.3949	2.1409	685.1832
1709	49.4209	2.1398	296.4908	1709	49.4209	2.1398	554.8436	1709	49.4209	2.1398	330.6815	1709	49.4209	2.1398	660.7944
1710	49.4469	2.1387	313.3255	1710	49.4469	2.1387	570.3424	1710	49.4469	2.1387	377.9951	1710	49.4469	2.1387	708.9883
1711	49.4729	2.1377	321.8258	1711	49.4729	2.1377	577.5068	1711	49.4729	2.1377	332.0279	1711	49.4729	2.1377	663.9014
1712	49.4989	2.1366	308.563	1712	49.4989	2.1366	562.9082	1712	49.4989	2.1366	330.2206	1712	49.4989	2.1366	662.9743
1713	49.5249	2.1356	305.7169	1713	49.5249	2.1356	558.7263	1713	49.5249	2.1356	412.61	1713	49.5249	2.1356	746.244
1714	49.5509	2.1345	286.3732	1714	49.5509	2.1345	538.0467	1714	49.5509	2.1345	354.4733	1714	49.5509	2.1345	688.9875
1715	49.5769	2.1335	302.5602	1715	49.5769	2.1335	552.8979	1715	49.5769	2.1335	349.6327	1715	49.5769	2.1335	685.0272
1716	49.6029	2.1324	305.9648	1716	49.6029	2.1324	554.9665	1716	49.6029	2.1324	332.0096	1716	49.6029	2.1324	668.2844
1717	49.6289	2.1314	288.8405	1717	49.6289	2.1314	536.5064	1717	49.6289	2.1314	374.6455	1717	49.6289	2.1314	711.8006
1718	49.6549	2.1303	274.2552	1718	49.6549	2.1303	520.5852	1718	49.6549	2.1303	385.5623	1718	49.6549	2.1303	723.5977
1719	49.6809	2.1293	348.4254	1719	49.6809	2.1293	593.4196	1719	49.6809	2.1293	363.1538	1719	49.6809	2.1293	702.0695
1720	49.7069	2.1283	286.3476	1720	49.7069	2.1283	530.0059	1720	49.7069	2.1283	328.1788	1720	49.7069	2.1283	667.9747
1721	49.7329	2.1272	292.0804	1721	49.7329	2.1272	534.4029	1721	49.7329	2.1272	358.0018	1721	49.7329	2.1272	698.678
1722	49.7589	2.1262	353.1324	1722	49.7589	2.1262	594.119	1722	49.7589	2.1262	341.8926	1722	49.7589	2.1262	683.449
1723	49.7849	2.1251	262.4851	1723	49.7849	2.1251	502.1359	1723	49.7849	2.1251	350.529	1723	49.7849	2.1251	692.9657

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1724	49.8109	2.1241	298.9757	1724	49.8109	2.1241	537.2906	1724	49.8109	2.1241	383.223	1724	49.8109	2.1241	726.54
1725	49.8369	2.1231	327.3701	1725	49.8369	2.1231	564.3492	1725	49.8369	2.1231	393.8484	1725	49.8369	2.1231	738.0457
1726	49.8629	2.122	281.8503	1726	49.8629	2.122	517.4935	1726	49.8629	2.122	303.7498	1726	49.8629	2.122	648.8274
1727	49.8889	2.121	295.0492	1727	49.8889	2.121	529.3566	1727	49.8889	2.121	326.8812	1727	49.8889	2.121	672.839
1728	49.9149	2.12	343.1028	1728	49.9149	2.12	576.0742	1728	49.9149	2.12	337.2113	1728	49.9149	2.12	684.0494
1729	49.9409	2.1189	273.625	1729	49.9409	2.1189	505.2607	1729	49.9409	2.1189	380.8498	1729	49.9409	2.1189	728.5682
1730	49.9669	2.1179	305.7023	1730	49.9669	2.1179	537.5952	1730	49.9669	2.1179	415.3182	1730	49.9669	2.1179	762.175
1731	49.9929	2.1169	324.6975	1731	49.9929	2.1169	556.8476	1731	49.9929	2.1169	399.3094	1731	49.9929	2.1169	745.3047
1732	50.0189	2.1158	301.0327	1732	50.0189	2.1158	533.4401	1732	50.0189	2.1158	358.7632	1732	50.0189	2.1158	703.897
1733	50.0449	2.1148	283.1165	1733	50.0449	2.1148	515.7812	1733	50.0449	2.1148	377.7947	1733	50.0449	2.1148	722.0669
1734	50.0709	2.1138	305.0227	1734	50.0709	2.1138	537.9447	1734	50.0709	2.1138	411.1434	1734	50.0709	2.1138	754.554
1735	50.0969	2.1127	340.2263	1735	50.0969	2.1127	573.4056	1735	50.0969	2.1127	388.2506	1735	50.0969	2.1127	730.7997
1736	50.1229	2.1117	299.6893	1736	50.1229	2.1117	533.1258	1736	50.1229	2.1117	373.4642	1736	50.1229	2.1117	715.1518
1737	50.1489	2.1107	287.0811	1737	50.1489	2.1107	520.7749	1737	50.1489	2.1107	378.3732	1737	50.1489	2.1107	719.1992
1738	50.1749	2.1097	288.5789	1738	50.1749	2.1097	522.53	1738	50.1749	2.1097	436.1139	1738	50.1749	2.1097	776.0784
1739	50.2009	2.1087	293.322	1739	50.2009	2.1087	527.5303	1739	50.2009	2.1087	467.4881	1739	50.2009	2.1087	806.591
1740	50.2269	2.1076	310.9274	1740	50.2269	2.1076	545.3929	1740	50.2269	2.1076	457.856	1740	50.2269	2.1076	796.0973
1741	50.2529	2.1066	332.4518	1741	50.2529	2.1066	567.1746	1741	50.2529	2.1066	461.7075	1741	50.2529	2.1066	799.0873
1742	50.2789	2.1056	314.8107	1742	50.2789	2.1056	549.7908	1742	50.2789	2.1056	482.8887	1742	50.2789	2.1056	819.4069
1743	50.3049	2.1046	287.8785	1743	50.3049	2.1046	523.1158	1743	50.3049	2.1046	526.827	1743	50.3049	2.1046	862.4837
1744	50.3309	2.1036	322.832	1744	50.3309	2.1036	558.3266	1744	50.3309	2.1036	566.8954	1744	50.3309	2.1036	901.6905
1745	50.3569	2.1025	311.0362	1745	50.3569	2.1025	546.7881	1745	50.3569	2.1025	631.6216	1745	50.3569	2.1025	965.5552
1746	50.3829	2.1015	293.1916	1746	50.3829	2.1015	529.2008	1746	50.3829	2.1015	745.0559	1746	50.3829	2.1015	1078.1279
1747	50.4089	2.1005	284.6525	1747	50.4089	2.1005	520.9189	1747	50.4089	2.1005	928.006	1747	50.4089	2.1005	1260.2165
1748	50.4349	2.0995	279.479	1748	50.4349	2.0995	516.0027	1748	50.4349	2.0995	1245.6434	1748	50.4349	2.0995	1576.9923
1749	50.4609	2.0985	284.7774	1749	50.4609	2.0985	521.5583	1749	50.4609	2.0985	1963.7294	1749	50.4609	2.0985	2294.2168
1750	50.4869	2.0975	304.7554	1750	50.4869	2.0975	541.7937	1750	50.4869	2.0975	2854.7557	1750	50.4869	2.0975	3184.3816
1751	50.5129	2.0965	332.1482	1751	50.5129	2.0965	569.4437	1751	50.5129	2.0965	3248.2823	1751	50.5129	2.0965	3577.0466
1752	50.5389	2.0955	361.2292	1752	50.5389	2.0955	598.782	1752	50.5389	2.0955	3105.5296	1752	50.5389	2.0955	3433.4324
1753	50.5649	2.0945	358.0187	1753	50.5649	2.0945	595.8287	1753	50.5649	2.0945	2787.9346	1753	50.5649	2.0945	3114.9758
1754	50.5909	2.0935	341.6581	1754	50.5909	2.0935	579.7253	1754	50.5909	2.0935	2585.8613	1754	50.5909	2.0935	2912.041
1755	50.6169	2.0925	352.1792	1755	50.6169	2.0925	590.5038	1755	50.6169	2.0925	2572.6709	1755	50.6169	2.0925	2897.989
1756	50.6429	2.0914	345.4133	1756	50.6429	2.0914	583.9951	1756	50.6429	2.0914	2359.0609	1756	50.6429	2.0914	2683.5175
1757	50.6689	2.0904	312.4086	1757	50.6689	2.0904	551.2476	1757	50.6689	2.0904	1949.1413	1757	50.6689	2.0904	2272.7363
1758	50.6949	2.0894	320.1315	1758	50.6949	2.0894	559.2278	1758	50.6949	2.0894	1554.2848	1758	50.6949	2.0894	1877.0183
1759	50.7209	2.0884	326.5142	1759	50.7209	2.0884	565.8678	1759	50.7209	2.0884	1235.5038	1759	50.7209	2.0884	1557.3757

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1760	50.7469	2.0874	307.002	1760	50.7469	2.0874	546.6129	1760	50.7469	2.0874	1053.854	1760	50.7469	2.0874	1374.8644
1761	50.7729	2.0864	293.8377	1761	50.7729	2.0864	533.7059	1761	50.7729	2.0864	917.3584	1761	50.7729	2.0864	1237.5073
1762	50.7989	2.0854	290.9283	1762	50.7989	2.0854	531.0537	1762	50.7989	2.0854	866.4206	1762	50.7989	2.0854	1185.7079
1763	50.8249	2.0845	296.7865	1763	50.8249	2.0845	537.1692	1763	50.8249	2.0845	842.0514	1763	50.8249	2.0845	1160.4772
1764	50.8509	2.0835	291.2201	1764	50.8509	2.0835	531.86	1764	50.8509	2.0835	740.117	1764	50.8509	2.0835	1057.6812
1765	50.8769	2.0825	306.9507	1765	50.8769	2.0825	547.8479	1765	50.8769	2.0825	710.1395	1765	50.8769	2.0825	1026.8421
1766	50.9029	2.0815	305.0778	1766	50.9029	2.0815	546.2322	1766	50.9029	2.0815	732.3131	1766	50.9029	2.0815	1048.1542
1767	50.9289	2.0805	255.5445	1767	50.9289	2.0805	496.9563	1767	50.9289	2.0805	719.3847	1767	50.9289	2.0805	1034.3643
1768	50.9549	2.0795	240.8079	1768	50.9549	2.0795	482.4769	1768	50.9549	2.0795	665.1511	1768	50.9549	2.0795	979.2691
1769	50.9809	2.0785	276.5169	1769	50.9809	2.0785	518.4432	1769	50.9809	2.0785	630.1242	1769	50.9809	2.0785	943.3807
1770	51.0069	2.0775	308.8164	1770	51.0069	2.0775	551	1770	51.0069	2.0775	619.8351	1770	51.0069	2.0775	932.23
1771	51.0329	2.0765	294.9954	1771	51.0329	2.0765	537.4362	1771	51.0329	2.0765	581.4666	1771	51.0329	2.0765	893
1772	51.0589	2.0755	262.3352	1772	51.0589	2.0755	505.0333	1772	51.0589	2.0755	569.4996	1772	51.0589	2.0755	880.1714
1773	51.0849	2.0746	250.3986	1773	51.0849	2.0746	493.354	1773	51.0849	2.0746	544.4181	1773	51.0849	2.0746	854.2284
1774	51.1109	2.0736	271.574	1774	51.1109	2.0736	514.7866	1774	51.1109	2.0736	539.1679	1774	51.1109	2.0736	848.1166
1775	51.1369	2.0726	293.4872	1775	51.1369	2.0726	536.9571	1775	51.1369	2.0726	523.0524	1775	51.1369	2.0726	831.1396
1776	51.1629	2.0716	295.5746	1776	51.1629	2.0716	539.3017	1776	51.1629	2.0716	496.4123	1776	51.1629	2.0716	803.6379
1777	51.1889	2.0706	272.4554	1777	51.1889	2.0706	516.4398	1777	51.1889	2.0706	485.0173	1777	51.1889	2.0706	791.3813
1778	51.2149	2.0696	271.9052	1778	51.2149	2.0696	516.1468	1778	51.2149	2.0696	419.6698	1778	51.2149	2.0696	725.1723
1779	51.2409	2.0687	286.7704	1779	51.2409	2.0687	531.2694	1779	51.2409	2.0687	395.508	1779	51.2409	2.0687	700.149
1780	51.2669	2.0677	291.2182	1780	51.2669	2.0677	535.9744	1780	51.2669	2.0677	406.4889	1780	51.2669	2.0677	710.2683
1781	51.2929	2.0667	310.5285	1781	51.2929	2.0667	555.542	1781	51.2929	2.0667	423.142	1781	51.2929	2.0667	726.0598
1782	51.3189	2.0657	281.2502	1782	51.3189	2.0657	526.5209	1782	51.3189	2.0657	415.1954	1782	51.3189	2.0657	717.2518
1783	51.3449	2.0648	273.625	1783	51.3449	2.0648	519.1531	1783	51.3449	2.0648	380.8498	1783	51.3449	2.0648	682.0446
1784	51.3709	2.0638	300.8602	1784	51.3709	2.0638	547.2007	1784	51.3709	2.0638	386.6053	1784	51.3709	2.0638	686.4796
1785	51.3969	2.0628	282.1183	1785	51.3969	2.0628	529.2712	1785	51.3969	2.0628	391.6954	1785	51.3969	2.0628	690.2493
1786	51.4229	2.0618	281.8879	1786	51.4229	2.0618	529.8533	1786	51.4229	2.0618	384.2228	1786	51.4229	2.0618	681.4563
1787	51.4489	2.0609	249.8463	1787	51.4489	2.0609	498.6242	1787	51.4489	2.0609	423.0203	1787	51.4489	2.0609	718.9334
1788	51.4749	2.0599	262.9803	1788	51.4749	2.0599	512.5707	1788	51.4749	2.0599	423.3978	1788	51.4749	2.0599	717.9904
1789	51.5009	2.0589	277.4455	1789	51.5009	2.0589	527.8483	1789	51.5009	2.0589	410.5833	1789	51.5009	2.0589	703.8556
1790	51.5269	2.058	274.824	1790	51.5269	2.058	526.0393	1790	51.5269	2.058	332.9854	1790	51.5269	2.058	624.9372
1791	51.5529	2.057	248.0369	1791	51.5529	2.057	500.0646	1791	51.5529	2.057	388.346	1791	51.5529	2.057	678.9774
1792	51.5789	2.056	261.764	1792	51.5789	2.056	514.6042	1792	51.5789	2.056	403.1889	1792	51.5789	2.056	692.4998
1793	51.6049	2.0551	260.4275	1793	51.6049	2.0551	514.0802	1793	51.6049	2.0551	390.1753	1793	51.6049	2.0551	678.1658
1794	51.6309	2.0541	250.6759	1794	51.6309	2.0541	505.1411	1794	51.6309	2.0541	406.3299	1794	51.6309	2.0541	693
1795	51.6569	2.0531	282.9603	1795	51.6569	2.0531	538.2379	1795	51.6569	2.0531	413.2337	1795	51.6569	2.0531	698.5834

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1796	51.6829	2.0522	235.647	1796	51.6829	2.0522	491.7371	1796	51.6829	2.0522	431.0967	1796	51.6829	2.0522	715.126
1797	51.7089	2.0512	256.5339	1797	51.7089	2.0512	513.4365	1797	51.7089	2.0512	399.9291	1797	51.7089	2.0512	682.6379
1798	51.7349	2.0502	267.3742	1798	51.7349	2.0502	525.0892	1798	51.7349	2.0502	365.2366	1798	51.7349	2.0502	646.625
1799	51.7609	2.0493	288.7573	1799	51.7609	2.0493	547.2848	1799	51.7609	2.0493	371.383	1799	51.7609	2.0493	651.451
1800	51.7869	2.0483	271.5629	1800	51.7869	2.0483	530.9029	1800	51.7869	2.0483	446.8194	1800	51.7869	2.0483	725.567
1801	51.8129	2.0474	260.8058	1801	51.8129	2.0474	520.9582	1801	51.8129	2.0474	374.3558	1801	51.8129	2.0474	651.7829
1802	51.8389	2.0464	267.7467	1802	51.8389	2.0464	528.7116	1802	51.8389	2.0464	357.8426	1802	51.8389	2.0464	633.9493
1803	51.8649	2.0455	236.4222	1803	51.8649	2.0455	498.1996	1803	51.8649	2.0455	374.0141	1803	51.8649	2.0455	648.8004
1804	51.8909	2.0445	228.3559	1804	51.8909	2.0445	490.9458	1804	51.8909	2.0445	385.7815	1804	51.8909	2.0445	659.2473
1805	51.9169	2.0436	272.1914	1805	51.9169	2.0436	535.5937	1805	51.9169	2.0436	369.5632	1805	51.9169	2.0436	641.7087
1806	51.9429	2.0426	242.3197	1806	51.9429	2.0426	506.5345	1806	51.9429	2.0426	413.2652	1806	51.9429	2.0426	684.0903
1807	51.9689	2.0417	254.0805	1807	51.9689	2.0417	519.1078	1807	51.9689	2.0417	414.7723	1807	51.9689	2.0417	684.2769
1808	51.9949	2.0407	222.4136	1808	51.9949	2.0407	488.2534	1808	51.9949	2.0407	406.7596	1808	51.9949	2.0407	674.9437
1809	52.0209	2.0398	252.7997	1809	52.0209	2.0398	519.4519	1809	52.0209	2.0398	393.2893	1809	52.0209	2.0398	660.1531
1810	52.0469	2.0388	273.625	1810	52.0469	2.0388	541.0897	1810	52.0469	2.0388	380.8498	1810	52.0469	2.0388	646.3931
1811	52.0729	2.0379	257.7465	1811	52.0729	2.0379	524.8537	1811	52.0729	2.0379	367.5861	1811	52.0729	2.0379	634.5528
1812	52.0989	2.0369	277.0213	1812	52.0989	2.0369	543.7709	1812	52.0989	2.0369	357.73	1812	52.0989	2.0369	626.1202
1813	52.1249	2.036	238.8992	1813	52.1249	2.036	505.2913	1813	52.1249	2.036	422.6869	1813	52.1249	2.036	692.5007
1814	52.1509	2.035	252.7914	1814	52.1509	2.035	518.8259	1814	52.1509	2.035	397.4907	1814	52.1509	2.035	668.7279
1815	52.1769	2.0341	237.3423	1815	52.1769	2.0341	503.0192	1815	52.1769	2.0341	371.3528	1815	52.1769	2.0341	644.0135
1816	52.2029	2.0331	257.5014	1816	52.2029	2.0331	522.8208	1816	52.2029	2.0331	383.7904	1816	52.2029	2.0331	657.8745
1817	52.2289	2.0322	271.7738	1817	52.2289	2.0322	536.7356	1817	52.2289	2.0322	394.2658	1817	52.2289	2.0322	669.7734
1818	52.2549	2.0313	230.6343	1818	52.2549	2.0313	495.2386	1818	52.2549	2.0313	349.3652	1818	52.2549	2.0313	626.2963
1819	52.2809	2.0303	250.9012	1819	52.2809	2.0303	515.148	1819	52.2809	2.0303	367.7935	1819	52.2809	2.0303	646.148
1820	52.3069	2.0294	227.3757	1820	52.3069	2.0294	491.2649	1820	52.3069	2.0294	331.0707	1820	52.3069	2.0294	610.8487
1821	52.3329	2.0284	232.1169	1821	52.3329	2.0284	495.6486	1821	52.3329	2.0284	415.3513	1821	52.3329	2.0284	696.5528
1822	52.3589	2.0275	244.9354	1822	52.3589	2.0275	508.1096	1822	52.3589	2.0275	391.4299	1822	52.3589	2.0275	674.0548
1823	52.3849	2.0266	224.987	1823	52.3849	2.0266	487.8036	1823	52.3849	2.0266	377.8142	1823	52.3849	2.0266	661.8626
1824	52.4109	2.0256	266.389	1824	52.4109	2.0256	528.8481	1824	52.4109	2.0256	401.9663	1824	52.4109	2.0256	687.4382
1825	52.4369	2.0247	247.4533	1825	52.4369	2.0247	509.5548	1825	52.4369	2.0247	407.6134	1825	52.4369	2.0247	694.5087
1826	52.4629	2.0238	274.6859	1826	52.4629	2.0238	536.4299	1826	52.4629	2.0238	410.2485	1826	52.4629	2.0238	698.5673
1827	52.4889	2.0228	259.2119	1827	52.4889	2.0228	520.5983	1827	52.4889	2.0228	377.5096	1827	52.4889	2.0228	667.2518
1828	52.5149	2.0219	242.1476	1828	52.5149	2.0219	503.1765	1828	52.5149	2.0219	414.5609	1828	52.5149	2.0219	705.7266
1829	52.5409	2.021	292.0516	1829	52.5409	2.021	552.723	1829	52.5409	2.021	391.8252	1829	52.5409	2.021	684.4144
1830	52.5669	2.0201	268.3053	1830	52.5669	2.0201	528.6192	1830	52.5669	2.0201	368.9448	1830	52.5669	2.0201	662.9575
1831	52.5929	2.0191	268.9391	1831	52.5929	2.0191	528.8954	1831	52.5929	2.0191	356.1418	1831	52.5929	2.0191	651.578

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1832	52.6189	2.0182	242.9359	1832	52.6189	2.0182	502.5347	1832	52.6189	2.0182	360.631	1832	52.6189	2.0182	657.4905
1833	52.6449	2.0173	236.1141	1833	52.6449	2.0173	495.3553	1833	52.6449	2.0173	345.9145	1833	52.6449	2.0173	644.1975
1834	52.6709	2.0163	228.8044	1834	52.6709	2.0163	487.6881	1834	52.6709	2.0163	388.4149	1834	52.6709	2.0163	688.1214
1835	52.6969	2.0154	265.1921	1835	52.6969	2.0154	523.7182	1835	52.6969	2.0154	367.3744	1835	52.6969	2.0154	668.5044
1836	52.7229	2.0145	260.5647	1836	52.7229	2.0145	518.7333	1836	52.7229	2.0145	371.1281	1836	52.7229	2.0145	673.6815
1837	52.7489	2.0136	273.625	1837	52.7489	2.0136	531.4361	1837	52.7489	2.0136	380.8498	1837	52.7489	2.0136	684.8267
1838	52.7749	2.0127	268.9218	1838	52.7749	2.0127	526.727	1838	52.7749	2.0127	331.1506	1838	52.7749	2.0127	635.2258
1839	52.8009	2.0117	263.9121	1839	52.8009	2.0117	521.7115	1839	52.8009	2.0117	401.263	1839	52.8009	2.0117	705.4365
1840	52.8269	2.0108	242.1251	1840	52.8269	2.0108	499.9187	1840	52.8269	2.0108	382.5539	1840	52.8269	2.0108	686.8258
1841	52.8529	2.0099	290.1929	1841	52.8529	2.0099	547.9806	1841	52.8529	2.0099	366.8869	1841	52.8529	2.0099	671.257
1842	52.8789	2.009	264.5015	1842	52.8789	2.009	522.2834	1842	52.8789	2.009	380.4597	1842	52.8789	2.009	684.9281
1843	52.9049	2.0081	267.7487	1843	52.9049	2.0081	525.5247	1843	52.9049	2.0081	356.5078	1843	52.9049	2.0081	661.0745
1844	52.9309	2.0072	301.6188	1844	52.9309	2.0072	559.3889	1844	52.9309	2.0072	360.3125	1844	52.9309	2.0072	664.9775
1845	52.9569	2.0062	296.7632	1845	52.9569	2.0062	554.5276	1845	52.9569	2.0062	393.6651	1845	52.9569	2.0062	698.4284
1846	52.9829	2.0053	265.2802	1846	52.9829	2.0053	523.0387	1846	52.9829	2.0053	423.166	1846	52.9829	2.0053	728.0276
1847	53.0089	2.0044	281.5852	1847	53.0089	2.0044	539.3379	1847	53.0089	2.0044	454.9607	1847	53.0089	2.0044	759.9207
1848	53.0349	2.0035	324.5618	1848	53.0349	2.0035	582.3087	1848	53.0349	2.0035	431.5919	1848	53.0349	2.0035	736.6502
1849	53.0609	2.0026	318.6873	1849	53.0609	2.0026	576.4283	1849	53.0609	2.0026	383.6541	1849	53.0609	2.0026	688.8106
1850	53.0869	2.0017	325.9142	1850	53.0869	2.0017	583.6494	1850	53.0869	2.0017	372.9746	1850	53.0869	2.0017	678.2294
1851	53.1129	2.0008	323.683	1851	53.1129	2.0008	581.4123	1851	53.1129	2.0008	394.3158	1851	53.1129	2.0008	699.669
1852	53.1389	1.9999	320.4457	1852	53.1389	1.9999	578.1692	1852	53.1389	1.9999	374.1244	1852	53.1389	1.9999	679.5758
1853	53.1649	1.999	328.5215	1853	53.1649	1.999	586.2391	1853	53.1649	1.999	407.6112	1853	53.1649	1.999	713.161
1854	53.1909	1.9981	331.0602	1854	53.1909	1.9981	588.772	1854	53.1909	1.9981	380.0227	1854	53.1909	1.9981	685.6708
1855	53.2169	1.9971	339.9591	1855	53.2169	1.9971	597.6651	1855	53.2169	1.9971	368.0205	1855	53.2169	1.9971	673.7669
1856	53.2429	1.9962	339.7642	1856	53.2429	1.9962	597.4644	1856	53.2429	1.9962	397.2265	1856	53.2429	1.9962	703.0712
1857	53.2689	1.9953	350.4956	1857	53.2689	1.9953	608.1899	1857	53.2689	1.9953	396.1252	1857	53.2689	1.9953	702.0682
1858	53.2949	1.9944	342.9339	1858	53.2949	1.9944	600.6223	1858	53.2949	1.9944	370.0067	1858	53.2949	1.9944	676.048
1859	53.3209	1.9935	291.5039	1859	53.3209	1.9935	549.1865	1859	53.3209	1.9935	346.2659	1859	53.3209	1.9935	652.4055
1860	53.3469	1.9926	297.2541	1860	53.3469	1.9926	554.9309	1860	53.3469	1.9926	324.9006	1860	53.3469	1.9926	631.1385
1861	53.3729	1.9917	324.24	1861	53.3729	1.9917	581.9109	1861	53.3729	1.9917	327.2772	1861	53.3729	1.9917	633.6134
1862	53.3989	1.9908	306.7619	1862	53.3989	1.9908	564.427	1862	53.3989	1.9908	353	1862	53.3989	1.9908	659.4346
1863	53.4249	1.9899	286.5691	1863	53.4249	1.9899	544.2284	1863	53.4249	1.9899	392.2264	1863	53.4249	1.9899	698.7593
1864	53.4509	1.989	273.625	1864	53.4509	1.989	531.2785	1864	53.4509	1.989	380.8498	1864	53.4509	1.989	687.4809
1865	53.4769	1.9881	276.7771	1865	53.4769	1.9881	534.0969	1865	53.4769	1.9881	375.0529	1865	53.4769	1.9881	680.7569
1866	53.5029	1.9873	262.2675	1866	53.5029	1.9873	519.2538	1866	53.5029	1.9873	378.9618	1866	53.5029	1.9873	683.7386
1867	53.5289	1.9864	241.7123	1867	53.5289	1.9864	498.365	1867	53.5289	1.9864	346.9353	1867	53.5289	1.9864	650.785

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1868	53.5549	1.9855	263.3087	1868	53.5549	1.9855	519.6278	1868	53.5549	1.9855	336.1772	1868	53.5549	1.9855	639.0997
1869	53.5809	1.9846	257.8263	1869	53.5809	1.9846	513.8118	1869	53.5809	1.9846	342.4472	1869	53.5809	1.9846	644.4425
1870	53.6069	1.9837	232.169	1870	53.6069	1.9837	487.8209	1870	53.6069	1.9837	335.5434	1870	53.6069	1.9837	636.6115
1871	53.6329	1.9828	244.4785	1871	53.6329	1.9828	499.7969	1871	53.6329	1.9828	331.9997	1871	53.6329	1.9828	632.1406
1872	53.6589	1.9819	261.8045	1872	53.6589	1.9819	516.7893	1872	53.6589	1.9819	362.671	1872	53.6589	1.9819	661.8848
1873	53.6849	1.981	256.8611	1873	53.6849	1.981	511.5124	1873	53.6849	1.981	375.586	1873	53.6849	1.981	673.8727
1874	53.7109	1.9801	263.2907	1874	53.7109	1.9801	517.6084	1874	53.7109	1.9801	370.3162	1874	53.7109	1.9801	667.6756
1875	53.7369	1.9792	285.4978	1875	53.7369	1.9792	539.4819	1875	53.7369	1.9792	366.5677	1875	53.7369	1.9792	663
1876	53.7629	1.9784	272.9538	1876	53.7629	1.9784	526.6043	1876	53.7629	1.9784	354.4367	1876	53.7629	1.9784	649.9419
1877	53.7889	1.9775	260.3381	1877	53.7889	1.9775	513.6551	1877	53.7889	1.9775	347.767	1877	53.7889	1.9775	642.3449
1878	53.8149	1.9766	250.0372	1878	53.8149	1.9766	503.0206	1878	53.8149	1.9766	377.7457	1878	53.8149	1.9766	671.3964
1879	53.8409	1.9757	259.1293	1879	53.8409	1.9757	511.7791	1879	53.8409	1.9757	384.7621	1879	53.8409	1.9757	677.4857
1880	53.8669	1.9748	255.092	1880	53.8669	1.9748	507.4082	1880	53.8669	1.9748	362.0833	1880	53.8669	1.9748	653.8798
1881	53.8929	1.9739	267.7095	1881	53.8929	1.9739	519.6922	1881	53.8929	1.9739	356.3604	1881	53.8929	1.9739	647.2296
1882	53.9189	1.9731	268.6786	1882	53.9189	1.9731	520.3277	1882	53.9189	1.9731	380.4876	1882	53.9189	1.9731	670.4297
1883	53.9449	1.9722	278.1244	1883	53.9449	1.9722	529.4399	1883	53.9449	1.9722	391.2615	1883	53.9449	1.9722	680.2764
1884	53.9709	1.9713	287.9978	1884	53.9709	1.9713	538.9797	1884	53.9709	1.9713	359.2695	1884	53.9709	1.9713	647.3572
1885	53.9969	1.9704	264.1901	1885	53.9969	1.9704	514.8384	1885	53.9969	1.9704	341.8562	1885	53.9969	1.9704	629.0168
1886	54.0229	1.9695	268.6852	1886	54.0229	1.9695	519	1886	54.0229	1.9695	348.887	1886	54.0229	1.9695	635.1204
1887	54.0489	1.9687	273.0306	1887	54.0489	1.9687	523.0118	1887	54.0489	1.9687	386.84	1887	54.0489	1.9687	672.1462
1888	54.0749	1.9678	265.3712	1888	54.0749	1.9678	515.0188	1888	54.0749	1.9678	384.535	1888	54.0749	1.9678	668.9141
1889	54.1009	1.9669	237.8892	1889	54.1009	1.9669	487.2032	1889	54.1009	1.9669	369.0147	1889	54.1009	1.9669	652.4666
1890	54.1269	1.966	286.9109	1890	54.1269	1.966	535.8914	1890	54.1269	1.966	375.4086	1890	54.1269	1.966	657.9333
1891	54.1529	1.9652	273.625	1891	54.1529	1.9652	522.2719	1891	54.1529	1.9652	380.8498	1891	54.1529	1.9652	662.4474
1892	54.1789	1.9643	264.8036	1892	54.1789	1.9643	512.9719	1892	54.1789	1.9643	338.2896	1892	54.1789	1.9643	624.9517
1893	54.2049	1.9634	253.4454	1893	54.2049	1.9634	501.1351	1893	54.2049	1.9634	379.1218	1893	54.2049	1.9634	670.8484
1894	54.2309	1.9626	260.1769	1894	54.2309	1.9626	507.3881	1894	54.2309	1.9626	401.2357	1894	54.2309	1.9626	698.0268
1895	54.2569	1.9617	263.2593	1895	54.2569	1.9617	509.9918	1895	54.2569	1.9617	333.8817	1895	54.2569	1.9617	635.7374
1896	54.2829	1.9608	249.4252	1896	54.2829	1.9608	495.6792	1896	54.2829	1.9608	361.543	1896	54.2829	1.9608	668.4631
1897	54.3089	1.96	280.3539	1897	54.3089	1.96	526.1293	1897	54.3089	1.96	343.0733	1897	54.3089	1.96	655.058
1898	54.3349	1.9591	255.9775	1898	54.3349	1.9591	501.2744	1898	54.3349	1.9591	360.483	1898	54.3349	1.9591	677.5322
1899	54.3609	1.9582	235.6645	1899	54.3609	1.9582	480.4827	1899	54.3609	1.9582	354.2015	1899	54.3609	1.9582	676.3152
1900	54.3869	1.9574	224.1751	1900	54.3869	1.9574	468.5148	1900	54.3869	1.9574	338.0698	1900	54.3869	1.9574	665.2481
1901	54.4129	1.9565	251.4813	1901	54.4129	1.9565	495.3424	1901	54.4129	1.9565	371.1667	1901	54.4129	1.9565	703.4094
1902	54.4389	1.9556	241.7132	1902	54.4389	1.9556	485.0957	1902	54.4389	1.9556	356.633	1902	54.4389	1.9556	693.9402
1903	54.4649	1.9548	274.8628	1903	54.4649	1.9548	517.7668	1903	54.4649	1.9548	314.6506	1903	54.4649	1.9548	657.0224

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1904	54.4909	1.9539	283.8752	1904	54.4909	1.9539	526.3006	1904	54.4909	1.9539	319.5106	1904	54.4909	1.9539	666.9469
1905	54.5169	1.953	308.2975	1905	54.5169	1.953	550.2443	1905	54.5169	1.953	342.0049	1905	54.5169	1.953	694.5057
1906	54.5429	1.9522	304.6885	1906	54.5429	1.9522	546.1567	1906	54.5429	1.9522	377.435	1906	54.5429	1.9522	735.0003
1907	54.5689	1.9513	324.3055	1907	54.5689	1.9513	565.2951	1907	54.5689	1.9513	320.2906	1907	54.5689	1.9513	682.9204
1908	54.5949	1.9505	318.5054	1908	54.5949	1.9505	559.0164	1908	54.5949	1.9505	260.9845	1908	54.5949	1.9505	628.6789
1909	54.6209	1.9496	331.0358	1909	54.6209	1.9496	571.0683	1909	54.6209	1.9496	353.5308	1909	54.6209	1.9496	726.2897
1910	54.6469	1.9488	331.0458	1910	54.6469	1.9488	570.5998	1910	54.6469	1.9488	287.0938	1910	54.6469	1.9488	664.9172
1911	54.6729	1.9479	311.3457	1911	54.6729	1.9479	550.4211	1911	54.6729	1.9479	329.6447	1911	54.6729	1.9479	712.5326
1912	54.6989	1.947	358.0173	1912	54.6989	1.947	596.614	1912	54.6989	1.947	334.3931	1912	54.6989	1.947	722.3455
1913	54.7249	1.9462	324.9963	1913	54.7249	1.9462	563.1145	1913	54.7249	1.9462	313.4403	1913	54.7249	1.9462	706.4572
1914	54.7509	1.9453	363.8267	1914	54.7509	1.9453	601.4664	1914	54.7509	1.9453	325.4855	1914	54.7509	1.9453	723.567
1915	54.7769	1.9445	389.1097	1915	54.7769	1.9445	626.2707	1915	54.7769	1.9445	402.8453	1915	54.7769	1.9445	805.9913
1916	54.8029	1.9436	420.2806	1916	54.8029	1.9436	656.9631	1916	54.8029	1.9436	396.7907	1916	54.8029	1.9436	805.0012
1917	54.8289	1.9428	488.0405	1917	54.8289	1.9428	724.2443	1917	54.8289	1.9428	394.6917	1917	54.8289	1.9428	807.9667
1918	54.8549	1.9419	466.7585	1918	54.8549	1.9419	702.4838	1918	54.8549	1.9419	380.8498	1918	54.8549	1.9419	799.1893
1919	54.8809	1.9411	526.8339	1919	54.8809	1.9411	762.0807	1919	54.8809	1.9411	446.6756	1919	54.8809	1.9411	867.802
1920	54.9069	1.9402	497.5809	1920	54.9069	1.9402	732.349	1920	54.9069	1.9402	401.008	1920	54.9069	1.9402	824.9213
1921	54.9329	1.9394	501.4564	1921	54.9329	1.9394	735.746	1921	54.9329	1.9394	448.5057	1921	54.9329	1.9394	875.2059
1922	54.9589	1.9385	564.1812	1922	54.9589	1.9385	797.9922	1922	54.9589	1.9385	411.8811	1922	54.9589	1.9385	841.3682
1923	54.9849	1.9377	575.1731	1923	54.9849	1.9377	808.5055	1923	54.9849	1.9377	378.8454	1923	54.9849	1.9377	811.1194
1924	55.0109	1.9369	517.3025	1924	55.0109	1.9369	750.1564	1924	55.0109	1.9369	487.9486	1924	55.0109	1.9369	923.0095
1925	55.0369	1.936	524.4484	1925	55.0369	1.936	756.8236	1925	55.0369	1.936	500.6092	1925	55.0369	1.936	938.4571
1926	55.0629	1.9352	535.9988	1926	55.0629	1.9352	767.8955	1926	55.0629	1.9352	600.0186	1926	55.0629	1.9352	1040.6533
1927	55.0889	1.9343	603.4171	1927	55.0889	1.9343	834.8352	1927	55.0889	1.9343	617.475	1927	55.0889	1.9343	1060.8966
1928	55.1149	1.9335	620.8579	1928	55.1149	1.9335	851.7974	1928	55.1149	1.9335	621.0699	1928	55.1149	1.9335	1067.2785
1929	55.1409	1.9326	623.4089	1929	55.1409	1.9326	853.8698	1929	55.1409	1.9326	665.9748	1929	55.1409	1.9326	1114.9703
1930	55.1669	1.9318	589.6217	1930	55.1669	1.9318	819.6041	1930	55.1669	1.9318	707.1933	1930	55.1669	1.9318	1158.9756
1931	55.1929	1.931	550.4972	1931	55.1929	1.931	780.001	1931	55.1929	1.931	821.7775	1931	55.1929	1.931	1276.3468
1932	55.2189	1.9301	598.7382	1932	55.2189	1.9301	827.7634	1932	55.2189	1.9301	1044.4569	1932	55.2189	1.9301	1501.813
1933	55.2449	1.9293	587.0398	1933	55.2449	1.9293	815.5865	1933	55.2449	1.9293	1124.0237	1933	55.2449	1.9293	1584.1668
1934	55.2709	1.9285	605.0776	1934	55.2709	1.9285	833.1456	1934	55.2709	1.9285	1107.9244	1934	55.2709	1.9285	1570.8544
1935	55.2969	1.9276	499.4013	1935	55.2969	1.9276	726.9908	1935	55.2969	1.9276	1087.3186	1935	55.2969	1.9276	1553.0354
1936	55.3229	1.9268	497.0996	1936	55.3229	1.9268	724.2106	1936	55.3229	1.9268	980.6504	1936	55.3229	1.9268	1449.1541
1937	55.3489	1.926	477.2831	1937	55.3489	1.926	703.9154	1937	55.3489	1.926	1004.8785	1937	55.3489	1.926	1476.1691
1938	55.3749	1.9251	448.9917	1938	55.3749	1.9251	675.1455	1938	55.3749	1.9251	909.7718	1938	55.3749	1.9251	1383.8494
1939	55.4009	1.9243	430.9953	1939	55.4009	1.9243	656.6704	1939	55.4009	1.9243	870.2002	1939	55.4009	1.9243	1347.0646

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1940	55.4269	1.9235	427.0427	1940	55.4269	1.9235	652.2393	1940	55.4269	1.9235	739.8373	1940	55.4269	1.9235	1219.4887
1941	55.4529	1.9226	349.2037	1941	55.4529	1.9226	573.9217	1941	55.4529	1.9226	694.5587	1941	55.4529	1.9226	1176.997
1942	55.4789	1.9218	340.7996	1942	55.4789	1.9218	565.0391	1942	55.4789	1.9218	617.4326	1942	55.4789	1.9218	1102.6578
1943	55.5049	1.921	328.2355	1943	55.5049	1.921	551.9964	1943	55.5049	1.921	574.3698	1943	55.5049	1.921	1062.3818
1944	55.5309	1.9201	328.2066	1944	55.5309	1.9201	551.4889	1944	55.5309	1.9201	553.9443	1944	55.5309	1.9201	1044.7432
1945	55.5569	1.9193	312.7086	1945	55.5569	1.9193	535.5124	1945	55.5569	1.9193	565.6128	1945	55.5569	1.9193	1059.1987
1946	55.5829	1.9185	305.6975	1946	55.5829	1.9185	527.2989	1946	55.5829	1.9185	663.1056	1946	55.5829	1.9185	1156.0449
1947	55.6089	1.9177	334.9409	1947	55.6089	1.9177	555.34	1947	55.6089	1.9177	750.7839	1947	55.6089	1.9177	1243.0765
1948	55.6349	1.9168	361.748	1948	55.6349	1.9168	580.9446	1948	55.6349	1.9168	937.5464	1948	55.6349	1.9168	1429.1924
1949	55.6609	1.916	333.4228	1949	55.6609	1.916	551.4172	1949	55.6609	1.916	1206.3422	1949	55.6609	1.916	1697.3416
1950	55.6869	1.9152	358.218	1950	55.6869	1.9152	575.01	1950	55.6869	1.9152	1634.6804	1950	55.6869	1.9152	2125.0332
1951	55.7129	1.9144	351.7431	1951	55.7129	1.9144	567.3327	1951	55.7129	1.9144	1956.7972	1951	55.7129	1.9144	2446.5033
1952	55.7389	1.9135	349.8033	1952	55.7389	1.9135	564.1905	1952	55.7389	1.9135	1972.4965	1952	55.7389	1.9135	2461.5561
1953	55.7649	1.9127	382.4508	1953	55.7649	1.9127	595.6357	1953	55.7649	1.9127	1898.686	1953	55.7649	1.9127	2387.0989
1954	55.7909	1.9119	363.8205	1954	55.7909	1.9119	575.8031	1954	55.7909	1.9119	1912.6742	1954	55.7909	1.9119	2400.4405
1955	55.8169	1.9111	349.1145	1955	55.8169	1.9111	559.8947	1955	55.8169	1.9111	1988.7223	1955	55.8169	1.9111	2475.842
1956	55.8429	1.9103	348.0048	1956	55.8429	1.9103	557.5827	1956	55.8429	1.9103	1989.2176	1956	55.8429	1.9103	2475.6907
1957	55.8689	1.9095	353.9124	1957	55.8689	1.9095	562.2879	1957	55.8689	1.9095	1883.7022	1957	55.8689	1.9095	2369.5286
1958	55.8949	1.9086	329.9769	1958	55.8949	1.9086	537.1501	1958	55.8949	1.9086	1734.2705	1958	55.8949	1.9086	2219.4503
1959	55.9209	1.9078	307.3127	1959	55.9209	1.9078	513.2835	1959	55.9209	1.9078	1477.3683	1959	55.9209	1.9078	1961.9015
1960	55.9469	1.907	297.6736	1960	55.9469	1.907	502.4421	1960	55.9469	1.907	1231.1011	1960	55.9469	1.907	1714.9877
1961	55.9729	1.9062	280.94	1961	55.9729	1.9062	484.5062	1961	55.9729	1.9062	1098.2909	1961	55.9729	1.9062	1581.5309
1962	55.9989	1.9054	287.1958	1962	55.9989	1.9054	489.5596	1962	55.9989	1.9054	997.8292	1962	55.9989	1.9054	1480.4225
1963	56.0249	1.9046	294.5139	1963	56.0249	1.9046	495.6754	1963	56.0249	1.9046	897.4045	1963	56.0249	1.9046	1379.3512
1964	56.0509	1.9038	283.7253	1964	56.0509	1.9038	483.6844	1964	56.0509	1.9038	781.112	1964	56.0509	1.9038	1262.4121
1965	56.0769	1.9029	278.2432	1965	56.0769	1.9029	477	1965	56.0769	1.9029	670.211	1965	56.0769	1.9029	1150.8644
1966	56.1029	1.9021	279.4456	1966	56.1029	1.9021	477	1966	56.1029	1.9021	593.8153	1966	56.1029	1.9021	1073.8221
1967	56.1289	1.9013	279.6624	1967	56.1289	1.9013	476.0145	1967	56.1289	1.9013	537.0011	1967	56.1289	1.9013	1016.3614
1968	56.1549	1.9005	289.0244	1968	56.1549	1.9005	484.1742	1968	56.1549	1.9005	531.1176	1968	56.1549	1.9005	1009.8312
1969	56.1809	1.8997	289.6482	1969	56.1809	1.8997	483.5956	1969	56.1809	1.8997	526.3949	1969	56.1809	1.8997	1004.4619
1970	56.2069	1.8989	268.6058	1970	56.2069	1.8989	461.3509	1970	56.2069	1.8989	515.7109	1970	56.2069	1.8989	993.1312
1971	56.2329	1.8981	258.8166	1971	56.2329	1.8981	450.3593	1971	56.2329	1.8981	509.9474	1971	56.2329	1.8981	986.7211
1972	56.2589	1.8973	273.625	1972	56.2589	1.8973	463.9654	1972	56.2589	1.8973	473.555	1972	56.2589	1.8973	949.6821
1973	56.2849	1.8965	292.8403	1973	56.2849	1.8965	482.4659	1973	56.2849	1.8965	492.6474	1973	56.2849	1.8965	968.1279
1974	56.3109	1.8957	287.5062	1974	56.3109	1.8957	476.4171	1974	56.3109	1.8957	512.1967	1974	56.3109	1.8957	987.0305
1975	56.3369	1.8949	290.753	1975	56.3369	1.8949	478.9492	1975	56.3369	1.8949	505.3878	1975	56.3369	1.8949	979.575

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
1976	56.3629	1.8941	294.1345	1976	56.3629	1.8941	481.616	1976	56.3629	1.8941	489.3747	1976	56.3629	1.8941	962.9153
1977	56.3889	1.8933	264.0204	1977	56.3889	1.8933	450.7871	1977	56.3889	1.8933	458.4222	1977	56.3889	1.8933	931.3162
1978	56.4149	1.8925	271.3188	1978	56.4149	1.8925	457.3708	1978	56.4149	1.8925	450.4589	1978	56.4149	1.8925	922.7063
1979	56.4409	1.8917	298.6006	1979	56.4409	1.8917	483.9379	1979	56.4409	1.8917	372.3506	1979	56.4409	1.8917	843.9514
1980	56.4669	1.8909	307.9142	1980	56.4669	1.8909	492.5368	1980	56.4669	1.8909	354.235	1980	56.4669	1.8909	825.1892
1981	56.4929	1.8901	293.0315	1981	56.4929	1.8901	476.9394	1981	56.4929	1.8901	375.0151	1981	56.4929	1.8901	845.3226
1982	56.5189	1.8893	324.8645	1982	56.5189	1.8893	508.0576	1982	56.5189	1.8893	355.3709	1982	56.5189	1.8893	825.0318
1983	56.5449	1.8885	310.5257	1983	56.5449	1.8885	493.0041	1983	56.5449	1.8885	339.6148	1983	56.5449	1.8885	808.6291
1984	56.5709	1.8877	294.1702	1984	56.5709	1.8877	475.9339	1984	56.5709	1.8877	307.1974	1984	56.5709	1.8877	775.565
1985	56.5969	1.8869	276.3989	1985	56.5969	1.8869	457.4479	1985	56.5969	1.8869	319.6774	1985	56.5969	1.8869	787.3984
1986	56.6229	1.8861	323.234	1986	56.6229	1.8861	503.5683	1986	56.6229	1.8861	334.7936	1986	56.6229	1.8861	801.868
1987	56.6489	1.8853	294.7279	1987	56.6489	1.8853	474.3475	1987	56.6489	1.8853	362.7602	1987	56.6489	1.8853	829.188
1988	56.6749	1.8845	279.3704	1988	56.6749	1.8845	458.2752	1988	56.6749	1.8845	396.8151	1988	56.6749	1.8845	862.5963
1989	56.7009	1.8837	291.0251	1989	56.7009	1.8837	469.2152	1989	56.7009	1.8837	395.3937	1989	56.7009	1.8837	860.5283
1990	56.7269	1.8829	303.6727	1990	56.7269	1.8829	481.1481	1990	56.7269	1.8829	430.4805	1990	56.7269	1.8829	894.9684
1991	56.7529	1.8821	298.9847	1991	56.7529	1.8821	475.7454	1991	56.7529	1.8821	441.3948	1991	56.7529	1.8821	905.2361
1992	56.7789	1.8813	303.6036	1992	56.7789	1.8813	479.6496	1992	56.7789	1.8813	465.011	1992	56.7789	1.8813	928.2057
1993	56.8049	1.8805	318.6688	1993	56.8049	1.8805	494	1993	56.8049	1.8805	600.2719	1993	56.8049	1.8805	1062.82
1994	56.8309	1.8798	311.7379	1994	56.8309	1.8798	486.3544	1994	56.8309	1.8798	834.8956	1994	56.8309	1.8798	1296.797
1995	56.8569	1.879	289.3224	1995	56.8569	1.879	463.2242	1995	56.8569	1.879	1119.6025	1995	56.8569	1.879	1580.8573
1996	56.8829	1.8782	314.7296	1996	56.8829	1.8782	487.9167	1996	56.8829	1.8782	1673.9936	1996	56.8829	1.8782	2134.6018
1997	56.9089	1.8774	354.992	1997	56.9089	1.8774	527.4644	1997	56.9089	1.8774	2233.5214	1997	56.9089	1.8774	2693.483
1998	56.9349	1.8766	319.4644	1998	56.9349	1.8766	491.2221	1998	56.9349	1.8766	2432.3521	1998	56.9349	1.8766	2891.667
1999	56.9609	1.8758	358.4417	1999	56.9609	1.8758	529.4846	1999	56.9609	1.8758	2330.4242	1999	56.9609	1.8758	2789.0926
2000	56.9869	1.875	383.389	2000	56.9869	1.875	553.7172	2000	56.9869	1.875	2210.2487	2000	56.9869	1.875	2664.8368
2001	57.0129	1.8743	345.7037	2001	57.0129	1.8743	515.3172	2001	57.0129	1.8743	2131.5813	2001	57.0129	1.8743	2582.0893
2002	57.0389	1.8735	310.2467	2002	57.0389	1.8735	479.1455	2002	57.0389	1.8735	2259.734	2002	57.0389	1.8735	2706.1618
2003	57.0649	1.8727	315.8831	2003	57.0649	1.8727	484.0671	2003	57.0649	1.8727	2190.5731	2003	57.0649	1.8727	2632.9208
2004	57.0909	1.8719	342.1537	2004	57.0909	1.8719	509.6231	2004	57.0909	1.8719	1950.9383	2004	57.0909	1.8719	2389.2059
2005	57.1169	1.8711	337.2365	2005	57.1169	1.8711	503.9911	2005	57.1169	1.8711	1687.4658	2005	57.1169	1.8711	2121.6533
2006	57.1429	1.8704	309.7757	2006	57.1429	1.8704	475.8156	2006	57.1429	1.8704	1365.0767	2006	57.1429	1.8704	1795.184
2007	57.1689	1.8696	273.9618	2007	57.1689	1.8696	439.287	2007	57.1689	1.8696	1143.7818	2007	57.1689	1.8696	1569.8089
2008	57.1949	1.8688	342.8738	2008	57.1949	1.8688	507.4842	2008	57.1949	1.8688	1065.44	2008	57.1949	1.8688	1487.387
2009	57.2209	1.868	338.2563	2009	57.2209	1.868	502.1521	2009	57.2209	1.868	906.3014	2009	57.2209	1.868	1324.1682
2010	57.2469	1.8672	340.3562	2010	57.2469	1.8672	503.5372	2010	57.2469	1.8672	807.3457	2010	57.2469	1.8672	1221.1324
2011	57.2729	1.8665	334.7023	2011	57.2729	1.8665	497.1686	2011	57.2729	1.8665	701.1925	2011	57.2729	1.8665	1110.8991

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2012	57.2989	1.8657	335.8424	2012	57.2989	1.8657	497.594	2012	57.2989	1.8657	714.266	2012	57.2989	1.8657	1119.8924
2013	57.3249	1.8649	287.2539	2013	57.3249	1.8649	448.2908	2013	57.3249	1.8649	593.5805	2013	57.3249	1.8649	995.1268
2014	57.3509	1.8641	295.7307	2014	57.3509	1.8641	456.0529	2014	57.3509	1.8641	627.0846	2014	57.3509	1.8641	1024.5508
2015	57.3769	1.8634	298.0955	2015	57.3769	1.8634	457.7029	2015	57.3769	1.8634	615.2081	2015	57.3769	1.8634	1008.5941
2016	57.4029	1.8626	281.4889	2016	57.4029	1.8626	440.3817	2016	57.4029	1.8626	653.9835	2016	57.4029	1.8626	1043.2893
2017	57.4289	1.8618	339.6282	2017	57.4289	1.8618	497.8062	2017	57.4289	1.8618	551.1352	2017	57.4289	1.8618	936.3609
2018	57.4549	1.8611	283.306	2018	57.4549	1.8611	440.7693	2018	57.4549	1.8611	532.1595	2018	57.4549	1.8611	913.3051
2019	57.4809	1.8603	280.321	2019	57.4809	1.8603	437.0696	2019	57.4809	1.8603	601.3811	2019	57.4809	1.8603	978.4465
2020	57.5069	1.8595	360.2512	2020	57.5069	1.8595	516.2851	2020	57.5069	1.8595	556.7364	2020	57.5069	1.8595	929.7217
2021	57.5329	1.8587	341.6706	2021	57.5329	1.8587	496.9897	2021	57.5329	1.8587	530.3858	2021	57.5329	1.8587	899.2909
2022	57.5589	1.858	304.4608	2022	57.5589	1.858	459.0652	2022	57.5589	1.858	530.3339	2022	57.5589	1.858	895.1589
2023	57.5849	1.8572	334.9725	2023	57.5849	1.8572	488.8622	2023	57.5849	1.8572	488.3361	2023	57.5849	1.8572	849.0809
2024	57.6109	1.8564	338.7522	2024	57.6109	1.8564	491.9272	2024	57.6109	1.8564	476.3545	2024	57.6109	1.8564	833.0192
2025	57.6369	1.8557	281.7511	2025	57.6369	1.8557	434.2114	2025	57.6369	1.8557	424.3787	2025	57.6369	1.8557	776.9632
2026	57.6629	1.8549	273.625	2026	57.6629	1.8549	425.3706	2026	57.6629	1.8549	380.8498	2026	57.6629	1.8549	729.3542
2027	57.6889	1.8542	341.2359	2027	57.6889	1.8542	494.1025	2027	57.6889	1.8542	386.9659	2027	57.6889	1.8542	732.1795
2028	57.7149	1.8534	312.5118	2028	57.7149	1.8534	466.4995	2028	57.7149	1.8534	415.04	2028	57.7149	1.8534	756.9629
2029	57.7409	1.8526	313.912	2029	57.7409	1.8526	469.0207	2029	57.7409	1.8526	377.4884	2029	57.7409	1.8526	716.1205
2030	57.7669	1.8519	319.8439	2030	57.7669	1.8519	476.0737	2030	57.7669	1.8519	351.2316	2030	57.7669	1.8519	686.573
2031	57.7929	1.8511	311.0717	2031	57.7929	1.8511	468.4225	2031	57.7929	1.8511	351.8072	2031	57.7929	1.8511	683.8577
2032	57.8189	1.8503	298.3542	2032	57.8189	1.8503	456.8261	2032	57.8189	1.8503	328.9577	2032	57.8189	1.8503	657.7175
2033	57.8449	1.8496	312.165	2033	57.8449	1.8496	471.758	2033	57.8449	1.8496	319.9899	2033	57.8449	1.8496	645.4589
2034	57.8709	1.8488	320.9097	2034	57.8709	1.8488	481.6238	2034	57.8709	1.8488	378.1244	2034	57.8709	1.8488	700.3026
2035	57.8969	1.8481	301.5315	2035	57.8969	1.8481	463.3666	2035	57.8969	1.8481	335.8486	2035	57.8969	1.8481	654.736
2036	57.9229	1.8473	271.7997	2036	57.9229	1.8473	434.756	2036	57.9229	1.8473	341.7579	2036	57.9229	1.8473	657.3546
2037	57.9489	1.8465	280.8869	2037	57.9489	1.8465	444.9642	2037	57.9489	1.8465	351.8869	2037	57.9489	1.8465	664.1928
2038	57.9749	1.8458	288.5314	2038	57.9749	1.8458	453.7297	2038	57.9749	1.8458	322.8767	2038	57.9749	1.8458	631.8918
2039	58.0009	1.845	303.4695	2039	58.0009	1.845	469.789	2039	58.0009	1.845	310.2703	2039	58.0009	1.845	615.9947
2040	58.0269	1.8443	315.0124	2040	58.0269	1.8443	482.4529	2040	58.0269	1.8443	326.1669	2040	58.0269	1.8443	628.6005
2041	58.0529	1.8435	301.268	2041	58.0529	1.8435	469.8295	2041	58.0529	1.8435	344.4765	2041	58.0529	1.8435	643.6193
2042	58.0789	1.8428	310.2894	2042	58.0789	1.8428	479.972	2042	58.0789	1.8428	327.9413	2042	58.0789	1.8428	623.7934
2043	58.1049	1.842	289.8199	2043	58.1049	1.842	460.6236	2043	58.1049	1.842	339.6896	2043	58.1049	1.842	632.2509
2044	58.1309	1.8413	270.6014	2044	58.1309	1.8413	442.5262	2044	58.1309	1.8413	340.7132	2044	58.1309	1.8413	629.9837
2045	58.1569	1.8405	276.7366	2045	58.1569	1.8405	449.7825	2045	58.1569	1.8405	353.9593	2045	58.1569	1.8405	639.939
2046	58.1829	1.8398	280.542	2046	58.1829	1.8398	454.7089	2046	58.1829	1.8398	374.3625	2046	58.1829	1.8398	657.0515
2047	58.2089	1.839	281.809	2047	58.2089	1.839	457.097	2047	58.2089	1.839	334.3715	2047	58.2089	1.839	613.7697

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2048	58.2349	1.8383	289.8597	2048	58.2349	1.8383	466.2688	2048	58.2349	1.8383	325.1614	2048	58.2349	1.8383	601.2688
2049	58.2609	1.8375	282.2827	2049	58.2609	1.8375	459.8128	2049	58.2609	1.8375	373.6112	2049	58.2609	1.8375	646.4278
2050	58.2869	1.8368	299.1024	2050	58.2869	1.8368	477.7536	2050	58.2869	1.8368	391.7895	2050	58.2869	1.8368	661.3154
2051	58.3129	1.836	325.0509	2051	58.3129	1.836	504.8232	2051	58.3129	1.836	364.415	2051	58.3129	1.836	630.6501
2052	58.3389	1.8353	294.4427	2052	58.3389	1.8353	475.3361	2052	58.3389	1.8353	325.7818	2052	58.3389	1.8353	588.7261
2053	58.3649	1.8345	273.625	2053	58.3649	1.8345	455.6395	2053	58.3649	1.8345	380.8498	2053	58.3649	1.8345	640.5034
2054	58.3909	1.8338	291.2818	2054	58.3909	1.8338	473.6269	2054	58.3909	1.8338	374.0502	2054	58.3909	1.8338	631.4145
2055	58.4169	1.833	277.7789	2055	58.4169	1.833	460.4548	2055	58.4169	1.833	325.3798	2055	58.4169	1.833	580.4548
2056	58.4429	1.8323	279.455	2056	58.4429	1.8323	462.4616	2056	58.4429	1.8323	349.7956	2056	58.4429	1.8323	602.5813
2057	58.4689	1.8316	287.2636	2057	58.4689	1.8316	470.6009	2057	58.4689	1.8316	389.2982	2057	58.4689	1.8316	639.7946
2058	58.4949	1.8308	300.6679	2058	58.4949	1.8308	484.3359	2058	58.4949	1.8308	370.7108	2058	58.4949	1.8308	618.9179
2059	58.5209	1.8301	284.9048	2059	58.5209	1.8301	468.9035	2059	58.5209	1.8301	331.7849	2059	58.5209	1.8301	577.7027
2060	58.5469	1.8293	287.3305	2060	58.5469	1.8293	471.66	2060	58.5469	1.8293	338.1815	2060	58.5469	1.8293	581.81
2061	58.5729	1.8286	292.6983	2061	58.5729	1.8286	477.3585	2061	58.5729	1.8286	380.9844	2061	58.5729	1.8286	622.3236
2062	58.5989	1.8279	266.9543	2062	58.5989	1.8279	451.9452	2062	58.5989	1.8279	398.9987	2062	58.5989	1.8279	638.0486
2063	58.6249	1.8271	293.1958	2063	58.6249	1.8271	478.5175	2063	58.6249	1.8271	381.0324	2063	58.6249	1.8271	617.793
2064	58.6509	1.8264	308.2565	2064	58.6509	1.8264	493.9088	2064	58.6509	1.8264	384.3774	2064	58.6509	1.8264	618.8487
2065	58.6769	1.8256	306.6286	2065	58.6769	1.8256	492.6116	2065	58.6769	1.8256	396.6957	2065	58.6769	1.8256	628.8777
2066	58.7029	1.8249	321.1967	2066	58.7029	1.8249	507.5105	2066	58.7029	1.8249	413.4631	2066	58.7029	1.8249	643.3558
2067	58.7289	1.8242	292.8245	2067	58.7289	1.8242	479.469	2067	58.7289	1.8242	418.3814	2067	58.7289	1.8242	645.9848
2068	58.7549	1.8234	302.7838	2068	58.7549	1.8234	489.7591	2068	58.7549	1.8234	404.7234	2068	58.7549	1.8234	630.0375
2069	58.7809	1.8227	318.6591	2069	58.7809	1.8227	505.9651	2069	58.7809	1.8227	409.3015	2069	58.7809	1.8227	632.3263
2070	58.8069	1.822	306.0158	2070	58.8069	1.822	493.6525	2070	58.8069	1.822	398.375	2070	58.8069	1.822	619.1105
2071	58.8329	1.8212	312.2764	2071	58.8329	1.8212	500.2438	2071	58.8329	1.8212	386.084	2071	58.8329	1.8212	604.5303
2072	58.8589	1.8205	324.6994	2072	58.8589	1.8205	512.9975	2072	58.8589	1.8205	405.6654	2072	58.8589	1.8205	621.8224
2073	58.8849	1.8198	320.1774	2073	58.8849	1.8198	508.8063	2073	58.8849	1.8198	420.6914	2073	58.8849	1.8198	634.559
2074	58.9109	1.819	294.5596	2074	58.9109	1.819	483.5192	2074	58.9109	1.819	418.973	2074	58.9109	1.819	630.5513
2075	58.9369	1.8183	298.7054	2075	58.9369	1.8183	487.9957	2075	58.9369	1.8183	403.2337	2075	58.9369	1.8183	612.5227
2076	58.9629	1.8176	298.1749	2076	58.9629	1.8176	487.7959	2076	58.9629	1.8176	393.1689	2076	58.9629	1.8176	600.1686
2077	58.9889	1.8168	309.3836	2077	58.9889	1.8168	499.3353	2077	58.9889	1.8168	409.908	2077	58.9889	1.8168	614.6185
2078	59.0149	1.8161	293.0251	2078	59.0149	1.8161	483.3075	2078	59.0149	1.8161	401.0089	2078	59.0149	1.8161	603.4301
2079	59.0409	1.8154	301.1796	2079	59.0409	1.8154	491.7928	2079	59.0409	1.8154	367.5275	2079	59.0409	1.8154	567.6593
2080	59.0669	1.8147	273.625	2080	59.0669	1.8147	464.5689	2080	59.0669	1.8147	380.8498	2080	59.0669	1.8147	578.6923
2081	59.0929	1.8139	273.2535	2081	59.0929	1.8139	463.5722	2081	59.0929	1.8139	415.0132	2081	59.0929	1.8139	613.8082
2082	59.1189	1.8132	285.5137	2082	59.1189	1.8132	475.2073	2082	59.1189	1.8132	409.8666	2082	59.1189	1.8132	609.6141
2083	59.1449	1.8125	272.3242	2083	59.1449	1.8125	461.3925	2083	59.1449	1.8125	399.4015	2083	59.1449	1.8125	600.1014

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2084	59.1709	1.8118	278.5524	2084	59.1709	1.8118	466.9956	2084	59.1709	1.8118	401.7015	2084	59.1709	1.8118	603.3539
2085	59.1969	1.811	285.3673	2085	59.1969	1.811	473.1853	2085	59.1969	1.811	402.9851	2085	59.1969	1.811	605.5899
2086	59.2229	1.8103	297.6154	2086	59.2229	1.8103	484.8082	2086	59.2229	1.8103	405.2253	2086	59.2229	1.8103	608.7826
2087	59.2489	1.8096	300.8072	2087	59.2489	1.8096	487.3748	2087	59.2489	1.8096	379.2413	2087	59.2489	1.8096	583.751
2088	59.2749	1.8089	291.8889	2088	59.2749	1.8089	477.8313	2088	59.2749	1.8089	415.3899	2088	59.2749	1.8089	620.8521
2089	59.3009	1.8081	287.1425	2089	59.3009	1.8081	472.4597	2089	59.3009	1.8081	389.9239	2089	59.3009	1.8081	596.3386
2090	59.3269	1.8074	281.8526	2090	59.3269	1.8074	466.5447	2090	59.3269	1.8074	401.0969	2090	59.3269	1.8074	608.4641
2091	59.3529	1.8067	285.2451	2091	59.3529	1.8067	469.312	2091	59.3529	1.8067	373.7585	2091	59.3529	1.8067	582.0781
2092	59.3789	1.806	290.5682	2092	59.3789	1.806	474.0099	2092	59.3789	1.806	350.7578	2092	59.3789	1.806	560.0298
2093	59.4049	1.8053	290.7876	2093	59.4049	1.8053	473.6041	2093	59.4049	1.8053	352.2263	2093	59.4049	1.8053	562.4508
2094	59.4309	1.8046	279.1801	2094	59.4309	1.8046	461.3715	2094	59.4309	1.8046	354.5525	2094	59.4309	1.8046	565.7295
2095	59.4569	1.8038	274.2111	2095	59.4569	1.8038	455.7773	2095	59.4569	1.8038	416.2802	2095	59.4569	1.8038	628.4096
2096	59.4829	1.8031	263.8447	2096	59.4829	1.8031	444.7857	2096	59.4829	1.8031	360.4925	2096	59.4829	1.8031	573.5744
2097	59.5089	1.8024	230.5388	2097	59.5089	1.8024	410.8546	2097	59.5089	1.8024	370.9497	2097	59.5089	1.8024	584.984
2098	59.5349	1.8017	252.2909	2098	59.5349	1.8017	431.9815	2098	59.5349	1.8017	415.9965	2098	59.5349	1.8017	630.9832
2099	59.5609	1.801	273.1758	2099	59.5609	1.801	452.2412	2099	59.5609	1.801	391.3153	2099	59.5609	1.801	607.2545
2100	59.5869	1.8003	252.7328	2100	59.5869	1.8003	431.1731	2100	59.5869	1.8003	374.2999	2100	59.5869	1.8003	591.1916
2101	59.6129	1.7995	255.6536	2101	59.6129	1.7995	433.4687	2101	59.6129	1.7995	356.4613	2101	59.6129	1.7995	574.3055
2102	59.6389	1.7988	259.9785	2102	59.6389	1.7988	437.1684	2102	59.6389	1.7988	361.1305	2102	59.6389	1.7988	579.9272
2103	59.6649	1.7981	244.3089	2103	59.6649	1.7981	420.8736	2103	59.6649	1.7981	359.1245	2103	59.6649	1.7981	578.8736
2104	59.6909	1.7974	280.7314	2104	59.6909	1.7974	456.6709	2104	59.6909	1.7974	392.235	2104	59.6909	1.7974	612.9365
2105	59.7169	1.7967	316.1644	2105	59.7169	1.7967	491.4787	2105	59.7169	1.7967	416.5537	2105	59.7169	1.7967	638.2077
2106	59.7429	1.796	258.2416	2106	59.7429	1.796	432.9308	2106	59.7429	1.796	369.3243	2106	59.7429	1.796	591.9308
2107	59.7689	1.7953	273.625	2107	59.7689	1.7953	447.689	2107	59.7689	1.7953	380.8498	2107	59.7689	1.7953	604.4087
2108	59.7949	1.7946	270.9325	2108	59.7949	1.7946	444.7188	2108	59.7949	1.7946	358.3848	2108	59.7949	1.7946	581.6251
2109	59.8209	1.7939	265.4743	2109	59.8209	1.7939	438.9829	2109	59.8209	1.7939	354.324	2109	59.8209	1.7939	577.2457
2110	59.8469	1.7932	233.6557	2110	59.8469	1.7932	406.8866	2110	59.8469	1.7932	349.6478	2110	59.8469	1.7932	572.2509
2111	59.8729	1.7925	247.7972	2111	59.8729	1.7925	420.7504	2111	59.8729	1.7925	387.0696	2111	59.8729	1.7925	609.3541
2112	59.8989	1.7917	288.5406	2112	59.8989	1.7917	461.2162	2112	59.8989	1.7917	334.9527	2112	59.8989	1.7917	556.9187
2113	59.9249	1.791	290.8374	2113	59.9249	1.791	463.2353	2113	59.9249	1.791	351.6615	2113	59.9249	1.791	573.3088
2114	59.9509	1.7903	253.256	2114	59.9509	1.7903	425.3762	2114	59.9509	1.7903	357.577	2114	59.9509	1.7903	578.9057
2115	59.9769	1.7896	264.0847	2115	59.9769	1.7896	435.9272	2115	59.9769	1.7896	328.3734	2115	59.9769	1.7896	549.3836
2116	60.0029	1.7889	261.22	2116	60.0029	1.7889	432.7847	2116	60.0029	1.7889	384.6672	2116	60.0029	1.7889	605.3588
2117	60.0289	1.7882	246.9964	2117	60.0289	1.7882	418.2835	2117	60.0289	1.7882	409.4764	2117	60.0289	1.7882	629.8494
2118	60.0549	1.7875	310.639	2118	60.0549	1.7875	481.6484	2118	60.0549	1.7875	376.1324	2118	60.0549	1.7875	596.1868
2119	60.0809	1.7868	285.6691	2119	60.0809	1.7868	456.4008	2119	60.0809	1.7868	388.0792	2119	60.0809	1.7868	607.815

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2120	60.1069	1.7861	273.8501	2120	60.1069	1.7861	444.3041	2120	60.1069	1.7861	379.8108	2120	60.1069	1.7861	599.228
2121	60.1329	1.7854	252.5994	2121	60.1329	1.7854	422.7757	2121	60.1329	1.7854	427.1736	2121	60.1329	1.7854	646.2722
2122	60.1589	1.7847	272.1526	2122	60.1589	1.7847	442.0512	2122	60.1589	1.7847	380.5243	2122	60.1589	1.7847	599.3043
2123	60.1849	1.784	288.4974	2123	60.1849	1.784	458.1183	2123	60.1849	1.784	339.7979	2123	60.1849	1.784	558.2593
2124	60.2109	1.7833	267.2174	2124	60.2109	1.7833	436.5607	2124	60.2109	1.7833	382.7358	2124	60.2109	1.7833	600.8787
2125	60.2369	1.7826	275.185	2125	60.2369	1.7826	444.2505	2125	60.2369	1.7826	338.9982	2125	60.2369	1.7826	556.8224
2126	60.2629	1.7819	309.1568	2126	60.2629	1.7819	477.9446	2126	60.2629	1.7819	372.0995	2126	60.2629	1.7819	589.6051
2127	60.2889	1.7812	278.9972	2127	60.2889	1.7812	447.5074	2127	60.2889	1.7812	338.6995	2127	60.2889	1.7812	555.8866
2128	60.3149	1.7805	308.8931	2128	60.3149	1.7805	477.1255	2128	60.3149	1.7805	355.723	2128	60.3149	1.7805	572.5915
2129	60.3409	1.7798	342.2622	2129	60.3409	1.7798	510.2169	2129	60.3409	1.7798	346.9404	2129	60.3409	1.7798	563.4903
2130	60.3669	1.7792	325.3124	2130	60.3669	1.7792	492.9895	2130	60.3669	1.7792	411.4266	2130	60.3669	1.7792	627.6579
2131	60.3929	1.7785	333.8524	2131	60.3929	1.7785	501.2517	2131	60.3929	1.7785	395.9873	2131	60.3929	1.7785	611.9
2132	60.4189	1.7778	338.4451	2132	60.4189	1.7778	505.5668	2132	60.4189	1.7778	402.673	2132	60.4189	1.7778	618.2671
2133	60.4449	1.7771	340.8474	2133	60.4449	1.7771	507.6913	2133	60.4449	1.7771	392.0394	2133	60.4449	1.7771	607.3149
2134	60.4709	1.7764	373.1922	2134	60.4709	1.7764	539.7585	2134	60.4709	1.7764	380.8498	2134	60.4709	1.7764	595.8068
2135	60.4969	1.7757	372.279	2135	60.4969	1.7757	538.5676	2135	60.4969	1.7757	435.1853	2135	60.4969	1.7757	649.3305
2136	60.5229	1.775	337.537	2136	60.5229	1.775	503.5479	2136	60.5229	1.775	426.453	2136	60.5229	1.775	639.7865
2137	60.5489	1.7743	373.7899	2137	60.5489	1.7743	539.5231	2137	60.5489	1.7743	427.3142	2137	60.5489	1.7743	639.8359
2138	60.5749	1.7736	362.2548	2138	60.5749	1.7736	527.7103	2138	60.5749	1.7736	426.9019	2138	60.5749	1.7736	638.6118
2139	60.6009	1.7729	366.2559	2139	60.6009	1.7729	531.4337	2139	60.6009	1.7729	437.3216	2139	60.6009	1.7729	648.2198
2140	60.6269	1.7722	351.2469	2140	60.6269	1.7722	516.147	2140	60.6269	1.7722	441.6898	2140	60.6269	1.7722	651.7762
2141	60.6529	1.7716	407.6811	2141	60.6529	1.7716	572.3035	2141	60.6529	1.7716	394.4488	2141	60.6529	1.7716	603.7235
2142	60.6789	1.7709	388.0803	2142	60.6789	1.7709	552.425	2142	60.6789	1.7709	428.9449	2142	60.6789	1.7709	637.4078
2143	60.7049	1.7702	329.6531	2143	60.7049	1.7702	493.7201	2143	60.7049	1.7702	462.5172	2143	60.7049	1.7702	670.1683
2144	60.7309	1.7695	340.7256	2144	60.7309	1.7695	504.515	2144	60.7309	1.7695	451.484	2144	60.7309	1.7695	658.3234
2145	60.7569	1.7688	363.5672	2145	60.7569	1.7688	527.0789	2145	60.7569	1.7688	446.699	2145	60.7569	1.7688	652.7266
2146	60.7829	1.7681	342.2488	2146	60.7829	1.7681	505.4827	2146	60.7829	1.7681	470.718	2146	60.7829	1.7681	675.9338
2147	60.8089	1.7674	356.0736	2147	60.8089	1.7674	519.0298	2147	60.8089	1.7674	438.1903	2147	60.8089	1.7674	642.5944
2148	60.8349	1.7668	362.8373	2148	60.8349	1.7668	525.5158	2148	60.8349	1.7668	431.1634	2148	60.8349	1.7668	634.7557
2149	60.8609	1.7661	349.2347	2149	60.8609	1.7661	511.6355	2149	60.8609	1.7661	430.7241	2149	60.8609	1.7661	633.5047
2150	60.8869	1.7654	349.9698	2150	60.8869	1.7654	512.0929	2150	60.8869	1.7654	408.0443	2150	60.8869	1.7654	610.0132
2151	60.9129	1.7647	372.4996	2151	60.9129	1.7647	534.3451	2151	60.9129	1.7647	393.5063	2151	60.9129	1.7647	594.6634
2152	60.9389	1.764	369.2892	2152	60.9389	1.764	530.857	2152	60.9389	1.764	394.2832	2152	60.9389	1.764	594.6286
2153	60.9649	1.7634	340.7042	2153	60.9649	1.7634	501.9943	2153	60.9649	1.7634	450.8334	2153	60.9649	1.7634	650.367
2154	60.9909	1.7627	314.9669	2154	60.9909	1.7627	475.9793	2154	60.9909	1.7627	496.5735	2154	60.9909	1.7627	695.2953
2155	61.0169	1.762	344.9082	2155	61.0169	1.762	505.6429	2155	61.0169	1.762	454.0172	2155	61.0169	1.762	651.9273

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2156	61.0429	1.7613	367.543	2156	61.0429	1.7613	528	2156	61.0429	1.7613	407.8477	2156	61.0429	1.7613	604.9461
2157	61.0689	1.7606	324.078	2157	61.0689	1.7606	484.2573	2157	61.0689	1.7606	422.4074	2157	61.0689	1.7606	618.694
2158	61.0949	1.76	303.2698	2158	61.0949	1.76	463.1714	2158	61.0949	1.76	387.7279	2158	61.0949	1.76	583.2027
2159	61.1209	1.7593	334.2346	2159	61.1209	1.7593	493.8585	2159	61.1209	1.7593	366.0908	2159	61.1209	1.7593	560.7539
2160	61.1469	1.7586	347.4538	2160	61.1469	1.7586	506.8001	2160	61.1469	1.7586	380.9264	2160	61.1469	1.7586	574.7777
2161	61.1729	1.7579	321.2175	2161	61.1729	1.7579	480.2861	2161	61.1729	1.7579	380.8498	2161	61.1729	1.7579	573.8894
2162	61.1989	1.7573	305.6484	2162	61.1989	1.7573	463.5579	2162	61.1989	1.7573	382.0605	2162	61.1989	1.7573	574.4634
2163	61.2249	1.7566	311.0856	2163	61.2249	1.7566	467.836	2163	61.2249	1.7566	380.2056	2163	61.2249	1.7566	571.972
2164	61.2509	1.7559	321.8656	2164	61.2509	1.7559	477.457	2164	61.2509	1.7559	369.4133	2164	61.2509	1.7559	560.543
2165	61.2769	1.7552	314.3073	2165	61.2769	1.7552	468.7397	2165	61.2769	1.7552	356.0564	2165	61.2769	1.7552	546.5495
2166	61.3029	1.7546	288.7343	2166	61.3029	1.7546	442.0076	2166	61.3029	1.7546	343.9612	2166	61.3029	1.7546	533.8176
2167	61.3289	1.7539	288.0686	2167	61.3289	1.7539	440.1829	2167	61.3289	1.7539	360.1127	2167	61.3289	1.7539	549.3326
2168	61.3549	1.7532	283.0994	2168	61.3549	1.7532	434.0547	2168	61.3549	1.7532	378.9216	2168	61.3549	1.7532	567.5048
2169	61.3809	1.7526	292.6042	2169	61.3809	1.7526	442.4004	2169	61.3809	1.7526	377.0765	2169	61.3809	1.7526	565.0231
2170	61.4069	1.7519	338.0691	2170	61.4069	1.7519	486.7063	2170	61.4069	1.7519	364.7263	2170	61.4069	1.7519	552.0363
2171	61.4329	1.7512	310.7221	2171	61.4329	1.7512	458.2002	2171	61.4329	1.7512	373.8834	2171	61.4329	1.7512	560.5568
2172	61.4589	1.7506	270.9833	2172	61.4589	1.7506	417.3024	2172	61.4589	1.7506	379.239	2172	61.4589	1.7506	565.2758
2173	61.4849	1.7499	295.0204	2173	61.4849	1.7499	440.1805	2173	61.4849	1.7499	358.8438	2173	61.4849	1.7499	544.2439
2174	61.5109	1.7492	303.6824	2174	61.5109	1.7492	447.6834	2174	61.5109	1.7492	399.9783	2174	61.5109	1.7492	584.7418
2175	61.5369	1.7485	298.4397	2175	61.5369	1.7485	441.2817	2175	61.5369	1.7485	413.2714	2175	61.5369	1.7485	597.3983
2176	61.5629	1.7479	284.0987	2176	61.5629	1.7479	425.7817	2176	61.5629	1.7479	356.4534	2176	61.5629	1.7479	539.9437
2177	61.5889	1.7472	272.8851	2177	61.5889	1.7472	413.4091	2177	61.5889	1.7472	350.51	2177	61.5889	1.7472	533.3636
2178	61.6149	1.7466	275.4334	2178	61.6149	1.7466	414.7983	2178	61.6149	1.7466	346.2154	2178	61.6149	1.7466	528.4324
2179	61.6409	1.7459	278.9619	2179	61.6409	1.7459	417.1677	2179	61.6409	1.7459	332.3723	2179	61.6409	1.7459	513.9527
2180	61.6669	1.7452	289.1603	2180	61.6669	1.7452	426.2072	2180	61.6669	1.7452	341.7457	2180	61.6669	1.7452	522.6895
2181	61.6929	1.7446	281.4257	2181	61.6929	1.7446	417.3135	2181	61.6929	1.7446	339.6033	2181	61.6929	1.7446	519.9104
2182	61.7189	1.7439	275.3107	2182	61.7189	1.7439	410.0394	2182	61.7189	1.7439	361.8328	2182	61.7189	1.7439	541.5034
2183	61.7449	1.7432	322.2356	2183	61.7449	1.7432	455.8053	2183	61.7449	1.7432	363.7404	2183	61.7449	1.7432	542.7743
2184	61.7709	1.7426	301.3246	2184	61.7709	1.7426	433.7353	2184	61.7709	1.7426	346.6034	2184	61.7709	1.7426	525.0007
2185	61.7969	1.7419	285.2992	2185	61.7969	1.7419	416.5508	2185	61.7969	1.7419	393.4496	2185	61.7969	1.7419	571.2102
2186	61.8229	1.7413	311.4251	2186	61.8229	1.7413	441.5177	2186	61.8229	1.7413	392.8917	2186	61.8229	1.7413	570.0157
2187	61.8489	1.7406	304.573	2187	61.8489	1.7406	433.5066	2187	61.8489	1.7406	355.2172	2187	61.8489	1.7406	531.7046
2188	61.8749	1.7399	273.625	2188	61.8749	1.7399	401.3996	2188	61.8749	1.7399	380.8498	2188	61.8749	1.7399	556.7006
2189	61.9009	1.7393	289.7589	2189	61.9009	1.7393	418.3109	2189	61.9009	1.7393	364.9221	2189	61.9009	1.7393	540.0093
2190	61.9269	1.7386	311.6287	2190	61.9269	1.7386	440.9582	2190	61.9269	1.7386	359.3621	2190	61.9269	1.7386	533.6857
2191	61.9529	1.738	296.272	2191	61.9529	1.738	426.3789	2191	61.9529	1.738	397.1979	2191	61.9529	1.738	570.7578

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2192	61.9789	1.7373	288.7733	2192	61.9789	1.7373	419.6577	2192	61.9789	1.7373	386.3409	2192	61.9789	1.7373	559.1372
2193	62.0049	1.7367	276.3314	2193	62.0049	1.7367	407.9933	2193	62.0049	1.7367	377.966	2193	62.0049	1.7367	549.9987
2194	62.0309	1.736	270.8984	2194	62.0309	1.736	403.3377	2194	62.0309	1.736	373.5672	2194	62.0309	1.736	544.8363
2195	62.0569	1.7353	304.1661	2195	62.0569	1.7353	437.3829	2195	62.0569	1.7353	376.9446	2195	62.0569	1.7353	547.4501
2196	62.0829	1.7347	306.9029	2196	62.0829	1.7347	440.8972	2196	62.0829	1.7347	400.656	2196	62.0829	1.7347	570.3979
2197	62.1089	1.734	295.9089	2197	62.1089	1.734	430.6806	2197	62.1089	1.734	361.964	2197	62.1089	1.734	530.9422
2198	62.1349	1.7334	273.0566	2198	62.1349	1.7334	408.6058	2198	62.1349	1.7334	336.0114	2198	62.1349	1.7334	504.226
2199	62.1609	1.7327	277.5285	2199	62.1609	1.7327	413.8552	2199	62.1609	1.7327	374.5167	2199	62.1609	1.7327	541.9676
2200	62.1869	1.7321	274.0664	2200	62.1869	1.7321	411.1705	2200	62.1869	1.7321	407.7054	2200	62.1869	1.7321	574.3928
2201	62.2129	1.7314	283.4603	2201	62.2129	1.7314	421.3419	2201	62.2129	1.7314	387.6921	2201	62.2129	1.7314	553.6158
2202	62.2389	1.7308	287.4006	2202	62.2389	1.7308	426.0596	2202	62.2389	1.7308	411.0009	2202	62.2389	1.7308	576.161
2203	62.2649	1.7301	297.7279	2203	62.2649	1.7301	437.1644	2203	62.2649	1.7301	406.7101	2203	62.2649	1.7301	571.1066
2204	62.2909	1.7295	267.3858	2204	62.2909	1.7295	407.5998	2204	62.2909	1.7295	375.0731	2204	62.2909	1.7295	538.7059
2205	62.3169	1.7288	255.8153	2205	62.3169	1.7288	396.8067	2205	62.3169	1.7288	380.6558	2205	62.3169	1.7288	543.5251
2206	62.3429	1.7282	280.5951	2206	62.3429	1.7282	422.364	2206	62.3429	1.7282	387.1999	2206	62.3429	1.7282	549.3056
2207	62.3689	1.7275	280.7823	2207	62.3689	1.7275	423.3287	2207	62.3689	1.7275	399.3097	2207	62.3689	1.7275	560.6517
2208	62.3949	1.7269	269.8226	2208	62.3949	1.7269	413.1465	2208	62.3949	1.7269	359.4516	2208	62.3949	1.7269	520.03
2209	62.4209	1.7262	296.7155	2209	62.4209	1.7262	440.8168	2209	62.4209	1.7262	373.4232	2209	62.4209	1.7262	533.2379
2210	62.4469	1.7256	291.6715	2210	62.4469	1.7256	436.5503	2210	62.4469	1.7256	326.7039	2210	62.4469	1.7256	485.755
2211	62.4729	1.7249	264.8501	2211	62.4729	1.7249	410.5064	2211	62.4729	1.7249	327.0079	2211	62.4729	1.7249	485.2955
2212	62.4989	1.7243	283.8135	2212	62.4989	1.7243	430.2472	2212	62.4989	1.7243	363.2863	2212	62.4989	1.7243	520.8102
2213	62.5249	1.7237	286.5813	2213	62.5249	1.7237	433.7924	2213	62.5249	1.7237	449.2301	2213	62.5249	1.7237	605.9904
2214	62.5509	1.723	281.7176	2214	62.5509	1.723	429.7062	2214	62.5509	1.723	394.2899	2214	62.5509	1.723	550.2866
2215	62.5769	1.7224	273.625	2215	62.5769	1.7224	422.3912	2215	62.5769	1.7224	380.8498	2215	62.5769	1.7224	536.0829
2216	62.6029	1.7217	256.0772	2216	62.6029	1.7217	404.5752	2216	62.6029	1.7217	441.5514	2216	62.6029	1.7217	597.7612
2217	62.6289	1.7211	281.4896	2217	62.6289	1.7211	429.7194	2217	62.6289	1.7211	386.0698	2217	62.6289	1.7211	543.2562
2218	62.6549	1.7204	259.1113	2218	62.6549	1.7204	407.0729	2218	62.6549	1.7204	405.796	2218	62.6549	1.7204	563.959
2219	62.6809	1.7198	291.0619	2219	62.6809	1.7198	438.7554	2219	62.6809	1.7198	386.9979	2219	62.6809	1.7198	546.1376
2220	62.7069	1.7192	290.5923	2220	62.7069	1.7192	438.0176	2220	62.7069	1.7192	394.7255	2220	62.7069	1.7192	554.8419
2221	62.7329	1.7185	235.4098	2221	62.7329	1.7185	382.5669	2221	62.7329	1.7185	377.3743	2221	62.7329	1.7185	538.4673
2222	62.7589	1.7179	228.3355	2222	62.7589	1.7179	375.2245	2222	62.7589	1.7179	434.6482	2222	62.7589	1.7179	596.7179
2223	62.7849	1.7172	317.9298	2223	62.7849	1.7172	464.5506	2223	62.7849	1.7172	394.0364	2223	62.7849	1.7172	557.0827
2224	62.8109	1.7166	280.2239	2224	62.8109	1.7166	426.5765	2224	62.8109	1.7166	379.6641	2224	62.8109	1.7166	543.6871
2225	62.8369	1.716	264.8561	2225	62.8369	1.716	410.9405	2225	62.8369	1.716	397.5896	2225	62.8369	1.716	562.5892
2226	62.8629	1.7153	254.9548	2226	62.8629	1.7153	400.771	2226	62.8629	1.7153	339.8811	2226	62.8629	1.7153	505.8574
2227	62.8889	1.7147	290.971	2227	62.8889	1.7147	436.5191	2227	62.8889	1.7147	401.6073	2227	62.8889	1.7147	568.5603

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2228	62.9149	1.7141	279.3682	2228	62.9149	1.7141	424.6481	2228	62.9149	1.7141	356.4994	2228	62.9149	1.7141	524.4289
2229	62.9409	1.7134	285.1333	2229	62.9409	1.7134	430.1451	2229	62.9409	1.7134	354.5594	2229	62.9409	1.7134	523.4657
2230	62.9669	1.7128	295.0885	2230	62.9669	1.7128	439.8321	2230	62.9669	1.7128	328.504	2230	62.9669	1.7128	498.3869
2231	62.9929	1.7121	297.3979	2231	62.9929	1.7121	441.8733	2231	62.9929	1.7121	381.7774	2231	62.9929	1.7121	552.637
2232	63.0189	1.7115	289.1591	2232	63.0189	1.7115	433.3663	2232	63.0189	1.7115	300.2372	2232	63.0189	1.7115	472.0734
2233	63.0449	1.7109	266.7249	2233	63.0449	1.7109	410.6639	2233	63.0449	1.7109	327.0058	2233	63.0449	1.7109	499.8187
2234	63.0709	1.7102	259.1115	2234	63.0709	1.7102	402.7824	2234	63.0709	1.7102	353.455	2234	63.0709	1.7102	527.2445
2235	63.0969	1.7096	262.7653	2235	63.0969	1.7096	406.168	2235	63.0969	1.7096	377.0738	2235	63.0969	1.7096	551.84
2236	63.1229	1.709	268.8075	2236	63.1229	1.709	411.9421	2236	63.1229	1.709	344.0154	2236	63.1229	1.709	519.7583
2237	63.1489	1.7084	287.2225	2237	63.1489	1.7084	430.0888	2237	63.1489	1.7084	345.0456	2237	63.1489	1.7084	521.765
2238	63.1749	1.7077	271.306	2238	63.1749	1.7077	413.9042	2238	63.1749	1.7077	363.9882	2238	63.1749	1.7077	541.6843
2239	63.2009	1.7071	288.8994	2239	63.2009	1.7071	431.2295	2239	63.2009	1.7071	357.8003	2239	63.2009	1.7071	536.4731
2240	63.2269	1.7065	267.4986	2240	63.2269	1.7065	409.5605	2240	63.2269	1.7065	323.7751	2240	63.2269	1.7065	503.4245
2241	63.2529	1.7058	243.1769	2241	63.2529	1.7058	384.9706	2241	63.2529	1.7058	347.6587	2241	63.2529	1.7058	528.2848
2242	63.2789	1.7052	273.625	2242	63.2789	1.7052	415.1505	2242	63.2789	1.7052	380.8498	2242	63.2789	1.7052	562.4526
2243	63.3049	1.7046	283.3163	2243	63.3049	1.7046	423.7373	2243	63.3049	1.7046	351.5414	2243	63.3049	1.7046	531.5348
2244	63.3309	1.704	287.4048	2244	63.3309	1.704	426.7215	2244	63.3309	1.704	353.269	2244	63.3309	1.704	531.6531
2245	63.3569	1.7033	275.8347	2245	63.3569	1.7033	414.0469	2245	63.3569	1.7033	383.4597	2245	63.3569	1.7033	560.2344
2246	63.3829	1.7027	229.1495	2246	63.3829	1.7027	366.2573	2246	63.3829	1.7027	351.0919	2246	63.3829	1.7027	526.2573
2247	63.4089	1.7021	238.2907	2247	63.4089	1.7021	374.2941	2247	63.4089	1.7021	346.4475	2247	63.4089	1.7021	520.0034
2248	63.4349	1.7015	267.4209	2248	63.4349	1.7015	402.3198	2248	63.4349	1.7015	352.0534	2248	63.4349	1.7015	524
2249	63.4609	1.7008	267.1746	2249	63.4609	1.7008	400.9691	2249	63.4609	1.7008	348.1052	2249	63.4609	1.7008	518.4425
2250	63.4869	1.7002	277.3205	2250	63.4869	1.7002	410.0105	2250	63.4869	1.7002	385.6189	2250	63.4869	1.7002	554.3468
2251	63.5129	1.6996	249.9975	2251	63.5129	1.6996	381.5831	2251	63.5129	1.6996	409.6053	2251	63.5129	1.6996	576.7239
2252	63.5389	1.699	271.0894	2252	63.5389	1.699	401.5706	2252	63.5389	1.699	375.5904	2252	63.5389	1.699	541.0996
2253	63.5649	1.6983	270.9733	2253	63.5649	1.6983	400.3501	2253	63.5649	1.6983	378.4051	2253	63.5649	1.6983	542.3049
2254	63.5909	1.6977	235.9247	2254	63.5909	1.6977	364.197	2254	63.5909	1.6977	371.3572	2254	63.5909	1.6977	533.6478
2255	63.6169	1.6971	260.3061	2255	63.6169	1.6971	387.474	2255	63.6169	1.6971	360.4134	2255	63.6169	1.6971	521.0945
2256	63.6429	1.6965	287.9384	2256	63.6429	1.6965	414.0018	2256	63.6429	1.6965	356.5516	2256	63.6429	1.6965	515.6234
2257	63.6689	1.6959	276.6583	2257	63.6689	1.6959	401.6173	2257	63.6689	1.6959	349.3845	2257	63.6689	1.6959	506.8469
2258	63.6949	1.6952	280.2531	2258	63.6949	1.6952	404.1077	2258	63.6949	1.6952	396.1832	2258	63.6949	1.6952	552.0362
2259	63.7209	1.6946	292.2272	2259	63.7209	1.6946	414.9773	2259	63.7209	1.6946	398.7922	2259	63.7209	1.6946	553.0359
2260	63.7469	1.694	253.1953	2260	63.7469	1.694	374.841	2260	63.7469	1.694	392.8331	2260	63.7469	1.694	545.4674
2261	63.7729	1.6934	279.7181	2261	63.7729	1.6934	400.2594	2261	63.7729	1.6934	405.1262	2261	63.7729	1.6934	556.1512
2262	63.7989	1.6928	281.9644	2262	63.7989	1.6928	401.4012	2262	63.7989	1.6928	399.6646	2262	63.7989	1.6928	549.0802
2263	63.8249	1.6921	271.5639	2263	63.8249	1.6921	389.8963	2263	63.8249	1.6921	390.7475	2263	63.8249	1.6921	538.5538

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2264	63.8509	1.6915	285.5886	2264	63.8509	1.6915	402.8166	2264	63.8509	1.6915	398.0825	2264	63.8509	1.6915	544.2795
2265	63.8769	1.6909	272.0142	2265	63.8769	1.6909	388.1377	2265	63.8769	1.6909	413.8435	2265	63.8769	1.6909	558.4312
2266	63.9029	1.6903	274.0791	2266	63.9029	1.6903	389.0982	2266	63.9029	1.6903	400.5075	2266	63.9029	1.6903	543.4857
2267	63.9289	1.6897	285.5693	2267	63.9289	1.6897	399.4839	2267	63.9289	1.6897	390.8563	2267	63.9289	1.6897	532.2252
2268	63.9549	1.6891	267.9679	2268	63.9549	1.6891	380.7781	2268	63.9549	1.6891	389.1172	2268	63.9549	1.6891	528.8767
2269	63.9809	1.6885	273.625	2269	63.9809	1.6885	385.3308	2269	63.9809	1.6885	380.8498	2269	63.9809	1.6885	519
2270	64.0069	1.6878	280.1848	2270	64.0069	1.6878	391.9515	2270	64.0069	1.6878	398.6326	2270	64.0069	1.6878	537.4801
2271	64.0329	1.6872	265.5543	2271	64.0329	1.6872	377.382	2271	64.0329	1.6872	420.3136	2271	64.0329	1.6872	559.8584
2272	64.0589	1.6866	275.1085	2272	64.0589	1.6866	386.9971	2272	64.0589	1.6866	401.3002	2272	64.0589	1.6866	541.5422
2273	64.0849	1.686	273.0063	2273	64.0849	1.686	384.9559	2273	64.0849	1.686	395.6924	2273	64.0849	1.686	536.6317
2274	64.1109	1.6854	274.3883	2274	64.1109	1.6854	386.3989	2274	64.1109	1.6854	437.1218	2274	64.1109	1.6854	578.7584
2275	64.1369	1.6848	279.1374	2275	64.1369	1.6848	391.2089	2275	64.1369	1.6848	472.7673	2275	64.1369	1.6848	615.1012
2276	64.1629	1.6842	277.5246	2276	64.1629	1.6842	389.6571	2276	64.1629	1.6842	488.1152	2276	64.1629	1.6842	631.1464
2277	64.1889	1.6836	288.7199	2277	64.1889	1.6836	400.9133	2277	64.1889	1.6836	472.0982	2277	64.1889	1.6836	615.8267
2278	64.2149	1.683	283.6289	2278	64.2149	1.683	395.8833	2278	64.2149	1.683	474.7698	2278	64.2149	1.683	619.1956
2279	64.2409	1.6823	297.831	2279	64.2409	1.6823	410.1463	2279	64.2409	1.6823	494.7754	2279	64.2409	1.6823	639.8984
2280	64.2669	1.6817	284.6238	2280	64.2669	1.6817	397.0001	2280	64.2669	1.6817	472.6313	2280	64.2669	1.6817	618.4516
2281	64.2929	1.6811	267.6845	2281	64.2929	1.6811	380.1217	2281	64.2929	1.6811	456.2813	2281	64.2929	1.6811	602.7989
2282	64.3189	1.6805	291.1171	2282	64.3189	1.6805	403.6152	2282	64.3189	1.6805	417.6261	2282	64.3189	1.6805	564.841
2283	64.3449	1.6799	277.5155	2283	64.3449	1.6799	390.0746	2283	64.3449	1.6799	382.2986	2283	64.3449	1.6799	530.2108
2284	64.3709	1.6793	291.1592	2284	64.3709	1.6793	403.7792	2284	64.3709	1.6793	377.0335	2284	64.3709	1.6793	525.6429
2285	64.3969	1.6787	293.6191	2285	64.3969	1.6787	406.3001	2285	64.3969	1.6787	405.5425	2285	64.3969	1.6787	554.8493
2286	64.4229	1.6781	275.1556	2286	64.4229	1.6781	387.8975	2286	64.4229	1.6781	415.6525	2286	64.4229	1.6781	565.6566
2287	64.4489	1.6775	252.9616	2287	64.4489	1.6775	365.7646	2287	64.4489	1.6775	387.7808	2287	64.4489	1.6775	538.4821
2288	64.4749	1.6769	275.1371	2288	64.4749	1.6769	388.001	2288	64.4749	1.6769	398.5236	2288	64.4749	1.6769	549.9222
2289	64.5009	1.6763	296.4171	2289	64.5009	1.6763	409.3419	2289	64.5009	1.6763	371.1173	2289	64.5009	1.6763	523.2132
2290	64.5269	1.6757	268.9085	2290	64.5269	1.6757	381.8943	2290	64.5269	1.6757	368.7977	2290	64.5269	1.6757	521.5909
2291	64.5529	1.6751	246.7389	2291	64.5529	1.6751	359.7857	2291	64.5529	1.6751	368.3946	2291	64.5529	1.6751	521.8851
2292	64.5789	1.6745	280.1603	2292	64.5789	1.6745	393.268	2292	64.5789	1.6745	378.079	2292	64.5789	1.6745	532.2667
2293	64.6049	1.6739	292.188	2293	64.6049	1.6739	405.3566	2293	64.6049	1.6739	432.5962	2293	64.6049	1.6739	587.4813
2294	64.6309	1.6733	313.354	2294	64.6309	1.6733	426.5836	2294	64.6309	1.6733	381.1913	2294	64.6309	1.6733	536.7736
2295	64.6569	1.6727	278.7094	2295	64.6569	1.6727	392	2295	64.6569	1.6727	372.8647	2295	64.6569	1.6727	529.1443
2296	64.6829	1.6721	273.625	2296	64.6829	1.6721	386.9766	2296	64.6829	1.6721	380.8498	2296	64.6829	1.6721	537.8267
2297	64.7089	1.6715	256.7028	2297	64.7089	1.6715	369.5632	2297	64.7089	1.6715	386.6457	2297	64.7089	1.6715	541.5974
2298	64.7349	1.6709	261.8855	2298	64.7349	1.6709	374.2548	2298	64.7349	1.6709	374.4441	2298	64.7349	1.6709	527.3707
2299	64.7609	1.6703	291.4832	2299	64.7609	1.6703	403.3614	2299	64.7609	1.6703	366.4172	2299	64.7609	1.6703	517.3186

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2300	64.7869	1.6697	307.3875	2300	64.7869	1.6697	418.7746	2300	64.7869	1.6697	415.2556	2300	64.7869	1.6697	564.1319
2301	64.8129	1.6691	278.9593	2301	64.8129	1.6691	389.8553	2301	64.8129	1.6691	421.0765	2301	64.8129	1.6691	567.9276
2302	64.8389	1.6685	270.9456	2302	64.8389	1.6685	381.3504	2302	64.8389	1.6685	420.8749	2302	64.8389	1.6685	565.7009
2303	64.8649	1.6679	282.0583	2303	64.8649	1.6679	391.9721	2303	64.8649	1.6679	438.5825	2303	64.8649	1.6679	581.3832
2304	64.8909	1.6673	299.5554	2304	64.8909	1.6673	408.9781	2304	64.8909	1.6673	434.9023	2304	64.8909	1.6673	575.6779
2305	64.9169	1.6667	276.3733	2305	64.9169	1.6667	385.3048	2305	64.9169	1.6667	334.4742	2305	64.9169	1.6667	473.2246
2306	64.9429	1.6661	272.1722	2306	64.9429	1.6661	380.6127	2306	64.9429	1.6661	352.857	2306	64.9429	1.6661	489.5823
2307	64.9689	1.6655	269.6931	2307	64.9689	1.6655	377.6424	2307	64.9689	1.6655	373.7302	2307	64.9689	1.6655	508.4303
2308	64.9949	1.6649	268.5252	2308	64.9949	1.6649	375.9834	2308	64.9949	1.6649	389.2754	2308	64.9949	1.6649	521.9503
2309	65.0209	1.6643	280.1127	2309	65.0209	1.6643	387.0798	2309	65.0209	1.6643	411.6743	2309	65.0209	1.6643	542.3241
2310	65.0469	1.6637	307.3614	2310	65.0469	1.6637	413.8375	2310	65.0469	1.6637	384.6678	2310	65.0469	1.6637	513.2925
2311	65.0729	1.6632	297.5257	2311	65.0729	1.6632	403.5106	2311	65.0729	1.6632	425.3918	2311	65.0729	1.6632	551.9912
2312	65.0989	1.6626	310.4267	2312	65.0989	1.6626	415.9205	2312	65.0989	1.6626	371.5131	2312	65.0989	1.6626	496.0875
2313	65.1249	1.662	246.9945	2313	65.1249	1.662	351.9972	2313	65.1249	1.662	403.7776	2313	65.1249	1.662	526.3267
2314	65.1509	1.6614	309.0958	2314	65.1509	1.6614	413.6074	2314	65.1509	1.6614	440.9342	2314	65.1509	1.6614	561.4581
2315	65.1769	1.6608	283.9351	2315	65.1769	1.6608	387.9556	2315	65.1769	1.6608	413.541	2315	65.1769	1.6608	532.0398
2316	65.2029	1.6602	306.3945	2316	65.2029	1.6602	409.9239	2316	65.2029	1.6602	415.1812	2316	65.2029	1.6602	531.6548
2317	65.2289	1.6596	271.9817	2317	65.2289	1.6596	375.02	2317	65.2289	1.6596	374.3303	2317	65.2289	1.6596	488.7788
2318	65.2549	1.659	273.5131	2318	65.2549	1.659	376.0603	2318	65.2549	1.659	415.1394	2318	65.2549	1.659	527.5627
2319	65.2809	1.6584	279.9442	2319	65.2809	1.6584	382.0003	2319	65.2809	1.6584	472.5958	2319	65.2809	1.6584	582.994
2320	65.3069	1.6579	282.4155	2320	65.3069	1.6579	383.9804	2320	65.3069	1.6579	427.0972	2320	65.3069	1.6579	535.4702
2321	65.3329	1.6573	265.2811	2321	65.3329	1.6573	366.3549	2321	65.3329	1.6573	416.8888	2321	65.3329	1.6573	523.2366
2322	65.3589	1.6567	279.9727	2322	65.3589	1.6567	380.5554	2322	65.3589	1.6567	407.033	2322	65.3589	1.6567	511.3557
2323	65.3849	1.6561	302.038	2323	65.3849	1.6561	402.1296	2323	65.3849	1.6561	380.8498	2323	65.3849	1.6561	483.1473
2324	65.4109	1.6555	258.7253	2324	65.4109	1.6555	358.3258	2324	65.4109	1.6555	375.9647	2324	65.4109	1.6555	479.1485
2325	65.4369	1.6549	302.9796	2325	65.4369	1.6549	402.089	2325	65.4369	1.6549	451.118	2325	65.4369	1.6549	555.188
2326	65.4629	1.6543	287.7683	2326	65.4629	1.6543	386.3866	2326	65.4629	1.6543	391.7583	2326	65.4629	1.6543	496.7145
2327	65.4889	1.6538	273.9823	2327	65.4889	1.6538	372.1095	2327	65.4889	1.6538	393.5237	2327	65.4889	1.6538	499.366
2328	65.5149	1.6532	256.9691	2328	65.5149	1.6532	354.6051	2328	65.5149	1.6532	396.004	2328	65.5149	1.6532	502.7325
2329	65.5409	1.6526	319.8191	2329	65.5409	1.6526	416.9641	2329	65.5409	1.6526	407.9979	2329	65.5409	1.6526	515.6126
2330	65.5669	1.652	299.7257	2330	65.5669	1.652	396.3796	2330	65.5669	1.652	408.4991	2330	65.5669	1.652	517
2331	65.5929	1.6514	301.2425	2331	65.5929	1.6514	397.4053	2331	65.5929	1.6514	424.353	2331	65.5929	1.6514	533.7401
2332	65.6189	1.6508	282.2922	2332	65.6189	1.6508	377.9639	2332	65.6189	1.6508	403.9483	2332	65.6189	1.6508	514.2216
2333	65.6449	1.6503	293.5989	2333	65.6449	1.6503	388.7794	2333	65.6449	1.6503	394.6732	2333	65.6449	1.6503	505.8327
2334	65.6709	1.6497	288.6489	2334	65.6709	1.6497	383.3384	2334	65.6709	1.6497	329.1074	2334	65.6709	1.6497	441.1531
2335	65.6969	1.6491	286.1189	2335	65.6969	1.6491	380.3173	2335	65.6969	1.6491	359.1366	2335	65.6969	1.6491	472.0685

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2336	65.7229	1.6485	284.6299	2336	65.7229	1.6485	378.3371	2336	65.7229	1.6485	397.7769	2336	65.7229	1.6485	511.595
2337	65.7489	1.6479	281.4978	2337	65.7489	1.6479	374.7139	2337	65.7489	1.6479	398.3666	2337	65.7489	1.6479	513.0709
2338	65.7749	1.6474	306.4346	2338	65.7749	1.6474	399.1597	2338	65.7749	1.6474	384.2355	2338	65.7749	1.6474	499.826
2339	65.8009	1.6468	286.3106	2339	65.8009	1.6468	378.5446	2339	65.8009	1.6468	427.8224	2339	65.8009	1.6468	544.2991
2340	65.8269	1.6462	285.7995	2340	65.8269	1.6462	377.5423	2340	65.8269	1.6462	408.5503	2340	65.8269	1.6462	525.9132
2341	65.8529	1.6456	312.767	2341	65.8529	1.6456	404.0187	2341	65.8529	1.6456	417.7331	2341	65.8529	1.6456	535.9822
2342	65.8789	1.6451	297.082	2342	65.8789	1.6451	387.8426	2342	65.8789	1.6451	363.1993	2342	65.8789	1.6451	482.3346
2343	65.9049	1.6445	311.3043	2343	65.9049	1.6445	401.5738	2343	65.9049	1.6445	390.698	2343	65.9049	1.6445	510.7194
2344	65.9309	1.6439	281.3703	2344	65.9309	1.6439	371.1486	2344	65.9309	1.6439	415.3734	2344	65.9309	1.6439	536.281
2345	65.9569	1.6433	275.6499	2345	65.9569	1.6433	364.9372	2345	65.9569	1.6433	438.9862	2345	65.9569	1.6433	560.7801
2346	65.9829	1.6428	297.9739	2346	65.9829	1.6428	386.77	2346	65.9829	1.6428	371.3653	2346	65.9829	1.6428	494.0454
2347	66.0089	1.6422	289.082	2347	66.0089	1.6422	377.3871	2347	66.0089	1.6422	371.6035	2347	66.0089	1.6422	495.1698
2348	66.0349	1.6416	273.9251	2348	66.0349	1.6416	361.7391	2348	66.0349	1.6416	391.5209	2348	66.0349	1.6416	515.9733
2349	66.0609	1.641	282.6189	2349	66.0609	1.641	369.9418	2349	66.0609	1.641	390.4466	2349	66.0609	1.641	515.7853
2350	66.0869	1.6405	273.625	2350	66.0869	1.6405	360.4568	2350	66.0869	1.6405	380.8498	2350	66.0869	1.6405	507.0747
2351	66.1129	1.6399	279.2117	2351	66.1129	1.6399	366.287	2351	66.1129	1.6399	372.872	2351	66.1129	1.6399	500.5869
2352	66.1389	1.6393	287.3718	2352	66.1389	1.6393	374.6908	2352	66.1389	1.6393	400.7388	2352	66.1389	1.6393	529.9437
2353	66.1649	1.6388	306.3322	2353	66.1649	1.6388	393.8947	2353	66.1649	1.6388	381.8293	2353	66.1649	1.6388	512.5244
2354	66.1909	1.6382	297.567	2354	66.1909	1.6382	385.3732	2354	66.1909	1.6382	358.5921	2354	66.1909	1.6382	490.7772
2355	66.2169	1.6376	273.8059	2355	66.2169	1.6376	361.8557	2355	66.2169	1.6376	371.0408	2355	66.2169	1.6376	504.716
2356	66.2429	1.637	273.9356	2356	66.2429	1.637	362.229	2356	66.2429	1.637	391.4947	2356	66.2429	1.637	526.66
2357	66.2689	1.6365	307.1246	2357	66.2689	1.6365	395.6616	2357	66.2689	1.6365	405.4447	2357	66.2689	1.6365	542.1
2358	66.2949	1.6359	311.3431	2358	66.2949	1.6359	400.1237	2358	66.2949	1.6359	376.3573	2358	66.2949	1.6359	514.5027
2359	66.3209	1.6353	307.1984	2359	66.3209	1.6353	396.2226	2359	66.3209	1.6353	373.668	2359	66.3209	1.6353	513.3035
2360	66.3469	1.6348	283.0332	2360	66.3469	1.6348	372.301	2360	66.3469	1.6348	403.8604	2360	66.3469	1.6348	544.986
2361	66.3729	1.6342	288.4076	2361	66.3729	1.6342	377.919	2361	66.3729	1.6342	399.6329	2361	66.3729	1.6342	542.2485
2362	66.3989	1.6336	298.9368	2362	66.3989	1.6336	388.6919	2362	66.3989	1.6336	385.1739	2362	66.3989	1.6336	529.2796
2363	66.4249	1.6331	291.7472	2363	66.4249	1.6331	381.7458	2363	66.4249	1.6331	387.4761	2363	66.4249	1.6331	533.0719
2364	66.4509	1.6325	311.3491	2364	66.4509	1.6325	401.5913	2364	66.4509	1.6325	382.1634	2364	66.4509	1.6325	529.2493
2365	66.4769	1.6319	298.0669	2365	66.4769	1.6319	388.5528	2365	66.4769	1.6319	384.7544	2365	66.4769	1.6319	533.3303
2366	66.5029	1.6314	288.8177	2366	66.5029	1.6314	379.5471	2366	66.5029	1.6314	388.7313	2366	66.5029	1.6314	538.7973
2367	66.5289	1.6308	296.7407	2367	66.5289	1.6308	387.7137	2367	66.5289	1.6308	392.8256	2367	66.5289	1.6308	544.3817
2368	66.5549	1.6302	285.644	2368	66.5549	1.6302	376.8607	2368	66.5549	1.6302	405.635	2368	66.5549	1.6302	558.6811
2369	66.5809	1.6297	307.7563	2369	66.5809	1.6297	399.2166	2369	66.5809	1.6297	428.1042	2369	66.5809	1.6297	582.6404
2370	66.6069	1.6291	318.4853	2370	66.6069	1.6291	410.1892	2370	66.6069	1.6291	463.7373	2370	66.6069	1.6291	619.7636
2371	66.6329	1.6286	279.7809	2371	66.6329	1.6286	371.7283	2371	66.6329	1.6286	519.2803	2371	66.6329	1.6286	676.7967

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2372	66.6589	1.628	265.2938	2372	66.6589	1.628	357.4849	2372	66.6589	1.628	621.0166	2372	66.6589	1.628	780.023
2373	66.6849	1.6274	287.1734	2373	66.6849	1.6274	379.6081	2373	66.6849	1.6274	711.8623	2373	66.6849	1.6274	872.3588
2374	66.7109	1.6269	284.8721	2374	66.7109	1.6269	377.5504	2374	66.7109	1.6269	773.183	2374	66.7109	1.6269	935.1696
2375	66.7369	1.6263	283.4127	2375	66.7369	1.6263	376.3346	2375	66.7369	1.6263	810.8562	2375	66.7369	1.6263	974.3328
2376	66.7629	1.6258	304.3999	2376	66.7629	1.6258	397.5654	2376	66.7629	1.6258	762.7925	2376	66.7629	1.6258	927.7591
2377	66.7889	1.6252	308.6865	2377	66.7889	1.6252	402.0956	2377	66.7889	1.6252	703.8998	2377	66.7889	1.6252	870.3566
2378	66.8149	1.6246	295.4412	2378	66.8149	1.6246	389.0939	2378	66.8149	1.6246	688.7355	2378	66.8149	1.6246	856.6823
2379	66.8409	1.6241	288.1527	2379	66.8409	1.6241	382.049	2379	66.8409	1.6241	697.9451	2379	66.8409	1.6241	867.382
2380	66.8669	1.6235	300.6962	2380	66.8669	1.6235	394.8362	2380	66.8669	1.6235	699.7246	2380	66.8669	1.6235	870.6516
2381	66.8929	1.623	281.4702	2381	66.8929	1.623	375.8537	2381	66.8929	1.623	651.6454	2381	66.8929	1.623	824.0625
2382	66.9189	1.6224	293.8728	2382	66.9189	1.6224	388.4999	2382	66.9189	1.6224	612.9673	2382	66.9189	1.6224	786.8744
2383	66.9449	1.6218	295.5104	2383	66.9449	1.6218	390.3812	2383	66.9449	1.6218	556.9976	2383	66.9449	1.6218	732.3948
2384	66.9709	1.6213	290.0993	2384	66.9709	1.6213	385.2136	2384	66.9709	1.6213	508.2268	2384	66.9709	1.6213	685.114
2385	66.9969	1.6207	275.2734	2385	66.9969	1.6207	370.6314	2385	66.9969	1.6207	505.4425	2385	66.9969	1.6207	683.8198
2386	67.0229	1.6202	284.0211	2386	67.0229	1.6202	379.6227	2386	67.0229	1.6202	439.4679	2386	67.0229	1.6202	619.3353
2387	67.0489	1.6196	267.5278	2387	67.0489	1.6196	363.373	2387	67.0489	1.6196	448.0794	2387	67.0489	1.6196	629.4369
2388	67.0749	1.6191	279.0546	2388	67.0749	1.6191	375.1434	2388	67.0749	1.6191	439.967	2388	67.0749	1.6191	622.8145
2389	67.1009	1.6185	296.6949	2389	67.1009	1.6185	393.0273	2389	67.1009	1.6185	391.1349	2389	67.1009	1.6185	575.4725
2390	67.1269	1.618	266.563	2390	67.1269	1.618	363.139	2390	67.1269	1.618	403.4856	2390	67.1269	1.618	589.3133
2391	67.1529	1.6174	279.3233	2391	67.1529	1.6174	376.1429	2391	67.1529	1.6174	379.9679	2391	67.1529	1.6174	567.2856
2392	67.1789	1.6169	281.4208	2392	67.1789	1.6169	378.484	2392	67.1789	1.6169	361.4698	2392	67.1789	1.6169	550.2776
2393	67.2049	1.6163	270.9472	2393	67.2049	1.6163	368.254	2393	67.2049	1.6163	348.7419	2393	67.2049	1.6163	539.0398
2394	67.2309	1.6157	293.7115	2394	67.2309	1.6157	391.262	2394	67.2309	1.6157	363.5096	2394	67.2309	1.6157	555.2976
2395	67.2569	1.6152	310.952	2395	67.2569	1.6152	408.746	2395	67.2569	1.6152	350.7458	2395	67.2569	1.6152	544.0238
2396	67.2829	1.6146	273.1706	2396	67.2829	1.6146	371.2083	2396	67.2829	1.6146	396.2458	2396	67.2829	1.6146	591.0139
2397	67.3089	1.6141	305.6592	2397	67.3089	1.6141	403.9404	2397	67.3089	1.6141	399.5991	2397	67.3089	1.6141	595.8573
2398	67.3349	1.6135	308.5547	2398	67.3349	1.6135	407.0795	2398	67.3349	1.6135	374.1445	2398	67.3349	1.6135	571.8928
2399	67.3609	1.613	285.295	2399	67.3609	1.613	384.0634	2399	67.3609	1.613	382.4285	2399	67.3609	1.613	581.6668
2400	67.3869	1.6124	297.3092	2400	67.3869	1.6124	396.3212	2400	67.3869	1.6124	362.8967	2400	67.3869	1.6124	563.6251
2401	67.4129	1.6119	305.4194	2401	67.4129	1.6119	404.6751	2401	67.4129	1.6119	354.1031	2401	67.4129	1.6119	556.3215
2402	67.4389	1.6114	269.9746	2402	67.4389	1.6114	369.4738	2402	67.4389	1.6114	359.9472	2402	67.4389	1.6114	563.6558
2403	67.4649	1.6108	292.424	2403	67.4649	1.6108	392.1669	2403	67.4649	1.6108	417.3022	2403	67.4649	1.6108	622.5008
2404	67.4909	1.6103	273.625	2404	67.4909	1.6103	373.6115	2404	67.4909	1.6103	380.8498	2404	67.4909	1.6103	587.5385
2405	67.5169	1.6097	255.1564	2405	67.5169	1.6097	354.4043	2405	67.5169	1.6097	441.2585	2405	67.5169	1.6097	646.4851
2406	67.5429	1.6092	282.5858	2406	67.5429	1.6092	381.0951	2406	67.5429	1.6092	407.3347	2406	67.5429	1.6092	611.0993
2407	67.5689	1.6086	291.626	2407	67.5689	1.6086	389.3966	2407	67.5689	1.6086	497.5705	2407	67.5689	1.6086	699.873

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2408	67.5949	1.6081	304.3088	2408	67.5949	1.6081	401.3408	2408	67.5949	1.6081	507.6399	2408	67.5949	1.6081	708.4804
2409	67.6209	1.6075	317.8863	2409	67.6209	1.6075	414.1796	2409	67.6209	1.6075	587.7985	2409	67.6209	1.6075	787.177
2410	67.6469	1.607	278.9312	2410	67.6469	1.607	374.486	2410	67.6469	1.607	667.551	2410	67.6469	1.607	865.4675
2411	67.6729	1.6064	286.5403	2411	67.6729	1.6064	381.3564	2411	67.6729	1.6064	865.3317	2411	67.6729	1.6064	1061.7861
2412	67.6989	1.6059	311.7678	2412	67.6989	1.6059	405.8453	2412	67.6989	1.6059	1139.3896	2412	67.6989	1.6059	1334.382
2413	67.7249	1.6054	310.7286	2413	67.7249	1.6054	404.0674	2413	67.7249	1.6054	1314.8998	2413	67.7249	1.6054	1508.4301
2414	67.7509	1.6048	313.0323	2414	67.7509	1.6048	405.6326	2414	67.7509	1.6048	1506.1554	2414	67.7509	1.6048	1698.2236
2415	67.7769	1.6043	324.5191	2415	67.7769	1.6043	416.3807	2415	67.7769	1.6043	1344.729	2415	67.7769	1.6043	1535.3352
2416	67.8029	1.6037	332.538	2416	67.8029	1.6037	423.661	2416	67.8029	1.6037	1289.0141	2416	67.8029	1.6037	1478.1583
2417	67.8289	1.6032	325.0595	2417	67.8289	1.6032	415.4439	2417	67.8289	1.6032	1192.2069	2417	67.8289	1.6032	1379.889
2418	67.8549	1.6026	340.891	2418	67.8549	1.6026	430.5367	2418	67.8549	1.6026	1190.4035	2418	67.8549	1.6026	1376.6237
2419	67.8809	1.6021	316.164	2419	67.8809	1.6021	405.0711	2419	67.8809	1.6021	1226.3446	2419	67.8809	1.6021	1411.1027
2420	67.9069	1.6016	325.8133	2420	67.9069	1.6016	413.9818	2420	67.9069	1.6016	1240.6776	2420	67.9069	1.6016	1423.9737
2421	67.9329	1.601	331.5104	2421	67.9329	1.601	418.9403	2421	67.9329	1.601	1095.9343	2421	67.9329	1.601	1277.7683
2422	67.9589	1.6005	300.0305	2422	67.9589	1.6005	386.7217	2422	67.9589	1.6005	949.8867	2422	67.9589	1.6005	1130.2587
2423	67.9849	1.5999	319.4115	2423	67.9849	1.5999	405.3641	2423	67.9849	1.5999	887.093	2423	67.9849	1.5999	1066.0029
2424	68.0109	1.5994	333.2437	2424	68.0109	1.5994	418.4577	2424	68.0109	1.5994	773.4745	2424	68.0109	1.5994	950.9224
2425	68.0369	1.5989	348.7501	2425	68.0369	1.5989	433.2254	2425	68.0369	1.5989	745.3567	2425	68.0369	1.5989	921.3426
2426	68.0629	1.5983	309.9103	2426	68.0629	1.5983	393.6471	2426	68.0629	1.5983	626.2942	2426	68.0629	1.5983	800.8181
2427	68.0889	1.5978	342.3571	2427	68.0889	1.5978	425.3552	2427	68.0889	1.5978	637.5801	2427	68.0889	1.5978	810.6418
2428	68.1149	1.5973	304.4037	2428	68.1149	1.5973	386.6632	2428	68.1149	1.5973	574.2614	2428	68.1149	1.5973	745.8611
2429	68.1409	1.5967	301.4791	2429	68.1409	1.5967	383	2429	68.1409	1.5967	530.7893	2429	68.1409	1.5967	700.927
2430	68.1669	1.5962	302.2178	2430	68.1669	1.5962	383	2430	68.1669	1.5962	469.9055	2430	68.1669	1.5962	638.5812
2431	68.1929	1.5957	273.625	2431	68.1929	1.5957	353.6686	2431	68.1929	1.5957	453.2316	2431	68.1929	1.5957	620.4452
2432	68.2189	1.5951	329.8848	2432	68.2189	1.5951	409.7657	2432	68.2189	1.5951	454.1273	2432	68.2189	1.5951	619.8789
2433	68.2449	1.5946	322.6402	2433	68.2449	1.5946	402.3583	2433	68.2449	1.5946	433.1169	2433	68.2449	1.5946	597.4064
2434	68.2709	1.5941	267.1828	2434	68.2709	1.5941	346.7381	2434	68.2709	1.5941	420.0047	2434	68.2709	1.5941	582.8322
2435	68.2969	1.5935	301.0644	2435	68.2969	1.5935	380.457	2435	68.2969	1.5935	462.9407	2435	68.2969	1.5935	624.3061
2436	68.3229	1.593	299.5387	2436	68.3229	1.593	378.7686	2436	68.3229	1.593	451.9554	2436	68.3229	1.593	611.8588
2437	68.3489	1.5925	275.5419	2437	68.3489	1.5925	354.609	2437	68.3489	1.5925	436.2899	2437	68.3489	1.5925	594.7313
2438	68.3749	1.5919	299.7737	2438	68.3749	1.5919	378.6781	2438	68.3749	1.5919	433.3819	2438	68.3749	1.5919	590.3613
2439	68.4009	1.5914	304.6395	2439	68.4009	1.5914	383.3811	2439	68.4009	1.5914	450.6717	2439	68.4009	1.5914	606.189
2440	68.4269	1.5909	283.6334	2440	68.4269	1.5909	362.2123	2440	68.4269	1.5909	439.9542	2440	68.4269	1.5909	594.0094
2441	68.4529	1.5903	317.2746	2441	68.4529	1.5903	395.6907	2441	68.4529	1.5903	453.1989	2441	68.4529	1.5903	605.7921
2442	68.4789	1.5898	305.9155	2442	68.4789	1.5898	384.1689	2442	68.4789	1.5898	466.6657	2442	68.4789	1.5898	617.7968
2443	68.5049	1.5893	259.112	2443	68.5049	1.5893	337.2026	2443	68.5049	1.5893	477.2587	2443	68.5049	1.5893	626.9279

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2444	68.5309	1.5887	282.7846	2444	68.5309	1.5887	360.7124	2444	68.5309	1.5887	516.5054	2444	68.5309	1.5887	664.7124
2445	68.5569	1.5882	330.9808	2445	68.5569	1.5882	408.7459	2445	68.5569	1.5882	475.2609	2445	68.5569	1.5882	622.006
2446	68.5829	1.5877	311.5778	2446	68.5829	1.5877	389.1802	2446	68.5829	1.5877	497.1967	2446	68.5829	1.5877	642.4797
2447	68.6089	1.5872	310.0513	2447	68.6089	1.5872	387.4909	2447	68.6089	1.5872	480.7859	2447	68.6089	1.5872	624.6069
2448	68.6349	1.5866	321.6448	2448	68.6349	1.5866	398.9217	2448	68.6349	1.5866	489.365	2448	68.6349	1.5866	631.7239
2449	68.6609	1.5861	307.1302	2449	68.6609	1.5861	384.2443	2449	68.6609	1.5861	452.6485	2449	68.6609	1.5861	593.5454
2450	68.6869	1.5856	277.6388	2450	68.6869	1.5856	354.5902	2450	68.6869	1.5856	418.7578	2450	68.6869	1.5856	558.1927
2451	68.7129	1.585	290.3036	2451	68.7129	1.585	367.0923	2451	68.7129	1.585	405.433	2451	68.7129	1.585	543.4058
2452	68.7389	1.5845	293.5695	2452	68.7389	1.5845	370.1954	2452	68.7389	1.5845	434.7904	2452	68.7389	1.5845	571.3012
2453	68.7649	1.584	283.1609	2453	68.7649	1.584	359.6241	2453	68.7649	1.584	471.738	2453	68.7649	1.584	606.7867
2454	68.7909	1.5835	280.3602	2454	68.7909	1.5835	356.6606	2454	68.7909	1.5835	435.8489	2454	68.7909	1.5835	569.4356
2455	68.8169	1.5829	282.1637	2455	68.8169	1.5829	358.3014	2455	68.8169	1.5829	416.1288	2455	68.8169	1.5829	548.2535
2456	68.8429	1.5824	272.7728	2456	68.8429	1.5824	348.7477	2456	68.8429	1.5824	400.755	2456	68.8429	1.5824	531.4176
2457	68.8689	1.5819	273.4963	2457	68.8689	1.5819	349.3085	2457	68.8689	1.5819	380.4441	2457	68.8689	1.5819	509.6447
2458	68.8949	1.5814	273.625	2458	68.8949	1.5814	349.2744	2458	68.8949	1.5814	380.8498	2458	68.8949	1.5814	508.5883
2459	68.9209	1.5809	300.6419	2459	68.9209	1.5809	376.9392	2459	68.9209	1.5809	400.5528	2459	68.9209	1.5809	526.6641
2460	68.9469	1.5803	296.2136	2460	68.9469	1.5803	373.1589	2460	68.9469	1.5803	405.5051	2460	68.9469	1.5803	529.9892
2461	68.9729	1.5798	275.0864	2461	68.9729	1.5798	352.6796	2461	68.9729	1.5798	396.6404	2461	68.9729	1.5798	519.4972
2462	68.9989	1.5793	275.9901	2462	68.9989	1.5793	354.2311	2462	68.9989	1.5793	407.7202	2462	68.9989	1.5793	528.9497
2463	69.0249	1.5788	284.2529	2463	69.0249	1.5788	363.1418	2463	69.0249	1.5788	403.9722	2463	69.0249	1.5788	523.5745
2464	69.0509	1.5782	295.884	2464	69.0509	1.5782	375.4209	2464	69.0509	1.5782	411.4281	2464	69.0509	1.5782	529.4032
2465	69.0769	1.5777	305.6755	2465	69.0769	1.5777	385.8603	2465	69.0769	1.5777	409.5566	2465	69.0769	1.5777	525.9044
2466	69.1029	1.5772	302.7518	2466	69.1029	1.5772	383.5845	2466	69.1029	1.5772	408.652	2466	69.1029	1.5772	523.3725
2467	69.1289	1.5767	292.2031	2467	69.1289	1.5767	373.6837	2467	69.1289	1.5767	375.7817	2467	69.1289	1.5767	488.875
2468	69.1549	1.5762	295.2188	2468	69.1549	1.5762	377.3473	2468	69.1549	1.5762	374.0098	2468	69.1549	1.5762	485.4759
2469	69.1809	1.5756	284.823	2469	69.1809	1.5756	367.5994	2469	69.1809	1.5756	412.7672	2469	69.1809	1.5756	522.606
2470	69.2069	1.5751	271.0887	2470	69.2069	1.5751	354.513	2470	69.2069	1.5751	417.7847	2470	69.2069	1.5751	525.9963
2471	69.2329	1.5746	286.2262	2471	69.2329	1.5746	370.2984	2471	69.2329	1.5746	410.0527	2471	69.2329	1.5746	516.6371
2472	69.2589	1.5741	296.3518	2472	69.2589	1.5741	381.0719	2472	69.2589	1.5741	413.1652	2472	69.2589	1.5741	518.1223
2473	69.2849	1.5736	291.7436	2473	69.2849	1.5736	377.1116	2473	69.2849	1.5736	407.2585	2473	69.2849	1.5736	510.5884
2474	69.3109	1.5731	287.5975	2474	69.3109	1.5731	373.6135	2474	69.3109	1.5731	374.8945	2474	69.3109	1.5731	476.5971
2475	69.3369	1.5725	298.9036	2475	69.3369	1.5725	385.5674	2475	69.3369	1.5725	370.4219	2475	69.3369	1.5725	470.4972
2476	69.3629	1.572	285.4947	2476	69.3629	1.572	372.8065	2476	69.3629	1.572	365.8589	2476	69.3629	1.572	464.307
2477	69.3889	1.5715	259.7152	2477	69.3889	1.5715	347.6749	2477	69.3889	1.5715	367.2317	2477	69.3889	1.5715	464.0526
2478	69.4149	1.571	268.0552	2478	69.4149	1.571	356.6628	2478	69.4149	1.571	410.4808	2478	69.4149	1.571	505.6744
2479	69.4409	1.5705	274.0092	2479	69.4409	1.5705	363.2647	2479	69.4409	1.5705	414.1689	2479	69.4409	1.5705	507.7353

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2480	69.4669	1.57	297.5124	2480	69.4669	1.57	387.4158	2480	69.4669	1.57	407.3479	2480	69.4669	1.57	499.287
2481	69.4929	1.5695	294.1653	2481	69.4929	1.5695	384.7166	2481	69.4929	1.5695	421.2265	2481	69.4929	1.5695	511.5384
2482	69.5189	1.5689	288.7771	2482	69.5189	1.5689	379.9763	2482	69.5189	1.5689	407.4874	2482	69.5189	1.5689	496.1721
2483	69.5449	1.5684	286.0854	2483	69.5449	1.5684	377.9325	2483	69.5449	1.5684	406.6713	2483	69.5449	1.5684	493.7287
2484	69.5709	1.5679	265.6014	2484	69.5709	1.5679	358.0964	2484	69.5709	1.5679	393.156	2484	69.5709	1.5679	478.5861
2485	69.5969	1.5674	273.625	2485	69.5969	1.5674	366.768	2485	69.5969	1.5674	380.8498	2485	69.5969	1.5674	464.6527
2486	69.6229	1.5669	284.3989	2486	69.6229	1.5669	376.9035	2486	69.6229	1.5669	415.8658	2486	69.6229	1.5669	500.1086
2487	69.6489	1.5664	266.7956	2487	69.6489	1.5664	358.6618	2487	69.6489	1.5664	387.9895	2487	69.6489	1.5664	472.6723
2488	69.6749	1.5659	290.3884	2488	69.6749	1.5659	381.6163	2488	69.6749	1.5659	371.9284	2488	69.6749	1.5659	457.0512
2489	69.7009	1.5654	290.3371	2489	69.7009	1.5654	380.9266	2489	69.7009	1.5654	386.6771	2489	69.7009	1.5654	472.24
2490	69.7269	1.5649	289.9376	2490	69.7269	1.5649	379.8888	2490	69.7269	1.5649	383.7621	2490	69.7269	1.5649	469.7649
2491	69.7529	1.5643	293.1322	2491	69.7529	1.5643	382.4449	2491	69.7529	1.5643	390.9809	2491	69.7529	1.5643	477.4237
2492	69.7789	1.5638	253.7735	2492	69.7789	1.5638	342.4479	2492	69.7789	1.5638	401.2206	2492	69.7789	1.5638	488.1034
2493	69.8049	1.5633	262.1936	2493	69.8049	1.5633	350.2296	2493	69.8049	1.5633	442.522	2493	69.8049	1.5633	529.8447
2494	69.8309	1.5628	292.9543	2494	69.8309	1.5628	380.352	2494	69.8309	1.5628	401.7863	2494	69.8309	1.5628	489.549
2495	69.8569	1.5623	282.3928	2495	69.8569	1.5623	369.1521	2495	69.8569	1.5623	423.6908	2495	69.8569	1.5623	511.8935
2496	69.8829	1.5618	304.3432	2496	69.8829	1.5618	390.4642	2496	69.8829	1.5618	401.6257	2496	69.8829	1.5618	490.2684
2497	69.9089	1.5613	276.8797	2497	69.9089	1.5613	362.3623	2497	69.9089	1.5613	402.4267	2497	69.9089	1.5613	491.5094
2498	69.9349	1.5608	275.2922	2498	69.9349	1.5608	360.1365	2498	69.9349	1.5608	406.9803	2498	69.9349	1.5608	496.503
2499	69.9609	1.5603	282.9401	2499	69.9609	1.5603	367.146	2499	69.9609	1.5603	387.6773	2499	69.9609	1.5603	477.6399
2500	69.9869	1.5598	273.5163	2500	69.9869	1.5598	357.0838	2500	69.9869	1.5598	392.8381	2500	69.9869	1.5598	483.2407
2501	70.0129	1.5593	294.3447	2501	70.0129	1.5593	377.2739	2501	70.0129	1.5593	363.5173	2501	70.0129	1.5593	454.3599
2502	70.0389	1.5588	310.3127	2502	70.0389	1.5588	392.6035	2502	70.0389	1.5588	376.8286	2502	70.0389	1.5588	468.1112
2503	70.0649	1.5583	299.8243	2503	70.0649	1.5583	381.4767	2503	70.0649	1.5583	404.6028	2503	70.0649	1.5583	496.3253
2504	70.0909	1.5578	289.1028	2504	70.0909	1.5578	370.1169	2504	70.0909	1.5578	374.582	2504	70.0909	1.5578	466.7446
2505	70.1169	1.5573	249.88	2505	70.1169	1.5573	330.2557	2505	70.1169	1.5573	411.489	2505	70.1169	1.5573	504.0916
2506	70.1429	1.5567	274.7783	2506	70.1429	1.5567	354.5156	2506	70.1429	1.5567	420.7246	2506	70.1429	1.5567	513.7671
2507	70.1689	1.5562	252.8083	2507	70.1689	1.5562	331.9073	2507	70.1689	1.5562	381.5595	2507	70.1689	1.5562	475.042
2508	70.1949	1.5557	276.0431	2508	70.1949	1.5557	354.5037	2508	70.1949	1.5557	400.3376	2508	70.1949	1.5557	494.2601
2509	70.2209	1.5552	259.1777	2509	70.2209	1.5552	337	2509	70.2209	1.5552	358.4969	2509	70.2209	1.5552	452.8594
2510	70.2469	1.5547	264.0148	2510	70.2469	1.5547	341.1987	2510	70.2469	1.5547	399.7336	2510	70.2469	1.5547	494.5361
2511	70.2729	1.5542	297.6981	2511	70.2729	1.5542	374.2437	2511	70.2729	1.5542	370.708	2511	70.2729	1.5542	465.9505
2512	70.2989	1.5537	273.625	2512	70.2989	1.5537	349.5322	2512	70.2989	1.5537	380.8498	2512	70.2989	1.5537	476.5322
2513	70.3249	1.5532	290.0437	2513	70.3249	1.5532	366.3008	2513	70.3249	1.5532	398.7149	2513	70.3249	1.5532	494.6544
2514	70.3509	1.5527	294.1111	2514	70.3509	1.5527	370.7181	2514	70.3509	1.5527	417.0409	2514	70.3509	1.5527	513.2375
2515	70.3769	1.5522	301.4968	2515	70.3769	1.5522	378.4536	2515	70.3769	1.5522	390.4393	2515	70.3769	1.5522	486.8929

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2516	70.4029	1.5517	258.2385	2516	70.4029	1.5517	335.5452	2516	70.4029	1.5517	371.0622	2516	70.4029	1.5517	467.7728
2517	70.4289	1.5512	270.0537	2517	70.4289	1.5512	347.7102	2517	70.4289	1.5512	367.3817	2517	70.4289	1.5512	464.3495
2518	70.4549	1.5507	288.5329	2518	70.4549	1.5507	366.5394	2518	70.4549	1.5507	403.0843	2518	70.4549	1.5507	500.3091
2519	70.4809	1.5502	271.2077	2519	70.4809	1.5502	349.564	2519	70.4809	1.5502	376.1265	2519	70.4809	1.5502	473.6083
2520	70.5069	1.5497	306.1674	2520	70.5069	1.5497	384.8736	2520	70.5069	1.5497	351.129	2520	70.5069	1.5497	448.8679
2521	70.5329	1.5492	284.0358	2521	70.5329	1.5492	363.0919	2521	70.5329	1.5492	328.1001	2521	70.5329	1.5492	426.0961
2522	70.5589	1.5488	263.876	2522	70.5589	1.5488	343.282	2522	70.5589	1.5488	390.8446	2522	70.5589	1.5488	489.0976
2523	70.5849	1.5483	289.5956	2523	70.5849	1.5483	369.3514	2523	70.5849	1.5483	370.9944	2523	70.5849	1.5483	469.5045
2524	70.6109	1.5478	283.1319	2524	70.6109	1.5478	363.2376	2524	70.6109	1.5478	339.3191	2524	70.6109	1.5478	438.0862
2525	70.6369	1.5473	281.5883	2525	70.6369	1.5473	362.0439	2525	70.6369	1.5473	381.958	2525	70.6369	1.5473	480.9821
2526	70.6629	1.5468	261.3241	2526	70.6629	1.5468	342.1296	2526	70.6629	1.5468	393.1809	2526	70.6629	1.5468	492.4621
2527	70.6889	1.5463	258.9084	2527	70.6889	1.5463	340.0637	2527	70.6889	1.5463	366.3093	2527	70.6889	1.5463	465.8476
2528	70.7149	1.5458	276.0958	2528	70.7149	1.5458	357.601	2528	70.7149	1.5458	386.4375	2528	70.7149	1.5458	486.2328
2529	70.7409	1.5453	301.8889	2529	70.7409	1.5453	383.744	2529	70.7409	1.5453	397.112	2529	70.7409	1.5453	497.1644
2530	70.7669	1.5448	285.6646	2530	70.7669	1.5448	367.8696	2530	70.7669	1.5448	336.9536	2530	70.7669	1.5448	437.263
2531	70.7929	1.5443	234.1322	2531	70.7929	1.5443	316.687	2531	70.7929	1.5443	377.9533	2531	70.7929	1.5443	478.5198
2532	70.8189	1.5438	270.6558	2532	70.8189	1.5438	353.5605	2532	70.8189	1.5438	379.6297	2532	70.8189	1.5438	480.4533
2533	70.8449	1.5433	245.9357	2533	70.8449	1.5433	329.1903	2533	70.8449	1.5433	354.3702	2533	70.8449	1.5433	455.4509
2534	70.8709	1.5428	264.8	2534	70.8709	1.5428	348.4045	2534	70.8709	1.5428	382.7351	2534	70.8709	1.5428	484.0728
2535	70.8969	1.5423	279.1855	2535	70.8969	1.5423	363.1398	2535	70.8969	1.5423	408.828	2535	70.8969	1.5423	510.4228
2536	70.9229	1.5418	273.0729	2536	70.9229	1.5418	357.3771	2536	70.9229	1.5418	396.0554	2536	70.9229	1.5418	497.9072
2537	70.9489	1.5413	268.8347	2537	70.9489	1.5413	353.4888	2537	70.9489	1.5413	375.3127	2537	70.9489	1.5413	477.4216
2538	70.9749	1.5409	258.0703	2538	70.9749	1.5409	343.0743	2538	70.9749	1.5409	392.3127	2538	70.9749	1.5409	494.6786
2539	71.0009	1.5404	273.625	2539	71.0009	1.5404	358.9789	2539	71.0009	1.5404	380.8498	2539	71.0009	1.5404	483.4728
2540	71.0269	1.5399	251.4931	2540	71.0269	1.5399	337.1664	2540	71.0269	1.5399	341.7085	2540	71.0269	1.5399	445.2861
2541	71.0529	1.5394	285.6734	2541	71.0529	1.5394	371.6662	2541	71.0529	1.5394	329.2783	2541	71.0529	1.5394	433.8105
2542	71.0789	1.5389	286.2382	2542	71.0789	1.5389	372.5505	2542	71.0789	1.5389	329.0881	2542	71.0789	1.5389	434.5749
2543	71.1049	1.5384	287.2558	2543	71.1049	1.5384	373.8877	2543	71.1049	1.5384	361.215	2543	71.1049	1.5384	467.6564
2544	71.1309	1.5379	289.5839	2544	71.1309	1.5379	376.5352	2544	71.1309	1.5379	367.3012	2544	71.1309	1.5379	474.6972
2545	71.1569	1.5374	276.8485	2545	71.1569	1.5374	364.1193	2545	71.1569	1.5374	391.4108	2545	71.1569	1.5374	499.7614
2546	71.1829	1.5369	232.0303	2546	71.1829	1.5369	319.6207	2546	71.1829	1.5369	382.244	2546	71.1829	1.5369	491.5492
2547	71.2089	1.5365	255.7201	2547	71.2089	1.5365	343.63	2547	71.2089	1.5365	402.3026	2547	71.2089	1.5365	512.5624
2548	71.2349	1.536	302.9829	2548	71.2349	1.536	391.2123	2548	71.2349	1.536	367.1104	2548	71.2349	1.536	478.3247
2549	71.2609	1.5355	293.1932	2549	71.2609	1.5355	381.742	2549	71.2609	1.5355	353.421	2549	71.2609	1.5355	465.59
2550	71.2869	1.535	285.5478	2550	71.2869	1.535	374.4162	2550	71.2869	1.535	379.3672	2550	71.2869	1.535	492.4907
2551	71.3129	1.5345	238.3377	2551	71.3129	1.5345	327.5255	2551	71.3129	1.5345	344.9381	2551	71.3129	1.5345	459.0163

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2552	71.3389	1.534	249.8395	2552	71.3389	1.534	339.3469	2552	71.3389	1.534	346.9907	2552	71.3389	1.534	462.0234
2553	71.3649	1.5335	282.4875	2553	71.3649	1.5335	372.3144	2553	71.3649	1.5335	334.985	2553	71.3649	1.5335	450.9724
2554	71.3909	1.5331	281.4962	2554	71.3909	1.5331	371.6426	2554	71.3909	1.5331	362.1561	2554	71.3909	1.5331	479.0981
2555	71.4169	1.5326	279.168	2555	71.4169	1.5326	369.6339	2555	71.4169	1.5326	380.7619	2555	71.4169	1.5326	498.6585
2556	71.4429	1.5321	291.8884	2556	71.4429	1.5321	382.6738	2556	71.4429	1.5321	376.2576	2556	71.4429	1.5321	495.1087
2557	71.4689	1.5316	281.291	2557	71.4689	1.5316	372.3959	2557	71.4689	1.5316	378.9418	2557	71.4689	1.5316	498.7476
2558	71.4949	1.5311	289.1792	2558	71.4949	1.5311	380.6035	2558	71.4949	1.5311	393.1849	2558	71.4949	1.5311	513.9453
2559	71.5209	1.5306	295.5435	2559	71.5209	1.5306	387.2873	2559	71.5209	1.5306	406.7104	2559	71.5209	1.5306	528.4253
2560	71.5469	1.5302	285.6304	2560	71.5469	1.5302	377.6938	2560	71.5469	1.5302	416.419	2560	71.5469	1.5302	539.0885
2561	71.5729	1.5297	262.0502	2561	71.5729	1.5297	354.4331	2561	71.5729	1.5297	418.178	2561	71.5729	1.5297	541.8021
2562	71.5989	1.5292	264.0228	2562	71.5989	1.5292	356.7252	2562	71.5989	1.5292	412.8872	2562	71.5989	1.5292	537.4659
2563	71.6249	1.5287	258.9218	2563	71.6249	1.5287	351.9438	2563	71.6249	1.5287	441.3164	2563	71.6249	1.5287	566.8498
2564	71.6509	1.5282	292.6226	2564	71.6509	1.5282	385.964	2564	71.6509	1.5282	454.9746	2564	71.6509	1.5282	581.4625
2565	71.6769	1.5278	299.4955	2565	71.6769	1.5278	393.1564	2565	71.6769	1.5278	473.2826	2565	71.6769	1.5278	600.7251
2566	71.7029	1.5273	273.625	2566	71.7029	1.5273	367.6054	2566	71.7029	1.5273	599.7202	2566	71.7029	1.5273	728.1173
2567	71.7289	1.5268	276.6662	2567	71.7289	1.5268	369.9334	2567	71.7289	1.5268	734.1152	2567	71.7289	1.5268	863.467
2568	71.7549	1.5263	287.2114	2568	71.7549	1.5263	379.7653	2568	71.7549	1.5263	875.3529	2568	71.7549	1.5263	1005.6592
2569	71.7809	1.5258	302.5505	2569	71.7809	1.5258	394.3911	2569	71.7809	1.5258	936.1637	2569	71.7809	1.5258	1067.4246
2570	71.8069	1.5254	305.2282	2570	71.8069	1.5254	396.3555	2570	71.8069	1.5254	889.4185	2570	71.8069	1.5254	1021.634
2571	71.8329	1.5249	298.586	2571	71.8329	1.5249	389	2571	71.8329	1.5249	835.35	2571	71.8329	1.5249	968.5201
2572	71.8589	1.5244	273.3406	2572	71.8589	1.5244	363.0414	2572	71.8589	1.5244	792.5285	2572	71.8589	1.5244	926.6532
2573	71.8849	1.5239	285.8815	2573	71.8849	1.5239	374.8689	2573	71.8849	1.5239	762.8067	2573	71.8849	1.5239	897.886
2574	71.9109	1.5235	299.5895	2574	71.9109	1.5235	387.8636	2574	71.9109	1.5235	761.5233	2574	71.9109	1.5235	897.5572
2575	71.9369	1.523	287.6799	2575	71.9369	1.523	375.2408	2575	71.9369	1.523	803.4922	2575	71.9369	1.523	940.4807
2576	71.9629	1.5225	293.2483	2576	71.9629	1.5225	380.0959	2576	71.9629	1.5225	793.8006	2576	71.9629	1.5225	931.7437
2577	71.9889	1.522	256.7801	2577	71.9889	1.522	342.9144	2577	71.9889	1.522	711.7643	2577	71.9889	1.522	850.662
2578	72.0149	1.5215	245.6025	2578	72.0149	1.5215	331.0235	2578	72.0149	1.5215	645.4032	2578	72.0149	1.5215	785.2555
2579	72.0409	1.5211	248.8279	2579	72.0409	1.5211	333.5357	2579	72.0409	1.5211	614.4376	2579	72.0409	1.5211	755.2445
2580	72.0669	1.5206	251.0344	2580	72.0669	1.5206	335.029	2580	72.0669	1.5206	571.0534	2580	72.0669	1.5206	712.8149
2581	72.0929	1.5201	277.5343	2581	72.0929	1.5201	360.8155	2581	72.0929	1.5201	537.0703	2581	72.0929	1.5201	679.7864
2582	72.1189	1.5197	284.934	2582	72.1189	1.5197	367.502	2582	72.1189	1.5197	546.6687	2582	72.1189	1.5197	690.3394
2583	72.1449	1.5192	271.0936	2583	72.1449	1.5192	352.9483	2583	72.1449	1.5192	594.0843	2583	72.1449	1.5192	738.7096
2584	72.1709	1.5187	272.4442	2584	72.1709	1.5187	353.5856	2584	72.1709	1.5187	603.5323	2584	72.1709	1.5187	749.1122
2585	72.1969	1.5182	267.0662	2585	72.1969	1.5182	347.4943	2585	72.1969	1.5182	592.1984	2585	72.1969	1.5182	738.7329
2586	72.2229	1.5178	277.5308	2586	72.2229	1.5178	357.2456	2586	72.2229	1.5178	562.1426	2586	72.2229	1.5178	709.6317
2587	72.2489	1.5173	291.0231	2587	72.2489	1.5173	370.0247	2587	72.2489	1.5173	547.5563	2587	72.2489	1.5173	696

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2588	72.2749	1.5168	307.8154	2588	72.2749	1.5168	386.1037	2588	72.2749	1.5168	545.2776	2588	72.2749	1.5168	694.6759
2589	72.3009	1.5163	276.4983	2589	72.3009	1.5163	354.0734	2589	72.3009	1.5163	542.9315	2589	72.3009	1.5163	693.2844
2590	72.3269	1.5159	280.2955	2590	72.3269	1.5159	357.1572	2590	72.3269	1.5159	549.0491	2590	72.3269	1.5159	700.3566
2591	72.3529	1.5154	295.3452	2591	72.3529	1.5154	371.4937	2591	72.3529	1.5154	559.5455	2591	72.3529	1.5154	711.8076
2592	72.3789	1.5149	285.2813	2592	72.3789	1.5149	360.7165	2592	72.3789	1.5149	550.2557	2592	72.3789	1.5149	703.4724
2593	72.4049	1.5145	273.625	2593	72.4049	1.5145	348.3469	2593	72.4049	1.5145	510.3862	2593	72.4049	1.5145	664.5575
2594	72.4309	1.514	284.9749	2594	72.4309	1.514	359.285	2594	72.4309	1.514	486.2005	2594	72.4309	1.514	638.9276
2595	72.4569	1.5135	284.6409	2595	72.4569	1.5135	358.5393	2595	72.4569	1.5135	484.0412	2595	72.4569	1.5135	635.324
2596	72.4829	1.5131	294.4539	2596	72.4829	1.5131	367.9406	2596	72.4829	1.5131	490.8107	2596	72.4829	1.5131	640.6493
2597	72.5089	1.5126	276.6273	2597	72.5089	1.5126	349.7022	2597	72.5089	1.5126	456.5165	2597	72.5089	1.5126	604.9109
2598	72.5349	1.5121	301.5552	2598	72.5349	1.5121	374.2183	2598	72.5349	1.5121	487.1954	2598	72.5349	1.5121	634.1456
2599	72.5609	1.5117	296.0768	2599	72.5609	1.5117	368.3283	2599	72.5609	1.5117	490.7038	2599	72.5609	1.5117	636.2097
2600	72.5869	1.5112	299.6819	2600	72.5869	1.5112	371.5215	2600	72.5869	1.5112	525.8134	2600	72.5869	1.5112	669.8751
2601	72.6129	1.5107	270.5925	2601	72.6129	1.5107	342.0204	2601	72.6129	1.5107	555.6865	2601	72.6129	1.5107	698.304
2602	72.6389	1.5103	281.6735	2602	72.6389	1.5103	352.6896	2602	72.6389	1.5103	588.2209	2602	72.6389	1.5103	729.3941
2603	72.6649	1.5098	291.3914	2603	72.6649	1.5098	361.9959	2603	72.6649	1.5098	548.5422	2603	72.6649	1.5098	688.2712
2604	72.6909	1.5093	280.5678	2604	72.6909	1.5093	350.7605	2604	72.6909	1.5093	545.8538	2604	72.6909	1.5093	684.1386
2605	72.7169	1.5089	271.1932	2605	72.7169	1.5089	340.9741	2605	72.7169	1.5089	541.0489	2605	72.7169	1.5089	677.8894
2606	72.7429	1.5084	280.8988	2606	72.7429	1.5084	350.268	2606	72.7429	1.5084	523.8298	2606	72.7429	1.5084	659.2262
2607	72.7689	1.5079	301.9074	2607	72.7689	1.5079	370.8649	2607	72.7689	1.5079	489.7432	2607	72.7689	1.5079	623.6953
2608	72.7949	1.5075	280.5375	2608	72.7949	1.5075	349.0832	2608	72.7949	1.5075	539.4808	2608	72.7949	1.5075	671.9887
2609	72.8209	1.507	264.9326	2609	72.8209	1.507	333.0665	2609	72.8209	1.507	555.4082	2609	72.8209	1.507	686.4719
2610	72.8469	1.5065	283.3319	2610	72.8469	1.5065	351.0541	2610	72.8469	1.5065	561.7436	2610	72.8469	1.5065	691.3631
2611	72.8729	1.5061	253.6149	2611	72.8729	1.5061	320.9253	2611	72.8729	1.5061	516.5628	2611	72.8729	1.5061	644.738
2612	72.8989	1.5056	264.2379	2612	72.8989	1.5056	331.1366	2612	72.8989	1.5056	494.2745	2612	72.8989	1.5056	621.0056
2613	72.9249	1.5052	287.4214	2613	72.9249	1.5052	353.9084	2613	72.9249	1.5052	456.7132	2613	72.9249	1.5052	582
2614	72.9509	1.5047	309.29	2614	72.9509	1.5047	375.3652	2614	72.9509	1.5047	460.8603	2614	72.9509	1.5047	584.7028
2615	72.9769	1.5042	312.1902	2615	72.9769	1.5042	377.8537	2615	72.9769	1.5042	491.9302	2615	72.9769	1.5042	614.3286
2616	73.0029	1.5038	279.3117	2616	73.0029	1.5038	344.5635	2616	73.0029	1.5038	423.4606	2616	73.0029	1.5038	544.4147
2617	73.0289	1.5033	254.5063	2617	73.0289	1.5033	319.3463	2617	73.0289	1.5033	412.4991	2617	73.0289	1.5033	532.009
2618	73.0549	1.5028	262.1381	2618	73.0549	1.5028	326.5663	2618	73.0549	1.5028	371.6691	2618	73.0549	1.5028	489.7347
2619	73.0809	1.5024	250.5226	2619	73.0809	1.5024	314.5391	2619	73.0809	1.5024	422.3473	2619	73.0809	1.5024	538.9687
2620	73.1069	1.5019	273.625	2620	73.1069	1.5019	337.2298	2620	73.1069	1.5019	380.8498	2620	73.1069	1.5019	496.027
2621	73.1329	1.5015	290.3699	2621	73.1329	1.5015	354.097	2621	73.1329	1.5015	384.1868	2621	73.1329	1.5015	498.0862
2622	73.1589	1.501	316.9795	2622	73.1589	1.501	380.8291	2622	73.1589	1.501	409.2265	2622	73.1589	1.501	521.8481
2623	73.1849	1.5005	261.9381	2623	73.1849	1.5005	325.9101	2623	73.1849	1.5005	398.8512	2623	73.1849	1.5005	510.195

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2624	73.2109	1.5001	319.3352	2624	73.2109	1.5001	383.4296	2624	73.2109	1.5001	373.6407	2624	73.2109	1.5001	483.7067
2625	73.2369	1.4996	261.0211	2625	73.2369	1.4996	325.2379	2625	73.2369	1.4996	397.3455	2625	73.2369	1.4996	506.1337
2626	73.2629	1.4992	293.9581	2626	73.2629	1.4992	358.2973	2626	73.2629	1.4992	392.8117	2626	73.2629	1.4992	500.3221
2627	73.2889	1.4987	304.9789	2627	73.2889	1.4987	369.4406	2627	73.2889	1.4987	427.7536	2627	73.2889	1.4987	533.9862
2628	73.3149	1.4983	321.2962	2628	73.3149	1.4983	385.8803	2628	73.3149	1.4983	431.9793	2628	73.3149	1.4983	536.9341
2629	73.3409	1.4978	312.1271	2629	73.3409	1.4978	376.8336	2629	73.3409	1.4978	409.2934	2629	73.3409	1.4978	512.9704
2630	73.3669	1.4973	314.8282	2630	73.3669	1.4973	379.6572	2630	73.3669	1.4973	395.8007	2630	73.3669	1.4973	498.1999
2631	73.3929	1.4969	284.3001	2631	73.3929	1.4969	349.2514	2631	73.3929	1.4969	403.1136	2631	73.3929	1.4969	504.235
2632	73.4189	1.4964	286.2929	2632	73.4189	1.4964	351.3667	2632	73.4189	1.4964	425.7287	2632	73.4189	1.4964	525.5723
2633	73.4449	1.496	297.4181	2633	73.4449	1.496	362.6143	2633	73.4449	1.496	412.6282	2633	73.4449	1.496	511.194
2634	73.4709	1.4955	275.0671	2634	73.4709	1.4955	340.3857	2634	73.4709	1.4955	398.593	2634	73.4709	1.4955	495.8809
2635	73.4969	1.4951	274.153	2635	73.4969	1.4951	339.594	2635	73.4969	1.4951	373.7788	2635	73.4969	1.4951	469.7889
2636	73.5229	1.4946	317.1745	2636	73.5229	1.4946	382.738	2636	73.5229	1.4946	396.9104	2636	73.5229	1.4946	491.6428
2637	73.5489	1.4942	275.3136	2637	73.5489	1.4942	340.9995	2637	73.5489	1.4942	351.0104	2637	73.5489	1.4942	444.465
2638	73.5749	1.4937	267.0266	2638	73.5749	1.4937	332.8349	2638	73.5749	1.4937	397.9276	2638	73.5749	1.4937	490.1044
2639	73.6009	1.4933	274.4942	2639	73.6009	1.4933	340.4249	2639	73.6009	1.4933	402.6761	2639	73.6009	1.4933	493.5751
2640	73.6269	1.4928	306.9195	2640	73.6269	1.4928	372.9727	2640	73.6269	1.4928	391.7829	2640	73.6269	1.4928	481.4041
2641	73.6529	1.4924	275.9825	2641	73.6529	1.4924	342.1581	2641	73.6529	1.4924	418.8368	2641	73.6529	1.4924	507.1802
2642	73.6789	1.4919	268.2925	2642	73.6789	1.4919	334.5905	2642	73.6789	1.4919	392.7398	2642	73.6789	1.4919	479.8053
2643	73.7049	1.4914	279.5739	2643	73.7049	1.4914	345.9942	2643	73.7049	1.4914	374.218	2643	73.7049	1.4914	460.0058
2644	73.7309	1.491	275.4788	2644	73.7309	1.491	342.0216	2644	73.7309	1.491	404.2807	2644	73.7309	1.491	488.7906
2645	73.7569	1.4905	277.1621	2645	73.7569	1.4905	343.8273	2645	73.7569	1.4905	375.7295	2645	73.7569	1.4905	458.9616
2646	73.7829	1.4901	247.2354	2646	73.7829	1.4901	314.023	2646	73.7829	1.4901	379.4009	2646	73.7829	1.4901	461.3552
2647	73.8089	1.4896	273.625	2647	73.8089	1.4896	340.5351	2647	73.8089	1.4896	380.8498	2647	73.8089	1.4896	461.5263
2648	73.8349	1.4892	300.0138	2648	73.8349	1.4892	366.9781	2648	73.8349	1.4892	363.6887	2648	73.8349	1.4892	444.5505
2649	73.8609	1.4887	264.3384	2649	73.8609	1.4887	331.3569	2649	73.8609	1.4887	386.2579	2649	73.8609	1.4887	467.305
2650	73.8869	1.4883	284.0037	2650	73.8869	1.4883	351.0765	2650	73.8869	1.4883	368.8496	2650	73.8869	1.4883	450.082
2651	73.9129	1.4878	283.7544	2651	73.9129	1.4878	350.8815	2651	73.9129	1.4878	382.9956	2651	73.9129	1.4878	464.4133
2652	73.9389	1.4874	281.9947	2652	73.9389	1.4874	349.176	2652	73.9389	1.4874	368.341	2652	73.9389	1.4874	449.9439
2653	73.9649	1.4869	287.1948	2653	73.9649	1.4869	354.4304	2653	73.9649	1.4869	353.0953	2653	73.9649	1.4869	434.8835
2654	73.9909	1.4865	310.3472	2654	73.9909	1.4865	377.6371	2654	73.9909	1.4865	355.7596	2654	73.9909	1.4865	437.7331
2655	74.0169	1.4861	276.6844	2655	74.0169	1.4861	344.0285	2655	74.0169	1.4861	372.4984	2655	74.0169	1.4861	454.6572
2656	74.0429	1.4856	272.3221	2656	74.0429	1.4856	339.7205	2656	74.0429	1.4856	361.9355	2656	74.0429	1.4856	444.2795
2657	74.0689	1.4852	272.4979	2657	74.0689	1.4852	339.9505	2657	74.0689	1.4852	368.6304	2657	74.0689	1.4852	451.1598
2658	74.0949	1.4847	257.9461	2658	74.0949	1.4847	325.453	2658	74.0949	1.4847	362.6466	2658	74.0949	1.4847	445.3612
2659	74.1209	1.4843	269.9822	2659	74.1209	1.4843	337.5433	2659	74.1209	1.4843	360.3655	2659	74.1209	1.4843	443.2655

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2660	74.1469	1.4838	266.2023	2660	74.1469	1.4838	333.8176	2660	74.1469	1.4838	393.5127	2660	74.1469	1.4838	476.598
2661	74.1729	1.4834	273.7113	2661	74.1729	1.4834	341.3809	2661	74.1729	1.4834	392.3151	2661	74.1729	1.4834	475.5855
2662	74.1989	1.4829	299.7924	2662	74.1989	1.4829	367.5163	2662	74.1989	1.4829	390.883	2662	74.1989	1.4829	474.3388
2663	74.2249	1.4825	292.6161	2663	74.2249	1.4825	360.3943	2663	74.2249	1.4825	387.2087	2663	74.2249	1.4825	470.8497
2664	74.2509	1.482	290.5524	2664	74.2509	1.482	358.3848	2664	74.2509	1.482	384.3661	2664	74.2509	1.482	468.1924
2665	74.2769	1.4816	303.2165	2665	74.2769	1.4816	371.1031	2665	74.2769	1.4816	382.8853	2665	74.2769	1.4816	466.8969
2666	74.3029	1.4812	310.9587	2666	74.3029	1.4812	378.8996	2666	74.3029	1.4812	423.3703	2666	74.3029	1.4812	507.5672
2667	74.3289	1.4807	293.2124	2667	74.3289	1.4807	361.2076	2667	74.3289	1.4807	407.7312	2667	74.3289	1.4807	492.1134
2668	74.3549	1.4803	259.8332	2668	74.3549	1.4803	327.8826	2668	74.3549	1.4803	362.7463	2668	74.3549	1.4803	447.3138
2669	74.3809	1.4798	250.1149	2669	74.3809	1.4798	318.2186	2669	74.3809	1.4798	359.7199	2669	74.3809	1.4798	444.4727
2670	74.4069	1.4794	256.4291	2670	74.4069	1.4794	324.587	2670	74.4069	1.4794	356.4749	2670	74.4069	1.4794	441.413
2671	74.4329	1.4789	254.728	2671	74.4329	1.4789	322.9402	2671	74.4329	1.4789	381.788	2671	74.4329	1.4789	466.9113
2672	74.4589	1.4785	258.1969	2672	74.4589	1.4785	326.4633	2672	74.4589	1.4785	404.2134	2672	74.4589	1.4785	489.522
2673	74.4849	1.4781	269.5804	2673	74.4849	1.4781	337.9011	2673	74.4849	1.4781	375.1244	2673	74.4849	1.4781	460.6183
2674	74.5109	1.4776	273.625	2674	74.5109	1.4776	342	2674	74.5109	1.4776	380.8498	2674	74.5109	1.4776	466.529
2675	74.5369	1.4772	272.5058	2675	74.5369	1.4772	340.1288	2675	74.5369	1.4772	379.2028	2675	74.5369	1.4772	465.9158
2676	74.5629	1.4767	280.2863	2676	74.5629	1.4767	347.1573	2676	74.5629	1.4767	373.0511	2676	74.5629	1.4767	460.7979
2677	74.5889	1.4763	277.5467	2677	74.5889	1.4763	343.6658	2677	74.5889	1.4763	397.5413	2677	74.5889	1.4763	486.3219
2678	74.6149	1.4759	259.7568	2678	74.6149	1.4759	325.124	2678	74.6149	1.4759	394.2685	2678	74.6149	1.4759	484.0829
2679	74.6409	1.4754	258.5286	2679	74.6409	1.4754	323.1438	2679	74.6409	1.4754	410.0146	2679	74.6409	1.4754	500.8628
2680	74.6669	1.475	261.4822	2680	74.6669	1.475	325.3454	2680	74.6669	1.475	435.5723	2680	74.6669	1.475	527.4543
2681	74.6929	1.4745	255.8658	2681	74.6929	1.4745	318.9771	2681	74.6929	1.4745	476.1852	2681	74.6929	1.4745	569.1009
2682	74.7189	1.4741	240.6407	2682	74.7189	1.4741	303	2682	74.7189	1.4741	505.0955	2682	74.7189	1.4741	599.045
2683	74.7449	1.4737	263.5321	2683	74.7449	1.4737	325.1394	2683	74.7449	1.4737	542.5381	2683	74.7449	1.4737	637.5215
2684	74.7709	1.4732	280.9772	2684	74.7709	1.4732	341.8325	2684	74.7709	1.4732	544.6405	2684	74.7709	1.4732	640.6576
2685	74.7969	1.4728	265.165	2685	74.7969	1.4728	325.2684	2685	74.7969	1.4728	567.7808	2685	74.7969	1.4728	664.8318
2686	74.8229	1.4724	274.6614	2686	74.8229	1.4724	334.0129	2686	74.8229	1.4724	531.9573	2686	74.8229	1.4724	630.042
2687	74.8489	1.4719	253.539	2687	74.8489	1.4719	312.1385	2687	74.8489	1.4719	548.184	2687	74.8489	1.4719	647.3026
2688	74.8749	1.4715	265.2345	2688	74.8749	1.4715	323.082	2688	74.8749	1.4715	522.8093	2688	74.8749	1.4715	622.9616
2689	74.9009	1.471	273.2734	2689	74.9009	1.471	330.369	2689	74.9009	1.471	482.0759	2689	74.9009	1.471	583.262
2690	74.9269	1.4706	290.9833	2690	74.9269	1.4706	347.3269	2690	74.9269	1.4706	488.5905	2690	74.9269	1.4706	590.8104
2691	74.9529	1.4702	328.5922	2691	74.9529	1.4702	384.1838	2691	74.9529	1.4702	479.8192	2691	74.9529	1.4702	583.0729
2692	74.9789	1.4697	285.1199	2692	74.9789	1.4697	339.9596	2692	74.9789	1.4697	469.2347	2692	74.9789	1.4697	573.5222
2693	75.0049	1.4693	251.9257	2693	75.0049	1.4693	306.0135	2693	75.0049	1.4693	453.5706	2693	75.0049	1.4693	558.8919
2694	75.0309	1.4689	290.8081	2694	75.0309	1.4689	344.1439	2694	75.0309	1.4689	457.6901	2694	75.0309	1.4689	564.0451
2695	75.0569	1.4684	297.4505	2695	75.0569	1.4684	350.0343	2695	75.0569	1.4684	431.949	2695	75.0569	1.4684	539.3379

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2696	75.0829	1.468	282.3233	2696	75.0829	1.468	334.1551	2696	75.0829	1.468	371.8701	2696	75.0829	1.468	480.2927
2697	75.1089	1.4676	305.4391	2697	75.1089	1.4676	356.519	2697	75.1089	1.4676	378.246	2697	75.1089	1.4676	487.7024
2698	75.1349	1.4671	277.9116	2698	75.1349	1.4671	328.2396	2698	75.1349	1.4671	428.8644	2698	75.1349	1.4671	539.3547
2699	75.1609	1.4667	286.084	2699	75.1609	1.4667	335.66	2699	75.1609	1.4667	367.7725	2699	75.1609	1.4667	479.2965
2700	75.1869	1.4663	310.2746	2700	75.1869	1.4663	359.0987	2700	75.1869	1.4663	374.0027	2700	75.1869	1.4663	486.5605
2701	75.2129	1.4658	312.62	2701	75.2129	1.4658	360.6921	2701	75.2129	1.4658	380.8498	2701	75.2129	1.4658	494.4415
2702	75.2389	1.4654	298.2835	2702	75.2389	1.4654	345.6036	2702	75.2389	1.4654	407.4332	2702	75.2389	1.4654	519.6058
2703	75.2649	1.465	273.2419	2703	75.2649	1.465	319.81	2703	75.2649	1.465	361.5474	2703	75.2649	1.465	472.301
2704	75.2909	1.4645	280.0255	2704	75.2909	1.4645	325.8416	2704	75.2909	1.4645	339.7456	2704	75.2909	1.4645	449.0803
2705	75.3169	1.4641	306.1517	2705	75.3169	1.4641	351.2159	2705	75.3169	1.4641	348.6361	2705	75.3169	1.4641	456.5518
2706	75.3429	1.4637	277.4061	2706	75.3429	1.4637	321.7184	2706	75.3429	1.4637	366.9889	2706	75.3429	1.4637	473.4856
2707	75.3689	1.4633	270.8386	2707	75.3689	1.4633	314.3989	2707	75.3689	1.4633	392.824	2707	75.3689	1.4633	497.9017
2708	75.3949	1.4628	276.4725	2708	75.3949	1.4628	319.2809	2708	75.3949	1.4628	396.9553	2708	75.3949	1.4628	500.614
2709	75.4209	1.4624	323.6394	2709	75.4209	1.4624	365.6958	2709	75.4209	1.4624	379.5865	2709	75.4209	1.4624	481.8262
2710	75.4469	1.462	294.1289	2710	75.4469	1.462	335.4334	2710	75.4469	1.462	353.7818	2710	75.4469	1.462	454.6025
2711	75.4729	1.4615	284.9957	2711	75.4729	1.4615	325.5482	2711	75.4729	1.4615	356.723	2711	75.4729	1.4615	456.1247
2712	75.4989	1.4611	298.7028	2712	75.4989	1.4611	338.5033	2712	75.4989	1.4611	338.1379	2712	75.4989	1.4611	436.1206
2713	75.5249	1.4607	302.1366	2713	75.5249	1.4607	341.1851	2713	75.5249	1.4607	370.9752	2713	75.5249	1.4607	467.539
2714	75.5509	1.4603	284.6226	2714	75.5509	1.4603	322.9192	2714	75.5509	1.4603	402.6019	2714	75.5509	1.4603	497.7467
2715	75.5769	1.4598	284.1718	2715	75.5769	1.4598	321.7164	2715	75.5769	1.4598	344.1325	2715	75.5769	1.4598	437.8582
2716	75.6029	1.4594	281.5732	2716	75.6029	1.4594	318.3659	2716	75.6029	1.4594	345.2786	2716	75.6029	1.4594	437.5854
2717	75.6289	1.459	288.0614	2717	75.6289	1.459	324.1021	2717	75.6289	1.459	370.0912	2717	75.6289	1.459	460.9789
2718	75.6549	1.4585	291.3693	2718	75.6549	1.4585	326.6581	2718	75.6549	1.4585	353.5184	2718	75.6549	1.4585	442.9871
2719	75.6809	1.4581	307.4008	2719	75.6809	1.4581	341.9376	2719	75.6809	1.4581	377.0764	2719	75.6809	1.4581	465.1262
2720	75.7069	1.4577	304.789	2720	75.7069	1.4577	338.5738	2720	75.7069	1.4577	351.6247	2720	75.7069	1.4577	438.2554
2721	75.7329	1.4573	240.5921	2721	75.7329	1.4573	273.625	2721	75.7329	1.4573	365.1292	2721	75.7329	1.4573	450.3409
2722	75.7589	1.4568	295.8272	2722	75.7589	1.4568	328.1081	2722	75.7589	1.4568	396.1481	2722	75.7589	1.4568	479.9409
2723	75.7849	1.4564	370.835	2723	75.7849	1.4564	402.364	2723	75.7849	1.4564	356.9739	2723	75.7849	1.4564	439.3477
2724	75.8109	1.456	277.9896	2724	75.8109	1.456	308.7667	2724	75.8109	1.456	369.8244	2724	75.8109	1.456	450.7792
2725	75.8369	1.4556	296.4085	2725	75.8369	1.4556	326.4335	2725	75.8369	1.4556	350.0873	2725	75.8369	1.4556	429.6231
2726	75.8629	1.4551	292.9181	2726	75.8629	1.4551	322.1912	2726	75.8629	1.4551	373.9653	2726	75.8629	1.4551	452.0821
2727	75.8889	1.4547	295.3825	2727	75.8889	1.4547	323.9037	2727	75.8889	1.4547	365.8321	2727	75.8889	1.4547	442.5299
2728	75.9149	1.4543	273.625	2728	75.9149	1.4543	301.3942	2728	75.9149	1.4543	380.8498	2728	75.9149	1.4543	456.1286
2729	75.9409	1.4539	292.4079	2729	75.9409	1.4539	320.5037	2729	75.9409	1.4539	382.5237	2729	75.9409	1.4539	458.864
2730	75.9669	1.4535	299.1101	2730	75.9669	1.4535	327.5324	2730	75.9669	1.4535	401.8837	2730	75.9669	1.4535	479.2854
2731	75.9929	1.453	348.5067	2731	75.9929	1.453	377.2556	2731	75.9929	1.453	416.219	2731	75.9929	1.453	494.6821

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2732	76.0189	1.4526	317.738	2732	76.0189	1.4526	346.8135	2732	76.0189	1.4526	371.3645	2732	76.0189	1.4526	450.889
2733	76.0449	1.4522	329.6593	2733	76.0449	1.4522	359.0613	2733	76.0449	1.4522	370.7678	2733	76.0449	1.4522	451.3538
2734	76.0709	1.4518	303.0354	2734	76.0709	1.4518	332.764	2734	76.0709	1.4518	388.8825	2734	76.0709	1.4518	470.5299
2735	76.0969	1.4513	316.3939	2735	76.0969	1.4513	346.449	2735	76.0969	1.4513	369.3523	2735	76.0969	1.4513	452.0611
2736	76.1229	1.4509	307.4054	2736	76.1229	1.4509	337.7871	2736	76.1229	1.4509	347.1166	2736	76.1229	1.4509	430.8869
2737	76.1489	1.4505	306.9969	2737	76.1489	1.4505	337.7052	2737	76.1489	1.4505	383.2408	2737	76.1489	1.4505	468.0726
2738	76.1749	1.4501	317.92	2738	76.1749	1.4501	348.9549	2738	76.1749	1.4501	390.7922	2738	76.1749	1.4501	476.6854
2739	76.2009	1.4497	285.4953	2739	76.2009	1.4497	316.8567	2739	76.2009	1.4497	381.7178	2739	76.2009	1.4497	468.6724
2740	76.2269	1.4492	297.2373	2740	76.2269	1.4492	328.9253	2740	76.2269	1.4492	383.0982	2740	76.2269	1.4492	471.1142
2741	76.2529	1.4488	303.4242	2741	76.2529	1.4488	335.4388	2741	76.2529	1.4488	378.0451	2741	76.2529	1.4488	467.1225
2742	76.2789	1.4484	329.3547	2742	76.2789	1.4484	361.6959	2742	76.2789	1.4484	395.133	2742	76.2789	1.4484	485.2719
2743	76.3049	1.448	320.2639	2743	76.3049	1.448	352.9316	2743	76.3049	1.448	344.8707	2743	76.3049	1.448	436.071
2744	76.3309	1.4476	308.1742	2744	76.3309	1.4476	341.1685	2744	76.3309	1.4476	369.679	2744	76.3309	1.4476	461.9407
2745	76.3569	1.4472	301.813	2745	76.3569	1.4472	335.1339	2745	76.3569	1.4472	395.1414	2745	76.3569	1.4472	488.4646
2746	76.3829	1.4467	304.1691	2746	76.3829	1.4467	337.8165	2746	76.3829	1.4467	380.296	2746	76.3829	1.4467	474.6806
2747	76.4089	1.4463	327.6275	2747	76.4089	1.4463	361.6015	2747	76.4089	1.4463	392.3886	2747	76.4089	1.4463	487.8346
2748	76.4349	1.4459	299.0132	2748	76.4349	1.4459	333.3138	2748	76.4349	1.4459	406.4141	2748	76.4349	1.4459	502.9215
2749	76.4609	1.4455	328.9182	2749	76.4609	1.4455	363.5453	2749	76.4609	1.4455	404.0299	2749	76.4609	1.4455	501.5988
2750	76.4869	1.4451	309.3126	2750	76.4869	1.4451	344.2663	2750	76.4869	1.4451	424.5254	2750	76.4869	1.4451	523.1558
2751	76.5129	1.4447	314.2758	2751	76.5129	1.4447	349.5561	2751	76.5129	1.4447	394.4824	2751	76.5129	1.4447	494.1741
2752	76.5389	1.4442	341.0988	2752	76.5389	1.4442	376.7056	2752	76.5389	1.4442	383.1732	2752	76.5389	1.4442	483.9264
2753	76.5649	1.4438	351.842	2753	76.5649	1.4438	387.7754	2753	76.5649	1.4438	416.1025	2753	76.5649	1.4438	517.9171
2754	76.5909	1.4434	327.4346	2754	76.5909	1.4434	363.6946	2754	76.5909	1.4434	448.9579	2754	76.5909	1.4434	551.8339
2755	76.6169	1.443	273.625	2755	76.6169	1.443	310.2116	2755	76.6169	1.443	500.8729	2755	76.6169	1.443	604.8104
2756	76.6429	1.4426	275.0393	2756	76.6429	1.4426	311.9148	2756	76.6429	1.4426	580.1046	2756	76.6429	1.4426	685.1035
2757	76.6689	1.4422	297.6106	2757	76.6689	1.4422	334.7749	2757	76.6689	1.4422	656.6935	2757	76.6689	1.4422	762.7538
2758	76.6949	1.4418	329.3164	2758	76.6949	1.4418	366.7696	2758	76.6949	1.4418	841.9381	2758	76.6949	1.4418	949.0599
2759	76.7209	1.4413	337.549	2759	76.7209	1.4413	375.2911	2759	76.7209	1.4413	1007.2035	2759	76.7209	1.4413	1115.3867
2760	76.7469	1.4409	323.3543	2760	76.7469	1.4409	361.3853	2760	76.7469	1.4409	1130.0535	2760	76.7469	1.4409	1239.2981
2761	76.7729	1.4405	332.0419	2761	76.7729	1.4405	370.3618	2761	76.7729	1.4405	1089.4388	2761	76.7729	1.4405	1199.7449
2762	76.7989	1.4401	328.0911	2762	76.7989	1.4401	366.6999	2762	76.7989	1.4401	1015.496	2762	76.7989	1.4401	1126.8635
2763	76.8249	1.4397	318.5077	2763	76.8249	1.4397	357.4054	2763	76.8249	1.4397	960.9471	2763	76.8249	1.4397	1073.376
2764	76.8509	1.4393	330.0923	2764	76.8509	1.4393	369.2788	2764	76.8509	1.4393	900.5202	2764	76.8509	1.4393	1014.0106
2765	76.8769	1.4389	329.3281	2765	76.8769	1.4389	368.8035	2765	76.8769	1.4389	844.6855	2765	76.8769	1.4389	959.2373
2766	76.9029	1.4385	309.2439	2766	76.9029	1.4385	349.0082	2766	76.9029	1.4385	845.3704	2766	76.9029	1.4385	960.9836
2767	76.9289	1.438	304.4962	2767	76.9289	1.438	344.5494	2767	76.9289	1.438	862.1056	2767	76.9289	1.438	978.7802

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2768	76.9549	1.4376	313.0181	2768	76.9549	1.4376	353.3601	2768	76.9549	1.4376	868.5292	2768	76.9549	1.4376	986.2653
2769	76.9809	1.4372	314.2287	2769	76.9809	1.4372	354.8596	2769	76.9809	1.4372	817.4123	2769	76.9809	1.4372	936.2098
2770	77.0069	1.4368	293.174	2770	77.0069	1.4368	334.0938	2770	77.0069	1.4368	736.7314	2770	77.0069	1.4368	856.5904
2771	77.0329	1.4364	288.1573	2771	77.0329	1.4364	329.366	2771	77.0329	1.4364	674.5579	2771	77.0329	1.4364	795.4783
2772	77.0589	1.436	315.1676	2772	77.0589	1.436	356.6651	2772	77.0589	1.436	598.0654	2772	77.0589	1.436	720.0472
2773	77.0849	1.4356	308.9111	2773	77.0849	1.4356	350.6976	2773	77.0849	1.4356	561.397	2773	77.0849	1.4356	684.4403
2774	77.1109	1.4352	300.0327	2774	77.1109	1.4352	342.108	2774	77.1109	1.4352	526.6002	2774	77.1109	1.4352	650.7049
2775	77.1369	1.4348	323.6226	2775	77.1369	1.4348	365.9868	2775	77.1369	1.4348	465.2381	2775	77.1369	1.4348	590.4043
2776	77.1629	1.4344	325.9654	2776	77.1629	1.4344	368.6185	2776	77.1629	1.4344	439.6504	2776	77.1629	1.4344	565.878
2777	77.1889	1.434	300.108	2777	77.1889	1.434	343.0499	2777	77.1889	1.434	424.9638	2777	77.1889	1.434	552.2528
2778	77.2149	1.4335	295.0345	2778	77.2149	1.4335	338.2654	2778	77.2149	1.4335	429.3608	2778	77.2149	1.4335	557.7112
2779	77.2409	1.4331	310.7368	2779	77.2409	1.4331	354.2565	2779	77.2409	1.4331	440.0501	2779	77.2409	1.4331	569.4619
2780	77.2669	1.4327	304.3578	2780	77.2669	1.4327	348.1665	2780	77.2669	1.4327	414.7666	2780	77.2669	1.4327	545.2399
2781	77.2929	1.4323	299.3185	2781	77.2929	1.4323	343.416	2781	77.2929	1.4323	397.8736	2781	77.2929	1.4323	529.4083
2782	77.3189	1.4319	304.0808	2782	77.3189	1.4319	348.4671	2782	77.3189	1.4319	380.8498	2782	77.3189	1.4319	513.4459
2783	77.3449	1.4315	307.5515	2783	77.3449	1.4315	352.2267	2783	77.3449	1.4315	369.7611	2783	77.3449	1.4315	500.3938
2784	77.3709	1.4311	298.4007	2784	77.3709	1.4311	343.3649	2784	77.3709	1.4311	406.6483	2784	77.3709	1.4311	535.3176
2785	77.3969	1.4307	294.134	2785	77.3969	1.4307	339.387	2785	77.3969	1.4307	407.7781	2785	77.3969	1.4307	534.4839
2786	77.4229	1.4303	288.8321	2786	77.4229	1.4303	334.374	2786	77.4229	1.4303	401.5247	2786	77.4229	1.4303	526.2672
2787	77.4489	1.4299	279.438	2787	77.4489	1.4299	325.2688	2787	77.4489	1.4299	415.0547	2787	77.4489	1.4299	537.8337
2788	77.4749	1.4295	297.9598	2788	77.4749	1.4295	344.0794	2788	77.4749	1.4295	429.4407	2788	77.4749	1.4295	550.2563
2789	77.5009	1.4291	302.2648	2789	77.5009	1.4291	348.6733	2789	77.5009	1.4291	405.4248	2789	77.5009	1.4291	524.277
2790	77.5269	1.4287	285.3326	2790	77.5269	1.4287	332.0301	2790	77.5269	1.4287	390.8837	2790	77.5269	1.4287	507.7724
2791	77.5529	1.4283	258.785	2791	77.5529	1.4283	305.7713	2791	77.5529	1.4283	374.4714	2791	77.5529	1.4283	489.3967
2792	77.5789	1.4279	274.3597	2792	77.5789	1.4279	321.6348	2792	77.5789	1.4279	357.5831	2792	77.5789	1.4279	470.5449
2793	77.6049	1.4275	273.7687	2793	77.6049	1.4275	321.3328	2793	77.6049	1.4275	353.4076	2793	77.6049	1.4275	464.4061
2794	77.6309	1.4271	309.8508	2794	77.6309	1.4271	357.7037	2794	77.6309	1.4271	353.3909	2794	77.6309	1.4271	462.4259
2795	77.6569	1.4267	300.2557	2795	77.6569	1.4267	348.3975	2795	77.6569	1.4267	355.5911	2795	77.6569	1.4267	462.6627
2796	77.6829	1.4263	279.6144	2796	77.6829	1.4263	328.0451	2796	77.6829	1.4263	367.7701	2796	77.6829	1.4263	472.8782
2797	77.7089	1.4259	257.513	2797	77.7089	1.4259	306.2326	2797	77.7089	1.4259	381.7389	2797	77.7089	1.4259	484.8837
2798	77.7349	1.4255	285.1964	2798	77.7349	1.4255	334.2049	2798	77.7349	1.4255	373.0554	2798	77.7349	1.4255	474.2367
2799	77.7609	1.4251	284.1694	2799	77.7609	1.4251	333.4668	2799	77.7609	1.4251	380.6815	2799	77.7609	1.4251	479.8994
2800	77.7869	1.4247	251.5614	2800	77.7869	1.4247	301.1477	2800	77.7869	1.4247	384.423	2800	77.7869	1.4247	481.6774
2801	77.8129	1.4243	293.6941	2801	77.8129	1.4243	343.5692	2801	77.8129	1.4243	373.8848	2801	77.8129	1.4243	469.1758
2802	77.8389	1.4239	305.4752	2802	77.8389	1.4239	355.6392	2802	77.8389	1.4239	402.9847	2802	77.8389	1.4239	496.3122
2803	77.8649	1.4235	279.649	2803	77.8649	1.4235	330.1019	2803	77.8649	1.4235	487.534	2803	77.8649	1.4235	578.8981

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2804	77.8909	1.4231	254.1514	2804	77.8909	1.4231	304.8932	2804	77.8909	1.4231	522.0308	2804	77.8909	1.4231	611.4315
2805	77.9169	1.4227	300.9694	2805	77.9169	1.4227	352	2805	77.9169	1.4227	518.1688	2805	77.9169	1.4227	605.6062
2806	77.9429	1.4223	298.6648	2806	77.9429	1.4223	349.9844	2806	77.9429	1.4223	560.4948	2806	77.9429	1.4223	645.9687
2807	77.9689	1.4219	287.7594	2807	77.9689	1.4219	339.3678	2807	77.9689	1.4219	539.3286	2807	77.9689	1.4219	622.8391
2808	77.9949	1.4215	287.8058	2808	77.9949	1.4215	339.7031	2808	77.9949	1.4215	521.0461	2808	77.9949	1.4215	602.5931
2809	78.0209	1.4211	306.879	2809	78.0209	1.4211	359.0652	2809	78.0209	1.4211	507.1479	2809	78.0209	1.4211	586.7315
2810	78.0469	1.4207	296.6553	2810	78.0469	1.4207	348.5394	2810	78.0469	1.4207	531.5081	2810	78.0469	1.4207	610.3848
2811	78.0729	1.4203	300.3165	2811	78.0729	1.4203	351.8985	2811	78.0729	1.4203	530.6875	2811	78.0729	1.4203	608.8575
2812	78.0989	1.4199	247.9369	2812	78.0989	1.4199	299.2169	2812	78.0989	1.4199	501.1875	2812	78.0989	1.4199	578.6506
2813	78.1249	1.4195	253.7657	2813	78.1249	1.4195	304.7435	2813	78.1249	1.4195	513.4501	2813	78.1249	1.4195	590.2063
2814	78.1509	1.4191	286.198	2814	78.1509	1.4191	336.8738	2814	78.1509	1.4191	570.2418	2814	78.1509	1.4191	646.2913
2815	78.1769	1.4187	267.4584	2815	78.1769	1.4187	317.8321	2815	78.1769	1.4187	563.6574	2815	78.1769	1.4187	639
2816	78.2029	1.4183	300.5847	2816	78.2029	1.4183	350.6563	2816	78.2029	1.4183	560.6519	2816	78.2029	1.4183	635.2877
2817	78.2289	1.4179	293.9363	2817	78.2289	1.4179	343.7059	2817	78.2289	1.4179	509.8946	2817	78.2289	1.4179	583.8235
2818	78.2549	1.4175	259.2441	2818	78.2549	1.4175	308.7116	2818	78.2549	1.4175	490.5554	2818	78.2549	1.4175	563.7775
2819	78.2809	1.4171	291.6263	2819	78.2809	1.4171	340.7916	2819	78.2809	1.4171	466.5102	2819	78.2809	1.4171	539.0255
2820	78.3069	1.4167	263.1247	2820	78.3069	1.4167	311.9879	2820	78.3069	1.4167	443.4531	2820	78.3069	1.4167	515.2615
2821	78.3329	1.4163	296.5727	2821	78.3329	1.4163	345.1339	2821	78.3329	1.4163	452.7262	2821	78.3329	1.4163	523.8278
2822	78.3589	1.4159	303.3263	2822	78.3589	1.4159	351.5854	2822	78.3589	1.4159	444.7526	2822	78.3589	1.4159	515.1474
2823	78.3849	1.4155	259.0749	2823	78.3849	1.4155	307.0319	2823	78.3849	1.4155	461.3007	2823	78.3849	1.4155	530.9886
2824	78.4109	1.4151	301.8879	2824	78.4109	1.4151	349.5428	2824	78.4109	1.4151	441.2422	2824	78.4109	1.4151	510.2233
2825	78.4369	1.4147	254.6543	2825	78.4369	1.4147	302.0072	2825	78.4369	1.4147	417.2396	2825	78.4369	1.4147	485.5139
2826	78.4629	1.4143	248.132	2826	78.4629	1.4143	295.1829	2826	78.4629	1.4143	441.6707	2826	78.4629	1.4143	509.2381
2827	78.4889	1.4139	275.1201	2827	78.4889	1.4139	321.8688	2827	78.4889	1.4139	387.4825	2827	78.4889	1.4139	454.3431
2828	78.5149	1.4136	299.3456	2828	78.5149	1.4136	345.7923	2828	78.5149	1.4136	383.9469	2828	78.5149	1.4136	450.1006
2829	78.5409	1.4132	283	2829	78.5409	1.4132	329.1446	2829	78.5409	1.4132	413.6855	2829	78.5409	1.4132	479.1325
2830	78.5669	1.4128	281.2277	2830	78.5669	1.4128	327.0702	2830	78.5669	1.4128	383.7157	2830	78.5669	1.4128	448.4558
2831	78.5929	1.4124	280.5397	2831	78.5929	1.4124	326.0801	2831	78.5929	1.4124	418.7632	2831	78.5929	1.4124	482.7965
2832	78.6189	1.412	280.7617	2832	78.6189	1.412	326	2832	78.6189	1.412	389.004	2832	78.6189	1.412	452.3304
2833	78.6449	1.4116	254.9618	2833	78.6449	1.4116	299.898	2833	78.6449	1.4116	459.2859	2833	78.6449	1.4116	521.9055
2834	78.6709	1.4112	290.6421	2834	78.6709	1.4112	335.2762	2834	78.6709	1.4112	380.853	2834	78.6709	1.4112	442.7658
2835	78.6969	1.4108	296.5481	2835	78.6969	1.4108	340.8802	2835	78.6969	1.4108	381.3568	2835	78.6969	1.4108	442.5627
2836	78.7229	1.4104	294.3591	2836	78.7229	1.4104	338.3891	2836	78.7229	1.4104	394.8148	2836	78.7229	1.4104	455.3139
2837	78.7489	1.41	284.8079	2837	78.7489	1.41	328.5358	2837	78.7489	1.41	422.1587	2837	78.7489	1.41	481.951
2838	78.7749	1.4096	269.1164	2838	78.7749	1.4096	312.5422	2838	78.7749	1.4096	389.4945	2838	78.7749	1.4096	448.5799
2839	78.8009	1.4093	276.9626	2839	78.8009	1.4093	320.0864	2839	78.8009	1.4093	381.9403	2839	78.8009	1.4093	440.3189

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2840	78.8269	1.4089	286.6538	2840	78.8269	1.4089	329.4755	2840	78.8269	1.4089	390.6344	2840	78.8269	1.4089	448.3061
2841	78.8529	1.4085	292.5838	2841	78.8529	1.4085	335.1034	2841	78.8529	1.4085	387.2903	2841	78.8529	1.4085	444.2552
2842	78.8789	1.4081	273.5133	2842	78.8789	1.4081	315.7308	2842	78.8789	1.4081	400.5249	2842	78.8789	1.4081	456.783
2843	78.9049	1.4077	267.4828	2843	78.9049	1.4077	309.3983	2843	78.9049	1.4077	370.0124	2843	78.9049	1.4077	425.5637
2844	78.9309	1.4073	272.1321	2844	78.9309	1.4073	313.7455	2844	78.9309	1.4073	383.5105	2844	78.9309	1.4073	438.3549
2845	78.9569	1.4069	268.2217	2845	78.9569	1.4069	309.533	2845	78.9569	1.4069	433.5984	2845	78.9569	1.4069	487.736
2846	78.9829	1.4065	286.2677	2846	78.9829	1.4065	327.2769	2846	78.9829	1.4065	442.7139	2846	78.9829	1.4065	496.1446
2847	79.0089	1.4061	318.1721	2847	79.0089	1.4061	358.8793	2847	79.0089	1.4061	398.1291	2847	79.0089	1.4061	450.853
2848	79.0349	1.4058	265.745	2848	79.0349	1.4058	306.1501	2848	79.0349	1.4058	436.818	2848	79.0349	1.4058	488.8351
2849	79.0609	1.4054	253.3101	2849	79.0609	1.4054	293.4131	2849	79.0609	1.4054	412.435	2849	79.0609	1.4054	463.7453
2850	79.0869	1.405	265.7071	2850	79.0869	1.405	305.5081	2850	79.0869	1.405	409.3674	2850	79.0869	1.405	459.9708
2851	79.1129	1.4046	292.5881	2851	79.1129	1.4046	332.0869	2851	79.1129	1.4046	384.5233	2851	79.1129	1.4046	434.4199
2852	79.1389	1.4042	286.1493	2852	79.1389	1.4042	325.346	2852	79.1389	1.4042	380.9257	2852	79.1389	1.4042	430.1154
2853	79.1649	1.4038	277.2988	2853	79.1649	1.4038	316.1935	2853	79.1649	1.4038	350.8392	2853	79.1649	1.4038	399.3222
2854	79.1909	1.4034	313.7592	2854	79.1909	1.4034	352.3518	2854	79.1909	1.4034	333.0737	2854	79.1909	1.4034	380.8498
2855	79.2169	1.4031	312.9833	2855	79.2169	1.4031	351.2738	2855	79.2169	1.4031	358.5201	2855	79.2169	1.4031	405.5893
2856	79.2429	1.4027	278.8092	2856	79.2429	1.4027	316.7977	2856	79.2429	1.4027	381.7154	2856	79.2429	1.4027	428.0778
2857	79.2689	1.4023	272.271	2857	79.2689	1.4023	309.9574	2857	79.2689	1.4023	394.6257	2857	79.2689	1.4023	440.2813
2858	79.2949	1.4019	273.6597	2858	79.2949	1.4019	311.044	2858	79.2949	1.4019	394.4872	2858	79.2949	1.4019	439.4359
2859	79.3209	1.4015	296.033	2859	79.3209	1.4015	333.1152	2859	79.3209	1.4015	392.116	2859	79.3209	1.4015	436.3579
2860	79.3469	1.4011	292.7836	2860	79.3469	1.4011	329.5637	2860	79.3469	1.4011	376.0286	2860	79.3469	1.4011	419.5637
2861	79.3729	1.4008	301.567	2861	79.3729	1.4008	338.0451	2861	79.3729	1.4008	381.4834	2861	79.3729	1.4008	424.3116
2862	79.3989	1.4004	296.9037	2862	79.3989	1.4004	333.0797	2862	79.3989	1.4004	381.0815	2862	79.3989	1.4004	423.2029
2863	79.4249	1.4	282.3069	2863	79.4249	1.4	318.1808	2863	79.4249	1.4	359.9231	2863	79.4249	1.4	401.3376
2864	79.4509	1.3996	280.0207	2864	79.4509	1.3996	315.5925	2864	79.4509	1.3996	378.7311	2864	79.4509	1.3996	419.4389
2865	79.4769	1.3992	271.4094	2865	79.4769	1.3992	306.6791	2865	79.4769	1.3992	390.8433	2865	79.4769	1.3992	430.8442
2866	79.5029	1.3988	276.485	2866	79.5029	1.3988	311.4526	2866	79.5029	1.3988	387.4238	2866	79.5029	1.3988	426.7179
2867	79.5289	1.3985	282.5209	2867	79.5289	1.3985	317.1865	2867	79.5289	1.3985	400.6669	2867	79.5289	1.3985	439.2542
2868	79.5549	1.3981	277.8726	2868	79.5549	1.3981	312.2361	2868	79.5549	1.3981	414.5419	2868	79.5549	1.3981	452.4223
2869	79.5809	1.3977	305.7962	2869	79.5809	1.3977	339.8576	2869	79.5809	1.3977	386.7974	2869	79.5809	1.3977	423.971
2870	79.6069	1.3973	311.5218	2870	79.6069	1.3973	345.2811	2870	79.6069	1.3973	382.3839	2870	79.6069	1.3973	418.8506
2871	79.6329	1.3969	311.8024	2871	79.6329	1.3969	345.2597	2871	79.6329	1.3969	415.8386	2871	79.6329	1.3969	451.5985
2872	79.6589	1.3966	346.8295	2872	79.6589	1.3966	379.9846	2872	79.6589	1.3966	401.7527	2872	79.6589	1.3966	436.8058
2873	79.6849	1.3962	359.612	2873	79.6849	1.3962	392.4651	2873	79.6849	1.3962	378.6665	2873	79.6849	1.3962	413.0127
2874	79.7109	1.3958	322.8808	2874	79.7109	1.3958	355.4318	2874	79.7109	1.3958	396.6515	2874	79.7109	1.3958	430.2909
2875	79.7369	1.3954	278.6678	2875	79.7369	1.3954	310.9167	2875	79.7369	1.3954	412.5841	2875	79.7369	1.3954	445.5167

Table I. part 4: *Continued*

E028_ConstCompExp_BackgrndRmvod				E028_ConstCompExp_raw				E015_sample3_ConstCompExp_BackgrdRmovd				E015_sample3_ConstCompExp_raw			
No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]	No.	Pos. [°2θ]	D spacings	Intensity [Counts]
2876	79.7629	1.395	252.3243	2876	79.7629	1.395	284.2711	2876	79.7629	1.395	384.8431	2876	79.7629	1.395	417.0689
2877	79.7889	1.3947	276.2881	2877	79.7889	1.3947	307.9329	2877	79.7889	1.3947	349.8462	2877	79.7889	1.3947	381.3651
2878	79.8149	1.3943	325.2858	2878	79.8149	1.3943	356.6285	2878	79.8149	1.3943	375.1232	2878	79.8149	1.3943	405.9352
2879	79.8409	1.3939	314.8756	2879	79.8409	1.3939	345.9162	2879	79.8409	1.3939	395.9237	2879	79.8409	1.3939	426.0289
2880	79.8669	1.3935	298.4301	2880	79.8669	1.3935	329.1686	2880	79.8669	1.3935	393.9504	2880	79.8669	1.3935	423.3488
2881	79.8929	1.3932	313.4299	2881	79.8929	1.3932	343.8663	2881	79.8929	1.3932	414.7656	2881	79.8929	1.3932	443.4572
2882	79.9189	1.3928	306.6886	2882	79.9189	1.3928	336.823	2882	79.9189	1.3928	388.4244	2882	79.9189	1.3928	416.4091
2883	79.9449	1.3924	267.3005	2883	79.9449	1.3924	297.1328	2883	79.9449	1.3924	371.4763	2883	79.9449	1.3924	398.7542
2884	79.9709	1.392	273.323	2884	79.9709	1.392	303.1553	2884	79.9709	1.392	380.143	2884	79.9709	1.392	407.4209

I

Appendix I

I.1 The complete MATLAB code used to plot saturation states, activities and other geochemical relations in the figures shown in Chapter 4 is provided in this appendix.

An updated version of the code will be eventually uploaded and made available on github.com under the repository "raphapietzsch/alkaline_lakes".

```
% "alkaline_lakes_of_the_world_vFinal": A script that computes chemical
% properties of several lakes from around the world
% Authors: Raphael Pietzsch and Nick Tosca
% Created: 25 April 2021
% Modified: 09 OCT 2021; 14 APR 2022; 16 MAY 2022
%
% Directly calls a dataset of estimated activities (not concentrations),
% calculated with GWB based on a thermodynamic database that considers the
% Pitzer ion interaction model for this purpose:
% "thermo_phrqpitz_CaP_OCP_HAP_MHC__CO3_basis.tdat"

%% Mineral equilibria

load('alkaline_lakes_of_the_world.mat'); % (database from appendix G)
load('Sascha_experiments.mat');

a_h = 10.^(-pH); % Activity from real pH measurements reported in the database
a_h2 = a_h.^2;
aMg_aH_ratio = aMg./a_h2;

dic_molal = conc_CO3./1000; % from mmol/kg to mol/kg
alk_molal = ALK./1000;

x = [0, 0.25, 0.5]; % Mole fraction of Mg in ACMC
x_matrix = repmat(x',1, 1000);
MgACMC = x_matrix.*100; % Percentage of Mg in ACMC
Ksp_ACMC = 10.^((0.0175.*MgACMC)-6.277); % ACMC solubility determination from
Purgstaller et al. 2019, Solubility investigations in the amorphous calcium
magnesium carbonate system, CrystEngComm 21.
Ksp_Calcite = 10^(-8.48); % Appelo and Postma (2005), p. 176; Fukushi and Matsumiya
(2018), p. 741.
Ksp_Aragonite = 10^(-8.34); % Appelo and Postma (2005), p. 176; Fukushi and
Matsumiya (2018), p. 741.
Ksp_Dolomite = 10^(-17.09); % Appelo and Postma (2005), p. 176.
Ksp_Vaterite = 10^(-7.91); % Fukushi and Matsumiya (2018), p. 741.
Ksp_Monohydrocalcite = 10^(-7.65); % Fukushi and Matsumiya (2018), p. 741.
Ksp_AMC1 = 10^(-5.2); % Fukushi and Matsumiya (2018), p. 741.
Ksp_AMC2 = 10^(-5.59); % Fukushi and Matsumiya (2018), p. 741.

aCa_ACMC = logspace(-8,0, 1000); % changing the lower boundary affects calculation
of Omega_HAP lines below
aMg_ACMC = aCa_ACMC./0.1974; %aMg_ACMC = aCa_ACMC./1.1957; % Average aCa/aMg ratio
from lake analyses(wrong value: 1.1957 is incorrect; possibly originally a typo)
aCO3_ACMC = Ksp_ACMC./((aCa_ACMC.^(1-x_matrix)).*(aMg_ACMC.^x_matrix)); %
Relationship between ACMC and aCO3
aCO3_calcite = Ksp_Calcite./aCa_ACMC;
aCO3_aragonite = Ksp_Aragonite./aCa_ACMC;
aCO3_dolomite = (Ksp_Dolomite./(aCa_ACMC.*aMg_ACMC)).^(1/2);
aCO3_vaterite = Ksp_Vaterite./aCa_ACMC;
aCO3_monohydrocalcite = Ksp_Monohydrocalcite./aCa_ACMC;
```

```
aCO3_AMC1_ca = Ksp_AMC1./aCa_ACMC; % this will create an artificial solubility line
for reference only, since there's no Ca in AMC
aCO3_AMC2_ca = Ksp_AMC2./aCa_ACMC; % this will create an artificial solubility line
for reference only, since there's no Ca in AMC
IAP_ACMC = aCO3_ACMC.*((aCa_ACMC.^(1-x_matrix)).*(aMg_ACMC.^x_matrix)); %
Relationship between ACMC and aCO3

%-------Saturation state calculations-------%

pH_1 = linspace(4,11, 1000);
a_H1 = 10.^(-pH_1); % Activity from pH points created above

KspOCP = 10^(-48.4); % Solubility product of OCP at 23.5oC (Tung et al., 1988)
%log_Ca4PO43 = pH_1+log10(KspOCP);
aPO4_OCP = ((KspOCP)./(a_H1.*aCa_ACMC.^4)).^(1/3); % Table 2 in Li et al. (2017,
Chemosphere 183).

KspACP = 10^(-25.5); % Solubility product of amorphous calcium phosphate
aPO4_ACP = sqrt(KspACP./(aCa_ACMC.^3));

KspHAP = 10^(-44.33); % Solubility product of hydroxyapatite (Li et al., 2017,
Chemosphere 183).
aPO4_HAP = ((a_H1.*KspHAP)./(aCa_ACMC.^5)).^(1/3);

% Na2CO3.10H2O, Natron:
Ksp_Natron = 10^(-0.825);
a_Na = logspace(-10,10, 1000);
aCO3_Natron = Ksp_Natron./((a_Na.^2).*(0.96.^10)); % Average H2O activity in saline
lakes precipitating natron

Ksp_Nesq = 10^(-5.167); % MgCO3.3H2O
Ksp_Mag = 10^(-7.834); % MgCO3
a_Mg = logspace(-8,0, 1000);
aCO3_Nesq = Ksp_Nesq./(a_Mg);
aCO3_Mag = Ksp_Mag./(a_Mg);
aCO3_Dol = (Ksp_Dolomite./(aCa_ACMC.*a_Mg)).^(1/2); % Differs from the above
dolomite: uses a_Mg instead of aMg_ACMC.
aCO3_AMC1 = Ksp_AMC1./a_Mg; % this creates a correct solubility line for the AMC1,
because it's based on a_Mg instead of aCa_ACMC as before
aCO3_AMC2 = Ksp_AMC2./a_Mg; % this creates a correct solubility line for the AMC2,
because it's based on a_Mg instead of aCa_ACMC as before

% MgCO3.5H2O, Lansfordite: From Marion (2001), GCA 65, Table 6.
a1lans = 9.556371E2;
a2lans = -1.003715E1;
a3lans = 3.464409E-2;
a4lans = -3.978274E-5;
a5lans = 0;
a6lans = 0;
a7lans = 0;
T = 298.15;
```

```
KspLans =
exp((a1lans)+(a2lans.*T)+(a3lans.*(T.^2))+(a4lans.*(T.^3))+(a5lans./T)+(a6lans.*(lo
g(T)))+(a7lans./(T.^2)));
aCO3_Lans = KspLans./(a_Mg);

% NaHCO3, Nahcolite: From Marion et al. (2011), Icarus 212, Table 1.
a1nahc = 1.479309E1;
a2nahc = -2.427724E-1;
a3nahc = 1.002818-3;
a4nahc = -1.224329E-6;
a5nahc = 0;
a6nahc = 0;
a7nahc = 0;
T = 298.15;
Ksp_Nahc =
exp((a1nahc)+(a2nahc.*T)+(a3nahc.*(T.^2))+(a4nahc.*(T.^3))+(a5nahc./T)+(a6nahc.*(lo
g(T)))+(a7nahc./(T.^2)));
aHCO3_Nahc = Ksp_Nahc./(a_Na);

% Na3H(CO3)2.2H2O, Trona: From Marion (2001), GCA 65, Table 6.
a1trona = -9.986743E0;
a2trona = 2.563766E-2;
a3trona = 0;
a4trona = 0;
a5trona = 0;
a6trona = 0;
a7trona = 0;
T = 298.15;
Ksp_Trona =
exp((a1trona)+(a2trona.*T)+(a3trona.*(T.^2))+(a4trona.*(T.^3))+(a5trona./T)+(a6tron
a.*(log(T)))+(a7trona./(T.^2)));
aCO3_Trona = sqrt(Ksp_Trona./(a_Na.^3.*0.96.^2)); % Assuming H2O activity = 0.96

% 5MgO.4CO2.5H2O, Hydromagnesite: From Marion (2001), GCA 65, Table 6.
% Mineral formula from Konigsberger et al., (1999) GCA 63, p. 8.
a1hmg = -9.986743E0;
a2hmg = 2.563766E-2;
a3hmg = 0;
a4hmg = 0;
a5hmg = 0;
a6hmg = 0;
a7hmg = 0;
T = 298.15;
Ksp_HMG =
exp((a1hmg)+(a2hmg.*T)+(a3hmg.*(T.^2))+(a4hmg.*(T.^3))+(a5hmg./T)+(a6hmg.*(log(T)))
+(a7hmg./(T.^2)));
aCO3_HMG = Ksp_HMG./(a_Mg);

% Na2CO3.H2O, Thermonatrite: From Marion et al. (2011), Icarus 212, Table 1.
a1tnt = -6.625585E1;
a2tnt = 4.250286E-1;
```

```
a3tnt = -6.681267E-4;
a4tnt = 0;
a5tnt = 0;
a6tnt = 0;
a7tnt = 0;
T = 298.15;
Ksp_TNT =
exp((a1tnt)+(a2tnt.*T)+(a3tnt.*(T.^2))+(a4tnt.*(T.^3))+(a5tnt./T)+(a6tnt.*(log(T)))
+(a7tnt./(T.^2)));
aCO3_TNT = Ksp_TNT./(a_Na.*0.96); % Assuming H2O activity = 0.96

%-------Make legend text-------%

lineA = ['ACMC (',num2str(x(1).*100),'mol % Mg)']; % Text lines that update with x
values
lineB = ['ACMC (',num2str(x(2).*100),'mol % Mg)']; % Text lines that update with x
values
lineC = ['ACMC (',num2str(x(3).*100),'mol % Mg)']; % Text lines that update with x
values
lineD = ['Calcite']; % Text lines
lineE = ['Nesquehonite']; % Text lines
lineF = ['Lansfordite']; % Text lines
lineG = ['Magnesite']; % Text lines
lineH = ['Amorphous Ca-phosphate']; % Text lines
lineI = ['Aragonite']; % Text lines
lineJ = ['Dolomite']; % Text lines
lineK = ['Dolomite']; % Text lines; uses other Mg activity values, see above.
lineL = ['OCP']; % Text lines
lineM = ['HAP']; % Text lines
lineN = ['Vaterite']; % Text lines
lineO = ['MHC']; % Text lines
lineP = ['Natron']; % Text lines
lineQ = ['Nahcolite']; % Text lines
lineR = ['Trona']; % Text lines
lineS = ['Hydromagnesite']; % Text lines
lineT = ['Thermonatrite']; % Text lines
lineU = ['AMC1']; % Text lines
lineV = ['AMC2']; % Text lines


%% ----------Removing outliers from charge balance errors----------%
% (step 1)
% Remove 'not a number' (a water sample was forced to charge balance, hence
% GWB didn't care to output the charge balance error value (which becomes
% zero, in this case)
CBnan = fillmissing(ChBalError,'constant',0);

%% Identify samples whose charge balance error lies above 10%:
% (step 2.a)
% plot 1
plot(aCO3,CBnan,'rs');
```

```
hold on;
plot(aCa,CBnan,'bo');
hold on;
plot(aMg,CBnan,'yd');
hold on;
plot(aPO4,CBnan,'g+');
hold on;
plot(aNa,CBnan,'cx');
hold on;
plot(aSiO2aq,CBnan,'m*');
hold off;

legend('aCO3','aCa','aMg','aPO4','aNa','aSiO2aq');

f = fittype({'x'});
aCO3fit = fit(aCO3,CBnan,f,'Robust','on');
aCafit = fit(aCa,CBnan,f,'Robust','on');
aMgfit = fit(aMg,CBnan,f,'Robust','on');
aPO4fit = fit(aPO4,CBnan,f,'Robust','on');
aNafit = fit(aNa,CBnan,f,'Robust','on');
aSiO2fit = fit(aSiO2aq,CBnan,f,'Robust','on');

figure;
plot(aCO3fit,aCO3,CBnan,'rs','residuals');
hold on;
plot(aCafit,aCa,CBnan,'bo','residuals');
hold on;
plot(aMgfit,aMg,CBnan,'yd','residuals');
hold on;
plot(aPO4fit,aPO4,CBnan,'g+','residuals');
hold on;
plot(aNafit,aNa,CBnan,'cx','residuals');
hold on;
plot(aSiO2fit,aSiO2aq,CBnan,'m*','residuals');
hold off;

aCO3res = CBnan - feval(aCO3fit,aCO3);
aCares = CBnan - feval(aCafit,aCa);
aMgres = CBnan - feval(aMgfit,aMg);
aPO4res = CBnan - feval(aPO4fit,aPO4);
aNares = CBnan - feval(aNafit,aNa);
aSiO2res = CBnan - feval(aSiO2fit,aSiO2aq);

aCO3outliers = excludedata(aCO3,aCO3res,'range',[-0.1 0.1]);
aCaoutliers = excludedata(aCa,aCares,'range',[-0.1 0.1]);
aMgoutliers = excludedata(aMg,aMgres,'range',[-0.1 0.1]);
aPO4outliers = excludedata(aPO4,aPO4res,'range',[-0.1 0.1]);
aNaoutliers = excludedata(aNa,aNares,'range',[-0.1 0.1]);
aSiO2outliers = excludedata(aSiO2aq,aSiO2res,'range',[-0.1 0.1]);
```

```
%%
% (step 2.b)
% plot 2
plot(pH_range1,CBnan,'k*');

legend('pH_range1');

f = fittype({'x'});
pH_range1fit = fit(pH_range1,CBnan,f,'Robust','on');

figure;
plot(pH_range1fit,pH_range1,CBnan,'rs','residuals');
hold off;

pH_range1res = CBnan - feval(pH_range1fit,pH_range1);

pH_range1outliers = excludedata(pH_range1,pH_range1res,'range',[-0.1 0.1]);


%%
% (step 2.c)
% plot 3
plot(SI_Calcite,CBnan,'m*');

legend('SI_Calcite');

f = fittype({'x'});
SI_Calcitefit = fit(SI_Calcite,CBnan,f,'Robust','on');

figure;
plot(SI_Calcitefit,SI_Calcite,CBnan,'rs','residuals');
hold off;

SI_Calciteres = CBnan - feval(SI_Calcitefit,SI_Calcite);

SI_Calciteoutliers = excludedata(SI_Calcite,SI_Calciteres,'range',[-0.1 0.1]);


%%
% (step 2.d)
% plot 4
plot(SI_Natron,CBnan,'g*');

legend('SI_Natron');

f = fittype({'x'});
SI_Natronfit = fit(SI_Natron,CBnan,f,'Robust','on');

figure;
plot(SI_Natronfit,SI_Natron,CBnan,'rs','residuals');
hold off;
```

```
SI_Natronres = CBnan - feval(SI_Natronfit,SI_Natron);

SI_Natronoutliers = excludedata(SI_Natron,SI_Natronres,'range',[-0.1 0.1]);


%%
% (step 2.e)
% plot 5
plot(SI_Amrphsilica,CBnan,'m*');

legend('SI_Amorphous SiO2');

f = fittype({'x'});
SI_Amrphsilicafit = fit(SI_Amrphsilica,CBnan,f,'Robust','on');

figure;
plot(SI_Amrphsilicafit,SI_Amrphsilica,CBnan,'m*','residuals');
hold off;

SI_Amrphsilicares = CBnan - feval(SI_Amrphsilicafit,SI_Amrphsilica);

SI_Amrphsilicaoutliers = excludedata(SI_Amrphsilica,SI_Amrphsilicares,'range',[-0.1
0.1]);


%%
% (step 2.f)
% plot 6
plot(SI_Sepiolite,CBnan,'g*');

legend('SI_Sepiolite');

f = fittype({'x'});
SI_Sepiolitefit = fit(SI_Sepiolite,CBnan,f,'Robust','on');

figure;
plot(SI_Sepiolitefit,SI_Sepiolite,CBnan,'rs','residuals');
hold off;

SI_Sepioliteres = CBnan - feval(SI_Sepiolitefit,SI_Sepiolite);

SI_Sepioliteoutliers = excludedata(SI_Sepiolite,SI_Sepioliteres,'range',[-0.1
0.1]);


%% ------- Make final plots -------%

% (step 3)

ax1=subplot(3,3,1); % Make a 3 x 3 grid of plots
```

```
loglog((aCO3_ACMC),(aCa_ACMC),(aCO3_calcite),(aCa_ACMC),(aCO3_aragonite),(aCa_ACMC)
,(aCO3_dolomite),(aCa_ACMC),(aCO3_vaterite),(aCa_ACMC),(aCO3_monohydrocalcite),(aCa
_ACMC),(aCO3_AMC1_ca),(aCa_ACMC),(aCO3_AMC2_ca),(aCa_ACMC),'LineWidth',1.5);
%loglog((aCO3_AMC1_ca),(aCa_ACMC),(aCO3_AMC2_ca),(aCa_ACMC),'LineWidth',1.5);
%loglog((aCO3_ACMC),(aCa_ACMC),(aCO3_calcite),(aCa_ACMC),(aCO3_aragonite),(aCa_ACMC
),(aCO3_dolomite),(aCa_ACMC),(aCO3_vaterite),(aCa_ACMC),(aCO3_monohydrocalcite),(aC
a_ACMC),'LineWidth',1.5);
hold on;
%gscatter(aCO3(~aCO3outliers & pH>8),aCa(~aCO3outliers &
pH>8),pH_range1(~aCO3outliers & pH>8));
%gscatter(aCO3(~aCO3outliers),aCa(~aCO3outliers),pH_range1(~aCO3outliers));
%gscatter(aCO3(~aCO3outliers),aCa(~aCO3outliers),ratioMgCa_new_rank2(~aCO3outliers)
);
gscatter(aCO3(~aCO3outliers),aCa(~aCO3outliers),aCa_rank(~aCO3outliers));
%gscatter(aCO3(~aCO3outliers),aCa(~aCO3outliers),ALKtoMgCa_rank(~aCO3outliers));
%gscatter(aCO3(~aCO3outliers),aCa(~aCO3outliers),Lake(~aCO3outliers));
%gscatter(aCO3(~aCO3outliers),aCa(~aCO3outliers),DeltaCO2_rank2(~aCO3outliers));
%gscatter(aCO3(~aCO3outliers),aCa(~aCO3outliers),SI_cal_rank(~aCO3outliers));
%gscatter(aCO3(~aCO3outliers),aCa(~aCO3outliers),country(~aCO3outliers));
%colorbar;
hold off;
axis([1E-7 1 1E-7 1E-1])
xlabel('a_{CO3}'); % x-axis label
ylabel('a_{Ca}'); % y-axis label
%set(gca,'Ydir','reverse');
%set(gca,'Xdir','reverse');
%legend(lineA,lineB,lineC,lineD,lineI,lineJ,lineN,lineO,lineU,lineV,'Location','nor
theast'); % legend text


ax2=subplot(3,3,2); % Make a 3 x 3 grid of plots
loglog(aCO3_Nesq,a_Mg,aCO3_Lans,a_Mg,aCO3_Mag,a_Mg,aCO3_Dol,a_Mg,(aCO3_AMC1),(a_Mg)
,(aCO3_AMC2),(a_Mg),'LineWidth',1.5);
%loglog((aCO3_AMC1),(a_Mg),(aCO3_AMC2),(a_Mg),'LineWidth',1.5);
%loglog(aCO3_Nesq,a_Mg,aCO3_Lans,a_Mg,aCO3_Mag,a_Mg,aCO3_Dol,a_Mg,'LineWidth',1.5);
hold on;
%gscatter(aCO3(~aCO3outliers),aMg(~aCO3outliers),pH_range1(~aCO3outliers));
%gscatter(aCO3(~aCO3outliers),aMg(~aCO3outliers),ratioMgCa_new_rank2(~aCO3outliers)
);
%gscatter(aCO3(~aCO3outliers),aMg(~aCO3outliers),aCa_rank(~aCO3outliers));
%gscatter(aCO3(~aCO3outliers),aMg(~aCO3outliers),aSiO2aq_rank(~aCO3outliers));
%gscatter(aCO3(~aCO3outliers),aMg(~aCO3outliers),ALKtoMgCa_rank(~aCO3outliers));
%gscatter(aCO3(~aCO3outliers),aMg(~aCO3outliers),DeltaCO2_rank2(~aCO3outliers));
%gscatter(aCO3(~aCO3outliers),aMg(~aCO3outliers),SI_cal_rank(~aCO3outliers));
gscatter(aCO3(~aCO3outliers),aMg(~aCO3outliers),country(~aCO3outliers));
%gscatter(aCO3(~aCO3outliers),aMg(~aCO3outliers),Lake(~aCO3outliers));
hold off;
axis([1E-7 1 1E-7 1E-1])
xlabel('a_{CO3}'); % x-axis label
ylabel('a_{Mg}'); % y-axis label
%legend(lineE,lineF,lineG,lineK,lineU,lineV,'Location','northeast'); % legend text
```

```
ax3=subplot(3,3,3); % Make a 3 x 3 grid of plots
omega_HAP = [1e-40 1e-30 1e-20 1e-15 1e-10 1e-5 1 1e5 1e10];
omegaHAPmatrix = repmat(omega_HAP', 1, 1000);
aPO4HAP = linspace(10^-15,10^-1, 1000); % changing the upper boundary affects
calculation of SI_HAP lines below
aCa_HAPlines = ((KspHAP.*a_H1.*omegaHAPmatrix)./(aPO4HAP.^3)).^(1/5);
omegaCC = aCa_HAPlines.*(aCO3_calcite./Ksp_Calcite); % Calcite saturation at
different Omega(HAP) values
SI_HAPlines = log10(omegaCC);

%-------Make legend text-------%

line1 = ['\Omega_{HAP} = 1e',num2str(log10(omega_HAP(1)))]; % Text lines that
update with Omega values
line2 = ['\Omega_{HAP} = 1e',num2str(log10(omega_HAP(2)))]; % Text lines that
update with Omega values
line3 = ['\Omega_{HAP} = 1e',num2str(log10(omega_HAP(3)))]; % Text lines that
update with Omega values
line4 = ['\Omega_{HAP} = 1e',num2str(log10(omega_HAP(4)))]; % Text lines that
update with Omega values
line5 = ['\Omega_{HAP} = 1e',num2str(log10(omega_HAP(5)))]; % Text lines that
update with Omega values
line6 = ['\Omega_{HAP} = 1e',num2str(log10(omega_HAP(6)))]; % Text lines that
update with Omega values
line7 = ['\Omega_{HAP} = 1e',num2str(log10(omega_HAP(7)))]; % Text lines that
update with Omega values
line8 = ['\Omega_{HAP} = 1e',num2str(log10(omega_HAP(8)))]; % Text lines that
update with Omega values
line9 = ['\Omega_{HAP} = 1e',num2str(log10(omega_HAP(9)))]; % Text lines that
update with Omega values

%plot(log10(aPO4HAP),SI_HAPlines);
%hold on;

outliersPO4 = excludedata(log10(aPO4),SI_Calcite,'domain',[-13 -5]); %
"outliersPO4a" if the 2nd and 3rd condition below are applied
%outliersPO4b = excludedata(log10(aPO4),SI_Calcite,'range',[-2 3]);
%outliersPO4 = outliersPO4a|outliersPO4b|aPO4outliers;

%gscatter(log10(aPO4(~outliersPO4)),SI_Calcite(~outliersPO4),pH_range1(~outliersPO4
));
%gscatter(log10(aPO4),SI_Calcite,pH_range1);
%gscatter(log10(aPO4(~outliersPO4)),SI_Calcite(~outliersPO4),ratioMgCa_new_rank2(~o
utliersPO4));
%gscatter(log10(aPO4(~outliersPO4)),SI_Calcite(~outliersPO4),conc_Ca_rank(~outliers
PO4));
gscatter(log10(aPO4(~outliersPO4)),SI_Calcite(~outliersPO4),aCa_rank(~outliersPO4))
;
```

```
%gscatter(log10(aPO4(~outliersPO4)),SI_Calcite(~outliersPO4),ALKtoMgCa_rank(~outlie
rsPO4));
%gscatter(log10(aPO4(~outliersPO4)),SI_Calcite(~outliersPO4),DeltaCO2_rank2(~outlie
rsPO4));
%gscatter(log10(aPO4(~outliersPO4)),SI_Calcite(~outliersPO4),SI_cal_rank(~outliersP
O4));
%gscatter(log10(aPO4(~outliersPO4)),SI_Calcite(~outliersPO4),country(~outliersPO4))
;
%gscatter(log10(aPO4(~outliersPO4)),SI_Calcite(~outliersPO4),Original_source(~outli
ersPO4));
%gscatter(log10(aPO4(~outliersPO4)),SI_Calcite(~outliersPO4),Lake(~outliersPO4));
hold on;
plot(logaPO4,SICalcite,'o');
hold off;

%legend(line1,line2,line3,line4,line5,line6,line7,line8,line9,'Location','best');
axis([-13 -5 -2 3])
xlabel('log(a_{PO4})'); % x-axis label
ylabel('Saturation Index (Calcite)'); % y-axis label


ax4 = subplot(3,3,4); % Make a 3 x 3 grid of plots
loglog(aCO3_Natron,a_Na,aCO3_Trona,a_Na,aCO3_TNT,a_Na,'LineWidth',1.5);
hold on;
%gscatter(aCO3(~aCO3outliers), aNa(~aCO3outliers), pH_range1(~aCO3outliers));
%gscatter(aCO3(~aCO3outliers), aNa(~aCO3outliers),
ratioMgCa_new_rank2(~aCO3outliers));
%gscatter(aCO3(~aCO3outliers), aNa(~aCO3outliers), aCa_rank(~aCO3outliers));
gscatter(aCO3(~aCO3outliers), aNa(~aCO3outliers), ALKtoMgCa_rank(~aCO3outliers));
%gscatter(aCO3(~aCO3outliers), aNa(~aCO3outliers), DeltaCO2_rank2(~aCO3outliers));
%gscatter(aCO3(~aCO3outliers), aNa(~aCO3outliers), SI_cal_rank(~aCO3outliers));
%gscatter(aCO3(~aCO3outliers), aNa(~aCO3outliers), country(~aCO3outliers));
hold off;
axis([1E-7 1e0 1E-7 1E4])
xlabel('a_{CO3}'); % x-axis label
ylabel('a_{Na}'); % y-axis label
%legend(lineP,lineR,lineT,'Location','best'); % legend text


ax5=subplot(3,3,5); % Make a 3 x 3 grid of plots
%gscatter(log10(aCa(~aCaoutliers)),SI_Natron(~aCaoutliers),pH_range1(~aCaoutliers))
;
%gscatter(log10(aCa(~aCaoutliers)),SI_Natron(~aCaoutliers),ratioMgCa_new_rank2(~aCa
outliers));
gscatter(log10(aCa(~aCaoutliers)),SI_Natron(~aCaoutliers),aCa_rank(~aCaoutliers));
%gscatter(log10(aCa(~aCaoutliers)),SI_Natron(~aCaoutliers),ALKtoMgCa_rank(~aCaoutli
ers));
%gscatter(log10(aCa(~aCaoutliers)),SI_Natron(~aCaoutliers),DeltaCO2_rank2(~aCaoutli
ers));
%gscatter(log10(aCa(~aCaoutliers)),SI_Natron(~aCaoutliers),SI_cal_rank(~aCaoutliers
));
```

```
%gscatter(log10(aCa(~aCaoutliers)),SI_Natron(~aCaoutliers),country(~aCaoutliers));
axis([-8 0 -18 0])
xlabel('log(a_{Ca})'); % x-axis label
ylabel('Saturation Index (Natron)'); % y-axis label


ax6=subplot(3,3,6); % Make a 3 x 3 grid of plots
%gscatter(log10(aMg(~aMgoutliers)),SI_Calcite(~aMgoutliers),pH_range1(~aMgoutliers)
);
%gscatter(log10(aMg(~aMgoutliers)),SI_Calcite(~aMgoutliers),ratioMgCa_new_rank2(~aM
goutliers));
gscatter(log10(aMg(~aMgoutliers)),SI_Calcite(~aMgoutliers),aCa_rank(~aMgoutliers));
%gscatter(log10(aMg(~aMgoutliers)),SI_Calcite(~aMgoutliers),pH_range1(~aMgoutliers)
);
%gscatter(log10(aMg(~aMgoutliers)),SI_Calcite(~aMgoutliers),ALKtoMgCa_rank(~aMgoutl
iers));
%gscatter(log10(aMg(~aMgoutliers)),SI_Calcite(~aMgoutliers),DeltaCO2_rank2(~aMgoutl
iers));
%gscatter(log10(aMg(~aMgoutliers)),SI_Calcite(~aMgoutliers),SI_cal_rank(~aMgoutlier
s));
%gscatter(log10(aMg(~aMgoutliers)),SI_Calcite(~aMgoutliers),ratioMgCa_new_rank2(~aM
goutliers));
%gscatter(log10(aMg(~aMgoutliers)),SI_Calcite(~aMgoutliers),country(~aMgoutliers));
%axis([-6 1 0 600])
axis([-6 1 -3 3])
xlabel('log(a_{Mg})'); % x-axis label
%ylabel('\Omega (Calcite)'); % y-axis label
ylabel('Saturation Index (Calcite)'); % y-axis label


ax7=subplot(3,3,7); % Make a 3 x 3 grid of plots
%gscatter(log10(aSiO2aq(~aSiO2outliers)),log10(aMg_aH_ratio(~aSiO2outliers)),pH_ran
ge1(~aSiO2outliers));
%gscatter(log10(aSiO2aq(~aSiO2outliers)),log10(aMg_aH_ratio(~aSiO2outliers)),ratioM
gCa_new_rank2(~aSiO2outliers));
gscatter(log10(aSiO2aq(~aSiO2outliers)),log10(aMg_aH_ratio(~aSiO2outliers)),aCa_ran
k(~aSiO2outliers));
%gscatter(log10(aSiO2aq(~aSiO2outliers)),log10(aMg_aH_ratio(~aSiO2outliers)),ALKtoM
gCa_rank(~aSiO2outliers));
%gscatter(log10(aSiO2aq(~aSiO2outliers)),log10(aMg_aH_ratio(~aSiO2outliers)),IonStr
_rank(~aSiO2outliers));
%gscatter(log10(aSiO2aq(~aSiO2outliers)),log10(aMg_aH_ratio(~aSiO2outliers)),conc_C
a_rank(~aSiO2outliers));
%gscatter(log10(aSiO2aq(~aSiO2outliers)),log10(aMg_aH_ratio(~aSiO2outliers)),DeltaC
O2_rank2(~aSiO2outliers));
%gscatter(log10(aSiO2aq(~aSiO2outliers)),log10(aMg_aH_ratio(~aSiO2outliers)),SI_cal
_rank(~aSiO2outliers));
%gscatter(log10(aSiO2aq(~aSiO2outliers)),log10(aMg_aH_ratio(~aSiO2outliers)),countr
y(~aSiO2outliers));
axis([-8 1 0 20])
xlabel('log(a_{SiO_2})'); % x-axis label
```

```
ylabel('log(a_{Mg}/a_{H^2})'); % y-axis label


% ax8=subplot(3,3,8); % Make a 3 x 3 grid of plots
% outliers_PO4a = excludedata(log10(aPO4),10.^(SI_Calcite),'domain',[-13 -5]);
% outliers_PO4sum = outliers_PO4a|aPO4outliers;
%
%gscatter(log10(aPO4(~outliers_PO4sum)),10.^SI_Calcite(~outliers_PO4sum),pH_range1(
~outliers_PO4sum));
%
%gscatter(log10(aPO4(~outliers_PO4sum)),10.^SI_Calcite(~outliers_PO4sum),ratioMgCa_
rank(~outliers_PO4sum));
%
gscatter(log10(aPO4(~outliers_PO4sum)),10.^SI_Calcite(~outliers_PO4sum),DeltaCO2_ra
nk2(~outliers_PO4sum));
% hold on;
% plot(logaPO4,10.^SICalcite,'o');
% hold off;
% axis([-13 -5  0 200])
% xlabel('log(a_{PO4})'); % x-axis label
% ylabel('\Omega (Calcite)'); % y-axis label


ax8=subplot(3,3,8); % Make a 3 x 3 grid of plots
outliersHPO4 = excludedata(log10(dic_molal),log10(conc_HPO4./1000),'range',[-10 -
8]);
gscatter(log10(dic_molal(outliersHPO4 &
~aCO3outliers)),log10((conc_HPO4(outliersHPO4 &
~aCO3outliers)./1000)),country(outliersHPO4 & ~aCO3outliers));
%gscatter(log10(dic_molal(outliersHPO4)),log10((conc_HPO4(outliersHPO4)./1000)),pH_
range1(outliersHPO4));
%gscatter(log10(dic_molal(outliersHPO4)),log10((conc_HPO4(outliersHPO4)./1000)),SI_
cal_rank(outliersHPO4));
%gscatter(log10(dic_molal(outliersHPO4)),log10((conc_HPO4(outliersHPO4)./1000)),ALK
toMgCa_rank(outliersHPO4));
%gscatter(log10(dic_molal(outliersHPO4)),log10((conc_HPO4(outliersHPO4)./1000)),aCa
_rank(outliersHPO4));
%gscatter(log10(dic_molal(outliersHPO4)),log10((conc_HPO4(outliersHPO4)./1000)),rat
ioMgCa_new_rank2(outliersHPO4));
%gscatter(log10(dic_molal(outliersHPO4)),log10((conc_HPO4(outliersHPO4)./1000)),Del
taCO2_rank2(outliersHPO4));
hold off;
axis([-4 1 -7 -1])
xlabel('log(DIC) (molal)'); % x-axis label
ylabel('log[\SigmaPO_4]'); % y-axis label


ax9=subplot(3,3,9); % Make a 3 x 3 grid of plots
loglog(aCa_ACMC,aPO4_ACP,aCa_ACMC,aPO4_OCP,aCa_ACMC,aPO4_HAP,'LineWidth',1.5);
axis([1e-8 1 1e-20 1])
hold on;
outliersA = ~excludedata(aCa,aPO4,'box',[1e-6 1e-1 1e-25 1e-16]);
```

```
outliersSum = outliersA|aCaoutliers;

%gscatter(aCa(~outliersSum), aPO4(~outliersSum), pH_range1(~outliersSum));
%gscatter(aCa(~outliersSum), aPO4(~outliersSum),
ratioMgCa_new_rank2(~outliersSum));
%gscatter(aCa(~outliersSum), aPO4(~outliersSum), ALKtoMgCa_rank(~outliersSum));
gscatter(aCa(~outliersSum), aPO4(~outliersSum), aCa_rank(~outliersSum));
%gscatter(aCa(~outliersSum), aPO4(~outliersSum), DeltaCO2_rank2(~outliersSum));
%gscatter(aCa(~outliersSum), aPO4(~outliersSum), SI_cal_rank(~outliersSum));
%gscatter(aCa(~outliersSum), aPO4(~outliersSum), country(~outliersSum));
axis([1e-8 1 1e-20 1])
hold off;
xlabel('a_{Ca}'); % x-axis label
ylabel('a_{PO4}'); % y-axis label


%% Extract list of samples and labels, whose CBE ≤ 10%, to show their Mg/Ca ratios
:
country_new = country(~aCaoutliers);
Lake_new = Lake(~aCaoutliers);
ratioMgCa_new_rank2_new = ratioMgCa_new_rank2(~aCaoutliers);
```

References

[1] Keisuke Fukushi and Haruna Matsumiya. "Control of water chemistry in alkaline lakes: solubility of monohydrocalcite and amorphous magnesium carbonate in $CaCl_2$–$MgCl_2$–Na_2CO_3 solutions". In: *ACS Earth and Space Chemistry* 2.7 (2018), pp. 735–744.

[2] Carlos Rodriguez-Navarro et al. "Direct nanoscale imaging reveals the growth of calcite crystals via amorphous nanoparticles". In: *Crystal Growth & Design* 16.4 (2016), pp. 1850–1860.

[3] LN Plummer et al. "PHRQPITZ, a computer program incorporating Pitzer's equations for calculation of geochemical reactions in brines". In: *US Geological Survey Water Resources Investigation Report* 88 (1988), p. 4153.

[4] CM Bethke, B Farrell, and M Sharifi. "The Geochemist's Workbench®, release 14: GWB essentials." In: *Aqueous Solutions, LLC, Champaign, IL* (2020).

[5] Robert A Berner. *Principles of chemical sedimentology*. Vol. 240. McGraw-Hill New York, 1971.

[6] Heinrich D Holland. *The chemical evolution of the atmosphere and oceans*. Princeton University Press, 1984.

[7] John P Grotzinger and Noel P James. "Precambrian carbonates: Evolution of understanding". In: *Carbonate Sedimentation and Diagenesis in the Evolving Precambrian World, SEPM Special Publication* 67 (2000), pp. 123–144.

[8] Dawn Y Sumner and John P Grotzinger. "Late Archean aragonite precipitation: petrography, facies associations, and environmental significance". In: *Carbonate Sedimentation and Diagenesis in the Evolving Precambrian World, SEPM Special Publication* 67 (2000), pp. 123–144.

[9] John P Grotzinger et al. "Geochemical model for Proterozoic stromatolite decline". In: *American Journal of Science* 290.80 (1990), e103.

[10] Nicholas T Arndt and Euan G Nisbet. "Processes on the young Earth and the habitats of early life". In: *Annual Review of Earth and Planetary Sciences* 40.521 (2012), p. 2012.

[11] Jihua Hao et al. "Cycling phosphorus on the Archean Earth: Part I. Continental weathering and riverine transport of phosphorus". In: *Geochimica et Cosmochimica Acta* 273 (2020), pp. 70–84.

[12] Dawn Y Sumner and John P Grotzinger. "Herringbone calcite; petrography and environmental significance". In: *Journal of Sedimentary Research* 66.3 (1996), pp. 419–429.

[13] Terry T Sami and Noel P James. "Synsedimentary cements as Paleoproterozoic platform building blocks, Pethei Group, northwestern Canada". In: *Journal of Sedimentary Research* 66.1 (1996).

[14] Henry S Chafetz and Sean A Guidry. "Bacterial shrubs, crystal shrubs, and ray-crystal shrubs: bacterial vs. abiotic precipitation". In: *Sedimentary Geology* 126.1-4 (1999), pp. 57–74.

[15] Michael C Pope and John P Grotzinger. "Controls on fabric development and morphology of tufas and stromatolites, uppermost Pethel Group (1.8 Ga), Great Slave Lake, northwest Canada". In: *Carbonate Sedimentation and Diagenesis in the Evolving Precambrian World, SEPM Special Publication* 67 (2000), pp. 103–121.

[16] DK Richter et al. "Radiaxial-fibrous calcites: A new look at an old problem". In: *Sedimentary Geology* 239.1-2 (2011), pp. 23–36.

[17] Javier Garcıa-Veigas et al. "A genetic model for Na-carbonate mineral precipitation in the Miocene Beypazarı trona deposit, Ankara province, Turkey". In: *Sedimentary Geology* 294 (2013), pp. 315–327.

[18] V Paul Wright and Andrew J Barnett. "An abiotic model for the development of textures in some South Atlantic early Cretaceous lacustrine carbonates". In: *Geological Society, London, Special Publications* 418.1 (2015), pp. 209–219.

[19] Juan Manuel Garcıa-Ruiz. "Geochemical scenarios for the precipitation of biomimetic inorganic carbonates". In: *Carbonate Sedimentation and Diagenesis in the Evolving Precambrian World, SEPM Special Publication* 67 (2000), pp. 75–89.

[20] Philippe Stephane Van Cappellen. "The formation of marine apatite: A kinetic study". PhD thesis. Yale University, 1991.

[21] James J De Yoreo and Peter G Vekilov. "Principles of crystal nucleation and growth". In: *Reviews in mineralogy and geochemistry* 54.1 (2003), pp. 57–93.

[22] James J De Yoreo et al. "Crystallization by particle attachment in synthetic, biogenic, and geologic environments". In: *Science* 349.6247 (2015), aaa6760.

[23] D Wang et al. "Revisiting geochemical controls on patterns of carbonate deposition through the lens of multiple pathways to mineralization". In: *Faraday Discussions* 159.1 (2012), pp. 371–386.

[24] W-K Burton, N Cabrera, and FC Frank. "The growth of crystals and the equilibrium structure of their surfaces". In: *Philosophical Transactions of the Royal Society of London. Series A, Mathematical and Physical Sciences* 243.866 (1951), pp. 299–358.

[25] Kevin J Davis, Patricia M Dove, and James J De Yoreo. "The role of Mg^{2+} as an impurity in calcite growth". In: *Science* 290.5494 (2000), pp. 1134–1137.

[26] John W Morse, Rolf S Arvidson, and Andreas Lüttge. "Calcium carbonate formation and dissolution". In: *Chemical reviews* 107.2 (2007), pp. 342–381.

[27] Giovanna Della Porta. "Carbonate build-ups in lacustrine, hydrothermal and fluvial settings: comparing depositional geometry, fabric types and geochemical signature". In: *Geological Society, London, Special Publications* 418.1 (2015), pp. 17–68.

[28] Benjamin M Tutolo and Nicholas J Tosca. "Experimental examination of the Mg-silicate-carbonate system at ambient temperature: Implications for alkaline chemical sedimentation and lacustrine carbonate formation". In: *Geochimica et Cosmochimica Acta* 225 (2018), pp. 80–101.

[29] Dario Fussmann et al. "Authigenic formation of Ca–Mg carbonates in the shallow alkaline Lake Neusiedl, Austria". In: *Biogeosciences* 17.7 (2020), pp. 2085–2106.

[30] Robert Jellison et al. "Meromixis in hypersaline Mono Lake, California. 2. Nitrogen fluxes". In: *Limnology and oceanography* 38.5 (1993), pp. 1020–1039.

[31] Miquela Ingalls et al. "P/Ca in carbonates as a proxy for alkalinity and phosphate levels". In: *Geophysical Research Letters* 47.21 (2020), e2020GL088804.

[32] Michael M Reddy. "Crystallization of calcium carbonate in the presence of trace concentrations of phosphorus-containing anions: I. Inhibition by phosphate and glycerophosphate ions at pH 8.8 and 25°C". In: *Journal of Crystal Growth* 41.2 (1977), pp. 287–295.

[33] Alfonso Mucci and John W Morse. "The incorporation of Mg^{2+} and Sr^{2+} into calcite overgrowths: influences of growth rate and solution composition". In: *Geochimica et Cosmochimica Acta* 47.2 (1983), pp. 217–233.

[34] Andrew J Gratz and Paul E Hillner. "Poisoning of calcite growth viewed in the atomic force microscope (AFM)". In: *Journal of crystal growth* 129.3-4 (1993), pp. 789–793.

[35] Yi-Pin Lin and Philip C Singer. "Inhibition of calcite precipitation by orthophosphate: speciation and thermodynamic considerations". In: *Geochimica et Cosmochimica Acta* 70.10 (2006), pp. 2530–2539.

[36] Ramon Mercedes-Martın et al. "Growing spherulitic calcite grains in saline, hyperalkaline lakes: experimental evaluation of the effects of Mg-clays and organic acids". In: *Sedimentary Geology* 335 (2016), pp. 93–102.

[37] Hans P Eugster and Blair F Jones. "Behavior of major solutes during closed-basin brine evolution". In: *American journal of science* 279.6 (1979), pp. 609–631.

[38] Abdallah Al-Droubi et al. "Generalized residual alkalinity concept; application to prediction of the chemical evolution of natural waters by evaporation". In: *American Journal of Science* 280.6 (1980), pp. 560–572.

[39] Allan Pentecost. "The formation of travertine shrubs: mammoth hot springs, Wyoming". In: *Geological Magazine* 127.2 (1990), pp. 159–168.

[40] Brian Jones. "Review of aragonite and calcite crystal morphogenesis in thermal spring systems". In: *Sedimentary Geology* 354 (2017), pp. 9–23.

[41] Denis Gebauer, Antje Volkel, and Helmut Colfen. "Stable prenucleation calcium carbonate clusters". In: *Science* 322.5909 (2008), pp. 1819–1822.

[42] Juan Diego Rodriguez-Blanco et al. "The role of Mg in the crystallization of monohydrocalcite". In: *Geochimica et Cosmochimica Acta* 127 (2014), pp. 204–220.

[43] Bettina Purgstaller et al. "Transformation of Mg-bearing amorphous calcium carbonate to Mg-calcite–In situ monitoring". In: *Geochimica et Cosmochimica Acta* 174 (2016), pp. 180–195.

[44] Christina R Blue et al. "Chemical and physical controls on the transformation of amorphous calcium carbonate into crystalline $CaCO_3$ polymorphs". In: *Geochimica et Cosmochimica Acta* 196 (2017), pp. 179–196.

[45] Marzena Prus et al. "Electrophoretic and potentiometric signatures of multistage $CaCO_3$ nucleation". In: *Journal of colloid and interface science* 544 (2019), pp. 249–256.

[46] Vanessa Schoeppler et al. "Crystallization by Amorphous Particle Attachment: On the Evolution of Texture". In: *Advanced Materials* 33.37 (2021), p. 2101358.

[47] Alison Lewis et al. *Industrial crystallization: fundamentals and applications*. Cambridge University Press, 2015.

[48] Robert L Folk and Riccardo Assereto. "Comparative fabrics of length-slow and length-fast calcite and calcitized aragonite in a Holocene speleothem, Carlsbad Caverns, New Mexico". In: *Journal of Sedimentary Research* 46.3 (1976), pp. 486–496.

[49] Maurice E Tucker. "Diagenesis, geochemistry, and origin of a Precambrian dolomite; the Beck Spring Dolomite of eastern California". In: *Journal of Sedimentary Research* 53.4 (1983), pp. 1097–1119.

[50] Katja Henzler et al. "Supersaturated calcium carbonate solutions are classical". In: *Science advances* 4.1 (2018), eaao6283.

[51] J Hershey, Marino Fernandez, and Frank J Millero. "The dissociation of phosphoric acid in NaCl and NaMgCl solutions at 25^{o}C". In: *Journal of solution chemistry* 18.9 (1989), pp. 875–891.

[52] Robert M Garrels and Charles L Christ. *Solutions, minerals, and equilibria*. Harper & Row, 1965.

[53] Alfred H Truesdell and Blair F Jones. "WATEQ, a computer program for calculating chemical equilibria of natural waters". In: *J. Res. US Geol. Surv* 2.2 (1974), pp. 233–248.

[54] Kenneth S Pitzer. *A thermodynamic model for aqueous solutions of liquid-like density*. Lawrence Berkeley Laboratory, University of California, Berkeley, 1987.

[55] Werner Stumm and James J Morgan. *Aquatic chemistry: chemical equilibria and rates in natural waters*. John Wiley & Sons, 1996.

[56] JI Drever. *The Geochemistry of Natural Waters: Surface and Groundwater Environments*. Prentice Hall, New Jersey, USA, 1997.

[57] Patrick Brezonik and William Arnold. *Water chemistry: an introduction to the chemistry of natural and engineered aquatic systems*. OUP USA, 2011.

[58] Gregor Munro Anderson. *Thermodynamics of natural systems: Theory and Applications in Geochemistry and Environmental Science. 3rd ed*. Cambridge University Press, 2017.

[59] L Niel Plummer and Eurybiades Busenberg. "The solubilities of calcite, aragonite and vaterite in CO_2-H_2O solutions between 0 and 90^{o}C, and an evaluation of the aqueous model for the system $CaCO_3$-CO_2-H_2O". In: *Geochimica et cosmochimica acta* 46.6 (1982), pp. 1011–1040.

[60] Gregor Munro Anderson and David A Crerar. *Thermodynamics in geochemistry: the equilibrium model*. Oxford University Press, 1993.

[61] Peter William Atkins and Julio de Paula. *Atkins' physical chemistry*. Oxford university press, 2014.

[62] C W Davies. *Ion Association*. Butterworths, 1962.

[63] Robert Anthony Robinson and Robert Harold Stokes. *Electrolyte solutions*. Butterworths Scientific Publications, 1955.

[64] Harold C Helgeson. "Thermodynamics of hydrothermal systems at elevated temperatures and pressures". In: *American journal of science* 267.7 (1969), pp. 729–804.

[65] Harold C Helgeson and David H Kirkham. "Theoretical prediction of the thermodynamic behavior of aqueous electrolytes at high pressures and temperatures; II, Debye-Huckel parameters for activity coefficients and relative partial molal properties". In: *American Journal of Science* 274.10 (1974), pp. 1199–1261.

[66] Craig M Bethke. *Geochemical and biogeochemical reaction modeling*. Cambridge university press, 2008.

[67] Charles E Harvie, Nancy Møller, and John H Weare. "The prediction of mineral solubilities in natural waters: The $Na\text{-}K\text{-}Mg\text{-}Ca\text{-}H\text{-}Cl\text{-}SO_4\text{-}OH\text{-}HCO_3\text{-}CO_3\text{-}CO_2\text{-}H_2O$ system to high ionic strengths at 25^oC". In: *Geochimica et Cosmochimica Acta* 48.4 (1984), pp. 723–751.

[68] MS Tung et al. "Octacalcium phosphate solubility product from 4 to 37^oC". In: *Journal of Research of the National Bureau of Standards* 93.5 (1988), p. 613.

[69] Jonathan D Toner and David C Catling. "Alkaline lake settings for concentrated prebiotic cyanide and the origin of life". In: *Geochimica et Cosmochimica Acta* 260 (2019), pp. 124–132.

[70] John D Sutherland. "The origin of life—out of the blue". In: *Angewandte Chemie International Edition* 55.1 (2016), pp. 104–121.

[71] Francois MM Morel and Janet G Hering. *Principles and applications of aquatic chemistry*. John Wiley & Sons, 1993.

[72] Richard E Zeebe and Dieter Wolf-Gladrow. *CO2 in seawater: equilibrium, kinetics, isotopes*. 65. Elsevier, 2001.

[73] Ulrich Theodore Hammer. *Saline lake ecosystems of the world*. Vol. 59. Springer Science & Business Media, 1986.

[74] Giovannella Pecoraino, Walter D'Alessandro, and Salvatore Inguaggiato. "The other side of the coin: geochemistry of alkaline lakes in volcanic areas". In: *Volcanic lakes*. Springer, 2015, pp. 219–237.

[75] Marie Edmonds et al. "Magmatic carbon outgassing and uptake of CO_2 by alkaline waters". In: *American Mineralogist: Journal of Earth and Planetary Materials* 105.1 (2020), pp. 28–34.

[76] Abraham Lerman and Werner Stumm. "CO_2 storage and alkalinity trends in lakes". In: *Water Research* 23.2 (1989), pp. 139–146.

[77] Kerri Finlay et al. "Decrease in CO_2 efflux from northern hardwater lakes with increasing atmospheric warming". In: *Nature* 519.7542 (2015), pp. 215–218.

[78] Jasmine E Chase, Maria L Arizaleta, and Benjamin M Tutolo. "A series of data-driven hypotheses for inferring biogeochemical conditions in alkaline lakes and their deposits based on the behavior of Mg and SiO_2". In: *Minerals* 11.2 (2021), p. 106.

[79] Andreas Reimer, Günter Landmann, and Stephan Kempe. "Lake Van, eastern Anatolia, hydrochemistry and history". In: *Aquatic Geochemistry* 15.1 (2009), pp. 195–222.

[80] Fadila Darragi and Yves Tardy. "Authigenic trioctahedral smectites controlling pH, alkalinity, silica and magnesium concentrations in alkaline lakes". In: *Chemical Geology* 63.1-2 (1987), pp. 59–72.

[81] Dieter A Wolf-Gladrow et al. "Total alkalinity: The explicit conservative expression and its application to biogeochemical processes". In: *Marine Chemistry* 106.1-2 (2007), pp. 287–300.

[82] Andrew G Dickson. "An exact definition of total alkalinity and a procedure for the estimation of alkalinity and total inorganic carbon from titration data". In: *Deep Sea Research Part A. Oceanographic Research Papers* 28.6 (1981), pp. 609–623.

[83] John W Morse and Fred T Mackenzie. *Geochemistry of sedimentary carbonates*. Elsevier, 1990.

[84] Jonathan D Sharp and Robert H Byrne. "Excess alkalinity in carbonate system reference materials". In: *Marine Chemistry* 233 (2021), p. 103965.

[85] Ian Clark. *Groundwater geochemistry and isotopes*. CRC press, 2015.

[86] Metrohm. *916 Ti-Touch Manual*. Metrohm. Herisau, Switzerland, 2017.

[87] BB Cael, AJ Heathcote, and DA Seekell. "The volume and mean depth of Earth's lakes". In: *Geophysical Research Letters* 44.1 (2017), pp. 209–218.

[88] JF Talling et al. "The upper limit of photosynthetic productivity by phytoplankton: evidence from Ethiopian soda lakes". In: *Freshwater Biology* 3.1 (1973), pp. 53–76.

[89] Robin W Renaut and Peter R Long. "Sedimentology of the saline lakes of the Cariboo plateau, Interior British Columbia, Canada". In: *Sedimentary Geology* 64.4 (1989), pp. 239–264.

[90] LA Hardie and Hans P. Eugster. "The evolution of closed basin brines". In: *Mineral. Soc. Spec. Paper* 3 (1970), pp. 273–290.

[91] C Hillaire-Marcel and Joel Casanova. "Isotopic hydrology and paleohydrology of the Madagi (Kenya)-Natron (Tanzania) basin during the late Quaternary". In: *Palaeogeography, Palaeoclimatology, Palaeoecology* 58.3-4 (1987), pp. 155–181.

[92] Larry Benson, Lloyd D White, and Robert Rye. "Carbonate deposition, Pyramid Lake Subbasin, Nevada: 4. Comparison of the stable isotope values of carbonate deposits (tufas) and the Lahontan lake-level record". In: *Palaeogeography, Palaeoclimatology, Palaeoecology* 122.1-4 (1996), pp. 45–76.

[93] John M Melack and Peter Kilham. "Photosynthetic rates of phytoplankton in East African alkaline, saline lakes 1". In: *Limnology and oceanography* 19.5 (1974), pp. 743–755.

[94] Jonathan D Toner and David C Catling. "A carbonate-rich lake solution to the phosphate problem of the origin of life". In: *Proceedings of the National Academy of Sciences* 117.2 (2020), pp. 883–888.

[95] Dimitar D Sasselov, John P Grotzinger, and John D Sutherland. "The origin of life as a planetary phenomenon". In: *Science Advances* 6.6 (2020), eaax3419.

[96] Hans P Eugster. "Chemistry and origin of the brines of Lake Magadi, Kenya". In: *Mineral. Soc. Amer., Spec. Pap.;(United States)* 3 (1970).

[97] Blair F Jones, Hans P Eugster, and Shirley L Rettig. "Hydrochemistry of the lake Magadi basin, Kenya". In: *Geochimica et Cosmochimica Acta* 41.1 (1977), pp. 53–72.

[98] Johannes F Imhoff et al. "The Wadi Natrun: chemical composition and microbial mass developments in alkaline brines of eutrophic desert lakes". In: *Geomicrobiology Journal* 1.3 (1979), pp. 219–234.

[99] PJ Ashton and FR Schoeman. "Limnological studies on the Pretoria Salt Pan, a hypersaline maar lake". In: *Hydrobiologia* 99.1 (1983), pp. 61–73.

[100] Joanne Frances Hirst. "Sedimentology, diagenesis and hydrochemistry of the saline, alkaline lakes on the Cariboo Plateau, Interior British Columbia, Canada". MA thesis. University of Saskatchewan, 1995.

[101] SL Shvartsev et al. "Geochemistry and chemical evolution of saline lakes of Western Mongolia". In: *Geochemistry International* 52.5 (2014), pp. 388–403.

[102] Renato L Guerreiro et al. "The soda lakes of Nhecolândia: a conservation opportunity for the Pantanal wetlands". In: *Perspectives in ecology and conservation* 17.1 (2019), pp. 9–18.

[103] Nicholas J Tosca et al. "Geochemical modeling of evaporation processes on Mars: Insight from the sedimentary record at Meridiani Planum". In: *Earth and Planetary Science Letters* 240.1 (2005), pp. 122–148.

[104] Nicholas J Tosca and Scott M McLennan. "Experimental constraints on the evaporation of partially oxidized acid-sulfate waters at the martian surface". In: *Geochimica et Cosmochimica Acta* 73.4 (2009), pp. 1205–1222.

[105] Nicholas J Tosca et al. "Physicochemical properties of concentrated Martian surface waters". In: *Journal of Geophysical Research: Planets* 116.E5 (2011).

[106] Rotem Golan et al. "The determination of pH in hypersaline lakes with a conventional combination glass electrode". In: *Limnology and Oceanography: Methods* 12.11 (2014), pp. 810–815.

[107] Bettina Purgstaller et al. "Solubility investigations in the amorphous calcium magnesium carbonate system". In: *CrystEngComm* 21.1 (2019), pp. 155–164.

[108] Giles M Marion. "Carbonate mineral solubility at low temperatures in the Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system". In: *Geochimica et Cosmochimica Acta* 65.12 (2001), pp. 1883–1896.

[109] GM Marion et al. "Modeling hot spring chemistries with applications to martian silica formation". In: *Icarus* 212.2 (2011), pp. 629–642.

[110] HC Whitehead and JH Feth. "Recent chemical analyses of waters from several closed-basin lakes and their tributaries in the western United States". In: *Geological Society of America Bulletin* 72.9 (1961), pp. 1421–1425.

[111] Kenneth N Phillips and AS Van Denburgh. *Hydrology and geochemistry of Abert, Summer, and Goose Lakes and other closed-basin lakes in south-central Oregon*. US Government Printing Office, 1971.

[112] John K Warren. "Evaporites through time: Tectonic, climatic and eustatic controls in marine and nonmarine deposits". In: *Earth-Science Reviews* 98.3-4 (2010), pp. 217–268.

[113] John de Kanel and John W Morse. "The chemistry of orthophosphate uptake from seawater on to calcite and aragonite". In: *Geochimica et Cosmochimica Acta* 42.9 (1978), pp. 1335–1340.

[114] Michael M Reddy and K Karin Wang. "Crystallization of calcium carbonate in the presence of metal ions: I. Inhibition by magnesium ion at pH 8.8 and 25°C". In: *Journal of Crystal Growth* 50.2 (1980), pp. 470–480.

[115] HJ Meyer. "The influence of impurities on the growth rate of calcite". In: *Journal of Crystal Growth* 66.3 (1984), pp. 639–646.

[116] Alfonso Mucci. "Growth kinetics and composition of magnesian calcite overgrowths precipitated from seawater: Quantitative influence of orthophosphate ions". In: *Geochimica et Cosmochimica Acta* 50.10 (1986), pp. 2255–2265.

[117] Elizabeth A Burton and Lynn M Walter. "The role of pH in phosphate inhibition of calcite and aragonite precipitation rates in seawater". In: *Geochimica et Cosmochimica Acta* 54.3 (1990), pp. 797–808.

[118] Patricia M Dove and Michael F Hochella Jr. "Calcite precipitation mechanisms and inhibition by orthophosphate: In situ observations by Scanning Force Microscopy". In: *Geochimica et cosmochimica acta* 57.3 (1993), pp. 705–714.

[119] Lawrence A Hardie. "Secular variation in seawater chemistry: An explanation for the coupled secular variation in the mineralogies of marine limestones and potash evaporites over the past 600 my". In: *Geology* 24.3 (1996), pp. 279–283.

[120] Friedrich Lippmann. *Sedimentary Carbonate Minerals*. Springer, 1973.

[121] E Atlas and RM Pytkowicz. "Solubility behavior of apatites in seawater". In: *Limnology and Oceanography* 22.2 (1977), pp. 290–300.

[122] Anneli Gunnars, Sven Blomqvist, and Cajsa Martinsson. "Inorganic formation of apatite in brackish seawater from the Baltic Sea: an experimental approach". In: *Marine Chemistry* 91.1-4 (2004), pp. 15–26.

[123] Matthew P Brady, Rosalie Tostevin, and Nicholas J Tosca. "Marine phosphate availability and the chemical origins of life on Earth". In: *Nature communications* 13.1 (2022), pp. 1–9.

[124] Sascha Roest-Ellis, Justin V Strauss, and Nicholas J Tosca. "Experimental constraints on nonskeletal $CaCO_3$ precipitation from Proterozoic seawater". In: *Geology* 49.5 (2021), pp. 561–565.

[125] Dawn Y Sumner and John P Grotzinger. "Were kinetics of Archean calcium carbonate precipitation related to oxygen concentration?" In: *Geology* 24.2 (1996), pp. 119–122.

[126] Frank J Millero and Denis Pierrot. "A chemical equilibrium model for natural waters". In: *Aquatic Geochemistry* 4.1 (1998), pp. 153–199.

[127] Arne Erik Nielsen. "Electrolyte crystal growth mechanisms". In: *Journal of Crystal Growth* 67.2 (1984), pp. 289–310.

[128] James L Bischoff. "Kinetics of calcite nucleation: magnesium ion inhibition and ionic strength catalysis". In: *Journal of Geophysical Research* 73.10 (1968), pp. 3315–3322.

[129] PM Gruzensky. "Growth of calcite crystals". In: *Crystal growth* (1967), pp. 365–367.

[130] Richard J Reeder, Richard O Fagioli, and William J Meyers. "Oscillatory zoning of Mn in solution-grown calcite crystals". In: *Earth-Science Reviews* 29.1-4 (1990), pp. 39–46.

[131] R Beck, M Seiersten, and J-P Andreassen. "The constant composition method for crystallization of calcium carbonate at constant supersaturation". In: *Journal of crystal growth* 380 (2013), pp. 187–196.

[132] RL Snyder and David L Bish. "Quantitative analysis". In: *Modern powder diffraction* 20 (1989), pp. 101–144.

[133] Thomas Degen et al. "The highscore suite". In: *Powder diffraction* 29.S2 (2014), S13–S18.

[134] German Montes-Hernandez and François Renard. "Time-resolved in situ raman spectroscopy of the nucleation and growth of siderite, magnesite, and calcite and their precursors". In: *Crystal Growth & Design* 16.12 (2016), pp. 7218–7230.

[135] Laura Borromeo et al. "Raman spectroscopy as a tool for magnesium estimation in Mg-calcite". In: *Journal of Raman Spectroscopy* 48.7 (2017), pp. 983–992.

[136] Bettina Purgstaller et al. "Control of Mg^{2+}/Ca^{2+} activity ratio on the formation of crystalline carbonate minerals via an amorphous precursor". In: *Crystal Growth & Design* 17.3 (2017), pp. 1069–1078.

[137] Florian Konrad et al. "Influence of aqueous Mg concentration on the transformation of amorphous calcium carbonate". In: *Journal of Crystal Growth* 498 (2018), pp. 381–390.

[138] Marco Bruno et al. "New estimates of the free energy of calcite/water interfaces for evaluating the equilibrium shape and nucleation mechanisms". In: *Crystal growth & design* 13.3 (2013), pp. 1170–1179.

[139] Laura C Nielsen and Donald J DePaolo. "Ca isotope fractionation in a high-alkalinity lake system: Mono Lake, California". In: *Geochimica et Cosmochimica Acta* 118 (2013), pp. 276–294.

[140] Brent Fultz. *Phase transitions in materials*. Cambridge University Press, 2020.

[141] Arne Erik Nielsen and J Christoffersen. "The mechanisms of chrystal growth and dissolution". In: *Biological mineralization and demineralization*. Springer, 1982, pp. 37–77.

[142] Arne Erik Nielsen and Jens M Toft. "Electrolyte crystal growth kinetics". In: *Journal of crystal growth* 67.2 (1984), pp. 278–288.

[143] Carl I Steefel and Philippe Van Cappellen. "A new kinetic approach to modeling water-rock interaction: The role of nucleation, precursors, and Ostwald ripening". In: *Geochimica et Cosmochimica Acta* 54.10 (1990), pp. 2657–2677.

[144] Wenhao Sun et al. "Nucleation of metastable aragonite CaCO3 in seawater". In: *Proceedings of the National Academy of Sciences* 112.11 (2015), pp. 3199–3204.

[145] Antonio C Lasaga. *Kinetic theory in the earth sciences*. Princeton, 1998.

[146] Barbara Myszka et al. "Phase-specific bioactivity and altered Ostwald ripening pathways of calcium carbonate polymorphs in simulated body fluid". In: *RSC advances* 9.32 (2019), pp. 18232–18244.

[147] Yaguang Zhu et al. "Sulfate-controlled heterogeneous CaCO3 nucleation and its non-linear interfacial energy evolution". In: *Environmental Science & Technology* 55.16 (2021), pp. 11455–11464.

[148] Ichiro Sunagawa. *Crystals: growth, morphology, & perfection*. Cambridge University Press, 2007.

[149] Ryoji Shiraki and Susan L Brantley. "Kinetics of near-equilibrium calcite precipitation at 100^{o}C: An evaluation of elementary reaction-based and affinity-based rate laws". In: *Geochimica et Cosmochimica Acta* 59.8 (1995), pp. 1457–1471.

[150] Clancy Zhijian Jiang and Nicholas J Tosca. "Growth kinetics of siderite at 298.15 K and 1 bar". In: *Geochimica et Cosmochimica Acta* 274 (2020), pp. 97–117.

[151] Raphael Pietzsch et al. "The role of phosphate on non-skeletal carbonate production in a Cretaceous alkaline lake". In: *Geochimica et Cosmochimica Acta* 317 (2022), pp. 365–394.

[152] Raymond H Bate, Nicholas R Cameron, and Mario GP Brandao. "The lower cretaceous (pre-salt) lithostratigraphy of the Kwanza basin, Angola". In: *Newsletters on Stratigraphy* (2001), pp. 117–127.

[153] GD Karner and LAP Gambôa. "Timing and origin of the South Atlantic pre-salt sag basins and their capping evaporites". In: *Geological Society, London, Special Publications* 285.1 (2007), pp. 15–35.

[154] Trond H Torsvik et al. "A new scheme for the opening of the South Atlantic Ocean and the dissection of an Aptian salt basin". In: *Geophysical Journal International* 177.3 (2009), pp. 1315–1333.

[155] Peter A Kukla, Frank Strozyk, and Webster U Mohriak. "South Atlantic salt basins–witnesses of complex passive margin evolution". In: *Gondwana Research* 53 (2018), pp. 41–57.

[156] Leonardo R Tedeschi et al. "New age constraints on Aptian evaporites and carbonates from the South Atlantic: Implications for Oceanic Anoxic Event 1a". In: *Geology* 45.6 (2017), pp. 543–546.

[157] JP Gomes et al. "Facies classification and patterns of lacustrine carbonate deposition of the Barra Velha Formation, Santos Basin, Brazilian Pre-salt". In: *Marine and Petroleum Geology* 113 (2020), p. 104176.

[158] Bruno Eustáquio Moreira Lima et al. "Deep-burial hydrothermal alteration of the Pre-Salt carbonate reservoirs from northern Campos Basin, offshore Brazil: evidence from petrography, fluid inclusions, Sr, C and O isotopes". In: *Marine and Petroleum Geology* 113 (2020), p. 104143.

[159] Anne-Claire Chaboureau et al. "Paleogeographic evolution of the central segment of the South Atlantic during Early Cretaceous times: Paleotopographic and geodynamic implications". In: *Tectonophysics* 604 (2013), pp. 191–223.

[160] Peter Szatmari and Edison J Milani. "Tectonic control of the oil-rich large igneous-carbonate-salt province of the South Atlantic rift". In: *Marine and Petroleum Geology* 77 (2016), pp. 567–596.

[161] Stephen F Poropat and Jean-Paul Colin. "Early Cretaceous ostracod biostratigraphy of eastern Brazil and western Africa: An overview". In: *Gondwana Research* 22.3-4 (2012), pp. 772–798.

[162] Daniel L Thompson, Jeffrey D Stilwell, and Mike Hall. "Lacustrine carbonate reservoirs from Early Cretaceous rift lakes of Western Gondwana: Pre-salt coquinas of Brazil and West Africa". In: *Gondwana Research* 28.1 (2015), pp. 26–51.

[163] MC Muniz and DWJ Bosence. "Pre-salt microbialites from the Campos Basin (offshore Brazil): image log facies, facies model and cyclicity in lacustrine carbonates". In: *Geological Society, London, Special Publications* 418.1 (2015), pp. 221–242.

[164] Teresa Sabato Ceraldi and Darryl Green. "Evolution of the South Atlantic lacustrine deposits in response to Early Cretaceous rifting, subsidence and lake hydrology". In: *Geological Society, London, Special Publications* 438.1 (2017), pp. 77–98.

[165] Jobel Lourenço Pinheiro Moreira et al. "Bacia de Santos". In: *Boletim de Geociencias da Petrobras* 15.2 (2007), pp. 531–549.

[166] V Paul Wright. "Lacustrine carbonates in rift settings: the interaction of volcanic and microbial processes on carbonate deposition". In: *Geological Society, London, Special Publications* 370.1 (2012), pp. 39–47.

[167] Nicholas J Tosca and V Paul Wright. "Diagenetic pathways linked to labile Mg-clays in lacustrine carbonate reservoirs: a model for the origin of secondary porosity in the Cretaceous pre-salt Barra Velha Formation, offshore Brazil". In: *Geological Society, London, Special Publications* 435.1 (2018), pp. 33–46.

[168] JL Dias et al. "Tectonic, stratigraphy and sedimentation during the Aptian along the Brazilian eastern margin". PhD thesis. 2005, pp. 7–25.

[169] WR Winter, RJ Jahnert, AB França, et al. "Bacia de campos". In: *Boletim de Geociencias da Petrobras* 15.2 (2007), pp. 511–529.

[170] CR Rodriguez et al. "Dual tectonic-climatic controls on salt giant deposition in the Santos Basin, offshore Brazil". In: *Geosphere* 14.1 (2018), pp. 215–242.

[171] Leonardo R Tedeschi et al. "Aptian carbon-isotope record from the Sergipe-Alagoas Basin: New insights into oceanic anoxic event 1a and the timing of seawater entry into the South Atlantic". In: *Newsletters on Stratigraphy* (2020).

[172] Andrew H Knoll. "Biomineralization and evolutionary history". In: *Reviews in mineralogy and geochemistry* 54.1 (2003), pp. 329–356.

[173] Marjorie D Cantine, Andrew H Knoll, and Kristin D Bergmann. "Carbonates before skeletons: A database approach". In: *Earth-Science Reviews* 201 (2020), p. 103065.

[174] Laura M Barge et al. "Pyrophosphate synthesis in iron mineral films and membranes simulating prebiotic submarine hydrothermal precipitates". In: *Geochimica et Cosmochimica Acta* 128 (2014), pp. 1–12.

[175] V Paul Wright. "The mantle, CO_2 and the giant Aptian chemogenic lacustrine carbonate factory of the South Atlantic: Some carbonates are made, not born". In: *Sedimentology* 69.1 (2022), pp. 47–73.

[176] Raphael Pietzsch. "Comment on "Evaporitic carbonates in the pre-salt of Santos Basin–Genesis and tectonic implications"". In: *Marine and Petroleum Geology* 133 (2021), p. 104963.

[177] Renato T Bertani and Albert V Carozzi. "Lagoa Feia Formation (Lower Cretaceous) Campos Basin, offshore Brazil: Rift valley type lacustrine carbonate reservoirs-I". In: *Journal of Petroleum Geology* 8.1 (1985), pp. 37–58.

[178] RT Bertani and AV Carozzi. "Lagoa Feia Formation (Lower Cretaceous) Campos Basin, offshore Brazil: Rift valley type lacustrine carbonate reservoirs—II". In: *Journal of Petroleum Geology* 8.2 (1985), pp. 199–220.

[179] Mario Carminatti, Breno Wolff, and Luiz Gamboa. "New exploratory frontiers in Brazil". In: *19th World Petroleum Congress*. OnePetro. 2008.

[180] Gerson Jose Salamoni Terra, Adali Ricardo Spadini, Almerio Barros Franca, et al. "Carbonate rock classification applied to brazilian sedimentary basins; Classificacao de rochas carbonaticas aplicavel as bacias sedimentares brasileiras". In: *Boletim de Geociências da Petrobras* 18 (2010).

[181] JP Buckley, D Bosence, and Chris Elders. "Tectonic setting and stratigraphic architecture of an Early Cretaceous lacustrine carbonate platform, Sugar Loaf High, Santos Basin, Brazil". In: *Geological Society, London, Special Publications* 418.1 (2015), pp. 175–191.

[182] RS Alvarenga et al. "Seismic characteristics and distribution of hydrothermal vent complexes in the Cretaceous offshore rift section of the Campos Basin, offshore Brazil". In: *Marine and Petroleum Geology* 74 (2016), pp. 12–25.

[183] G Armelenti et al. "Deposition, diagenesis and reservoir potential of non-carbonate sedimentary rocks from the rift section of Campos Basin, Brazil". In: *Petroleum Geoscience* 22.3 (2016), pp. 223–239.

[184] Arthur Saller et al. "Presalt stratigraphy and depositional systems in the Kwanza Basin, offshore Angola". In: *Aapg Bulletin* 100.7 (2016), pp. 1135–1164.

[185] Ronaldo Herlinger Jr, Eveline Ellen Zambonato, and Luiz Fernando De Ros. "Influence of diagenesis on the quality of Lower Cretaceous pre-salt lacustrine carbonate reservoirs from northern Campos Basin, offshore Brazil". In: *Journal of Sedimentary Research* 87.12 (2017), pp. 1285–1313.

[186] Pierre-Alexandre Teboul et al. "Volcanic rock alterations of the Kwanza Basin, offshore Angola-Insights from an integrated petrological, geochemical and numerical approach". In: *Marine and Petroleum Geology* 80 (2017), pp. 394–411.

[187] Henry Chafetz et al. "Origins of carbonate spherulites: implications for Brazilian Aptian pre-salt reservoir". In: *Sedimentary Geology* 365 (2018), pp. 21–33.

[188] Bruno Eustáquio Moreira Lima and Luiz Fernando De Ros. "Deposition, diagenetic and hydrothermal processes in the Aptian Pre-Salt lacustrine carbonate reservoirs of the northern Campos Basin, offshore Brazil". In: *Sedimentary Geology* 383 (2019), pp. 55–81.

[189] Ramon Mercedes-Martın et al. "The hydrochemical evolution of alkaline volcanic lakes: a model to understand the South Atlantic Pre-salt mineral assemblages". In: *Earth-Science Reviews* 198 (2019), p. 102938.

[190] Pierre-Alexandre Teboul et al. "Diversity and origin of quartz cements in continental carbonates: Example from the Lower Cretaceous rift deposits of the South Atlantic margin". In: *Applied geochemistry* 100 (2019), pp. 22–41.

[191] V Paul Wright and Andrew J Barnett. "The textural evolution and ghost matrices of the Cretaceous Barra Velha Formation carbonates from the Santos Basin, offshore Brazil". In: *Facies* 66.1 (2020), pp. 1–18.

[192] Raphael Pietzsch et al. "Palaeohydrology of the Lower Cretaceous pre-salt lacustrine system, from rift to post-rift phase, Santos Basin, Brazil". In: *Palaeogeography, Palaeoclimatology, Palaeoecology* 507 (2018), pp. 60–80.

[193] Raphael Pietzsch et al. "Environmental conditions of deposition of the Lower Cretaceous lacustrine carbonates of the Barra Velha Formation, Santos Basin (Brazil), based on stable carbon and oxygen isotopes: a continental record of pCO_2 during the onset of the Oceanic Anoxic Event 1a (OAE 1a) interval?" In: *Chemical Geology* 535 (2020), p. 119457.

[194] Victor Hugo G Pinto et al. "Seawater storage and element transfer associated with mantle serpentinization in magma-poor rifted margins: A quantitative approach". In: *Earth and Planetary Science Letters* 459 (2017), pp. 227–237.

[195] Felipe Farias et al. "Evaporitic carbonates in the pre-salt of Santos Basin–Genesis and tectonic implications". In: *Marine and Petroleum Geology* 105 (2019), pp. 251–272.

[196] Jeferson L Dias. "Análise sedimentológica e estratigráfica do andar aptiano em parte da margem leste do Brasil e no Platô das Malvinas: considerações sobre as primeiras incursões e ingressões marinhas do Oceano Atlântico Sul Meridional". In: *Brazil, Universidade Federal do Rio Grande do Sul* (1998).

[197] Leonardo Ribeiro Tedeschi. "Lower Cretaceous climate records and the correlation between marine and lacustrine settings (Europe and South America)". PhD thesis. University of Oxford, 2017.

[198] Daniel A Stolper and John M Eiler. "The kinetics of solid-state isotope-exchange reactions for clumped isotopes: A study of inorganic calcites and apatites from natural and experimental samples". In: *American Journal of Science* 315.5 (2015), pp. 363–411.

[199] Ian Z Winkelstern and Kyger C Lohmann. "Shallow burial alteration of dolomite and limestone clumped isotope geochemistry". In: *Geology* 44.6 (2016), pp. 467–470.

[200] Marco Romano. "Reviewing the term uniformitarianism in modern Earth sciences". In: *Earth-Science Reviews* 148 (2015), pp. 65–76.

[201] Noel P James and Brian Jones. *Origin of carbonate sedimentary rocks*. John Wiley & Sons, 2015.

[202] Desiree Liechoscki de Paula Faria, Antonio Tadeu dos Reis, and Olinto Gomes de Souza Jr. "Three-dimensional stratigraphic-sedimentological forward modeling of an Aptian carbonate reservoir deposited during the sag stage in the Santos basin, Brazil". In: *Marine and Petroleum Geology* 88 (2017), pp. 676–695.

[203] Ana Carolina Leonel Sartorato et al. "Caracterização faciológica, estratigráfica e diagenética dos reservatórios carbonáticos da Formação Barra Velha, Bacia de Santos". MA thesis. Universidade do Estado do Rio de Janeiro, 2018.

[204] Gerald Manfred Friedman. "Identification of carbonate minerals by staining methods". In: *Journal of Sedimentary Research* 29.1 (1959), pp. 87–97.

[205] RA Young. *The Rietveld Method*. Oxford University Press, 1995.

[206] Pn K Swart, SJ Burns, and JJ Leder. "Fractionation of the stable isotopes of oxygen and carbon in carbon dioxide during the reaction of calcite with phosphoric acid as a function of temperature and technique". In: *Chemical Geology: Isotope Geoscience section* 86.2 (1991), pp. 89–96.

[207] J Rosenbaum and SMF Sheppard. "An isotopic study of siderites, dolomites and ankerites at high temperatures". In: *Geochimica et cosmochimica acta* 50.6 (1986), pp. 1147–1150.

[208] RA Reyment and Enrico Savazzi. *Aspects of multivariate statistical analysis in geology*. Elsevier, 1999.

[209] Kurt Varmuza and Peter Filzmoser. *Introduction to multivariate statistical analysis in chemometrics*. CRC press, 2016.

[210] Raphael Pietzsch, Sambasiva R Patchineelam, and João PM Torres. "Polycyclic aromatic hydrocarbons in recent sediments from a subtropical estuary in Brazil". In: *Marine Chemistry* 118.1-2 (2010), pp. 56–66.

[211] Peter Filzmoser and Valentin Todorov. "Review of robust multivariate statistical methods in high dimension". In: *Analytica chimica acta* 705.1-2 (2011), pp. 2–14.

[212] John Aitchison. "The statistical analysis of compositional data". In: *Journal of the Royal Statistical Society: Series B (Methodological)* 44.2 (1982), pp. 139–160.

[213] Detlev K Richter et al. "Radiaxial-fibrous and fascicular-optic Mg-calcitic cave cements: a characterization using electron backscattered diffraction (EBSD)". In: *International Journal of Speleology* 44.1 (2015), p. 8.

[214] Ramon Mercedes-Martın et al. "Effects of salinity, organic acids and alkalinity on the growth of calcite spherulites: implications for evaporitic lacustrine sedimentation". In: *The Depositional Record* 8.1 (2022), pp. 143–164.

[215] Peter K Swart. "The geochemistry of carbonate diagenesis: The past, present and future". In: *Sedimentology* 62.5 (2015), pp. 1233–1304.

[216] Eva De Boever et al. "What do we really know about early diagenesis of non-marine carbonates?" In: *Sedimentary Geology* 361 (2017), pp. 25–51.

[217] H Elderfield. "Strontium isotope stratigraphy". In: *Palaeogeography, palaeoclimatology, palaeoecology* 57.1 (1986), pp. 71–90.

[218] Jay L Banner. "Radiogenic isotopes: systematics and applications to earth surface processes and chemical stratigraphy". In: *Earth-Science Reviews* 65.3-4 (2004), pp. 141–194.

[219] Stéphane Bodin et al. "Large igneous provinces and organic carbon burial: Controls on global temperature and continental weathering during the Early Cretaceous". In: *Global and Planetary Change* 133 (2015), pp. 238–253.

[220] Takashi Shimura et al. "In-situ analyses of phosphorus contents of carbonate minerals: reconstruction of phosphorus contents of seawater from the Ediacaran to early Cambrian". In: *Gondwana Research* 25.3 (2014), pp. 1090–1107.

[221] Guilherme Ferreira da Silva et al. "Qmin–A machine learning-based application for processing and analysis of mineral chemistry data". In: *Computers & Geosciences* 157 (2021), p. 104949.

[222] Guotao Sun, Qingdong Zeng, and Jia-Xi Zhou. "Machine learning coupled with mineral geochemistry reveals the origin of ore deposits". In: *Ore Geology Reviews* 142 (2022), p. 104753.

[223] Pedro Acosta-Góngora et al. "Uraninite chemistry of the Central Mineral Belt, Labrador, Canada: Application of grain-scale unsupervised machine-learning". In: *Journal of Geochemical Exploration* 233 (2022), p. 106910.

[224] Romain Guilbaud et al. "Phosphorus-limited conditions in the early Neoproterozoic ocean maintained low levels of atmospheric oxygen". In: *Nature Geoscience* 13.4 (2020), pp. 296–301.

[225] Ellery D Ingall et al. "Phosphorus K-edge XANES spectroscopy of mineral standards". In: *Journal of synchrotron radiation* 18.2 (2011), pp. 189–197.

[226] Jocelyn A Richardson et al. "Characterization and Geological Implications of Precambrian Calcite–hosted Phosphate". In: *Geophysical Research Letters* (), e2022GL100328.

[227] Harris E Mason et al. "Phosphorus speciation in calcite speleothems determined from solid-state NMR spectroscopy". In: *Earth and Planetary Science Letters* 254.3-4 (2007), pp. 313–322.

[228] Harris E Mason et al. "Phosphate defects and apatite inclusions in coral skeletal aragonite revealed by solid-state NMR spectroscopy". In: *Geochimica et Cosmochimica Acta* 75.23 (2011), pp. 7446–7457.

[229] Brian L Phillips et al. "NMR spectroscopic study of organic phosphate esters coprecipitated with calcite". In: *Geochimica et Cosmochimica Acta* 183 (2016), pp. 46–62.

[230] Steffen H Büttner et al. "Living phosphatic stromatolites in a low-phosphorus environment: Implications for the use of phosphorus as a proxy for phosphate levels in paleo-systems". In: *Geobiology* 19.1 (2021), pp. 35–47.

[231] Uwe Brand and Jan Veizer. "Chemical diagenesis of a multicomponent carbonate system; 1, Trace elements". In: *Journal of Sedimentary Research* 50.4 (1980), pp. 1219–1236.

[232] Craig Joseph et al. "Methane-derived authigenic carbonates from modern and paleoseeps on the Cascadia margin: Mechanisms of formation and diagenetic signals". In: *Palaeogeography, Palaeoclimatology, Palaeoecology* 390 (2013), pp. 52–67.

[233] Steven M Stanley, Justin B Ries, and Lawrence A Hardie. "Low-magnesium calcite produced by coralline algae in seawater of Late Cretaceous composition". In: *Proceedings of the National Academy of Sciences* 99.24 (2002), pp. 15323–15326.

[234] C Anthony J Appelo and Dieke Postma. *Geochemistry, groundwater and pollution*. CRC press, 2004.

[235] Lukas Wissler, Hanspeter Funk, and Helmut Weissert. "Response of Early Cretaceous carbonate platforms to changes in atmospheric carbon dioxide levels". In: *Palaeogeography, Palaeoclimatology, Palaeoecology* 200.1-4 (2003), pp. 187–205.

[236] Jens O Herrle et al. "Mid-Cretaceous High Arctic stratigraphy, climate, and oceanic anoxic events". In: *Geology* 43.5 (2015), pp. 403–406.

[237] Leon J Clarke and Hugh C Jenkyns. "New oxygen isotope evidence for long-term Cretaceous climatic change in the Southern Hemisphere". In: *Geology* 27.8 (1999), pp. 699–702.

[238] Alessio P Menegatti et al. "High-resolution δ13C stratigraphy through the early Aptian "Livello Selli" of the Alpine Tethys". In: *Paleoceanography* 13.5 (1998), pp. 530–545.

[239] Karl B Föllmi et al. "Interactions between environmental change and shallow water carbonate buildup along the northern Tethyan margin and their impact on the Early Cretaceous carbon isotope record". In: *Paleoceanography* 21.4 (2006).

[240] Robert L Folk. "The natural history of crystalline calcium carbonate; effect of magnesium content and salinity". In: *Journal of Sedimentary Research* 44.1 (1974), pp. 40–53.

[241] Jeanne Paquette and Richard J Reeder. "New type of compositional zoning in calcite: Insights into crystal-growth mechanisms". In: *Geology* 18.12 (1990), p. 1244.

[242] Jeanne Paquette and Richard J Reeder. "Relationship between surface structure, growth mechanism, and trace element incorporation in calcite". In: *Geochimica et cosmochimica acta* 59.4 (1995), pp. 735–749.

[243] Kevin J Davis et al. "Morphological consequences of differential Mg^{2+} incorporation at structurally distinct steps on calcite". In: *American Mineralogist* 89.5-6 (2004), pp. 714–720.

[244] Mina Hong, Jie Xu, and Henry H Teng. "Evolution of calcite growth morphology in the presence of magnesium: Implications for the dolomite problem". In: *Geochimica et Cosmochimica Acta* 172 (2016), pp. 55–64.

[245] Gary Lofgren. "An experimental study of plagioclase crystal morphology; isothermal crystallization". In: *American journal of Science* 274.3 (1974), pp. 243–273.

[246] László Gránásy et al. "Growth and form of spherulites". In: *Physical Review E* 72.1 (2005), p. 011605.

[247] Rong-Fu Xiao, J Iwan D Alexander, and Franz Rosenberger. "Morphological evolution of growing crystals: A Monte Carlo simulation". In: *Physical Review A* 38.5 (1988), p. 2447.

[248] Rong-Fu Xiao, J Iwan D Alexander, and Franz Rosenberger. "Growth morphology with anisotropic surface kinetics". In: *Journal of crystal growth* 100.3 (1990), pp. 313–329.

[249] Janice L Littlewood et al. "Mechanism of enhanced strontium uptake into calcite via an amorphous calcium carbonate crystallization pathway". In: *Crystal Growth & Design* 17.3 (2017), pp. 1214–1223.

[250] Nicholas J Tosca et al. "Sedimentary talc in Neoproterozoic carbonate successions". In: *Earth and Planetary Science Letters* 306.1-2 (2011), pp. 11–22.

[251] Andre Baldermann et al. "Effect of aqueous Si/Mg ratio and pH on the nucleation and growth of sepiolite at 25^{o}C". In: *Geochimica et Cosmochimica Acta* 227 (2018), pp. 211–226.

[252] Justin V Strauss and Nicholas J Tosca. "Mineralogical constraints on Neoproterozoic pCO_2 and marine carbonate chemistry". In: *Geology* 48.6 (2020), pp. 599–603.

[253] Matthew Haworth et al. "Mid-Cretaceous pCO_2 based on stomata of the extinct conifer Pseudofrenelopsis (Cheirolepidiaceae)". In: *Geology* 33.9 (2005), pp. 749–752.

[254] Bengt Boström et al. "Exchange of phosphorus across the sediment-water interface". In: *Phosphorus in freshwater ecosystems*. Springer, 1988, pp. 229–244.

[255] Kurt O Konhauser. *Introduction to geomicrobiology*. John Wiley & Sons, 2009.

[256] Ana C Azerêdo, Luis V Duarte, and Alexandre P Silva. "The challenging carbonates from the Pre-Salt reservoirs offshore Brazil: facies, palaeoenvironment and diagenesis". In: *Journal of South American Earth Sciences* 108 (2021), p. 103202.

[257] Karline Soetaert et al. "The effect of biogeochemical processes on pH". In: *Marine Chemistry* 105 (2007), pp. 30–51.

[258] Bertram Boehrer and Martin Schultze. "Stratification of lakes". In: *Reviews of Geophysics* 46.2 (2008).

[259] Ellery D Ingall, RM Bustin, and Philippe Van Cappellen. "Influence of water column anoxia on the burial and preservation of carbon and phosphorus in marine shales". In: *Geochimica et Cosmochimica Acta* 57.2 (1993), pp. 303–316.

[260] Ellery Ingall and Richard Jahnke. "Evidence for enhanced phosphorus regeneration from marine sediments overlain by oxygen depleted waters". In: *Geochimica et Cosmochimica Acta* 58.11 (1994), pp. 2571–2575.

[261] Jonathan D Toner and David C Catling. "High phosphate concentrations needed for prebiotic chemistry occur in alkaline lakes". In: (2019).

[262] Lieven Clarisse et al. "Atmospheric ammonia (NH_3) emanations from Lake Natron's saline mudflats". In: *Scientific reports* 9.1 (2019), pp. 1–12.

[263] David B Herbst. "Potential salinity limitations on nitrogen fixation in sediments from Mono Lake, California". In: *International Journal of Salt Lake Research* 7.3 (1998), pp. 261–274.

[264] EE Stüeken, R Buick, and AJ Schauer. "Nitrogen isotope evidence for alkaline lakes on late Archean continents". In: *Earth and Planetary Science Letters* 411 (2015), pp. 1–10.

[265] Michel Meybeck. "Global distribution of lakes". In: *Physics and chemistry of lakes*. Springer, 1995, pp. 1–35.

[266] Ayumi Koishi et al. "Surface wetting controls calcium carbonate crystallization kinetics". In: *Chemistry of Materials* 31.9 (2019), pp. 3340–3348.

[267] Sebastian T Mergelsberg et al. "Metastable solubility and local structure of amorphous calcium carbonate (ACC)". In: *Geochimica et Cosmochimica Acta* 289 (2020), pp. 196–206.

[268] John M Hayes. "An introduction to isotopic calculations". In: *Woods Hole Oceanographic Institution, Woods Hole, MA* (2004).

[269] Zachary Sharp. *Principles of stable isotope geochemistry*. Prentice Hall, 2007.

[270] Jochen Hoefs. *Stable isotope geochemistry*. Springer, 2015.

[271] Charles R McKinney et al. "Improvements in mass spectrometers for the measurement of small differences in isotope abundance ratios". In: *Review of Scientific Instruments* 21.8 (1950), pp. 724–730.

[272] Mark B Yunker et al. "Tracing the inputs and fate of marine and terrigenous organic matter in Arctic Ocean sediments: A multivariate analysis of lipid biomarkers". In: *Deep Sea Research Part II: Topical Studies in Oceanography* 52.24-26 (2005), pp. 3478–3508.

[273] Josep Antoni Martın-Fernández and S Thió-Henestrosa. "Rounded zeros: some practical aspects for compositional data". In: *Geological Society, London, Special Publications* 264.1 (2006), pp. 191–201.