Development and Understanding of Catalytic Functionalization of Amides and Other Organic Molecules



A thesis submitted in partial fulfilment of the requirement

for the degree of Doctor of Philosophy (D. Phil.)

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Abstract

This thesis describes the development and mechanistic studies of an iridium-catalyzed reductive functionalization of amides and other catalytic transformations. The aim is to reveal and address the details of a wide variety of organic reactions, including some transition metal-catalyzed and organocatalytic transformations.

Chapter 1 introduces organic synthesis and computational chemistry and their historical backgrounds. In particular, reactions involving amines and organocatalysis are described. Chapter 2 details the development of the iridium-catalyzed reductive synthesis of azomethine ylides for [3+2] cycloaddition reactions. The unique selectivity of the cyclization reaction was extensively interrogated and explained by means of density functional theory. Chapter 3 describes mechanistic insight into the iridium-catalyzed reductive functionalization of amides. The detailed kinetic and computational studies revealed a full picture of the catalytic cycle and the high chemoselectivity in keeping with all experimental data. Chapter 4 describes computational mechanistic studies of enantioselective catalytic desymmetrization reactions of variously 4-substituted cyclohexanones. Three distinct catalytic reactions are studied, and the origin of the enantio- and diastereoselectivities for the transformations have been uncovered using density functional theory calculations. Chapter 5 describes computational mechanistic studies of enantioselective bifunctional iminophosphorane (BIMP)-catalyzed reactions. Three transformations using the BIMP catalyst are studied, and the chiral induction mechanisms originating from the stabilizing interactions are explained in detail.

Declarations and Copyright

I declare that this thesis has been written by me, that it is the record of work carried out by me and that it has not been submitted in any previous application for a higher degree at this or any other university or institute of learning. Work that was done as part of a collaboration with a research colleague has been fully acknowledged and referenced within the text.

I was admitted as a probationer research student in October 2018 and as a candidate for the degree of Doctor of Philosophy in October 2019; the higher study for which this is a record was carried out in the University of Oxford between 2018 and 2023.

Ken Yamazaki

Date Signature of candidate

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Abbreviations

The following abbreviations are used throughout this report.

AcOH	acetic acid
MeCN	acetonitrile
ASA	activation strain analysis
ASM	activation strain model
ADF	Amsterdam Density Functional
Bn	benzyl
BIMP	bifunctional iminophosphorane
S_N2	bimolecular nucleophilic substitution
S_N2@Si	bimolecular nucleophilic substitution at silicon
br	broad
δ_C	carbon (^{13}C) NMR chemical shift
cat.	catalytic amount
COSMO	conductor-like screening model
CuAAC	copper-catalyzed azide-alkyne cycloaddition
CCSD(T)	coupled-cluster singles and doubles plus perturbative triples
J	coupling constant

CPME	cyclopentyl methyl ether
°C	degree(s) Celsius
DFT	density functional theory
dr	diastereomeric ratio
DBU	1,8-diazabicyclo[5.4.0]undec-7-ene
DDQ	2,3-dichloro-5,6-dicyano-1,4-benzoquinone
DCM	dichloromethane
DMSO	dimethyl sulfoxide
d	doublet
dd	doublet of doublets
ddd	doublet of doublet of doublets
ddt	doublet of doublet of triplets
dt	doublet of triplets
dtd	doublet of triplet of doublets
ES	Electrospray
EDA	energy decomposition analysis
EtOAc	ethyl acetate
XC	exchange-correlation
δ_F	fluorine (^{19}F) NMR chemical shift

FMO	frontier molecular orbital
GGA	generalized gradient approximation
HF	Hartree Fock
Hz	Hertz
HFIP	1,1,1,3,3,3-hexafluoro-2-propyl
HOMO	highest occupied molecular orbital
HRMS	high resolution mass spectrometry
h	hours
HB	hydrogen bond donor
HCN	hydrogen cyanide
IED	inverse electron demand
KS	Kohn Sham
LA	left arm
LDA	local density approximation
LUMO	lowest unoccupied molecular orbital
IR	infrared
ν_{max}	Infra-red absorption
MS	mass spectrometry
m/z	mass to charge ratio

MHz	megahertz
MeOH	methanol
MA	methyl acrylate
mp	melting point
µL	microliter(s)
µmol	micromole(s)
mg	milligram(s)
mL	milliliter(s)
mmol	millimole(s)
min	minute(s)
M	molar
mol	mole(s)
MEP	molecular electrostatic potential
$[M]^+$	molecular ion
MM	molecular mechanics
MO	molecular orbital
m	multiplet
nm	nanometer(s)
NCI	non-covalent interactions

NED	normal electron demand
NMR	nuclear magnetic resonance
PMP	*p*-methoxyphenyl
Ts	*p*-toluenesulfonyl
ppm	parts per million
^{i}PrOH	2-propanol
δ_H	proton (^{1}H) NMR chemical shift
QM	quantum mechanics
q	quartet
qd	quartet of doublets
RA	right arm
rt	room temperature
$AgNTf_2$	silver bis(trifluoromethanesulfonyl)imide
s	singlet
SoA	sum of angles
TBDPS	*tert*-butyldiphenylsilyl
THF	tetrahydrofuran
TMDS	1,1,3,3-tetramethyldisiloxane
TS	transition states

TFA	trifluoroacetic acid
TMS	trimethylsilyl
TMSCl	trimethylsilyl chloride
TMSCN	trimethylsilyl cyanide
t	triplet
td	triplet of doublets
UV	ultra-violet
VB	valence-bond
ZORA	zeroth-order regular approximation

Chapter 1

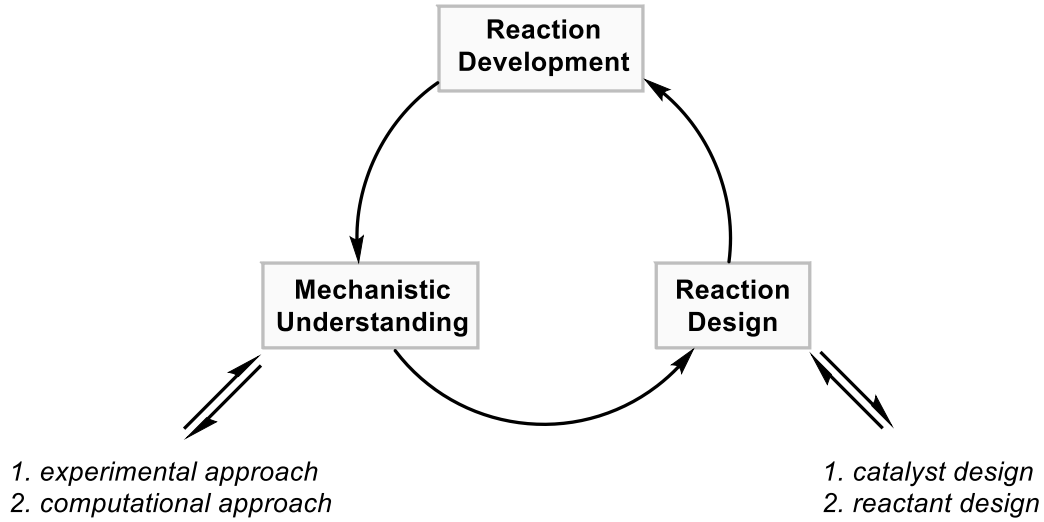
Introduction

1.1. Development of Organic Reactions

Organic chemistry has a very long and rich history. A large part of organic chemistry to date has involved development of new chemical reactions in ever increasing modes of sophistication leading to highly complex scaffolds and novel bonding types and arrangements. In parallel, the development of novel applications of these newly developed reactions has greatly contributed to the furtherment of society, for example, in the discovery of novel functional materials and complex drug molecules with beneficial biological properties.

Amongst the many kinds of functional groups known to date, some of them are still underutilized in organic synthesis. For example, amides are very stable and fundamental building blocks that are common in biology and chemistry. Although the formation and cleavage of amide bonds in peptides is facile within cells and living organisms, in chemical systems amide bonds are rather recognized as less reactive and usually harsh conditions are required to transform them into other functionalities. Therefore, many research groups continue to develop and understand fundamental reactions that can further expand potential applications in organic chemistry.

Innovations in the development of novel organic reactions have mainly been driven by understanding the mechanistic features (Scheme 1.1). A new reactivity or selectivity can be explained by illustrating a reaction mechanism, and the insight from the mechanistic study enables us to further design and predict more reactions. A catalytic reaction normally consists of multiple fundamental processes, and each step is essential for achieving the transformation.



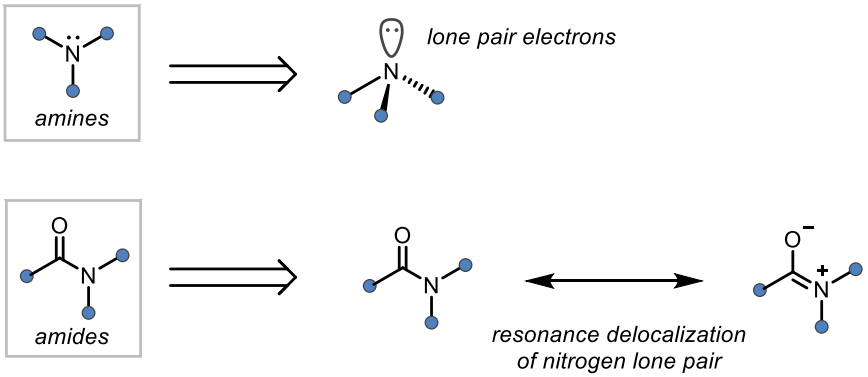
Scheme 1.1. Reaction development, mechanistic understanding, and reaction design.

In order to understand mechanistic details, two approaches are commonly used. Firstly, an experimental approach such as observation of reactive intermediates and kinetic studies is a very powerful and straightforward method. However, it is not always possible to take this approach due to the difficulties in the isolation of such short-lived species. In contrast, computational-based mechanistic studies are frequently utilized to overcome this problem. Recent rapid development in computational chemistry has enabled us to compare and disclose the most probable reaction mechanism.

This thesis is comprised of elements of development and mechanistic studies from both experimental and computational aspects. The experimental studies are based on the functionalization of amides, and the theoretical studies are based on various (organo)catalytic transformations. Since the research field in this thesis covers a large area of organic chemistry, brief introductions into nitrogen-containing molecules, organocatalysis, and computational chemistry are described in the following sections, and further details will be included in each chapter.

1.2. Amines and Amides: Compounds and Synthesis

Among the organic molecules known to exist, compounds containing nitrogen atoms are of great importance. Notably, amines and amides are the most frequently observed functionalities that are essential for building the biological environment in nature (Scheme 1.2). Amines have three substituents around the nitrogen atom, and the additional lone pair of electrons imparts it with Lewis or Brønsted basicity. The simplest source of amine is ammonia (NH_3), and it is one of the most important molecules that serves as a fertilizer and a precursor to half of the world's food and fertilizers. More complex natural products such as alkaloids also contains amine structures, and they are in many cases critical for various biological activities. Another class of nitrogen-containing molecules are amides, represented as the carbonyl group directly attached to a nitrogen atom. The character of amide bonds is unique and shows little similarity with other carbonyl groups because of the delocalization of lone pair of electrons on the nitrogen atom. Accordingly, the C–N bond length of amides is much shorter than the one of amines, which makes the amide bond stronger and less electrophilic than other carbonyl compounds. The amide groups are widely seen in peptides that can connect a large number of amino acids to build proteins with a variety of functions.



Scheme 1.2. Amines and amides.

Generally, amines are known to possess biological activity and can be found in a wide range of natural products and pharmaceutical compounds (Figure 1.1). Therefore, synthetic development of these compounds

is highly valued, and many groups have established various preparation methods of amines. An early approach includes numerous name reactions developed in the 20th century.[1] One of the classical reactions is the conversion of alkyl halides into primary amines by S_N2 reactions such as the Gabriel synthesis,[1a] Delépine reaction,[1b] and Staudinger reaction (Scheme 1.3a).[1c] The reduction of nitro,[1d] amide,[1e] and nitrile groups[1f] are also frequently used to obtain primary amines. Secondary or tertiary amines can be prepared from primary amines by reductive amination with aldehydes or the *N*-alkylation with alkyl halides (Scheme 1.3b and c).[1g-i]

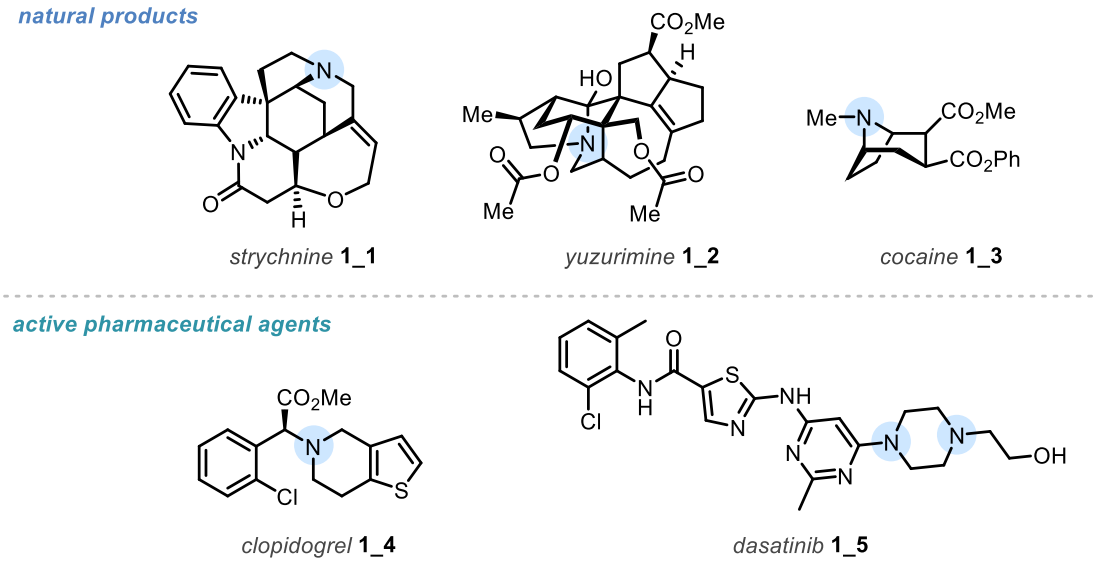
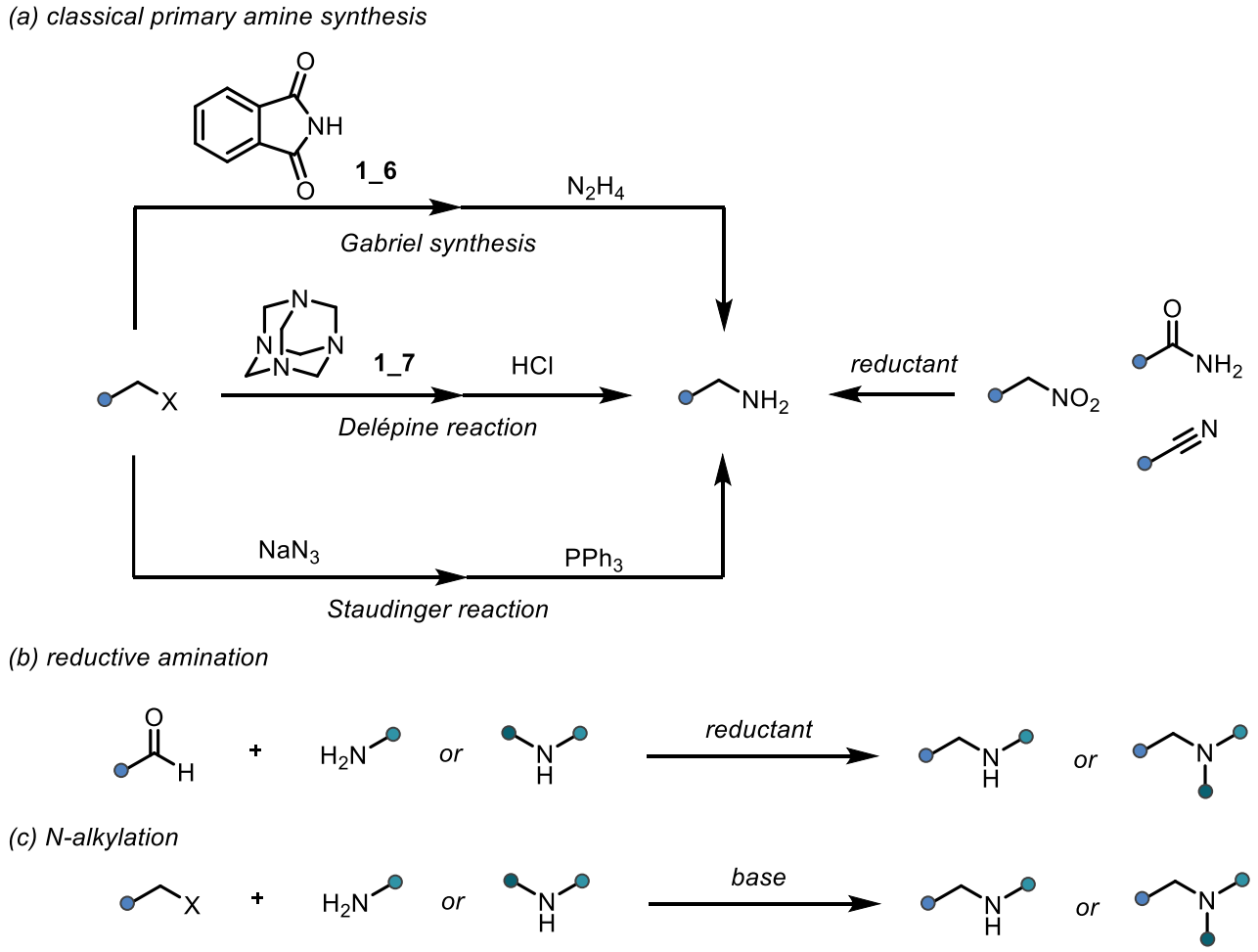
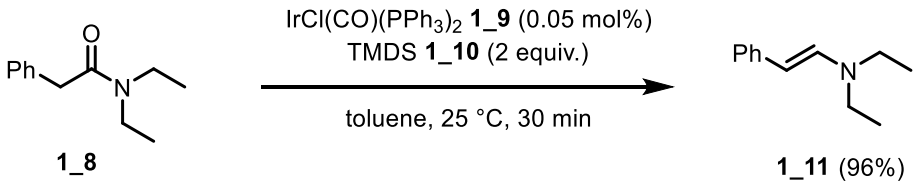


Figure 1.1. Amines in natural products and active pharmaceutical agents.

Considering the fact that naturally abundant amides are a good source of nitrogen atoms, a direct transformation of amides into amines is highly desired especially in late-stage functionalization.[2] In 2009, Nagashima discovered that an iridium complex can catalyze the reduction of an amide **1_8** into an enamine **1_11** using 1,1,3,3-tetramethyldisiloxane **1_10** (TMDS) (Scheme 1.4).[2a] The iridium complex $IrCl(CO)(PPh_3)_2$ (**1_9**) was found to be highly active, and the reaction can be performed with as low as 0.05 mol% of the catalyst loading in order to achieve such transformation in a quantitative yield.[3] This complex is also known as Vaska's complex, discovered in 1961, and since then it was mainly used to study organometallic processes such as oxidative addition but not applied into organic reactions.



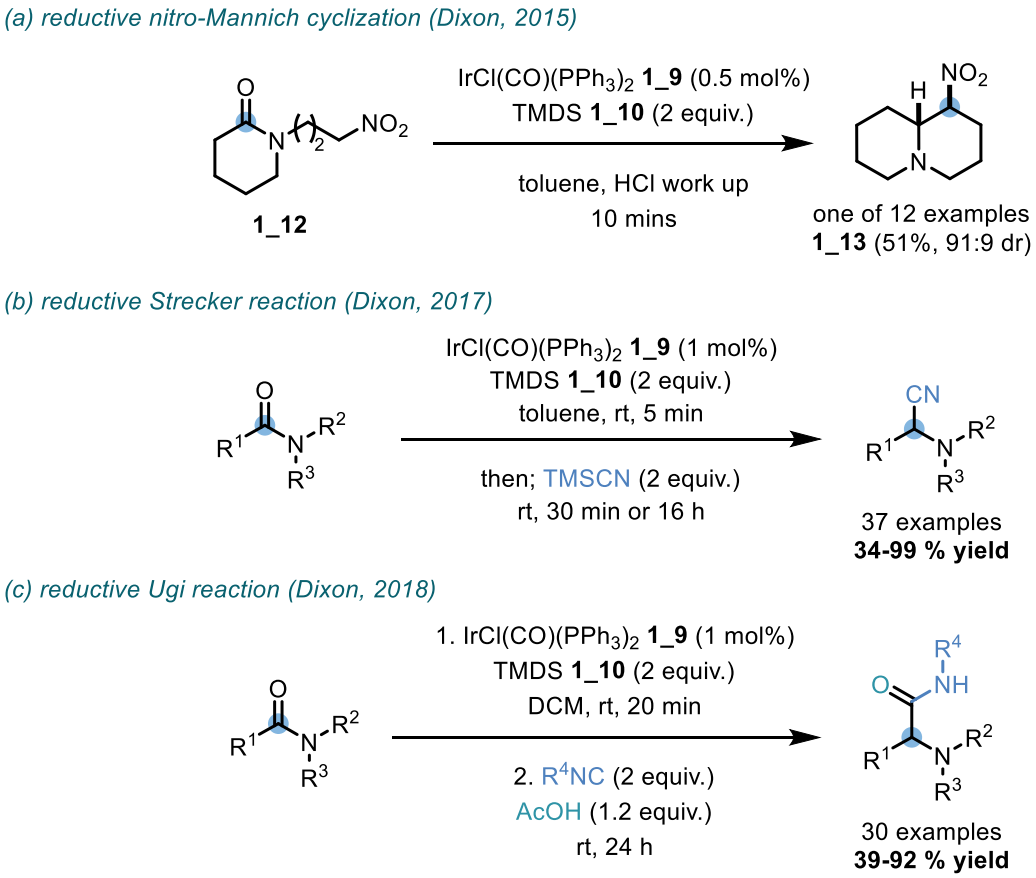
Scheme 1.3. Classical methods for amine synthesis.



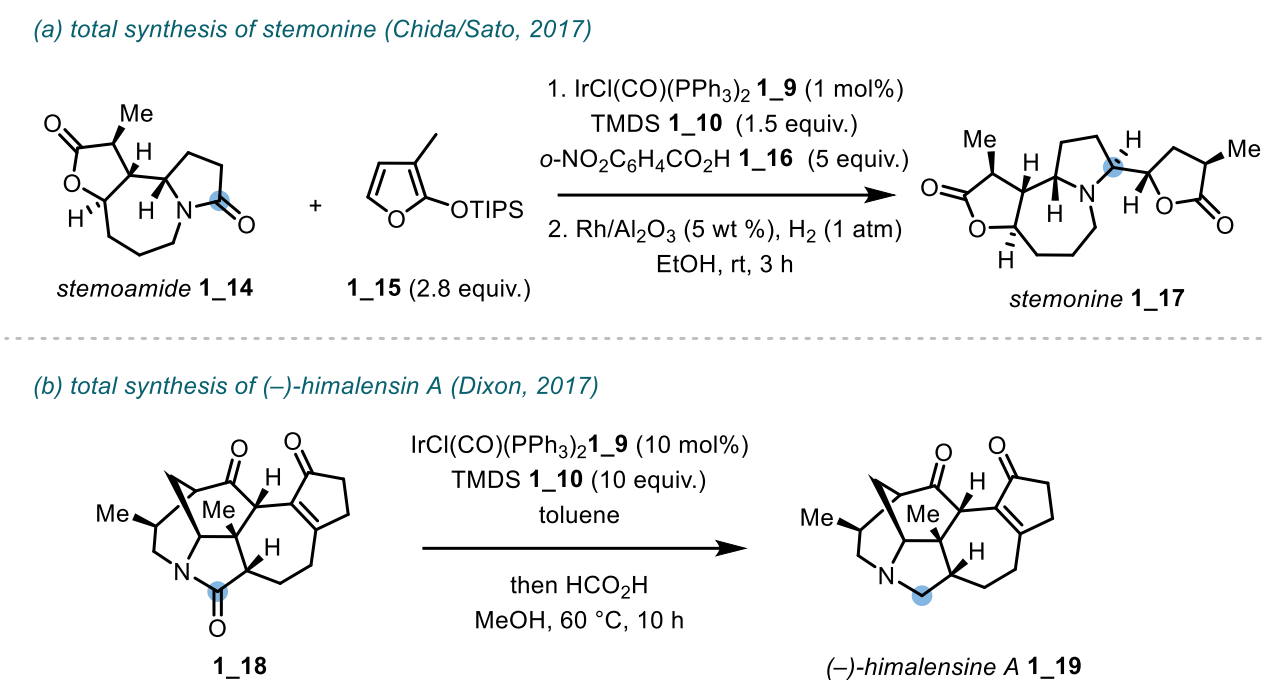
Scheme 1.4. Nagashima's iridium-catalyzed amide reduction reactions.

Several years later, Dixon applied this approach to wider reductive transformations of amides into complex amines.[4] The reduction of a nitro alkane-tethered lactam **1_12** using the standard amide reduction conditions with Vaska's complex in conjunction with TMDS **1_10** furnishes the bicyclic *β*-nitro amine product **1_13** in good diastereoselectivity (Scheme 1.5a).[4a] The initial reduction of the amide group leads to the

formation of cyclic enamine, and the iminium is formed upon treatment with acid, which subsequently cyclizes by an *in situ* formed nitronate by basification. If the reaction is carried out in the presence of trimethylsilyl cyanide (TMSCN) or isocyanide, amides are transformed into α-cyano amines or amino acid derivatives, respectively (Scheme 1.5b and c).[4c,g] These methods are comparable to the classical reactions such as Strecker reaction and Ugi reaction, but the use of chemically stable amides as a starting material and the high chemoselectivity of the reaction conditions enable more general and practical applications. Indeed, the reductive approach was successfully applied at the late stage of several total synthesis of complex natural products such as stemonine **1_17** and himalensine A **1_19** (Scheme 1.6).[4f,5]



Scheme 1.5. Iridium-catalyzed amide reduction reactions.



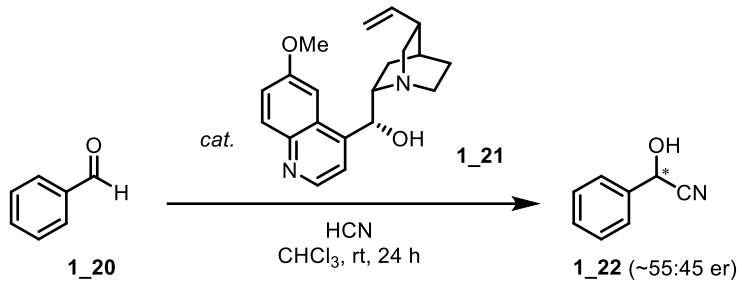
Scheme 1.6. Examples of the iridium-catalyzed amide reduction in total synthesis of natural products.

1.3. Organocatalysis

For more than a century, organic chemists have been developing novel synthetic methodologies for the construction of complex molecules. In particular, the controlled construction of stereogenic centers in a molecule is highly valuable to the pharmaceutical, chemical, and agrochemical industries. Historically, these were prepared by chiral resolution or chromatographic separation of racemic compounds.[6] The major issue with these methods is the loss of essentially half of the material. An alternative technique is to utilize a chiral auxiliary that can induce asymmetry into the molecule, which is then removed subsequently to afford a pure enantiomer.[7] However, the necessity of installation and cleavage of chiral auxiliaries increases the overall reaction step count, and the atom economy is poor.

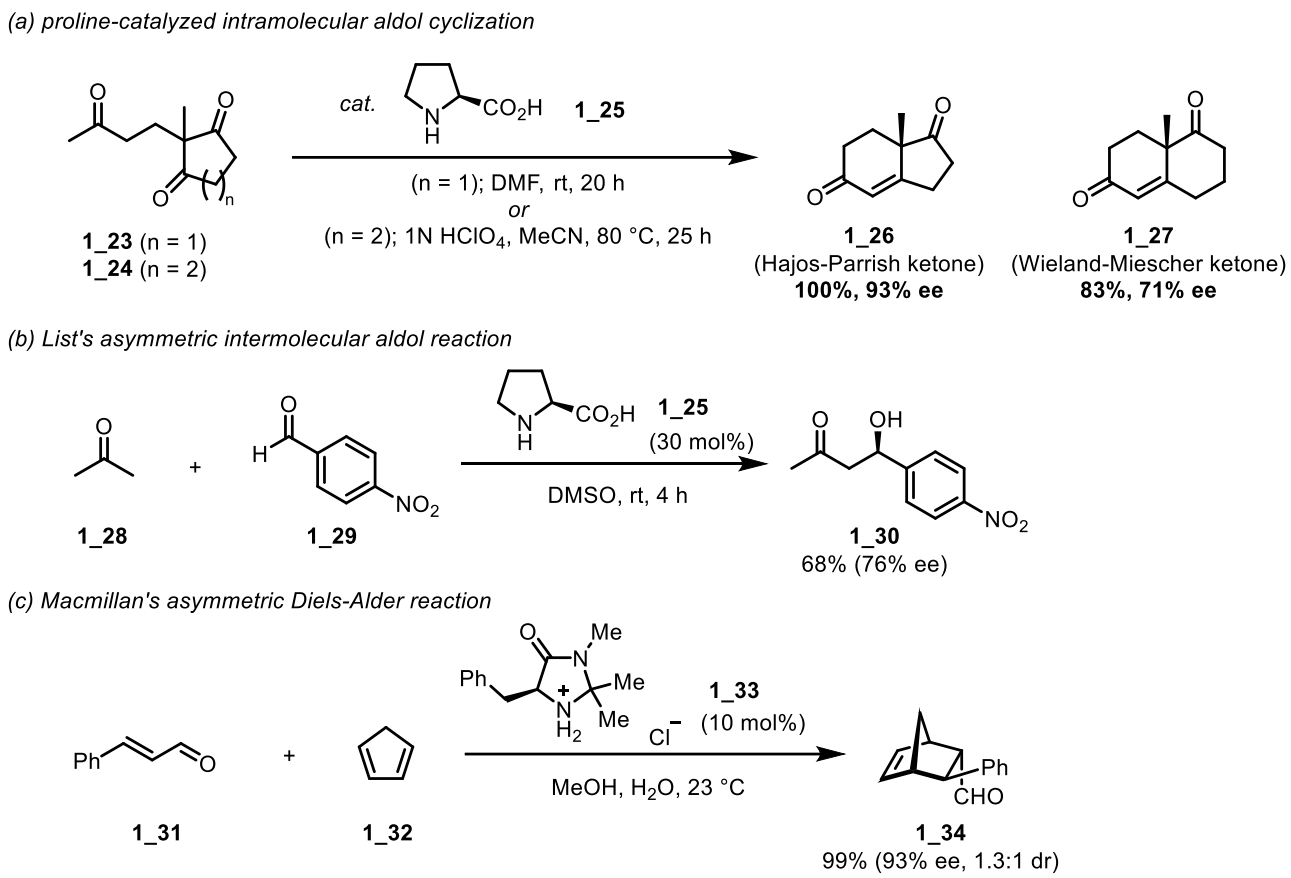
On the other hand, an asymmetric reaction, where an achiral compound is used as a starting material and only catalytic amounts of chiral "controller" molecules induce asymmetry in a product, is considered to be one of the most effective methodologies for the preparation of such compounds.[8] It is sometimes comparable

to enzymes, where extremely high selectivity towards a certain substrate is exhibited. Since the early 2000s, researchers have tried to mimic enzyme specificity by designing synthesizable chiral organic molecules that function as catalysts. This concept is called “organocatalysis”, and numerous types of catalysts have been developed for a wide variety of asymmetric reactions.[9] An early example of an enantioselective reaction that utilized a chiral molecule as a catalyst was reported in 1912 by Bredig, when the cyanation reaction of benzaldehyde **1_20** with hydrogen cyanide was carried in the presence of quinine **1_21** (Scheme 1.7).[10] The enantiomeric excess was measured to be less than 10% when Prelog reinvestigated this reaction in 1950s.[11]



Scheme 1.7. Bredig's hydrocyanation reaction of benzaldehyde.

Other milestone discoveries in asymmetric organocatalysis were reported in the 1970s when Eder, Sauer, Wiechert, Hajos, and Parrish found the proline-catalyzed intramolecular aldol cyclization for the synthesis of steroid precursors (Scheme 1.8a).[12] These remarkable reports suggested that the proline **1_25** can be recognized as a simplified model of a biological system in enzymes. Almost 30 years later, List, Barbas, and Macmillan reopened a new era of asymmetric organocatalysis when they used chiral secondary amines for an intermolecular aldol and Diels-Alder reactions (Scheme 1.8b and c).[13,14] The concepts of enamine and iminium catalysis are generally applicable due to the mild conditions and easily accessible catalyst structures, and activation methods accelerated the development of novel transformations of a wide variety of organic compounds and the precise construction of numerous complex molecules. This remarkable milestone in organic chemistry was awarded the Nobel Prize in Chemistry in 2021 jointly to List and Macmillan, and asymmetric organocatalysis is now a well-established and reliable synthetic tool.

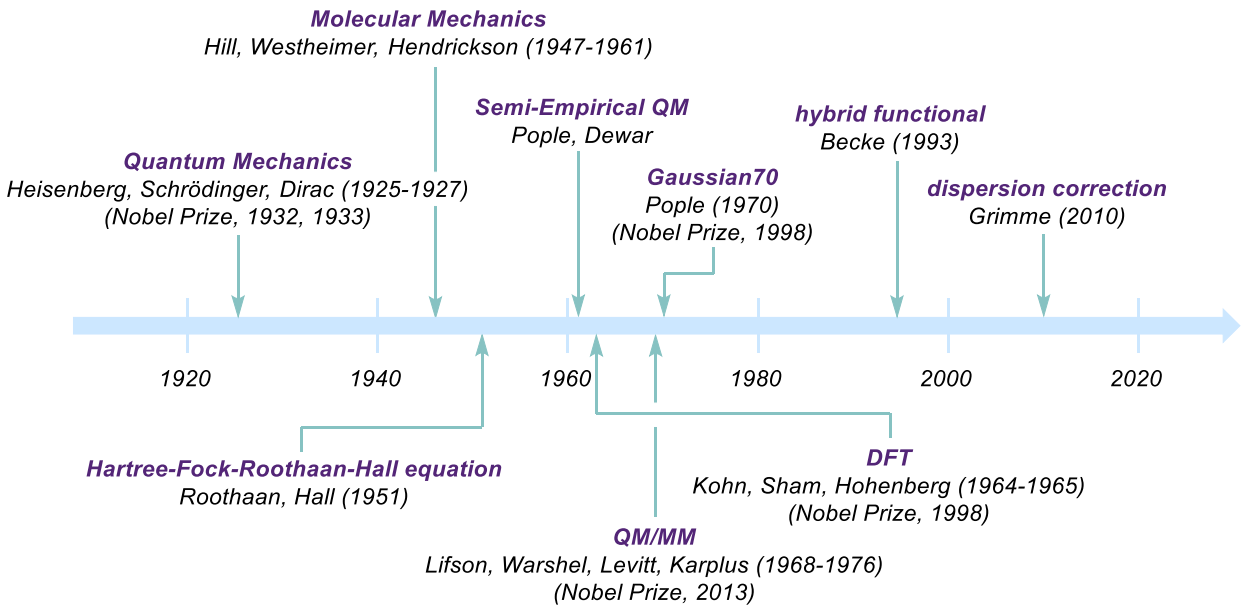


Scheme 1.8. Proline and imidazolidinone-catalyzed inter- and intramolecular reactions.

1.4. Computational Chemistry

Since the late 1960s, great achievements have been made in computational organic chemistry along with the development of computational resources, and it has become an indispensable tool in research like the frequently used nuclear magnetic resonance (NMR) spectroscopy, mass spectrometry (MS), and infrared (IR) spectroscopy.[15] A wide variety of research areas have benefited from the theoretical calculations of chemical reactions, and nowadays even experimental chemists utilize computational tools on their own for the rationalization of observations in their experiments.[16] Such advances and improvements could be achieved by the discovery of mathematical theories, development of computer programs and algorithms, and benchmark studies for higher accuracy.

The root of computational chemistry comes from the early discovery of quantum mechanics (QM) by physicists Heisenberg and Schrödinger, which was later reformulated and generalized by Dirac in the 1920s (Scheme 1.9).[17] In 1927, Hartree introduced the self-consistent field method to determine approximate wave functions and energies, which Fock later modified in 1930 to form the Hartree-Fock (HF) method.[18] The HF method approximates the wavefunction by one Slater determinant with one spin orbital for each electron. The numerical *ab initio* theory was revised in 1951 independently by Roothaan and Hall by representing the HF equation in a non-orthonormal basis set.[19] Since the full HF method without an approximation is computationally too expensive and time consuming, several approximations using empirical parameters have been developed and it is known as the semi-empirical QM method.[20] In the 1960s, Hohenberg, Kohn, and Sham reported density functional theory (DFT) where the energy is obtained from the electron density, and now is has become one of the most popular computational methods.[23] Other important breakthroughs in computational chemistry such as molecular mechanics (MM) or the combination of accurate QM calculations and fast MM calculations (QM/MM) has also accelerated the development and application of computational methodology for the representation of complex chemical systems.[22,23]



Scheme 1.9. Milestones in computational organic chemistry.

1.4.1. Density Functional Theory

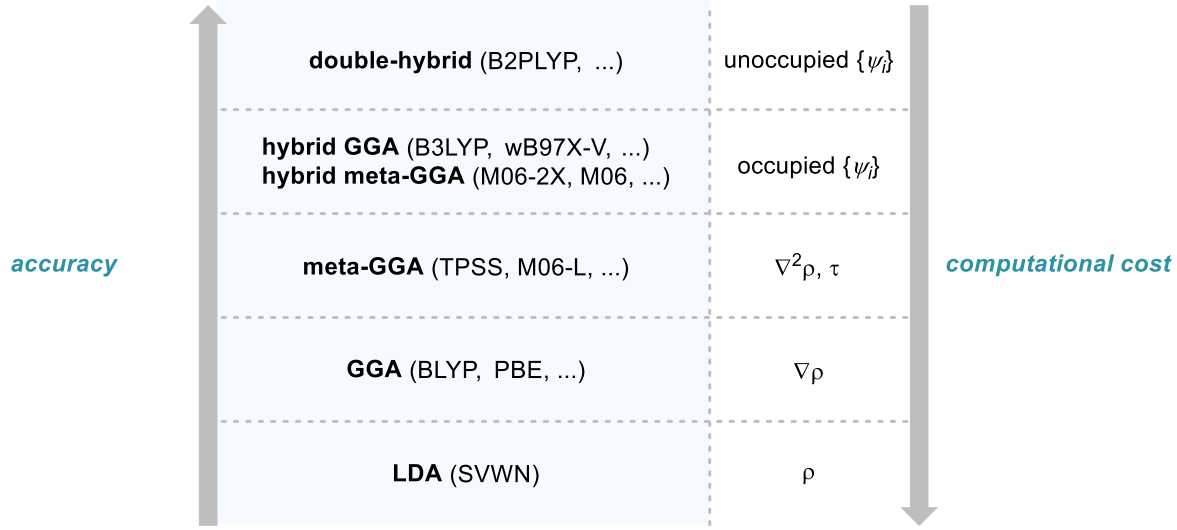
A coupled cluster method such as the coupled-cluster singles and doubles plus perturbative triples CCSD(T) method is well-established as the gold-standard for accurate calculations of molecular properties.[24] Nevertheless, such calculation methods are cost inefficient and not practical especially for a complex catalytic system. In contrast, density functional theory methods that have seen great progress over the last few decades give high accuracy with a relatively low computational cost, and they are one of the most used methodologies for the computational mechanistic studies of a wide variety of chemical reactions. The DFT methods originate from the theorem developed by Hohenberg and Kohn that the energy of a molecule can be determined from the electron density instead of a wave function.[21a] Subsequently, Kohn and Sham reported a practical application of this theory into a method that is similar in structure to the HF method (Kohn-Sham equation, eq. (1)).[21b] Kohn was then awarded the Nobel Prize in Chemistry in 1998 "for his development of the density-functional theory".

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + v_{eff}(\boldsymbol{r})\right)\varphi_i(\boldsymbol{r}) = \varepsilon_i\varphi_i(\boldsymbol{r}) \qquad (1)$$

The Kohn-Sham equation indicates that the electron density is expressed as a linear combination of basis functions. The energy of a molecule is calculated from the electron density from the determinant (known as Kohn-Sham orbitals) formed from these functions. Then, a density functional is used to collect the energy for the electron density. Since the exact density functional is unknown, a comprehensive list of various functionals with advantages or disadvantages exists. Some are based on fundamental quantum mechanics (*ab initio*), while some are based on the parametrized functions (semiempirical).

DFT approximations can be broken down into several classes, and it is now known as the "Jacob's ladder of DFT" (Scheme 1.10).[25] The lower rung of the ladder indicates that the accuracy is low, and the higher rung of the ladder indicates that the accuracy is high (usually within ±1 kcal mol^{-1}). One of the most successful functionals that has a high accuracy with relatively low computational cost are the hybrid functionals such as B3LYP,[26] PBE0,[27] and M06,[28] and these are regularly used in chemical reactions with or without transition

metals. DFT calculations are particularly useful for the mechanistic studies for observing and comparing short-lived intermediates and transition states that cannot be detected experimentally. Therefore, insights from computational analysis of catalytic systems are highly valuable for the development of novel organic reactions.



Scheme 1.10. Jacob's ladder of density functional theory methods.

1.4.2. Activation Strain Analysis and Energy Decomposition Analysis

Rational explanation of reaction mechanisms and selectivities are highly valuable for designing chemical transformations. One frequently employed method for mechanistic study is by using quantum chemical calculations. The substantial growth of computer technology in the past decades has enabled the utilization of such accurate and cost-effective models. To this end, many quantum chemical models such as frontier molecular orbital (FMO) theory and valence-bond (VB) theory have been developed for the rationalization of chemical reactions.[29,30]

A different model for analyzing chemical reactions, namely, the activation strain model (ASM), was developed in order to develop a deeper quantitative insight into the reaction mechanism that governs the fundamental processes.[31] ASM, also known as the distortion/interaction model, is a method that aims to

understand the chemical reactivity with regards to the properties of reactants and characters of mechanistic pathways. An electronic energy $\Delta E(\xi)$ of a potential energy surface can be decomposed into the strain energy $\Delta E_{\text{strain}}(\xi)$ and the interaction energy $\Delta E_{\text{int}}(\xi)$ between the fragments of choice (eq. (2)).

$$\Delta E(\xi) = \Delta E_{\text{strain}}(\xi) + \Delta E_{\text{int}}(\xi) \quad (2)$$

The strain energy $\Delta E_{\text{strain}}(\xi)$ is usually destabilizing (positive value) and caused by the penalty that is required to distort each reactant from their equilibrium structures during the course of the reaction, and this is directly related to the reactant rigidity. The $\Delta E_{\text{strain}}(\xi)$ can be further decomposed into the strain energies of the individual fragments (eq. (3)).

$$\Delta E_{\text{strain}}(\xi) = \Delta E_{\text{strain_fragment_A}}(\xi) + \Delta E_{\text{strain_fragment_B}}(\xi) \quad (3)$$

On the other hand, the interaction energy $\Delta E_{\text{int}}(\xi)$ accounts for any chemical interactions between the reactants when they are mutually oriented as they approach each other. The $\Delta E_{\text{int}}(\xi)$ is usually stabilizing (negative value) and directly related to the interaction between the distorted reactants along the reaction coordinates. The $\Delta E_{\text{int}}(\xi)$ is commonly decomposed into several terms that originates from different interaction types. Such an energy decomposition scheme plays a key role to quantitatively analyze and get deeper insights into the contributing interactions. The Amsterdam Density Functional (ADF) is one of the computational packages that implements the canonical energy decomposition analysis (EDA) scheme, and the decomposed energy components are easy to understand by means of Kohn–Sham molecular orbital (KS-MO) theory.[31,32] The decomposed physically meaningful energy terms are the sum of the Pauli repulsions ($\Delta E_{\text{Pauli}}(\xi)$), the electrostatic interactions ($\Delta V_{\text{elstat}}(\xi)$), and the orbital interactions ($\Delta E_{\text{oi}}(\xi)$) (eq. (4)). The $\Delta E_{\text{Pauli}}(\xi)$ comprises the destabilizing interaction between occupied orbitals that is responsible for the steric repulsion. The $\Delta V_{\text{elstat}}(\xi)$ corresponds from the classical stabilizing electrostatic interaction between unperturbed charge distributions. The $\Delta E_{\text{oi}}(\xi)$ accounts for the charge transfer and polarization between orbitals.

$$\Delta E_{\text{int}}(\xi) = \Delta E_{\text{Pauli}}(\xi) + \Delta V_{\text{elstat}}(\xi) + \Delta E_{\text{oi}}(\xi) \quad (4)$$

1.5. Conclusion and Thesis Aims

The remarkable expansion of the field of organic chemistry for more than a century has enabled the construction of complex molecules with desired properties. The most critical component of the development of novel organic reactions is to achieve high selectivity, and yet extensive and completely selective transformations of a specific target or a functional group has not been achieved. In pursuit of the desire to achieve such an extensive synthetic toolkit, we felt the need for understanding the origin of selectivity in a wide variety of organic reactions. Therefore, we aimed to develop and understand a number of novel reactions developed previously and concurrently in the Dixon group. In chapter 2 and 3, an iridium-catalyzed reductive functionalization of tertiary amides is described. The synthetic applicability of the reaction and the experimentally observed diastereo- and chemoselectivities are revealed. In chapter 4, three distinct catalytic systems for the synthesis of morphan cores are described. The origin of the chiral induction mechanism by desymmetrization is revealed. Finally, chapter 5 demonstrates the utility of novel bifunctional organocatalysis from a theoretical point of view.

1.6. References

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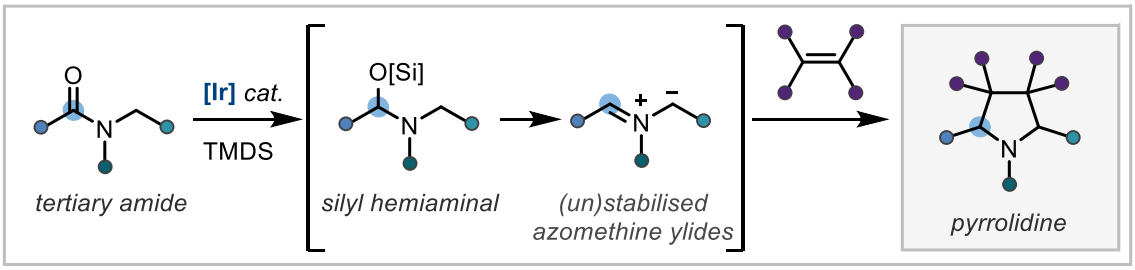
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Chapter 2

Iridium-Catalyzed Reductive Synthesis of Azomethine Ylides for [3+2] Cycloaddition

2.1. Chapter Overview

This chapter describes a new iridium-catalyzed reductive synthesis of azomethine ylides for [3+2] cycloaddition to afford functionalized pyrrolidines. The reaction proceeds under very mild conditions using a catalytic amount of Vaska's complex [$IrCl(CO)(PPh_3)_2$] and 1,1,3,3-tetramethyldisiloxane (TMDS) as a reductant for the activation of amides, and a wide variety of functional groups are tolerated. This new methodology can be applied to both inter- and intramolecular [3+2] cycloadditions to afford complex fused heterocycle structures that often feature in the structures of drug molecules and natural products. The regio- and diastereoselectivities can be controlled by the choice of dipolarophile, and the origin of the selectivities in the cycloaddition reaction was elucidated by means of density functional theory (DFT) computations. This reductive functionalization of amides has the potential to be used as a late-stage functionalization method to synthesize complex molecules possessing naturally abundant pyrrolidine scaffolds.

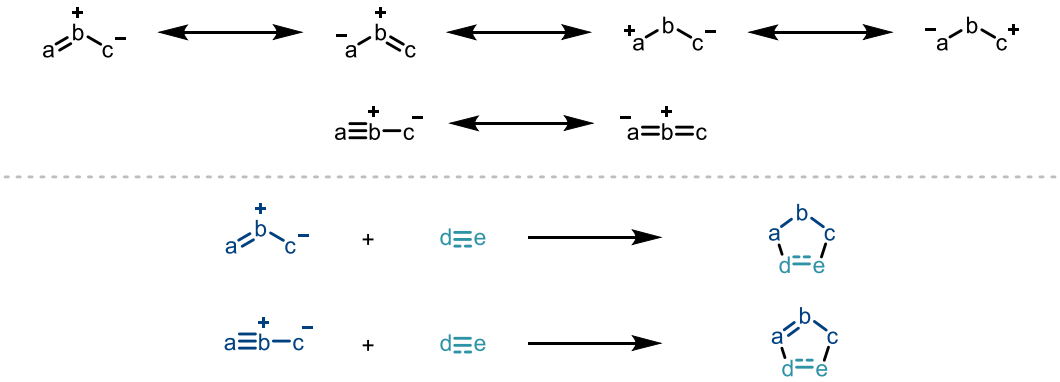


Scheme 2.1. Overview of the iridium-catalyzed reductive [3+2] cycloaddition of amides.

2.2. Introduction

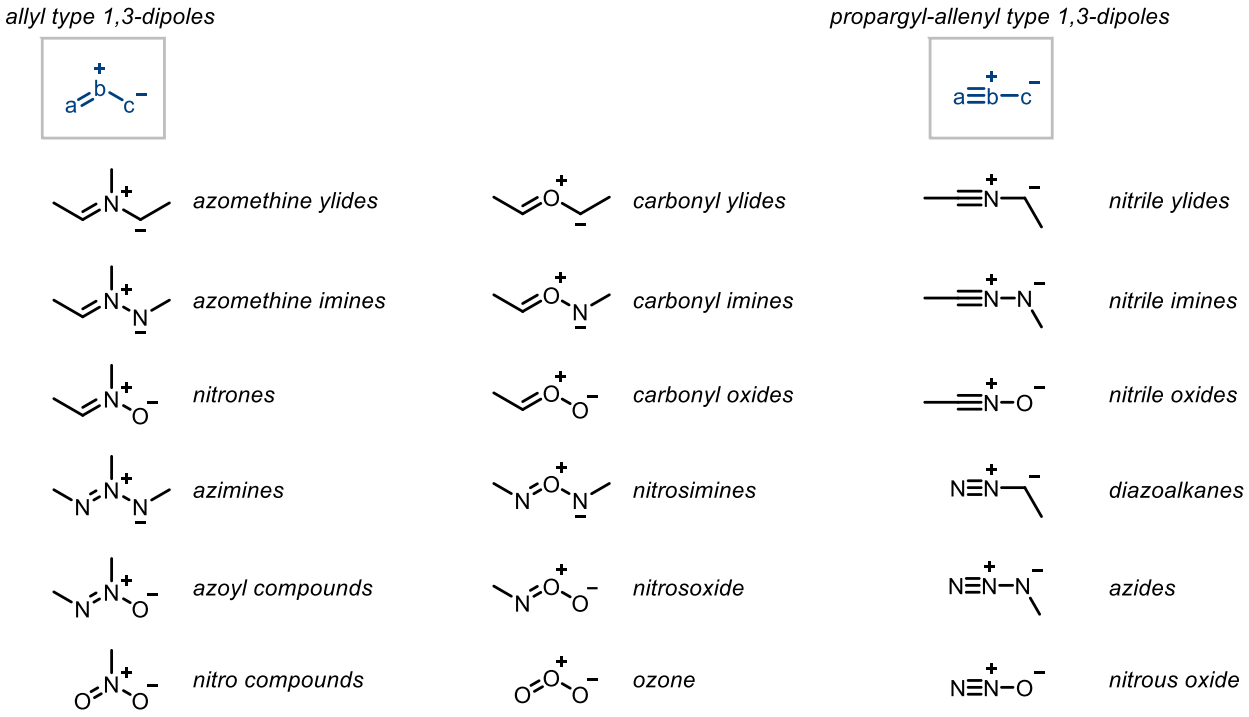
2.2.1. Nature of 1,3-Dipoles

In the 1960s, Huisgen first introduced the concept of 1,3-dipolar cycloadditions.[1] A 1,3-dipole can be described as a molecule with a general formula "*abc*" that acts as a 4π-electron system (Scheme 2.2).[2] The 1,3-dipoles "*abc*" usually bear a positive charge at the center "*b*" atom and a negative charge at the either "*a*" or "*c*" atom, in which the charges are delocalized because of the resonance structures that can be adopted. There are a number of types of 1,3-dipoles known to date, and they mostly contain carbon, nitrogen, or oxygen atoms (Scheme 2.3). These 4π-electron 1,3-dipoles react with dipolarophiles, which are described as "*de*" with 2π electrons, to give five-membered heterocyclic products. This type of reaction is often called a "[3+2] cycloaddition" because of the number of atoms involved during the cyclization process, and the possibility of obtaining a wide variety of five-membered ring systems that contain one or more heteroatoms is highly valuable for the field of synthetic chemistry.[3] One of the most famous and successful examples of the 1,3-dipolar cycloaddition is the reaction between an azide and an alkyne, which Meldal discovered in 2002 and where a copper catalyst can facilitate the cyclization (also known as a copper-catalyzed azide-alkyne cycloaddition, or CuAAC),[4] then later Sharpless defined the concept of "click chemistry" which is a form of simple and reliable chemistry that occurs rapidly without the formation of by-products.[5] Meldal and Sharpless received the Nobel Prize in Chemistry 2022 "for the development of click chemistry and bioorthogonal chemistry" together with Bertozzi, who utilized click chemistry inside living organisms.[6]



Scheme 2.2. Resonance forms of 1,3-dipoles and the [3+2] cycloaddition with dipolarophiles.

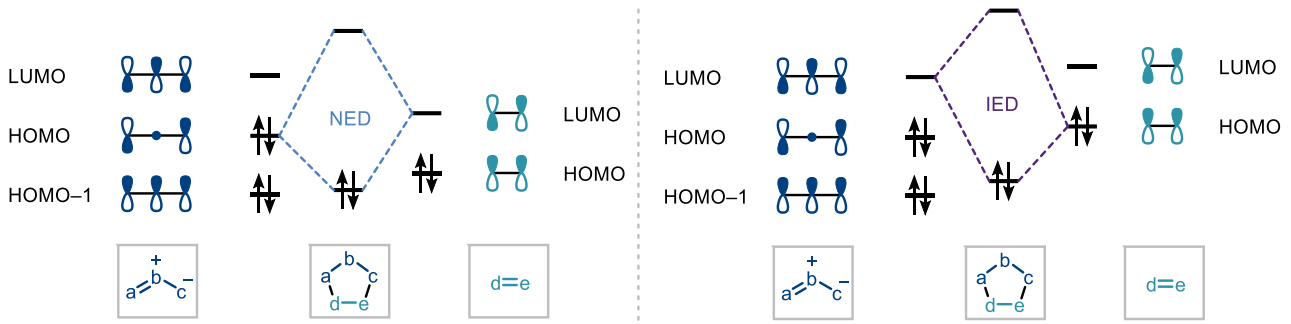
There are two different types of 1,3-dipoles "*abc*" depending on the shape of the molecule (Scheme 2.3). One is the allyl type 1,3-dipoles, where the species is bent at the central "*b*" atom and the angle between a-b-c is not linear. On the other hand, there is also the propargyl-allenyl type 1,3-dipole where all atoms are aligned, and only nitrogen is possible for the propargyl-allenyl type 1,3-dipole. These systematic classifications were used to identify unknown 1,3-dipoles.



Scheme 2.3. Types of 1,3-dipoles.

A reaction between a 1,3-dipole and a dipolarophile can potentially generate multiple isomeric cyclized products. In order to rationalize and predict the reactivity of 1,3-dipolar cycloaddition reactions, several models have been proposed. Sustmann applied frontier molecular orbital theory to explain the mechanism of the reaction between an azide and a dipolarophile, and a correlation between the second-order rate constants and the experimental ionization potentials of the dipolarophiles was observed.[7] Houk successfully confirmed this correlation by calculating the ionization energies using a combination of HF and DFT.[8] Based on these results, the 1,3-dipolar cycloaddition can be classified into three categories: (1) normal

electron demand (NED), (2) inverse electron demand (IED), and (3) combination of NED and IED (Scheme 2.4). The NED originates from the interaction between the HOMO of the 1,3-dipole and the LUMO of the dipolarophile, and the IED originates from the interaction between the LUMO of the 1,3-dipole and the HOMO of the dipolarophile.



Scheme 2.4. Normal electron demand and inverse electron demand 1,3-dipolar cycloaddition.

More recently, a different approach that accounts for distortion energies, which is the energy penalty associated with the deformation of reactants during the reaction process, has been recognized as a powerful method to analyze 1,3-dipolar cycloadditions.[9] The activation strain model (ASM) or distortion/interaction model that was proposed by Bickelhaupt and Houk decomposes the potential energy surface $\Delta E(\xi)$ into the reaction strain energy $\Delta E_{strain}(\xi)$, which is associated with the distortion of fragments, and the interaction energy $\Delta E_{int}(\xi)$ between the fragments (eq. (1)).[9d] The importance of strain energy for 1,3-dipolar cycloaddition reactions has been highlighted in many literature reports, and ASM is now frequently used for elucidating the origin of reactivity divergence.[10]

$$\Delta E(\xi) = \Delta E_{strain}(\xi) + \Delta E_{int}(\xi) \quad (1)$$

2.2.2. Classical Azomethine Ylide Generation and its Reactivity

An azomethine ylide is a 1,3-dipole that contains a nitrogen atom at the center ("*b*" = N) along with two terminal carbon atoms ("*a*" and "*c*" = C), and the [3+2] dipolar cycloadditions of azomethine ylides are synthetically useful and allow straightforward access to a pyrrolidine ring that is commonly seen in biologically active natural products and pharmaceutical compounds (Figure 2.1).[11-15] While relatively simple pyrrolidine derivatives are commercially available, the synthesis of polysubstituted pyrrolidines with excellent selectivity control is a non-trivial undertaking.

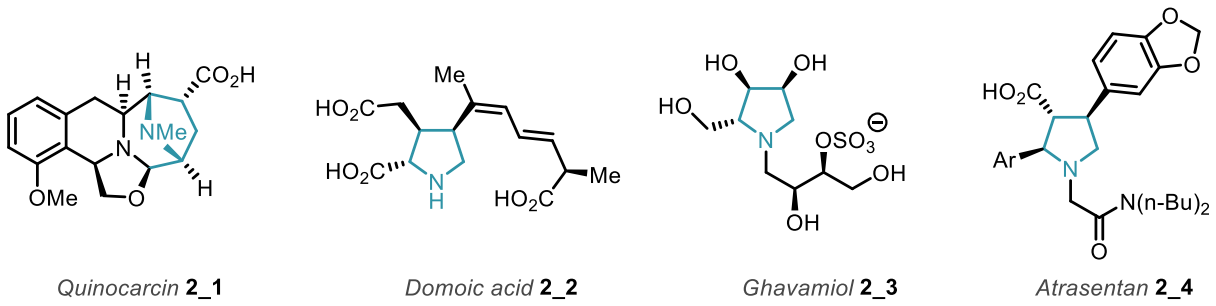
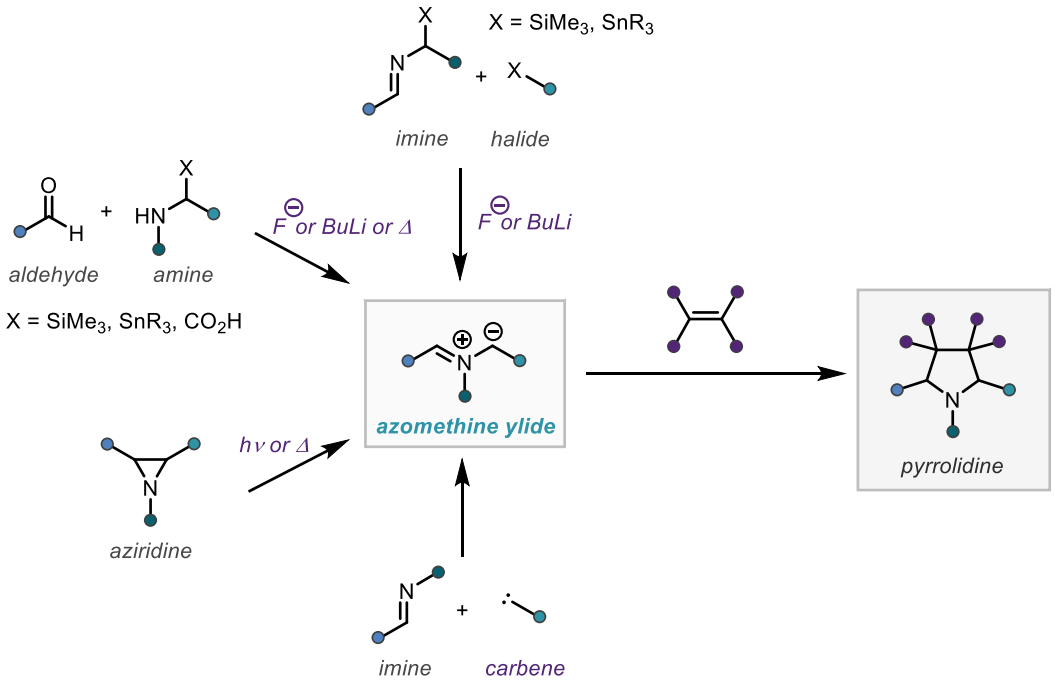


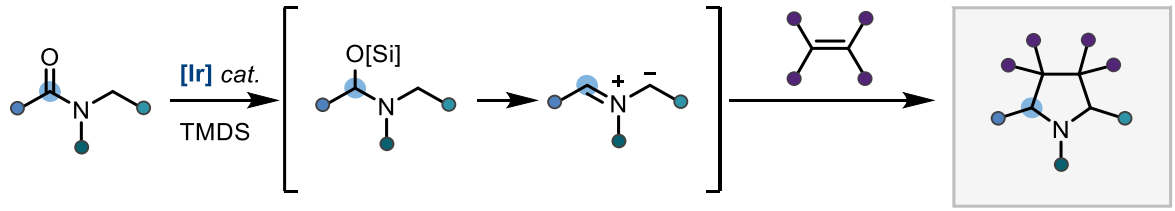
Figure 2.1. Pyrrolidine containing biologically active natural products and pharmaceutical compounds.



Scheme 2.5. Classical syntheses of azomethine ylides and the 1,3-dipolar cycloaddition.

There are a number of research reports that focus on the synthesis and further reaction of azomethine ylides (Scheme 2.5).[16-21] One common synthetic route to an azomethine ylide is the condensation of an aldehyde and a primary or secondary amine to form an imine either *in situ* or *ex situ*, followed by the elimination of an adjacent proton or leaving group such as silyl, stannyl, or carboxylate.[16] Alternatively, the ring opening of an aziridine by heat or light generates a dipole species.[17,18] Furthermore, the 1,3-dipole can be generated via an imidate species.[19] However, these methodologies require reactive intermediates or harsh conditions that ultimately limit the scope of amenable substrates.

In order to tackle the limitations associated with these classical synthetic methodologies, we aimed to develop a new transformation that involves a reduction of amides using an iridium catalyst as an alternative azomethine ylide generation methodology and described in this chapter (Scheme 2.6).[22]



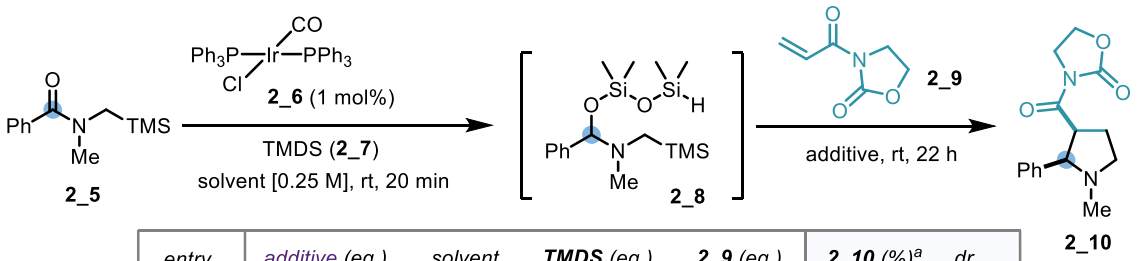
Scheme 2.6. Chapter aim and overview.

2.3. Reaction Development

2.3.1. Reaction Condition Optimization

In order to validate the hypothesis that the hemiaminal species after the hydrosilylation of amides converts to an azomethine ylide in the presence of the silyl group next to the nitrogen atom, the amide **2_5** was chosen as a model substrate for investigating conditions for partial reduction of the amide bond (Table 2.1). Vaska's complex [IrCl(CO)(PPh_3)$_2$] (**2_6**) and 1,1,3,3-tetramethyldisiloxane (TMDS, **2_7**) were added to the amide solution at room temperature and left to stir for 20 min, followed by the addition of an electron deficient dipolarophile **2_9** and an additive to assist the formation of the pyrrolidine **2_10**. The use of cesium fluoride

(CsF) as a source to trap the TMS group afforded the desired product **2_10** in a low yield (Table 2.1, entry 1). Use of trifluoroacetic acid (TFA) resulted in an increase in the product yield to 61% (Table 2.1, entry 2). Na_2CO_3 as a base was also shown to promote the reaction and slightly improved the yield to 76% (Table 2.1, entry 3). Unlike an acid, Na_2CO_3 was not expected to interfere in the catalytic activities of Vaska's complex **2_6**, and entries 4 and 5 were conducted with all components added before TMDS **2_7** was introduced for the purpose of simplifying the experimental procedure, however the yields were not improved in the presence or absence of Na_2CO_3 (Table 2.1, entries 4, 5). Further experiments demonstrated that a catalytic amount of trimethylsilyl chloride (TMSCl) also promotes the 1,3-dipole formation, and the crude NMR spectrum of the reaction product was very clean compared to the reactions with other additives (Table 2.1, entry 6). By reducing the amount of TMDS **2_7** to 1.0 equivalents, the formation of the over-reduced amide byproduct was suppressed, and the yield of **2_10** was significantly improved (Table 2.1, entries 7, 8). Solvent screening (Table 2.1, entries 9, 10) did not improve yields, and the conditions shown in entry 8 were identified as being optimal.



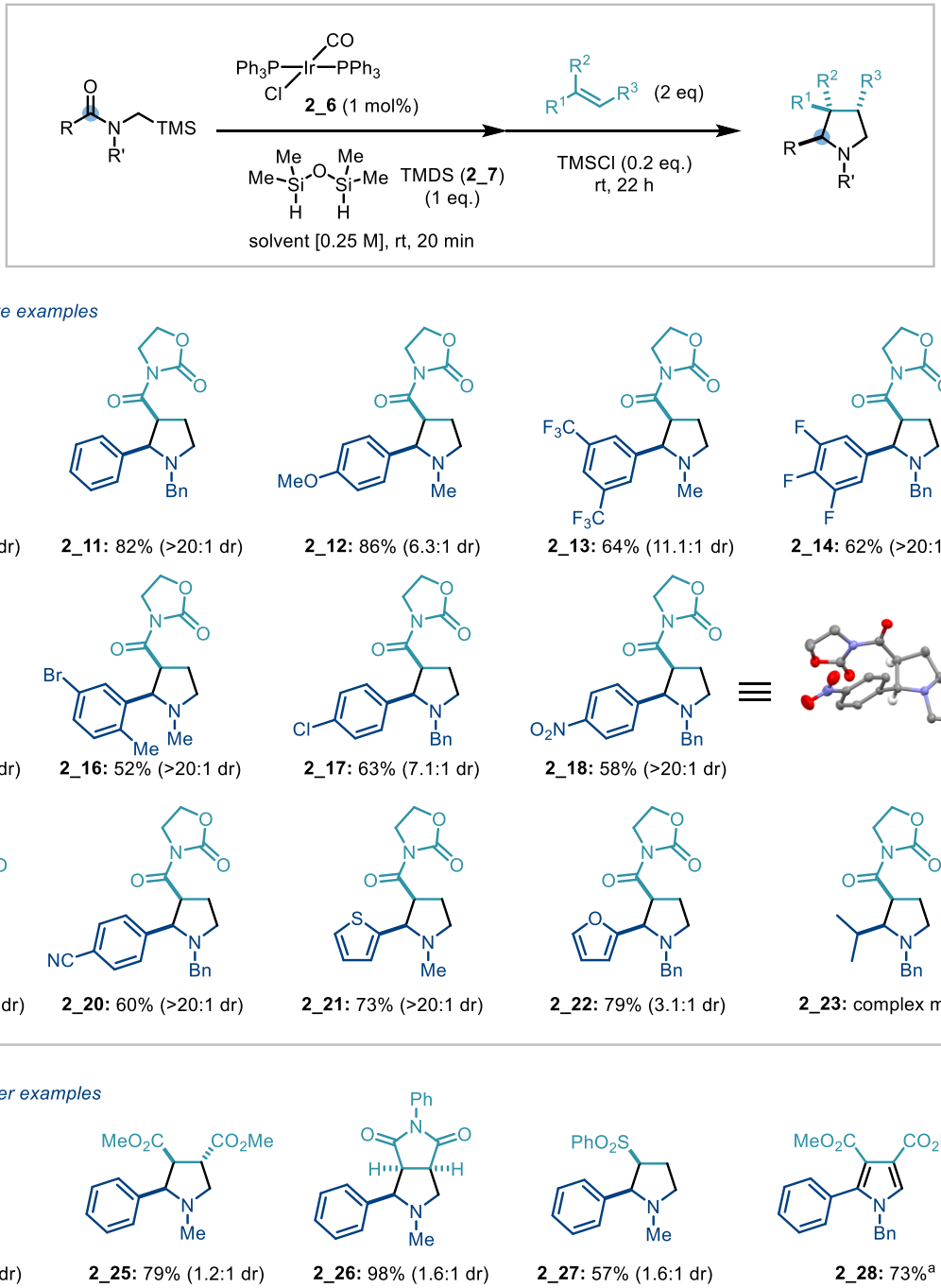
entry	*additive (eq.)*	*solvent*	***TMDS** (eq.)*	***2_9** (eq.)*	***2_10** (%)[a]*	*dr*
1	CsF (2.0)	toluene	2.0	1.1	19	n.d.
2	TFA (1.1)	toluene	2.0	1.1	61	3.0 : 1
3	Na_2CO_3 (1.1)	toluene	2.0	1.1	76	5.2 : 1
4[b]	Na_2CO_3 (1.1)	toluene	2.0	1.1	44	4.4 : 1
5[b]	---	toluene	2.0	1.1	44	3.7 : 1
6	TMSCl (0.2)	toluene	2.0	2.0	66	4.8 : 1
7	TMSCl (0.2)	toluene	1.5	2.0	68	7.7 : 1
8	**TMSCl (0.2)**	**toluene**	**1.0**	**2.0**	**88 (85)**	**7.7 : 1**
9	TMSCl (0.2)	DCM	1.0	2.0	trace	---
10	TMSCl (0.2)	THF	1.0	2.0	61	5.6 : 1

Table 2.1. Reaction condition optimization for the iridium-catalyzed reductive [3+2] cycloaddition of **2_5** and **2_9**. [a]Yield calculated by ^{1}H NMR with 1,3,5-trimethoxybenzene as an internal standard; isolated yield in parenthesis. [b]Alkene and additive were added before the addition of TMDS **2_7**.

2.3.2. Substrate Scope

With the optimal reaction conditions in hand, we explored the scope of the [3+2] cycloaddition reaction with a broad range of amides and dipolarophiles. As shown in Scheme 2.6, the reaction was found to be tolerant of a wide range of functionalized substrates. Diastereoselectivity was improved dramatically by changing the substituent on the amide nitrogen (R') from methyl (**2_10**, 7.7 : 1 dr) to benzyl (**2_11**, >20 : 1 dr). Aryl amides containing both electron donating and electron withdrawing groups afforded the corresponding pyrrolidines in good to excellent yields, and electron withdrawing groups were shown to increase the diastereoselectivity (**2_12**-**2_15**). An aryl chloride and aryl bromide on the amide moiety were also tolerated, indicating the possibility of combining this methodology with standard metal-catalyzed cross-coupling reactions (**2_16**, **2_17**). Aromatic amides with nitro and cyano groups also afforded the desired product in an excellent diastereoselectivity without any decomposition (**2_18**, **2_19**), and the relative stereochemical information in product **2_18** was confirmed by single crystal X-ray diffraction analysis. Heteroaromatic amides also underwent the transformation smoothly, although the diastereoselectivity decreased with the furan substituted substrate (**2_21**, **2_22**). An alkyl amide substrate was employed to extend the methodology to a broader range of scaffolds, however, the reaction gave a complex mixture of products, indicating lack of regio- and diastereoselectivities (**2_23**).

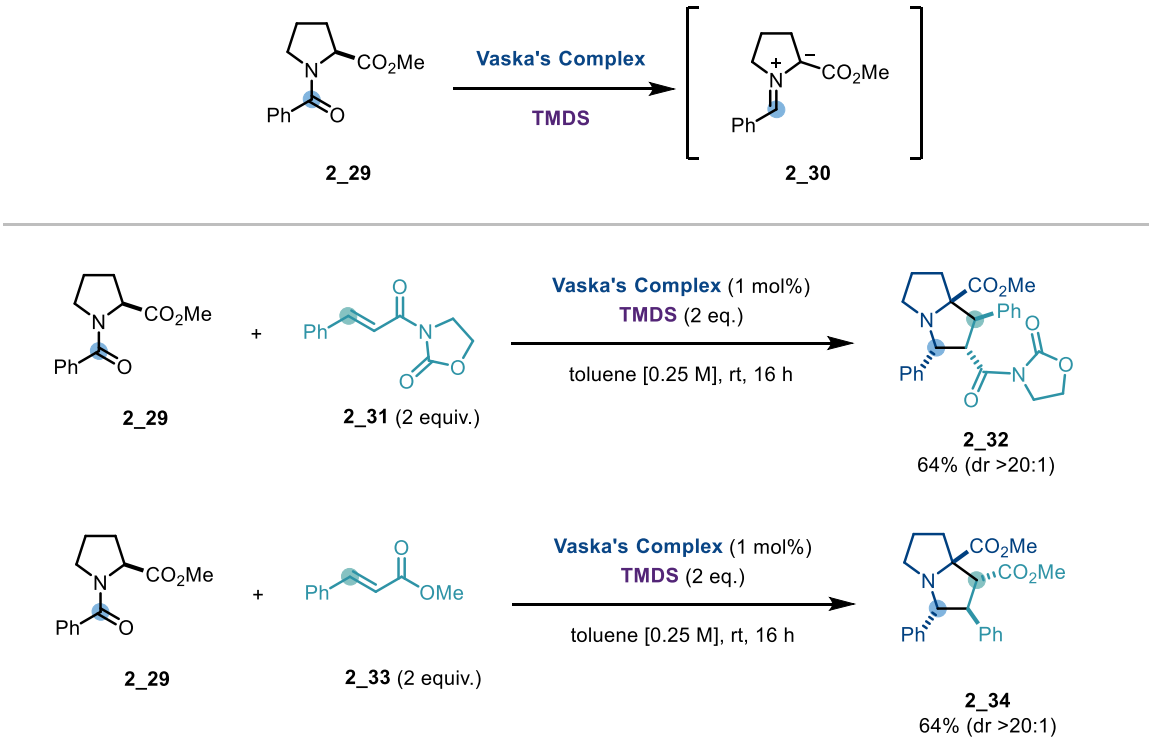
Although the diastereoselectivity was somewhat reduced, several other dipolarophiles were effective in the reaction leading to products derived from *tert*-butyl acrylate (**2_24**), dimethyl fumarate (**2_25**), *N*-phenyl maleimide (**2_26**), and phenyl vinyl sulfone (**2_27**). The pyrrole **2_28** was successfully obtained under the standard conditions using dimethyl acetylenecarboxylate as the dipolarophile, followed by oxidation of the resulting dihydropyrrolidine ring with DDQ. These examples have shown that many types of alkenes and alkynes can be used as the coupling partners in this methodology. This broad substrate scope coupled with the very mild reaction conditions employed, strongly support the potential applicability of this methodology to late-stage functionalization.



Scheme 2.6. Substrate scope of the [3+2] cycloaddition via non-stabilized azomethine ylides, with regards to the amides (A) and the dipolarophiles (B). Standard conditions: amide (0.3 mmol), dipolarophile (0.6 mmol), $IrCl(CO)(PPh_3)_2$ (1 mol%), TMDS (0.3 mmol), toluene (1 mL), rt; yields of purified product following flash column chromatography; [a]Overall yield following the oxidation by DDQ (2.0 equiv), 80 °C, 16 h.

2.3.3. Synthesis of Stabilized Azomethine Ylides and the Reactivities

In a related study, the preparation of stabilized azomethine ylides was also achieved by other members of the Dixon group (Scheme 2.7).[23] When the proline derivative **2_29** was subjected to the reductive conditions with Vaska's complex **2_6**, the *in situ* generated stabilized azomethine ylide **2_30** reacted smoothly with a wide variety of electron-deficient dipolarophiles. An interesting difference of the reaction conditions is that the dipolarophile can be added from the beginning of the reaction for the generation of stabilized azomethine ylides, giving an advantage of the easier synthetic operations. The unique selectivity was seen with dipolarophiles such as acrylate, furanone, nitroalkene, cinnamate, and vinyl sulfone, and only a single diastereomer of the corresponding polysubstituted nitrogen-containing [3.2.0] bicyclic compounds was observed in most of the cases.



Scheme 2.7. The generation of stabilized azomethine ylide **2_30** from the proline derivative **2_29** and the reactions with *N*-enoyl oxazolidinone **2_31** and methyl cinnamate **2_33**.

Two selected reaction examples with *N*-enoyl oxazolidinone **2_31** and methyl cinnamate **2_33** are shown in Scheme 2.7, and these two coupling partners demonstrated a completely different trend in the 1,3-dipolar cycloaddition reactions. Interestingly, *N*-enoyl oxazolidinone **2_31** gave the newly formed C–C bond between the carbonyl carbon atom of the substrate and the α position of the dipolarophile, whereas methyl cinnamate **2_33** gave the newly formed C–C bond between the carbonyl carbon atom of the substrate and the β position of the dipolarophile. These results suggested that the regio- and diastereoselectivities are highly dependent on the nature of the dipolarophile. The explanation of the trend is not possible using the simple FMO model, therefore we turned to utilize state-of-the-art density functional theory (DFT) calculations to further explore the controlling factors behind these 1,3-dipolar cycloadditions.

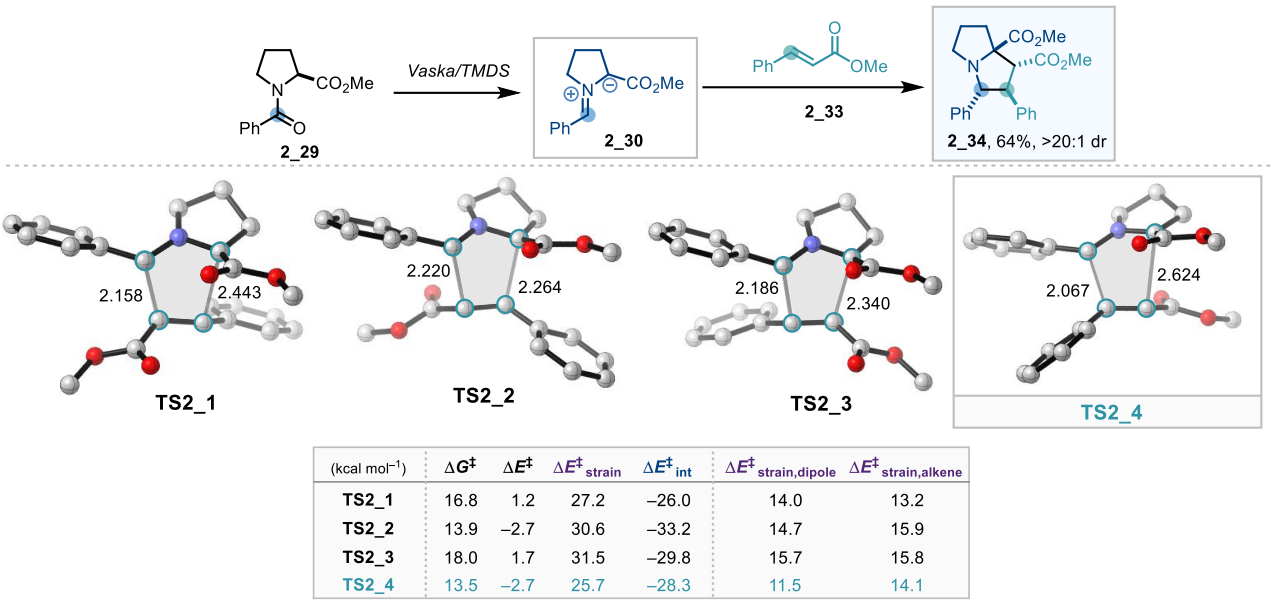
2.4. Computational Mechanistic Study

2.4.1. Computational Details

All calculations reported in this chapter were performed using the Amsterdam Density Functional (ADF) software[24], and COSMO(toluene)-M06-2X/TZ2P//BP86/TZ2P level of theory was used.[25-30]

2.4.2. Transition State Structures for the 1,3-Dipolar Cycloaddition

In order to investigate the regio- and diastereoselectivities involved in the cycloaddition reaction and to elucidate the origin of the inversion of selectivity between methyl cinnamate **2_33** and *N*-enoyl oxazolidinone **2_31**, DFT calculations were utilized. First, four cycloaddition transition state structures between the *in situ* generated azomethine ylide **2_30** and methyl cinnamate **2_33** as the dipolarophile were computed (Scheme 2.8). Among the four TSs, the energy barrier via **TS2_4** that leads to the experimentally confirmed product **2_32** is found to be the most favorable.



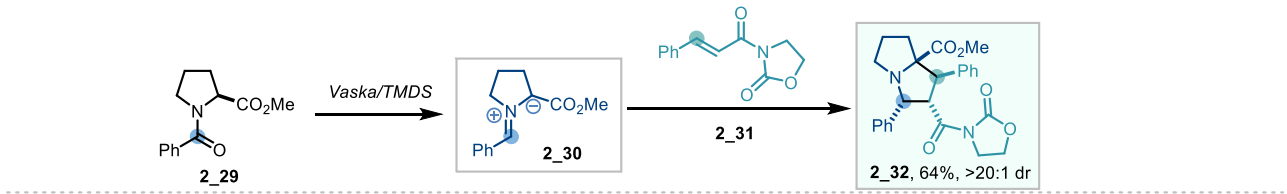
(kcal mol^{-1})	$\Delta G^{\ddagger}$	$\Delta E^{\ddagger}$	$\Delta E^{\ddagger}_{strain}$	$\Delta E^{\ddagger}_{int}$	$\Delta E^{\ddagger}_{strain,dipole}$	$\Delta E^{\ddagger}_{strain,alkene}$
TS2_1	16.8	1.2	27.2	–26.0	14.0	13.2
TS2_2	13.9	–2.7	30.6	–33.2	14.7	15.9
TS2_3	18.0	1.7	31.5	–29.8	15.7	15.8
TS2_4	13.5	–2.7	25.7	–28.3	11.5	14.1

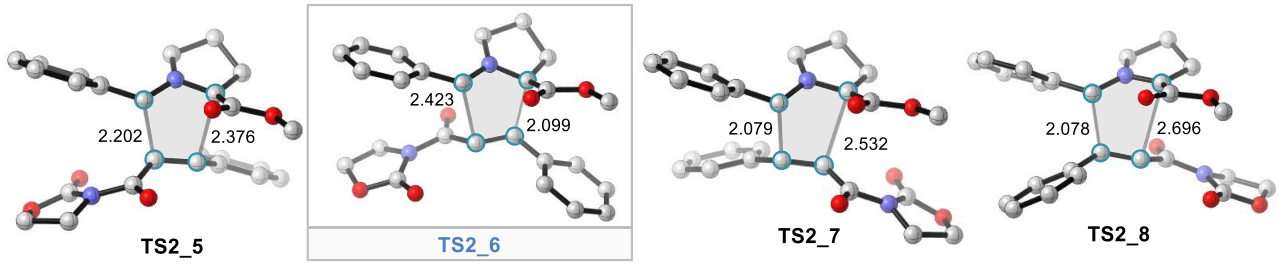
Scheme 2.8. Transition state structures for the 1,3-dipolar cycloaddition between the azomethine ylide **2_30** and methyl cinnamate **2_33**.

To elucidate the kinetic preference for this selectivity-determining step, the activation strain model that involves the decomposition of the electronic activation barrier ($\Delta E^{\ddagger}$) into the strain energy ($\Delta E^{\ddagger}_{strain}$) that results from the deformation of the individual reactants and the interaction energy ($\Delta E^{\ddagger}_{int}$) between the deformed reactants was applied (Scheme 2.8).[9] This analysis reveals that the most favored transition state **TS2_4** proceeds with the least strain energy ($\Delta E^{\ddagger}_{strain}$ = 25.7 kcal mol^{-1}). Especially, the reduced strain in the dipole is the main factor that contributes to lower the energy barrier ($\Delta E^{\ddagger}_{strain,dipole}$ = 11.5 kcal mol^{-1}).

On the other hand, the cycloaddition between the azomethine ylide **2_30** and *N*-enoyl oxazolidinone **2_31** preferably goes through the lowest transition state structure **TS2_6**, in which the relative stereochemical configuration of the product through the TS agrees with the experimentally confirmed product **2_32** (Scheme 2.9). The ASM on these four transition states revealed that the most preferred transition state structure **TS2_6** benefits from the more stabilizing interaction energy ($\Delta E^{\ddagger}_{int}$ = –35.2 kcal mol^{-1}). In other words, the interaction energy overrules the strain energy that was decisive in the case with methyl cinnamate **2_33**.

The important role of the interaction energy on the reactivity trends was analyzed using a canonical energy decomposition analysis (EDA) (Scheme 2.9).[31] The EDA breaks down the ΔE_{int} between the distorted reactants in the TS structure into three physically meaningful energy terms, namely the electrostatic interaction (ΔV_{elstat}), the Pauli repulsion (ΔE_{Pauli}), and the orbital interactions (ΔE_{oi}). Analysis of the EDA terms computed on the solution phase geometries in the gas phase revealed that the more stabilizing orbital interactions ($\Delta E^{\ddagger}_{oi}$ = –64.6 kcal mol^{-1}) and the electrostatic interactions ($\Delta V^{\ddagger}_{elstat}$ = –70.6 kcal mol^{-1}) for **TS2_6** determines the trend in ΔE_{int}, which ultimately contributes to the selectivity.





(kcal mol^{-1})	$\Delta G^{\ddagger}$	$\Delta E^{\ddagger}$	$\Delta E^{\ddagger}_{strain}$	$\Delta E^{\ddagger}_{int}$	$\Delta E^{\ddagger}_{int,gas}$	$\Delta E^{\ddagger}_{Pauli}$	$\Delta V^{\ddagger}_{elstat}$	$\Delta E^{\ddagger}_{oi}$
TS2_5	14.4	–1.3	28.8	–30.1	–31.7	79.4	–51.1	–60.0
TS2_6	11.4	–5.0	30.2	–35.2	–37.5	97.7	–64.6	–70.6
TS2_7	16.8	0.6	30.8	–30.2	–31.4	85.3	–52.2	–64.5
TS2_8	11.6	–4.9	24.1	–29.1	–31.5	82.2	–54.4	–59.2

Scheme 2.9. Transition state structures for the 1,3-dipolar cycloaddition between the azomethine ylide **2_30** and *N*-enoyl oxazolidinone **2_31**.

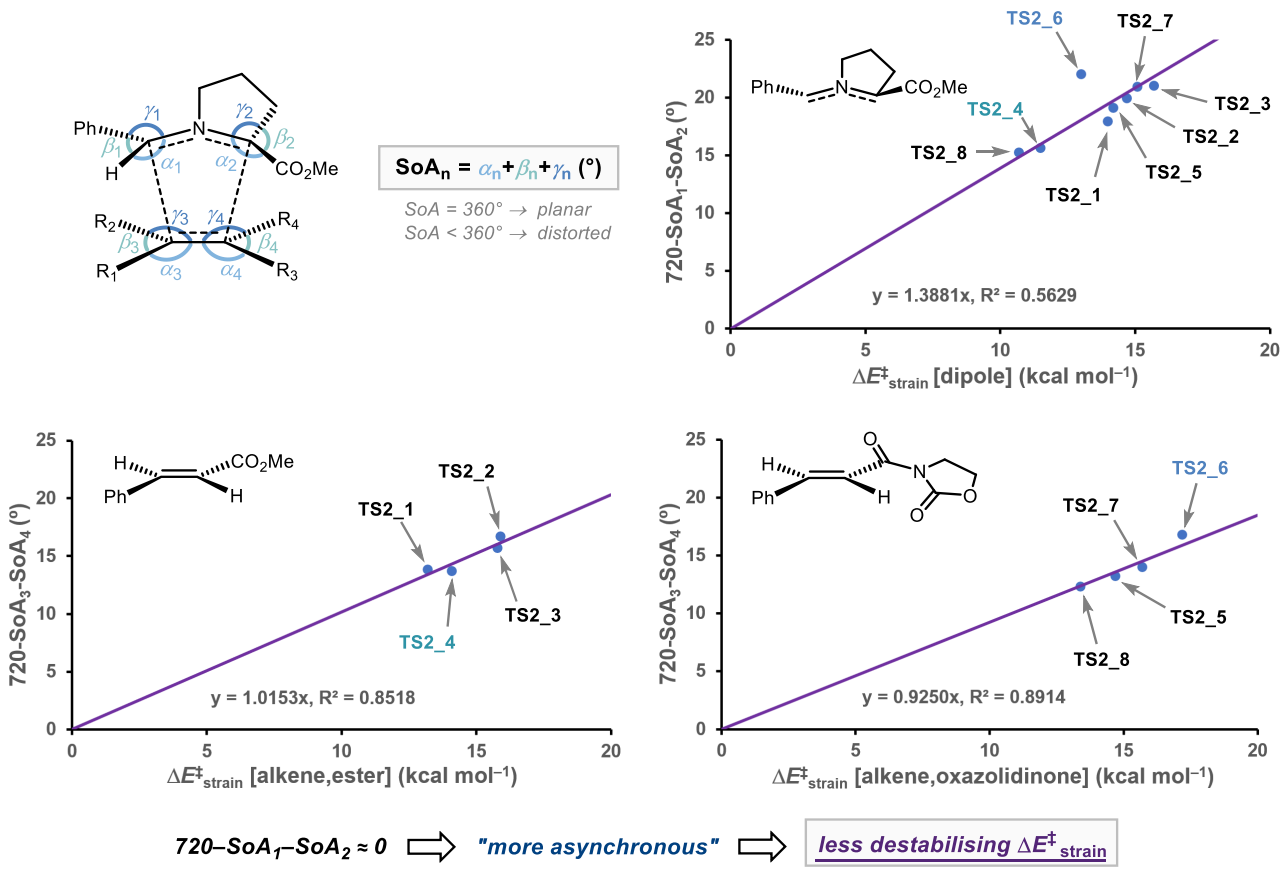
2.4.3. Origin of the Regio- and Diastereoselectivities

As described above, the strain energy becomes decisive for the stereochemical control when methyl cinnamate is used, whereas the interaction energy dominates and controls the selectivity when the dipolarophile

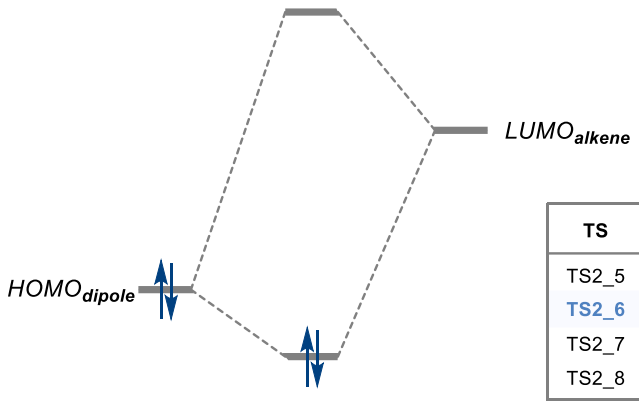
possesses an oxazolidinone group. The origin of the regio- and diastereoselectivities of this cycloaddition, which depends on the nature of dipolarophiles, is explained below.

All transition state structures form two different C−C bonds at the same time. However, the lengths of these two forming bonds are usually not the same, indicating that the TS is asynchronous and one bond forms faster than the other. The degree of asynchronicity was therefore defined as the bond length difference between two newly forming C−C bonds in the TS structures. The most favored transition state **TS2_4** with methyl cinnamate **2_33** has the least destabilizing strain energy on the dipole fragment, and this can be explained by the higher degree of asynchronicity, which is the result of a smaller degree of pyramidalization (sum of angles around an atom [SoA (°)]) at the reacting carbon atoms (Scheme 2.10). The relationship between the strain energies of each fragment and the normalized SoA at two reacting carbon atoms (720−SoA_1−SoA_2 [for the dipole fragment] or 720−SoA_3−SoA_4 [for the dipolarophile fragment]) showed an excellent correlation. Therefore, the TS that minimizes the pyramidalization of reacting carbon atoms benefits from a less destabilizing $\Delta E^{\ddagger}_{\text{strain}}$ by the asynchronicity, and thus the activation energy barrier decreases.

The bonding mechanism and the frontier molecular orbital (FMO) interactions were thoroughly analyzed, and the origin of more stabilizing ΔE_{oi} for **TS2_6** originates from a smaller normal electron demand (NED) energy gap between the HOMO of dipole and the LUMO of dipolarophile, in conjunction with the larger orbital overlap *S* compared to other TSs. The combination of these effects results in the most stabilizing orbital interactions ($S^2/\Delta\varepsilon \times 10^3 = 9.0$) for **TS2_6** (Scheme 2.11).[32]



Scheme 2.10. Correlation between the Sum of Angles (SoA in degrees) and the strain energies of the azomethine ylide **2_30** and the dipolarophiles.

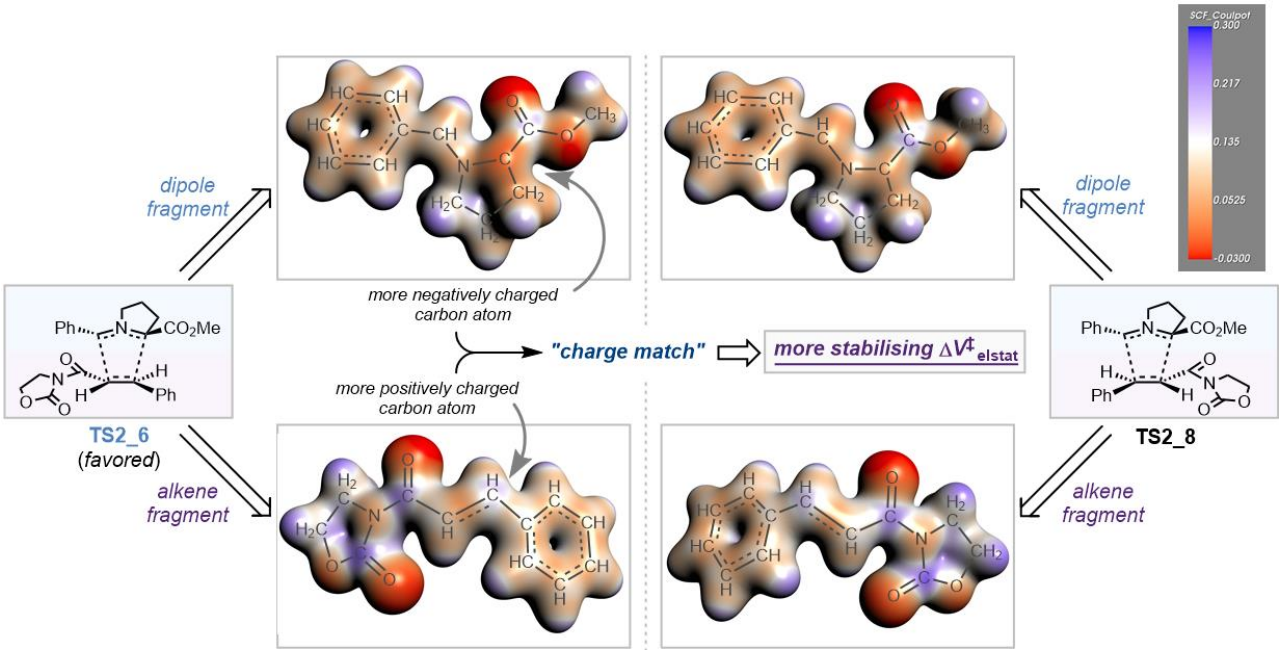


higher $S^2/\Delta\varepsilon \times 10^3$ ⇨ more stabilising $\Delta E^{\ddagger}_{oi}$

TS	$\Delta\varepsilon$ HOMO$_{dipole}$–LUMO$_{alkene}$ (eV)	Orbital Overlap S	$S^2/\Delta\varepsilon \times 10^3$
TS2_5	4.1	0.17	7.4
TS2_6	3.9	0.19	9.0
TS2_7	4.0	0.17	7.4
TS2_8	4.1	0.16	6.5

Scheme 2.11. Frontier molecular orbital diagrams with calculated key orbital energy gaps and overlaps of the normal electron demand $HOMO_{dipole}$–$LUMO_{alkene}$ interaction.

Finally, the ΔV_{elstat} in **TS2_6** also contributed to the energy trend, and this can be explained from the molecular electrostatic potential (MEP) maps (Scheme 2.12). There are two carbon atoms participating in the shorter newly forming C−C bond, and the lowest energy **TS2_6** benefits from the charge match between these two atoms compared to that of the second most favorable **TS2_8**. Particularly, the bond formation between the negatively charged carbon atom on the dipole and the positively charged carbon atom on the dipolarophile provides a more stabilizing electrostatic interaction. Therefore, the regio- and diastereoselectivities of the 1,3-dipolar cycloaddition between an *in situ* generated azomethine ylide **2_30** and a variety of dipolarophiles are determined by either the strain or the interaction energies of the cycloaddition TSs. The strain energy becomes decisive for stereochemical control when methyl cinnamate is used, whereas the interaction energy dominates and controls the selectivity when the dipolarophile possesses an oxazolidinone group.



Scheme 2.12. Molecular electrostatic potential map surfaces (at 0.03 $Bohr^{-3}$) from −0.03 (Red) to 0.03 (Blue) Hartree e^{-1} of distorted dipole and dipolarophile fragments for the 1,3-dipolar cycloadditions between the azomethine Ylide **2_30** and the *N*-enoyl oxazolidinone **2_31**.

2.5. Conclusion

In conclusion, a highly selective reductive [3+2] cycloaddition reaction of amides and conjugated alkenes for the synthesis of functionalized pyrrolidines was developed. This strategy, a cycloaddition proceeded by the initial partial reduction of amides with Vaska's complex and TMDS to generate a range of stabilized and non-stabilized azomethine ylides, afforded a wide variety of highly substituted pyrrolidines after the cyclization with dipolarophiles. The reaction proceeds under mild conditions in high regio- and diastereoselectivities. The origin of these selectivities in the [3+2] cycloaddition reaction were elucidated by means of state-of-the-art DFT calculations. Activation strain model and energy decomposition analysis revealed that the selectivity is determined by either the strain or the interaction energies depending on the nature of the dipolarophile. Highly asynchronous TSs are energetically preferred due to the lower strain energy, and the presence of a highly stabilizing interaction energy between the reactants can overrule the strain energy, in which the orbital and electrostatic interactions are decisive for the energy trend.

2.6. References

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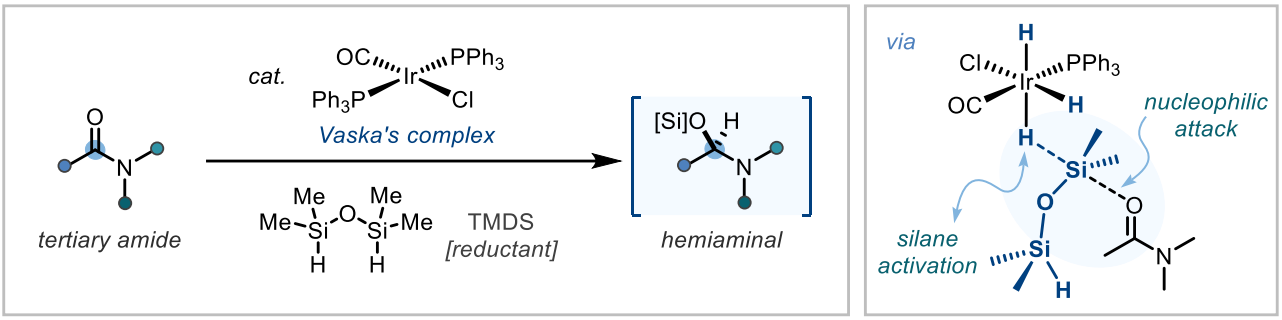
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Chapter 3

Mechanistic Studies of Iridium-Catalyzed Hydrosilylation of Amides

3.1. Chapter Overview

This chapter describes the combined experimental and computational mechanistic study of the iridium-catalyzed hydrosilylation of amides (Scheme 3.1). Vaska's complex was used as a catalyst and 1,1,3,3-tetramethyldisiloxane (TMDS) was used as a reductant, and the *in situ* generated dihydride iridium(III) complex was found to be the active catalyst. Several catalytic cycles were considered, and the silyl transfer mechanism was determined to be the optimal pathway. The high chemoselectivity was demonstrated by performing the reaction using compounds with a wide variety of functional groups. The current kinetic and computational mechanistic studies revealed the detailed mechanisms for the active catalyst generation and the hydrosilylation.

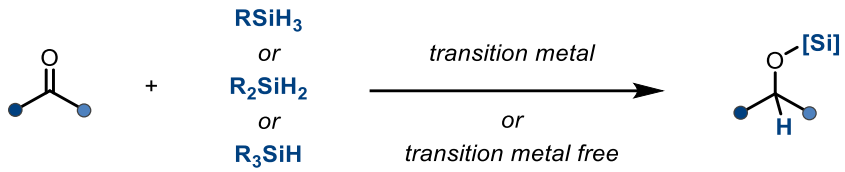


Scheme 3.1. Overview of the iridium-catalyzed hydrosilylation of amides.

3.2. Introduction

3.2.1. Hydrosilylation of Carbonyl Compounds

Reduction of carbonyl compounds with hydrosilanes has remarkably advanced the field of organic chemistry.[1] A hydrosilylation reaction is accompanied by the transformation of a reactive Si–H bond of hydrosilane into stable C–H and Si−O bonds, and numerous efforts have been made to develop this area of research in the last few decades.[2] Especially, the atom-economic transformation and user-friendly experimental procedures that derive from the use of chemically stable and easy-to-handle silanes accelerated the reaction as one of the first-choice methods for the reduction of carbonyl compounds (Scheme 3.2). Silanes may contain one to four Si–H bonds and metal-catalyzed and metal-free methods are known to date, leading to a wide variety of silyl ether products.

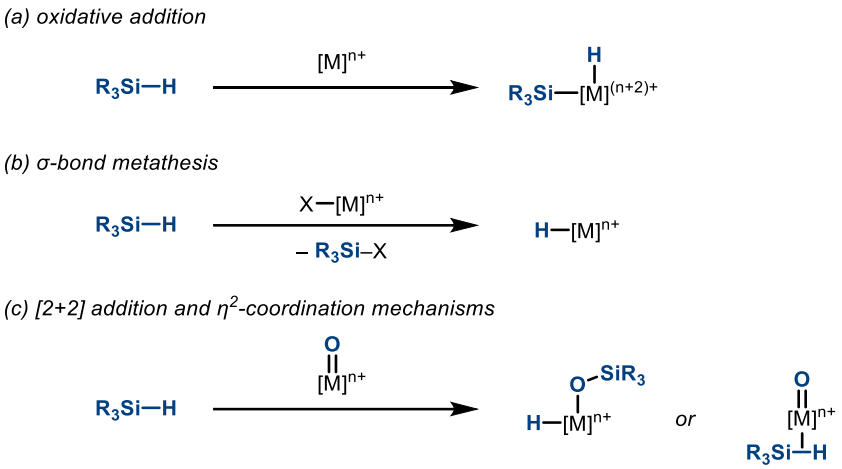


Scheme 3.2. General scheme for carbonyl hydrosilylation.

3.2.2. Diverse Mechanisms of Hydrosilylation of Carbonyl Compounds

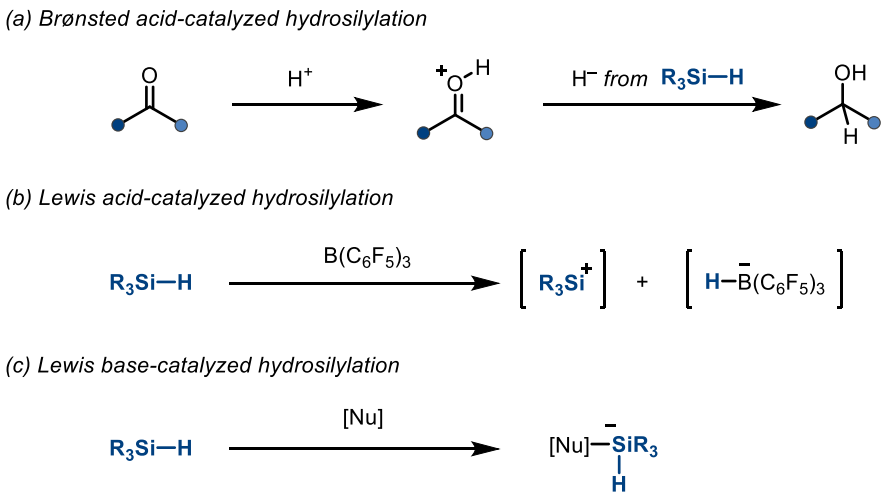
The mechanisms of hydrosilylation of carbonyl compounds depends on the catalytic system, and diverse modes of Si–H bond activation are proposed (Scheme 3.3).[3] A transition metal-catalyzed hydrosilylation usually involves the activation of the Si–H bond by an interaction with the transition metal center. The most common activation mode is the oxidative addition of Si–H bond into the transition metal that leads to the intermediate with hydride and silyl groups, which transfers both the silicon group and the hydride by migratory insertion and reductive elimination (Scheme 3.3a). This is widely seen with a group 8–10 transition metal complex, and the mechanism is similar to the one for the hydrogenation of unsaturated bonds. Another activation mode is the σ-bond metathesis that involves the exchange of Si–H and metal–X bonds into

metal–H and Si–X bonds via the four-membered transition state (Scheme 3.3b). This process is promoted by the formation of a stronger Si–X bond, and the generated metal hydride species reacts with a carbonyl group by hydrometallation. Catalytic reactions with transition metals of group 4, 11, and 12 usually proceed via hydrosilylation with this mechanism. In addition to these two modes of silane activation, a high-valent oxo complex exhibits a different reactivity, and the Si–H bond activation by [2+2] addition or by η^2-coordination are proposed (Scheme 3.3c).



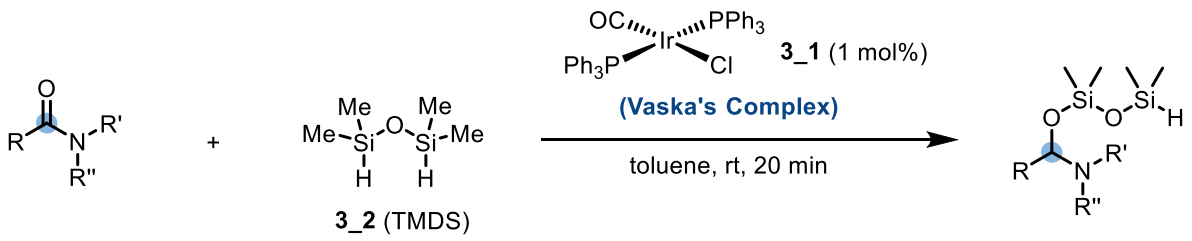
Scheme 3.3. Mechanisms for metal-catalyzed carbonyl hydrosilylation.

A transition metal-free hydrosilylation is promoted by Brønsted or Lewis acids or bases (Scheme 3.4).[4] The Brønsted acid-catalyzed reaction is initiated by the protonation of carbonyl compounds, followed by the hydride attack to the cationic species (Scheme 3.4a). Some Lewis acids are also known to activate silanes by interaction with the silane hydrogen atom (Scheme 3.4b). The commonly used tris(pentafluorophenyl)borane [$B(C_6F_5)_3$] is capable of abstracting hydride atom from silane to give a boron hydride anion and a silylium cation. Furthermore, the Lewis base-promoted silane activation is facilitated by the nucleophilic attack of the base to give the pentavalent silicate species as an intermediate (Scheme 3.4c). The nucleophilicity of hydride is dramatically increased compared to the neutral silane hydride atom to facilitate the hydride transfer from the silicon atom to the carbonyl carbon atom.



Scheme 3.3. Mechanisms for metal-free carbonyl reduction and hydrosilylation.

Despite decades of extensive mechanistic exploration for a variety of hydrosilylation reactions, there are still a number of catalytic systems where the mechanism is not yet fully understood. One example is the iridium-catalyzed hydrosilylation of amides using Vaska's complex **3_1** (Scheme 3.4).[5] The reaction proceeds under mild conditions and exhibits a high chemoselectivity. A tertiary amide is rapidly reduced to the corresponding hemiaminal, and other carbonyl groups such as ester, ketone, or aldehyde are usually unreactive. The current knowledge of mechanistic models for the transition metal-catalyzed hydrosilylation of carbonyl compounds such as the oxidative addition or σ-bond metathesis cannot describe the unique selectivity and illustrate the full catalytic process, since these mechanisms depend on the electrophilicity of carbonyl compounds and amides are one of the least electrophilic compounds. Therefore, a thorough combined kinetic and computational studies was performed and is described in this chapter.



Scheme 3.4. Iridium-catalyzed hydrosilylation of amides.

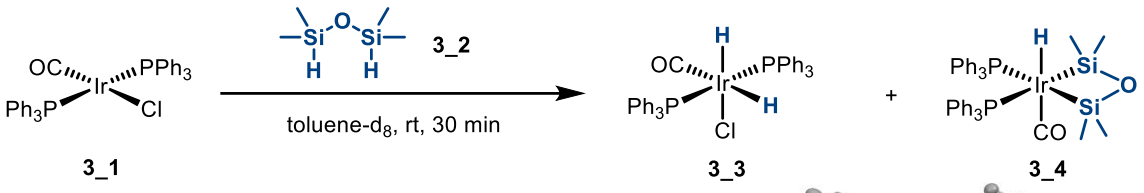
3.3. Computational Details

All calculations reported in this chapter were performed using the Amsterdam Density Functional (ADF) software,[6] and COSMO(toluene)-ZORA-M06/TZ2P//COSMO(toluene)-ZORA-BLYP-D3(BJ)/TZ2P level of theory was used.[7-13]

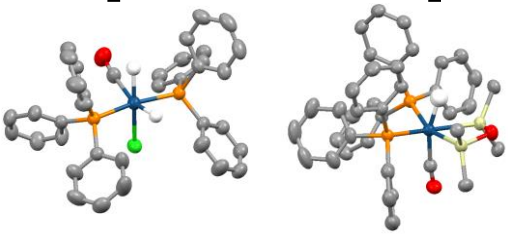
3.4. Results and Discussion

3.4.1. Determination of Active Species

In order to determine the *in situ* generated active species for the hydrosilylation of amides, the reaction between Vaska's complex **3_1** and TMDS **3_2** was conducted (Scheme 3.5).[14] An NMR study revealed that Vaska's complex **3_1** was immediately consumed, and the formation of two iridium complexes was confirmed by $^{31}P\{^{1}H\}$ NMR. After isolation and analysis by X-ray crystallography, these complexes were found to be **3_3** ($^{31}P\{^{1}H\}$ NMR: 9.16 ppm) and **3_4** ($^{31}P\{^{1}H\}$ NMR: 1.42 ppm). Complex **3_3** has two hydride atoms added on the Vaska's complex **3_1** to form the Ir(III) species, and **3_4** has a four-membered iridacycle with one hydride atom. As evidenced by the fact that **3_3** initially forms with less than the required equivalent amount of TMDS **3_2**, and that **3_4** is gradually generated with an increased amount of TMDS **3_2** after the full conversion of **3_3** to **3_4**, complex **3_4** is obtained via **3_3**. This was also proven by the observation that the dihydride complex **3_3** was gradually converted to the complex **3_4** in the presence of an excess of TMDS **3_2**, but that **3_4** remained unchanged under the same conditions.

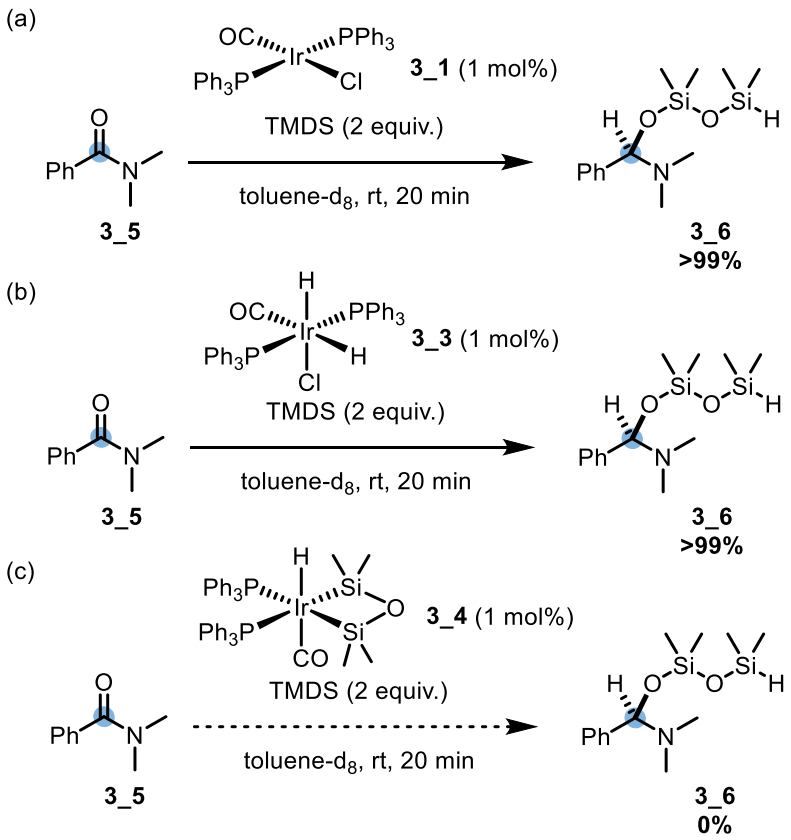


3_2 (equiv.)	**3_1** (%)	**3_3** (%)	**3_4** (%)
0	100	0	0
0.5	76	24	0
1	69	31	0
2	39	61	0
5	0	100	0
10	0	50	50
20	0	38	62
50	0	0	100
100	0	0	100
200	0	0	100



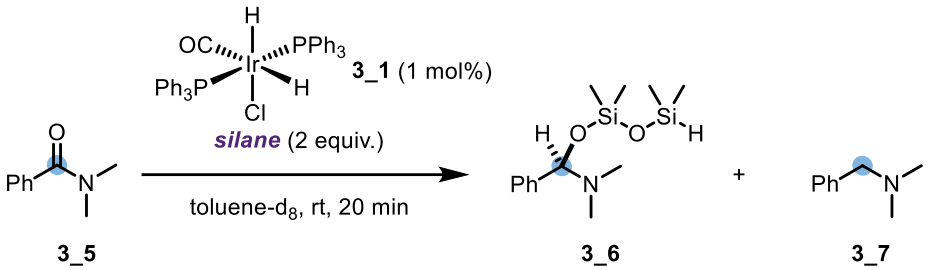
Scheme 3.5. Reaction between Vaska's complex **3_1** and TMDS **3_2**, and the X-ray crystal structures.

Then, the catalytic activities of these *in situ* generated iridium(III) complexes were examined (Scheme 3.6). The Vaska's complex **3_1** is highly active to convert *N*,*N*-dimethylbenzamide **3_5** into the corresponding hemiaminal **3_6** in quantitative yield within 20 minutes (Scheme 3.6a). Interestingly, the dihydride iridium complex **3_3** also showed a similar catalytic activity, and the amide was reduced rapidly (Scheme 3.6b). In contrast, the complex **3_4** did not promote the hydrosilylation of amides at all even after 24 hours of reaction time (Scheme 3.6c). These data strongly suggest that complex **3_3** is the active catalyst and the complex **3_4** is the deactivated catalyst, and the formation of a 16-electron iridium active species after the ligand dissociation from **3_3** is the key for promoting the catalytic cycle of the amide hydrosilylation.



Scheme 3.6. Comparison of catalytic activities of iridium complexes. Conversions were determined by ^{1}H NMR.

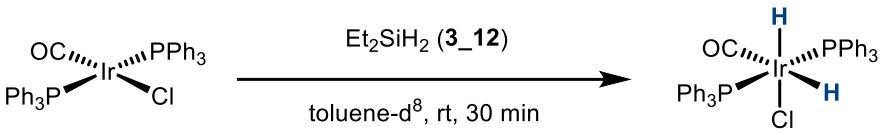
In order to compare the effect of silanes for the iridium-catalyzed hydrosilylation of amides, various silanes were tested using the dihydride iridium complex **3_3** (Scheme 3.7). The amide **3_5** was not reduced when Et_3SiH (**3_8**), Ph_3SiH (**3_9**), or $(EtO)_3SiH$ (**3_10**) was used, and $(MeO)Me_2SiH$ (**3_11**) only gave a trace amount of hydrosilylated product **3_6**. Interestingly, Et_2SiH_2 **3_12** gave a good conversion, but the overreduced product **3_7** could be observed. The formation of the dihydride complex **3_3** was also observed when Et_2SiH_2 **3_12** was used instead of TMDS **3_2** (Scheme 3.8), and the reaction proceeded in a similar fashion and the reaction was completed with 5 equivalents of Et_2SiH_2 **3_12**.



3_5 3_6 3_7

silane	conversion (%)	**3_6** (%)	**3_7** (%)
TMDS **3_2**	100	100	0
Et_3SiH **3_8**	0	0	0
Ph_3SiH **3_9**	0	0	0
$(EtO)_3SiH$ **3_10**	0	0	0
$(MeO)Me_2SiH$ **3_11**	2	2	0
Et_2SiH_2 **3_12**	74	59	15

Scheme 3.7. Comparison of reactivity of silanes. Conversions were determined by ^{1}H NMR.

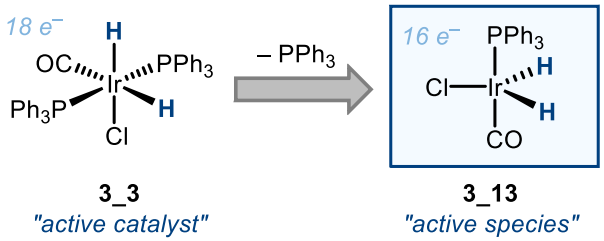


3_1 3_3

Et_2SiH_2 (equiv.)	**3_1** (%)	**3_3** (%)
0	100	0
0.5	84	16
1	77	23
2	32	68
5	0	100
10	0	100
20	0	100

Scheme 3.8. Reaction between Vaska's complex **3_1** and Et_2SiH_2 **3_12**. Conversions were determined by ^{1}H NMR.

The active species is formed from the 18-electron hexacoordinate iridium complex **3_3** by ligand dissociation (Figure 3.9). Extensive analysis of the pentacoordinate iridium complexes with various ligand orientation revealed that the 16-electron iridium(III) complex **3_13** is the active species that catalyzes the amide hydrosilylation.



Scheme 3.9. Generation of active species **3_13**.

3.4.2. Proposed Mechanisms

Based on these observations, three possible mechanisms were considered (Figure 3.1).[3] The first path is the Chalk-Harrod mechanism, in which the amide carbonyl group reacts with an iridium hydride bond via a migratory insertion (Path A, Figure 3.1a).[15] Another possible mechanism is where the iridium active species acts as the Lewis acid to activate the carbonyl group, and the silane hydride attacks the more electrophilic carbonyl carbon atom (Path B, Figure 3.1b). Alternatively, the iridium active species coordinates to the silane and increases the electrophilicity, and the amide oxygen attacks the silicon atom (Path C, Figure 3.1c).

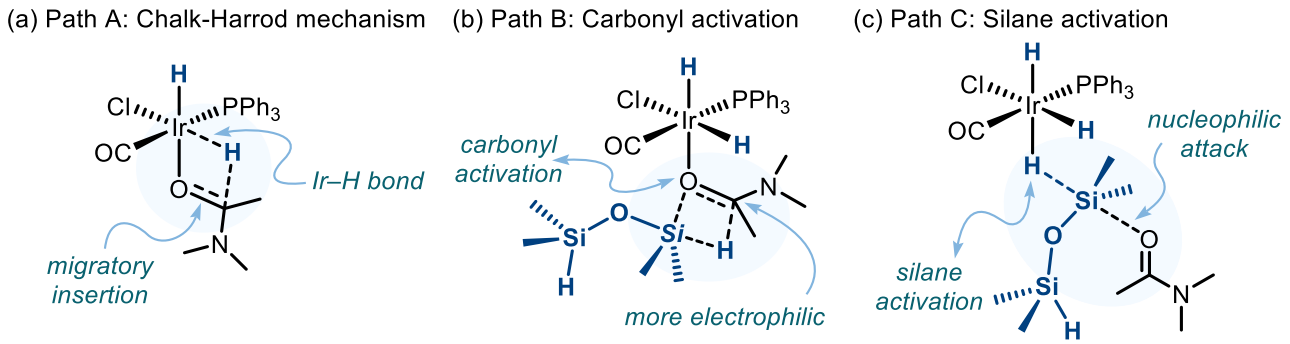
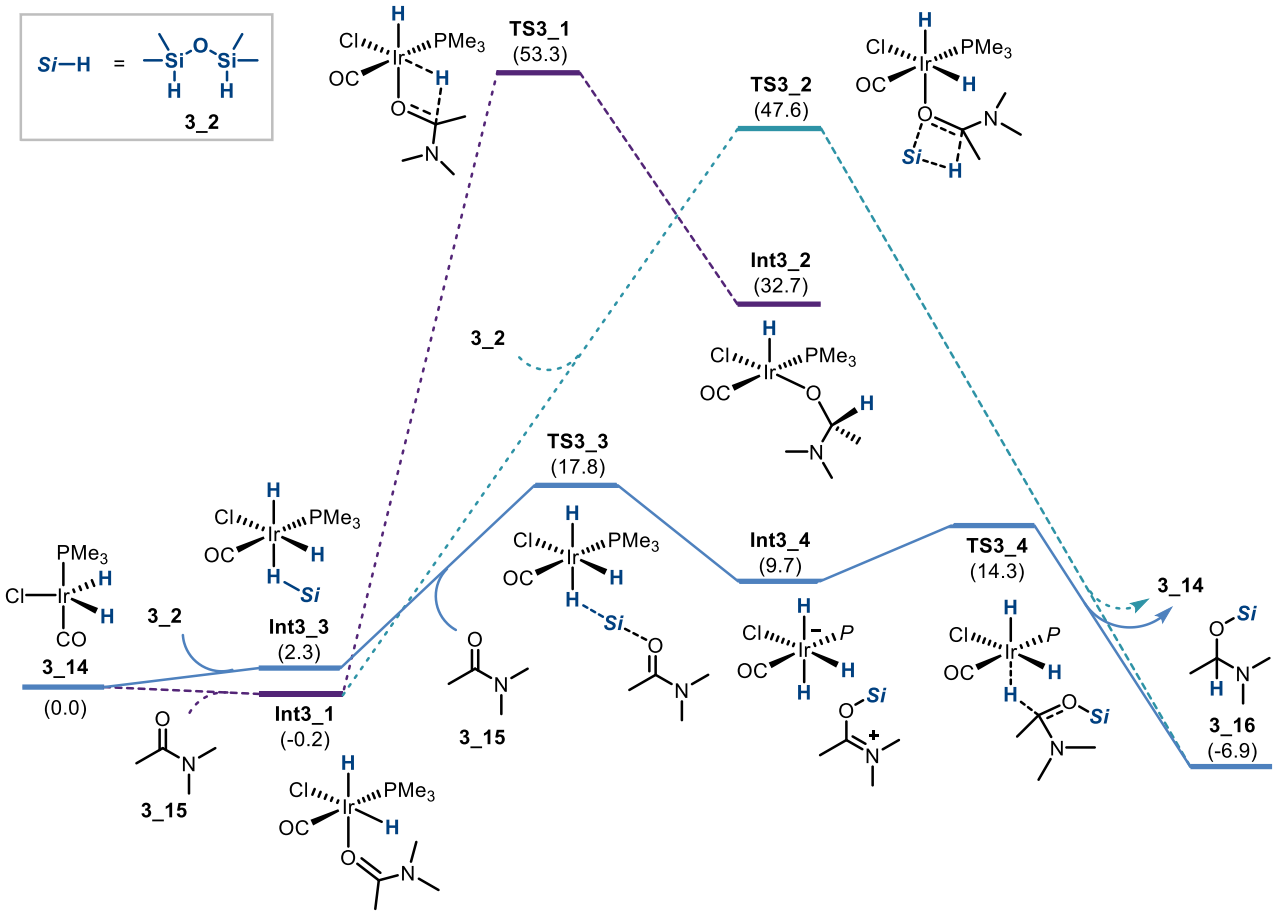


Figure 3.1. Key transition state structures of proposed mechanisms.

3.4.3. Computational Studies

In order to elucidate which mechanism is the most feasible pathway, density functional theory (DFT) calculations were employed (Scheme 3.10). Path A initiates from the amide coordination to **3_14** to form the complex **Int3_1**, and then the migratory insertion of carbonyl group of **3_15** into the Si–H bond proceeds via the transition state **TS3_1**, however the energy barrier for this step is high ($\Delta G^{\ddagger}$ = 53.3 kcal mol^{-1}). Path B goes through the transition state **TS3_2** with another molecule of TMDS **3_2**, and the four-membered TS geometry is also energetically demanding ($\Delta G^{\ddagger}$ = 47.6 kcal mol^{-1}). On the other hand, Path C is initiated from the complexation of the active species **3_14** and TMDS **3_2** to generate the intermediate **Int3_3**. Surprisingly, the nucleophilic attack of the amide **3_15** to the silicon atom through **TS3_3** requires a smaller energy barrier to obtain the iridium trihydride anion and the silylated amide cation pair **Int3_4** ($\Delta G^{\ddagger}$ = 17.6 kcal mol^{-1}). Finally, the hydride rapidly attacks the cationic species via the transition state **TS3_4** to furnish the silylated hemiaminal **3_16** and regenerate the active species **3_14**. Therefore, Path C is the most feasible mechanism, and the relatively low energy barrier for the rate-determining silyl transfer process agrees with the experimental results that the reaction can be performed at room temperature.



Scheme 3.10. Computed reaction energy profile (ΔG in kcal mol^{-1}) of the proposed mechanisms.

3.4.4. Kinetic Studies

Next, the kinetics of the reaction was studied. Since the reaction rapidly occurs with a simple amide such as *N*,*N*-dimethylbenzamide **3_5** which makes it difficult to measure the initial rates of the reaction, *N*-isopropyl-*N*-phenylbenzamide **3_17** was chosen as a standard substrate for the kinetic studies. In this study, the dihydrido iridium complex **3_3** was prepared *in situ* from the Vaska's complex under the H_2 atmosphere prior to the addition of **3_17** and **3_2** in order to simplify the catalytic system. The reaction rate is increased when the concentration of the iridium catalyst **3_3** is higher (Figure 3.2). The initial rate is linearly increased by the catalyst concentration, indicating that the reaction is first order on the catalyst. Next, the effect of concentration of the amide substrate **3_17** was examined, and it was revealed that the reaction is also first order

on the substrate (Figure 3.3). Interestingly, the concentration of TMDS did not affect the reaction rate, which suggests the zero-order kinetics on the silane (Figure 3.4). These results are in agreement with the computational results that the iridium complex **Int3_3** and the amide **3_15** are involved in the rate-determining transition state **TS3_3**, and the concentration of these two species are directly affecting the reaction rate.

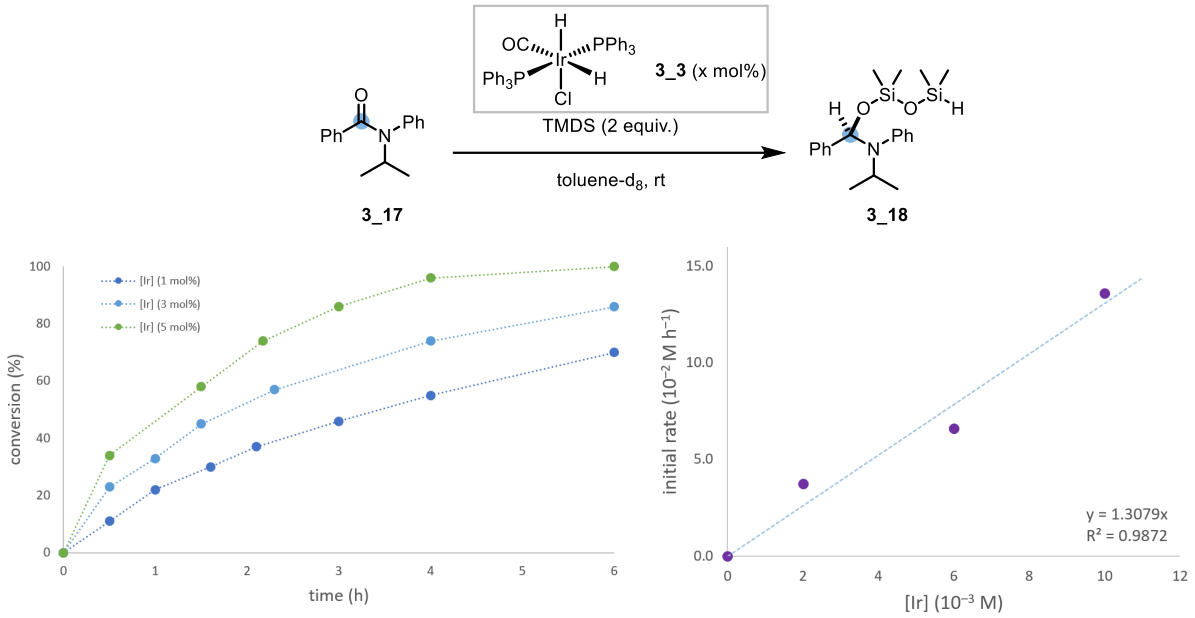


Figure 3.2. Reaction profile with various catalyst concentrations. Conversions were determined by ^{1}H NMR.

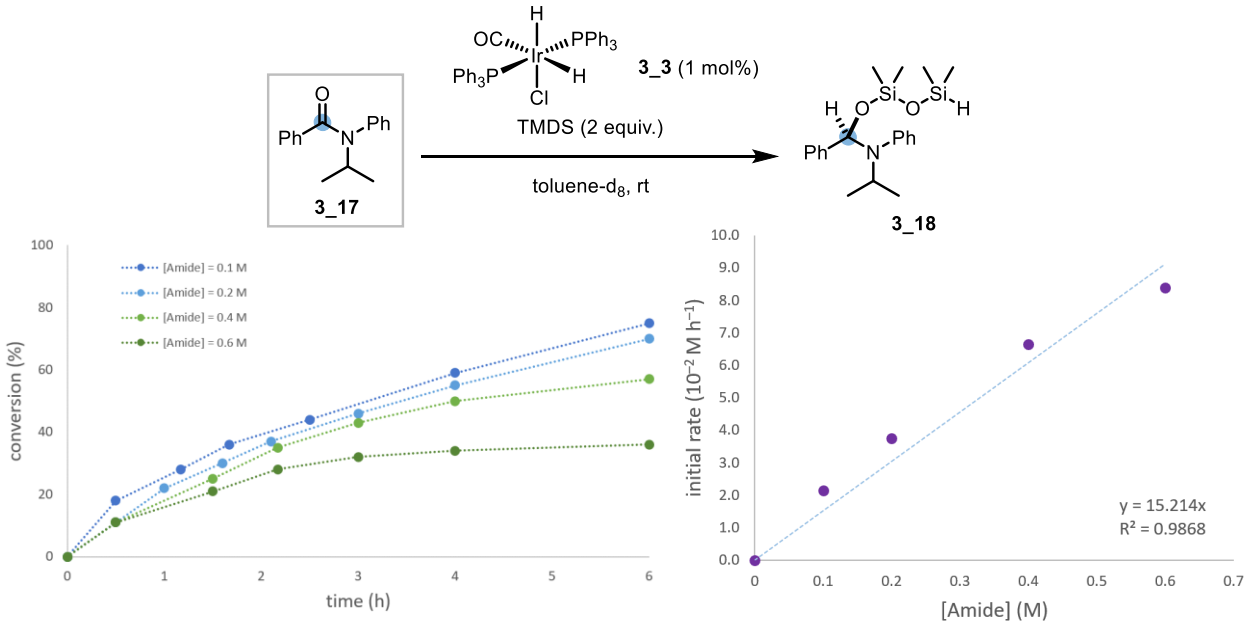


Figure 3.3. Reaction profile with various substrate concentrations. Conversions were determined by ^{1}H NMR.

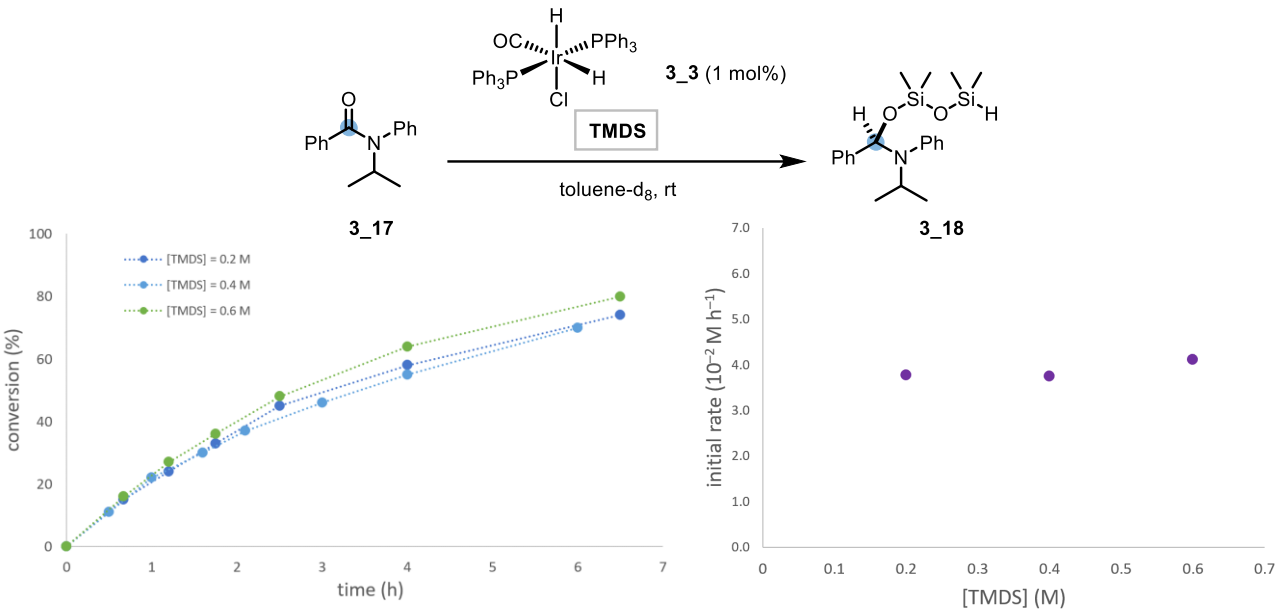


Figure 3.4. Reaction profile with various TMDS concentrations. Conversions were determined by ^{1}H NMR.

The electronic character of the key reduction process of amides was then examined through a Hammett analysis (Figure 3.5).[16] It was found that the *para*-substituent of the aryl group next to the carbonyl group has a great influence on the reaction rate, and the initial rate is accelerated in the presence of an electron-donating group such as a methoxy group (**3_19**). On the other hand, an electron-withdrawing group such as halides (**3_20**, **3_21**) and nitro groups (**3_22**) decreased the reactivity. These results indicate that the positive charge buildup occurs during the rate-determining transition state, in which the electron-donating group can stabilize the positively charged silylated amide cationic intermediate in **Int3_4**.

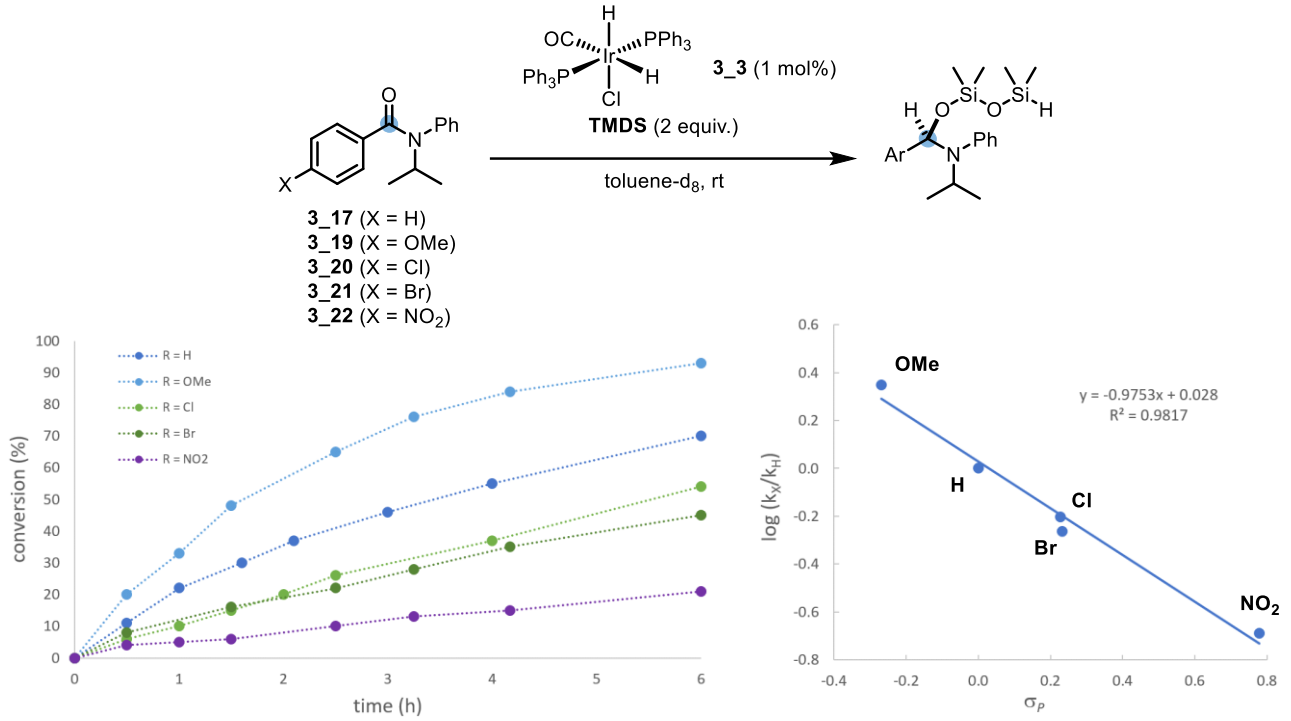


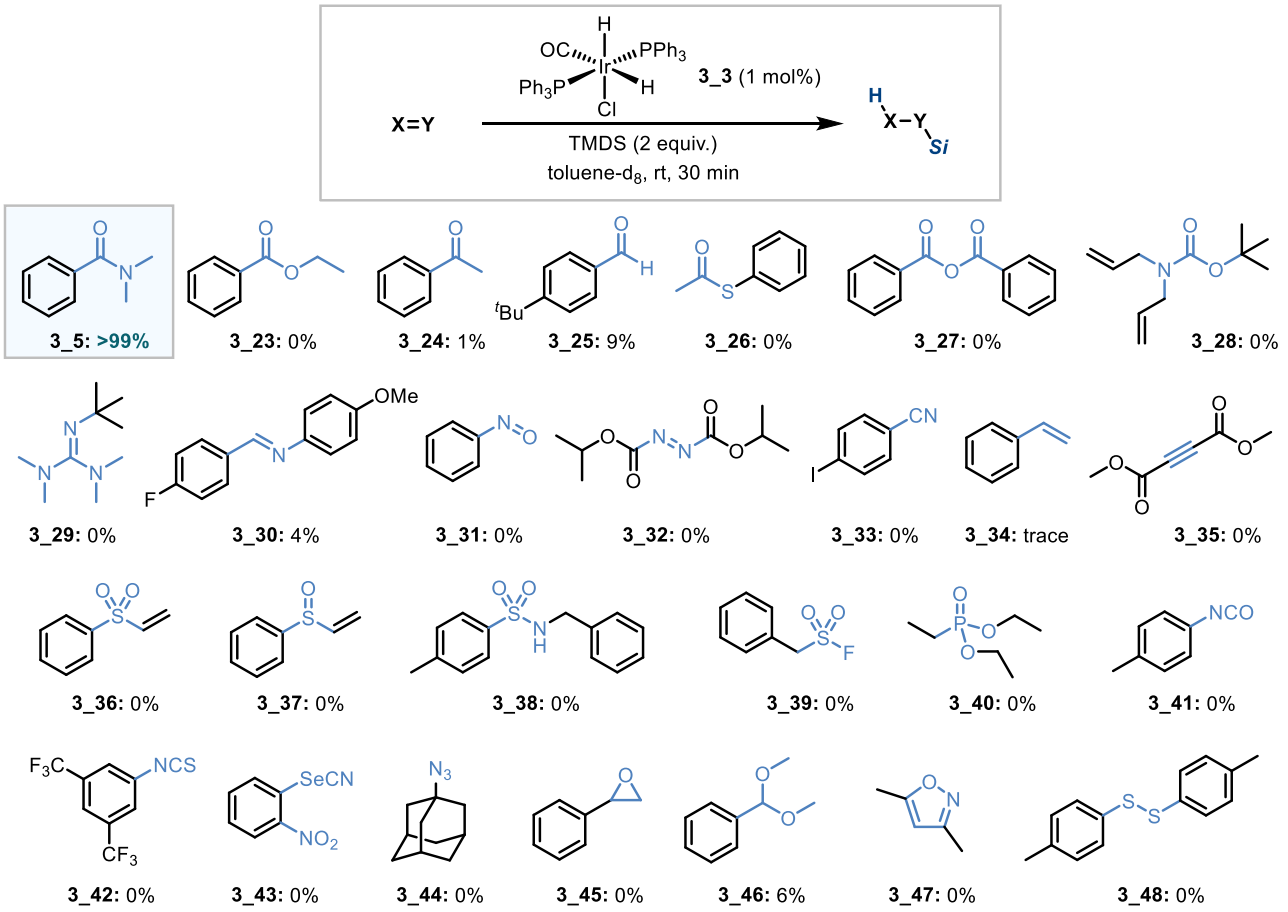
Figure 3.5. Hammett plot. Conversions were determined by ^{1}H NMR.

Overall, these kinetic studies agree with the computationally most preferred pathway through Path C which involves nucleophilic attack to the carbonyl oxygen and the hydride transfer from the iridium species. The reaction rate can be described as k_{obs}[iridium]^{1}[amide]^{1}, and Hammett analysis agrees with the formation of cationic intermediate. In other words, the reactivity depends on the nucleophilicity of the carbonyl group, thus the amides are more reactive than other carbonyl groups such as esters, ketones, and aldehydes.

3.4.5. Functional Group Selectivity

Inspired by the above-described mechanistic pathway, the generality and specificity of the iridium-catalyzed hydrosilylation of unsaturated compounds were examined (Scheme 3.11). The amide compound **3_5** rapidly reacts to furnish the hydrosilylated compound, while other carbonyl compounds such as ester (**3_23**), ketone (**3_24**), aldehyde (**3_25**), thioester (**3_26**), carboxylic anhydride (**3_27**), or carbamate (**3_28**) gave no

or extremely low conversions under the reaction conditions with **3_3** and TMDS **3_2**. Unsaturated nitrogen compounds such as guanidine (**3_29**), imine (**3_30**), nitroso (**3_31**), diazo (**3_32**), or nitrile (**3_33**) were also unreactive. Interestingly, alkene (**3_34**) or alkyne (**3_35**) remained intact under the standard conditions. Sulfur or phosphorus-containing unsaturated compounds (**3_36**-**3_40**) and various reactive functional groups such as isocyanate (**3_41**), thioisocyanate (**3_42**), selenocyanate (**3_43**), azide (**3_44**), epoxide (**3_45**), acetal (**3_46**), isoxazole (**3_47**), or disulfide (**3_48**) tolerated the reaction conditions. These results prove that this method is highly selective towards the amide group, and easily applicable for late-stage functionalization.



Scheme 3.11. Chemoselectivity of the hydrosilylation reaction.

3.4.6. Catalyst Modifications

Our mechanistic investigations revealed that the key transition state is the nucleophilic attack of the carbonyl group to the silane, and the reaction was accelerated by stabilizing the cationic silylated amide intermediate. This led to the inspiration about whether the reactivity can be controlled by changing the nature of the iridium catalyst. First, the key rate-determining transition state was theoretically analyzed with different phosphine ligands (Figure 3.6). As expected, the energy barriers with these electron-deficient phosphines such as $P(OMe)_3$ (**TS3_5**) or $P(OHFIP)_3$ (**TS3_6**, OHFIP = 1,1,1,3,3,3-hexafluoro-2-propoxyl) were significantly lowered to 13.2 kcal mol^{-1} and 12.2 kcal mol^{-1}, respectively. The energy trend derives from the stabilization of the anionic iridium trihydride intermediate.

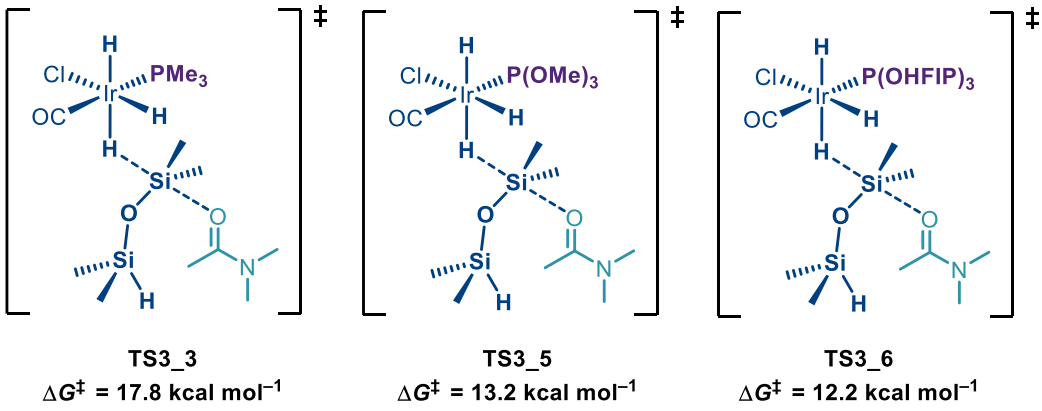
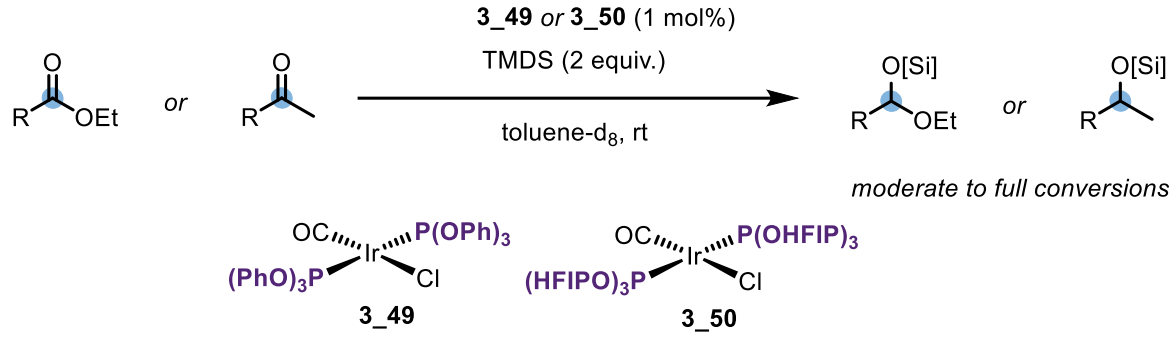


Figure 3.6. Nucleophilic attack transition state structures with different phosphines.

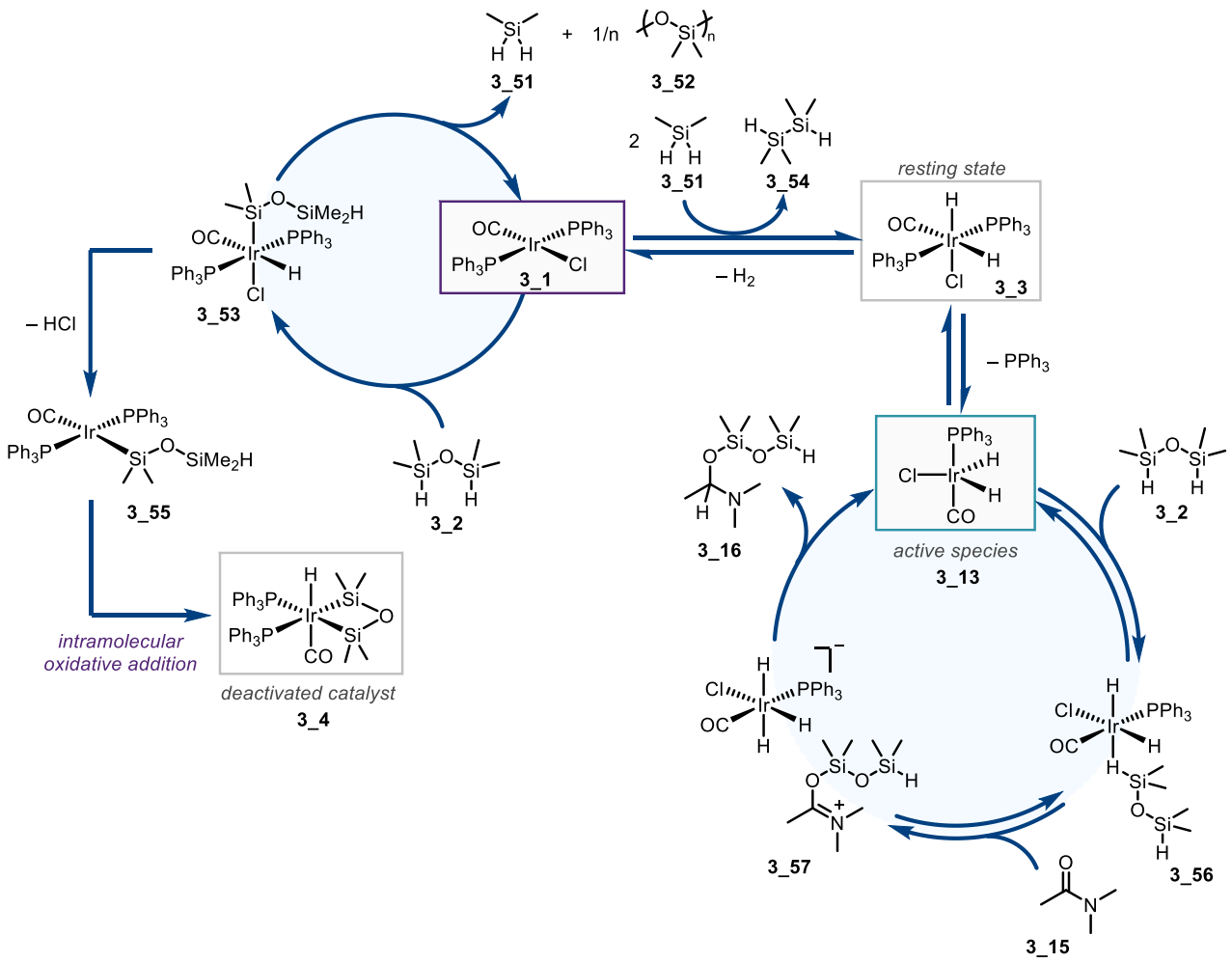
The hypothesis that the electron-deficient ligand can promote the hydrosilylation of other carbonyl groups was experimentally validated by using Vaska-type complexes (Scheme 3.12).[17] Indeed, the ester and ketone compounds reacted under these conditions with the phosphite-based Vaska's complexes such as **3_49** and **3_50**, and this demonstrates that the catalytic activities of such iridium complexes are tunable by controlling the electronic nature of the ligands.



Scheme 3.12. Carbonyl hydrosilylation with different iridium catalysts.

3.4.7. Catalytic Cycles

A summary of the combined experimental and computational mechanistic studies of the hydrosilylation of amides is shown in Scheme 3.13. The Vaska's complex **3_1** initially reacts rapidly to give the active catalyst **3_3** in the presence of TMDS **3_2**. As evidenced by the fact that the reaction also proceeds with Et_2SiH_2 **3_12** which also generate the iridium species **3_3** *in situ*, the Vaska's complex **3_1** degrades TMDS into Me_2SiH_2 **3_51** and siloxane **3_52** via oxidative addition through the intermediate **3_53**.[18] The active iridium complex **3_3** can gradually release hydrogen gas to regenerate Vaska's complex **3_1**, and the release of HCl from intermediate **3_53** by reductive elimination gives the intermediate **3_55** that further undergoes an intramolecular oxidative addition to furnish the deactivated catalyst **3_4**. Once the phosphine ligand is dissociated from the **3_3** to generate the 16-electron iridium(III) species **3_13**, the catalytic cycle is initiated by the coordination of TMDS **3_2** to give the intermediate **3_56**. Then, the amide substrate **3_15** attacks the activated silicon atom by the nucleophilic substitution at silicon (S_N2@Si) pathway to obtain the silylated amide cation and iridium trihydride anion pair **3_57**, and the final facile hydride transfer furnishes the silylated hemiaminal product **3_16** and regenerates the active species **3_3**.[19]



Scheme 3.13. Summary of the catalytic cycles of the amide hydrosilylation.

3.5. Conclusion

In conclusion, a detailed mechanistic study of the hydrosilylation of amides was performed computationally and experimentally. NMR studies and the isolation of iridium complexes enabled us to determine the actual catalyst that promotes the reaction, and the catalytic cycle was demonstrated to proceed via the nucleophilic attack of the amide to the activated silane. The key rate-determining transition state generates two ionic intermediates by the silyl transfer, namely the silylated amide cation and the trihydride iridium anion, and the reactivity is defined by the stability of these species. The high chemoselectivity was

also demonstrated using the discovered active catalyst, suggesting the high utility of this reaction. The insights from these studies can promote further reaction development and the understanding of catalytic systems.

3.6. References

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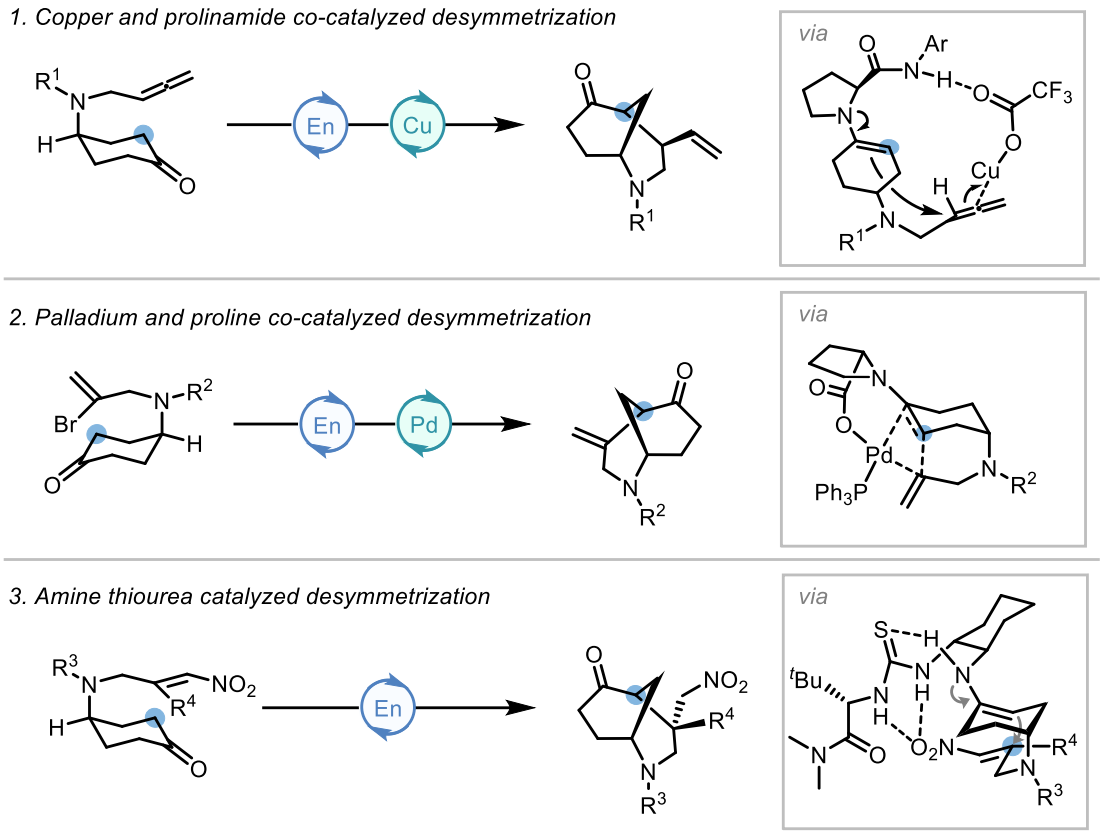
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Chapter 4

Mechanistic Studies of Enantioselective Desymmetrization of Cyclohexanones

4.1. Chapter Overview

This chapter describes mechanistic studies of enantioselective catalytic desymmetrization reactions of various 4-substituted cyclohexanones where the origin of the enantio- and diastereoselectivities for the transformations have been uncovered using density functional theory (DFT) calculations (Scheme 4.1). The products formed from the desymmetrization reactions possess morphan cores, which are widely seen in alkaloid natural products, with multiple stereocenters. A copper and prolinamide co-catalyzed desymmetrization of allene-tethered cyclohexanones set all three of the newly formed stereogenic centers during the key nucleophilic attack of an enamine to copper-coordinated allene in the intramolecular cyclization step by a key hydrogen bonding interaction between an amide N–H bond and an O atom in trifluoroacetate and the steric repulsion of the vinyl group. A palladium and proline-co-catalyzed desymmetrization of vinyl-bromide-tethered cyclohexanones set the enantioselectivity by the key migratory insertion of an enamine intermediate to a tethered Pd–C bond through a transition state structure that benefits from more stabilizing interaction energy and less destabilizing strain energy. An amine thiourea-catalyzed desymmetrization of nitro-olefin-tethered cyclohexanones set all three of the newly formed stereogenic centers by an irreversible intramolecular Michael addition of an enamine to a thiourea-activated nitro olefin through the lowest-energy conformation of the transition state structure that benefits from stabilization from several hydrogen bonds involving the thiourea, nitro group and the enamine moieties. These DFT calculations provide evidence for the kinetic preference for the formation of products, which were confirmed by X-ray crystallography.



Scheme 4.1. Overview of enantioselective catalytic desymmetrization of cyclohexanones investigated in this chapter.

4.2. Introduction

4.2.1. Morphan Core Containing Bioactive Compounds and Natural Products

The morphan scaffold (azabicyclo[3.3.1]nonane) is commonly found and is present in more than 300 natural products (Figure 4-1).[1] These are mainly the daphniphyllum, strychnos, and madangamine alkaloid families, and a variety of natural compounds such as morphine (**4_1**), strychnine (**4_2**), and himalensine A (**4_3**) can be found in this category. Furthermore, it is present in other biologically relevant molecules such as immunosuppressant FR901483 (**4_4**). Due to the potential applications of morphan core-containing biologically active compounds in pharmaceuticals, development of a wide variety of synthetic methods are desired.[2]

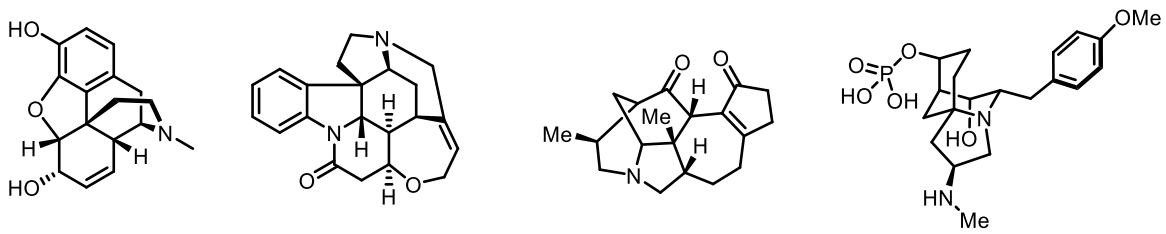
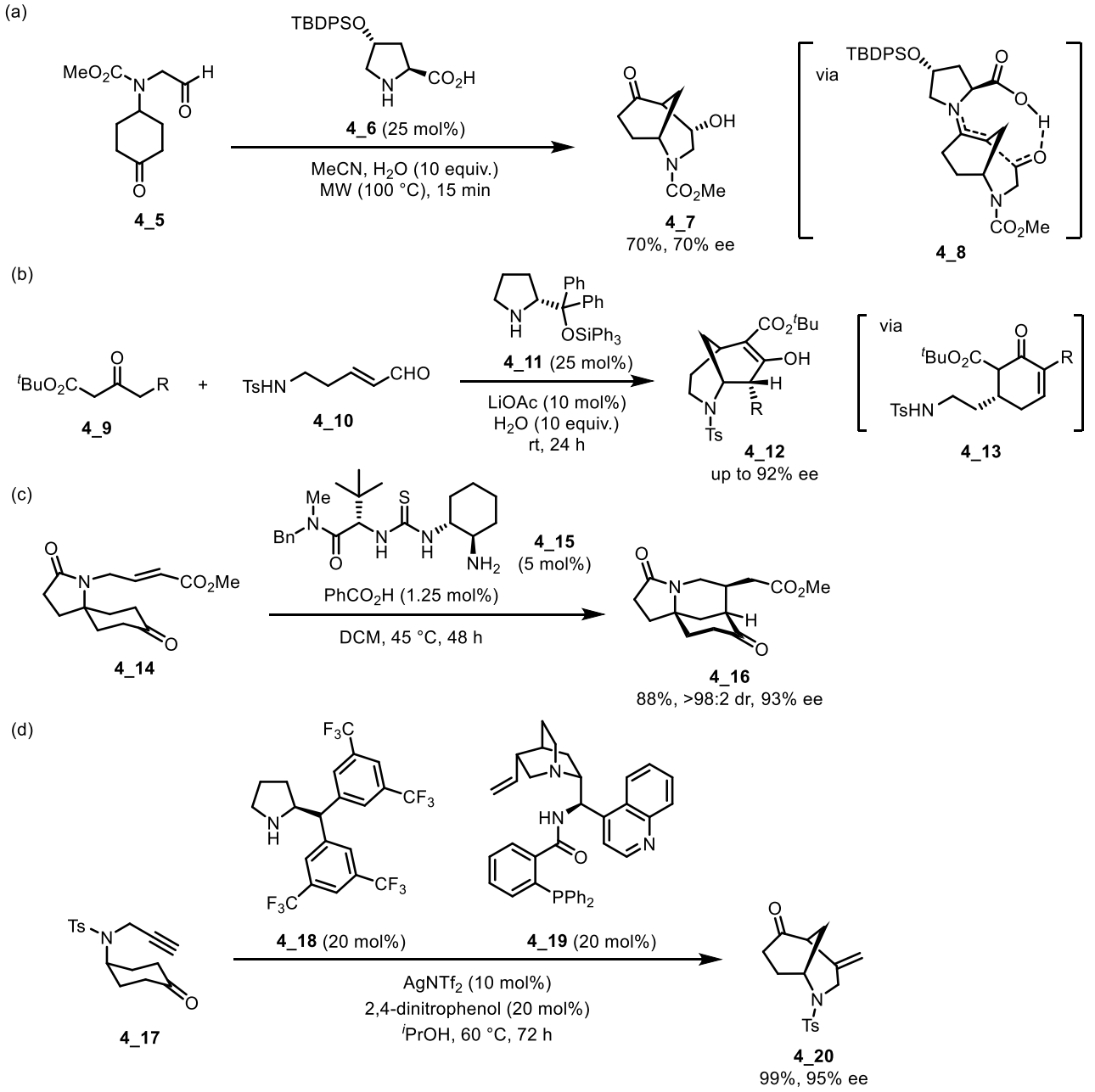


Figure 4.1. Natural products and biologically relevant molecules containing the morphan core.

4.2.2. Enantioselective Construction of Morphan Cores

While various reactions for constructing the morphan core as a racemate have been reported, enantioselective approaches have not been fully developed.[1e] The first example of an organocatalytic construction of the morphan core was achieved by Bonjoch and Diaba in 2009 by using the hydroxyproline derivative **4_6** as the catalyst to carry out a stereoselective intramolecular aldol reaction (Scheme 4.2a).[3] Furthermore, Bonjoch developed an organocatalytic cascade reaction of the *β*-ketoester **4_9** and the enal **4_10** using a catalytic amount of prolinol derivative **4_11** to achieve the Michael addition/Robinson annulation/aza-Michael addition sequence (Scheme 4.2b).[4] In 2015, Dixon and Paton reported the enantioselective desymmetrization of unsaturated ester-tethered cyclohexanone **4_14** with a bifunctional organocatalyst **4_15** (Scheme 4.2c).[5] This synthetic methodology provides a rapid construction of the morphan core with three stereo centers in an excellent chemical yield, and high diastereo- and enantioselectivities. A detailed mechanistic study was performed using DFT calculations, and it was revealed that the cyclization occurs via the stepwise Michael addition/intramolecular proton transfer sequence. The second proton transfer step is irreversible and determined the enantioselectivity, and the computed 96% ee was in excellent agreement with the experimentally observed 96% ee using a computationally simplified thiourea catalyst.



Scheme 4.2. Enantioselective organocatalytic syntheses of morphan cores.

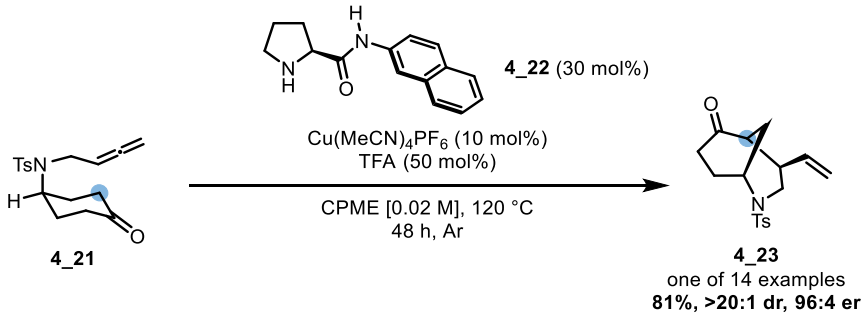
Enantioselective synthesis of morphan cores can also be achieved by using transition metal catalysis. In 2017, Dixon and Paton demonstrated the silver (I) and amine-cocatalyzed desymmetrization of 4-propargylamino cyclohexanones **4_17** (Scheme 4.2d).[6] This synthetic methodology provides access to methylene-substituted morphan cores **4_20** in excellent yields and enantioselectivities. The computational

analysis of the key C–C bond forming transition state revealed that the enamine formed from the ketone and the amine catalyst **4_18** undergoes nucleophilic attack to the alkyne-silver complex with the cinchona-derived ligand **4_19**. The chirality matching effect between the cinchona alkaloid-derived aminophosphine ligand and the amine catalyst was also rationalized by the DFT calculations.

4.3. Copper and Prolinamide Co-catalyzed Desymmetrization

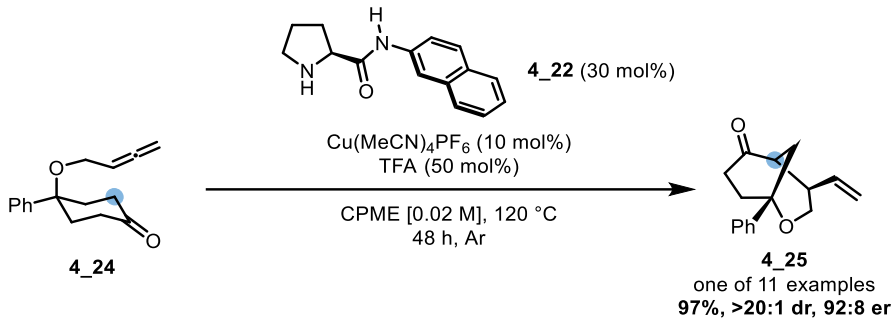
4.3.1. Previous Experimental Findings

Previously, our group discovered that 2-naphthylprolinamide **4_22** as an amine catalyst in conjunction with the copper(I) complex $Cu(MeCN)_4PF_6$ is optimal for the enantioselective desymmetrization of allene-tethered cyclohexanones **4_21**.[7,8] Interestingly, the addition of trifluoroacetic acid (TFA) substantially improved the enantioselectivity. The optimized conditions at 120 °C in CPME as solvent furnished the products in good to excellent yields with up to >20:1 dr and 96:4 er. The substrate scope with nitrogen-linked allene was explored with 14 examples, and the reaction was found to proceed in 75-90% yields with up to >20:1 dr and 96:4 er (Scheme 4.3). Several functional groups such as bromo, nitro, trifluoromethyl, pyridinyl and thiophenyl groups tolerated the conditions. An internal allene substrate also reacted smoothly under the optimized conditions.



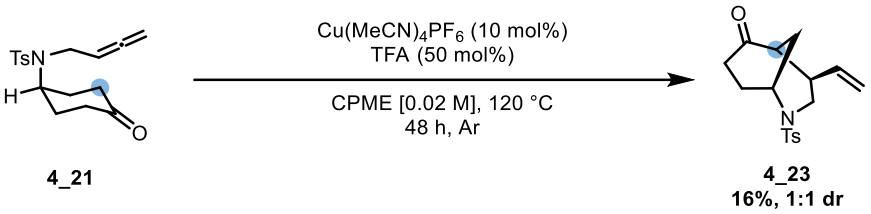
Scheme 4.3. Nitrogen-linked allene substrate **4_21** for the copper(I) and prolinamide **4_22** co-catalyzed desymmetrization.

In addition to the nitrogen-linked allene substrate, oxygen-substituted counterparts **4_24** to construct the analogous 2-oxabicyclo[3.3.1]nonane heterocycle **4_25** were also studied (Scheme 4.4). Although the substitution of -NTs group by an oxygen atom in the substrate did not furnish any desired product, installation of a substituent such as an alkyl or aryl group at the α-position to the oxygen atom provided the bicyclic compound as a single diastereomer in all cases in 67-98% yields and 81:19 to 94:6 er.

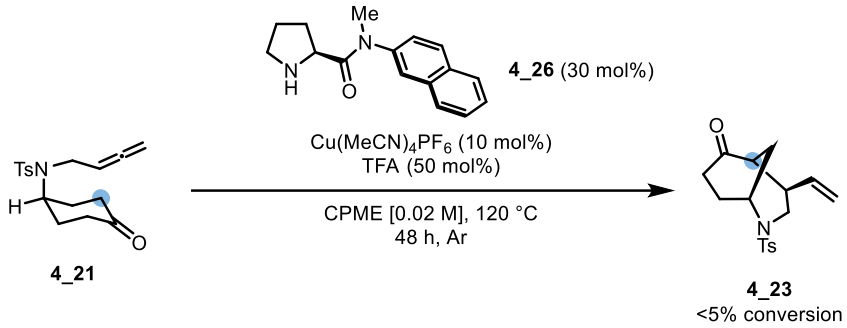


Scheme 4.4. Oxygen-linked allene substrate **4_24** for the copper(I) and prolinamide **4_22** co-catalyzed desymmetrization.

In order to uncover the mechanistic pathway of the dual-catalytic reaction to obtain the enantioenriched vinyl-substituted morphan core, mechanistic studies were performed. When the reaction was conducted without the copper catalyst, the formation of the enamine structure was confirmed by MS, however no cyclized product was observed. In the absence of the prolinamide catalyst **4_22**, the reactivity was suppressed substantially, and the product **4_23** was observed in poor yield (16%) with no diastereoselectivity (1:1 dr) (Scheme 4.5). This indicated that the organocatalyst is crucial not only for enantioselectivity, but also for reaction efficiency and diastereoselectivity. Finally, when the reaction was conducted with the *N*-methylated organocatalyst **4_26**, only a trace amount of the product was observed with almost quantitative recovery of the starting material, suggesting that the amide N–H bond plays an important role in the reaction mechanism to boost the reactivity and selectivity (Scheme 4.6).



Scheme 4.5. Reactivity in the absence of the prolinamide catalyst.



Scheme 4.6. Reactivity with *N*-methylated prolinamide catalyst **4_26**.

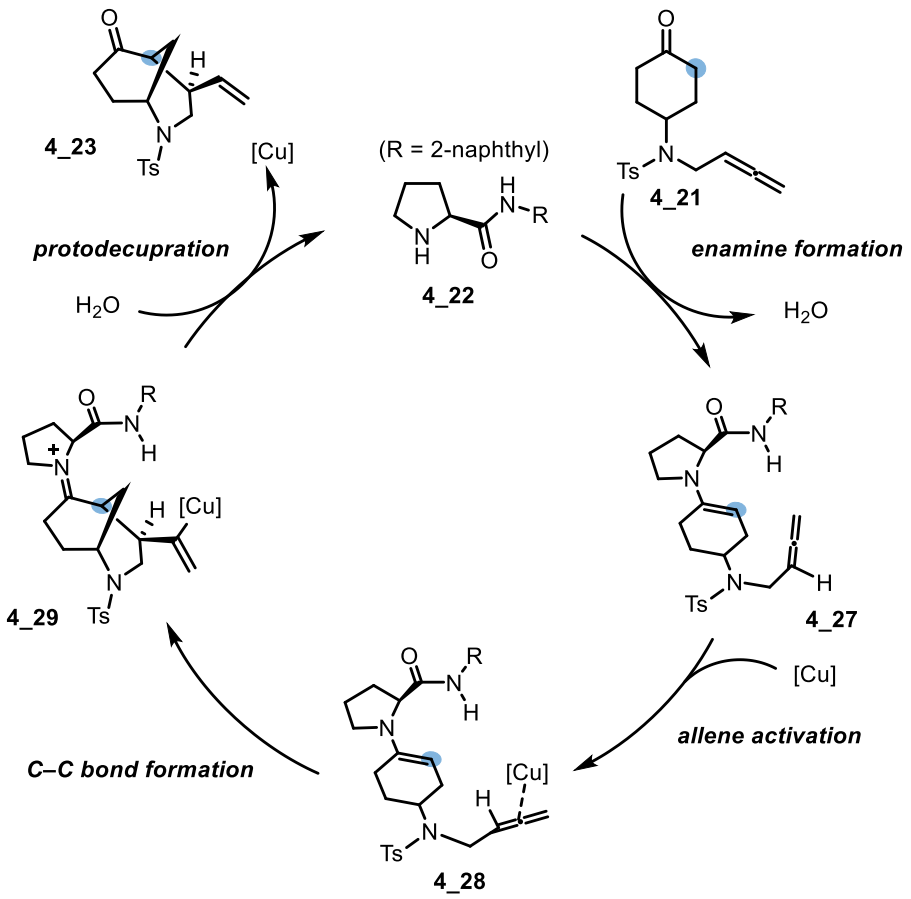
4.3.2. Computational Details

All calculations reported in this chapter were performed using the Amsterdam Density Functional (ADF) software,[9] and the COSMO(Et_2O)-ZORA-M06/TZ2P//COSMO(Et_2O)-ZORA-BLYP-D3(BJ)/TZ2P level of theory was used.[10-16]

4.3.3. Proposed Catalytic Cycle

Based on the experimental results described above, a plausible catalytic cycle was proposed (Scheme 4.7). The initial step is the formation of an enamine from the cyclohexanone substrate **4_21** and the prolinamide organocatalyst **4_22**. Then, the copper species activates the allene moiety by coordination prior to the subsequent cyclization step. The enamine undergoes intramolecular nucleophilic attack to the copper-coordinated allene to form a new C–C bond.[17] This process is the enantio- and diastereoselectivity-determining step which could lead to four possible products. Finally, the vinyl cuprate intermediate is protodemetalated,

and the iminium **4_29** is hydrolyzed to furnish the vinyl-substituted cyclized product **4_23**, and the prolinamide organocatalyst **4_22** is regenerated. The most important step in the proposed catalytic cycle that affects the stereoselectivity is the new C–C bond forming intramolecular nucleophilic attack of the enamine. Therefore, this step was the focus of the study to understand the origin of the unique reactivity of the reaction.



Scheme 4.7. Proposed catalytic cycle.

4.3.4. Intramolecular Nucleophilic Attack of Enamine

Considering the fact that the results of the experimental mechanistic study in Scheme 4.5 and 4.6 provided some evidence towards the roles of the copper and prolinamide catalysts as well as trifluoroacetic acid as an additive in this reaction system, the following model has been proposed for the computational mechanistic study: (1) $Cu^{I}(TFA)$ is the active species resulting from the reaction between $Cu(MeCN)_4PF_6$ and

trifluoroacetic acid, (2) hydrogen bonding between the prolinamide N–H bond and the oxygen atom of trifluoroacetate stabilizes the intermediates and transition state structures, and (3) the bulky substituent of the amide prevents reactivity from the top-surface of the enamine in each of the structures. From these hypotheses, the stereoselectivity-determining intramolecular nucleophilic attack of an enamine was studied.

In this computational study, the substituent of the prolinamide organocatalyst was chosen as phenyl group instead of 2-naphthyl group for the simplification of the calculations. The allene-tethered cyclohexanone substrate and the prolinamide organocatalyst initially react to form either *s-cis* enamine **Int4_1** or *s-trans* **Int4_2** (Figure 4.2). The energy difference between these species is small, indicating that the equilibrium between these conformations is rapid (ΔG = 0.9 kcal mol^{-1}). Then the copper(I) trifluoroacetate coordinates to the allene moiety of these enamine species to generate highly stabilized complexes **Int4_3** to **Int4_4**. The reactant complexes **Int4_3** and **Int4_4** are more stable compared to **Int4_5** and **Int4_6** due to the existence of hydrogen bonding between the N–H bond of the amide and the carbonyl oxygen atom of the trifluoroacetate ligand. The most favorable C–C bond forming transition state is **TS4_1** that proceeds with a stabilizing hydrogen bonding interaction. The second most favorable transition state **TS4_2** that forms a diastereomer is 2.2 kcal mol^{-1} higher in energy than **TS4_1** because of the steric clash between the prolinamide and the allene moiety.

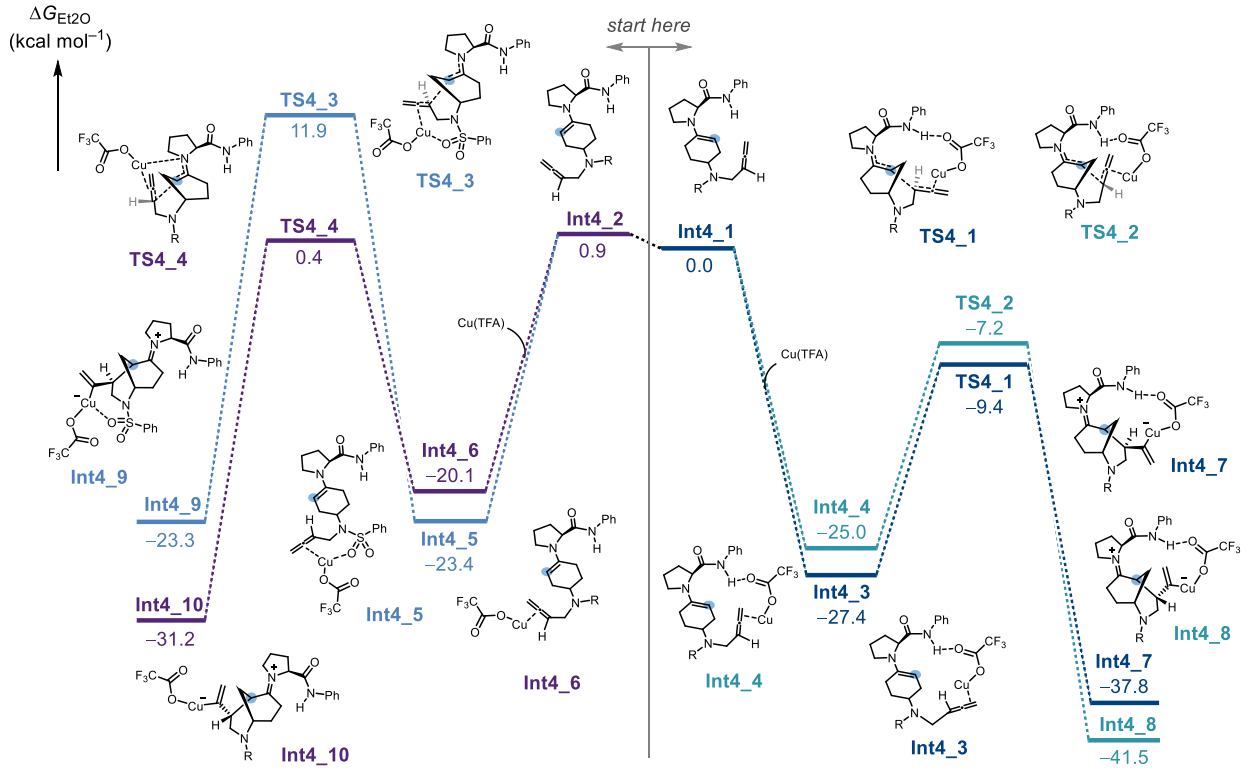


Figure 4.2. Computed reaction energy profile for the four possible pathways of the intramolecular nucleophilic attack of the enamine to the allene. R = SO_2Ph.

In order to quantitatively confirm this diastereoselectivity, the activation strain analysis (ASA) was performed on these two transition states using Cu(TFA) and the enamine substrate as the fragments, and the results are summarized in Figure 4.3.[18] The trend of energy barriers was consistent with the strain energy $\Delta E^{\ddagger}_{strain}$, and the favored transition state **TS4_1** is less distorted especially on the substrate fragment ($\Delta\Delta E^{\ddagger}_{strain}$ = 1.9 kcal mol^{-1}). The origin of the destabilized strain energy for **TS4_2** is that the enamine moiety is forced to rotate at the C–C bond between the pyrrolidine and cyclohexene rings, as evidenced by the larger dihedral angle ϕ (C(4)–C(5)–C(6)–C(7)) in **TS4_2**. This preferred nucleophilic attack step is highly exergonic (ΔG = –10.4 kcal mol^{-1}), and the reverse process requires a large energy barrier ($\Delta G^{\ddagger}$ = 28.4 kcal mol^{-1}) that indicates the irreversibility. Other possible intramolecular nucleophilic attack transition states from **Int4_5** or **Int4_6** can be excluded from the pathway because these structures are highly destabilized due to the absence of

hydrogen bonding between the N–H bond and the oxygen atom. Therefore, the enantio- and diastereoselectivities are set during the intramolecular nucleophilic attack.

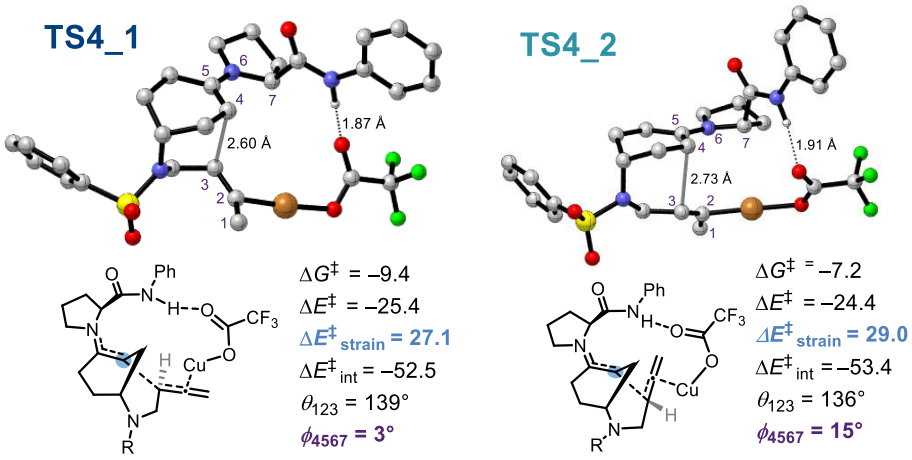


Figure 4.3. Transition state structures **TSB1-C1** and **TSB2-C2** of the intramolecular nucleophilic attack.

4.3.5. Protodecupration Process

After the intramolecular cyclization process, the intermediate **Int4_7** undergoes the protodecupration process (Figure 4.4). Since the most acidic proton source is trifluoroacetic acid, the acid coordinates to **Int4_7** prior to the protodecupration step. Initially, the proton coordinates to the C=C double bond to form **Int4_11**, and the complex is destabilized due to the entropic cost (ΔG = 9.9 kcal mol^{-1}). The energy barrier through the irreversible protodecupration transition state **TS4_5** from **Int4_7** is 18.0 kcal mol^{-1}, and the C–H bond formation and the C–Cu bond cleavage occur at the same time. Finally, the iminium moiety is hydrolyzed to give **Int4_15**, and the prolinamide organocatalyst and copper(I) trifluoroacetate species are regenerated. It is likely that the formal "Cu(TFA)" is transferred to another allene substrate or stabilized by solvent molecules, rather than dissociated to exist without any stabilization. This is evidenced by the energy change from **Int4_15** to **P4_1**, but the dissociation of "Cu(TFA)" is shown in the scheme for the simplicity of the calculated model.

The alternative protodecupration pathway from **Int4_8** is shown in the Figure 4.4. The energy change trend was identical to the pathway from **Int4_7**, and indeed the enantio- and diastereoselectivities are determined by the previous nucleophilic attack process.

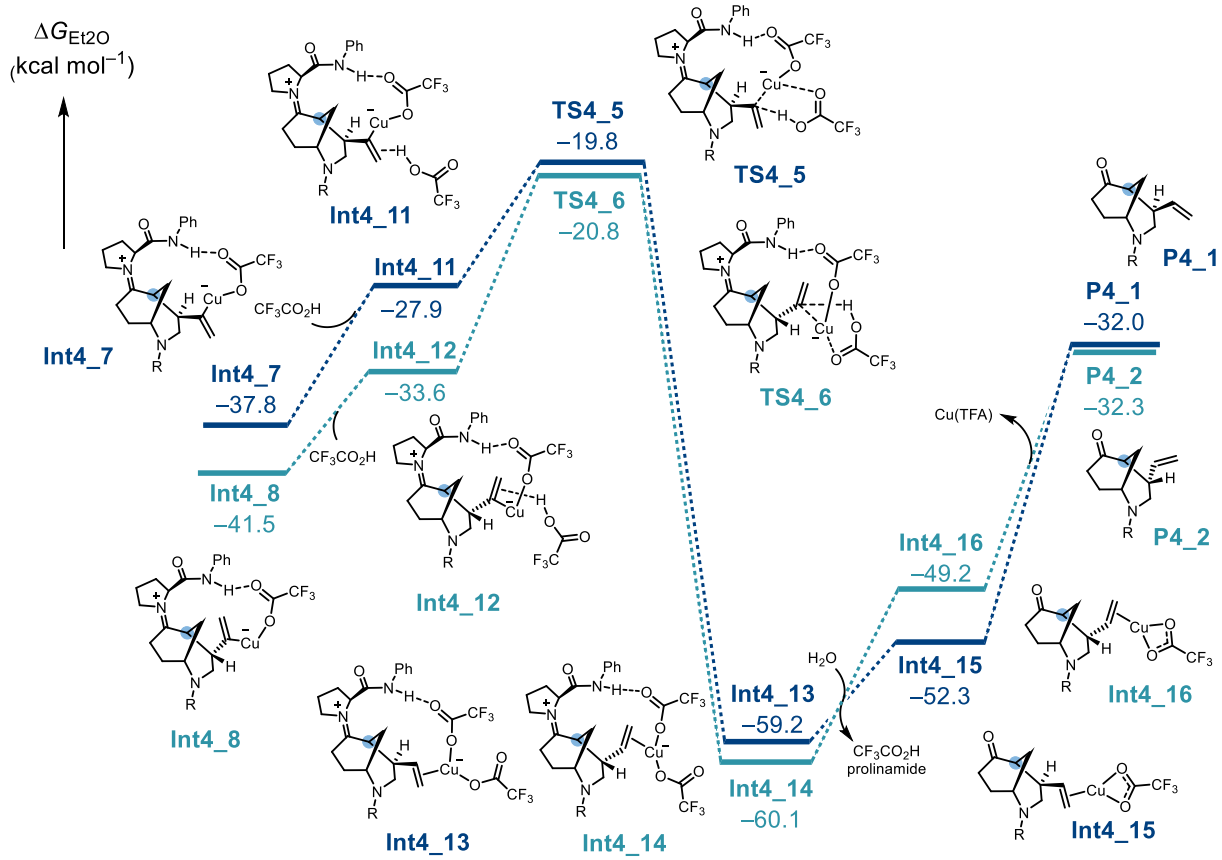


Figure 4.4. Computed reaction energy profile for the four possible pathways of the intramolecular nucleophilic attack of the enamine to the allene. R = SO_2Ph.

4.3.6. Summary

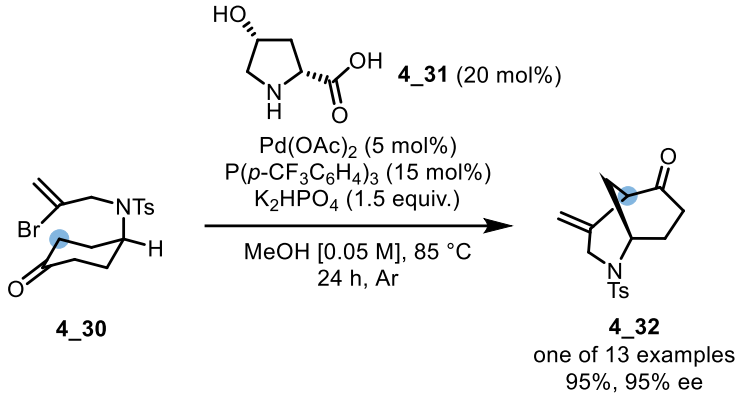
In summary, a detailed mechanistic study of the enantio- and diastereoselective copper and prolinamide co-catalyzed desymmetrization of allene-tethered cyclohexanones was performed using density functional theory calculations. All three of the newly formed stereogenic centers that arise from the cyclization reaction are set during the key intramolecular nucleophilic attack of the enamine to the copper-activated allene. The enantioselectivity can be controlled from the hydrogen bonding between an amide N–H bond and the

carbonyl oxygen of trifluoroacetate, while the diastereoselectivity is controlled from the distortion of the enamine moiety. The computational model used in this study successfully explained the origin of selectivities.

4.4. Palladium and Proline Co-catalyzed Desymmetrization

4.4.1. Previous Experimental Findings

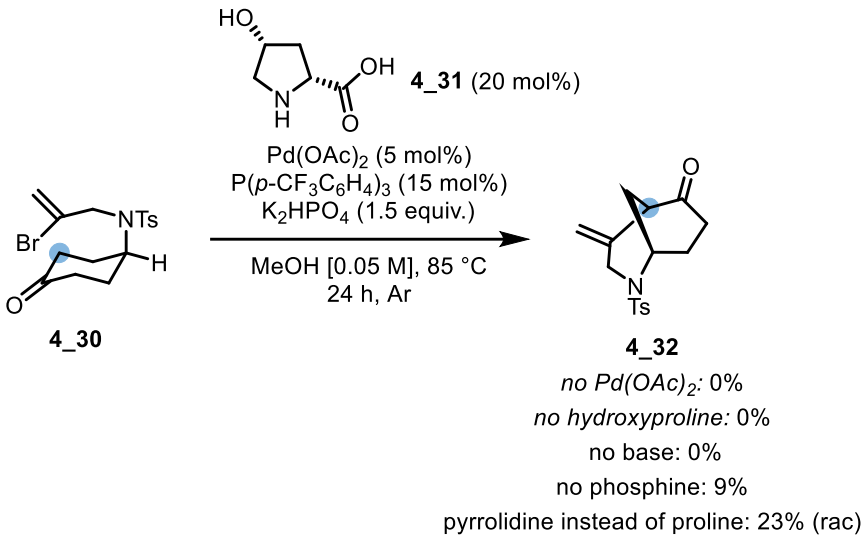
Previously, our group discovered that a hydroxyproline catalyst **4_31** in conjunction with palladium acetate $Pd(OAc)_2$ and a phosphine $P(p\text{-}CF_3C_6H_4)_3$ is optimal for the enantioselective desymmetrization of vinyl-bromide-tethered cyclohexanones **4_30** (Scheme 4.8).[19] The phosphine ligand is especially critical in this reaction, in that the electron withdrawing group at the *para*-position on the ligand improves the enantioselectivity as well as the reactivity. The optimized conditions at 85 °C in methanol as solvent furnished the products **4_32** in good to excellent yields with up to 95% ee. A wide range of functional groups tolerated the reaction conditions.



Scheme 4.8. Nitrogen-linked vinyl bromide substrate for the palladium and proline co-catalyzed desymmetrization.

In order to gain insight into the reaction mechanism, control experiments were also carried out (Scheme 4.9). The product was not obtained in the absence of $Pd(OAc)_2$ or the hydroxyproline, and a

significant drop in the yield was observed without the phosphine ligand. In addition, the use of pyrrolidine instead of the hydroxyproline also showed low reactivity to give the desired product in 23% yield as a racemic compound. Based on these experimental data, the computational studies are described below.



Scheme 4.9. Control experiments.

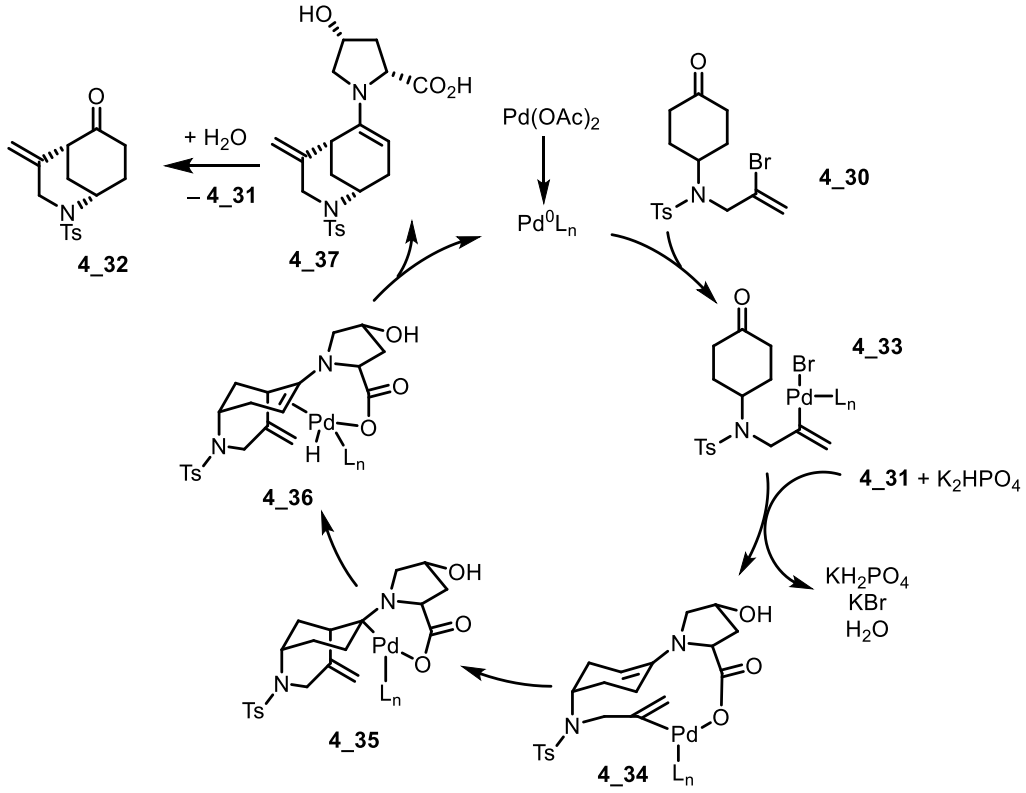
4.4.2. Computational Details

All calculations reported in this chapter were performed using the Amsterdam Density Functional (ADF) software,[9] and COSMO(MeOH)-ZORA-M06/TZ2P//COSMO(MeOH)-ZORA-BLYP-D3(BJ)/TZ2P level of theory was used.[10-16]

4.4.3. Proposed Reaction Pathway

Based on the experimental results described above, a plausible catalytic cycle is proposed (Scheme 4.10). Proline and PPh_3 are used as model systems instead of the hydroxyproline and P(*p*-$CF_3C_6H_4)_3$, respectively, in order to simplify the calculations. Initially, $Pd(OAc)_2$ reacts with the phosphine ligand to generate the palladium(0) active species.[20] An oxidative addition of vinyl bromide **4_30** to Pd(0) gives an intermediate **4_33** with the formation of a Pd–C bond. Then, enamine formation and ligand exchange are

accelerated by K_2HPO_4 to give the macrocyclic palladium complex **4_34**. The following step is a Heck-type C=C bond insertion into the Pd–C bond that furnishes the intermediate **4_35**, and this step is the stereoselectivity-determining C–C bond forming step. Finally, *β*-hydride elimination and a reductive elimination sequence regenerates the Pd(0) active species, and the cyclized enamine **4_37** is then hydrolyzed to complete the catalytic reaction pathway from the vinyl-bromide-tethered cyclohexanone to the vinyl-substituted morphan core.

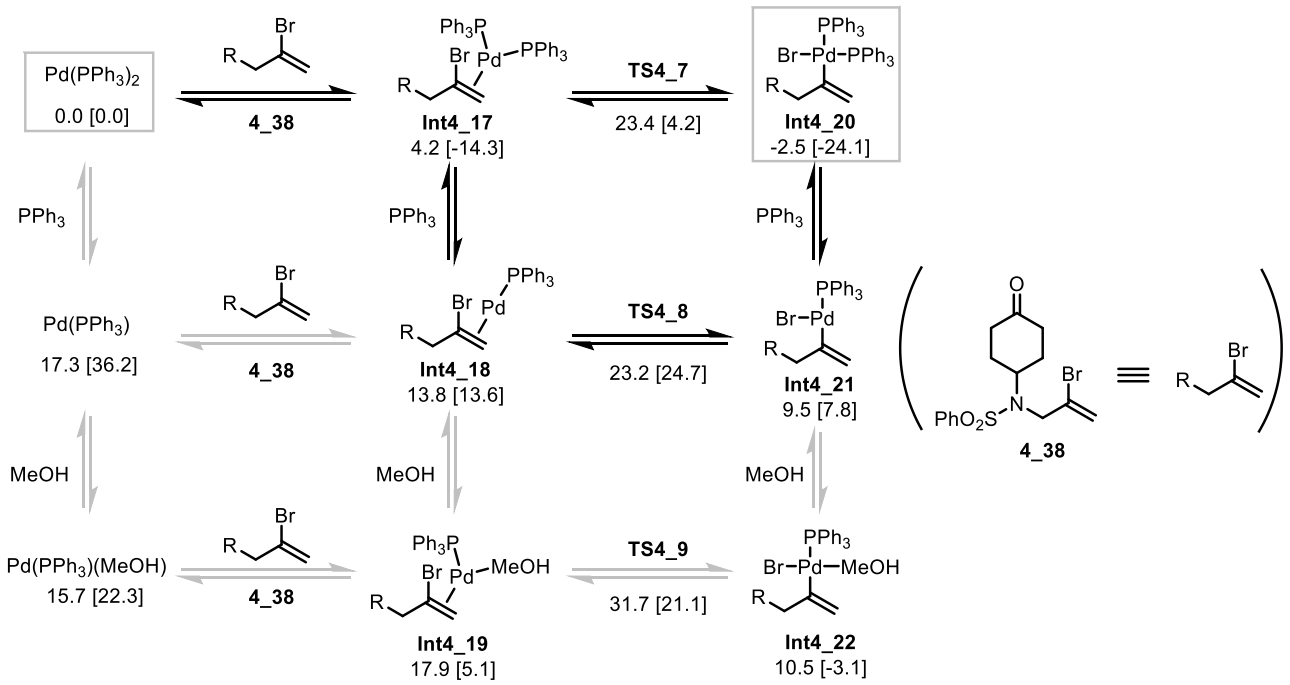


Scheme 4.10. Proposed catalytic cycle.

4.4.4. Calculated Catalytic Cycle

The initial step of the reaction is the oxidative addition, and the effect of coordinating ligands was studied (Scheme 4.11). Generally, $Pd(PPh_3)_2$ is known to behave as an active species for the oxidative addition step.[21] The vinyl bromide substrate coordinates to form a complex **Int4_17**, and the oxidative addition occurs

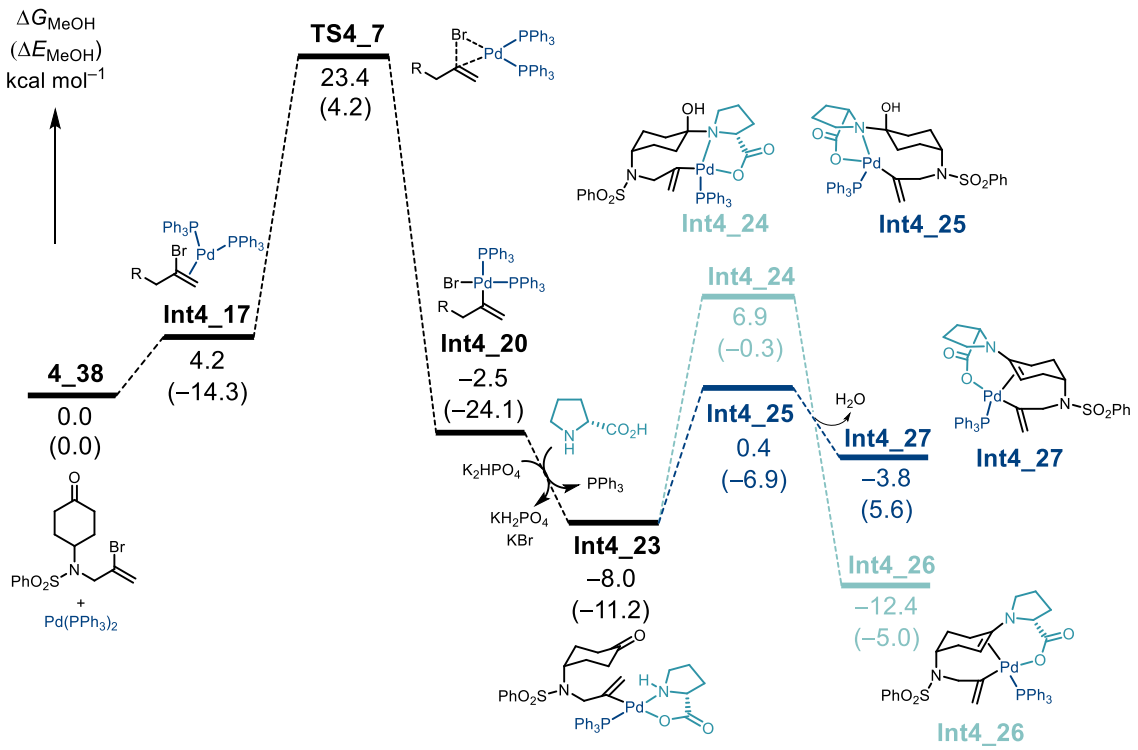
through the transition state **TS4_7** with an overall activation energy barrier of 23.4 kcal mol^{-1}. The dissociation of PPh_3 from **Int4_17** leads to the formation of less stable complex **Int4_18**, and the oxidative addition transition state **TS4_8** has an identical Gibbs free energy compared to **TS4_7**, indicating that the oxidative addition may proceed with either one or two PPh_3 ligands. Since methanol was used as the solvent, the involvement of MeOH molecule was also considered. Both intermediate **Int4_19** and transition state **TS4_9**, were destabilized, which indicates the non-participation of the solvent molecule during the oxidative addition step. For simplicity and consistency to other computational reports, the oxidative addition transition state **TS4_7** with two phosphines is shown in the following scheme.



Scheme 4.11. Energy changes (ΔG [ΔE] in kcal mol^{-1}) of the possible pathways for the oxidative addition of vinyl bromide to Pd(0) species.

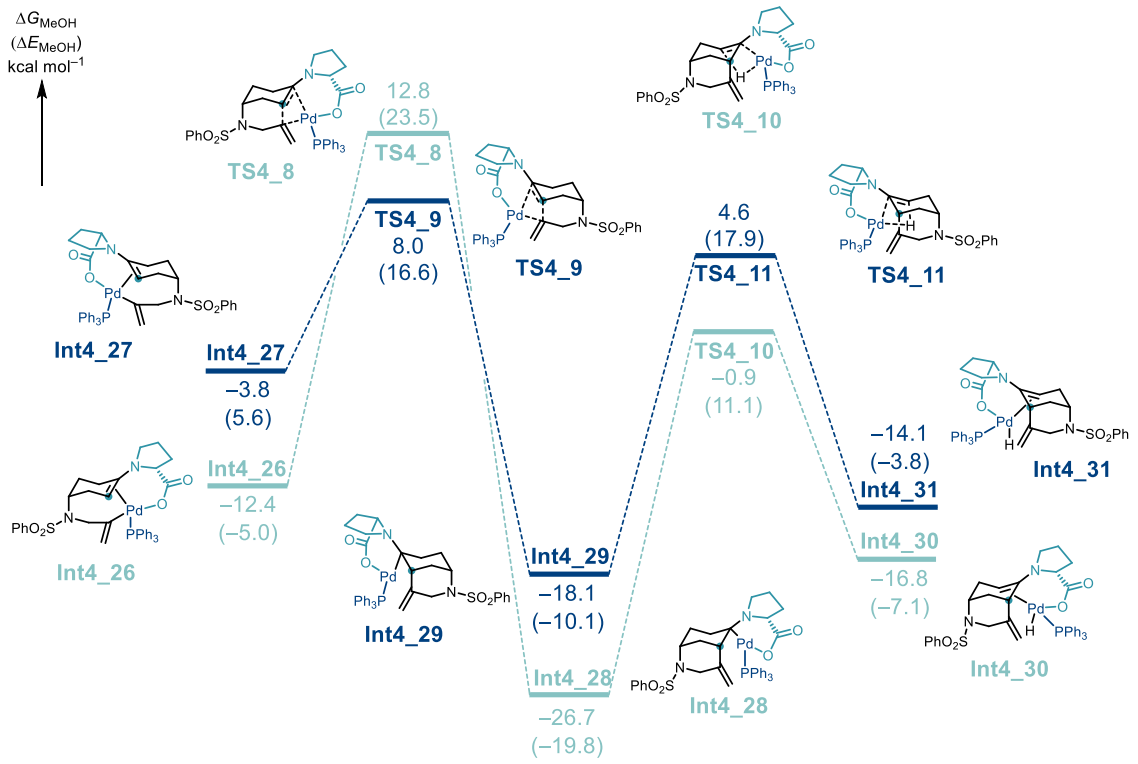
As mentioned above, the catalytic cycle initiates from the oxidative addition of vinyl bromide **4_38** to the active species $Pd(PPh_3)_2$, which is formed *in situ* from $Pd(OAc)_2$ (Scheme 4.12). After the exergonic Pd–C bond formation through **TS4_7**, tetracoordinated Pd(II) species **Int4_20** is generated. Then, proline chelates

to the palladium to furnish the stable complex **Int4_23**. The pyrrolidine nitrogen atom undergoes the nucleophilic attack to the ketone and generates either hemiaminals **Int4_24** or **Int4_25**, which then eliminates water to form enamines **Int4_26** or **Int4_27**.



Scheme 4.12. Computed reaction energy profile for the oxidative addition and the enamine formation.

Subsequently, the C=C bond of the enamine moiety proceeds to undergo migratory insertion into the Pd–C bond through either **TS4_8** or **TS4_9**. The transition state **TS4_9** from the precursor **Int4_27** has a lower energy barrier than **TS4_8** ($\Delta\Delta G^{\ddagger}$ = 4.8 kcal mol^{-1}), and the thermodynamically more stable intermediate **Int4_29** with a new C–C bond at the enamine *β* position is formed. The following step is the *β*-hydride elimination that regenerates an enamine, and the preferred pathway (dark blue line in Scheme 4.13) goes through the transition state **TS4_11** to furnish the Pd–H species **Int4_31**. The lower energy of **TS4_11** compared to **TS4_8** indicates that the previous migratory insertion step is indeed irreversible and the enantioselectivity-determining step.

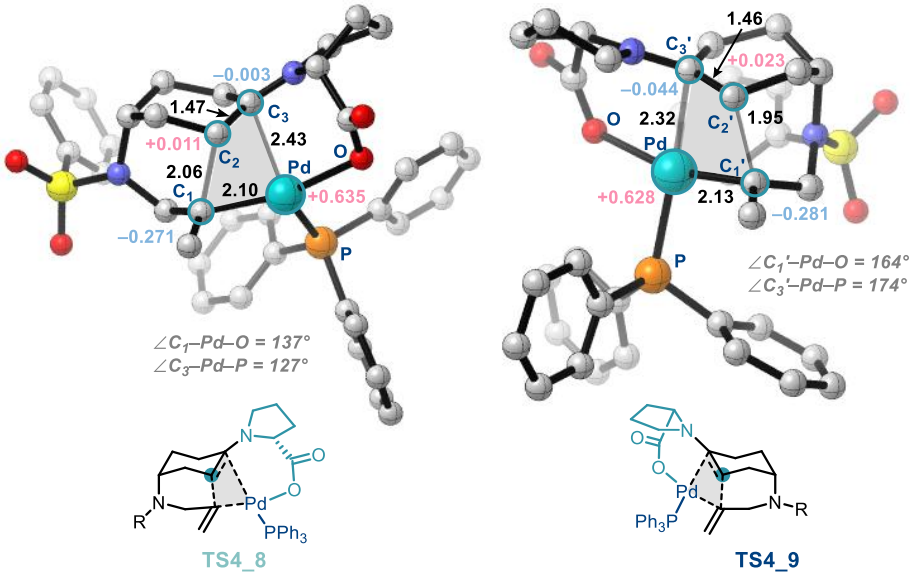


Scheme 4.13. Computed reaction energy profile for the migratory insertion and the *β*-hydride elimination.

In order to quantitatively elucidate the origin of the kinetic preference of the migratory insertion step, the activation strain model (ASM) was used (Scheme 4.14).[18] The energy barriers were recomputed in the gas phase ($\Delta E^{\ddagger}_{gas}$), and they were decomposed into the strain energy ($\Delta E^{\ddagger}_{strain}$) and the interaction energy ($\Delta E^{\ddagger}_{int}$) by using $Pd(PPh_3)^{2+}$ and the dianionic substrate as the fragments. The ASM revealed that the transition state **TS4_9** is favored mainly because of the more stabilizing interaction energy ($\Delta\Delta E^{\ddagger}_{int}$ = –11.6 kcal mol^{-1}) along with a small contribution from a less destabilizing strain energy ($\Delta\Delta E^{\ddagger}_{strain}$ = –3.0 kcal mol^{-1}). The interaction energies were further decomposed using a canonical energy decomposition analysis (EDA), and the electrostatic interaction energy ($\Delta V^{\ddagger}_{elstat}$) was identified as the decisive factor for setting the trend in the migratory insertion ($\Delta\Delta V^{\ddagger}_{elstat}$ = –27.7 kcal mol^{-1}).[22] The more stabilizing electrostatic interaction originates from the nearly square planar geometry that allows tighter bindings of the positively charged palladium atom and the negatively charged carbon atoms of the substrate.[23] The more distorted angles between ligands in *trans*

positions in **TS4_8** increases the destabilizing strain energy, which is combined with the less stabilizing interaction energy that leads to a higher energy barrier.

(kcal mol^{-1})	TS4_8	TS4_9
$\Delta G^{\ddagger}_{sol}$	12.8	8.0
$\Delta E^{\ddagger}_{sol}$	23.5	16.6
$\Delta E^{\ddagger}_{gas}$	42.6	28.1
$\Delta E^{\ddagger}_{strain}$	544.3	541.3
$\Delta E^{\ddagger}_{int}$	–501.7	–513.3
$\Delta E^{\ddagger}_{Pauli}$	162.7	169.9
$\Delta V^{\ddagger}_{elstat}$	–356.4	–384.1
$\Delta E^{\ddagger}_{oi}$	–308.0	–299.1



TS4_8

TS4_9

Scheme 4.14. Computed reaction energy profile for the migratory insertion and the *β*-hydride elimination.

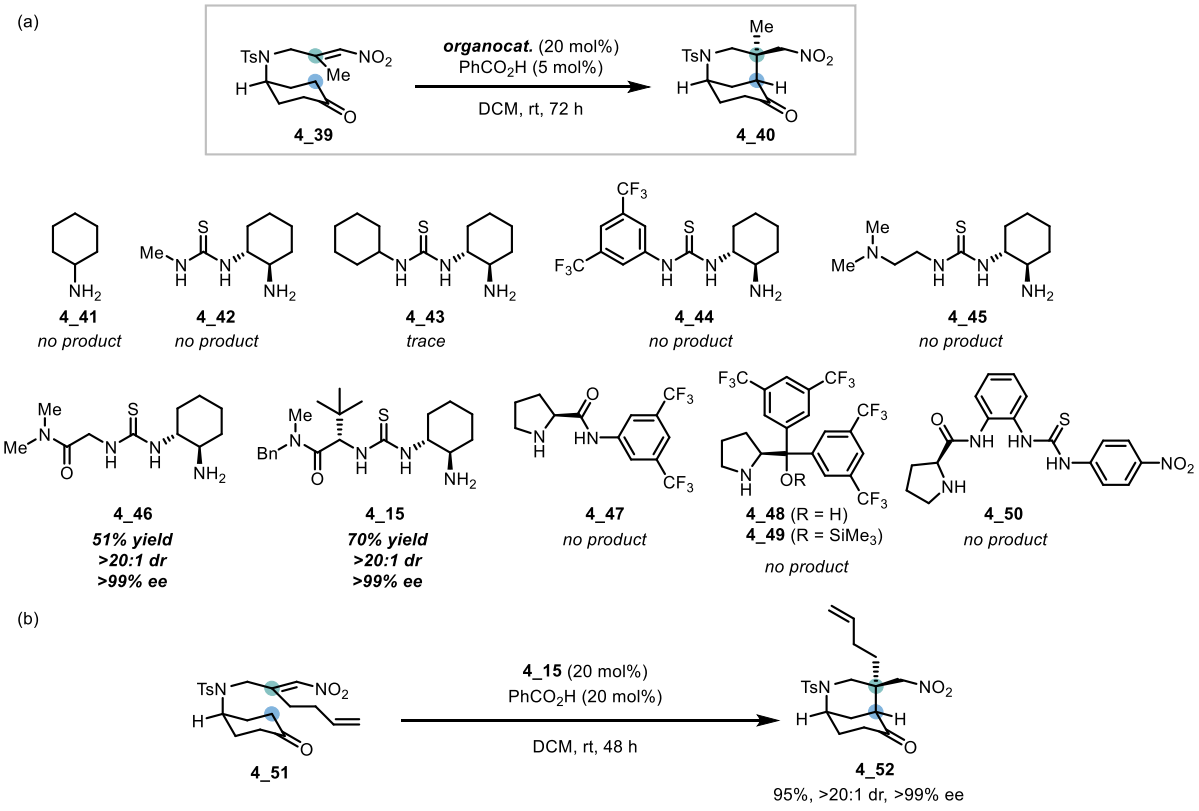
4.4.5. Summary

In summary, the detailed mechanism of the palladium and proline co-catalyzed desymmetrization of vinyl-bromide-tethered cyclohexanones was studied using density functional theory calculations. The reaction proceeds through a Heck-type mechanism via an oxidative addition/migratory insertion/*β*-hydride elimination sequence, and the stereoselectivity-determining C–C bond forming migratory insertion step proceeds through the square planar-like transition state structure that benefits from a more stabilizing interaction energy and a less destabilizing strain energy. This computational model successfully explained the experimental observations and provides a broad insight into these palladium-mediated reactions.

4.5. Amine Thiourea-Catalyzed Desymmetrization

4.5.1. Previous Experimental Findings

Following the study by Dixon and Paton on the amine thiourea-catalyzed desymmetrization of *α,β*-unsaturated ester-tethered cyclohexanones (Scheme 4.2c),[5a] our group discovered that the *β,β'*-disubstituted nitro-olefin-tethered cyclohexanones **4_39** can also be catalyzed to undergo intramolecular cyclization with amine thiourea organocatalysis, which leads to a product with three stereocenters including a quaternary carbon center (Scheme 4.15).[24,25] Screening of an amine catalyst library showed that the catalyst **4_15**, which is the same organocatalyst for the desymmetrization of *α,β*-unsaturated ester-tethered cyclohexanones, is optimal for this reaction, and furnished the desired product **4_40** in a good yield (70%) and the excellent enantio- and diastereoselectivities (>20:1 dr and >99% ee). Interestingly, the absence of the thiourea group, as well as the tertiary amide group completely inhibited the reaction.



Scheme 4.15. (a) Catalyst screening of the enantioselective desymmetrization of nitro-olefin-tethered cyclohexanones, and (b) Optimized conditions.

Further optimization with the suitable organocatalyst that was found in Scheme 4.15 expanded the reactivity by using an increased amount of benzoic acid. The *β,β'*-disubstituted nitro olefin substrate **4_51** was catalyzed by the primary amine thiourea organocatalyst **4_15** in the presence of 20 mol% of benzoic acid to furnish the product **4_52** in 95% yield, >20:1 dr and >99% ee.

4.5.2. Computational Details

All calculations reported in this chapter were performed using the Amsterdam Density Functional (ADF) software,[9] and COSMO(DCM)-ZORA-M06-2X/TZ2P//COSMO(DCM)-ZORA-BLYP-D3(BJ)/DZP level of theory was used.[10-16]

4.5.3. Proposed Reaction Pathway

Our mechanistic proposal is presented in Figure 4.5 according to the previously proposed mechanistic insight by experiments and computational results.[5a] The initial enamine formation between the cyclohexanone and the amine is assumed rapid and reversible, and the rotameric and diastereomeric forms of enamine **4_53** is obtained in equilibrium. The following step is the intramolecular Michael addition of the enamine to the tethered nitro olefin. A new C–C bond is formed during this process, and the relative and absolute stereochemical configurations of the three newly formed stereogenic centers are determined by this process, thus we focused on this step to elucidate the origin of the stereoselectivities for this transformation with several potential conformations.

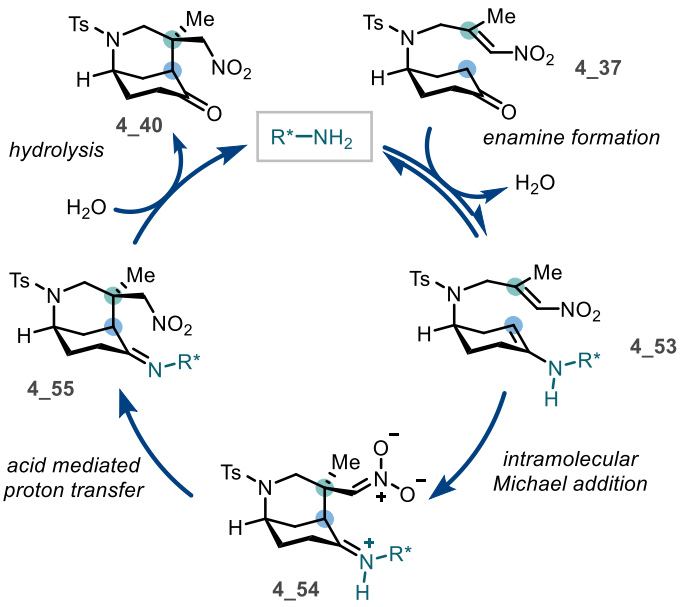


Figure 4.5. Proposed reaction pathway of the enantioselective desymmetrization of nitro-olefin-tethered cyclohexanones.

4.5.4. Conformational Analysis of the Amine-Thiourea Model Substrate

Initially, a conformational analysis on the thiourea-enamine model substrate was performed due to the existence of several free rotating single bonds that can diversify the conformations (Figure 4.6). The key rotating bonds are the C–N bond between the enamine nitrogen atom and the nitro-olefin-tethered cyclohexene ring (*s-cis* or *s-trans*), and the C–N bond between the enamine nitrogen atom and the thiourea-substituted cyclohexane ring, which can be distinguished by the position of the thiourea moiety (*up* or *down*). The *s-trans* enamines **4_58** and **4_59** are less stable than the *s-cis* enamines **4_56** and **4_57**, and this is caused by the steric repulsion between the thiourea-tethered cyclohexane ring and the CH or CH_2 group on the *β*-position of the enamine moiety. Importantly, the most preferred conformation is **4_56**, which has a stabilizing hydrogen bonding between the thiourea S atom and the enamine N–H bond.

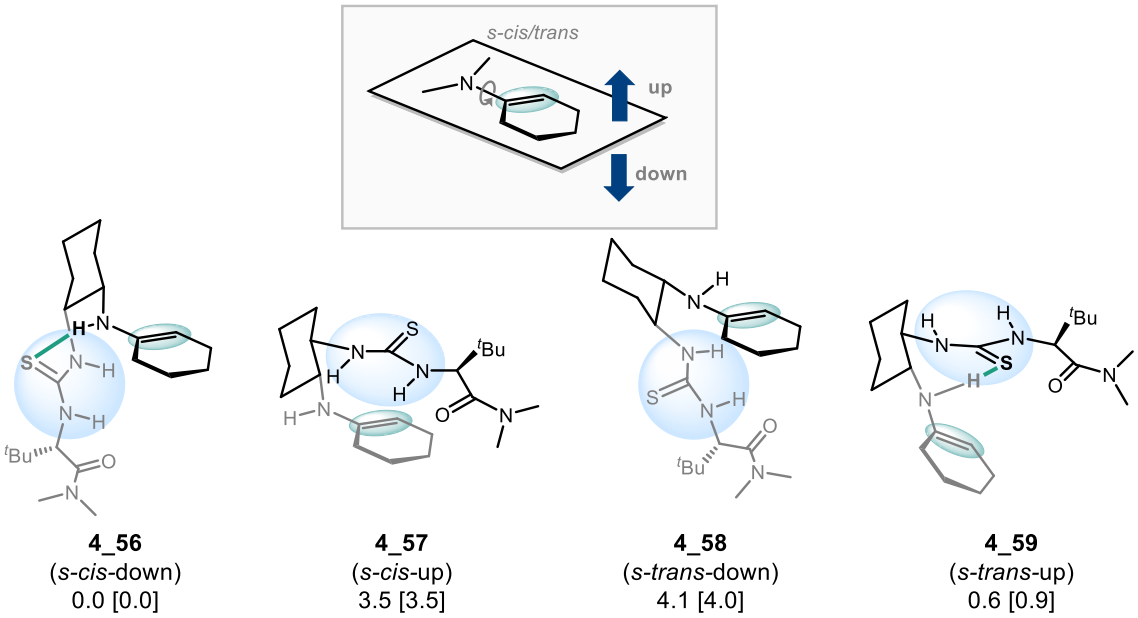
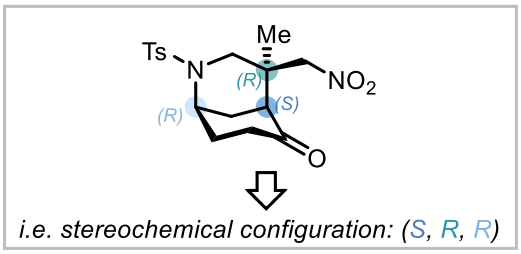


Figure 4.6. Relative stability (ΔG [ΔE] in kcal mol^{-1}) of thiourea-enamine substrate.

4.5.5. Intramolecular Michael Addition

Since the intramolecular conjugate addition step sets three newly formed stereocenters, the C–C bond forming event was extensively studied (Table 4.1). There are 16 possible transition state conformations leading to eight stereoisomers of the cyclized product. Among all considered TSs, the most favorable transition state is **TS4_12** with the *s-cis*-down conformation that leads to the experimentally obtained product. This transition state **TS4_12** benefits from two stabilizing hydrogen bonding interactions, namely the interactions between the thiourea and enamine groups and between thiourea and nitro groups, and these fulfill a cooperative push/pull-type mechanism, where the thiourea moiety activates both the electrophilic nitro olefin and the nucleophilic enamine. The second-lowest-energy transition state **TS4_20** has no stabilizing hydrogen bonding ($\Delta\Delta G^{\ddagger}$ = 3.0 kcal mol^{-1}), and it leads to the formation of an enantiomer, amounting to a computed 99% ee that is in excellent agreement with the experimental enantioselectivity (99% ee). TSs with only one or no intramolecular hydrogen bonding are generally less stable and have higher energy barriers. Overall, the transition state structure that benefits from a cooperative push/pull-type mechanism is the most preferred conformation.



TS	configuration	enamine	thiourea	ΔΔG‡	ΔΔE‡	interactions
TS4_12	(S, R, R)	s-cis	down	**0.0**	**0.0**	● ●
TS4_13	(S, R, R)	s-cis	up	7.9	7.9	
TS4_14	(S, R, R)	s-trans	down	4.8	5.1	● ○
TS4_15	(S, R, R)	s-trans	up	4.7	5.1	● ○
TS4_16	(S, S, R)	s-cis	down	3.2	4.1	●
TS4_17	(S, S, R)	s-cis	up	11.4	10.8	
TS4_18	(S, S, R)	s-trans	down	9.1	9.7	
TS4_19	(S, S, R)	s-trans	up	5.4	8.0	●
TS4_20	(R, S, S)	s-cis	down	**3.0**	**2.8**	
TS4_21	(R, S, S)	s-cis	up	14.1	16.0	● ●
TS4_22	(R, S, S)	s-trans	down	8.3	8.1	○
TS4_23	(R, S, S)	s-trans	up	10.7	9.8	●
TS4_24	(R, R, S)	s-cis	down	5.1	4.5	●
TS4_25	(R, R, S)	s-cis	up	14.9	16.2	
TS4_26	(R, R, S)	s-trans	down	9.7	9.2	
TS4_27	(R, R, S)	s-trans	up	4.6	4.5	●

● = thiourea•••NO_2 ● = thiourea•••enamine ○ = enamine•••NO_2

Table 4.1. Relative stability (in kcal mol^{-1}) of intramolecular Michael addition transition state structures.

In order to elucidate the key roles of hydrogen bonding interactions described above, the interaction energies between archetypal model functional groups were computed (Figure 4.7). The electronic energies of the thiourea-enamine complex **4_63**, the enamine-nitro complex **4_64**, and the thiourea-nitro complex **4_65** from each separated species were shown to be stabilized by 3.5, 2.6 and 3.2 kcal mol^{-1}, respectively. Interactions between the thiourea and enamine groups and between thiourea and nitro groups are notably strong, both of which exist in the most preferred intramolecular Michael addition transition state that is consistent with the cooperative push/pull-type mechanism.[26]

The computed reaction energy profile using the most preferred intramolecular Michael addition transition state described above is shown in Scheme 4.16. The primary amine **4_67** undergoes the addition reaction to the cyclohexanone substrate **4_66** to generate a hemiaminal intermediate **Int4_32**, which then forms an imine **Int4_33** after the elimination of water.[27] Although this process is endergonic, the thiourea moiety and its side chain promote the ketone activation and water elimination. The imine **Int4_33** tautomerizes to an enamine **Int4_34**, and the new C–C bond is formed through the intramolecular Michael addition transition state **TS4_12** to furnish the stable iminium-nitronate species **Int4_35** (ΔG_{rxn} = –19.4 kcal mol^{-1}). This type of intermediate has been proposed and observed by many groups in similar reaction systems.[28]

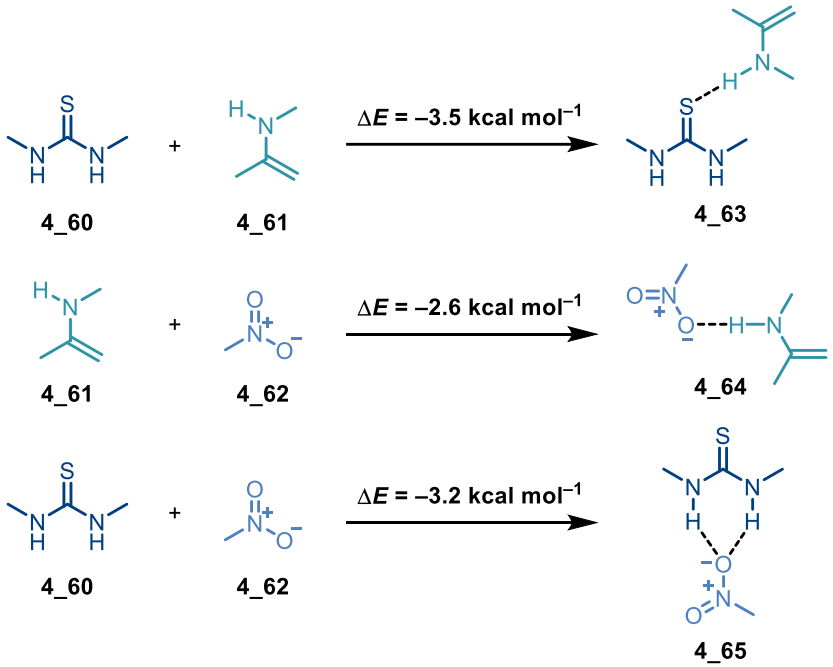
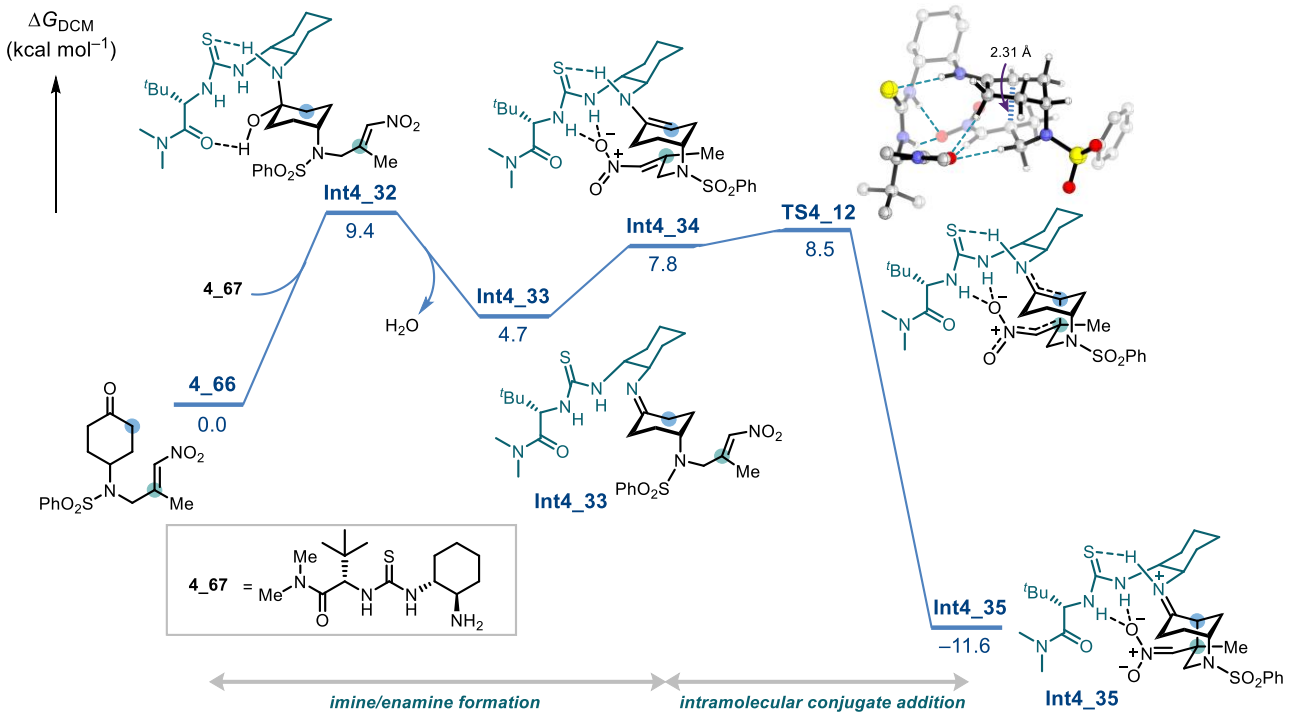


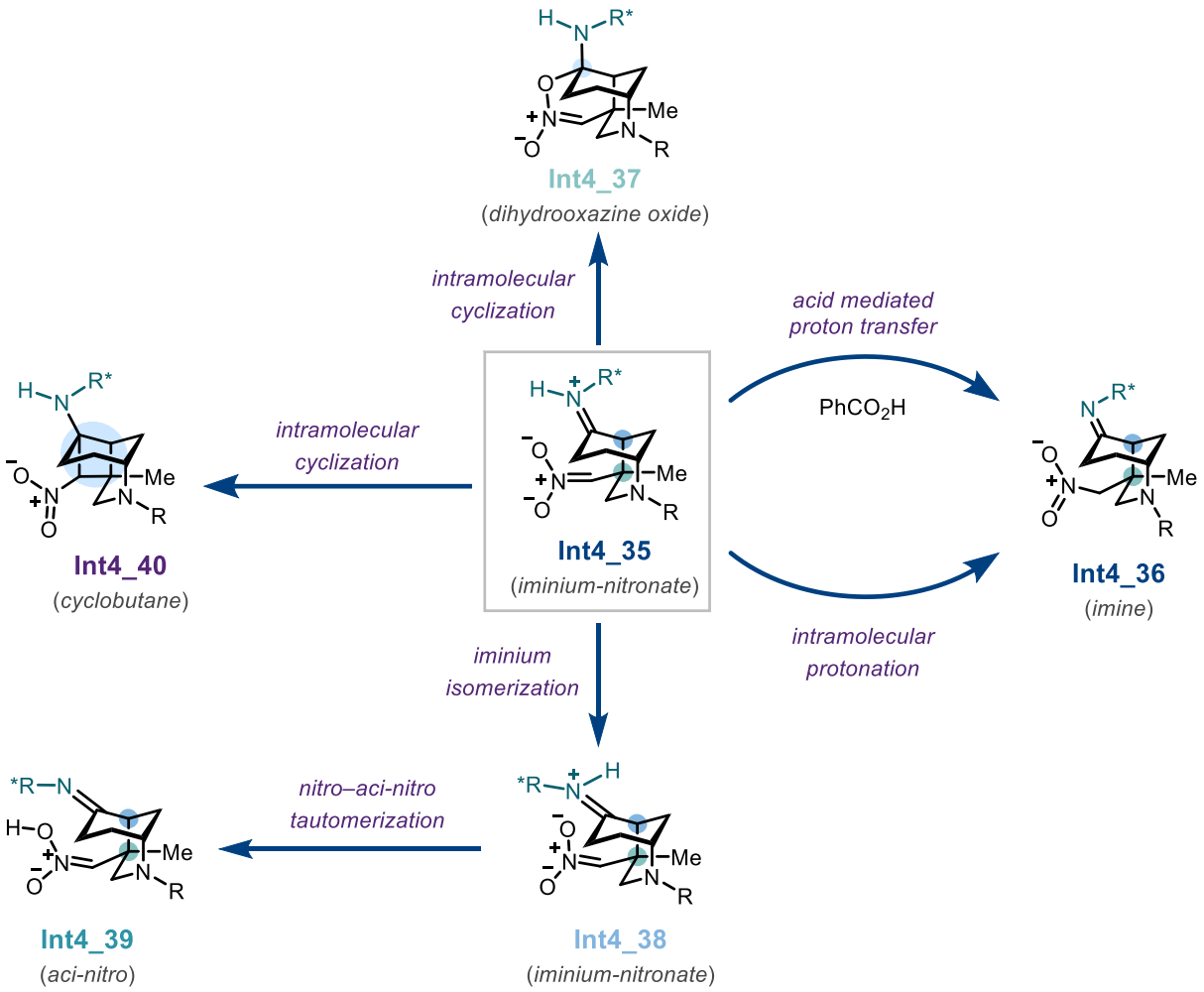
Figure 4.7. Total electronic energy (ΔE in kcal mol^{-1}) for the complexation between archetypal thiourea, enamine, and nitro moieties.



Scheme 4.16. Computed reaction energy profile (ΔG in kcal mol^{-1}) for the pathway through the lowest-energy intramolecular Michael addition transition state structure leading to the nitronate-iminium intermediate **Int4_35**.

4.5.6. Proton Transfer

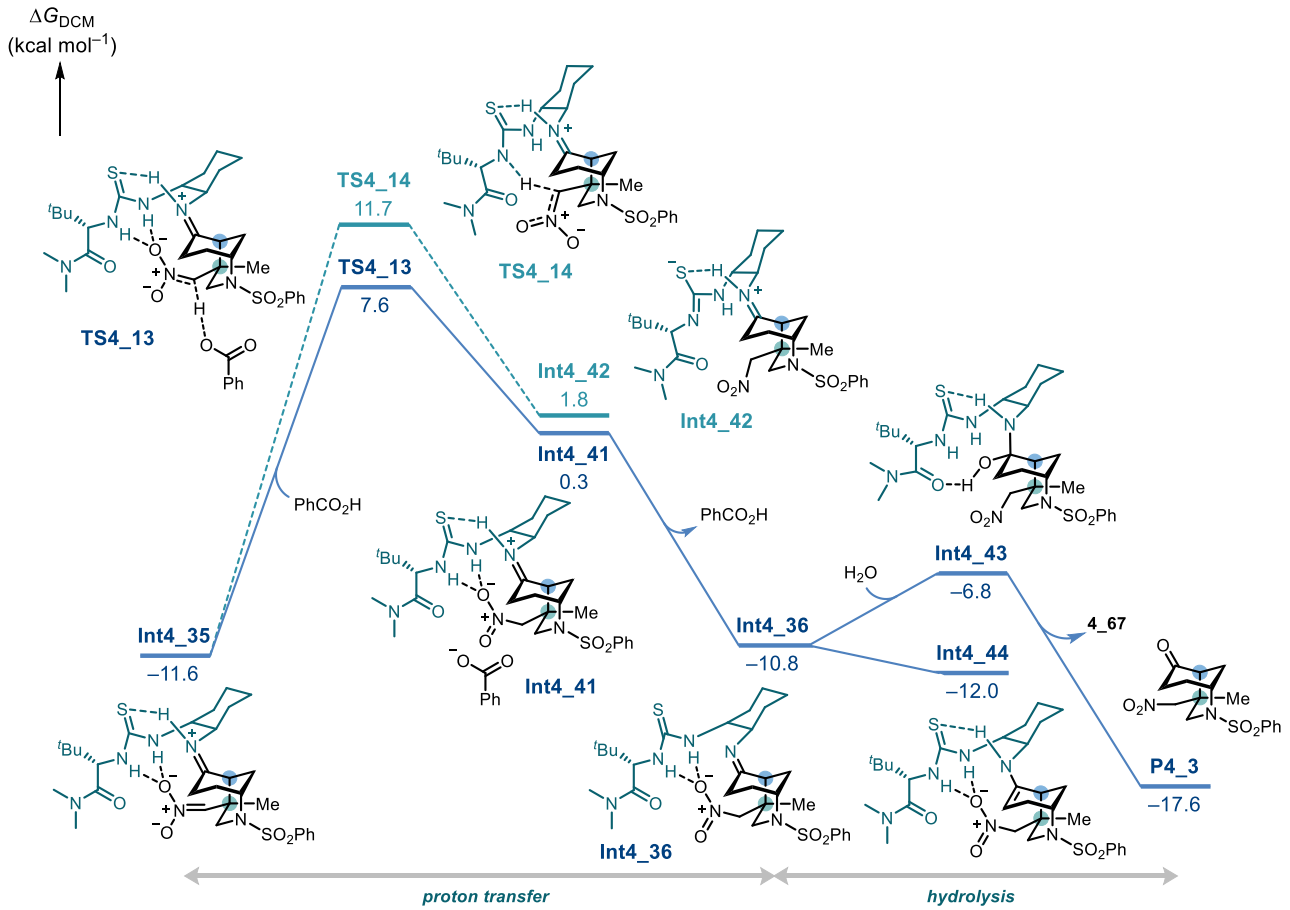
Following the C–C bond formation, several mechanistic pathways for the proton transfer from the iminium-nitronate intermediate **Int4_35** that arise from the existence of two reactive functional groups were considered and computed (Scheme 4.17). Firstly, both intermolecular and intramolecular proton transfer from **Int4_35** is described. Other possibilities after the isomerization of the iminium-nitronate species into a dihydrooxazine oxide **Int4_37**, cyclobutane intermediates **Int4_40**, or the aci-nitro intermediate **Int4_39** via **Int4_38** were also studied.



Scheme 4.17. Proposed reaction pathways from the intermediate **Int4_35**.

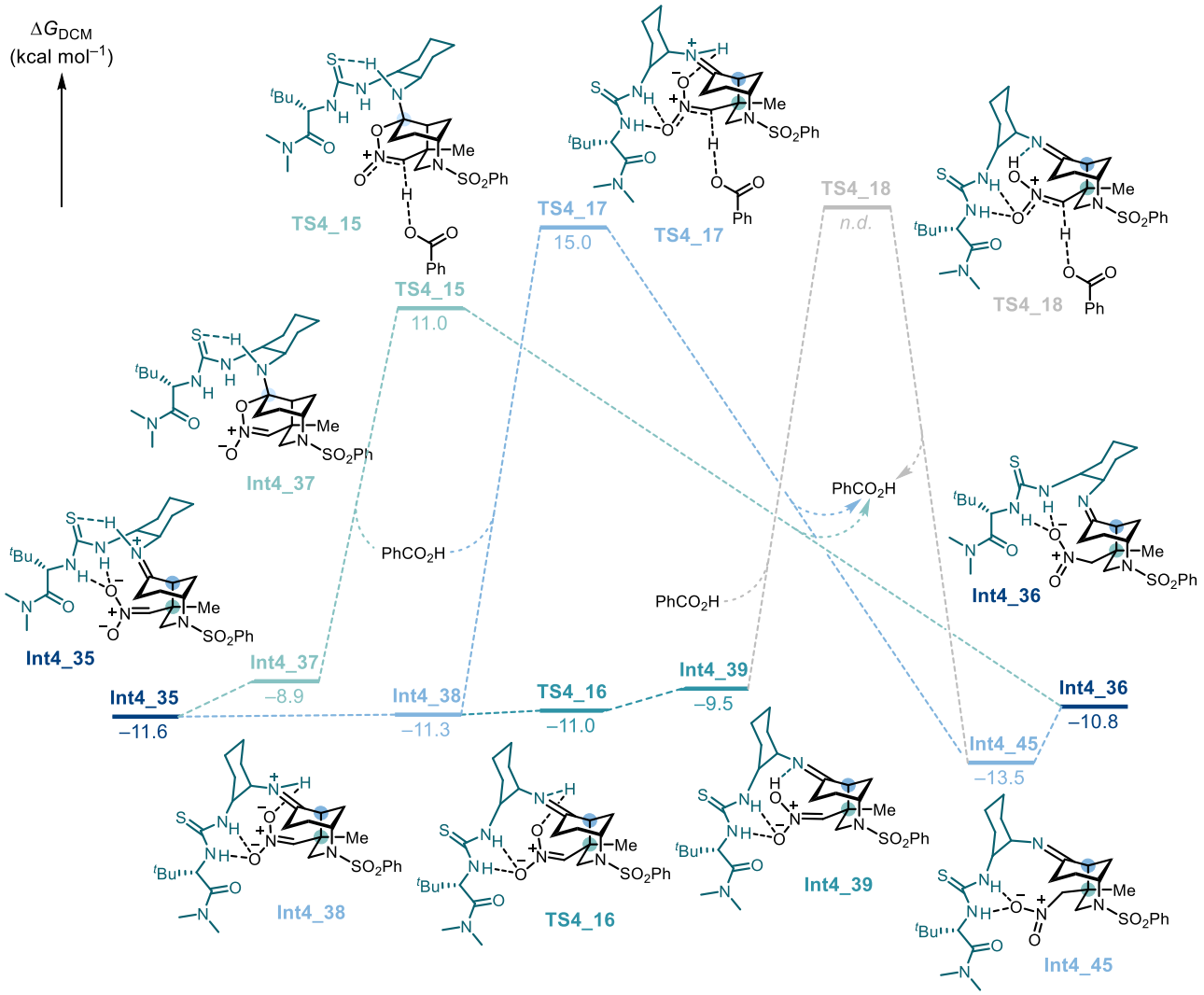
The intermolecular proton transfer goes through the transition state **TS4_13** and is facilitated by benzoic acid (Scheme 4.18). The residual benzoate anion after protonating the nitronate in **Int4_41** deprotonates the iminium to furnish the imine intermediate **Int4_36**. On the other hand, the intramolecular protonation from the thiourea N–H bond to the nitronate requires higher energy to overcome the transition state **TS4_14**, indicating that the acid-mediated proton transfer is more favorable. Moreover, the energy barrier through **TS4_13** is lower than the C–C bond cleaving retro-Michael addition process, and this confirms that the enantio- and diastereoselectivities are determined by the irreversible intramolecular Michael addition. Once the C–C bond is formed, the imine **Int4_36** or the enamine **Int4_44** after the tautomerization, are hydrolyzed

through the hemiaminal **Int4_43** and this releases the cyclized product with the experimentally confirmed stereochemical configuration. Interestingly, previous theoretical study on the enantioselective desymmetrization of *α,β*-unsaturated ester-tethered cyclohexanones indicated that intramolecular protonation reaction is preferred over intermolecular protonation.[5a] This difference can be attributed to the pK_a difference between nitronate and enolate [nitronate (pK_a = 17); thiourea (pK_a = 20); enolate (pK_a = 30)]. In other words, deprotonation of thiourea is favorable with an enolate but unfavorable with a nitronate, and this leads to the reactivity difference between these tethered cyclohexanone substrates.



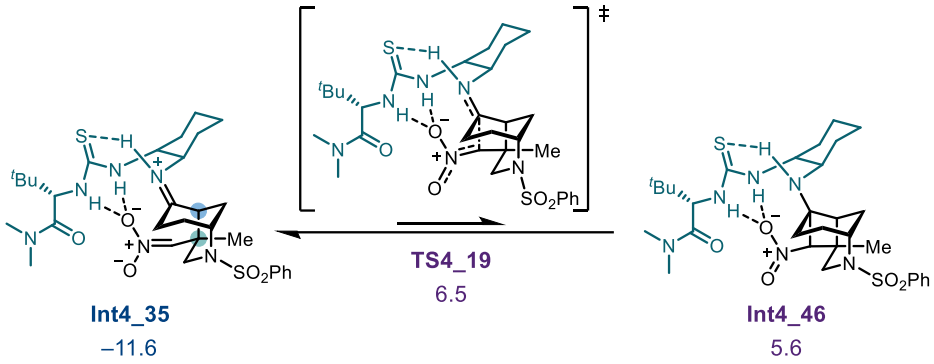
Scheme 4.18. Computed reaction energy profile (Δ*G* in kcal mol^{-1}) for the pathway from the nitronate-iminium intermediate **Int4_35**.

The formation of the six-membered dihydrooxazine oxide **Int4_37** from **Int4_35** is endergonic (ΔG_{rxn} = 2.7 kcal mol^{-1}), and the intermolecular protonation through **TS4_15** is less favorable than **TS4_13** ($\Delta\Delta G^{\ddagger}$ = 22.6 kcal mol^{-1}) (Scheme 4.19). In addition, the iminium rotation from **Int4_35** to **Int4_38** and the nitro–aci-nitro tautomerization from **Int4_38** to **Int4_39** through **TS4_16** both can occur rapidly, however the downstream proton transfer does not occur since the energy barrier is high (**TS4_17**) or the transition state could not be located (**TS4_18**).



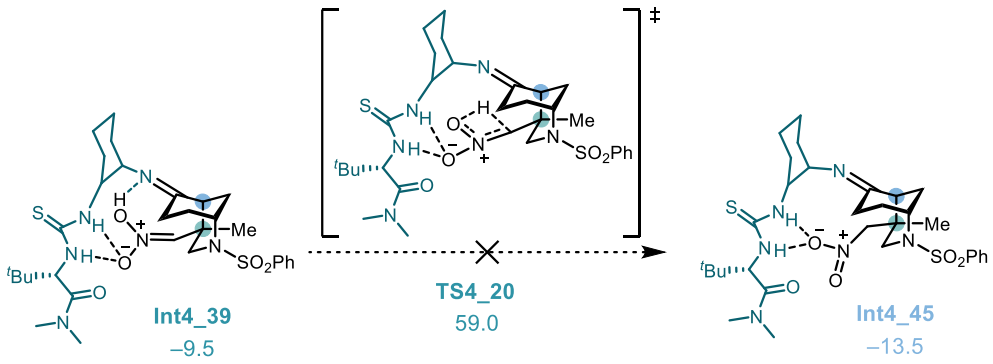
Scheme 4.19. Computed reaction energy profile (ΔG in kcal mol^{-1}) for the pathway from the nitronate-iminium intermediate **Int4_35**.

Since the nucleophilic nitronate and electrophilic iminium moieties exist in the intermediate **Int4_35**, an intramolecular cyclization for the formation of a cyclobutane ring can be considered (Scheme 4.20). Indeed, the activation energy barrier through **TS4_19** is lower than that of **TS4_13** for the intermolecular protonation and the cyclobutane intermediate **Int4_46** can be formed; however, the reverse ring opening process is almost barrierless because the ring is highly strained and energetically unstable.



Scheme 4.20. Computed reaction energy profile (Δ*G* in kcal mol^{-1}) for the cyclobutane intermediate formation.

An alternative pathway is the 1,3-proton shift from the aci-nitro species **Int4_39** (Scheme 4.21). The activation energy barrier through **TS4_20** is extremely high and this process does not occur. This is because the reaction should proceed via an antarafacial shift according to the Woodward-Hoffman rules, and this is geometrically impossible for such a thermal 1,3-shift.



Scheme 4.21. Computed reaction energy profile (Δ*G* in kcal mol^{-1}) for the 1,3-proton transfer from the imine-aci-nitro intermediate **Int4_39**.

4.5.7. Summary

In summary, an in-depth mechanistic pathway of the amine thiourea-catalyzed desymmetrization of nitro-olefin-tethered cyclohexanones was studied using density functional theory calculations. The flexible nature of the amine thiourea catalyst was fully considered during the lowest-energy transition state conformational search, and the results suggested that the most preferred transition state structure leads to the experimentally confirmed stereochemical configuration with three newly formed stereocenters. The enantio- and diastereoselectivity for the intramolecular Michael addition originates from a cooperative push/pull-type mechanism. After the C–C bond formation, several mechanisms were considered, and the pathway involving acid-mediated intermolecular proton transfer leads to the product with a morphan core. Overall, the full mechanistic picture of the catalytic cycle could be obtained from the calculations by considering all possible intermediates involving off-cycle species.

4.6. Conclusion

In conclusion, three computational mechanistic studies of enantioselective catalytic desymmetrization reactions of cyclohexanones using density functional theory calculations were described in this chapter. The origin of the selectivity in the copper and prolinamide co-catalyzed desymmetrization of allene-tethered cyclohexanones is the nucleophilic attack of an enamine to copper-coordinated allene in the intramolecular cyclization step, and the intramolecular hydrogen bonding was the key to realize such high enantio- and diastereoselectivities. The stereochemistry-determining migratory insertion step in the palladium and proline-co-catalyzed desymmetrization of vinyl-bromide-tethered cyclohexanones benefits from both more stabilizing interaction energy and less destabilizing strain energy. In the amine thiourea-catalyzed desymmetrization of nitro-olefin-tethered cyclohexanones, consideration of flexibility of the amine thiourea catalyst revealed the origins of both enantio- and diastereoselectivies during the key irreversible intramolecular Michael addition that benefits from a cooperative push/pull-type mechanism. These enantioselective reactions have similarities

in the product core, but the mechanisms and the key factors that determine the enantioselectivity were distinct from each other. The current study can provide insights for further reaction development.

4.7. References

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Chapter 5

Mechanistic Studies of Bifunctional Iminophosphorane-Catalyzed Reactions

5.1. Chapter Overview

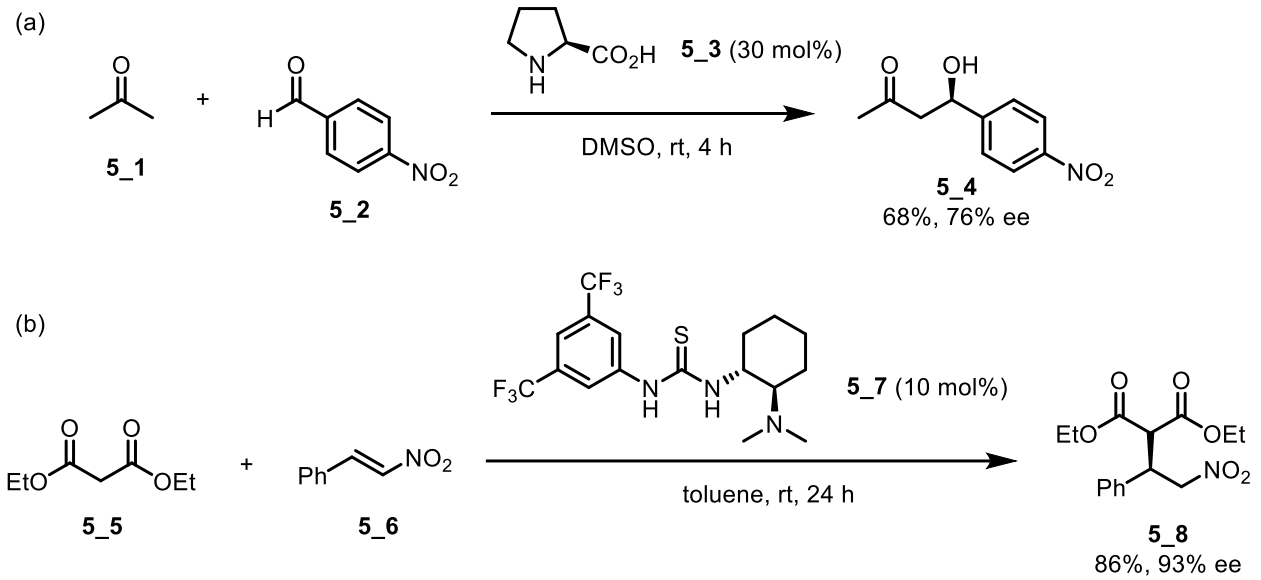
This chapter describes mechanistic studies of enantioselective bifunctional iminophosphorane (BIMP)-catalyzed reactions and studies into the origin of the enantioselectivity for those transformations using density functional theory (DFT) calculations. BIMP catalysts were previously demonstrated to be highly useful and tunable for a wide variety of organic reactions, and three distinct enantioselective transformations including a C–N bond formation, a C–S bond formation, and an alkene isomerization reaction were chosen for the detailed theoretical study. A conformational analysis of the catalyst structure at the key transition states provided detailed insight into the chiral induction mechanism in all computed reactions, and the existence of stabilizing inter- and intramolecular interactions were revealed as the most important controlling factor for the enantioselectivities.

5.2. Introduction

5.2.1. Bifunctional Catalysis in Organic Synthesis

Organic synthesis using organic molecules as a catalyst has been extensively studied for more than a century, and since Macmillan defined the term "organocatalysis" in 2000, the research field rapidly advanced.[1-3] The catalytic use of an organic molecule facilitates the performance of reactions under milder conditions, enabling chemoselective syntheses of complex molecules. In addition, organocatalysts are frequently used as an asymmetric catalyst which transfers chiral information from the catalyst to induce asymmetry in the product. This can be regarded as a simplified enzyme, in which high specificity can be created by tuning the structure

of the catalysts. One of the early examples of asymmetric organocatalysis was reported in 2000 by List, who was awarded the Nobel Prize in chemistry in 2021 jointly with MacMillan, where proline **5_3** was used for direct asymmetric aldol reactions.[2] Since this discovery, research activity into this fundamental area has dramatically increased (Scheme 5.1a).[3]



Scheme 5.1. (a) List's proline-catalyzed direct asymmetric aldol reaction. (b) Takemoto's bifunctional catalysis-catalyzed Michael addition reaction.

In 2003, Takemoto reported the first example of a bifunctional catalyst that functions to activate both an electrophile and a nucleophile (Scheme 5.1b).[4] The catalyst **5_7** has a thiourea moiety that activates the nitro styrene **5_6** by hydrogen bonding interactions and a tertiary amine that activates the malonate ester **5_5** by deprotonation. Both functionalities were crucial to achieve the enantioselective transformation. The authors postulated that the nitro-olefin is bound to the thiourea moiety, and the protonated tertiary amine is bound to the enol in the transition state (Figure 5.1a). In the computational studies by Pápai and Soós, it was revealed that the alternative mechanism, in which the enol is bound to the thiourea, and the tertiary ammonium salt

activates the nitro-olefin, is more favorable (Figure 5.1b).[5] The calculated transition state for the Pápai and Soós' model **5_10** was 2.7 kcal mol^{-1} lower than the model **5_9** proposed by Takemoto.

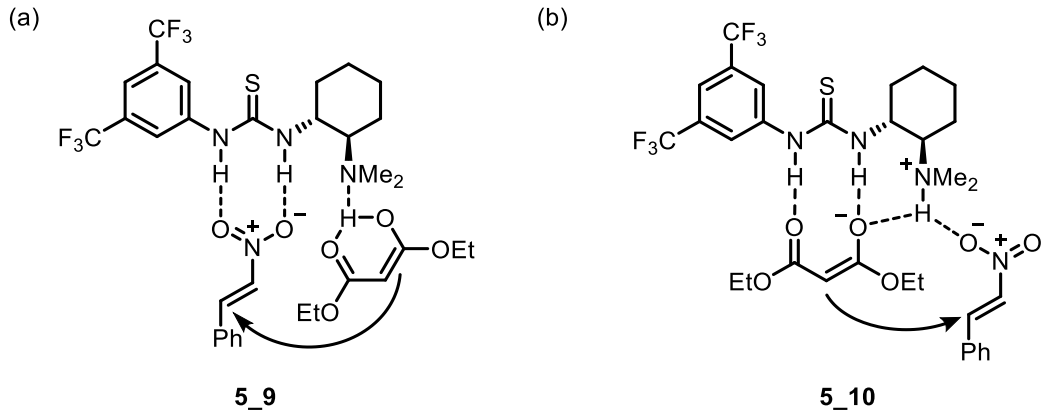


Figure 5.1. (a) Takemoto's proposed mechanism. (b) Pápai and Soós' proposed mechanism.

Since then, many research groups have independently developed bifunctional organocatalysts (Figure 5.2).[4,6] The cinchona-derived bifunctional thiourea organocatalysts, such as **5_12**, were shown to be highly useful for enantioselective conjugate addition reactions. A wide variety of asymmetric reactions with these types of catalysts have been reported to date, and comprehensive reviews can be found in the literature.

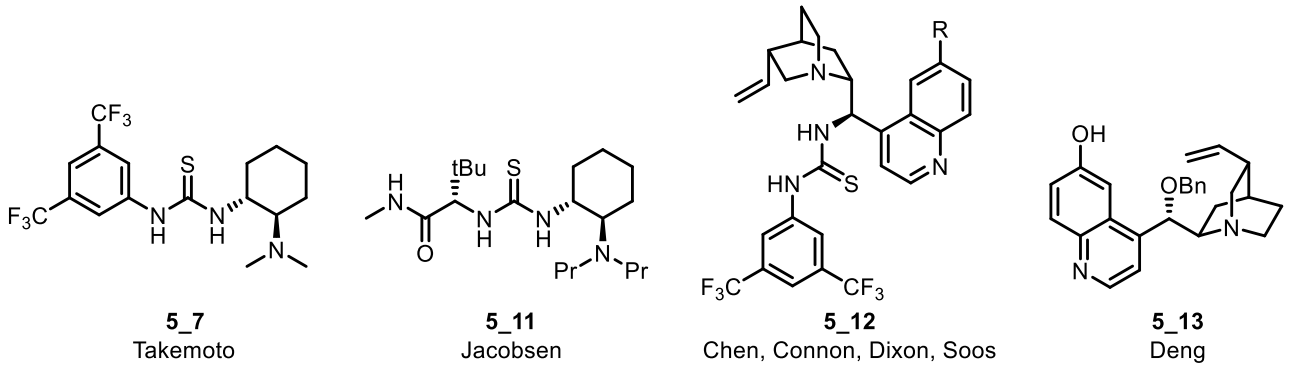
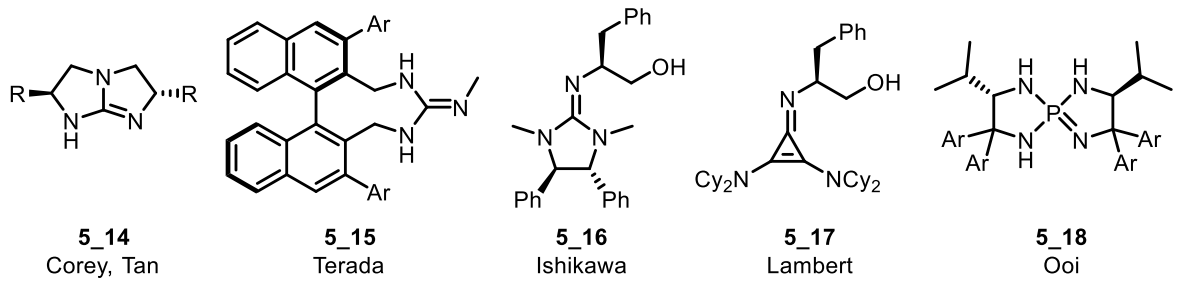


Figure 5.2. Representative bifunctional organocatalysts.

5.2.2. Bifunctional Iminophosphorane (BIMP) Catalysts

In comparison to tertiary amine organic catalysis, a stronger base, also known as “superbase”, exhibits unique reactivity in organic reactions.[7] Superbases are defined as a basic reagent created by combining the characteristics of several different bases, and amidines, guanidines and phosphazenes are the most widely used superbases.

Superbases are also useful for asymmetric reactions.[8] Several groups have designed and developed organosuperbases bearing chiral centers and representative examples are shown in Figure 5.3. In 1999, Corey reported the use of a bicyclic guanidine **5_14** as an effective organocatalyst_for the asymmetric Strecker reaction.[8b] The protonated guanidinium salt is proposed to function as the hydrogen bond donor, and the substrate is tightly bound to the catalyst to transfer the chiral information during the key transition state.

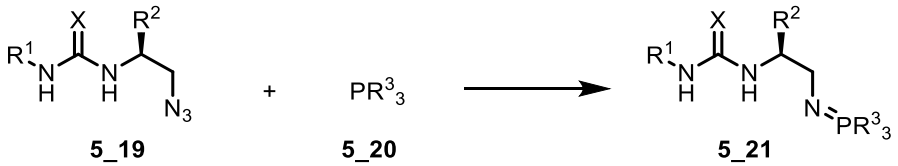


5_14 Corey, Tan | **5_15** Terada | **5_16** Ishikawa | **5_17** Lambert | **5_18** Ooi

Figure 5.3. Representative organosuperbases.

Although these superbases showed excellent catalytic activity, the preparation of these reactive catalysts is usually not straightforward. Also, the modification of the stereogenic centers in the catalysts is not trivial, limiting the tunability of the catalyst scaffold. In order to avoid and overcome these issues, Dixon discovered and utilized the iminophosphorane moiety as an alternative superbase accompanying a hydrogen bond donor (Scheme 5.4).[9] This catalyst was named “bifunctional iminophosphorane (BIMP),” and it showed superior catalytic activity for a wide variety of enantioselective reactions. The catalyst structure is easily modified, especially at the hydrogen bond donor, phosphine, and the chiral backbone. In particular, the basicity

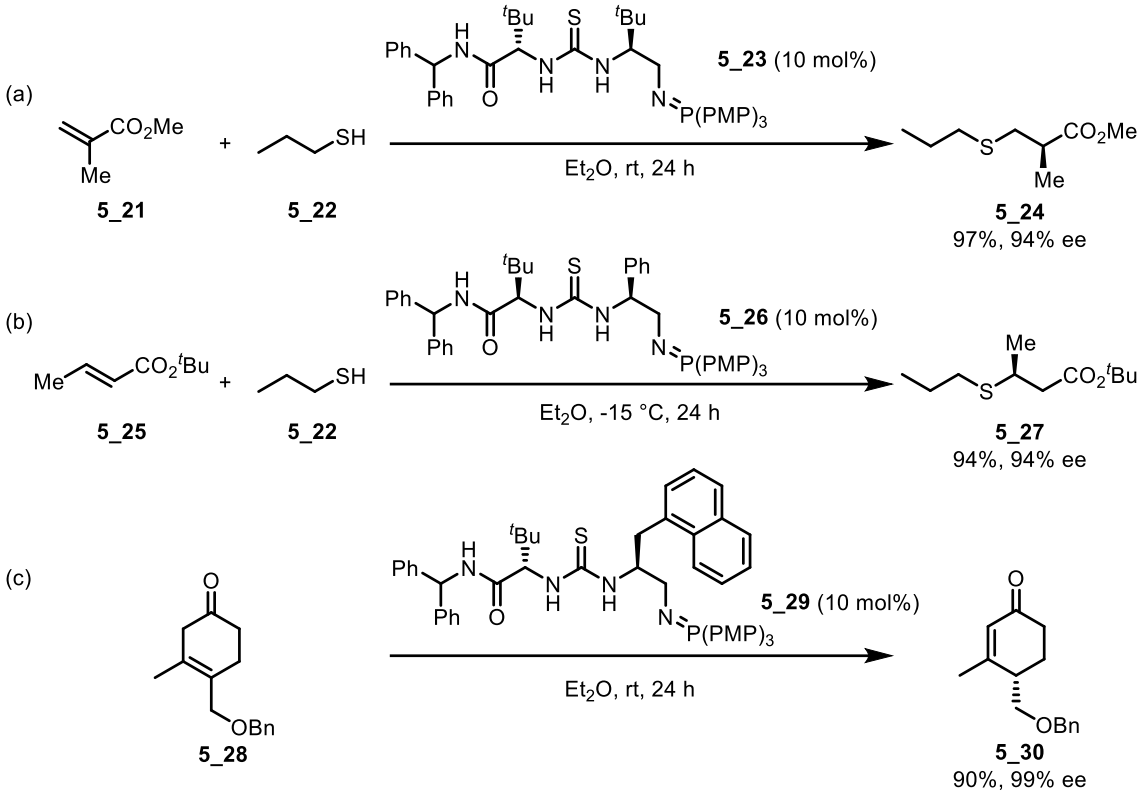
of the superbase moiety can be controlled by the choice of phosphine, enabling the late-stage tuning of the BIMP catalyst.



5_19 **5_20** **5_21**

Scheme 5.4. Synthesis of BIMP catalyst.

An early example of an asymmetric reaction catalyzed by a BIMP catalyst by Dixon was the enantioselective sulfa-Michael addition to unsaturated *α,β*-unsaturated esters (Scheme 5.5a).[9b] The *α*-substituted acrylate esters **5_21** gave the product **5_24** with a chiral center at the α position in excellent yield and enantioselectivity. In addition, a slight modification in the catalyst backbone enabled further application to the enantioselective sulfa-Michael addition to unsaturated *α,β*-unsaturated esters with *β*-substituents **5_25** (Scheme 5.5b).[9d] Furthermore, the BIMP catalysts are also effective for an enantioselective alkene isomerization (Scheme 5.5c).[9e] The *β,γ*-unsaturated cyclohexanones **5_28** with *γ*-substituents were transformed into *α,β*-unsaturated cyclohexanones **5_30** with a chiral center at the γ position. A detailed computational study was performed by the group, and the reprotonation step was found to be the rate- and enantio-determining step. These examples show the potential generality of the BIMP-catalyzed reactions.

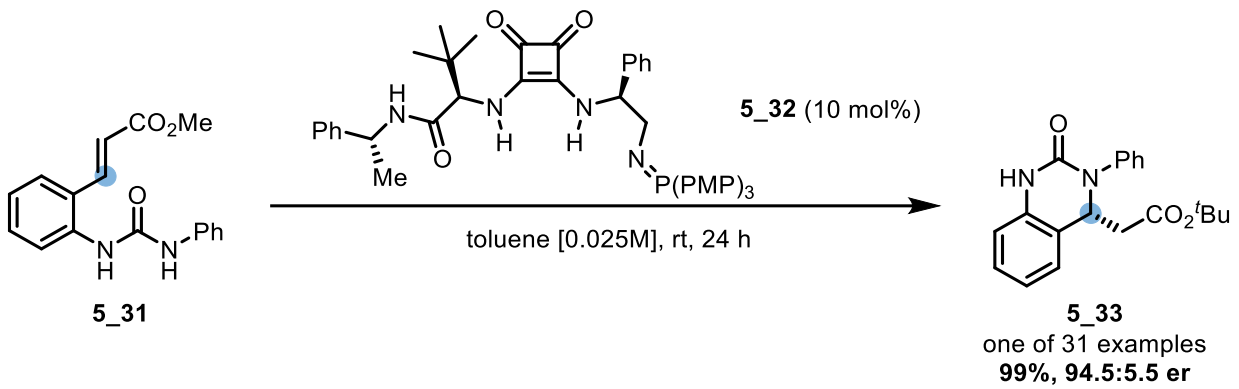


Scheme 5.5. Representative enantioselective organic reactions under BIMP catalysis.

5.3. Enantioselective Aza-Michael Addition to *α,β*-Unsaturated Esters

5.3.1. Previous Experimental Findings

Previously, our group discovered that bifunctional iminophosphorane catalyst **5_32** can lead to a highly enantioselective intramolecular aza-Michael addition of urea-tethered *α,β*-unsaturated esters **5_31** for the synthesis of hydroquinazoline cores **5_33** (Scheme 5.6).[10,11] The reaction proceeds at room temperature in toluene as the solvent to furnish the cyclized products in good to excellent yields with up to 97:3 er. A wide variety of functional groups such as halides, trifluoromethoxy, and alkyne tolerated the reaction conditions, and both aromatic and aliphatic ureas gave the desired products with high enantioselectivity. Interestingly, the hydrogen bond donor moiety had a large effect on the reactivity and enantioselectivity, and a squaramide moiety was superior to urea and thiourea.



Scheme 5.6. BIMP-catalyzed enantioselective intramolecular aza-Michael addition of *α,β*-unsaturated esters.

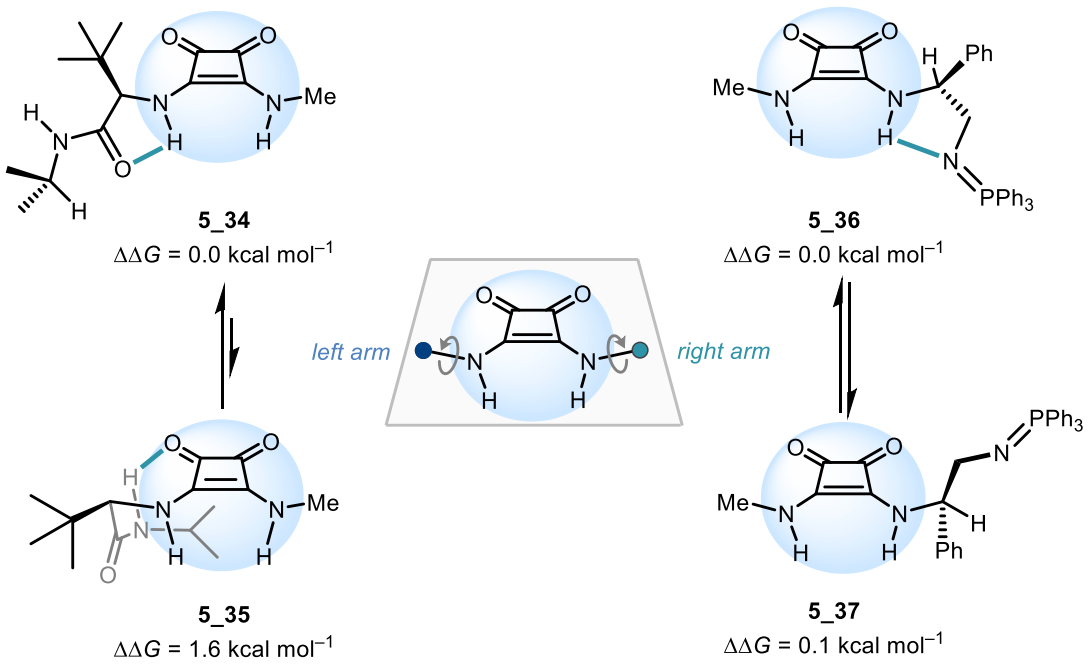
5.3.2. Computational Details

All calculations reported in this chapter were performed using the Amsterdam Density Functional (ADF) software,[12] and COSMO(toluene)-ZORA-M06-2X/TZ2P//COSMO(toluene)-ZORA-BLYP-D3(BJ)/DZP level of theory was used.[13-19]

5.3.3. Conformational Analysis of the BIMP Catalyst

Since the BIMP squaramide catalyst **5_32** is highly flexible with several freely rotating single bonds, conformational analysis on model substrates of the catalyst was performed (Scheme 5.7). There are two groups on the squaramide moiety of the organocatalyst, and the side chain that contains the amide moiety with the ^{t}Bu group was named "*left arm* (*LA*)" and the side chain that contains the iminophosphorane moiety with phenyl group was named "*right arm* (*RA*)." The *left arm* can mainly take two conformations that form hydrogen bonding between the amide and the squaramide, and the model substrate **5_34** that possesses O(amide)–H(squaramide) interaction is energetically more stable than the model substrate **5_35** that possesses O(squaramide)–H(amide) interaction by 1.6 kcal mol^{-1}. On the other hand, the *right arm* can mainly take two conformations where the iminophosphorane moiety is located either on the top or bottom side of the squaramide plane, and there is almost no stability difference between the model substrate **5_36** that possesses

N(iminophosphorane)–H(squaramide) interaction and the model substrate **5_37**. This conformational search indicates that the catalyst can take various conformations.



Scheme 5.7. Relative stability of the model squaramide catalyst. Energies (kcal mol^{-1}) are provided in the insert.

5.3.4. Transition State Structures of the Aza-Michael Addition Step

Generally, there are two coordination modes between a catalyst and a substrate in the transition state (Figure 5.4).[20] In mode A, a hydrogen bond donor (squaramide) coordinates to an electrophile (ester) and a protonated base (iminophosphorane) coordinates to a nucleophile (urea) (Figure 5.4a). In mode B, a hydrogen bond donor (squaramide) coordinates to a nucleophile (urea) and a protonated base (iminophosphorane) coordinates to an electrophile (ester) (Figure 5.4b). In order to consider all possibilities, both activation modes were studied in the following stereoselectivity-determining aza-Michael addition transition state.

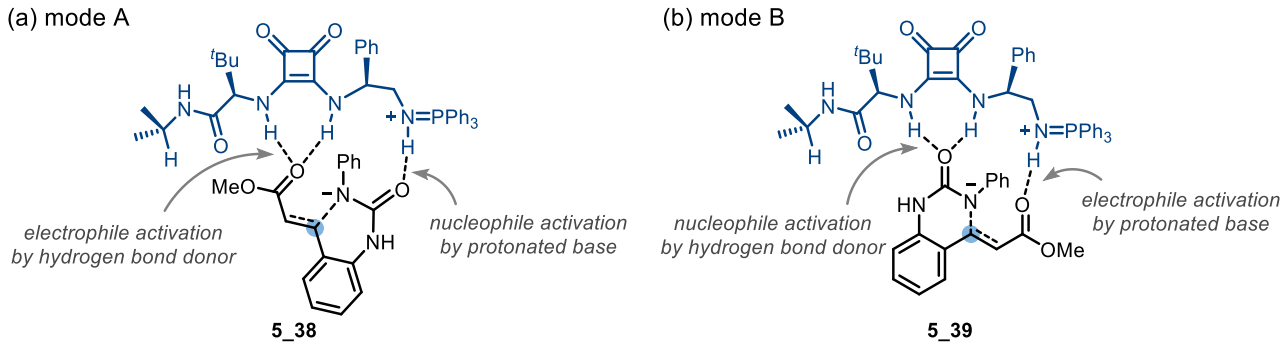
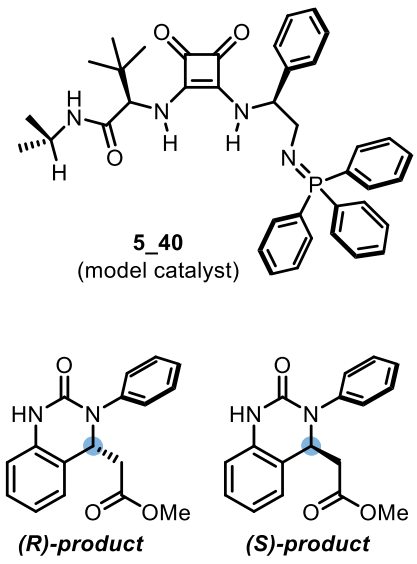


Figure 5.4. Activation modes of the BIMP catalyst.

There are 16 possible transition states for the aza-Michael addition step with the model catalyst **5_40** that originate from different activation mode, *left arm* conformation, *right arm* conformation, and the forming stereochemistry (Figure 5.5). The results showed that the lowest energy transition state for the (*R*)-product formation (**TS5_1** with mode A, LA1, RA1) is more stable than the one for the (*S*)-product formation (**TS5_12** with mode A, LA2, RA2) by 1.2 kcal mol^{-1}. This agrees with the experimentally confirmed absolute stereochemical configuration by single crystal X-ray diffraction studies, and the theoretical enantioselectivity (88:12 er) is in excellent agreement with the experimental enantioselectivity of 92:8 er for a similar substrate.



TS	*mode*	*left arm*	*right arm*	*stereochemisry*	$\Delta G^{\ddagger}$	$\Delta E^{\ddagger}$
TS5_1	A	LA1	RA1	*R*	15.1	–7.7
TS5_2	A	LA1	RA2	*R*	18.0	–4.2
TS5_3	A	LA2	RA1	*R*	16.6	–6.7
TS5_4	A	LA2	RA2	*R*	29.3	4.8
TS5_5	B	LA1	RA1	*R*	15.4	–6.5
TS5_6	B	LA1	RA2	*R*	24.0	–2.2
TS5_7	B	LA2	RA1	*R*	16.7	–6.2
TS5_8	B	LA2	RA2	*R*	27.2	2.1
TS5_9	A	LA1	RA1	*S*	27.7	3.3
TS5_10	A	LA1	RA2	*S*	17.6	–6.5
TS5_11	A	LA2	RA1	*S*	25.0	–0.8
TS5_12	A	LA2	RA2	*S*	16.3	–7.3
TS5_13	B	LA1	RA1	*S*	18.2	–6.3
TS5_14	B	LA1	RA2	*S*	19.7	–1.0
TS5_15	B	LA2	RA1	*S*	20.7	–3.3
TS5_16	B	LA2	RA2	*S*	21.3	–1.7

Figure 5.5. Relative stability of the possible intramolecular aza-Michael addition transition state structures. Energies (kcal mol^{-1}) are provided in the insert.

The preferred transition state **TS5_1** is stabilized by several non-covalent interactions (NCI) such as hydrogen bonding, CH–π, and CO–π interactions between the substrate and the catalyst and within the catalyst (Figure 5.6, left).[21] Interestingly, the intermolecular interactions exist from both *left arm* and *right arm*, creating the ideal-fit pocket of the catalyst where the substrate can strongly bind with more stabilizing interactions and less steric repulsion. These weak interactions can also be qualitatively visualized in the NCI plot (Figure 5.6, right). On the other hand, the less favored transition state **TS5_12** is also stabilized by several NCIs; however, the distinctive interactions are much less than with **TS5_1** (Scheme 5.7). Therefore, the aza-Michael addition step proceeds with a specific catalyst conformation where the substrate can perfectly fit.

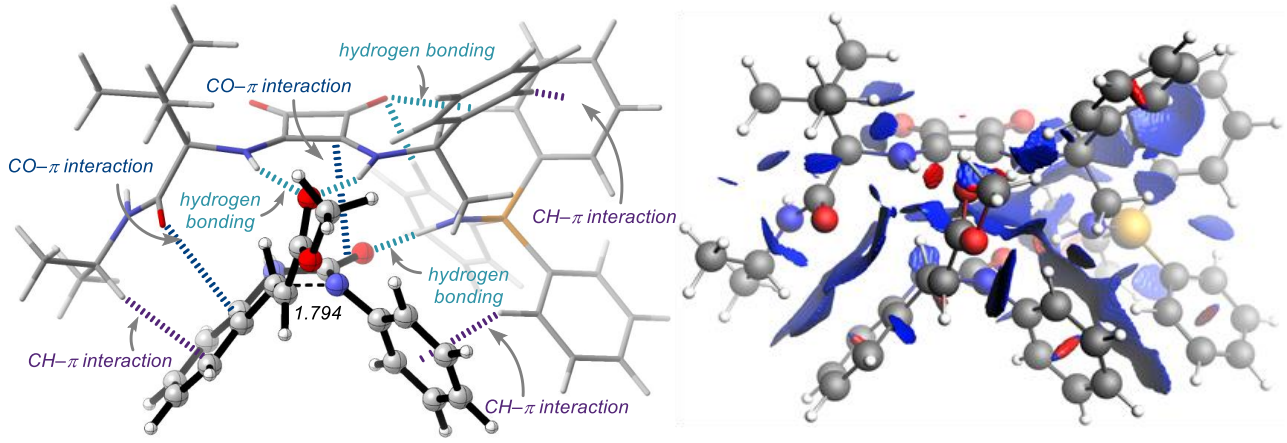


Figure 5.6. Transition state structure geometry of **TS5_1**, and the non-covalent interaction. A forming bond length (Å) in the TS geometry is provided in the insert.

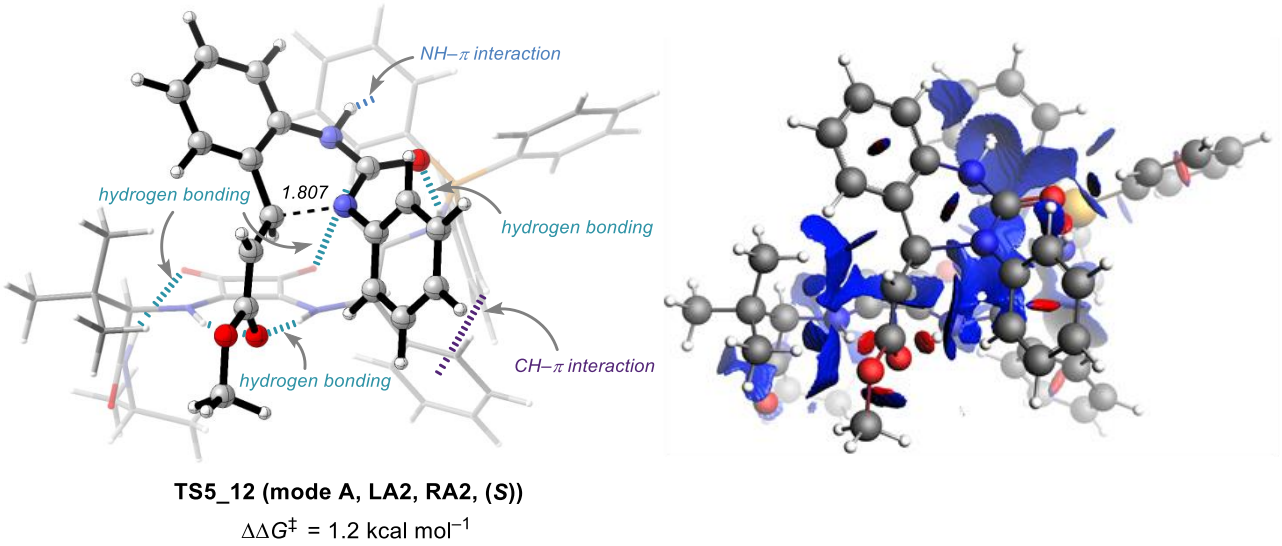
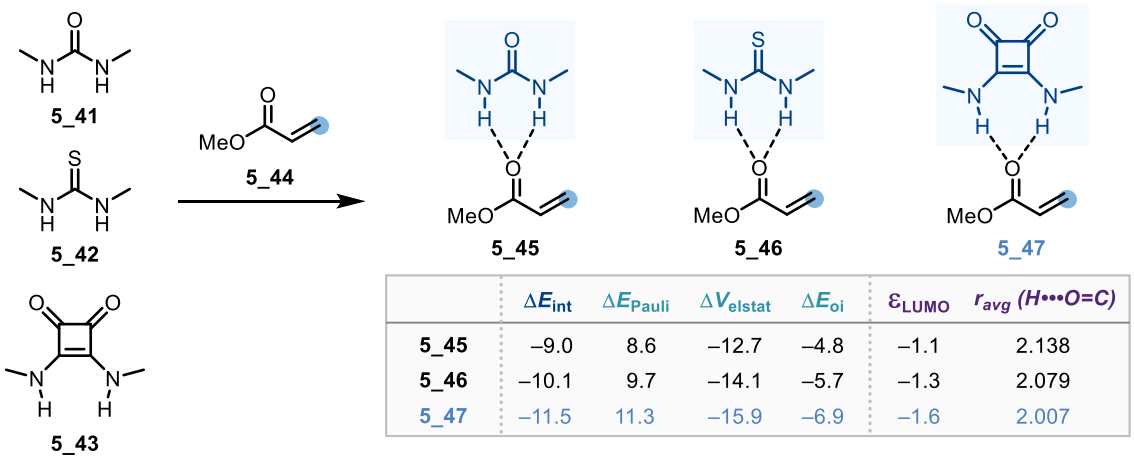


Figure 5.7. Transition state structure geometry of **TS5_12**, and the non-covalent interaction. A forming bond length (Å) in the TS geometry is provided in the insert.

5.3.5. Origin of Reactivity Enhancement of Squaramide Motif in BIMP Catalyst

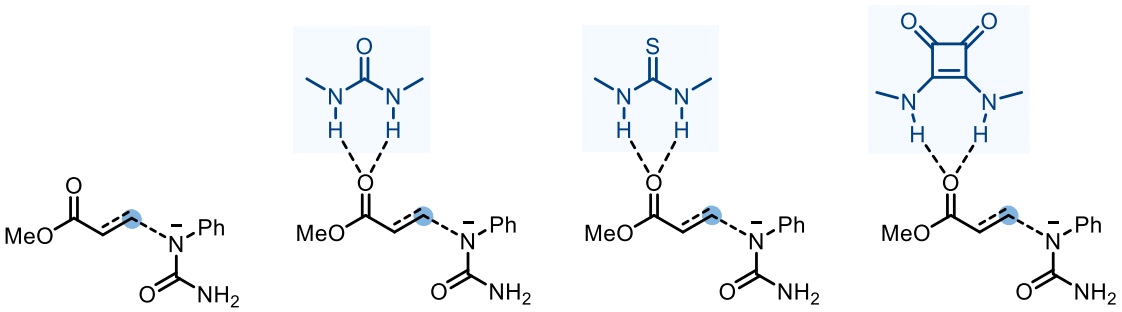
To obtain more insight into the origin of enhanced reactivity with the squaramide BIMP catalyst, activation strain analysis (ASA) and energy decomposition analysis (EDA) were performed on a model system (Figure 5.8).[22,23] First, the interaction between a hydrogen bond donor (HB) and methyl acrylate (MA) **5_44** was studied. The interaction energy between HB and MA changes from urea to squaramide (ΔE_{int} = –9.0 (urea), –10.1 (thiourea), –11.5 (squaramide) kcal mol^{-1}), and the squaramide had the most stabilizing ΔE_{int} because of the electrostatic interaction term (ΔV_{elstat}) by the nature of the hydrogen bonding interaction, as well as the orbital interaction term (ΔE_{oi}) that involves charge transfer from the carbonyl oxygen lone pair and the two σ* N–H orbitals.



	ΔE_{int}	ΔE_{Pauli}	ΔV_{elstat}	ΔE_{oi}	ε_{LUMO}	r_{avg} (H•••O=C)
5_45	–9.0	8.6	–12.7	–4.8	–1.1	2.138
5_46	–10.1	9.7	–14.1	–5.7	–1.3	2.079
5_47	–11.5	11.3	–15.9	–6.9	–1.6	2.007

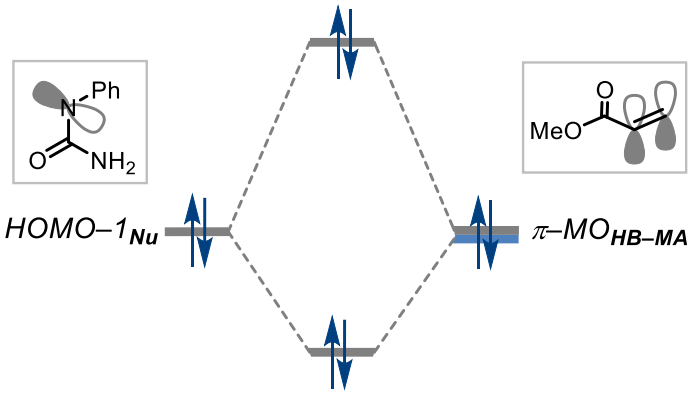
Figure 5.8. Interaction energies and the energy decomposition analysis of the hydrogen bond donor–methyl acrylate complexes (HB–MA). Energies (kcal mol^{-1}) are provided in the insert.

Next, in-depth analysis of the aza-Michael addition transition states was carried out (Figure 5.9). As expected, the uncatalyzed reaction proceeds with the highest activation energy barrier through **TS5_17** ($\Delta G^{\ddagger}$ = 16.3 kcal mol^{-1}), and the barriers are reduced when a hydrogen bond donor is coordinated to the ester group. Among the hydrogen bond donors, the squaramide-catalyzed aza-Michael addition proceeds with the lowest energy barrier through **TS5_20** ($\Delta G^{\ddagger}$ = 8.9 kcal mol^{-1}). Then, the ASA was performed on the HB–MA complex fragment and the deprotonated phenyl urea fragment. The energy barrier trend follows the trend of the interaction energy ($\Delta E^{\ddagger}_{int}$), and this originates from the Pauli repulsion ($\Delta E^{\ddagger}_{Pauli}$) between reactants. The enhanced reactivity with the squaramide catalyst is the result of lower destabilizing $\Delta E^{\ddagger}_{Pauli}$ between the lone pair of the nucleophile and the filled π orbital of the C=C double bond. A Kohn-Sham molecular orbital (KS-MO) analysis revealed that the size of the occupied C=C π orbital is diminished with the squaramide in **TS5_20** because of the charge polarization, and the orbital overlap *S* with the HOMO–1 of the nucleophile is minimized (Figure 5.10). Therefore, the BIMP squaramide catalyst can reduce the destabilizing Pauli repulsion between the reactants to enhance the reactivity of the novel intramolecular aza-Michael addition.



	$\Delta G^{\ddagger}$	$\Delta E^{\ddagger}$	$\Delta E^{\ddagger}_{strain}$	$\Delta E^{\ddagger}_{int}$	$\Delta E^{\ddagger}_{int,gas}$	$\Delta E^{\ddagger}_{Pauli}$	$\Delta V^{\ddagger}_{elstat}$	$\Delta E^{\ddagger}_{oi}$
TS5_17	16.3	2.9	23.0	–20.0	–27.6	146.3	–81.6	–92.2
TS5_18	12.0	–4.5	21.9	–26.4	–39.5	114.8	–75.2	–79.1
TS5_19	11.2	–5.7	21.5	–27.2	–41.4	109.4	–73.8	–77.0
TS5_20	8.9	–8.8	20.4	–29.2	–46.9	102.7	–76.1	–73.5

Figure 5.9. Energy barriers of the aza-Michael addition transition state structures and the activation strain analysis and the energy decomposition analysis. Energies (kcal mol^{-1}) are provided in the insert.



	π–$MO_{HB–MA}$	Orbital Overlap *S*
TS5_17	*HOMO*	0.141
TS5_18	*HOMO–2*	0.118
TS5_19	*HOMO–2*	0.111
TS5_20	*HOMO–2*	**0.106**

Figure 5.10. Molecular orbital diagram and the most significant occupied orbital overlaps.

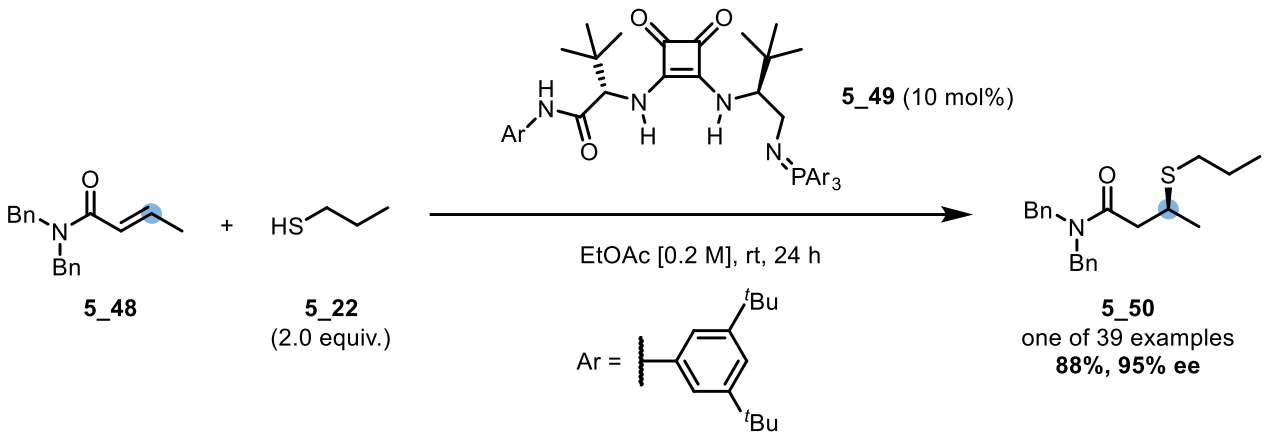
5.3.6. Summary

In summary, a detailed mechanistic study of the enantioselective intramolecular aza-Michael addition of urea-tethered α,β-unsaturated esters for the synthesis of hydroquinazoline cores was performed using density functional theory calculations. The stereoselectivity-determining aza-Michael addition proceeds through the transition state conformation where the substrate can strongly bind with more stabilizing interactions and less steric repulsion. The enantioselectivity is controlled by several non-covalent interactions, and the theoretical value is in excellent agreement with the experimental data. The activation strain analysis and the energy decomposition analysis revealed that the origin of reactivity enhancement with the squaramide motif is the reduced destabilizing Pauli repulsion between reactants. These computational studies shed light on further development of novel organocatalytic reactions.

5.4. Enantioselective Sulfa-Michael Addition to *α,β*-Unsaturated Amides

5.4.1. Previous Experimental Findings

Previously, our group discovered that bifunctional iminophosphorane catalyst **5_49** can promote a highly enantioselective intermolecular sulfa-Michael addition to unactivated *α,β*-unsaturated amide **5_48** (Scheme 5.8).[24,25] The reaction proceeds at room temperature in ethyl acetate as the solvent to generate a stereocenter at the *β*-position in good to excellent yield and enantioselectivity. A wide variety of substrates with reactive functional groups tolerated these mild reaction conditions to give the desired products with high enantioselectivity. Interestingly, an *α*-substituted unsaturated amide also gave the product with good enantioselectivity. The key improvement from the previous report on the BIMP-catalyzed sulfa-Michael addition to unactivated *α,β*-unsaturated esters was the use of a squaramide motif in the catalyst scaffold.



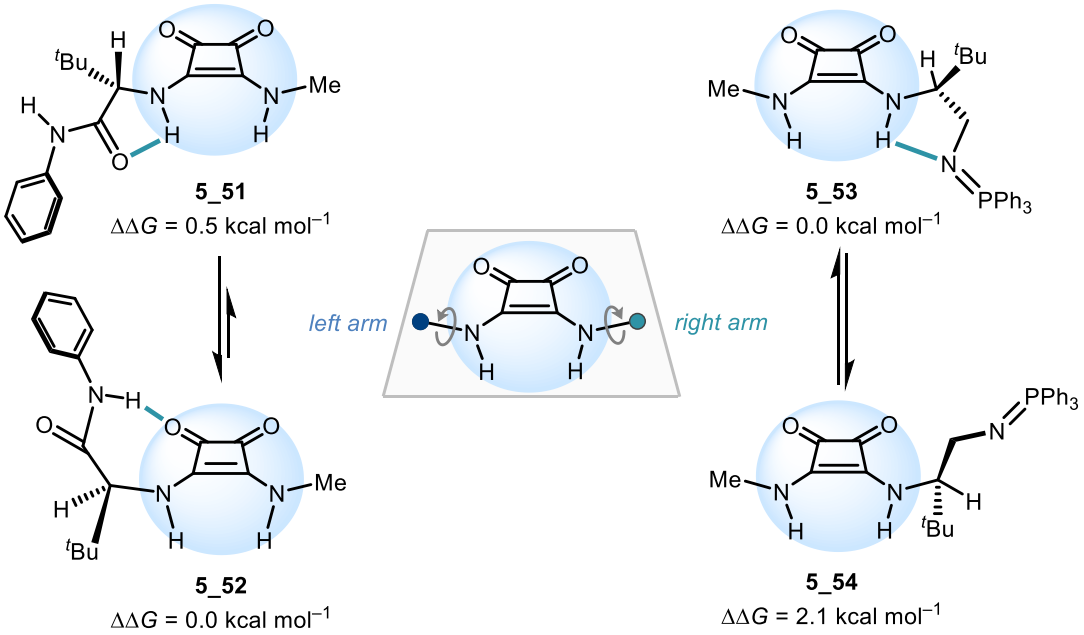
Scheme 5.8. BIMP-catalyzed enantioselective intermolecular sulfa-Michael addition to *α,β*-unsaturated amides.

5.4.2. Computational Details

All calculations reported in this chapter were performed using the Amsterdam Density Functional (ADF) software,[12] and COSMO(EtOAc)-ZORA-M06-2X/TZ2P//COSMO(EtOAc)-ZORA-BLYP-D3(BJ)/DZP level of theory was used.[13-19]

5.4.3. Conformational Analysis of the BIMP Catalyst

As described above, the BIMP catalyst has two flexible side chains with several freely rotating bonds, and the catalyst conformation was studied using model systems (Scheme 5.9). The side chain that contains the amide moiety with a ^{t}Bu group was named "*left arm* (*LA*)," and the side chain that contains the iminophosphorane moiety with ^{t}Bu group was named "*right arm* (*RA*)." The *LA* can form an intramolecular hydrogen bonding with the squaramide at the N–H bond in **5_51** or the carbonyl oxygen in **5_52**, and both conformations are energetically similar and exist in an equilibrium. On the other hand, the conformation of *RA* can be distinguished by the position of the iminophosphorane moiety which is either on the top side (**5_53**) or bottom side (**5_54**) of the squaramide, and **5_53** is stabilized due to the presence of an internal hydrogen bond.



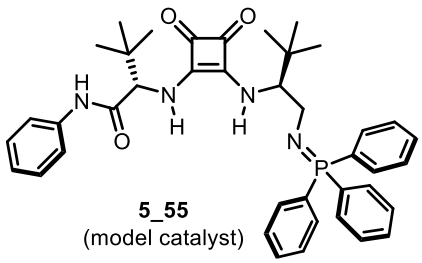
Scheme 5.9. Relative stability of the model catalysts. Energies (kcal mol^{-1}) are provided in the insert.

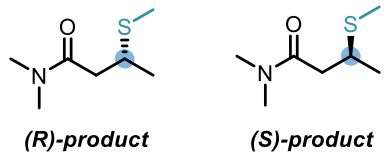
5.4.4. Transition State Structures of the Sulfa-Michael Addition Step

In order to elucidate the enhancement of both reactivity and enantioselectivity using the squaramide motif, a thorough transition state search was performed on the key C–S bond forming step based on the type of hydrogen bond donor, activation modes, *left arm* and *right arm* conformations, and the forming

stereochemical outcome (Figure 5.11). Among 16 possible transition states with the BIMP squaramide catalyst, the lowest energy TS is **TS5_31** for the formation of the (*S*)-product, which agrees with the experimentally confirmed absolute stereochemical configuration. The activation energy required to form the minor enantiomer is much higher through the **TS5_27** ($\Delta\Delta G^{\ddagger}$ = 4.1 kcal mol^{-1}), resulting in this highly enantioselective transformation.

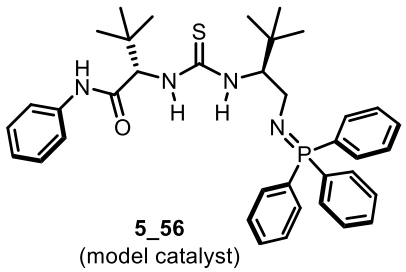
Replacement of the squaramide by a thiourea gave a similar trend, but the overall activation energy was increased (Figure 5.12). The lowest energy transition states for the formation of both enantiomers proceed with higher energy barriers ($\Delta G^{\ddagger}$ = 22.1 and 26.0 kcal mol^{-1} through **TS5_47** and **TS5_43**, respectively), and also the energy difference $\Delta\Delta G^{\ddagger}$ is smaller than the one with the squaramide catalyst **5_55**. Therefore, the calculations indicate that the squaramide motif can enhance both the reactivity and enantioselectivity.



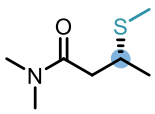


TS	mode	left arm	right arm	configuration	$\Delta G^{\ddagger}$	$\Delta E^{\ddagger}$
TS5_21	A	LA1	RA1	*R*	32.6	–4.9
TS5_22	A	LA1	RA2	*R*	26.4	–8.8
TS5_23	A	LA2	RA1	*R*	28.0	–8.0
TS5_24	A	LA2	RA2	*R*	30.0	–5.4
TS5_25	B	LA1	RA1	*R*	25.4	–8.6
TS5_26	B	LA1	RA2	*R*	29.6	–5.3
TS5_27	B	LA2	RA1	*R*	**24.6**	**–9.2**
TS5_28	B	LA2	RA2	*R*	35.7	1.0
TS5_29	A	LA1	RA1	*S*	24.1	–11.3
TS5_30	A	LA1	RA2	*S*	24.3	–10.7
TS5_31	A	LA2	RA1	*S*	**20.5**	**–15.4**
TS5_32	A	LA2	RA2	*S*	35.9	–0.4
TS5_33	B	LA1	RA1	*S*	23.9	–9.9
TS5_34	B	LA1	RA2	*S*	30.9	–4.1
TS5_35	B	LA2	RA1	*S*	23.6	–10.6
TS5_36	B	LA2	RA2	*S*	32.7	–2.4

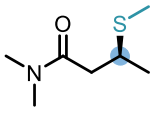
Figure 5.11. Relative stability of the possible intramolecular sulfa-Michael addition transition state structures with the BIMP squaramide catalyst **5_55**. Energies (kcal mol^{-1}) are provided in the insert.



5_56
(model catalyst)



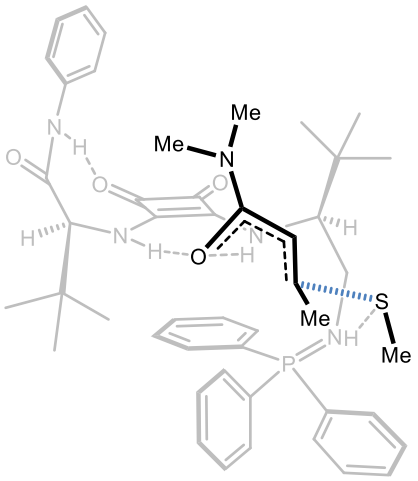
(R)-product



(S)-product

TS	*mode*	*left arm*	*right arm*	*configuration*	$\Delta G^{\ddagger}$	$\Delta E^{\ddagger}$
TS5_37	A	LA1	RA1	*R*	*n.d.*	*n.d.*
TS5_38	A	LA1	RA2	*R*	27.0	–3.8
TS5_39	A	LA2	RA1	*R*	28.5	–4.3
TS5_40	A	LA2	RA2	*R*	*n.d.*	*n.d.*
TS5_41	B	LA1	RA1	*R*	26.1	–4.1
TS5_42	B	LA1	RA2	*R*	30.6	–1.0
TS5_43	B	LA2	RA1	*R*	**26.0**	**–3.9**
TS5_44	B	LA2	RA2	*R*	33.7	3.0
TS5_45	A	LA1	RA1	*S*	27.5	–4.9
TS5_46	A	LA1	RA2	*S*	32.9	–0.3
TS5_47	A	LA2	RA1	*S*	**22.1**	**–9.9**
TS5_48	A	LA2	RA2	*S*	32.2	–0.3
TS5_49	B	LA1	RA1	*S*	27.1	–5.3
TS5_50	B	LA1	RA2	*S*	31.5	–1.2
TS5_51	B	LA2	RA1	*S*	26.1	–5.4
TS5_52	B	LA2	RA2	*S*	36.8	4.8

Figure 5.12. Relative stability of the possible intramolecular sulfa-Michael addition transition state structures with the BIMP thiourea catalyst **5_56**. Energies (kcal mol^{-1}) are provided in the insert.



TS5_31

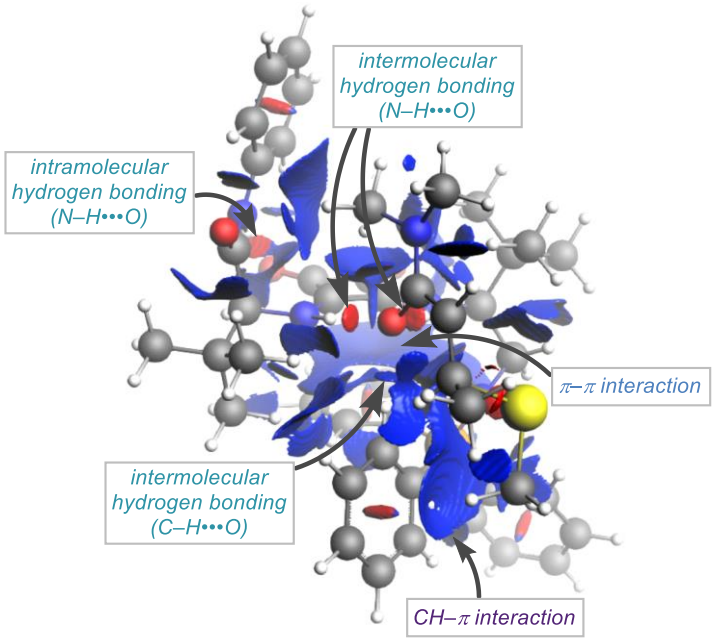


Figure 5.13. ADFview2020 plot of noncovalent interaction (NCI) regions materialized by reduced density gradient isosurfaces (all default settings were used) colored according to the sign of the signed density λ2ρ (red and blue colors are associated with negatively and positively signed terms) for the transition state structure geometry of **TS5_31**.

The most favored transition state **TS5_31** with the squaramide BIMP catalyst **5_55** has multiple stabilizing non-covalent interactions (Figure 5.13). The major NCIs are the inter- and intramolecular hydrogen bonding, CH–π, and π–π interactions between the substrate and the catalyst and within the catalyst.[21] Moreover, the catalyst conformation specifically prevents steric clash, and the ideal-fit pocket of the catalyst is created for a substrate to bind strongly.

5.4.5. Summary

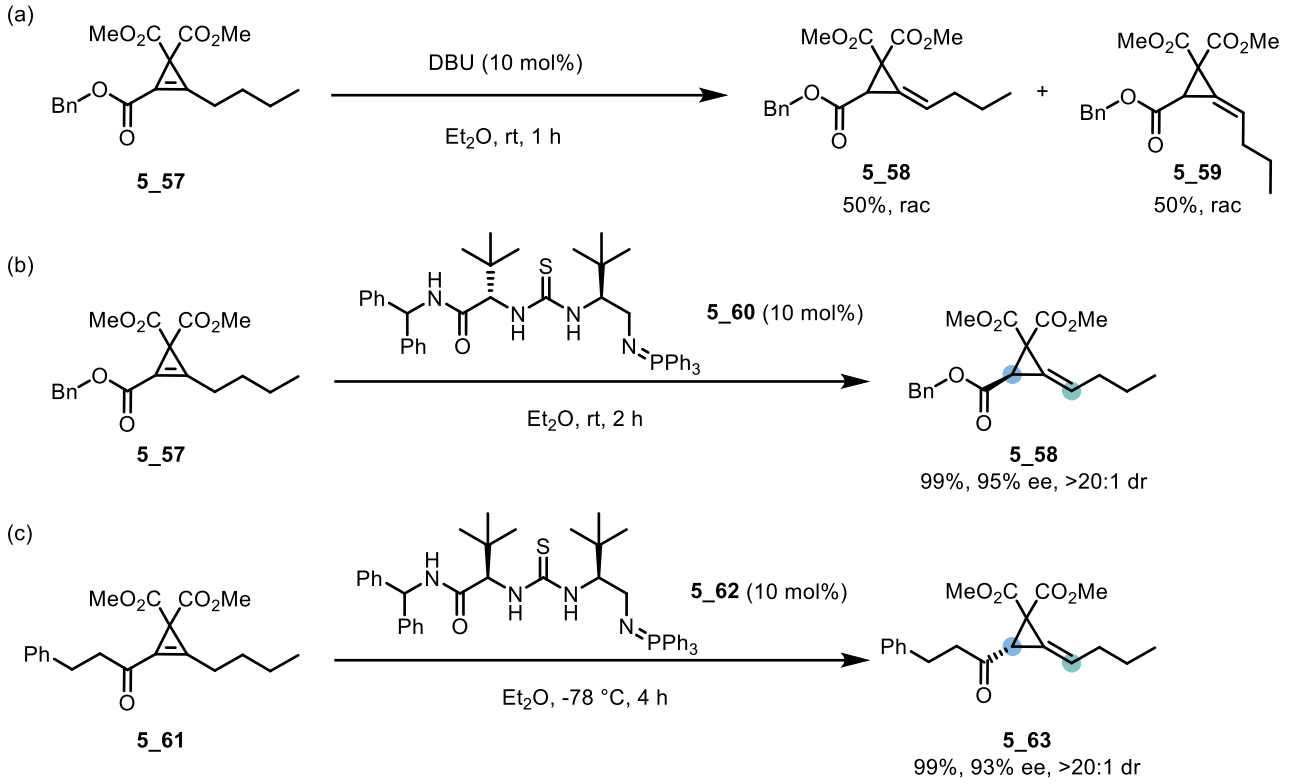
In conclusion, a detailed mechanistic study of the enantioselective sulfa-Michael addition to unactivated *α,β*-unsaturated amides was performed using density functional theory calculations. The stereoselectivity-determining sulfa-Michael addition proceeds through the lowest-energy transition state conformation, where the catalyst creates an ideal-fit pocket for the substrate to strongly bind with more stabilizing interactions and less steric repulsion. There are several non-covalent interactions that control the enantioselectivity, and the reactivity enhancement of the squaramide motif was supported by comparing with the model thiourea scaffold. These computational studies have demonstrated the potential to further improve and develop novel organocatalytic reactions.

5.5. Enantioselective 1,3-Prototropic Shift of Cyclopropenes

5.5.1. Previous Experimental Findings

Previously, our group reported that bifunctional iminophosphorane catalysis was highly useful for the enantioselective 1,3-prototropic shift for the synthesis of conjugated cyclohexenones.[9e] This methodology was then applied to the 1,3-prototropic shift of cyclopropenes, and a modest catalyst tuning enabled the formation of a chiral carbon center at the three-membered ring (Scheme 5.10).[26] The reaction proceeds under mild conditions to furnish the enantioenriched products in excellent yields and selectivity with up to >99% ee (Scheme 5.10b). A wide variety of functional groups such as ester, amides, ketones, and alkenes tolerated the

reaction conditions to give the desired products with high enantioselectivity. Interestingly, a slight modification of the catalyst stereocenter was required when the ketone-substituted cyclopropene substrate **5_61** was used. Furthermore, the BIMP catalyst controls not only the enantioselectivity, but also the diastereoselectivity at the C=C double bond.



Scheme 5.10. BIMP-catalyzed 1,3-prototropic shift of cyclopropenes.

5.5.2. Computational Details

All calculations reported in this chapter were performed using the Amsterdam Density Functional (ADF) software,[12] and COSMO(Et_2O)-ZORA-M06-2X/TZ2P//COSMO(Et_2O)-ZORA-BLYP-D3(BJ)/DZP level of theory was used.[13-19]

5.5.3. Conformational Analysis of BIMP Catalysts

In order to quantify the flexible nature of BIMP catalysts used in the 1,3-prototropic shift reactions, conformational analysis on the catalysts was performed (Figures 5.14 and 5.15). Both catalysts **5_60**, that is efficient for the reaction with ester-substituted cyclopropenes, and **5_62** that is efficient for the reaction with ketone-substituted cyclopropenes take the most stable conformations when the thiourea sulfur atom and the amide N–H bond creates an intramolecular hydrogen bonding and two *tert*-butyl groups are on the different side of the thiourea plane that are represented as **5_64** and **5_68**, respectively.

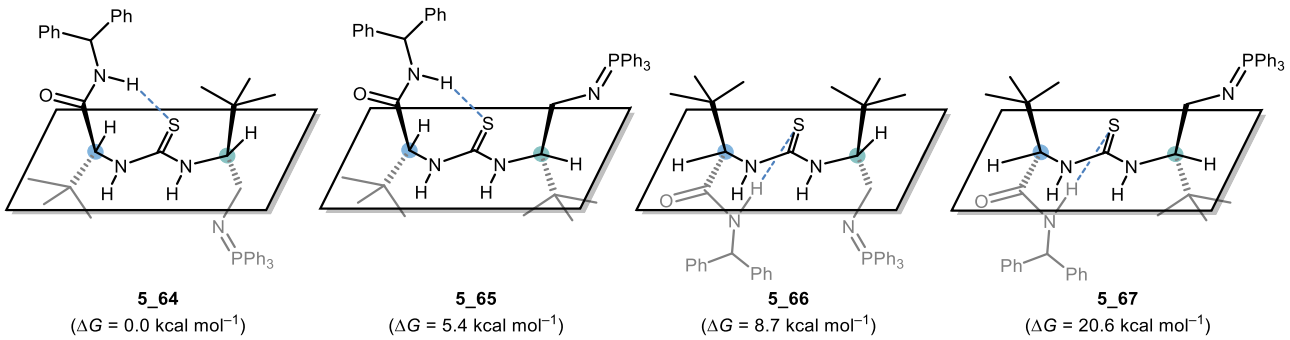


Figure 5.14. Relative stability (Δ*G* in kcal mol^{-1}) of the BIMP catalyst **5_60**.

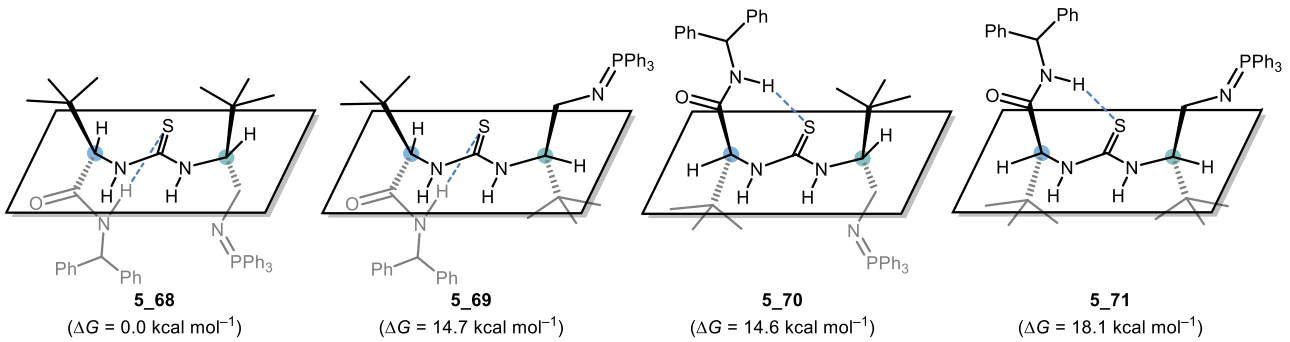


Figure 5.15. Relative stability (Δ*G* in kcal mol^{-1}) of the BIMP catalyst **5_62**.

5.5.4. Potential Energy Surfaces of BIMP-Catalyzed 1,3-Prototropic Shift

Since the catalyst can adopt several relevant conformational states, nomenclature was required (Figure 5.16). Both the left side of the catalyst chain that contains the amide moiety with a ^{t}Bu group (LA) and the right side of the catalyst chain that contains the iminophosphorane moiety with a ^{t}Bu group (RA) can take two conformations, and those were named as **LA1**, **LA2**, **LA3**, **RA1**, and **RA2**, respectively. In addition, there are two protons at the γ position of the cyclopropene substrate (H_a and H_b) with the model substrates **5_72** and **5_73**. Based on these defined rules, the key transition states of the deprotonation and reprotonation processes were extensively explored.

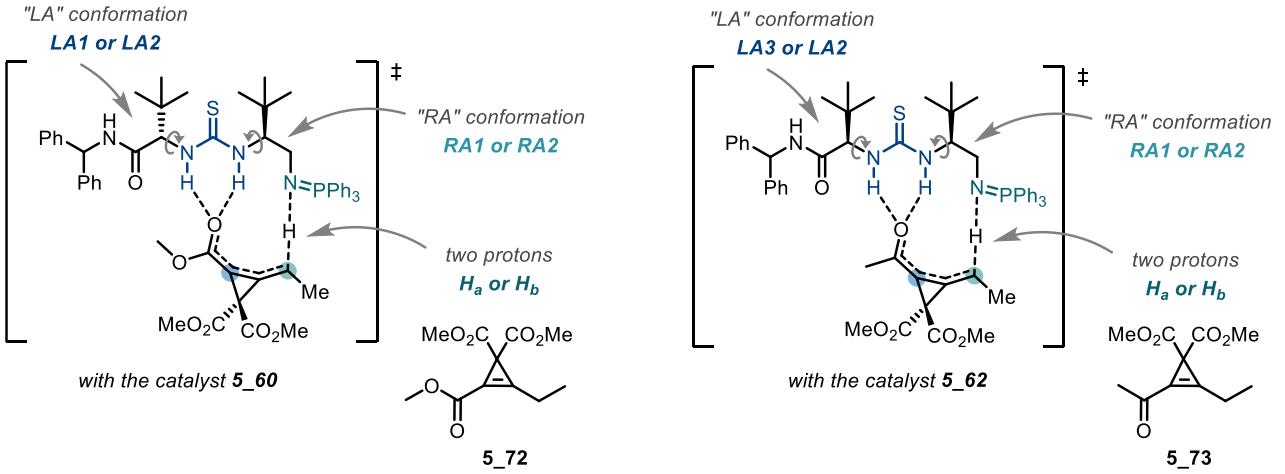
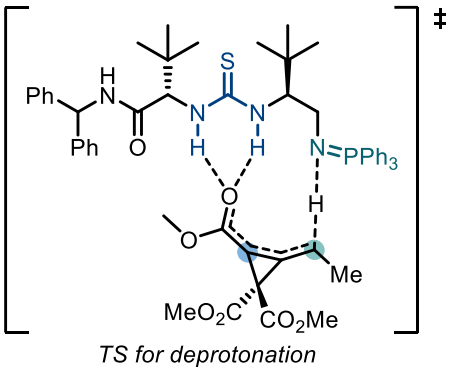


Figure 5.16. Catalyst conformations of BIMP catalysts **5_60** and **5_62**.

Initially, transition states for the deprotonation process were studied (Figure 5.17). The thiourea activates the ester carbonyl group, and the iminophosphorane superbase removes the acidic γ proton. Seven different TSs were located among the extensive calculations that were performed, and the lowest conformation was **TS5_53**. The activation energy barrier of 21.7 kcal mol^{-1} indicates that the reaction is indeed feasible at room temperature. The substrate at this transition state has no significant steric repulsion, and the methyl group

at the γ position is pointing away from the phosphine ligand, indicating that the *E/Z* selectivity is highly controlled at this deprotonation step (Figure 5.18).



TS	*left arm*	*right arm*	*proton*	$\Delta G^{‡}$	$\Delta E^{‡}$
TS5_53	LA1	RA1	H_a	**21.7**	**2.7**
TS5_54	LA1	RA2	H_a	22.1	4.8
TS5_55	LA2	RA1	H_a	36.2	17.9
TS5_56	LA2	RA2	H_a	33.1	13.0
TS5_57	LA1	RA1	H_b	22.5	4.1
TS5_58	LA1	RA2	H_b	26.6	7.0
TS5_59	LA2	RA1	H_b	*n.d.*	*n.d.*
TS5_60	LA2	RA2	H_b	35.5	15.1

Figure 5.17. Relative stability of the possible deprotonation transition state structures with ester-substituted cyclopropene **5_72** and the BIMP catalyst **5_60**. Energies (kcal mol^{-1}) are provided in the insert.

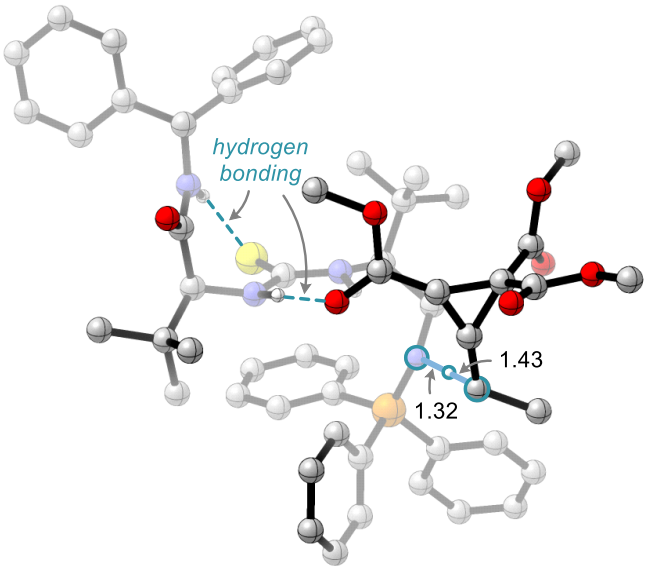
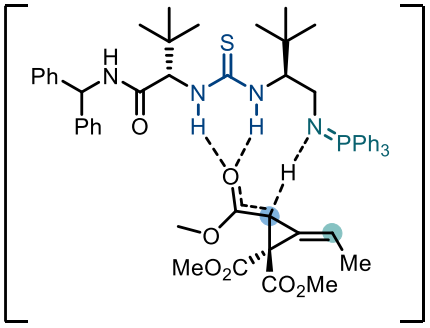


Figure 5.18. Transition state structure geometry of **TS5_53**. Forming and breaking bond lengths (Å) are provided in the insert.

The reprotonation step determines the enantioselectivity at the α position, and eight possible TS geometries were successfully located. The lowest energy TSs for the formation of (*R*)-product and (*S*)-product were **TS5_61** and **TS5_65**, respectively. Pleasingly, the computationally favored TS leads to the (*R*)-product, which agrees with the experimentally confirmed absolute stereochemical configuration by single crystal X-ray diffraction studies.

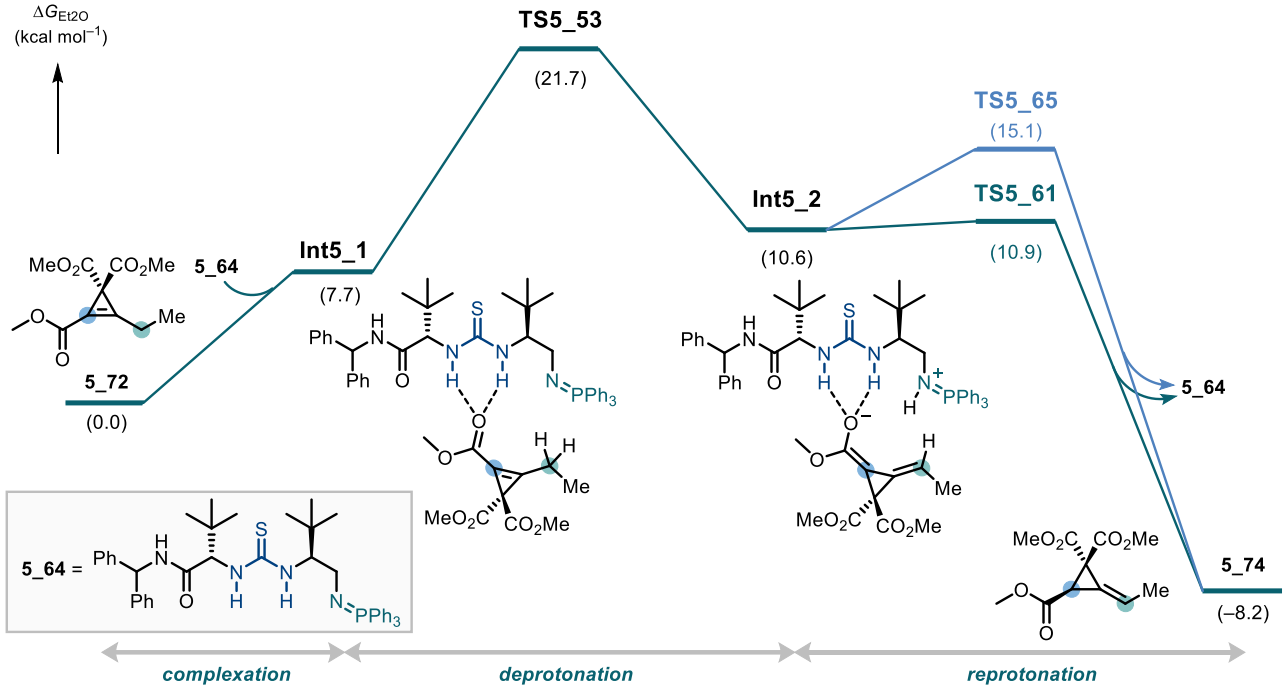


TS for reprotonation

TS	*left arm*	*right arm*	*configuration*	$\Delta G^{‡}$	$\Delta E^{‡}$
TS5_61	LA1	RA1	*R*	**10.9**	**–8.7**
TS5_62	LA1	RA2	*R*	26.5	7.9
TS5_63	LA2	RA1	*R*	13.7	–4.8
TS5_64	LA2	RA2	*R*	23.9	2.4
TS5_65	LA1	RA1	*S*	**15.1**	**–5.1**
TS5_66	LA1	RA2	*S*	20.2	5.0
TS5_67	LA2	RA1	*S*	20.1	0.8
TS5_68	LA2	RA2	*S*	28.2	7.6

Figure 5.19. Relative stability of the possible reprotonation transition state structures with ester-substituted cyclopropene **5_72** and the BIMP catalyst **5_60**. Energies (kcal mol^{-1}) are provided in the insert.

The complete potential energy surface of the 1,3-prototropic shift of ester-substituted cyclopropenes is shown in Scheme 5.11. The catalyst-substrate complex **Int5_1** is initially formed, and the deprotonation occurs through the transition state **TS5_53** to give the enolate intermediate **Int5_2**. The final reprotonation process preferably occurs via the **TS5_61** to furnish the product **5_74**. The large energy release by C=C double bond isomerization and strain release is the driving force of this reaction, and the enantioselectivity is determined by the reprotonation step after the rate-determining deprotonation step.



Scheme 5.11. Computed reaction energy profile (Δ*G* in kcal mol^{-1}) for the 1,3-prototropic shift of ester substituted cyclopropenes.

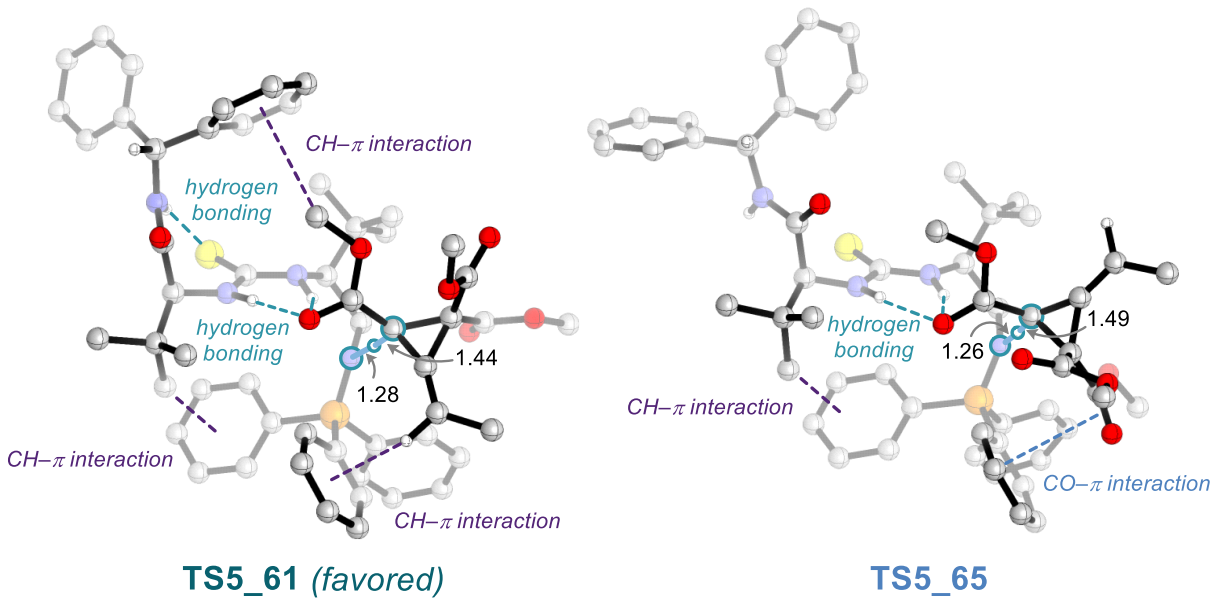
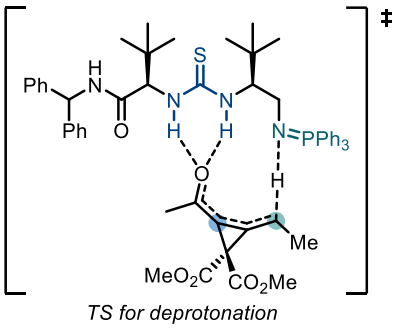


Figure 5.20. TS geometries of **TS5_61** and **TS5_65**. Bond lengths (Å) are provided in the insert.

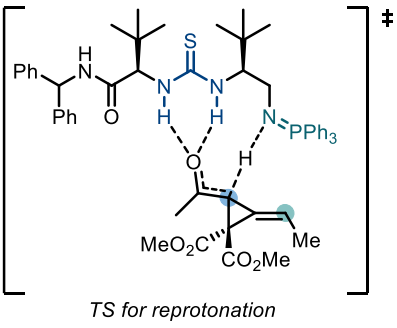
The preferred transition state **TS5_61** is highly stabilized by several NCIs such as hydrogen bonding between thiourea, ester carbonyl and amide N–H bond, and intermolecular CH–π interaction between the substrate and the catalyst (Figure 5.20). On the other hand, the unfavored TS has limited contact between these two species and mainly benefits from less sterically demanding catalyst conformations.



TS for deprotonation

TS	*left arm*	*right arm*	*proton*	$\Delta G^{‡}$	$\Delta E^{‡}$
TS5_69	LA1	RA1	H_a	**20.0**	**4.4**
TS5_70	LA1	RA2	H_a	33.1	15.4
TS5_71	LA2	RA1	H_a	28.0	12.6
TS5_72	LA2	RA2	H_a	*n.d.*	*n.d.*
TS5_73	LA1	RA1	H_b	23.5	9.1
TS5_74	LA1	RA2	H_b	*n.d.*	*n.d.*
TS5_75	LA2	RA1	H_b	38.3	20.7
TS5_76	LA2	RA2	H_b	33.5	18.0

Figure 5.20. Relative stability of the possible deprotonation transition state structures with ketone-substituted cyclopropene **5_73** and the BIMP catalyst **5_62**. Energies (kcal mol^{-1}) are provided in the insert.



TS for reprotonation

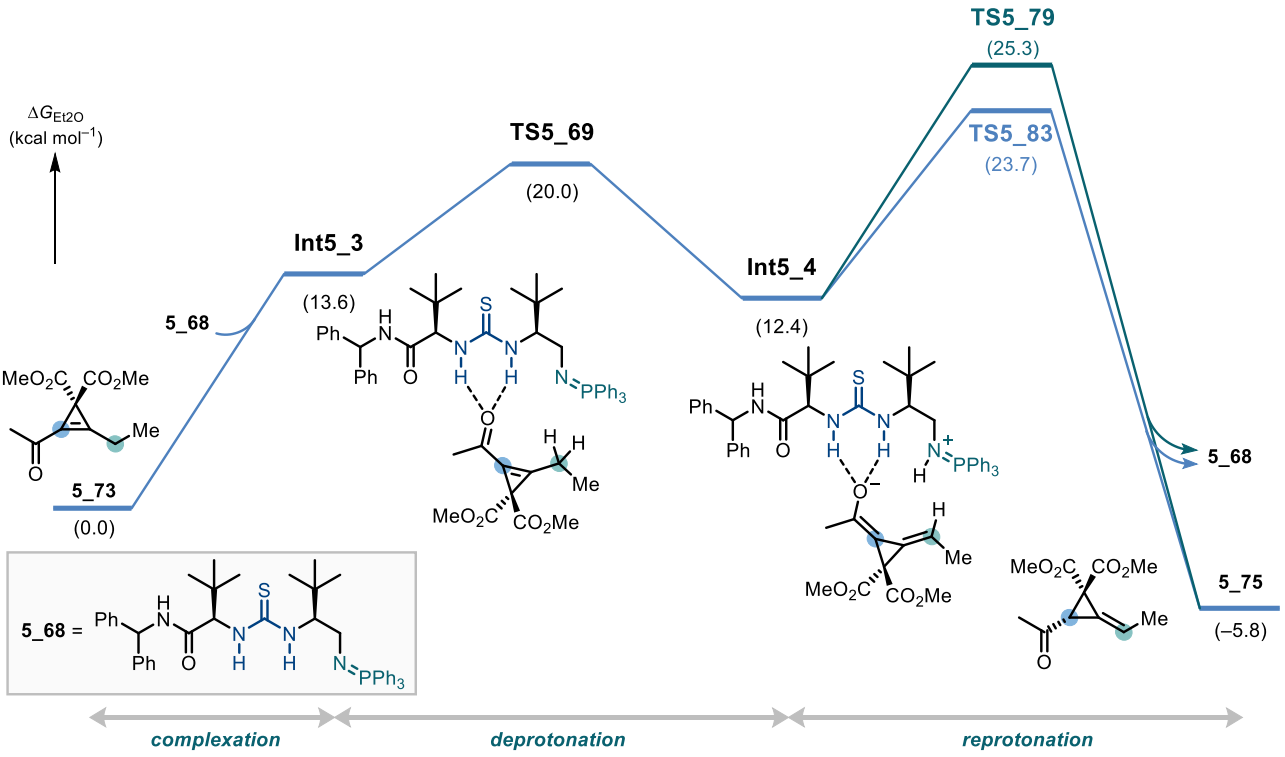
TS	*left arm*	*right arm*	*stereochemistry*	$\Delta G^{‡}$	$\Delta E^{‡}$
TS5_77	LA1	RA1	*R*	*n.d.*	*n.d.*
TS5_78	LA1	RA2	*R*	31.4	14.4
TS5_79	LA2	RA1	*R*	**25.3**	**9.0**
TS5_80	LA2	RA2	*R*	46.4	23.8
TS5_81	LA1	RA1	*S*	29.8	11.2
TS5_82	LA1	RA2	*S*	28.2	11.0
TS5_83	LA2	RA1	*S*	**23.7**	**7.0**
TS5_84	LA2	RA2	*S*	29.7	13.4

Figure 5.21. Relative stability of the possible reprotonation transition state structures with ketone-substituted cyclopropene **5_73** and the BIMP catalyst **5_62**. Energies (kcal mol^{-1}) are provided in the insert.

As described in Scheme 5.10, the ketone-substituted cyclopropenes showed different reactivity and required a slight change in the catalyst structure and reaction conditions. In order to elucidate the origin of the reactivity difference, the complete catalytic cycle was also computed with the ketone-substituted cyclopropene **5_73** and the corresponding BIMP catalyst **5_62** (Figures 5.20 and 5.21). These extensive calculations revealed

that the deprotonation proceeds through **TS5_69**, and the enantioselective reprotonation proceeds through either **TS5_79** or **TS5_83**. Interestingly, the rate-determining step is not the deprotonation step as seen in the previous calculations with the ester group, and instead the reprotonation is now controlling the reaction rate. The preferred transition state leads to the experimentally observed chirality of (*S*) conformation at the α-position of the carbonyl group.

The complete potential energy surface is shown in Scheme 5.12. Initial complexation between the catalyst and the substrate gives an intermediate **Int5_3**, and the facile deprotonation at the γ position through **TS5_69** furnishes the enolate-protonated catalyst complex **Int5_4**. Since the following step has a higher energy barrier, this first step is reversible. Then, the rate-determining reprotonation preferably proceeds through **TS5_83** to obtain the isomerized product **5_75** with a chiral center at the three-membered ring.



Scheme 5.12. Computed reaction energy profile (ΔG in kcal mol^{-1}) for the 1,3-prototropic shift of ketone-substituted cyclopropenes.

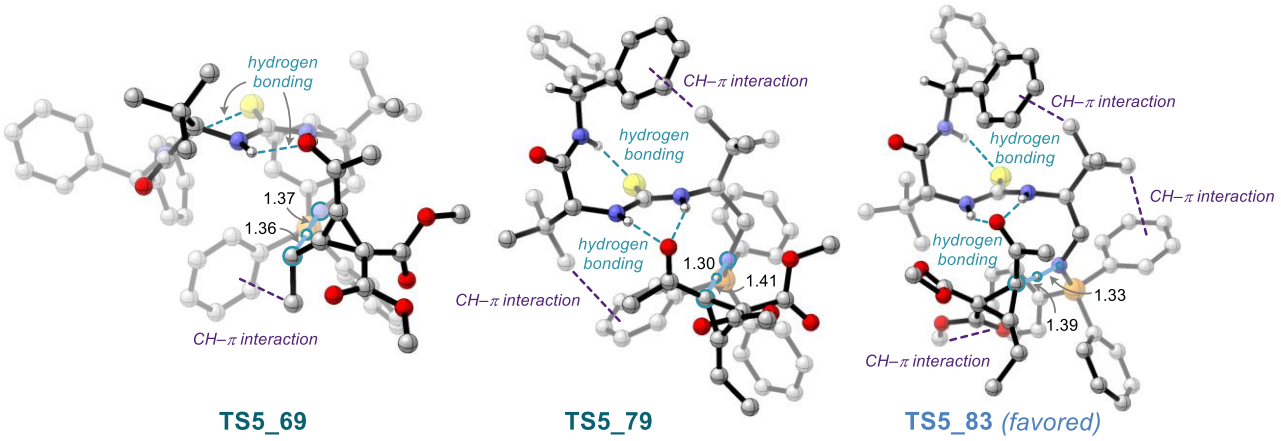
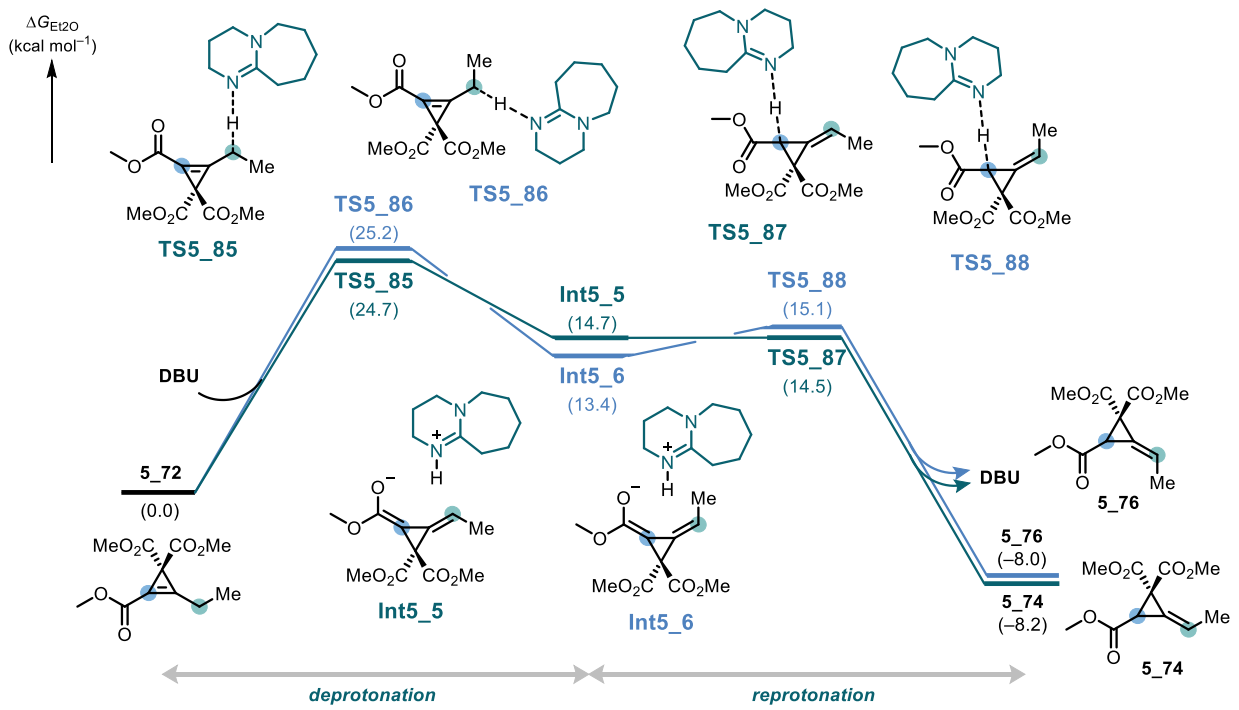


Figure 5.22. Transition state structure geometry of **TS5_69**, **TS5_79** and **TS5_83**. Forming and breaking bond lengths (Å) are provided in the insert.

5.5.5. Potential Energy Surfaces of DBU-Catalyzed 1,3-Prototropic Shift

One interesting experimental observation is that the BIMP catalyst is also controlling the diastereoselectivity at the forming C=C double bond. When the achiral base DBU was used, a 1:1 ratio of (*E*)- and (*Z*)-products were obtained. Therefore, the achiral pathway was also computed to support that the above computed enantioselective catalytic cycle is mechanistically correct (Scheme 5.13).

The initial deprotonation proceeds either through **TS5_85** or **TS5_86**, and the activation energy barrier is almost identical. The thermal stability of (*Z*)-enolate and (*E*)-enolate are also similar in **Int5_6** and **Int5_7**. The following reprotonation step is barrierless and the cyclopropane products **5_74** and **5_76** are rapidly formed with a large energy release. These results agree with the experimental fact that the DBU-catalyzed pathway is not diastereomerically selective due to the small energy difference ($\Delta\Delta G^{\ddagger}$ = 0.5 kcal mol^{-1}) in the rate-determining deprotonation process.



Scheme 5.13. Computed reaction energy profile (Δ*G* in kcal mol^{-1}) for the DBU-catalyzed 1,3-prototropic shift of ester-substituted cyclopropenes.

5.5.6. Relative pK_a Calculations

The primary difference in reactivity between the ester- and the ketone-substituted cyclopropenes was the rate-determining step. The initial deprotonation step has a higher energy barrier with the ester group, whereas the second reprotonation has a higher energy barrier with the ketone group. In order to rationalize these results, relative pK_a values were computed using methyl (*E*)-but-2-enoate **5_77** as the reference (pK_a = 20) (Figure 5.23).[27] The *α,β*-unsaturated butanoate has a higher pK_a value than the *β,γ*-unsaturated butanoate **5_80**, while the ester- and ketone-substituted cyclopropenes **5_78** and **5_79** have lower pK_a values than the corresponding cyclopropanes **5_81** and **5_82**, respectively. Changing the substituent from ester to ketone further lowers the pK_a values. These indicate that the ester-substituted cyclopropenes have the rate-determining step at the first stage because the *γ* position is relatively difficult to deprotonate, while the ketone-substituted

cyclopropenes have the rate-determining step at the second stage because the α position is relatively difficult to protonate.

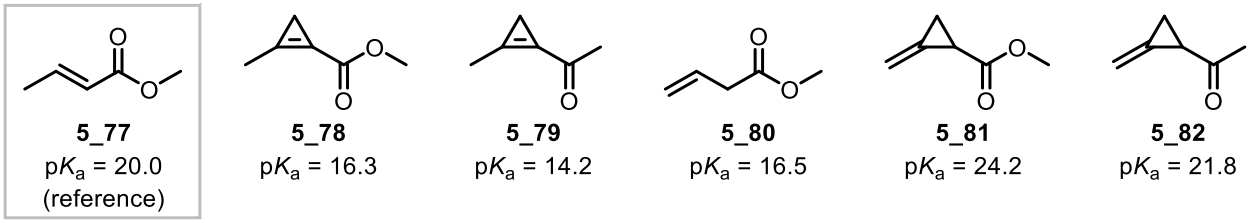


Figure 5.23. Relative pK_a values computed at COSMO(H_2O)-ZORA-M06-2X/TZ2P//COSMO(H_2O)-ZORA-BLYP-D3(BJ)/TZ2P level of theory.

5.5.7. Summary

In summary, a detailed mechanistic study of the enantioselective 1,3-prototropic shift of cyclopropenes was performed using density functional theory calculations. The reaction proceeds through a deprotonation-reprotonation sequence, and a conformational study on the enantioselectivity-determining reprotonation step explained the experimental trends with both ester- and ketone-substituted substrates. Analysis of the transition state structures proved that the existence of several non-covalent interactions is crucial for controlling the enantioselectivity. These computational studies show the potential for further development of novel organocatalytic reactions.

5.6. Conclusion

In conclusion, three computational mechanistic studies of enantioselective BIMP-catalyzed reactions using density functional theory calculations were described in this chapter. The intramolecular aza-Michael addition of urea-tethered α,β-unsaturated esters, the sulfa-Michael addition to unactivated α,β-unsaturated amides, and the 1,3-prototropic shift of cyclopropenes were computationally studied, and the enantioselectivities originated from the flexible nature of the BIMP catalysts that enables the formation of

stabilizing non-covalent interactions. These results strongly support the experimental data, and these insights into tunable BIMP catalysts can be used to further develop new transformations.

5.7. Thesis Summary and Future Direction

Over the course of the D.Phil. the development and mechanistic studies of a wide variety of novel organic reactions has been successfully achieved. Firstly, the methodology involving the iridium-catalyzed reductive functionalization of tertiary amides was applied for the synthesis of pyrrolidine derivatives in Chapter 2, and the experimentally observed diastereoselectivity was analyzed using the density functional theory. The detailed mechanism and the origin of the chemoselectivity were revealed using kinetic and computational analyses in Chapter 3, and the catalytic cycle was demonstrated to proceed via the nucleophilic attack of the amide to the activated silane. Then, the computational analysis of the distinct desymmetrization reactions for the synthesis of morphan cores and the enantioselective transformations with novel bifunctional organocatalysis were described in Chapter 4 and 5, respectively.

Throughout the projects, we developed and gained insights into various organic reactions, through the aid of kinetic, NMR, and computational studies. Future directions for the iridium-catalyzed reductive synthesis of azomethine ylide is to expand the methodology into other 1,3-dipoles and an enantioselective transformation. The conversion of an amide carbonyl carbon atom to a chiral sp^3-hybridized carbon atom is still challenging and requires more work to be done. In addition, the possibility of tunable chemoselectivity in the carbonyl reduction by designing ligands of the Vaska-type complexes has led to an inspiration to synthesize and perform further hydrosilylation reactions with novel iridium catalysts. The understanding of catalytic cycles and the chiral induction mechanisms of several reactions can be used to design both catalysts and substrates for related transformations. Furthermore, the insights from quantum mechanical analysis of reactions using flexible BIMP catalysts can be used to obtain the quantitative relationship of catalyst structures and the catalytic activity including enantioselectivity. We anticipate that the development of novel organic reactions and the

applications in the pharmaceutical, agrochemical, and fine chemical industries will continue with the knowledge obtained during the D.Phil. course and from around the world.

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Chapter 6

Experimental Details

6.1. General Experimental Details

Reagents and solvents were purchased at reagent-grade from Acros Organics, Sigma-Aldrich, Alfa Aeser, and Fluorochem and used without further purification unless stated. Solvents for extraction or column chromatography were of technical quality. All water used was purified via a Merck Millipore reverse osmosis purification system prior to use. All reactions were performed under N_2 atmosphere if not stated otherwise. Anhydrous solvents (toluene, dichloromethane, diethyl ether, dimethyl sulfoxide *N*,*N*-dimethyl formamide) were dried by filtration through activated alumina (Sigma-Aldrich, 58 Å pore size, powder 150 mesh, basic) columns and stored under N_2 atmosphere prior to use. Solvents were removed under reduced pressure using Büchi Rotavapor apparatus.

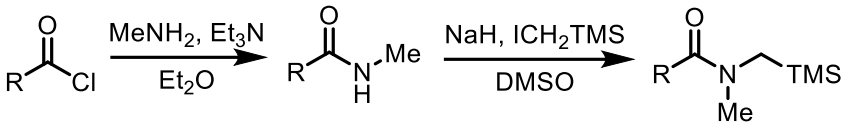
Thin-layer chromatography was performed on SiO_2-60 UV254 coated aluminium sheets from Merck (silica gel 60 F254). Visualization was achieved with a UV lamp at a wavelength of 254 nm, or with a $KMnO_4$ solution. **Flash column chromatography** was carried out on silica gel 60 (VWR, 40-63 μm). Solvents for extraction and chromatography were of technical quality. Solvent mixtures are individually reported in parenthesis. **Proton, Carbon, Fluorine, and Phosphorus nuclear magnetic resonance** (^{1}H, ^{13}C, ^{19}F, ^{31}P NMR) spectra were recorded on a Bruker AVIII HD (400, 101, 377, and 162 MHz) spectrometer at 25 °C. Chemical shifts (δ) are given in ppm, coupling constants (*J*) in Hz. The residual deuterated solvent was used as internal standard ($CDCl_3$: δ_H = 7.26 ppm). HSQC, COSY and HMBC experiments were used for ^{1}H and ^{13}C NMR signals assignment where required. **Melting points (m.p.)** were determined with a Leica Galen III Hot-stage melting point apparatus and microscope and on a Kofler hot block and are reported uncorrected. **Infrared (IR)** spectra were recorded on a Bruker Tensor 27 FT-IR spectrometer as a thin film. Selected absorption bands

are reported in wave numbers (cm^{-1}) with relative signal intensities described as s (strong), m (medium), or w (weak). When applicable, peak shape is characterized by br (broad). **High-resolution mass spectrometry (HR-MS-ESI)** was performed on a Bruker μTOF mass spectrometer. The molecular ion (M^+) is reported in m/z units.

6.2. Synthesis of Compounds in Chapter 2

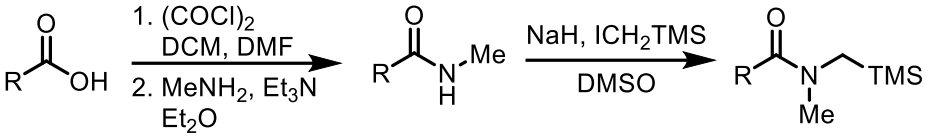
6.2.1. General Procedures

General procedure A for the synthesis of amides.



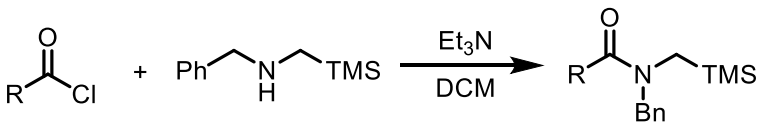
In a solution of triethylamine (8.3 mL, 60 mmol, 2.0 equiv.) in Et_2O (60 mL) under nitrogen atmosphere, acid chloride (30 mmol, 1.0 equiv.) was added dropwise at 0 °C. To the mixture was added methylamine solution 33 wt. % in EtOH (5.5 mL, 45 mmol, 1.5 equiv.) dropwise. The resulting mixture was allowed to warm to room temperature and stirred 1 h. Et_2O was added and the mixture was washed with 1M HCl, sat. aq. $NaHCO_3$ and brine. After drying over Na_2SO_4 and concentration under reduced pressure, the remaining crude was purified by flash column chromatography on silica gel to give *N*-methylamide. The amide (10 mmol, 1.0 equiv.) was added to a suspension of NaH (60 % w/w in mineral oil, 440 mg, 11 mmol, 1.1 equiv.) in DMSO (30 mL) at room temperature under nitrogen atmosphere. After 1.5 h, ICH_2TMS (1.5 mL, 10 mmol, 1.0 equiv.) was added and stirred at room temperature for 16 h. The reaction was then poured into water and extracted with Et_2O. The combined organic phase was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The crude was purified by flash column chromatography on silica gel.

General procedure B for the synthesis of amides.



To a stirred solution of a carboxylic acid (30 mmol, 1.0 equiv.) and DMF (10 drops) in DCM (20 mL), $(COCl)_2$ (3.0 mL, 36 mmol, 1.2 equiv.) was added dropwise. The solution was stirred at room temperature for 2 h. The solvent was then removed by evaporation under reduced pressure, and the resulting residue was dissolved in DCM (30 mL). After cooling the reaction mixture to 0 °C, to the mixture was added methylamine solution 33 wt. % in EtOH (5.5 mL, 45 mmol, 1.5 equiv.) dropwise. The resulting mixture was allowed to warm to room temperature and stirred 1 h. DCM was added and the mixture was washed with 1M HCl, sat. aq. $NaHCO_3$ and brine. After drying over Na_2SO_4 and concentration under reduced pressure, the remaining crude was purified by flash column chromatography on silica gel to give *N*-methylamide. The amide (10 mmol, 1.0 equiv.) was added to a suspension of NaH (60 % w/w in mineral oil, 440 mg, 11 mmol, 1.1 equiv.) in DMSO (30 mL) at room temperature under nitrogen atmosphere. After 1.5 h, ICH_2TMS (1.5 mL, 10 mmol, 1.0 equiv.) was added and stirred at room temperature for 16 h. The reaction was then poured into water and extracted with Et_2O. The combined organic phase was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The crude was purified by flash column chromatography on silica gel.

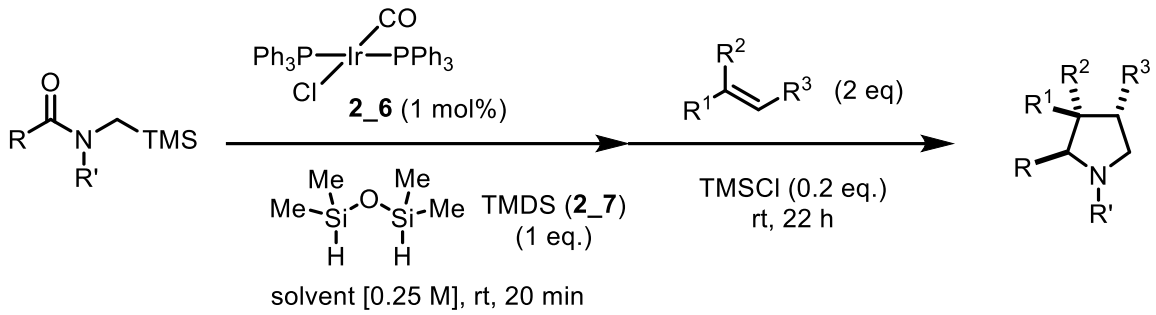
General procedure C for the synthesis of amides.



In a solution of triethylamine (0.14 mL, 2.0 mmol, 2.0 equiv.) in DCM (1.0 mL) under nitrogen atmosphere, acid chloride (1.0 mmol, 1.0 equiv.) was added dropwise at 0 °C. To the mixture was added *N*-[(Trimethylsilyl)methyl]benzylamine (0.19 mL, 1.0 mmol, 1.0 equiv.) dropwise. The resulting mixture was

allowed to warm to room temperature and stirred 1 h. DCM was added and the mixture was washed with 1M HCl, sat. aq. $NaHCO_3$ and brine. After drying over Na_2SO_4 and concentration under reduced pressure, the remaining crude was purified by flash column chromatography on silica gel to give the product.

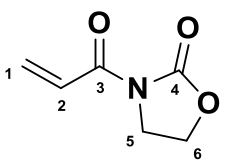
General procedure D for the [3+2] cycloaddition reactions.



To an oven-dried 5 ml round bottom flask was added an amide (0.25 mmol, 1.0 eq.), $IrCl(CO)(PPh_3)_2$ (2.0 mg, 0.0025 mmol, 0.01 eq.) and toluene (1.0 ml), followed by the addition of TMDS (44 μL, 0.25 mmol, 1.0 eq.). The mixture was stirred under nitrogen atmosphere at room temperature. After 20 min, dipolarophile (0.50 mmol, 2.0 eq.) and TMSCl (6.3 μL, 0.050 mmol, 0.2 eq.) were added and stirred at room temperature for 22 h. DCM was added and the mixture was washed with sat. aq. Na_2CO_3 and brine. After drying over Na_2SO_4 and concentration under reduced pressure, the remaining crude was purified by flash column chromatography on silica gel to give the product.

6.2.2. Synthesis and Characterization

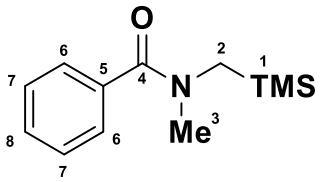
3-acryloyloxazolidin-2-one (**2_9**)



To a solution of oxazolidin-2-one (8.7 g, 100 mmol, 1.0 eq.), DMAP (1.2 g, 10 mmol, 0.10 eq.) and acrylic acid (10.3 ml, 150 mmol, 1.5 eq.) in dry DCM (100 ml) under N_2 atmosphere was added DCC (41.3 g, 200 mmol, 2.0 eq.) at 0 °C. The reaction was warmed up to room temperature and stirred overnight. DCM was added and the mixture was washed with sat. aq. $NaHCO_3$ and brine. After drying over Na_2SO_4 and concentration under reduced pressure, the remaining crude was purified by flash column chromatography on silica gel and recrystallized from EtOAc afforded the pure product (3.2 g, 23 %) as a white solid.

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.50 (dd, 1H *J* = 17.0, 10.5 Hz, C^2H), 6.56 (dd, 1H, *J* = 17.0, 1.8 Hz, C^1H), 5.90 (dd, 1H, *J* = 10.4, 1.8 Hz, C^1H), 4.44 (dd, 2H, *J* = 8.5, 7.5 Hz, C^6H_2), 4.09 (dd, 2H, *J* = 8.5, 7.5 Hz, C^5H_2) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 165.05 (C^3), 153.36 (C^4), 131.75 (C^2), 127.00 (C^1), 62.14 (C^6), 42.61 (C^5) ppm. Data is consistent with the reported literature.[1]

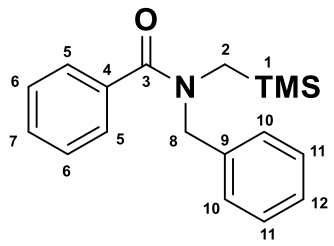
N-methyl-*N*-[(trimethylsilyl)methyl]benzamide (**2_5**)



Prepared following **General Procedure A** to afford the title compound as a pale yellow oil (1.6 g, 70%).

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.26 (bs, 5H, C^6H, C^7H, C^8H), 2.99 (s, 2H, C^2H_2), 2.85 (s, 3H, C^3H_3), 0.05 (s, 9H, C^1H_3) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 170.34 (C^4), 136.92 (C^5), 129.16 (C^8), 128.33 (C^7), 101.90 (C^6), 40.26 (C^3), -1.33 (C^1) ppm. Data is consistent with the published literature.[2]

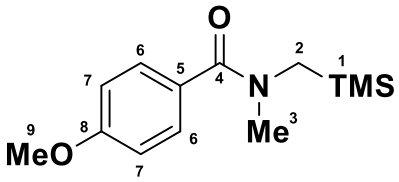
N-benzyl-*N*-((trimethylsilyl)methyl)benzamide (**2_11a**)



Prepared following **General Procedure C** to afford the title compound as a pale yellow oil (0.25 g, 84%), and as a 85(**A**):15(**B**) mixture of rotamers.

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.50-7.05 (m, 10H, C^5H, C^6H, C^7H, $C^{10}H$, $C^{11}H$, $C^{12}H$), 4.79 (s, 2H, C^8H_2 (**B**)), 4.50 (s, 2H, C^8H_2 (**A**)), 2.95 (s, 2H, C^2H_2 (**A**)), 2.86 (s, 2H, C^2H_2 (**B**)), 0.14 (s, 9H, C^1H_3 (**A**)), -0.01 (s, 9H, C^1H_3 (**B**)) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 170.34 (C^4), 136.92 (C^5), 129.16 (C^8), 128.33 (C^7), 101.90 (C^6), 40.26 (C^3), -1.33 (C^1) ppm. Data is consistent with the published literature.[2]

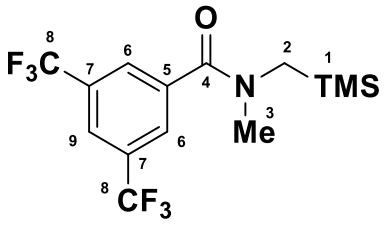
4-methoxy-*N*-methyl-*N*-((trimethylsilyl)methyl)benzamide (**2_12a**)



Prepared following **General Procedure A** to afford the title compound as a pale yellow solid (2.1 g, 83%).

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.38-7.30 (m, 2H, C^6H), 6.92-6.85 (m, 2H, C^7H), 3.82 (s, 3H, C^9H), 3.06 (s, 2H, C^2H_2), 3.00 (s, 3H, C^3H_3), 0.13 (s, 9H, C^1H_3) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 165.63 (C^4), 160.32 (C^9), 129.04 (C^5), 128.83 (C^6), 113.58 (C^7), 55.30 (C^9), 40.49 (C^2), 40.23 (C^3), -1.35 (C^1) ppm. **FT-IR** (thin film) ν_{max} 2953, 1608, 1482, 1394, 1246, 1172, 1029 cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{13}H_{22}NO_2Si^+$) requires m/z 252.1414, found m/z 252.1413. **m.p**.: 28-30 °C.

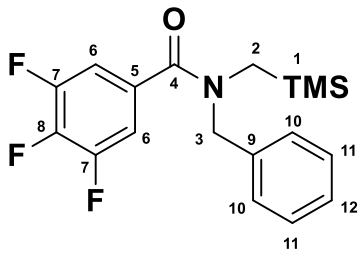
N-methyl-3,5-bis(trifluoromethyl)-*N*-((trimethylsilyl)methyl)benzamide (**2_13a**)



Prepared following **General Procedure A** to afford the title compound as a pale yellow oil (2.4 g, 68%), and as a 78(**A**):22(**B**) mixture of rotamers.

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.91 (s, 1H, C^9H), 7.82 (s, 2H, C^6H), 3.12 (s, 2H, C^2H_2), 2.97 (s, 3H, C^3H_3, (**A**), 2.82 (s, 3H, C^3H_3, (**B**), 0.18 (s, 9H, C^1H_3 (**A**)), 0.07 (s, 9H, C^1H_3, (**B**)) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 168.41 (C^4), 140.23 (C^5), 133.39 (q, J = 33.5 Hz, C^7), 128.64 (C^6), 125.05 (C^8), 122.96 (C^9), 41.95 (C^2), 41.44 (C^3), 0.00 (C^1) ppm. **^{19}F NMR** ($CDCl_3$, 377 MHz) δ_F: -63.02 ppm. **FT-IR** (thin film) ν_{max} 1636, 1366, 1277, 1129, 864 cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{14}H_{18}NOSi^+$) requires m/z 358.1056, found m/z 358.1054.

N-benzyl-3,4,5-trifluoro-*N*-((trimethylsilyl)methyl)benzamide (**2_14a**)

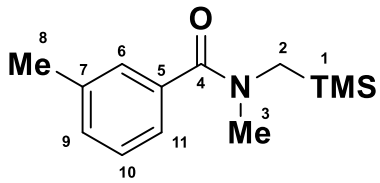


Prepared following **General Procedure C** to afford the title compound as a pale yellow oil (0.34 g, 98%), and as a 88(**A**):12(**B**) mixture of rotamers.

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.40-7.34 (m, 2H, ArH), 7.33-7.28 (m, 1H, ArH), 7.12 (d, J = 7.4 Hz, 2H, ArH), 7.08-7.01 (t, J = 6.8 Hz, 2H, ArH), 4.74 (s, 2H, C^3H_2, (**B**)), 4.48 (s, 2H, C^3H_2, (**A**)), 2.97 (s, 2H, C^2H_2,

(**A**)), 2.82 (s, 2H, C^2H_2, (**B**)), 0.13 (s, 9H, C^1H_3) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 169.02 (C^4), 152.33 (ddd, *J* = 253.0, 10.2, 3.7 Hz, C^7), 141.67 (dt, *J* = 255.1, 15.3 Hz, C^8), 137.12 (C^9), 133.65 – 133.32 (m, C^5), 130.25 (C^{11}), 129.17 (C^{12}), 127.80 (C^{10}), 113.55 – 111.99 (m, C^6), 56.26 (C^3), 39.25 (C^2), 0.00 (C^1) ppm. **^{19}F NMR** ($CDCl_3$, 377 MHz) δ_F: -132.50 (dd, *J* = 20.4, 7.3 Hz), -157.96 – -158.43 (m) ppm. **FT-IR** (thin film) ν_{max} 1626, 1451, 1247, 851 cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{18}H_{20}F_3NOSi^+$) requires m/z 351.1016, found m/z 351.1016.

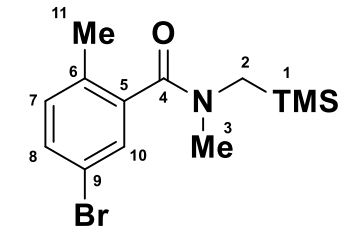
N,3-dimethyl-*N*-((trimethylsilyl)methyl)benzamide (**2_15a**)



Prepared following **General Procedure A** to afford the title compound as a pale yellow oil (0.93 g, 39%), and as a 80(**A**):20(**B**) mixture of rotamers.

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.30-7.10 (m, 4H, ArH), 3.09 (s, 2H, C^2H_2), 2.95 (s, 3H, C^3H_3 (**A**)), 2.89 (s, 3H, C^3H_3, (**B**)), 2.36 (s, 3H, C^8H_3), 0.16 (s, 9H, C^1H_3 (**A**)), 0.05 (s, 9H, C^1H_3 (**B**)) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 171.85 (C^4), 139.48 (C^7), 138.19 (C^5), 131.17 (C^9), 129.45 (C^{10}), 128.83 (C^6), 125.16 (C^{11}), 41.56 (C^3 or C^2), 41.34 (C^2 or C^3), 0.00 (C^1). **FT-IR** (thin film) ν_{max} 1624, 1393, 1247, 1074, 842 cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{13}H_{22}NOSi^+$) requires m/z 236.1465, found m/z 236.1465.

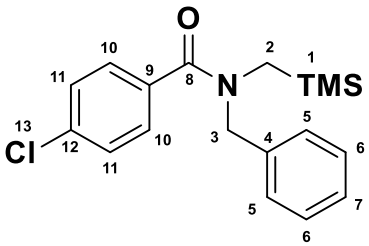
5-bromo-*N*,2-dimethyl-*N*-((trimethylsilyl)methyl)benzamide (**2_16a**)



Prepared following **General Procedure B** to afford the title compound as a white solid (2.1 g, 67%), and as a 87(**A**):13(**B**) mixture of rotamers.

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.36 (dd, *J* = 8.1, 2.0 Hz, 1H, C^8H), 7.29-7.21 (m, 1H, C^7H), 7.07 (d, *J* = 8.1 Hz, 1H, $C^{10}H$), 3.10 (s, 2H, C^2H_2), 2.82 (s, 3H, C^3H_3 (**A**)), 2.71 (s, 3H, C^3H_3 (**B**)), 2.23 (s, 3H, $C^{11}H_3$), 0.17 (s, 9H, C^1H_3 (**A**)), 0.05 (s, 9H, C^1H_3 (**B**)) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 169.74 (C^4), 140.30 (C^5), 134.31 (ArC), 133.29 (ArC), 132.79 (ArC), 130.42 (ArC), 130.28 (ArC), 130.04 (ArC), 129.47 (ArC), 101.55 (ArC), 120.72 (ArC), 43.73 (C^3, (**B**)), 40.72 (C^3, (**A**)), 40.22 (C^2, (**A**)), 36.02 (C^2, (**B**)), 19.89 (C^{11}), 0.00 (C^1, (**A**)), -0.25 (C^1, (**B**)) ppm. **FT-IR** (thin film) ν_{max} 2922, 1621, 1462, 1396, 1246, 840, 814 cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{13}H_{21}BrNOSi^+$) requires m/z 314.0570, 316.0550, found m/z314.0569, 316.0547. **m.p.**: 52-55 °C.

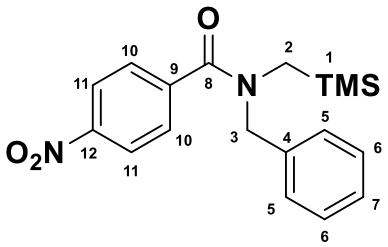
N-benzyl-4-chloro-*N*-((trimethylsilyl)methyl)benzamide (**2_17a**)



Prepared following **General Procedure C** to afford the title compound as a white solid (0.23 g, 97%), and as a 88(**A**):12(**B**) mixture of rotamers.

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.42-7.25 (m, 7H, ArH), 7.13 (d, *J* = 7.3 Hz, 2H, ArH), 4.77 (s, 2H, C^3H_2, (**B**)), 4.48 (s, 2H, C^3H_2, (**A**)), 2.96 (s, 2H, C^2H_2, (**A**)), 2.86 (s, 2H, C^2H_2, (**B**)), 0.13 (s, 9H, C^1H_3, (**A**)), 0.02 (s, 9H, C^1H_3, (**B**)) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 171.24 (C^8), 137.63 (ArC), 136.46 (ArC), 136.09 (ArC), 129.95 (ArC), 129.84 (ArC), 129.27 (ArC), 128.78 (ArC), 127.83 (ArC), 56.23 (C^3), 38.78 (C^2), 0.00 (C^1) ppm. **FT-IR** (thin film) ν_{max} 1627, 1452, 1436, 1397, 1247, 1089 cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{18}H_{23}ClNOSi^+$) requires m/z 332.1232, found m/z 332.1233. **m.p.**: 47-48 °C.

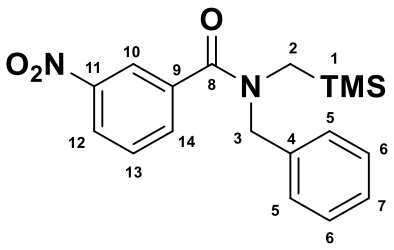
N-benzyl-4-nitro-*N*-((trimethylsilyl)methyl)benzamide (**2_18a**)



Prepared following **General Procedure C** to afford the title compound as a yellow oil (0.21 g, 44%), and as a 87(**A**):13(**B**) mixture of rotamers.

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 8.25-8.18 (m, 2H, $C^{11}H$), 7.61-7.52 (m, 2H, C^{10}), 7.42-7.28 (m, 3H, ArH), 7.12 (d, *J* = 7.3 Hz, 2H, ArH), 4.79 (s, 2H, C^3H_2, (**B**)), 4.43 (s, 2H, C^3H_2, (**A**)), 3.02 (s, 2H, C^2H_2, (**A**)), 2.78 (s, 2H, C^2H_2, (**B**)), 0.16 (s, 9H, C^1H_3, (**A**)), 0.02 (s, 9H, C^1H_3, (**B**)) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 170.01 (C^8), 149.31 (C^{12}), 144.01 (C^9), 137.06 (C^4), 130.17 (C^6), 129.10 (C^5), 128.81 (C^7), 127.75 (C^{10}), 125.01 (C^{11}), 56.04 (C^3), 38.99 (C^2), 0.00 (C^1) ppm. **FT-IR** (thin film) ν_{max} 1713, 1525, 1489, 1443, 1294, 1244, 1209, 1066 cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{18}H_{23}N_2O_3Si^+$) requires m/z 343.1473, found m/z 343.1475.

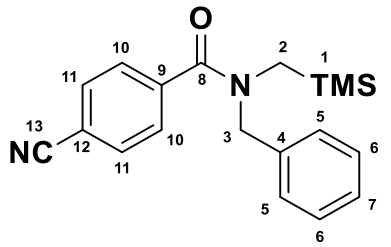
N-benzyl-3-nitro-*N*-((trimethylsilyl)methyl)benzamide (**2_19a**)



Prepared following **General Procedure C** to afford the title compound as a white solid (0.21 g, 44%), and as a 87(**A**):13(**B**) mixture of rotamers.

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 8.33-8.18 (m, 2H, C^{10}, C^{12}), 7.72 (d, *J* = 7.6 Hz, 1H, $C^{14}H$), 7.55 (t, *J* = 7.9 Hz, 1H, $C^{13}H$), 7.42-7.28 (m, 3H, ArH), 7.13 (d, *J* = 7.4 Hz, 2H, $C^{5}H$), 4.79 (s, 3H, $C^{3}H_2$, (**B**)), 4.47 (s, 3H, $C^{3}H_2$, (**A**)), 3.02 (s, 3H, $C^{2}H_2$, (**A**)), 2.82 (s, 3H, $C^{2}H_2$, (**B**)), 0.16 (s, 9H, $C^{1}H_3$, (**A**)), 0.04 (s, 9H, $C^{1}H_3$, (**B**)) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 169.38 (C^{8}), 149.23 (C^{11}), 139.41 (C^{9}), 137.13 (C^{4}), 133.67 (C^{14}), 130.84 (ArH), 130.15 (ArH), 129.09 (ArH), 127.78 (ArH), 125.26 (ArH), 123.11 (ArH), 56.26 (C^{3}), 39.17 (C^{2}), 0.00 (C^{1}) ppm. **FT-IR** (thin film) ν_{max} 1626, 1526, 1351, 1243, 842 cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{18}H_{23}N_2O_3Si^+$) requires m/z 343.1473, found m/z 343.1475. **m.p.**: 48-52 °C.

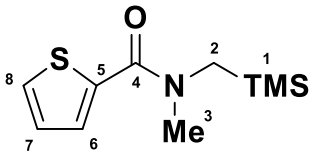
N-benzyl-4-cyano-*N*-((trimethylsilyl)methyl)benzamide (**2_20a**)



Prepared following **General Procedure C** to afford the title compound as a clear oil (0.36 g, 84%), and as a 86(**A**):14(**B**) mixture of rotamers.

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.64 (d, *J* = 8.0 Hz, 2H, $C^{10}H$), 7.49 (d, *J* = 8.1 Hz, 2H, $C^{11}H$), 7.41-7.27 (m, 3H, ArH), 7.11 (d, *J* = 7.3 Hz, 2H, ArH), 4.77 (s, 2H, $C^{3}H_2$, (**B**)), 4.42 (s, 2H, $C^{3}H_2$, (**A**)), 2.99 (s, 2H, $C^{2}H_2$, (**A**)), 2.77 (s, 2H, $C^{2}H_2$, (**B**)), 0.14 (s, 9H, $C^{1}H_3$, (**A**)), 0.01 (s, 9H, $C^{1}H_3$, (**B**)) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 170.24 (C^{8}), 142.21 (C^{9}), 137.18 (C^{4}), 133.52 (C^{11}), 130.11 (ArC), 129.04 (ArC), 128.52 (ArC), 127.79 (ArC), 119.21 (C^{13}), 114.33 (C^{12}), 56.08 (C^{3}), 38.95 (C^{2}), 0.00 (C^{1}) ppm. **FT-IR** (thin film) ν_{max} 1626, 1451, 1247, 851 cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{19}H_{23}N_2OSi^+$) requires m/z 323.1574, found m/z 323.1573.

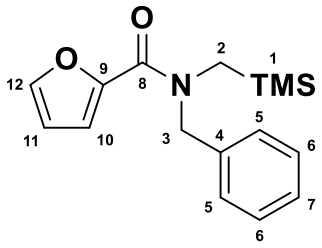
N-methyl-*N*-((trimethylsilyl)methyl)thiophene-2-carboxamide (**2_21a**)



Prepared following **General Procedure B** to afford the title compound as a yellow oil (1.5 g, 66%).

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.41 (dd, *J* = 5.1, 1.1 Hz, 1H, $C^{6}H$), 7.31 (dd, *J* = 3.7, 1.1 Hz, 1H, $C^{8}H$), 7.03 (dd, *J* = 5.0, 3.7 Hz, 1H, $C^{7}H$), 3.21 (s, 3H, $C^{3}H_3$), 3.12 (s, 2H, $C^{2}H_2$), 0.13 (s, 9H, $C^{1}H_3$). **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 172.40 (C^{4}), 139.62 (C^{5}), 130.06 (ArC), 129.65 (ArC), 127.98 (ArC), 43.06 (C^{2}), 41.55 (C^{3}), 0.00 (C^{1}) ppm. **FT-IR** (thin film) ν_{max} 1606, 1525, 1393, 1247, 841 cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{10}H_{18}NOSSi^+$) requires m/z 228.0873, found m/z 228.0875.

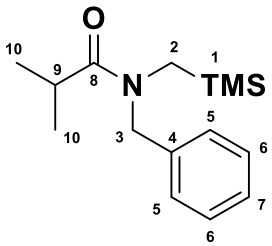
N-benzyl-*N*-((trimethylsilyl)methyl)furan-2-carboxamide (**2_22a**)



Prepared following **General Procedure C** to afford the title compound as a yellow oil (0.26 g, 89%), and as a 77(**A**):23(**B**) mixture of rotamers.

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.36 (s, 1H, $C^{12}H$), 7.32-7.11 (m, 5H, $C^{5}H$, $C^{6}H$ and $C^{7}H$), 6.84 (s, 1H, $C^{10}H$), 6.36 (s, 1H, $C^{11}H$), 4.74 (s, 2H, $C^{3}H_2$), 3.11 (s, 2H, $C^{2}H_2$ (**B**)), 2.85 (s, 2H, $C^{2}H_2$ (**A**)), 0.00 (s, 9H, $C^{1}H_3$) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 160.84 (C^{8}), 149.20 (C^{9}), 144.66 (C^{12}), 138.16 (C^{4}), 129.86 (ArC), 128.66 (ArC), 128.26 (ArC), 116.57 (C^{10}), 112.36 (C^{11}), 55.37 (C^{3}), 40.22 (C^{2}), 0.00 (C^{1}) ppm. **FT-IR** (thin film) ν_{max} 1614, 1489, 1436, 1247, 843 cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{16}H_{22}NO_2Si^+$) requires m/z 288.1414, found m/z 288.1415.

N-benzyl-*N*-((trimethylsilyl)methyl)isobutyramide (**2_23a**)

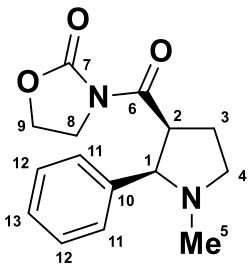


Prepared following **General Procedure C** to afford the title compound as a white solid (0.10 g, 81%), and as a 75(**A**):25(**B**) mixture of rotamers.

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.39-7.24 (m, 3H, ArH), 7.20-7.12 (m, 2H, ArH), 4.59 (s, 2H, $C^{3}H_2$, (**B**)), 4.54 (s, 2H, $C^{3}H_2$, (**A**)), 2.85 (s, 2H, $C^{2}H_2$), 2.84-2.74 (m, 1H, $C^{9}H$), 1.18 (d, J = 6.7 Hz, 2H, (**B**)), 1.13 (d, J =

6.7 Hz, 2H, (**A**)), 0.11 (s, 9H, C^1H_3, (**B**)), 0.06 (s, 9H, C^1H_3, (**A**)) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 177.64 (C^8), 138.99 (C^4), 138.37 (C^4), 130.04 (ArC), 129.73 (ArC), 129.02 (ArC), 128.70 (ArC), 128.36 (ArC), 127.48 (ArC), 54.42 (C^3, (**A**)), 51.14 (C^3, (**B**)), 39.91 (C^2, (**A**)), 39.05 (C^2, (**B**)), 31.50 (C^9, (**B**)), 31.33 (C^9, (**A**)), 21.06 (C^{10}, (**A**)), 20.52 (C^{10}, (**B**)), 0.00 (C^1, (**A**)), -0.38 (C^1, (**B**)) ppm. **FT-IR** (thin film) ν_{max} 1625, 1435, 1248, 1218, 845cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{15}H_{26}NOSi^+$) requires m/z 264.1778, found m/z 264.1779. **m.p.**: 30-32 °C.

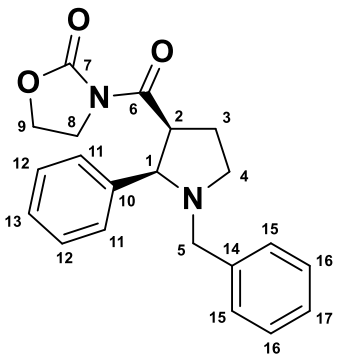
cis-3-(1-methyl-2-phenylpyrrolidine-3-carbonyl)oxazolidin-2-one (**2_10**)



Prepared following **General Procedure D** to afford the title compound as a white solid (65.6 mg, 85%). Crude dr = 7.7:1.

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.36-7.20 (m, 5H, ArH), 4.68 (ddd, *J* = 10.0, 8.8, 7.9 Hz, 1H, C^2H), 4.04 (ddd, *J* = 9.1, 8.2, 5.2 Hz, 1H, C^9H_a), 3.70-3.49 (m, 3H, C^1H, C^9H_b and C^8H), 3.30 (8.7, 7.4, 0.9 Hz, 1H, C^4H_a), 3.01 (ddd, *J* = 10.2, 8.8, 5.2 Hz, 1H, C^8H_b), 2.65 (ddt, *J* = 12.4, 11.3, 7.7 Hz, 1H, C^3H_a), 2.37 (ddd, *J* = 11.2, 8.8, 6.5 Hz, 1H, C^4H_b), 2.17 (s, 3H, C^5H_3), 1.91 (dddd, *J* = 12.3, 8.9, 6.6, 1.1 Hz, 1H, C^3H_b) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 172.97 (C^6), 153.00 (C^7), 139.39 (C^{10}), 128.56 (ArC), 127.87 (ArC), 127.58 (ArC), 73.20 (C^1), 61.66 (C^9), 56.06 (C^4), 47.88 (C^2), 42.64 (C^8), 40.23 (C^5), 25.41 (C^3) ppm. **FT-IR** (thin film) ν_{max} 1769, 1693, 1382, 1251, 1220, 1196, 1109, 753cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{15}H_{19}N_2O_3^+$) requires m/z 275.1390, found m/z 275.1390. **m.p.**: 118-120 °C.

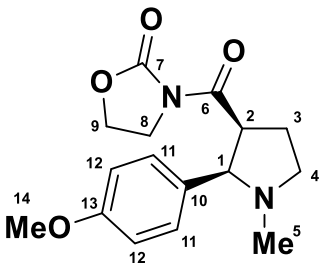
cis-3-(1-benzyl-2-phenylpyrrolidine-3-carbonyl)oxazolidin-2-one (**2_11**)



Prepared following **General Procedure D** to afford the title compound as a clear oil (71.8 mg, 82%). Crude dr = >20:1.

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.48-7.38 (m, 2H, ArH), 7.35-7.17 (m, 8H, ArH), 4.66 (dt, *J* = 10.3, 8.6 Hz, 1H, C^2H), 4.09-4.01 (m, 1H, C^9H_a), 3.93 (d, *J* = 10.2 Hz, 1H, C^1H), 3.79 (d, *J* = 13.3 Hz, 1H, C^5H_a), 3.70-3.55 (m, 2H, C^9H_b, C^8H_a), 3.17 (t, *J* = 8.2 Hz, 1H, C^4H_a), 3.11 (d, *J* = 13.3 Hz, 1H, C^5H_b), 3.04-2.94 (m, 1H, C^8H_b), 2.61 (tt, *J* = 11.8, 7.9 Hz, 1H, C^3H_a), 2.27 (ddd, *J* = 11.2, 8.7, 6.3 Hz, 1H, C^4H_b), 1.93-1.78 (m, 1H, C^3H_b) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 153.06 (C^6), 128.87 (ArC), 128.62 (ArC), 128.09 (ArC), 127.93 (ArC), 127.65 (ArC), 101.78 (ArC), 70.68 (C^1), 61.68 (C^9), 57.33 (C^5), 52.28 (C^4), 47.60 (C^2), 42.62 (C^8), 25.27 (C^3) ppm. **FT-IR** (thin film) ν_{max} 1769, 1694, 1384, 1220, 1038, 700cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{21}H_{23}N_2O_3^+$) requires m/z 351.1703, found m/z 351.1700.

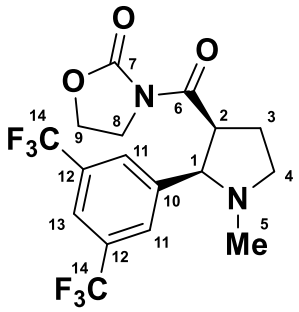
cis-3-(2-(4-methoxyphenyl)-1-methylpyrrolidine-3-carbonyl)oxazolidin-2-one (**2_12**)



Prepared following **General Procedure D** to afford the title compound as a white solid (65.6 mg, 86%). Crude dr = 6.3:1.

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.22-7.16 (m, 2H, $C^{11}H$), 6.83-6.77 (m, 2H, $C^{12}H$), 4.61 (dt, *J* = 9.9, 8.3 Hz, 1H, C^2H), 4.11-4.01 (m, 1H, C^9H_a), 3.76 (s, 3H, $C^{14}H_3$), 3.70-3.57 (m, 2H, C^8H_a, C^9H_b), 3.52 (d, *J* = 10.0 Hz, 1H, C^1H), 3.26 (t, *J* = 8.2 Hz, 1H, C^4H_a), 3.14-3.04 (m, 1H, C^8H_b), 2.61 (ddt, *J* = 12.3, 11.3, 7.7 Hz, 1H, C^3H_a), 2.32 (ddd, *J* = 11.4, 8.8, 6.5 Hz, 1H, C^4H_b), 2.13 (s, 3H, C^5H_3), 1.86 (dddd, *J* = 12.4, 8.8, 6.5, 1.0 Hz, 1H, C^3H_b) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 173.10 (C^6), 159.12 (C^{13}), 153.03 (C^7), 131.28 (C^{10}), 129.61 (C^{11}), 113.17 (C^{12}), 72.54 (C^1), 61.71 (C^9), 55.96 (C^4), 55.30 (C^{14}), 47.69 (C^2), 42.71 (C^8), 40.16 (C^5), 25.37 (C^3) ppm. **FT-IR** (thin film) ν_{max} 1759, 1694, 1387, 1240, 1219, 1023 831cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{16}H_{21}N_2O_4^+$) requires m/z 305.1496, found m/z 305.1494. **m.p.**: 80-85 °C.

cis-3-(2-(3,5-bis(trifluoromethyl)phenyl)-1-methylpyrrolidine-3-carbonyl)oxazolidin-2-one (**2_13**)

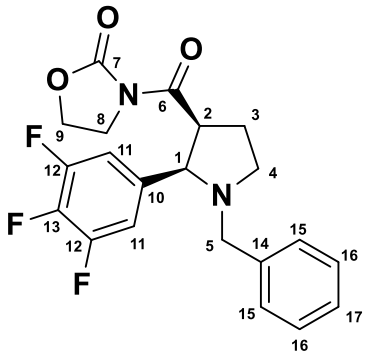


Prepared following **General Procedure D** to afford the title compound as a white solid (65.3 mg, 64%). Crude dr = 11.1:1.

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.80 (s, 2H, $C^{11}H$), 7.76 (s, 1H, $C^{13}H$), 4.67 (dt, *J* = 10.1, 8.4 Hz, 1H, C^2H), 4.14 (td, *J* = 8.7, 6.3 Hz, 1H, C^9H_a), 3.80 (d, *J* = 9.9 Hz, 1H, C^1H), 3.78-3.65 (m, 2H, C^9H_b, C^8H_a), 3.33 (t, *J* = 8.1 Hz, 1H, C^4H_a), 3.02 (ddd, *J* = 10.9, 8.8, 6.3 Hz, 1H, C^8H_b), 2.63 (dddd, *J* = 12.2, 11.2, 8.3, 7.4 Hz, 1H, C^3H_a), 2.46 (ddd, *J* = 11.2, 8.8, 6.3 Hz, 1H, C^4H_b), 2.19 (s, 3H, C^5H_3), 1.93 (dddd, *J* = 12.3, 8.6, 6.3, 1.1 Hz, 1H, C^3H_b) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 171.91 (C^6), 152.93 (C^7), 142.96 (C^{10}), 131.21 (q, *J* = 33.4

Hz, C^{12}), 128.88 (d, *J* = 3.8 Hz, C^{11}), 123.24 (q, *J* = 272.8 Hz, C^{14}), 121.55-121.21 (m, C^{13}), 71.75 (C^1), 61.67 (C^9), 55.84 (C^4), 48.32 (C^2), 42.29 (C^8), 40.13 (C^5), 26.01 (C^3) ppm. **^{19}F NMR** ($CDCl_3$, 377 MHz) δ_F: -62.81 ppm. **FT-IR** (thin film) ν_{max} 1768, 1686, 1390, 1256, 1123, 1007 cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{17}H_{17}F_6N_2O_3^+$) requires m/z 411.1138, found m/z 411.1135. **m.p.**: 40-44 °C.

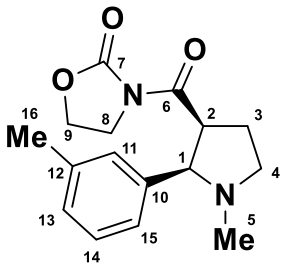
cis-3-(1-benzyl-2-(3,4,5-trifluorophenyl)pyrrolidine-3-carbonyl)oxazolidin-2-one (**2_14**)



Prepared following **General Procedure D** to afford the title compound as a pale yellow oil (62.8 mg, 62%). Crude dr = >20:1.

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.33-7.24 (m, 2H, ArH), 7.25-7.19 (m, 3H, ArH), 7.09 (dd, *J* = 8.8, 6.7 Hz, 2H, $C^{11}H$), 4.56 (ddd, *J* = 10.4, 9.5, 8.2 Hz, 1H, C^1H), 4.24 (td, *J* = 9.1, 6.7 Hz, 1H, C^9H_a), 4.04 (td, *J* = 9.1, 6.9 Hz, 1H, C^9H_b), 3.96 (d, *J* = 10.4 Hz, 1H, C^2H), 3.81 (ddd, *J* = 11.1, 9.3, 6.9 Hz, 1H, C^8H_a), 3.70 (d, *J* = 13.1 Hz, 1H, C^5H_a), 3.35-3.11 (m, 3H, C^8H_b, C^5H_b, C^4H_a), 2.64-2.47 (m, 1H, C^3H), 2.41-2.30 (m, 1H, C^4H_b), 1.92-1.79 (m, 1H, C^3H_b) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 171.76 (C^6), 153.16 (C^7), 150.63 (ddd, *J* = 249.7, 9.8, 3.7 Hz, C^{12}), 138.26 (C^{10}), 137.06 (bs, C^{13}), 128.62 (C^{15}), 128.25 (C^{16}), 127.12 (C^{17}), 11012 (d, *J* = 20.7 Hz, C^{11}), 68.90 (C^2), 61.92 (C^9), 57.62 (C^5), 52.21 (C^4), 47.90 (C^1), 42.53 (C^8), 26.03 (C^3) ppm. **^{19}F NMR** ($CDCl_3$, 377 MHz) δ_F: -134.19 (dd, *J* = 20.7, 9.2 Hz), -160.95 (dt, *J* = 20.8, 6.9 Hz) ppm. **FT-IR** (thin film) ν_{max} 1776, 1698, 1387, 1010, 1223 cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{21}H_{19}F_3N_2O_3^+$) requires m/z 404.1348, found m/z 404.1348.

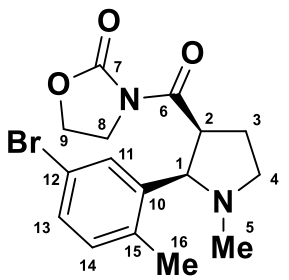
cis-3-(1-methyl-2-(m-tolyl)pyrrolidine-3-carbonyl)oxazolidin-2-one (**2_15**)



Prepared following **General Procedure D** to afford the title compound as a pale yellow oil (62.4 mg, 87%). Crude dr = 4.9:1.

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.15 (t, *J* = 7.4 Hz, 1H, $C^{14}H$), 7.11-7.00 (m, 3H, $C^{11}H$, $C^{13}H$, $C^{15}H$), 4.67 (ddd, *J* = 10.0, 8.8, 7.8 Hz, 1H, $C^{2}H$), 4.03 (ddd, *J* = 9.3, 8.3, 5.0 Hz, 1H, $C^{9}H_a$), 3.62 (dt, *J* = 10.4, 8.7 Hz, 1H, $C^{8}H_a$), 3.56-3.44 (m, 2H, $C^{1}H$, $C^{9}H_b$), 3.29 (ddd, *J* = 8.7, 7.5, 1.0 Hz, 1H, $C^{4}H_a$), 2.98 (ddd, *J* = 10.4, 8.9, 5.0 Hz, 1H, $C^{8}H_b$), 2.63 (ddt, *J* = 12.4, 11.3, 7.7 Hz, 1H, $C^{3}H_a$), 2.34 (ddd, *J* = 11.2, 8.8, 6.6 Hz, 1H, $C^{4}H_b$), 2.30 (s, 3H, $C^{16}H_3$), 2.16 (s, 3H, $C^{5}H_3$), 1.89 (dddd, *J* = 12.3, 8.8, 6.6, 1.0 Hz, 1H, $C^{3}H_b$) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 173.03 (C^{6}), 153.04 (C^{7}), 139.29 (C^{10}), 137.47 (C^{12}), 129.08 (ArC), 128.21 (ArC), 127.82 (C^{14}), 125.65 (ArC), 73.24 (C^{1}), 61.66 (C^{9}), 56.08 (C^{4}), 47.86 (C^{2}), 42.68 (C^{8}), 40.29 (C^{5}), 25.32 (C^{3}), 21.22 (C^{16}) ppm. **FT-IR** (thin film) ν_{max} 1780, 1699, 1388, 1259 cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{16}H_{21}N_2O_3^+$) requires m/z 289.1547, found m/z 289.1547.

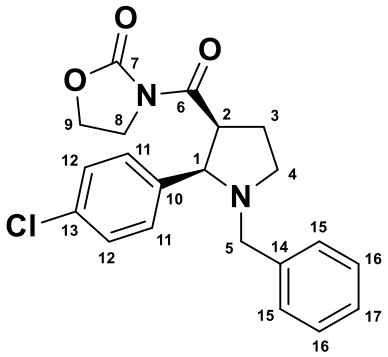
cis-3-(2-(5-bromo-2-methylphenyl)-1-methylpyrrolidine-3-carbonyl)oxazolidin-2-one (**2_16**)



Prepared following **General Procedure D** to afford the title compound as a pale yellow oil (48.0 mg, 52%). Crude dr = >20:1.

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.45 (d, *J* = 2.2 Hz, 1H, $C^{11}H$), 7.25 (dd, *J* = 8.0, 2.4 Hz, 1H, $C^{13}H$), 7.00 (d, *J* = 8.1 Hz, 1H, $C^{14}H$), 4.72 (td, *J* = 8.8, 5.1 Hz, 1H, $C^{9}H_a$), 4.10 (m, 1H, $C^{8}H_a$), 3.79-3.68 (m, 2H, $C^{1}H$, $C^{9}H_b$), 3.62 (q, *J* = 8.7 Hz, 1H, $C^{8}H_b$), 3.43-3.33 (m, 2H, $C^{4}H_a$), 2.59 (dddd, *J* = 12.7, 9.6, 8.3, 5.2 Hz, 1H, $C^{3}H_a$), 2.39-2.29 (m, 4H, $C^{16}H_3$, $C^{4}H_b$), 2.11 (s, 3H, $C^{5}H_3$), 1.98 (dtd, *J* = 12.7, 8.6, 2.0 Hz, 1H, $C^{3}H_b$) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 172.29 (C^{9}), 152.00 (C^{8}), 138.15 (C^{10}), 135.66 (C^{15}), 131.06 (C^{11}), 129.35 (C^{14}), 128.94 (C^{13}), 118.30 (C^{12}), 68.26 (C^{1}), 60.85 (C^{9}), 54.72 (C^{4}), 45.53 (C^{2}), 41.84 (C^{8}), 39.10 (C^{5}), 24.04 (C^{3}), 17.88 (C^{16}) ppm. **FT-IR** (thin film) ν_{max} 1774, 1697, 1386, 1258, 1222, 1039 cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{16}H_{20}BrN_2O_3^+$) requires m/z 367.0652, 369.0632, found m/z 367.0653, 369.0633.

cis-3-(1-benzyl-2-(4-chlorophenyl)pyrrolidine-3-carbonyl)oxazolidin-2-one (**2_17**)

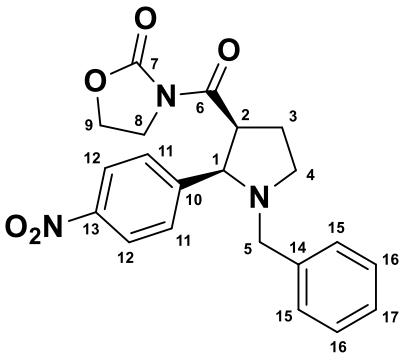


Prepared following **General Procedure D** to afford the title compound as a pale yellow oil (63.1 mg, 73%). Crude dr = >20:1.

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.43-7.35 (m, 2H, $C^{12}H$), 7.31-7.25 (m, 4H, ArH), 7.23 (d, *J* = 7.3 Hz, 3H, ArH), 4.63 (dt, *J* = 10.3, 8.6 Hz, 1H, $C^{2}H$), 4.14 (td, *J* = 8.3, 7.7, 5.8 Hz, 1H, $C^{9}H_a$), 3.94 (d, *J* = 10.3 Hz, 1H, $C^{1}H$), 3.82-3.66 (m, 3H, $C^{9}H_b$, $C^{8}H_a$, $C^{5}H_a$), 3.21-3.07 (m, 3H, $C^{8}H_b$, $C^{5}H_b$, $C^{4}H_a$), 2.60 (dddd, *J* = 12.3, 11.3, 8.6, 7.4 Hz, 1H, $C^{3}H_a$), 2.30 (ddd, *J* = 11.3, 8.8, 6.2 Hz, 1H, $C^{4}H_b$), 1.87 (dddd, *J* = 12.3, 8.6, 6.3, 1.1 Hz, 1H,

C^3H_b) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 172.50 (C^6), 153.05 (C^7), 138.67 (C^{10} or C^{14}), 138.57 (C^{10} or C^{14}), 133.33 (C^{13}), 130.26 (C^{12}), 128.59 (ArC), 128.14 (ArC), 128.03 (ArC), 101.90 (ArC), 69.84 (C^1), 61.77 (C^9), 57.35 (C^5), 52.28 (C^4), 47.68 (C^2), 42.63 (C^8), 25.46 (C^3) ppm. **FT-IR** (thin film) ν_{max} 1775, 1699, 1386, 1258, 1222 cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{21}H_{22}ClN_2O_3^+$) requires m/z 385.1313, found m/z 385.1313.

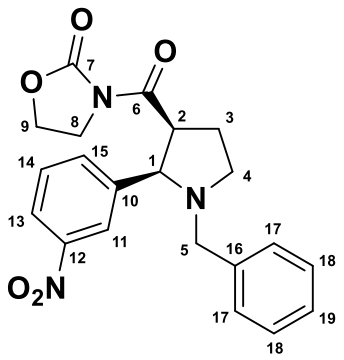
cis-3-(1-benzyl-2-(4-nitrophenyl)pyrrolidine-3-carbonyl)oxazolidin-2-one (**2_18**)



Prepared following **General Procedure D** to afford the title compound as a pale yellow oil (57.3 mg, 58%). Crude dr = >20:1.

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 8.18–8.10 (m, 2H, $C^{12}H$), 7.64-7.57 (m, 2H, $C^{11}H$), 7.30–7.14 (m, 5H, $C^{15}H$, $C^{16}H$, $C^{17}H$), 4.64 (ddd, *J* = 10.4, 9.2, 8.3 Hz, 1H, C^2H), 4.15 (td, *J* = 9.1, 6.6 Hz, 1H, C^9H_a), 4.12 (d, *J* = 10.4 Hz, 1H, C^1H) 3.85 (td, *J* = 9.0, 6.9 Hz, 1H, C^9H_b), 3.73 (ddd, *J* = 11.3, 9.4, 7.0 Hz, 1H, C^8H_a), 3.67 (d, *J* = 13.3. Hz, 1H, C^5H_a), 3.25 (d, *J* = 13.2 Hz, 1H, C^5H_b), 3.21 (d, *J* = 8.0 Hz, 1H, C^8H_b), 3.08 (ddd, *J* = 11.0, 9.2, 6.7 Hz, 1H, C^4H_a), 2.69–2.57 (m, 1H, C^3H_a), 2.39 (ddd, *J* = 11.6, 8.9, 6.0 Hz, 1H, C^4H_b), 1.91 (dddd, *J* = 12.3, 8.3, 6.0, 1.0 Hz, 1H, C^3H_b) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 171.8 (C^8), 153.0 (C^7), 148.2 (C^{10}), 147.5 (C^{13}), 138.2 (C^{14}), 129.9 (C^{11}), 128.6 (ArC), 128.2 (ArC), 127.1 (ArC), 123.0 (C^{12}), 69.6 (C^1), 61.8 (C^9), 57.8 (C^5), 52.56 (C^4), 48.2 (C^2), 42.4 (C^8), 26.2 (C^3) ppm. **FT-IR** (thin film) ν_{max} 1780, 1692, 1530, 1210 cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{21}H_{22}N_3O_5^+$) requires m/z 396.1554, found m/z 396.1555.

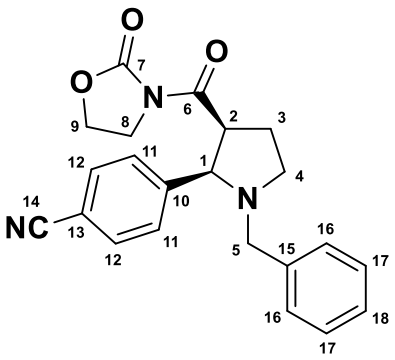
cis-3-(1-benzyl-2-(3-nitrophenyl)pyrrolidine-3-carbonyl)oxazolidin-2-one (**2_19**)



Prepared following **General Procedure D** to afford the title compound as a brown oil (53.1 mg, 54%). Crude dr = >20:1.

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 8.27 (t, *J* = 2.0 Hz, 1H, $C^{11}H$), 8.08 (ddd, *J* = 8.1, 2.3, 1.1 Hz, 1H, $C^{13}H$), 7.76 (dt, *J* = 7.7, 1.4 Hz, 1H, $C^{15}H$), 7.45 (t, *J* = 7.9 Hz, 1H, $C^{14}H$), 7.29-7.16 (m, 5H, ArH), 4.63 (ddd, *J* = 10.3, 9.3, 8.2 Hz, 1H, $C^{2}H$), 4.20-4.12 (m, 2H, $C^{1}H$, $C^{9}H_a$), 3.85 (td, *J* = 9.0, 7.0 Hz, 1H, $C^{9}H_b$), 3.76-3.67 (m, 2H, $C^{5}H_a$, $C^{8}H_a$), 3.30 (d, *J* = 13.2 Hz, 1H, $C^{5}H_b$), 3.23 (dd, *J* = 8.8, 7.1 Hz, 1H, $C^{4}H_a$), 3.07 (ddd, *J* = 11.0, 9.2, 6.6 Hz, 1H, $C^{8}H_b$), 2.63 (tdd, *J* = 12.0, 9.3, 7.2 Hz, 1H, $C^{3}H_a$), 2.41 (ddd, *J* = 11.5, 8.8, 5.9 Hz, 1H, $C^{4}H_b$), 1.91 (dddd, *J* = 12.4, 8.2, 5.9, 1.0 Hz, 1H, $C^{3}H_b$) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 161.80 (C^{6}), 154.15 (C^{7}), 148.03 (C^{12}), 142.98 (C^{10}), 134.99 (C^{15}), 131.74 (ArC), 128.66 (C^{14}), 128.23 (ArC), 127.00 (ArC), 123.68 (C^{11}), 122.55 (C^{13}), 69.38 (C^{1}), 61.80 (C^{9}), 57.88 (C^{5}), 52.52 (C^{4}), 48.13 (C^{2}), 42.40 (C^{8}), 26.08 (C^{3}) ppm. **FT-IR** (thin film) ν_{max} 1774, 1696, 1529, 1338, 1351, 1224 cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{21}H_{22}N_3O_5^+$) requires m/z 396.1554, found m/z 396.1555.

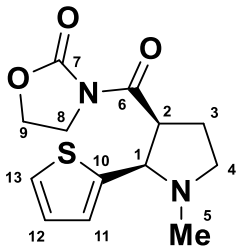
cis-4-(1-benzyl-3-(2-oxooxazolidine-3-carbonyl)pyrrolidin-2-yl)benzonitrile (**2_20**)



Prepared following **General Procedure D** to afford the title compound as a pale yellow oil (56.4 mg, 60%). Crude dr = >20:1.

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.62-7.52 (m, 4H, $C^{11}H$, $C^{12}H$), 7.30-7.16 (m, 5H, $C^{16}H$, $C^{17}H$, $C^{18}H$), 4.63 (dt, *J* = 10.4, 8.7 Hz, 1H, $C^{2}H$), 4.20-4.09 (m, 1H, $C^{9}H_a$), 4.05 (d, *J* = 10.4 Hz, 1H, $C^{1}H$), 3.84 (td, *J* = 9.0, 7.1 Hz, 1H, $C^{9}H_b$), 3.77-3.64 (m, 2H, $C^{8}H_a$, $C^{5}H_a$), 3.26-3.17 (m, 2H, $C^{5}H_b$, $C^{4}H_a$), 3.06 (ddd, *J* = 10.9, 9.2, 6.5 Hz, 1H, $C^{8}H_b$), 2.62 (tdd, *J* = 11.9, 9.0, 7.2 Hz, 1H, $C^{3}H_a$), 2.36 (ddd, *J* = 11.5, 8.9, 6.0 Hz, 1H, $C^{4}H_b$), 1.95-1.84 (m, 1H $C^{3}H_b$) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 131.60 (ArC), 129.79 (ArC), 128.60 (ArC), 128.22 (ArC), 69.94 (C^{1}), 61.79 (C^{9}), 57.68 (C^{5}), 52.51 (C^{4}), 48.10 (C^{2}), 42.43 (C^{8}), 25.98 (C^{3}) ppm. **FT-IR** (thin film) ν_{max} 1776, 1698, 1387, 1010, 1223 cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{22}H_{22}N_3O_3^+$) requires m/z 376.1656, found m/z 376.1654.

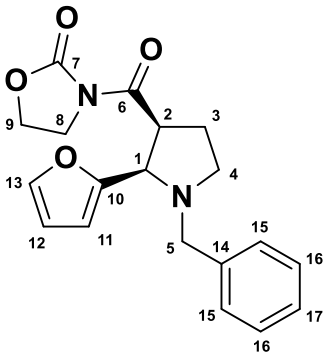
cis-3-(1-methyl-2-(thiophen-2-yl)pyrrolidine-3-carbonyl)oxazolidin-2-one (**2_21**)



Prepared following **General Procedure D** to afford the title compound as a white solid (44.2 mg, 63%). Crude dr = 7.1:1.

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.20 (ddd, *J* = 5.1, 1.3, 0.6 Hz, 1H, $C^{11}H$), 6.96 (td, *J* = 3.4, 0.8 Hz, 1H, $C^{13}H$), 6.91 (dd, *J* = 5.0, 3.5 Hz, 1H, $C^{12}H$), 4.61 (dt, *J* = 10.1, 8.6 Hz, 1H, $C^{2}H$), 4.16 (ddd, *J* = 9.1, 8.4, 5.6 Hz, 1H, $C^{9}H_a$), 4.01 (d, *J* = 10.1 Hz, 1H, $C^{1}H$), 3.86 (dt, *J* = 8.9, 8.1 Hz, 1H, $C^{9}H_b$), 3.75 (ddd, *J* = 10.8, 9.1, 7.9 Hz, 1H, $C^{8}H_a$), 3.34-3.22 (m, 2H, $C^{8}H_b$, $C^{4}H_a$), 2.66 (dddd, *J* = 12.3, 11.3, 8.5, 7.4 Hz, 1H, $C^{3}H_a$), 2.37 (ddd, *J* = 11.3, 9.0, 6.3 Hz, 1H, $C^{4}H_b$), 2.27 (s, 3H, $C^{5}H_3$), 1.88 (dddd, *J* = 12.4, 8.6, 6.3, 1.1 Hz, 1H, $C^{3}H_b$) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 172.43 (C^{6}), 153.28 (C^{7}), 144.37 (C^{10}), 101.15 (C^{11}), 125.90 (C^{12}), 125.21 (C^{13}), 67.96 (C^{1}), 61.94 (C^{9}), 55.74 (C^{4}), 48.13 (C^{2}), 42.91 (C^{8}), 40.52 (C^{5}), 25.30 (C^{3}) ppm. **FT-IR** (thin film) ν_{max} 1770, 1697, 1386, 1220, 1038, 701 cm^{-1}. HRMS (ES^+) exact mass calculated for $[M+H]^+$ ($C_{13}H_{17}N_2O_3S^+$) requires m/z 281.0954, found m/z 281.0951. **m.p.**: 95-100 °C.

cis-3-(1-benzyl-2-(furan-2-yl)pyrrolidine-3-carbonyl)oxazolidin-2-one (**2_22**)

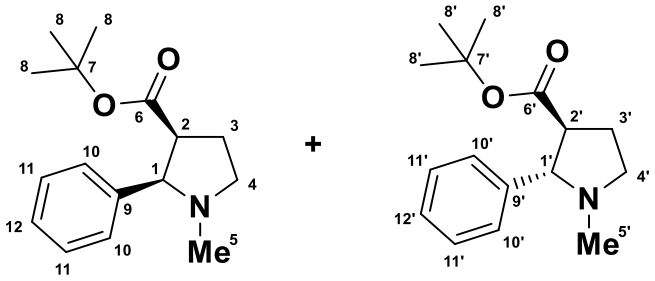


Prepared following **General Procedure D** to afford the title compound as a pale yellow oil (67.6 mg, 79%). Crude dr = 3.1:1.

^{1}H NMR ($CDCl_3$, 400 MHz) (for major isomer) δ_H: 7.43–7.18 (m, 6H, $C^{15}H$, $C^{16}H$, $C^{17}H$, $C^{13}H$), 6.36–6.27 (m, 2H, $C^{11}H$, $C^{12}H$), 4.55–4.44 (m, 1H, $C^{2}H$), 4.42-4.32 (m, 1H, $C^{9}H_a$), 4.29–4.19 (m, 1H, $C^{1}H$), 4.09–3.97 (m, 2H, $C^{9}H_b$, $C^{8}H_a$), 3.88–3.79 (m, 2H, $C^{5}H_a$), 3.47 (ddd, *J* = 10.8, 9.2, 5.6 Hz, 1H, $C^{8}H_b$), 3.35 (d, *J* = 13.4

Hz, 1H, C^5H_b), 3.11 (ddd, *J* = 8.9, 7.4, 1.6 Hz, 1H, C^4H_a), 2.63 (dddd, *J* = 12.3, 10.7, 9.1, 7.3 Hz, 1H, C^3H_b), 2.45–2.33 (m, 1H, C^4H_b), 1.87 (dddd, *J* = 12.1, 8.0, 6.0, 1.5 Hz, 1H, C^3H_b) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) (for major isomer) δ_C: 172.0 (C^6), 154.0 (C^7), 142.0 (C^{14}), 128.8 (ArC), 128.2 (ArC), 128.1 (ArC), 101.9 (ArC), 110.4 (C^{12}), 110.1 (C^{10}), 108.7 (C^{11}), 63.0 (C^1), 62.0 (C^9), 57.4 (C^6), 51.8 (C^4), 46.6 (C^2), 42.8 (C^8), 25.2 (C^3) ppm. **FT-IR** (thin film) ν_{max} 1777, 1699, 1387, 1224 cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{19}H_{21}N_2O_4^+$) requires m/z 341.1496, found m/z 341.1496.

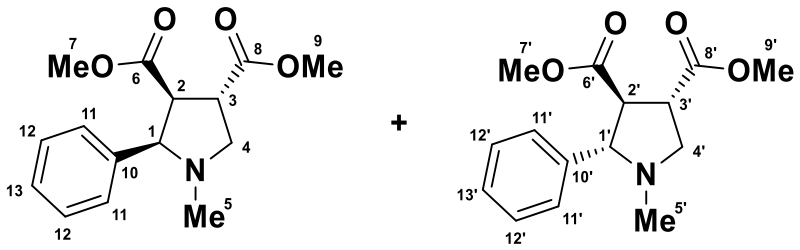
cis- and *trans-tert*-butyl 1-methyl-2-phenylpyrrolidine-3-carboxylate (**2_24**)



Prepared following **General Procedure D** to afford the inseparable mixtures of title compounds as a pale yellow oil (50.9 mg, 78%). Crude dr = 5.4:1.

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.33-7.13 (m, 6.8H, ArH), 3.45-3.38 (m, 1H, C^1H (**A**)), 3.25-3.00 (m, 2.5H), 2.78 (ddd, *J* = 10.8, 8.7, 5.5 Hz, 1H, C^2H (**B**)), 2.43-2.23 (m, 2H), 2.21-2.07 (m, 6H), 2.06-1.81 (m, 2H), 1.29 (s, 9H, C^8H_3 (**B**)), 0.90 (s, 2.2H, C^8H_3 (**A**)) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 173.79 (C^6 (**B**)), 141.32 (C^6 (**A**)), 128.92 (ArC), 128.48 (ArC), 128.35 (ArC), 127.95 (ArC), 127.84 (ArC), 127.54 (ArC), 127.47 (ArC), 127.22 (ArC), 80.43 (C^7 (**B**)), 79.81 (C^7 (**A**)), 74.78 (C^1 (**B**)), 72.97 (C^1 (**A**)), 56.13 (C^4 (**B**)), 56.03 (C^4 (**A**)), 53.42 (C^2 (**B**)), 50.25 (C^2 (**A**)), 40.51 (C^5 (**A**)), 40.16 (C^5 (**B**)), 28.01 (C^8 (**B**)), 27.43 (C^8 (**A**)), 27.12 (C^3 (**B**)), 26.98 (C^3 (**A**)). **FT-IR** (thin film) ν_{max} 1728, 1367, 1151 cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{16}H_{24}NO_2^+$) requires m/z 262.1802, found m/z 262.1802.

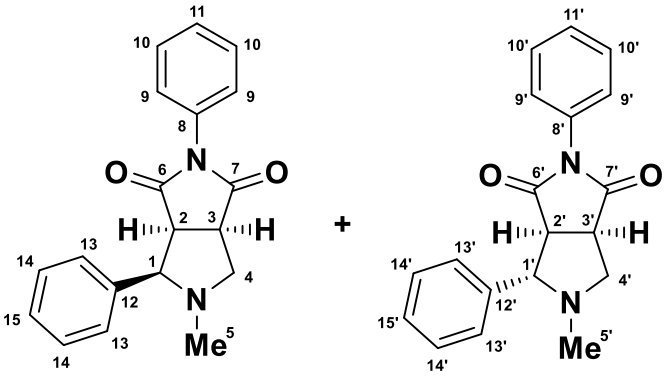
cis- and *trans*-dimethyl 1-methyl-2-phenylpyrrolidine-3,4-dicarboxylate (**2_25**)



Prepared following **General Procedure D** to afford the inseparable mixtures of title compounds as a colorless oil (87.7 mg, 79%). Crude dr = 1.2:1.

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.39-7.16 (m, 5H, ArH), 3.80-3.71 (m, 1H), 3.74 (s, 3H, C^7H_3, (**B**)), 3.69 (s, 3H, C^7H_3 (**A**)), 3.60 (s, 3H, C^9H_3, (**B**)), 3.63-3.44 (m, 5H), 3.33 (ddd, *J* = 8.8, 5.4, 1.9 Hz, 1H, C^4H_a, (**B**)), 3.25 (d, *J* = 8.8 Hz, 1H, (**B**)), 3.05 (s, 3H, C^9H_3, (**A**)), 2.66 (dd, *J* = 9.7, 8.7 Hz, 1H, C^4H_b, (**B**)), 2.49 (dd, *J* = 10.4, 9.0 Hz, 1H, C^4H_b, (**A**)), 2.16 (s, 3H, C^5H_3, (**A**)), 2.08 (s, 3H, C^5H_3, (**B**)) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 173.96 (C^8), 173.61 (C^8), 173.45 (C^6), 172.23 (C^6), 140.24 (C^{10}), 138.25 (C^{10}), 128.48 (ArC), 128.18 (ArC), 128.07 (ArC), 127.95 (ArC), 127.87 (ArC), 127.72 (ArC), 74.69 (C^1), 73.07 (C^1), 58.75 (C^2), 58.61 (C^2), 54.87, 52.75, 52.41, 52.11, 52.03, 51.42, 45.00 (C^5), 44.23 (C^5), 39.96 (C^3), 39.62 (C^3) ppm. **FT-IR** (thin film) ν_{max} 1732, 1436, 1170, 1006, 701 cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{15}H_{20}NO_4^+$) requires m/z 278.1387, found m/z 278.1388.

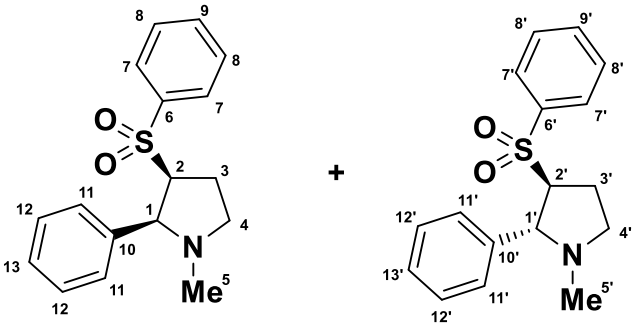
cis- and *trans*-5-methyl-2,4-diphenyltetrahydropyrrolo[3,4-c]pyrrole-1,3(2H,3aH)-dione (**2_26**)



Prepared following **General Procedure D** to afford the inseparable mixtures of title compounds as a pale yellow oil (78.1 mg, 98%). Crude dr = 1.2:1.

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.51-7.20 (m, 28H, ArH), 3.72 (d, *J* = 9.5 Hz, 1H, C^4H_a (**A**)), 3.68-3.54 (m, 5.9H, C^4H_a (**B**), C^3H (**B**), C^1H (**A**, **B**)), 3.49 (dd, *J* = 8.9, 7.9 Hz, 1H, C^2H (**A**)), 3.42 (dd, *J* = 8.7, 6.1 Hz, 1.6H, C^2H (**B**)), 3.35 (ddd, *J* = 7.7, 6.8, 0.6 Hz, 1H, C^3H (**A**)), 2.73 (dd, *J* = 9.2, 6.1 Hz, 1.6H, C^4H_b (**B**)), 2.63 (dd, *J* = 9.5, 6.7 Hz, 1H, C^4H_b (**A**)), 2.21 (s, 3H, C^5H_3 (**A**)), 2.17 (s, 4.8H, C^5H_3 (**B**)) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 178.22 (C(C=O)), 177.01 (C(C=O)), 176.40 (C(C=O)), 174.79 (C(C=O)), 136.74 (ArC), 132.10 (ArC), 131.84 (ArC), 129.20 (ArC), 129.14 (ArC), 129.02 (ArC), 128.75 (ArC), 128.63 (ArC), 128.52 (ArC), 128.33 (ArC), 128.24 (ArC), 128.13 (ArC), 127.95 (ArC), 127.83 (ArC), 101.49 (ArC), 101.24 (ArC), 73.42 (C^1 (**A**)), 72.74 (C^1 (**B**)), 58.33 (C^4 (**A**)), 57.48 (C^4 (**B**)), 53.61 (C^2 (**B**)), 50.65 (C^2 (**A**)), 44.62 (C^3 (**A**)), 44.26 (C^3 (**B**)), 39.74 (C^5 (**A**)), 38.77 (C^5 (**B**)) ppm. **FT-IR** (thin film) ν_{max} 1712, 1499, 1382, 1184 cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{19}H_{19}N_2O_2^+$) requires m/z 307.1441, found m/z 307.1441.

cis- and *trans*-1-methyl-2-phenyl-3-(phenylsulfonyl)pyrrolidine (**2_27**)

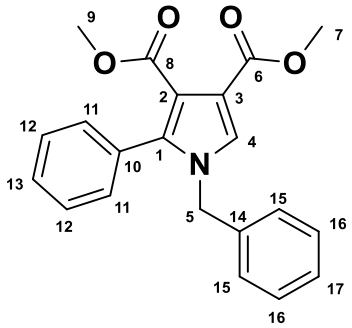


Prepared following **General Procedure D** to afford the inseparable mixtures of title compounds as a pale yellow oil (43.3 mg, 57%). Crude dr = 1.6:1.

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.96-7.90 (m, 2H, ArH), 7.79-7.72 (m, 3H, ArH), 7.69-7.62 (m, 1H, ArH), 7.60-7.49 (m, 3H, ArH), 7.45-7.37 (m, 3H, ArH), 7.34-7.21 (m, 5H, ArH), 7.19-7.13 (m, 4H, ArH), 7.13-7.06

(m, 3H, ArH), 3.92-3.82 (m, 1H, C^2H), 3.67 (ddd, *J* = 10.4, 7.1, 3.3 Hz, 1H, C^2H), 3.54 (d, *J* = 7.1 Hz, 1H, C^1H), 3.35 (dt, *J* = 9.8, 7.6 Hz, 2H), 3.18 (ddt, *J* = 9.0, 7.1, 0.9 Hz, 1H), 2.82 (dd, *J* = 9.9, 8.8 Hz, 1H), 2.65 (ddd, *J* = 13.9, 7.2, 4.2 Hz, 1H), ddd, *J* = 11.1, 9.0, 6.7 Hz, 1H), 2.45-2.25 (m, 3H), 2.15 (s, 3H), 2.15 (s, 3H), 2.00 (ddd, *J* = 14.0, 10.7, 9.6 Hz, 1H) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 140.83 (C^{10}), 140.37 (C^{10}), 138.69 (C^6), 138.46 (C^6), 133.83 (C^9), 133.55 (C^9), 129.37 (ArC), 129.06 (ArC), 129.04 (ArC), 128.60 (ArC), 128.51 (ArC), 128.40 (ArC), 128.35 (ArC), 127.74 (ArC), 127.68 (ArC), 127.41 (ArC), 70.87 (C^2), 70.82 (C^2), 70.17 (C^1), 60.98 (C^1), 56.19 (C^4), 55.56 (C^4), 39.77 (C^5), 39.75 (C^5), 36.27 (C^3), 25.89 (C^3) ppm. **FT-IR** (thin film) ν_{max} 1447, 1305, 1144, 1086 cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{17}H_{20}NO_2S^+$) requires m/z 302.1209, found m/z 302.1208.

dimethyl 1-benzyl-2-phenyl-1H-pyrrole-3,4-dicarboxylate (**2_28**)



To an oven-dried 5 ml round bottom flask was added **2_11a** (0.25 mmol, 1.0 eq.), $IrCl(CO)(PPh_3)_2$ (2.0 mg, 0.0025 mmol, 0.01 eq.) and toluene (1.0 ml), followed by the addition of **2_7** (44 μL, 0.25 mmol, 1.0 eq.). The mixture was stirred under nitrogen atmosphere at room temperature. After 20 min, dimethyl acetylenecarboxylate (0.50 mmol, 2.0 eq.) and TMSCl (6.3 μL, 0.050 mmol, 0.2 eq.) were added and stirred at room temperature for 22 h. DDQ (0.5 mmol) was then added and stirred at 80 °C for 16 h. DCM was added and the mixture was washed with sat. aq. Na_2CO_3 and brine. After drying over Na_2SO_4 and concentration under reduced pressure, the remaining crude was purified by flash column chromatography on silica gel to give a colorless oil (63.8 mg, 67%).

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.42-7.33 (m, 3H, ArH), 7.32-7.23 (m, 7H, ArH), 7.00-6.91 (m, 1H, C^4H), 4.93 (s, 2H, C^5H_2), 3.81 (s, 3H, C^7H_3 or C^9H_3), 3.66 (s, 3H, C^7H_3 or C^9H_3) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 164.10 (C^7 or C^9), 137.27 (C^{14}), 136.35 (C^{10}), 130.46 (ArC), 130.08 (ArC), 128.87 (ArC), 128.27 (ArC), 128.05 (ArC), 127.01 (ArC), 101.93 (ArC), 115.62 (ArC), 115.10 (ArC), 51.71 (C^5), 51.45 (C^7 or C^9), 51.20 (C^7 or C^9) ppm. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{21}H_{20}NO_4^+$) requires m/z 350.1392, found m/z 350.1392. Data is consistent with the published literature.[3]

6.2.3. Crystallographic Data

X-ray diffraction data has been made available in the Cambridge Crystallographic Data Centre as CCDC 2056517 (**2_18**).

Crystal data

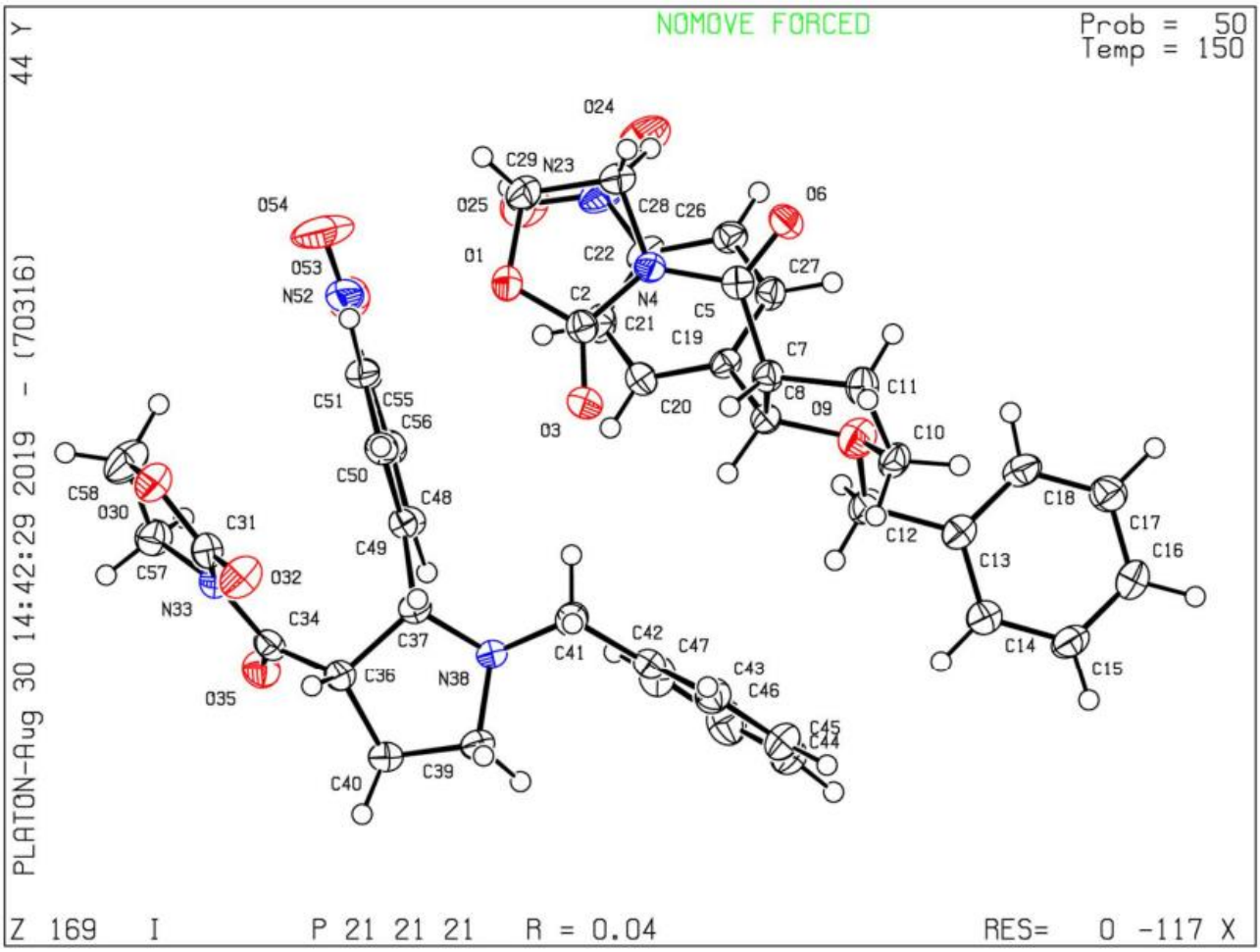
Chemical formula	$C_{10.50}H_{10.50}N_{1.50}O_{2.50}$
M_r	197.71
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	150
a, b, c (Å)	8.2586 (2), 10.4558 (3), 44.1264 (11)
V (Å^3)	3810.33 (17)
Z	16
Radiation type	Cu Kα
U (mm^{-1})	0.83
Crystal size (mm)	0.15 × 0.15 × 0.10

Data collection

Diffractometer	Oxford Diffraction SuperNova
Absorption correction	Multi-scan CrysAlis PRO (Rigaku Oxford Diffraction, 2017)
T_{min}, T_{max}	0.75, 0.92
No. of measured, independent and observed [I > 2.0σ(I)] reflections	24644, 4545, 4167
R_{int}	0.037
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.633

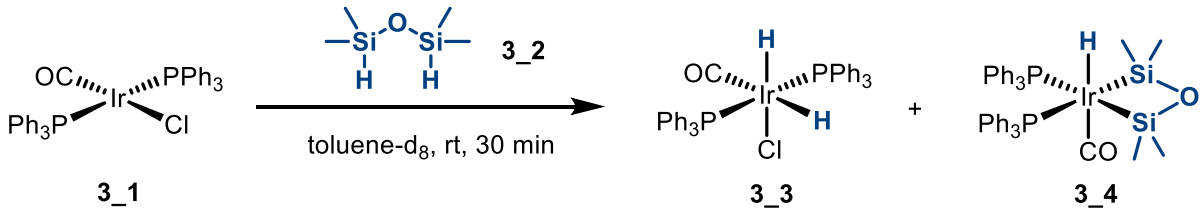
Refinement

R[$F^2 > 2\sigma(F^2)$], $wR(F^2)$, S	0.034, 0.086, 1.01
No. of reflections	4545
No. of parameters	523
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.21, -0.20



6.3. Synthesis of Compounds in Chapter 3

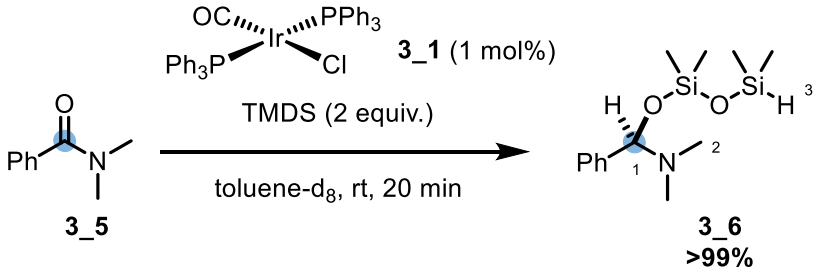
6.3.1. Reaction between Vaska's Complex and TMDS



To a solution of $IrCl(CO)(PPh_3)_2$ **3_1** (0.8 mg, 0.001 mmol) in 0.5 mL of toluene-d_8 was added TMDS **3_2** in an NMR tube at room temperature. After 30 min, the formation of **3_3** and **3_4** was confirmed by ^1H and $^{31}P\{^1H\}$ NMR spectra. **3_3**: **$^{31}P\{^1H\}$ NMR** ($CDCl_3$, 162 MHz) δ_P: 9.16 (d, J = 2.2 Hz, 2P). **3_4**: **$^{31}P\{^1H\}$ NMR**

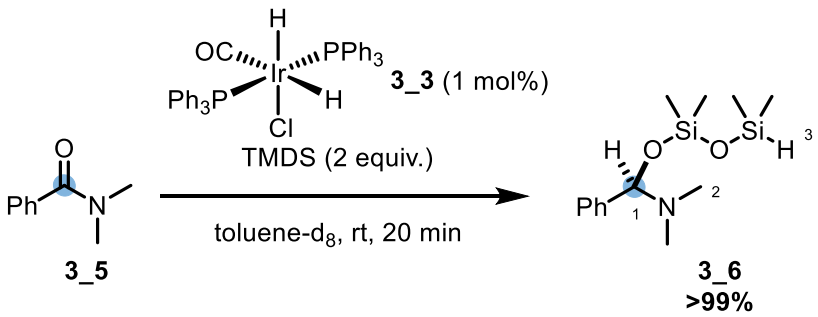
($CDCl_3$, 162 MHz) δ_P: 1.42 (s, 2P). **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{41}H_{44}IrO_2P_2Si_2^+$) requires m/z 879.1979, found m/z 879.1973. Data is consistent with the published literature.[4,5]

6.3.2. Amide Reduction with Vaska's Complex and TMDS



To a solution of $IrCl(CO)(PPh_3)_2$ **3_1** (0.4 mg, 0.0005 mmol) and *N*,*N*-dimethylbenzamide **3_5** (7.5 mg, 0.05 mmol) in 0.5 mL of toluene-d_8 was added TMDS **3_2** (17.8 µL, 0.1 mmol) in an NMR tube at room temperature. After 20 min, the starting material **3_5** was fully converted to the hemiaminal **3_6**, which was confirmed by ^1H NMR spectrum. **3_6**: **^1H NMR** ($CDCl_3$, 400 MHz) δ_H: 7.55 (ddt, *J* = 7.2, 1.3, 0.7 Hz, 2H, ArH), 7.24–7.16 (m, 2H, ArH), 7.09 (ttd, *J* = 6.8, 1.3, 0.5 Hz, 1H, ArH), 5.57 (s, 1H, C^1H), 4.90 (hept, *J* = 2.8 Hz, 1H, Si^3H), 2.25 (s, 6H, C^2H_3).

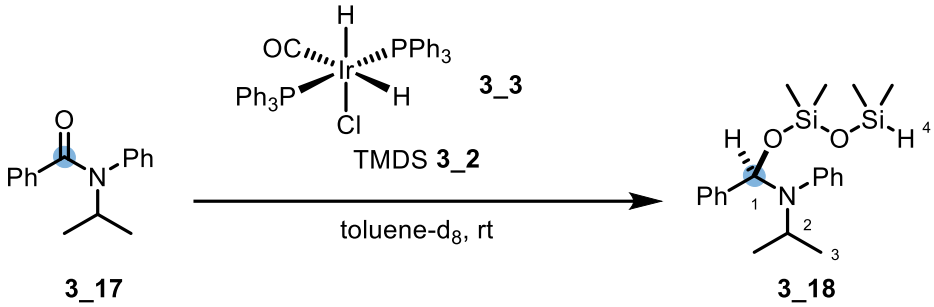
6.3.3. Amide Reduction with 3_3 and TMDS



A solution of $IrCl(CO)(PPh_3)_2$ **3_1** (0.4 mg, 0.0005 mmol) in 0.5 mL of toluene-d_8 in an NMR tube was kept under H_2 atmosphere (1 atm) at room temperature for 1 h. The full conversion of **3_1** to **3_3** was confirmed by

$^{31}P\{^{1}H\}$ NMR spectrum. Then, *N*,*N*-dimethylbenzamide **3_5** (7.5 mg, 0.05 mmol) and TMDS **3_2** (17.8 μL, 0.1 mmol) was added to the NMR tube at room temperature. After 20 min, the starting material **3_5** was fully converted to the hemiaminal **3_6**, which was confirmed by ^{1}H NMR spectrum.

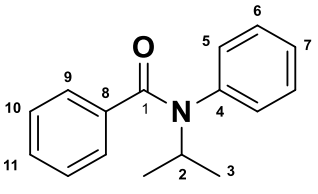
6.3.4. Kinetic Studies



A solution of $IrCl(CO)(PPh_3)_2$ **3_1** (0.4 mg, 0.0005 mmol) in 0.5 mL of toluene-d_8 in an NMR tube was kept under H_2 atmosphere (1 atm) at room temperature for 1 h. The full conversion of **3_1** to **3_3** was confirmed by $^{31}P\{^{1}H\}$ NMR spectrum. Then, **3_17** (7.5 mg, 0.05 mmol) and TMDS **3_2** (17.8 μL, 0.1 mmol) was added to the NMR tube at room temperature. After 20 min, the starting material **3_17** was fully converted to the hemiaminal **3_18**, which was confirmed by ^{1}H NMR spectrum. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ_H: 7.49–7.34 (m, 2H, ArH), 7.25–6.94 (m, 7H, ArH), 6.91–6.77 (m, 1H, ArH), 6.33 (s, 0.3H, $C^{1}H$), 6.14 (m, 0.7H, $C^{1}H$), 4.98-4.85 (m, 1H, $Si^{4}H$), 3.77-3.61 (m, 1H, $C^{2}H$), 1.28 (d, J = 6.6 Hz, 0.9H, $C^{3}H_3$), 1.24 (d, J = 6.7 Hz, 2.1H, $C^{3}H_3$), 1.02 (d, J = 6.6 Hz, 0.9H, $C^{3}H_3$), 1.01 (d, J = 6.7 Hz, 2.1H, $C^{3}H_3$), 0.22–0.05 (m, 12H).

6.3.5. Synthesis and Characterization

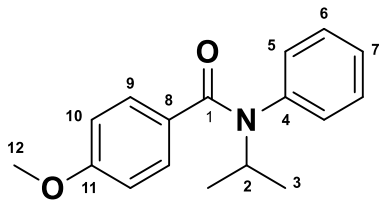
N-isopropyl-*N*-phenylbenzamide (**3_17**)



In a solution of triethylamine (0.83 mL, 6 mmol, 2.0 equiv.) in DCM (3 mL) under nitrogen atmosphere, benzoyl chloride (0.35 mL, 3.0 mmol, 1.0 equiv.) was added dropwise at 0 °C. To the mixture was added *N*-isopropylaniline (0.43 mL, 3.0 mmol, 1.0 equiv.) dropwise. The resulting mixture was allowed to warm to room temperature and stirred for 24 h. DCM was added and the mixture was washed with 1M HCl, sat. aq. $NaHCO_3$ and brine. After drying over Na_2SO_4 and concentration under reduced pressure, the remaining crude was purified by flash column chromatography on silica gel to give the title compound as a white solid (709.5 mg, 99%).

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.33–7.06 (m, 8H, ArH), 7.06–6.97 (m, 2H, ArH), 5.10 (bs, 1H, C^2H), 1.21 (d, J = 6.8 Hz, 6H, C^3H_3) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 130.66 (ArC), 128.90 (ArC), 128.60 (ArC), 128.12 (ArC), 127.58 (ArC), 127.35 (ArC), 21.12 (C^2) ppm. **FT-IR** (thin film) ν_{max} 2975, 2932, 1641, 1593, 1494, 1390, 1342, 1253, 1117, 701 cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{16}H_{18}NO^+$) requires m/z 240.1383, found m/z 240.1382. Data is consistent with the published literature.[6]

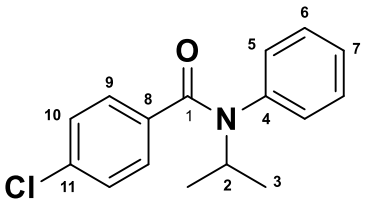
N-isopropyl-4-methoxy-*N*-phenylbenzamide (**3_19**)



In a solution of triethylamine (0.83 mL, 6 mmol, 2.0 equiv.) in DCM (3 mL) under nitrogen atmosphere, 4-methoxybenzoyl chloride (0.51 mg, 3.0 mmol, 1.0 equiv.) was added dropwise at 0 °C. To the mixture was added *N*-isopropylaniline (0.43 mL, 3.0 mmol, 1.0 equiv.) dropwise. The resulting mixture was allowed to warm to room temperature and stirred for 24 h. DCM was added and the mixture was washed with 1M HCl, sat. aq. $NaHCO_3$ and brine. After drying over Na_2SO_4 and concentration under reduced pressure, the remaining crude was purified by flash column chromatography on silica gel to give the title compound as a white solid (802.9 mg, 99%).

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.28-7.16 (m, 5H, ArH), 7.05-6.99 (m, 2H, ArH), 6.65-6.59 (m, 2H, ArH), 5.09 (hept, *J* = 6.8 Hz, 1H, C^2H), 3.71 (s, 3H, $C^{12}H_3$), 1.20 (d, *J* = 6.8 Hz, 6H, C^3H_3) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 170.23 (C^1), 160.04 (C^{11}), 140.23 (C^4), 130.53 (ArC), 130.34 (ArC), 129.45 (ArC), 128.64 (ArC), 127.18 (ArC), 112.83 (C^{10}), 55.12 (C^2), 47.89 (C^{12}), 21.11 (C^3) ppm. **FT-IR** (thin film) ν_{max} 2974, 2935, 1637, 1606, 1511, 1495, 1388, 1341, 1251, 1176, 1117, 1031, 844, 762, 704 cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{17}H_{20}NO_2^+$) requires m/z 270.1489, found m/z 270.1485.

4-chloro-*N*-isopropyl-*N*-phenylbenzamide (**3_20**)

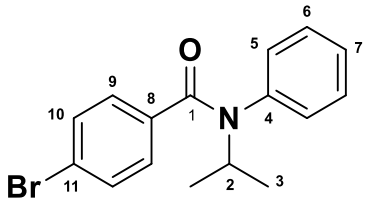


In a solution of triethylamine (0.83 mL, 6 mmol, 2.0 equiv.) in DCM (3 mL) under nitrogen atmosphere, 4-chlorobenzoyl chloride (0.38 mL, 3.0 mmol, 1.0 equiv.) was added dropwise at 0 °C. To the mixture was added *N*-isopropylaniline (0.43 mL, 3.0 mmol, 1.0 equiv.) dropwise. The resulting mixture was allowed to warm to room temperature and stirred for 24 h. DCM was added and the mixture was washed with 1M HCl, sat. aq. $NaHCO_3$ and brine. After drying over Na_2SO_4 and concentration under reduced pressure, the remaining crude

was purified by flash column chromatography on silica gel to give the title compound as a white solid (813.5 mg, 99%).

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.28–7.14 (m, 5H, ArH), 7.13–7.05 (m, 2H, ArH), 7.03–6.96 (m, 2H, ArH), 5.07 (bs, 1H, C^2H), 1.20 (d, J = 6.8 Hz, 6H, C^3H_3) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 169.48 (C^1), 135.69 (C^4), 134.95 (C^8), 130.52 (ArC), 129.68 (ArC), 128.81 (ArC), 127.85 (ArC), 127.60 (ArC), 47.92 (C^2), 21.03 (C^3) ppm. **FT-IR** (thin film) ν_{max} 2975, 2361, 1638, 1592, 1496, 1402, 1350, 1250, 1120, 1016, 708 cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{16}H_{17}ClNO^+$) requires m/z 274.0993, 276.0964, found m/z 274.0993, 276.0964.

4-bromo-*N*-isopropyl-*N*-phenylbenzamide (**3_21**)

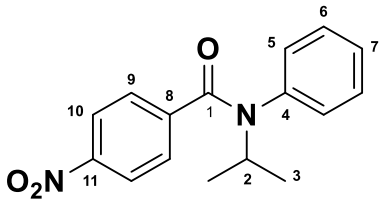


In a solution of triethylamine (0.83 mL, 6 mmol, 2.0 equiv.) in DCM (3 mL) under nitrogen atmosphere, 4-bromobenzoyl chloride (0.66 mg, 3.0 mmol, 1.0 equiv.) was added dropwise at 0 °C. To the mixture was added *N*-isopropylaniline (0.43 mL, 3.0 mmol, 1.0 equiv.) dropwise. The resulting mixture was allowed to warm to room temperature and stirred for 24 h. DCM was added and the mixture was washed with 1M HCl, sat. aq. $NaHCO_3$ and brine. After drying over Na_2SO_4 and concentration under reduced pressure, the remaining crude was purified by flash column chromatography on silica gel to give the title compound as a white solid (774.8 mg, 81%).

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.29–7.18 (m, 5H, ArH), 7.14–7.08 (m, 2H, ArH), 7.03–6.97 (m, 2H, ArH), 5.07 (s, 1H, C^2H), 1.20 (d, J = 6.8 Hz, 6H, C^3H_3) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 169.51 (C^1), 139.38 (C^4), 136.15 (C^8), 130.81 (ArC), 130.52 (ArC), 129.89 (ArC), 128.83 (ArC), 127.63 (ArC), 123.31 (ArC),

47.94 (C^2), 21.02 (C^3) ppm. **FT-IR** (thin film) ν_{max} 2975, 2934, 1642, 1591, 1494, 1396, 1344, 1253, 1117, 1012, 754, 703 cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{16}H_{17}BrNO^+$) requires m/z 318.0488, 320.0468, found m/z 318.0490, 320.0469.

N-isopropyl-4-nitro-*N*-phenylbenzamide (**3_22**)



In a solution of triethylamine (0.83 mL, 6 mmol, 2.0 equiv.) in DCM (3 mL) under nitrogen atmosphere, 4-nitrobenzoyl chloride (0.56 mg, 3.0 mmol, 1.0 equiv.) was added dropwise at 0 °C. To the mixture was added *N*-isopropylaniline (0.43 mL, 3.0 mmol, 1.0 equiv.) dropwise. The resulting mixture was allowed to warm to room temperature and stirred for 24 h. DCM was added and the mixture was washed with 1M HCl, sat. aq. $NaHCO_3$ and brine. After drying over Na_2SO_4 and concentration under reduced pressure, the remaining crude was purified by flash column chromatography on silica gel to give the title compound as a white solid (316.2 mg, 37%).

^{1}H NMR ($CDCl_3$, 400 MHz) δ_H: 7.98 (d, *J* = 8.3 Hz, 2H), 7.38 (d, *J* = 8.3 Hz, 2H), 7.28-7.18 (m, 3H, ArH), 7.05–6.96 (m, 2H, ArH), 5.11 (bs, 1H, C^2H), 1.23 (d, *J* = 6.8 Hz, 6H, C^3H_3) ppm. **^{13}C NMR** ($CDCl_3$, 101 MHz) δ_C: 130.56, 129.06, 128.15, 122.95, 20.96 (C^3) ppm. **FT-IR** (thin film) ν_{max} 3378, 2938, 1640, 1592, 1521, 1495, 1345, 1117, 704 cm^{-1}. **HRMS** (ES^+) exact mass calculated for $[M+H]^+$ ($C_{16}H_{17}NO_3^+$) requires m/z 285.1234, found m/z 285.1233.

6.4. References

[1] Pirenne, V; Traboulsi, I; Rouviere, L; Lusseau, J; Massip, S; Bassani, D. M.; Robert, F.; Landais, Y. p-Anisaldehyde-Photosensitized Sulfonylcyanation of Chiral Cyclobutenes: Enantioselective Access to Cyclic and Acyclic Systems Bearing All-Carbon Quaternary Stereocenters. *Org. Lett.*, **2020**, *22*, 575–579.

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Chapter 7

Computational Details

7.1. Computational Details for Chapter 2

Table 7.1. Cartesian coordinates (in Å), energies (in kcal mol^{-1}), and number of imaginary frequencies computed at COSMO(toluene)-M06-2X/TZ2P//BP86/TZ2P.

TS2_1
E = -10546.82
G = -10318.39
N_{imag} = 1, 281i cm^{-1}

C	0.01054977	-1.29732312	-2.15866440
C	1.06329817	0.63117079	-1.33381145
C	2.11545693	-0.12918397	-2.10547621
C	1.28260536	-1.08739248	-2.97948724
H	0.14831767	-2.09681552	-1.41552118
H	-0.88383846	-1.51708151	-2.75130140
H	2.75697215	0.53799968	-2.69106352
H	2.77171447	-0.68687207	-1.41739229
H	1.03447382	-0.60929872	-3.93674774
H	1.79376339	-2.03355257	-3.19015473
C	1.14374129	2.07687799	-1.11379665
O	0.21223966	2.85712725	-0.96715965
O	2.45644166	2.48383044	-1.10527811
C	2.63561735	3.89753479	-0.87558923
H	2.17882228	4.19542782	0.07580743
H	3.71786200	4.05273250	-0.85293267
H	2.17972517	4.48189066	-1.68426270
C	-1.20931732	0.31567955	-0.64944208
C	-2.53533586	-0.32064003	-0.75434337
C	-2.76154426	-1.71048666	-0.76825415
C	-3.65915331	0.52892909	-0.77148001
C	-4.05579552	-2.22435610	-0.82951085
H	-1.92455547	-2.40306732	-0.70271742
C	-4.95220513	0.01450187	-0.83285309
H	-3.50427707	1.60803400	-0.74558783
C	-5.15710375	-1.36641646	-0.86770395
H	-4.20550270	-3.30421346	-0.83520487
H	-5.80355974	0.69511213	-0.85374732
H	-6.16761172	-1.77211470	-0.91381417
H	-1.23165640	1.38258915	-0.43323221
N	-0.15883250	0.00258599	-1.46605555
C	1.10180454	0.17446316	1.06631598
C	-0.26792836	-0.10863125	1.24545151
H	1.40992200	1.18505776	1.33856862
H	-0.59085990	-1.14674366	1.32700980
C	2.16774297	-0.82356597	1.06920176
C	3.51125632	-0.39612799	1.15516314
C	1.93800628	-2.21580172	1.01435648
C	4.56488558	-1.30663484	1.19179260
H	3.71808389	0.67388712	1.19686881
C	2.99210651	-3.12572479	1.04782026
H	0.91675589	-2.59507335	0.96919978
C	4.31430401	-2.68011021	1.13817095
H	5.58966105	-0.94134477	1.26628596
H	2.77991507	-4.19503605	1.01402372
H	5.13655212	-3.39442504	1.17067713
C	-1.06358474	0.82655855	2.06854914
O	-0.82999383	2.00728811	2.26410932
O	-2.15072243	0.18472019	2.60607627
C	-2.99221648	1.01736386	3.42961964
H	-3.80782856	0.36958792	3.76276953
H	-2.43002111	1.40398627	4.28868391
H	-3.38233852	1.86513569	2.85343474

TS2_2
E = -10550.67
G = -10321.24
Nimag = 1, 290i cm-1

C	-1.22289195	1.76498498	-1.80849935
C	0.82129373	1.38232930	-0.68451306
C	1.16122294	1.91922845	-2.06490860
C	-0.14941474	2.59071882	-2.51443524
H	-1.46516521	0.85423305	-2.37349341
H	-2.14159844	2.32011848	-1.59084090
H	2.01178846	2.60644358	-2.04141210
H	1.42567870	1.09462579	-2.74499602
H	-0.18070813	3.63156195	-2.16408240
H	-0.28369716	2.58975860	-3.60226499
C	1.67332238	1.66404578	0.48151771
O	1.35146735	1.59737238	1.66270375
O	2.93498878	2.00314292	0.08312348
C	3.87276784	2.21615200	1.16111047
H	3.98615263	1.30015276	1.75196039
H	4.81552722	2.47927729	0.67412928
H	3.53201697	3.02936591	1.81294301
C	-1.13751085	0.67502842	0.47577876
C	-2.58214428	0.60513762	0.73976328
C	-3.59124349	0.46998001	-0.23538445
C	-2.97549989	0.62653643	2.09422035
C	-4.93322717	0.39154645	0.13530395
H	-3.33104236	0.38843772	-1.28723216
C	-4.31580496	0.54738897	2.46086214
H	-2.20851985	0.71878784	2.86405728
C	-5.30456412	0.43572283	1.48054616
H	-5.69608992	0.28741380	-0.63672890
H	-4.59005474	0.57552043	3.51549565
H	-6.35549013	0.37550333	1.76303772
H	-0.51806669	0.68278845	1.36875881
N	-0.56194316	1.38718705	-0.53246900
C	1.02587018	-0.87246545	-0.64080980
C	-0.18791993	-1.26732019	-0.02667748
H	1.00539755	-0.86603214	-1.73286355
H	-0.16163542	-1.69198642	0.97568261
C	2.34308812	-1.18069796	-0.06426473
C	3.46009149	-1.27989800	-0.91833514
C	2.54964173	-1.41040573	1.31081427
C	4.72234378	-1.60485081	-0.42733276
H	3.32386786	-1.11129955	-1.98769015
C	3.81277556	-1.73521156	1.80208491
H	1.71487390	-1.33091578	2.00574904
C	4.90694359	-1.83615890	0.93829819
H	5.56544823	-1.68404263	-1.11436241
H	3.94359750	-1.91370542	2.86995896
H	5.89185017	-2.09763584	1.32515771
C	-1.25758657	-1.79849677	-0.87777418
O	-1.45382253	-1.53934661	-2.06124947

O	-2.05065322	-2.66876759	-0.17774210
C	-3.11793928	-3.26818850	-0.93845838
H	-2.71737762	-3.81694778	-1.79961178
H	-3.62090097	-3.94974137	-0.24676105
H	-3.81691195	-2.50299148	-1.29702912

TS2_3

E = -10546.28

G = -10317.11

Nimag = 1, 300i cm-1

C	-0.36704465	-1.16808564	2.21611056
C	1.55146566	-0.87741590	0.88197630
C	2.00328455	-0.74040119	2.32445080
C	0.85173928	-1.39747106	3.11072608
H	-0.82965627	-0.18774912	2.40405241
H	-1.13821910	-1.94133727	2.30213942
H	2.97146797	-1.22034599	2.49865045
H	2.11772907	0.31945010	2.59835467
H	1.03665737	-2.47455407	3.21950340
H	0.71230281	-0.97227280	4.11133662
C	2.44051983	-1.42806581	-0.16027116
O	2.10315898	-2.03459138	-1.16568820
O	3.75077294	-1.18944389	0.15206482
C	4.68834403	-1.66653849	-0.83897532
H	4.47006161	-1.21635062	-1.81434628
H	5.67332353	-1.36114756	-0.47533697
H	4.63237082	-2.75824448	-0.92785839
C	-0.50495555	-1.04444373	-0.30747769
C	-1.91371532	-1.42885687	-0.47063667
C	-2.95351250	-1.14446109	0.43721770
C	-2.25294631	-2.08656209	-1.67195415
C	-4.26282071	-1.54345974	0.17099498
H	-2.75431928	-0.57830299	1.34346154
C	-3.56162564	-2.47937577	-1.93770231
H	-1.46513987	-2.30232194	-2.39467021
C	-4.57402096	-2.21695065	-1.01126583
H	-5.04929149	-1.31036908	0.88888953
H	-3.79161272	-2.99600363	-2.86968709
H	-5.59953066	-2.52512348	-1.21460271
H	0.11503299	-1.26530209	-1.17222461
N	0.20934501	-1.19680173	0.85222978
C	1.15719237	1.23821941	-0.03667596
C	-0.11971888	1.08480158	-0.62088660
H	1.24720630	1.70140532	0.94499032
H	-0.11156863	0.98287897	-1.70823323
C	-1.32480153	1.75084239	-0.08861656
C	-2.44515633	1.90778334	-0.92788983
C	-1.41420303	2.28119645	1.21410105
C	-3.59797412	2.55760016	-0.49018851
H	-2.40018782	1.51665487	-1.94508972
C	-2.56908474	2.92376306	1.65633093
H	-0.56103333	2.21197306	1.88975322
C	-3.67095578	3.06632952	0.80766949
H	-4.44455945	2.66681172	-1.16858556
H	-2.60485859	3.32947388	2.66816292
H	-4.57044477	3.57587289	1.15265313
C	2.32519024	1.43777497	-0.89929295
O	2.44247066	1.10565696	-2.07005374
O	3.32242239	2.09256400	-0.21095897
C	4.50155099	2.37488072	-0.98635772
H	4.25287109	2.98722894	-1.86222186
H	5.17187418	2.91876325	-0.31449024
H	4.97441000	1.44665209	-1.33016911

TS2_4

E = -10550.66

G = -10321.66

Nimag = 1, 298i cm-1

C	0.75398563	-2.72257519	-0.06087138
C	1.76252289	-0.79324596	-0.92386158
C	2.88602726	-1.74738957	-0.60331219
C	2.16540540	-3.10506302	-0.50380731
H	0.69685676	-2.61238369	1.02998728
H	-0.03168098	-3.40143129	-0.40770820
H	3.67293379	-1.72521712	-1.36461298
H	3.35185047	-1.48249292	0.35841289
H	2.13486439	-3.59114387	-1.48846886
H	2.64095296	-3.79148734	0.20524431
C	1.91676027	0.37639927	-1.78365205
O	1.03355398	1.00383965	-2.36350149
O	3.24614980	0.68696719	-1.91596930
C	3.51407743	1.84265079	-2.73444126
H	3.04107404	2.73631632	-2.30889169
H	4.60215889	1.95005066	-2.73641565
H	3.13723977	1.69337315	-3.75357355
C	-0.62079942	-0.67663227	-0.63109258
C	-1.93060983	-1.34051273	-0.45693920
C	-2.24534911	-2.20561920	0.60851090
C	-2.95268188	-1.01872356	-1.36974349
C	-3.52143830	-2.75449663	0.72994485
H	-1.49809729	-2.43564335	1.36606810
C	-4.22799771	-1.56646481	-1.24636908
H	-2.73430324	-0.33038708	-2.18656453
C	-4.51677336	-2.44323732	-0.19883743
H	-3.74246061	-3.42075189	1.56412528
H	-4.99994148	-1.30471615	-1.97015709
H	-5.51398898	-2.87162682	-0.09899439
H	-0.61845394	0.13377985	-1.35767360
N	0.55714952	-1.38391743	-0.68345375
C	1.09257629	0.91583520	0.95056246
C	-0.28066986	0.60169691	0.95773001
H	1.44304467	1.85385388	0.52483698
H	-0.56531725	-0.12177794	1.72689220
C	-1.30401814	1.64980535	0.70694935
C	-2.45899881	1.68765006	1.50562144
C	-1.15960271	2.61884213	-0.30115694
C	-3.42708078	2.67563922	1.32274570
H	-2.59061607	0.93841720	2.28735809
C	-2.12765536	3.60520149	-0.48407338
H	-0.29068421	2.58617020	-0.95962829
C	-3.26413644	3.64191730	0.32886604
H	-4.31171695	2.68941128	1.96005848
H	-1.99648581	4.34814274	-1.27149391
H	-4.01929633	4.41451735	0.18344217
C	2.00959537	0.22072003	1.83330222
O	1.79936639	-0.82703870	2.44486969
O	3.20862919	0.89270666	1.93767710
C	4.14505220	0.32043295	2.86883859
H	5.03648686	0.95190653	2.81238694
H	3.73349935	0.32836044	3.88637470
H	4.39151372	-0.71455342	2.60062644

TS2_5

E = -11789.69

G = -11542.01

Nimag = 1, 271i cm-1

C	-1.09417693	1.56433450	-2.17724519
C	-1.83992913	-0.49527258	-1.32346806
C	-3.07947534	0.28930461	-1.69270949
C	-2.53966706	1.38131329	-2.63792925
H	-1.03289376	2.26351516	-1.32926385
H	-0.40392113	1.89868715	-2.95906022
H	-3.83962104	-0.34464962	-2.16140011
H	-3.53817328	0.73292790	-0.79480185
H	-2.55848135	1.02851790	-3.67793907
H	-3.10748720	2.31687090	-2.58248189
C	-1.82833005	-1.96322048	-1.30897871
O	-0.87623417	-2.69942937	-1.52804432
O	-3.07916335	-2.44440469	-1.00859492
C	-3.15956169	-3.88410735	-0.94079745
H	-2.45855984	-4.27534310	-0.19369932
H	-4.19251322	-4.10391391	-0.65715815
H	-2.92394377	-4.33123308	-1.91426249
C	0.52247349	-0.13585354	-1.27035094
C	1.76060497	0.55213038	-1.67907458
C	1.97347180	1.94119240	-1.59642170
C	2.82433614	-0.25471700	-2.13174118
C	3.18922836	2.50102844	-1.98541695
H	1.20198072	2.58999845	-1.18755100
C	4.03798442	0.30718245	-2.52277377

H	2.68057612	-1.33427923	-2.18751314
C	4.22357173	1.69008885	-2.45757432
H	3.33446640	3.57799935	-1.90258536
H	4.84077093	-0.33715989	-2.88208044
H	5.17269731	2.13250132	-2.75987771
H	0.61769547	-1.21310062	-1.14473302
N	-0.71427477	0.20589419	-1.72494503
C	-1.27965232	-0.33457862	0.98040860
C	0.06379247	0.09397867	0.87104246
H	-1.41823791	-1.39662115	1.18975922
H	0.29139394	1.15185844	0.97763943
C	-2.37500508	0.52897162	1.42688022
C	-3.60964263	-0.05544160	1.78275258
C	-2.26261113	1.93036512	1.54924453
C	-4.67523152	0.71734155	2.23905095
H	-3.72227295	-1.13671225	1.69572481
C	-3.32996356	2.70258930	2.00251420
H	-1.31788326	2.42212617	1.31733147
C	-4.54410038	2.10373032	2.35109309
H	-5.61370510	0.23371324	2.51203443
H	-3.20854987	3.78221845	2.09720623
H	-5.37467597	2.71009842	2.71181011
C	1.11935890	-0.80820336	1.34066901
O	1.04515940	-2.03415155	1.38832699
C	3.42753106	-1.10230219	2.19768462
C	4.57929082	-0.10729644	2.36639302
H	3.62954716	-1.87897643	1.45311699
H	5.23588932	-0.07678956	1.48584825
C	2.65311477	1.12074364	2.02500749
O	1.95816988	2.10519016	1.91541185
O	3.94107393	1.18703804	2.49580037
N	2.35164424	-0.21841563	1.74667835
H	3.14719250	-1.59718725	3.13840973
H	5.17852386	-0.28003361	3.26612954

TS2_6

E = -11793.40

G = -11545.10

Nimag = 1, 268i cm-1

C	-0.29560838	2.33910067	-1.75674688
C	1.56072764	1.38064200	-0.61670960
C	2.04678294	1.87165881	-1.97779031
C	0.97330948	2.88773899	-2.40366820
H	-0.74429347	1.54197787	-2.36521412
H	-1.04736777	3.10249227	-1.52997361
H	3.04959118	2.30287353	-1.92413030
H	2.08511221	1.03551995	-2.69223533
H	1.20602229	3.88180453	-1.99736291
H	0.87169332	2.97610828	-3.49166985
C	2.42427685	1.55085134	0.57917872
O	2.05600056	1.55735916	1.74616846
O	3.73296729	1.67342823	0.22151334
C	4.65901584	1.74407972	1.32933398
H	4.59656186	0.83081089	1.93180389
H	5.64732785	1.83780102	0.87196102
H	4.43739272	2.61261133	1.96050417
C	-0.54236328	1.28038951	0.52371021
C	-1.96955003	1.50800600	0.73005442
C	-2.94201799	1.64441249	-0.28439445
C	-2.40837064	1.54290682	2.07249648
C	-4.28302897	1.84522563	0.04018476
H	-2.66174016	1.55597997	-1.32988238
C	-3.74696858	1.74496920	2.39056299
H	-1.67562432	1.41274165	2.86910130
C	-4.69248919	1.90674150	1.37406760
H	-5.01644039	1.95105990	-0.75978009
H	-4.05466170	1.77518761	3.43562450
H	-5.74179609	2.06955868	1.61988883
H	0.03700159	1.06081755	1.41434298
N	0.20986070	1.75657479	-0.48705224
C	1.33132923	-0.70521842	-0.66302064
C	0.10920034	-0.99341700	-0.00111870
H	1.24830618	-0.69102420	-1.75311577
H	0.10429567	-1.41100793	1.00106465
C	2.60480610	-1.29645743	-0.18355665
C	3.62672369	-1.56977086	-1.11098015
C	2.83428007	-1.62754577	1.16463125
C	4.82868579	-2.15361566	-0.71348829
H	3.46514245	-1.33270239	-2.16376274
C	4.03586827	-2.21171205	1.56284216
H	2.06542882	-1.43133822	1.91054690
C	5.04000280	-2.47837095	0.62811045
H	5.59971673	-2.36312336	-1.45556889
H	4.18566584	-2.46825072	2.61209584
H	5.97502923	-2.94252683	0.94200026
C	-1.08449091	-1.18522066	-0.79158265
O	-1.23145996	-0.84308784	-1.97608825
C	-3.37656125	-2.12723597	-0.99195206
C	-4.37176549	-2.58986061	0.07662193
H	-3.14246104	-2.91141810	-1.72659974
H	-4.96006492	-3.46354315	-0.22249850
C	-2.30768015	-2.39985786	1.09403909
O	-1.49606851	-2.44531584	1.98966026
O	-3.55748535	-2.96373561	1.21336692
N	-2.20011103	-1.82779752	-0.17675673
H	-3.71005818	-1.23846307	-1.53639407
H	-5.04604512	-1.78107702	0.39160796

TS2_7

E = -11787.79

G = -11539.62

Nimag = 1, 300i cm-1

C	-1.41488470	-0.32832372	2.45961559
C	0.67025692	-0.79277599	1.48033491
C	0.96972089	-0.15815859	2.82073810
C	-0.36655181	-0.31292225	3.57411679
H	-1.76115781	0.68344262	2.20562302
H	-2.28749133	-0.95373997	2.67792603
H	1.80670068	-0.64936959	3.32740351
H	1.24920996	0.89764732	2.69370478
H	-0.38465018	-1.26723198	4.11727272
H	-0.55000848	0.49190241	4.29467442
C	1.58589609	-1.72612033	0.81271463
O	1.29548481	-2.59018877	-0.00266298
O	2.86871561	-1.54354283	1.26684414
C	3.82750939	-2.46253101	0.70340624
H	3.81189775	-2.41480349	-0.39187762
H	4.79751969	-2.14945599	1.09949917
H	3.60291940	-3.49115969	1.01197164
C	-1.21615468	-1.06881279	0.04308890
C	-2.62942767	-1.41986048	-0.19730551
C	-3.74472452	-0.79968990	0.39918382
C	-2.87104962	-2.42725240	-1.15404145
C	-5.04102911	-1.20628142	0.08277437
H	-3.61188371	0.02654049	1.09280093
C	-4.16602314	-2.82599766	-1.47422535
H	-2.02069100	-2.90948024	-1.63752422
C	-5.25962586	-2.22242630	-0.84858964
H	-5.88765872	-0.71219972	0.55958628
H	-4.32151872	-3.61515230	-2.21001370
H	-6.27490379	-2.53452518	-1.09310925
H	-0.52796230	-1.63908043	-0.57769473
N	-0.68164968	-0.90152506	1.30429902
C	0.67357819	0.92940421	-0.37640280
C	-0.63630307	0.70886983	-0.86606394
H	0.87368509	1.67284147	0.38864759
H	-0.67073098	0.26017615	-1.86180704
C	-1.72100442	1.69110551	-0.62344142
C	-2.83348567	1.70658210	-1.48516975
C	-1.68091994	2.65128199	0.40628590
C	-3.86387473	2.63273643	-1.32473097
H	-2.88089461	0.98304565	-2.29973290
C	-2.71371916	3.57207184	0.57326685
H	-0.81873299	2.70056157	1.07156571
C	-3.81361747	3.56772072	-0.28994860
H	-4.70855708	2.62410980	-2.01403187
H	-2.65183762	4.31015944	1.37364357
H	-4.61574678	4.29466009	-0.16302410
C	1.79979618	0.53119099	-1.19566671
O	1.74347591	-0.19505654	-2.19220463

C	3.45782323	1.91859662	0.17170519
O	2.77872764	2.41635830	1.04267524
O	4.80252635	2.18705475	0.05857404
C	4.20624718	0.79182968	-1.76056045
H	4.05289956	1.33442498	-2.70471814
H	4.28808874	-0.27394356	-1.99705320
C	5.39007727	1.32937211	-0.94883238
H	6.08877085	1.92934911	-1.54107741
H	5.94147884	0.52951828	-0.43479527
N	3.09225603	1.04046471	-0.84686307

TS2_8

E = -11793.29

G = -11544.83

Nimag = 1, 286i cm-1

C	0.17639247	-2.83459967	0.04833016
C	-0.85523151	-1.13894882	1.29063318
C	-1.90051754	-2.20404530	1.08577069
C	-1.06190535	-3.43914391	0.70832918
H	0.00442028	-2.63511006	-1.01700078
H	1.09168378	-3.42168265	0.17379681
H	-2.51837528	-2.34973839	1.97818229
H	-2.57413761	-1.92402407	0.25961531
H	-0.77767878	-3.99409296	1.61264721
H	-1.58654641	-4.12487485	0.03402630
C	-0.98078207	-0.04672102	2.25359368
O	-0.07938747	0.64956262	2.71282559
O	-2.28789357	0.07565819	2.64103330
C	-2.55792753	1.18801054	3.52279408
H	-2.45740110	2.13062440	2.97128369
H	-3.59162260	1.05193369	3.85185091
H	-1.87089721	1.18119977	4.37633738
C	1.39649779	-0.68053852	0.56630096
C	2.71079887	-1.16614193	0.09508197
C	2.91031150	-1.88317371	-1.10011008
C	3.84481732	-0.81601656	0.85200259
C	4.19073301	-2.26615818	-1.49811910
H	2.06406242	-2.12465939	-1.74123605
C	5.12369509	-1.19956607	0.45340878
H	3.71186664	-0.23811784	1.76683937
C	5.30236611	-1.93268900	-0.72132975
H	4.32107994	-2.81970810	-2.42825202
H	5.98440975	-0.92090554	1.06147941
H	6.30185936	-2.23199436	-1.03645508
H	1.44411490	0.06159957	1.36108535
N	0.33068800	-1.52919190	0.75187386
C	-0.71759188	0.86751215	-0.50406166
C	0.64604068	0.68727469	-0.80647005
H	-1.04860444	1.71646412	0.08661492
H	0.83867894	0.05711149	-1.67894610
C	1.61334034	1.80144005	-0.63788871
C	2.61724016	1.99099166	-1.60212797
C	1.56207128	2.68506800	0.45424378
C	3.52836860	3.04204934	-1.49333151
H	2.67536541	1.30911127	-2.45153147
C	2.47307360	3.73418597	0.56275701
H	0.81376598	2.53716563	1.23350818
C	3.45887653	3.92022677	-0.41085862
H	4.29527760	3.17369798	-2.25715019
H	2.41630346	4.40928740	1.41712145
H	4.16999472	4.74173147	-0.32267087
C	-1.72143098	0.12291327	-1.22031111
O	-1.51407384	-0.84504907	-1.97068556
C	-3.62881777	1.61849977	-0.39636203
O	-3.07768990	2.45103970	0.28682190
O	-4.98731824	1.64331945	-0.61967668
C	-4.09828887	-0.11611149	-1.92157981
H	-4.02382832	-1.20658068	-1.86629071
H	-3.96245471	0.17953719	-2.97239126
C	-5.38865116	0.43749326	-1.31210519
H	-5.82901602	-0.24977064	-0.57527299
H	-6.14408311	0.70769072	-2.05704740
N	-3.08797376	0.52542864	-1.07926637

2_30

E = -6111.38

G = -5981.32

Nimag = 0

C	-0.99133222	0.76721814	2.67722570
C	0.25265637	-1.05111280	1.89059000
C	1.24566773	-0.08425630	2.47294093
C	0.36469727	0.78933634	3.37987552
H	-1.05660402	1.54014543	1.89822281
H	-1.85054670	0.86372170	3.34728631
H	2.04519542	-0.59568623	3.02169572
H	1.73650707	0.52182235	1.68976652
H	0.27466116	0.33107479	4.37395851
H	0.73904848	1.81184872	3.50639817
C	0.55357407	-2.29794146	1.26708176
O	-0.24428078	-3.12203979	0.80387045
O	1.92460503	-2.50592485	1.22904665
C	2.31507675	-3.74885552	0.62202317
H	1.97325180	-3.80199748	-0.41966059
H	3.40825277	-3.76524396	0.66672566
H	1.89634651	-4.60276016	1.17035001
C	-2.17443904	-1.16217766	1.62994925
C	-3.52731155	-0.66756710	1.69206938
C	-3.95763504	0.67991049	1.80004244
C	-4.54267172	-1.65438532	1.57052742
C	-5.31233920	1.00258368	1.82453374
H	-3.23778364	1.49292357	1.82422093
C	-5.89056031	-1.32413631	1.59808156
H	-4.24456491	-2.69774640	1.46261213
C	-6.29043963	0.00981867	1.73464940
H	-5.60704364	2.04966697	1.90192718
H	-6.63801684	-2.11311541	1.51121666
H	-7.34764525	0.27217980	1.75545957
H	-2.01265334	-2.16445577	1.23660330
N	-1.03624778	-0.56849116	2.00953570

2_31

E = -5676.98

G = -5575.14

Nimag = 0

C	4.33423159	-0.53793785	0.70684800
H	5.42193334	-0.49927838	0.55764956
H	4.09158113	-1.32070530	1.43236224
N	3.17434445	0.71767275	-0.85990022
C	2.19738854	2.44553985	-2.32620125
C	1.66580912	2.80865037	-3.51351194
H	2.34833093	3.13943191	-1.50290022
H	1.55950485	2.02205671	-4.26639387
C	1.22063383	4.13882527	-3.90710202
C	0.73022457	4.32691773	-5.21472887
C	1.25654194	5.25222938	-3.04157207
C	0.29624451	5.57831556	-5.64677289
H	0.69557342	3.47303643	-5.89277339
C	0.82163423	6.49971891	-3.47336998
H	1.62594901	5.13507202	-2.02325481
C	0.34065016	6.66939372	-4.77723131
H	-0.07825617	5.70279456	-6.66276086
H	0.85523824	7.34944111	-2.79148158
H	0.00110092	7.64994800	-5.11075465
C	2.59480274	1.04694144	-2.11057958
O	2.47649510	0.14278462	-2.93520896
C	3.32292813	1.50115473	0.29642466
O	3.00111489	2.65009104	0.48669276
O	3.91395775	0.73236861	1.26479443
C	3.56792185	-0.66966500	-0.61409608
H	4.18105084	-1.04828747	-1.43854129
H	2.67748770	-1.30872576	-0.53200214

2_33

E = -4436.62

G = -4353.82

Nimag = 0

H	3.04733425	-3.93121960	1.93843356
H	5.23556758	-3.05696870	1.13353803
C	-1.17221870	1.12764875	2.15533106
O	-0.99987500	2.29796424	1.85913532

O	-2.36705020	0.63852973	2.61477133
C	-3.41646514	1.62186727	2.72456664
H	-4.28852608	1.07967428	3.09965847
H	-3.12583526	2.41861714	3.42029212
H	-3.62872284	2.06911694	1.74565562
C	1.07860698	0.29609242	1.65928863
C	-0.17551953	0.04450012	2.08234245
H	1.29826261	1.33143077	1.38138212
H	-0.50959055	-0.94675734	2.38700028
C	2.18249764	-0.64854020	1.53005648
C	3.42787417	-0.17264931	1.07532563
C	2.06772757	-2.01958072	1.83820752
C	4.51790365	-1.02899224	0.93359256
H	3.53154324	0.88584521	0.83268257
C	3.15527692	-2.87393449	1.69592974
H	1.11741731	-2.41929871	2.19117499
C	4.38570690	-2.38350083	1.24356197
H	5.47226974	-0.63865142	0.58030840

7.2. Computational Details for Chapter 3

Table 7.2. Cartesian coordinates (in Å), energies (in kcal mol^{-1}), and number of imaginary frequencies computed at COSMO(toluene)-ZORA-M06/TZ2P//COSMO(toluene)-ZORA-BLYP-D3(BJ)/TZ2P

3_14
E = -2803.65
G = -2743.99
N_{imag} = 0

Ir	-2.39463801	-0.49071231	1.31885032
C	0.93808171	0.23388904	2.24323759
H	-2.57858982	-0.56922009	-0.24455922
H	0.14822674	-2.75963413	-0.07246446
H	-2.37801854	0.94694708	0.66944324
Cl	-1.97931528	-1.76887421	3.34183219
O	-5.43631925	-0.21328925	1.51929687
P	-0.05867806	-0.55025367	0.91300098
C	0.62555376	-2.25016916	0.77029247
C	0.48724186	0.29102269	-0.62697695
H	0.39518767	-2.79539241	1.68975924
H	1.57472354	0.22392829	-0.73956736
H	0.18652182	1.34228517	-0.58827866
C	-4.28717214	-0.34623355	1.49232310
H	0.00011684	-0.18152311	-1.48533575
H	2.00783326	0.15227033	2.02139795
H	0.71167225	-0.26919075	3.18753952
H	0.65887791	1.28859196	2.32766442
H	1.70932110	-2.21601334	0.61434044

3_2
E = -2949.20
G = -2949.20
N_{imag} = 0

Si	-2.52508569	-1.23991259	0.11984149
C	-2.42428575	-3.02007776	-0.48430344
H	-3.67580239	-0.55687844	-0.55554946
C	-2.73897940	-1.16094774	1.98437312
O	-1.12594042	-0.42685928	-0.26796925
Si	-0.35363536	0.26217707	-1.57027063
C	1.19289821	1.11754895	-0.93441391
H	-1.27464752	1.27061058	-2.18778506
C	0.06676455	-1.05216772	-2.85087574
H	-2.32178421	-3.06524970	-1.57520399
H	-3.33152148	-3.57225981	-0.20513676
H	-1.56265707	-3.53408305	-0.03884177
H	-1.89346112	-1.64392684	2.49129870
H	-3.65927830	-1.67508150	2.29099134
H	-2.79642252	-0.12149592	2.32997086
H	1.88139925	0.39159598	-0.48283109
H	0.94141657	1.86833504	-0.17522830
H	1.72017807	1.62356323	-1.75364519
H	0.60444035	-0.60473856	-3.69731808
H	-0.83814119	-1.53287906	-3.24243058
H	0.70564914	-1.83040720	-2.41384983

3_15
E = -2340.50
G = -2131.73
N_{imag} = 0

O	-0.57487045	-0.56229232	0.53661178
C	-1.81512702	-0.59977471	0.62311970
C	-2.54046835	-1.93810605	0.75044728
N	-2.57744184	0.54043693	0.61038853
C	-1.93305759	1.85106685	0.47778108
H	-0.85300306	1.71105577	0.44884151
H	-2.20223513	2.48858665	1.33014236
H	-2.26592102	2.34478272	-0.44531253
C	-4.03939161	0.57514356	0.68454131
H	-4.45628875	1.00711685	-0.23617795
H	-4.35611178	1.20148512	1.52941056
H	-4.45237616	-0.42268000	0.81873099
H	-1.78365980	-2.72402015	0.74962214
H	-3.22916090	-2.10459654	-0.08617133
H	-3.11739914	-1.99809356	1.68057596

3_16
E = -5314.41
G = -5194.42
N_{imag} = 0

H	-2.02679329	1.05496179	2.76417887
C	-2.69496498	-0.59378091	1.51107990
Si	-4.58739326	0.39254480	-0.29113679
C	-2.65302828	0.16102745	2.83907968
H	-3.44746467	-1.39138625	1.57098233
H	-2.26385358	-0.48666158	3.63206899
H	-0.14995499	0.26081350	1.91464478
N	-1.44360650	-1.24523071	1.17511664
C	-1.57364280	-2.14385278	0.01762891
H	-2.41095959	-2.83107062	0.17913254
H	-0.65595819	-2.73281200	-0.08569210
H	-1.74579018	-1.59984056	-0.92837181
C	-0.29737645	-0.33428691	1.01000577
O	-3.10519103	0.35092743	0.45948684
O	-5.76506975	0.90335401	0.76650487
C	-5.12604210	-1.30623033	-0.88562238
C	-4.40087692	1.62525795	-1.69132409
Si	-6.03966141	2.09986836	1.88956709
C	-4.76408308	3.47564611	1.72688519
H	-5.91821282	1.47933892	3.24691961
C	-7.78967343	2.74622701	1.65991833
H	-4.86873389	3.99669500	0.76677346
H	-3.74694417	3.07144804	1.78730435
H	-4.89068020	4.21414173	2.52916535
H	-8.02772322	3.49689701	2.42497503
H	-8.52093795	1.93262565	1.74169861
H	-7.90689250	3.21441418	0.67404378
H	-6.09710302	-1.23703043	-1.39193325
H	-5.23704936	-2.00886493	-0.05079624
H	-4.40028319	-1.72578358	-1.59213007
H	-4.03736514	2.58781086	-1.31238327
H	-5.36380371	1.79376204	-2.18933318
H	-3.68608721	1.26361642	-2.44063603
H	-0.42132650	0.34953151	0.15286693
H	0.60447870	-0.93417980	0.84846628
H	-3.66415461	0.47831951	3.10942979

Int3_1

E = -5159.15
G = -5026.32
N_{imag} = 0

Ir	-3.86661187	-0.78432479	0.12807918
C	-2.49772273	-2.00583756	-2.94597404
H	-5.17372624	-1.57572561	-0.26837264
H	-0.40034637	-1.77193813	-0.65137367
H	-4.04756794	0.04447737	-1.22737019
Cl	-3.40731394	-2.30533275	2.11955683
O	-5.71071312	1.22091023	1.50142222
P	-2.68855019	-2.39730967	-1.15709689
C	-0.96888647	-2.70339048	-0.58338258
C	-3.47105356	-4.05828863	-1.14163287
H	-2.86049568	-4.78245818	-1.69190579
H	-4.46338762	-3.98844431	-1.59747944
H	-3.58175410	-4.37028404	-0.09915378
C	-4.98102400	0.45906967	1.01409888
N	-0.40049833	1.60086453	1.58240376
H	-1.95322776	-1.06169523	-3.04713704
H	-3.48977591	-1.88536451	-3.39177338
C	0.38265190	0.50018613	2.16642261
H	1.31128183	0.34925180	1.59993814
H	-0.21248246	-0.41178225	2.14148545
H	0.63759802	0.75428024	3.20028906
H	-2.79136904	3.05154200	0.99797746
H	-3.03042286	2.04220846	-0.44609462
C	0.15394669	2.94640580	1.76762921
H	-0.58488206	3.71116459	1.53452650
H	1.03829039	3.09421626	1.13241867
H	0.45564713	3.06340227	2.81387877
H	-0.49224834	-3.48172467	-1.18910127
H	-1.01382314	-3.00985586	0.46531573
H	-1.63248132	3.14494022	-0.34189148
O	-1.83520986	0.12413357	0.66400165
C	-1.49646268	1.32619900	0.83432537
C	-2.28189859	2.46807796	0.22197816
H	-1.95340333	-2.80158892	-3.46651295

TS3_1
E = -5105.88
G = -4972.79
N_{imag} = 1, 139i cm^{-1}

Ir	-3.18582731	-1.10841585	0.92450569
C	-3.42813883	-1.06252013	-2.63242579
H	-4.69421195	-1.17822498	0.42000658
H	-0.45405020	-1.82934952	-1.56955494
H	-2.71017418	0.48719394	0.37827697
Cl	-3.32399769	-3.36675561	1.81993447
O	-4.66843101	-0.19674102	3.43133124
P	-2.86585400	-2.10939956	-1.22141596
C	-1.15740993	-2.66093659	-1.62324460
C	-3.85203017	-3.64040762	-1.46149481
H	-3.85480713	-3.90603657	-2.52417385
H	-4.87507594	-3.46982492	-1.11661088
H	-3.41722629	-4.44932298	-0.87180654
C	-3.99003979	-0.49139089	2.54179220
N	-1.22952429	1.71446809	1.51495113
H	-3.07741799	-0.03380488	-2.52461032
H	-4.52287498	-1.05518974	-2.62697819
C	-0.05342925	1.58085673	2.40013195
H	0.82616192	1.29890868	1.81460217
H	-0.19626606	0.83369707	3.19758185
H	0.13214688	2.55780033	2.85915216
H	-1.07269343	1.89575754	-1.01871302
H	-1.20652143	0.19378469	-1.52983805
C	-2.39272534	2.19462728	2.26286107
H	-2.66915834	1.53393130	3.10086718
H	-3.25255833	2.31174924	1.59760052
H	-2.15259685	3.17906643	2.68063835
H	-1.13121702	-3.11318587	-2.62054751
H	-0.86765063	-3.40376290	-0.87334074
H	0.26317790	0.75277536	-0.72059477
O	-0.97827345	-0.65599516	1.13350583
C	-1.35501935	0.50867594	0.64511893
C	-0.82614668	0.86376227	-0.76123722
H	-3.07216888	-1.47503911	-3.58262154

Int3_2
E = -5129.84
G = -4993.43
N_{imag} = 0

Ir	-3.10512014	-0.57977139	0.90610286
C	-1.45858549	-1.80387957	-2.02310868
H	-4.29876961	-0.48507152	-0.11019718
H	-0.35243511	-3.10032329	0.61005460
H	-1.64880638	2.07136069	1.34652738
Cl	-4.27493070	-2.33203287	2.16849737
O	-4.60000966	1.50570923	2.57534009
P	-2.37100656	-2.34639634	-0.52549479
C	-1.28234624	-3.58134233	0.29405334
C	-3.75938697	-3.34794990	-1.18704146
H	-3.37705720	-4.17048846	-1.80066709
H	-4.40437980	-2.70458497	-1.79299776
H	-4.33817195	-3.73906802	-0.34641301
C	-3.96681593	0.75813863	1.95795658
N	-0.05368454	0.76884991	1.48026474
H	-0.58570047	-1.21819326	-1.72863267
H	-2.11442125	-1.16029283	-2.61656454
C	0.89670648	-0.07583629	0.73963441
H	1.43323273	0.52056748	-0.00121208
H	0.40331863	-0.91259317	0.22031243
H	1.62695213	-0.48744217	1.44331094
H	0.36626639	3.12839408	0.23732664
H	-1.09630329	3.12926597	-0.78183065
C	-0.71095932	0.04812898	2.53249039
H	-1.45476603	-0.75178494	2.14465951
H	-1.27482277	0.71406382	3.18762769
H	-0.00203445	-0.54192384	3.12099464
H	-1.05359758	-4.40585172	-0.39012624
H	-1.80382206	-3.96379354	1.17642385
H	0.19911676	1.96883043	-1.11100299
O	-1.83618485	0.64238822	-0.15476038
C	-1.02760152	1.50801732	0.62911087
C	-0.33668640	2.49528464	-0.31485971
H	-1.15399757	-2.67310546	-2.61535086

TS3_2
E = -8077.63
G = -7848.20
N_{imag} = 1, 640i cm^{-1}

Si	-4.38491490	0.07150792	0.98576678
C	-2.79895046	-1.44176039	-0.25747368
H	-2.55591402	0.42553249	2.64809190
C	-1.65624046	-1.88821729	0.64334160
H	-3.88425936	-1.49465245	0.70181385
O	-2.91813975	-0.11887116	-0.53385897
H	-3.89217706	1.56530971	2.85471876
N	-3.17550700	-2.32101388	-1.25796107
C	-4.37170189	-1.97286060	-2.03264165
H	-1.45848748	-1.10513633	1.37364307
H	-0.75553201	-2.02883196	0.03667994
H	-1.88864695	-2.81484210	1.17326354
H	-2.71340192	1.80972086	1.53140932
H	-4.85799372	1.71590894	-0.79644214
H	-6.24379328	1.52389506	0.32337341
H	-5.96563717	0.32111118	-0.94246710
C	-3.01611078	-3.76861404	-1.04325224
C	-5.46518834	0.99630550	-0.24159985
C	-3.26458653	1.06284275	2.10827784
O	-5.51201761	-0.60116350	2.06832693
H	-3.70883988	-4.13866578	-0.27034928
H	-3.23832873	-4.28043381	-1.98260258
H	-1.99211678	-4.00678699	-0.75512418
H	-4.36497750	-2.51918467	-2.97900829
H	-4.37842596	-0.90398888	-2.22406328
H	-5.28394153	-2.24342393	-1.47535342
Si	-6.52291991	-1.91642986	2.10371800
C	-7.29885065	-2.02992247	3.81049200
H	-5.70284927	-3.14716484	1.83975041
C	-7.83651533	-1.78998157	0.75611971

H	-8.43102166	-0.87540584	0.87517419
H	-8.51806644	-2.64978089	0.79782804
H	-7.38264493	-1.76807087	-0.24229167
H	-6.52738405	-2.10859158	4.58614515
H	-7.94827490	-2.91210346	3.88221326
H	-7.90635398	-1.14056671	4.02126557
H	-3.81693217	2.52694045	-3.33639404
Ir	-1.09173416	1.09292010	-1.25037868
C	-1.73972963	-0.57001714	-4.33475604
H	0.09477919	1.93528855	-1.86316192
H	-4.32700350	0.84163136	-3.17055609
H	-0.29416862	-0.23539757	-1.64353004
Cl	-2.45925871	3.20905918	-0.89726502
O	0.52240309	1.16550819	1.33275450
P	-1.91406938	1.05240489	-3.47996424
C	-3.67701351	1.51668492	-3.72969760
C	-1.03066586	2.22711368	-4.58434466
H	-1.44005486	2.19263275	-5.59992610
H	0.03267631	1.97124069	-4.60399549
H	-1.14294215	3.23462504	-4.17243870
C	-0.14461888	1.14138292	0.38087035
H	-2.22262161	-1.34459737	-3.73355569
H	-0.67443751	-0.80918636	-4.41046752
H	-3.93334434	1.48026903	-4.79398213
H	-2.18315309	-0.54073168	-5.33605364

Int3_3

E = -5766.69

G = -5611.37

N_{imag} = 0

Ir	-4.38108680	-0.86055920	0.46053606
C	-2.51556597	-1.53288530	-2.49864138
H	-4.98178819	0.33422987	-0.44754091
H	-3.27859817	-4.11572559	-0.90438001
H	-2.99838388	-0.11370002	0.17889031
Cl	-6.68019562	-1.96716728	0.50751615
O	-4.89677825	0.94965203	2.88183610
P	-4.07645613	-1.94698109	-1.62755393
C	-4.10661385	-3.78013781	-1.53212600
C	-5.39469330	-1.53854741	-2.83560584
H	-5.25841017	-2.11195349	-3.75876948
H	-5.35631343	-0.46742274	-3.05473277
H	-6.36101989	-1.77390943	-2.38135030
C	-4.70319966	0.23829392	1.99216252
Si	-2.44827882	-2.24621620	1.75181084
C	-0.74518045	-5.57408244	0.11374807
C	-2.74178918	-3.65731857	2.97162704
H	0.12220551	-6.24516489	0.06375082
H	-1.32090611	-5.69839119	-0.81192436
H	0.25381274	-3.30831941	-2.07915734
H	1.74024504	-3.78661657	-1.23766234
H	1.09759459	-2.14344025	-1.03175901
H	-1.79306303	-3.97954275	3.42072790
H	-3.20814252	-4.52018829	2.48213555
H	-3.40688377	-3.32857843	3.78032444
H	-2.22810754	-0.43464422	3.44872186
H	-1.28732435	-0.04539321	1.99170511
H	0.63753569	-3.67756645	1.57760483
C	0.81807127	-3.19858417	-1.14468292
O	-1.51508078	-2.79839236	0.49195575
H	-4.01255433	-2.34151760	1.28212200
C	-1.58450288	-0.85299520	2.66650545
H	-1.37293061	-5.89381272	0.95388891
H	-2.44489312	-2.07771086	-3.44635529
H	-1.67602471	-1.79407723	-1.85202775
H	-2.49609253	-0.45606515	-2.69209436
H	-4.01965964	-4.22110085	-2.53083438
H	-5.05331060	-4.07906264	-1.07280624
H	-0.68738238	-1.26311773	3.15032742
Si	-0.18044947	-3.79429833	0.32949092

TS3_3

E = -8107.45

G = -7878.01

N_{imag} = 1, 47i cm^{-1}

Ir	0.96115647	-0.24049879	0.90960598
P	1.87961043	1.92771053	1.04358651
O	0.53848465	-3.24609907	0.61762456
Cl	-0.27604995	0.11417085	3.12533587
C	2.35972269	2.43995104	2.74300351
C	-1.62081343	0.04046917	-4.70005016
H	-0.96681912	-0.33886220	-5.49615605
H	-6.92388769	0.23893866	-3.18907303
H	1.31378391	1.23558773	-2.18522909
H	0.51039750	2.24736674	-3.41316354
H	1.50952458	0.86203798	-3.90991191
H	-0.49340030	0.33183488	0.06497524
Si	-2.12711236	0.43928736	-0.32282405
O	-4.15020202	0.68051141	-1.00276605
C	-5.28443597	0.59060018	-0.45548235
N	-6.39519669	0.72886460	-1.21378977
C	-6.28167518	0.95451993	-2.66357604
C	-5.44260877	0.32823022	1.03201825
C	-7.76896660	0.67199494	-0.70081532
Si	-0.70559605	0.10120153	-3.05643444
C	0.63276723	-2.09513368	0.74802369
C	0.91305379	3.37763267	0.44436986
C	3.45380279	2.10667412	0.10310010
H	-0.28840209	-1.28021789	-2.66714922
H	-1.96653945	1.04111937	-4.98993136
C	-2.32712741	1.97655447	0.74089352
C	-2.51509973	-1.31687172	0.23088125
O	-1.76696004	0.69091466	-1.91950287
H	1.73681539	-0.32610388	-0.48070213
H	-3.55920880	-1.60817372	0.09626319
H	-1.75514598	1.84353377	1.66491568
H	-1.90785079	2.81983973	0.18130771
H	-3.36424947	2.21802496	0.98304146
C	0.80134544	1.22170864	-3.15231242
H	-2.49578312	-0.61810393	-4.63443743
H	-7.78575244	0.61978855	0.38537452
H	-8.28459893	-0.20621805	-1.10945448
H	-8.31018068	1.57151122	-1.01729082
H	-5.24492087	0.82125166	-2.96781833
H	-6.61024638	1.97179423	-2.91046791
H	2.34595498	-0.60926021	1.66165211
H	-4.46375980	0.19889387	1.48828459
H	-6.03523111	-0.57463914	1.21172233
H	-5.94747804	1.16728260	1.52310177
H	-1.89078301	-2.00225043	-0.35156669
H	-2.23279365	-1.42491963	1.28417842
H	3.89987622	3.09242547	0.27985992
H	3.25640319	1.98297421	-0.96650370
H	4.14735527	1.32286226	0.42247347
H	1.53196020	4.28228928	0.47119488
H	0.03929863	3.51546876	1.08603321
H	0.57510516	3.19455736	-0.58030363
H	3.08705047	1.72172445	3.13471749
H	1.47186768	2.41129538	3.38132209
H	2.79485135	3.44592331	2.73559508

Int3_4

E = -8112.43

G = -7886.14

N_{imag} = 0

Ir	-1.79245532	-0.77192018	1.98564377
P	-0.38045612	0.91802580	2.82717118
O	-3.33130375	-3.08000681	0.73207634
Cl	-2.54340260	-1.19602887	4.45273206
C	0.67141755	0.40472064	4.24815050
C	-3.09399063	2.61521827	-3.46984585
H	-2.05933054	2.79645070	-3.78950948
H	-5.76955237	3.65984811	2.32829806
H	-2.31575653	2.02397250	0.44651752
H	-2.80390980	3.58103471	-0.29868400
H	-1.24858535	2.83583585	-0.72317346
H	-3.00831991	0.38265196	1.79753867
Si	-5.89455856	0.70934066	-0.57166988
O	-5.60968324	1.27418262	1.03745889
C	-5.37632204	0.87902760	2.26414746

N	-5.04355300	1.82809890	3.11864556
C	-4.82026792	3.20281435	2.62520876
C	-5.61356258	-0.52357042	2.71573947
C	-4.82538585	1.52175475	4.55121334
Si	-3.12007506	1.66206430	-1.85068593
C	-2.75483684	-2.19032211	1.22881381
C	-1.20056055	2.44173892	3.47242523
C	0.85016259	1.58804697	1.62873451
H	-2.47732420	0.32816472	-2.02245838
H	-3.58927616	3.58807692	-3.35427141
C	-5.85155073	-1.14462497	-0.71446182
C	-7.55096186	1.46142616	-0.98085206
O	-4.72955983	1.41620682	-1.46165186
H	-1.89478592	2.14365257	4.26301895
H	-0.46889784	3.15153395	3.87447882
H	1.46402824	0.75963045	1.26262431
H	1.49016758	2.34162395	2.10154573
H	0.32326108	2.03254937	0.78068950
H	-1.76300054	2.91287544	2.66226205
H	-3.60438638	2.06208717	-4.26758591
H	-5.74000608	1.11347755	4.99149558
H	-4.57183905	2.45015623	5.06089439
H	-4.01063877	0.79621647	4.65683111
H	-4.15312273	3.17634350	1.76158257
H	-4.36645204	3.78492303	3.42538561
H	-0.43632667	-1.72883656	2.22233798
H	-5.67860527	-1.19002413	1.85958088
H	-6.55871007	-0.56492602	3.27530545
H	-4.79997466	-0.85856101	3.36926353
H	-7.52441043	2.55159859	-0.86803124
H	-7.82397802	1.23103461	-2.01806155
H	-8.33617366	1.06314415	-0.32629734
H	-6.67044488	-1.62084397	-0.16313481
H	-5.97505142	-1.39866579	-1.77562131
H	-4.90331488	-1.57134747	-0.37759448
H	1.33676640	-0.39687341	3.91412097
H	0.01864884	0.00939849	5.03152106
H	1.25994172	1.24707709	4.62903009
H	-1.26202402	-0.39005312	0.53692561
C	-2.29471204	2.62406341	-0.46949154

TS3_4

E = -8109.46

G = -7881.57

N_{imag} = 1, 186i cm^{-1}

Ir	-6.31417989	-1.64751859	0.38187727
P	-6.48639729	-2.20133926	-1.90487157
O	-6.41618603	-1.00676223	3.36093639
Cl	-4.01655814	-2.83553858	0.31035892
C	-6.50860128	-4.00841093	-2.24901150
C	-5.22074017	1.89086245	5.01867044
H	-5.00895862	1.96722741	6.09305708
H	-7.93581105	1.39954454	5.33421860
H	-8.40350858	4.39914265	5.00218954
H	-6.69585176	4.83242150	4.76623620
H	-7.24279317	4.19755108	6.33156954
H	-5.59714913	-0.15079834	-0.08035555
Si	-6.86813232	2.69467073	1.53309865
O	-5.36620775	1.89398775	1.31698726
C	-4.66546511	1.41711547	0.29395286
N	-3.46250979	0.91120670	0.59502544
C	-2.61059428	0.35454976	-0.47291381
C	-4.94951791	1.95233201	-1.08756115
C	-3.20844824	0.38423380	1.94852292
Si	-7.00691078	2.35778121	4.67139936
H	-4.52984975	2.56000928	4.48992899
C	-5.12666929	-1.60274184	-2.99719340
C	-8.00016247	-1.57794918	-2.75229535
H	-5.02450722	0.86123589	4.70225952
H	-3.77548297	0.95420201	2.67963773
C	-6.46751829	4.52056642	1.44348608
C	-8.15595028	2.12961976	0.30861478
O	-7.32787056	2.25228600	3.03502159
H	-4.17802089	-1.95836925	-2.58553963
H	-5.25288312	-1.97470616	-4.02005956
H	-8.88117426	-1.97696728	-2.24063215
H	-8.01714144	-1.87969865	-3.80555721
H	-8.02360676	-0.48596144	-2.68245528
H	-5.12722233	-0.50938530	-3.00589024
H	-2.13935158	0.46766481	2.15632408
H	-3.50906438	-0.67068885	1.97531202
H	-3.06822832	-0.55867030	-0.86892165
H	-1.64647462	0.09842824	-0.03217383
H	-2.45105758	1.09097942	-1.26226854
C	-6.34862224	-1.25579761	2.22287978
H	-7.06778446	-3.09646565	0.63283478
H	-4.50239811	2.95273043	-1.17898526
H	-6.02518656	2.03072887	-1.23432776
H	-4.54366587	1.30917769	-1.86541037
H	-8.07718279	2.65326829	-0.65080253
H	-8.07329059	1.05078876	0.13780055
H	-9.14843626	2.34052943	0.72599411
H	-5.67752242	4.78341199	2.15730772
H	-6.12747252	4.80248472	0.43923435
H	-7.35585184	5.11898277	1.68075646
H	-7.38565396	-4.44727650	-1.76455165
H	-5.60878908	-4.44586819	-1.80642490
H	-6.53551414	-4.20792572	-3.32617313
H	-7.75408956	-0.98320545	0.24383979
C	-7.37276287	4.11304107	5.24466692

TS3_5

E = -8768.01

G = -8535.91

N_{imag} = 1, 47i cm^{-1}

Ir	1.02081988	-0.09383199	1.78866953
P	1.51419751	2.00810394	0.92094520
O	0.70423391	-3.00578960	2.66320006
Cl	0.07748742	0.96858769	3.91083346
O	2.73644300	2.85892371	1.58725880
C	-1.55716724	-0.69955030	-3.48543467
H	-1.09757236	-1.00155590	-4.43571396
H	-5.45073440	1.55539912	-3.78693575
H	0.66804151	2.63476580	-2.90599957
H	-0.89426706	2.53310909	-3.75159231
H	0.53402949	1.71940051	-4.42650699
H	-0.59290338	0.02798944	1.10697754
Si	-1.93722485	0.30225170	0.19809944
O	-3.69717220	0.64544630	-1.01459095
C	-4.94458155	0.66434220	-0.83882943
N	-5.72959655	1.35111250	-1.70151036
C	-5.13445809	2.04257345	-2.85585681
C	-5.59840768	-0.07490196	0.31457694
C	-7.19554683	1.38539533	-1.63796785
Si	-0.40139440	0.43042871	-2.51304333
C	0.80307221	-1.89130567	2.35927067
O	0.23602553	2.98652450	0.91181103
O	1.98378533	2.11110814	-0.63211215
H	0.84642433	-0.32593852	-2.19353631
H	-2.50323661	-0.18904505	-3.70353122
C	-2.63822575	1.55297809	1.40947546
C	-2.31144511	-1.54751255	0.22378916
O	-1.13232388	0.90530004	-1.10456403
H	1.59801146	-0.66613877	0.41330297
C	0.24897707	4.28776940	0.25577365
C	3.18282496	1.41792867	-1.07881978
C	2.89786191	2.91844719	3.04018601
H	3.21085263	1.53626160	-2.16335505
C	0.01700648	1.97845177	-3.49334196
H	-1.78804208	-1.60819215	-2.91636507
H	-7.55630387	1.05240635	-0.66677133
H	-7.62904328	0.74882538	-2.42083039
H	-7.53335324	2.41451063	-1.80056029
H	-4.04976957	2.00580365	-2.77233166
H	-5.47519128	3.08374026	-2.86993119
H	2.52268474	-0.11260681	2.39446777
H	-4.83536888	-0.62059443	0.86659756
H	-6.34686316	-0.78673623	-0.04873150
H	-6.09742478	0.62212455	0.99669867
H	-1.40961948	-2.08355430	-0.09321766

H	-2.52060405	-1.85714446	1.25583124
H	-3.14570935	-1.84076987	-0.41880116
H	-3.56968226	1.18711041	1.85473269
H	-1.91838625	1.74547202	2.20943741
H	-2.85109668	2.48722104	0.87845664
H	3.12207573	0.35627150	-0.81978971
H	1.17209580	4.82821002	0.48547465
H	-0.61168462	4.83064927	0.65111119
H	0.14929162	4.15090778	-0.82432362
H	4.06854218	1.87044133	-0.62312699
H	3.80213716	3.50541510	3.21128347
H	3.00548200	1.90980202	3.44641849
H	2.02991123	3.40075368	3.49706059

TS3_6

E = -12155.04

G = -11921.54

N_{imag} = 1, 41i cm^{-1}

Ir	1.00589774	-0.15282585	0.95834553
P	1.84511358	1.94765161	1.30844542
O	0.60353529	-3.08626837	0.21267223
Cl	0.15360089	-0.38107245	3.34359103
O	2.92913696	2.21035883	2.52654015
C	-2.02833521	-0.31926208	-4.35390099
H	-1.54008590	-0.82503615	-5.19690734
H	-6.63304597	-0.23538648	-3.49792287
H	1.32897125	1.11520757	-2.57799481
H	0.37319705	1.90057072	-3.85128897
H	1.25712508	0.39861068	-4.20071966
H	-0.54688717	0.47658836	0.44092892
Si	-2.10431268	0.53094492	-0.15648027
O	-4.16774982	0.65942159	-1.09755269
C	-5.35521254	0.61522773	-0.68213450
N	-6.37635387	0.57148698	-1.57150732
C	-6.09987078	0.59204935	-3.01643933
C	-5.67742091	0.60645633	0.80314397
C	-7.79879555	0.58796039	-1.21245762
Si	-0.82398122	-0.07555218	-2.92952956
C	0.70648763	-1.97718712	0.51045161
O	0.87438923	3.27050034	1.53421627
O	2.68787841	2.38611512	-0.01773095
H	-0.39961038	-1.41071212	-2.40622246
H	-2.40768935	0.64777395	-4.70799347
C	-2.44624215	2.11313243	0.77989829
C	-2.56479697	-1.17975903	0.46799872
O	-1.62316082	0.73324807	-1.71170992
H	1.54597986	0.03204623	-0.52880401
C	0.82272795	4.16475861	2.64326416
C	3.36961974	3.61598345	-0.26551999
C	3.28713925	1.21594772	3.49690822
C	4.86348951	3.28485715	-0.52535587
C	0.67495157	0.93047720	-3.43690839
H	-2.88345385	-0.92908886	-4.03776048
H	-7.93700527	0.52361600	-0.13553365
H	-8.30392177	-0.26297601	-1.68467879
H	-8.26501211	1.51315858	-1.57541053
H	-5.02812472	0.49056889	-3.17772804
H	-6.44956814	1.53702483	-3.45121443
H	2.47832287	-0.65107591	1.40106951
H	-4.74917809	0.60587423	1.37153680
H	-6.25990257	-0.27850593	1.07964779
H	-6.25645740	1.49343437	1.08268785
H	-2.02054851	-1.92647053	-0.12117334
H	-2.23592197	-1.27336789	1.50977329
H	-3.63063861	-1.40261033	0.39698310
H	-2.45354126	1.90501579	1.85482426
H	-1.62852499	2.81367587	0.58532630
H	-3.38894726	2.58304070	0.49170036
H	3.33279020	4.30073818	0.58272002
C	-0.50413814	3.96675705	3.43737498
C	0.97539132	5.61475869	2.10759520
H	1.63952738	3.98865670	3.34639895
C	2.66651939	4.31725403	-1.46119203
C	3.13231959	1.86740928	4.89464309
C	4.72577006	0.71249987	3.20419417
H	2.60256778	0.35760582	3.45959048
F	5.02431161	2.32598381	-1.47035599
F	5.43093314	2.83890805	0.62671215
F	5.54158742	4.39687953	-0.92346423
F	3.17820932	5.56437956	-1.65033454
F	1.33892160	4.44703126	-1.19913817
F	2.79686404	3.62074995	-2.61920519
F	5.66531686	1.68365353	3.36240210
F	4.80841838	0.26445561	1.92436600
F	5.04049831	-0.32020763	4.03187977
F	3.49823632	1.01024226	5.87767414
F	1.82883451	2.21059861	5.09516525
F	3.87004766	3.00676933	5.02181136
F	-1.58358906	4.49456934	2.79579220
F	-0.40426447	4.57484794	4.65417729
F	-0.73293573	2.65282865	3.64066795
F	0.15408649	5.87503206	1.06597679
F	2.26411222	5.80928658	1.67673184
F	0.73807911	6.52548223	3.08525852

$IrH_2Cl(CO)(P(OMe)_3)$

E = -3461.66

G = -3397.32

N_{imag} = 0

Ir	-2.00429653	-0.41870021	1.26093621
O	1.27672756	0.33268233	1.80677243
H	-2.15586421	-1.26240828	-0.06464816
C	-3.91677933	-0.30155763	1.33245652
H	-2.04734266	0.52944709	0.00142434
Cl	-1.64975264	-0.50947459	3.65230468
O	-5.06699476	-0.22706980	1.27515807
P	0.30684296	-0.56112462	0.87994023
O	0.97772769	-2.02257683	1.01174918
O	0.82398154	-0.12827655	-0.58967260
C	0.67968222	-2.89090354	2.15657004
C	0.92815507	1.72137732	2.12177405
C	0.28252067	-0.74921831	-1.79639224
H	0.48091495	-1.82477996	-1.78454982
H	1.00689863	-2.41163723	3.08237862
H	0.96990477	2.32887006	1.21298203
H	0.80448145	-0.27794588	-2.63013110
H	-0.79261837	-0.56095255	-1.86932264
H	1.68097534	2.05664160	2.83581471
H	-0.06649145	1.76474259	2.57270279
H	1.24127395	-3.80834370	1.97815150
H	-0.39227560	-3.09861914	2.20177516

$IrH_2Cl(CO)(P(OHFIP)_3)$

E = -6846.26

G = -6781.94

N_{imag} = 0

Ir	-2.17977878	-0.16920309	1.82311735
O	1.18693044	0.40376324	1.43729684
H	-2.71293868	-0.85822955	0.51331605
C	-4.01809188	0.14516187	2.29578643
H	-2.36412619	0.89015964	0.66308078
Cl	-1.45184446	-0.67398634	4.08070898
O	-5.13355049	0.33912760	2.48849777
P	-0.08271868	-0.52126119	0.95342084
O	0.67246204	-1.94994537	1.12114187
O	-0.12553509	-0.39732008	-0.66703858
C	0.53551556	-2.81812714	2.25557346
C	1.28413465	1.82813273	1.35277887
C	0.97541078	-0.50871932	-1.58066561
C	2.75796691	2.14921716	0.96307027
C	0.86580093	2.47474498	2.70731602
H	0.64116934	2.24453614	0.57274828
C	0.90341863	0.72760510	-2.52344097
C	0.86554161	-1.86190382	-2.34301468
H	1.94205441	-0.48513859	-1.07102712
C	1.94977321	-3.02674698	2.85029074
C	-0.17199243	-4.11099050	1.77619784
H	-0.09027134	-2.37003553	3.03835752
F	2.41947928	-1.83372700	3.30666788
F	2.83582815	-3.49919703	1.93539506

F	1.90798327	-3.89446453	3.89464284
F	0.55038326	-4.80217169	0.85876333
F	-1.36247076	-3.77454771	1.20156630
F	-0.42925559	-4.93105054	2.82738948
F	0.78839719	1.86805599	-1.77800460
F	-0.16129233	0.68017453	-3.36002084
F	2.03408091	0.83044197	-3.26354700
F	-0.38192136	-2.06690478	-2.83380481
F	1.16064204	-2.89045852	-1.50896911
F	1.74717286	-1.89326254	-3.37865869
F	3.13739749	1.37775911	-0.09777019
F	3.62277693	1.90619775	1.97735316
F	2.87711474	3.44808069	0.59078010
F	1.39094986	1.82036415	3.76636104
F	-0.49183985	2.44956743	2.82197999
F	1.25944001	3.77557755	2.76066507

7.3. Computational Details for Chapter 4

Table 7.3. Cartesian coordinates (in Å), energies (in kcal mol^{-1}), and number of imaginary frequencies computed at COSMO(Et_2O)-ZORA-M06/TZ2P//COSMO(Et_2O)-ZORA-BLYP-D3(BJ)/TZ2P.

Int4_1
E = -11072.01
G = -10783.10
N_{imag} = 0

C	0.06306410	-1.26086666	2.16448745
C	-0.63610709	-0.79777579	3.42416712
H	-1.91383683	0.22710625	0.25396355
H	0.08109200	-0.30195202	4.09828365
C	-1.77459477	0.21189999	3.17926356
C	-0.09033228	-0.67440354	0.94729185
C	-0.99218401	0.53530676	0.77107253
C	-1.33984567	1.21852978	2.10148200
H	-1.95225647	0.75917842	4.10585883
H	-2.12907633	1.96107626	1.95096852
H	-0.45485682	1.74671173	2.48193352
C	-5.87204773	-1.54900773	5.07355623
H	-0.51126359	1.26662050	0.11285201
H	-1.01234443	-1.65629710	3.99434037
N	-3.08573580	-0.43157466	2.81820171
C	-3.18093966	-1.74704773	2.13354488
H	-2.24871953	-1.86422157	1.57716469
H	-4.00777725	-1.70880118	1.42243760
C	-3.35757503	-2.93419353	3.06874390
C	-4.37761638	-3.74983586	3.01883866
C	-5.41597387	-4.54271988	2.97147619
S	-4.48153289	0.21255116	3.44376410
O	-5.57565882	-0.12126151	2.52808124
O	-4.19926282	1.61352478	3.77150885
H	-3.16144077	0.30757592	6.02545764
H	5.56098994	-6.41395923	3.42411058
H	7.37364441	-2.65649994	2.34877580
H	7.53491823	-4.88341238	3.45591280
N	0.50703079	-1.15787680	-0.20782884
C	1.21088385	-2.42867528	-0.22404933
H	-3.54163913	-0.94794740	8.13239975

Int4_2
E = -11070.93
G = -10782.17
N_{imag} = 0

C	-0.45914742	-1.35487854	2.10733240
C	-0.88908642	-0.39520288	3.23187504
H	-1.13540340	-2.21794135	2.05226097
H	-0.01803115	0.20379934	3.52834159
C	-1.99016972	0.61161567	2.84720814
C	-0.38593724	-0.70427398	0.73846720
C	-0.91049325	0.52662757	0.51153865
C	-1.59687768	1.37267020	1.56053521
H	-2.06540065	1.34592571	3.64997540
H	-2.49791596	1.84100477	1.14290458
H	-0.94368230	2.20800906	1.86214978
H	-0.85411908	0.96148632	-0.48228527
H	0.51933647	-1.76929643	2.37719165
H	-1.19284787	-0.96863339	4.11373795
N	-3.36676411	0.03407041	2.75311554
C	-3.74605907	-0.94447802	1.70367906
H	-2.97649946	-0.84986145	0.93190717
H	-4.69955798	-0.64821813	1.26201261
C	-3.83554665	-2.38226606	2.18826947
C	-4.86675857	-3.15586222	1.97098753
C	-5.91673336	-3.90630045	1.76141163
S	-4.43902956	0.32858287	3.98874816
O	-5.76315383	-0.06413807	3.50324531
O	-4.20748483	1.69387828	4.47153001
H	-2.53818027	0.59438466	6.15751682
H	5.17114867	-6.40434396	3.96765905
H	6.81113197	-2.53904369	3.00373646
H	7.03157601	-4.74648278	4.13919541
C	0.34440105	-0.57820681	-1.55584439
H	0.60571756	0.48498615	-1.56474472
H	-0.69478721	-0.67650360	-1.90847838
C	1.31101278	-2.78597507	-1.73215465
C	1.30642661	-1.40810749	-2.42127615
H	2.19817657	-3.38277882	-1.96340825
H	0.42553529	-3.36603057	-2.01645996
H	2.30876558	-0.96943097	-2.38550753
H	0.98347352	-1.45877427	-3.46531907
C	2.62515439	-2.32369442	0.40502462
H	-5.42922104	-5.43486134	2.34567023
C	-6.08942664	-2.24220694	6.26758450
H	-6.30793241	-4.33907600	3.56428765
O	3.33522396	-1.32577499	0.26542985
N	3.00689862	-3.46842159	1.06476125
H	2.30139413	-4.19758034	1.11645702
H	5.27333656	-1.95915533	1.22554183
C	-5.24781178	-2.03315306	7.36557062
C	-4.19061094	-1.11818186	7.27702032
C	-3.96955287	-0.41393681	6.09151869
H	-2.58037156	-3.09761976	3.81589532
H	-6.50785775	-1.70705593	4.20940943
H	-6.91419767	-2.94703866	6.33755141
H	-5.41709430	-2.57745141	8.29127256
H	0.63106039	-3.18748547	0.32483030
C	4.23518273	-3.79218260	1.68759156
C	4.32606736	-5.05006533	2.31370304
C	5.50682580	-5.43895738	2.94548242
C	6.61410142	-4.58094938	2.96343838
C	6.52091946	-3.33183028	2.34131938
C	5.34365935	-2.92676205	1.70382715
H	3.46770158	-5.71972104	2.30096879
C	-4.81138619	-0.64296562	4.99590946
H	0.73001454	-2.10920606	2.28617005
N	0.17038546	-1.48048408	-0.27105493
C	0.86606117	-2.74110053	-0.05364498
H	-1.82531276	-0.97927198	7.94831783
C	0.36652057	-0.95617372	-1.63177483
H	0.85009381	0.02991599	-1.60083928
H	-0.60776719	-0.83383270	-2.13007138
C	1.05559107	-3.28447887	-1.49385857
C	1.25596120	-2.00434294	-2.33045323
H	1.89162079	-3.98603990	-1.56980227
H	0.13954419	-3.80721015	-1.79124548
H	2.30330676	-1.69019608	-2.28779674
H	0.98256050	-2.14596133	-3.38006905
C	2.24064368	-2.55347498	0.64376785
H	-6.00741318	-4.53014619	0.87219514
C	-4.22584492	-2.89726877	6.46306013
H	-6.74319128	-3.93442681	2.47240857
O	2.91431188	-1.53032458	0.50259497
N	2.61990627	-3.64335967	1.39269282
H	1.94955624	-4.40604668	1.42446547
H	4.76518109	-1.98750979	1.71198593
C	-3.21348352	-2.52776387	7.35668789
C	-2.60229623	-1.27277975	7.24701411
C	-2.99445936	-0.38670725	6.24034874
H	-2.98979252	-2.76955447	2.75653452
H	-5.40251109	-2.29546352	4.74719799
H	-4.70990613	-3.86624346	6.55609464
H	-2.90670850	-3.21339592	8.14269865
H	0.25435234	-3.43092272	0.54056750
C	3.81677427	-3.88359642	2.10844108
C	3.94046239	-5.13003632	2.75142258
C	5.09077524	-5.43707028	3.47724937
C	6.13431632	-4.50751075	3.57390722
C	6.00826536	-3.26964069	2.93534384

C	4.86074472	-2.94620514	2.20377336
H	3.13174307	-5.85511054	2.67751544
C	-3.99690875	-0.77525953	5.34316505
C	-4.62225999	-2.02205243	5.44818225

Cu(TFA)

E = -1388.43

G = -1395.06

N_{imag} = 0

O	-2.31479210	-1.94800062	0.00000000
C	-2.19199413	-3.17077043	0.00000000
C	-3.46929460	-4.08519738	0.00000000
F	-4.61351488	-3.35591101	0.00000000
F	-3.49306885	-4.89334751	-1.10402120
F	-3.49306885	-4.89334751	1.10402120
O	-1.10805732	-3.88629671	0.00000000
Cu	0.45907336	-2.82914781	0.00000000

Int4_3

E = -12501.77

G = -12205.60

N_{imag} = 0

C	2.43482053	-2.75469638	1.26899554
C	1.53446533	-3.71818937	0.46380757
H	2.04204917	-2.62608491	2.28767861
H	2.15346902	-4.25633931	-0.26507685
C	0.42260203	-3.03533709	-0.35289207
C	2.61122437	-1.38551657	0.63427074
C	1.99287879	-1.04888740	-0.52731820
C	1.03832467	-1.95647984	-1.26389951
H	-0.02966935	-3.79868179	-0.99087120
H	0.23503683	-1.36919154	-1.72282702
H	1.53966105	-2.47966698	-2.09486212
H	2.14448221	-0.06558490	-0.95997637
H	3.41807242	-3.22365345	1.40163176
H	1.10065436	-4.47032481	1.13144738
N	-0.70682916	-2.53332516	0.49202317
C	-0.57428678	-1.40674381	1.42177782
H	-1.38817049	-1.46796625	2.14932405
H	0.36340373	-1.51367025	1.96382528
C	-0.59223671	-0.01861668	0.77582865
C	-1.38499024	0.29092822	-0.21918621
C	-2.24106067	0.30406875	-1.26330575
S	-2.21833081	-3.12798534	0.13204341
O	-3.16459388	-2.44938034	1.02465132
O	-2.46027968	-3.10076677	-1.31415542
H	-2.38601144	-5.60509605	-1.37792348
H	4.25344346	4.65605565	-4.84706838
H	7.72007847	2.21349331	-4.08729617
H	6.53791991	3.88813901	-5.50611321
N	3.36522674	-0.48883017	1.37885806
C	3.56120025	0.88949804	0.95149376
H	2.59664827	1.35014141	0.71105797
C	4.27474955	-0.87244898	2.48112070
H	3.69842365	-1.20144006	3.35705919
H	4.93902619	-1.69360985	2.18474623
C	4.21320208	1.54901892	2.19188204
C	5.07632314	0.41329391	2.78029094
H	3.42112087	1.84375505	2.88982154
H	4.79307261	2.44082850	1.93647750
H	5.26231965	0.54054740	3.85092722
H	6.03973973	0.37505150	2.26421328
C	4.50527504	1.00445646	-0.27584355
H	-1.94316329	-0.08376462	-2.23886725
Cu	-1.27225736	2.13478422	-1.08060454
H	-3.30494364	0.49255355	-1.11268279
O	5.48064562	0.25806171	-0.41439058
N	4.17204109	2.03012254	-1.12378591
H	3.28673043	2.50575733	-0.92631366
H	6.64229899	1.31254991	-2.04335205
F	0.45987773	6.36663129	-0.43160220
F	2.50254241	5.56672491	-0.57447971
F	1.29809616	5.82174560	-2.40057167
H	0.08314184	0.72002939	1.20079032
O	-0.57755419	3.92886113	-1.18564780
O	1.46580016	3.07823830	-0.67335933
C	0.68605009	3.99749886	-0.95044752
C	1.24443472	5.45786819	-1.07749589
C	4.84247154	2.47681994	-2.28547346
C	4.17572426	3.42189795	-3.09007773
C	4.78319564	3.92585100	-4.23951004
C	6.06398570	3.49576891	-4.60976123
C	6.72480515	2.55571741	-3.81177967
C	6.12872676	2.04171621	-2.65560745
H	3.18203885	3.75735133	-2.80806629
C	-2.09319101	-4.85579493	0.61990120
C	-1.86599011	-5.15223497	1.96960677
C	-1.75809247	-6.48678793	2.36125645
C	-1.87109933	-7.51014389	1.40938194
C	-2.09549292	-7.19939483	0.06491807
C	-2.21001192	-5.86402075	-0.33911831
H	-1.77442424	-4.35243390	2.69875955
H	-1.58428119	-6.72916856	3.40649214
H	-1.78249289	-8.54855870	1.71883232
H	-2.18223971	-7.99256390	-0.67319960

Int4_4

E = -12502.67

G = -12203.12

N_{imag} = 0

C	3.50256257	-2.75307816	-0.46356889
C	2.99850567	-3.27297183	-1.82892106
H	3.02188174	-3.29334066	0.36326108
H	3.80614561	-3.16100215	-2.56247954
C	1.79613408	-2.52305494	-2.43145410
C	3.29169169	-1.26919629	-0.23753462
C	2.61854388	-0.49494480	-1.12283263
C	2.03723230	-1.00316714	-2.41773777
H	1.71995764	-2.82665726	-3.47614654
H	1.08929682	-0.49807213	-2.63857867
H	2.70584379	-0.76796788	-3.26324514
H	2.48095201	0.56330054	-0.92703266
H	4.57006866	-2.99109967	-0.37936191
H	2.78535034	-4.34635677	-1.76748486
N	0.45814553	-2.87787369	-1.83544419
C	0.29208937	-3.17277402	-0.40440647
H	-0.67880682	-3.66092090	-0.28832898
H	1.05657145	-3.86839197	-0.04285613
C	0.26975749	-1.91278233	0.45433845
C	0.64413497	-1.93183805	1.70979333
C	1.11521534	-2.23470619	2.93839780
S	-0.61081558	-3.63485563	-2.88516168
O	-1.88397075	-3.77984351	-2.17536280
O	-0.55951982	-2.91050292	-4.15456739
H	1.05632235	-4.72201988	-4.99691765
H	2.39806208	7.04632177	-0.72972945
H	6.33443845	5.65555223	-1.79355090
H	4.62165891	7.46566493	-1.78772999
N	3.73348988	-0.79983173	0.99377356
C	3.45671632	0.55768090	1.43575909
H	2.38031487	0.75532298	1.35381027
C	4.72141231	-1.48645440	1.84999357
H	4.27591162	-2.37481883	2.32483238
H	5.59048898	-1.82227787	1.27242111
C	3.93082838	0.55869832	2.90939757
C	5.11745397	-0.42613047	2.89800510
H	3.11968544	0.18943574	3.54993916
H	4.20280889	1.55727469	3.26222872
H	5.30677667	-0.86825801	3.88056516
H	6.02257279	0.09367247	2.57142892
C	4.21859114	1.64162870	0.62596738
H	0.47386115	-2.69953678	3.68978069
Cu	0.51809220	-0.25024451	2.89821861
H	2.18496325	-2.21462122	3.15023976
O	5.38101555	1.47399645	0.24332328
N	3.48080989	2.78359029	0.44647399
H	2.52074556	2.75072894	0.79741560
H	5.84073519	3.45324710	-0.75880252
F	1.21686758	4.14383152	4.23415770
F	0.12255449	4.93010367	2.49224408

F	-0.98140657	3.95924053	4.12640251
H	-0.13418346	-1.01652646	-0.00899728
O	0.13920384	1.53305428	3.48321544
O	0.72044146	2.49503200	1.50181987
C	0.35753320	2.51755897	2.68316988
C	0.16187795	3.90780484	3.38598113
C	3.84415042	4.00777124	-0.16043952
C	2.87541500	5.03108390	-0.15742042
C	3.15583443	6.26619428	-0.74033171
C	4.40315345	6.50232778	-1.33344080
C	5.36275200	5.48460736	-1.33515028
C	5.09764268	4.23952982	-0.75501285
H	1.90760930	4.84887283	0.30441578
C	0.07679454	-5.27425517	-3.15434106
C	-0.15624292	-6.27272329	-2.19933389
C	0.45895190	-7.51687110	-2.35510366
C	1.29810420	-7.75544113	-3.45077641
C	1.51617797	-6.75209119	-4.40142307
C	0.90530314	-5.50289478	-4.25904627
H	-0.81810920	-6.08459105	-1.35991826
H	0.27866970	-8.30032145	-1.62346117
H	1.77484262	-8.72547626	-3.56694339
H	2.15802462	-6.94039237	-5.25823757

Int4_5

E = -12498.51

G = -12201.52

N_{imag} = 0

C	-3.45462436	-3.38357884	1.29359249
C	-4.37184920	-3.26065650	2.51924164
H	-4.05930477	-3.43631448	0.37488269
H	-3.80467340	-3.50890221	3.42583217
C	-4.91558057	-1.83616159	2.70318530
C	-2.46218128	-2.23568184	1.18171913
C	-2.59098856	-1.11463382	1.94140354
C	-3.72690834	-0.88139003	2.91359475
H	-5.54523557	-1.80764061	3.59225999
H	-4.07381545	0.15776550	2.86777391
H	-3.39107186	-1.02961329	3.95252491
H	-1.86390798	-0.31323762	1.85071805
H	-2.91836734	-4.33756193	1.35298200
H	-5.19244630	-3.98180580	2.45646057
N	-5.80705431	-1.40403754	1.57048655
C	-5.32969675	-0.72904839	0.33830482
H	-6.09171239	-0.87187921	-0.43346686
H	-4.42630482	-1.23358217	-0.00226563
C	-5.02250427	0.75190949	0.49098667
C	-5.87371811	1.73582758	0.32948407
C	-6.49408100	2.92936735	0.21042403
S	-7.44563125	-1.61739125	1.67228514
O	-8.13589504	-0.33647524	1.41473061
O	-7.72754811	-2.30971879	2.93003696
H	-6.59484052	-4.29802654	1.01298935
H	-0.81238043	-10.51326816	-0.53593940
H	1.65190739	-8.76711987	2.53630934
H	0.80362044	-10.78711748	1.34889275
N	-1.47897959	-2.37515116	0.21490217
C	-1.23378319	-3.58805984	-0.55315291
H	-2.16347346	-3.97305798	-0.98899586
C	-0.43119326	-1.36086875	0.02001348
H	-0.87618996	-0.43751166	-0.38301624
H	0.04745350	-1.10972922	0.97624137
C	-0.26923946	-3.10267741	-1.66720105
C	0.56244426	-2.01184140	-0.96232598
H	-0.86534956	-2.67513571	-2.48126953
H	0.33949976	-3.91404131	-2.07664916
H	0.98269588	-1.28808148	-1.66636910
H	1.38698346	-2.46984818	-0.40742796
C	-0.56909495	-4.70655871	0.29462475
H	-6.42570325	3.50934517	-0.71066574
Cu	-7.87540064	1.43758837	-0.15257507
H	-6.89544702	3.43999198	1.08785667
O	0.15528604	-4.45514793	1.26014364
N	-0.85048609	-5.97112962	-0.16610912
H	-1.48361485	-6.01714537	-0.95927398
H	0.89970308	-6.50130097	1.85947453
F	-13.05036840	1.24094842	-0.79027763
F	-11.87339408	-0.53183015	-1.34859233
F	-11.87208503	1.25289747	-2.64861525
H	-3.99232670	1.00723613	0.74528954
O	-9.52410000	0.96397666	-1.07944580
O	-10.79450677	2.16534100	0.38379847
C	-10.62379037	1.40373774	-0.56947648
C	-11.87354747	0.84057728	-1.33929756
C	-0.37703591	-7.22854470	0.28029128
C	-0.85638767	-8.36943066	-0.39080557
C	-0.43331003	-9.64180714	-0.00740873
C	0.47313237	-9.79572732	1.04945083
C	0.94775587	-8.66043039	1.71414048
C	0.53272288	-7.37743847	1.34209120
H	-1.56001890	-8.25318644	-1.21351350
C	-7.85780651	-2.69799315	0.28884350
C	-8.74965834	-2.26211121	-0.69467283
C	-9.06125721	-3.12301228	-1.75330308
C	-8.48857064	-4.39622551	-1.81940228
C	-7.59964598	-4.82133021	-0.82215087
C	-7.27945576	-3.97242889	0.23747052
H	-9.18949781	-1.27299465	-0.64368437
H	-9.75274321	-2.79123219	-2.52329553
H	-8.73346963	-5.06029572	-2.64462604
H	-7.15776751	-5.81332963	-0.86920980

Int4_6

E = -12498.23

G = -12198.30

N_{imag} = 0

C	-0.01928831	-1.90103415	2.33776090
C	-0.33439492	-1.36458486	3.75360405
H	-0.63004440	-2.78319491	2.11092821
H	0.56680532	-0.87572754	4.14269245
C	-1.43369097	-0.29153640	3.84850820
C	-0.20456133	-0.88730099	1.22697718
C	-0.73052541	0.33608724	1.46250528
C	-1.15681492	0.82682706	2.82223725
H	-1.36972160	0.14267218	4.84667968
H	-2.03922172	1.46595715	2.72357569
H	-0.37954753	1.47569691	3.25982586
H	-0.86705338	1.03160101	0.64013323
H	1.01787446	-2.25824449	2.34626470
H	-0.55117045	-2.19812838	4.43087662
N	-2.82289308	-0.87028073	3.79482742
C	-3.18545764	-2.04391498	2.98993632
H	-4.18459319	-2.35540846	3.30607548
H	-2.51334629	-2.86866697	3.24365855
C	-3.17144191	-1.81297189	1.47904145
C	-2.87353009	-2.78005964	0.64436513
C	-2.47813765	-3.97193403	0.12113621
S	-4.08474002	0.01707805	4.44734167
O	-3.49671008	0.95971993	5.39907487
O	-5.10541265	-0.93743590	4.89016959
H	-5.98686275	-0.70303066	2.37946573
H	6.43212517	-6.29316769	1.61321831
H	7.31818988	-2.08010695	1.77350863
H	8.04885979	-4.44420621	2.06745764
N	0.09711083	-1.33262383	-0.06489240
C	0.98002707	-2.46935209	-0.32146047
H	-6.88306089	0.55985803	0.43642298
C	0.15013861	-0.36370258	-1.18673302
H	0.69211850	0.54046777	-0.88003601
H	-0.86757932	-0.06964057	-1.46678942
C	0.95554177	-2.57470912	-1.86483407
C	0.89339711	-1.10198664	-2.32292284
H	1.81975729	-3.11403852	-2.26269242
H	0.05078759	-3.11338954	-2.16730382
H	1.90409689	-0.69748743	-2.42827118
H	0.38809044	-0.99709008	-3.28614336
C	2.42670228	-2.24445326	0.18995351
H	-3.19959314	-4.76311828	-0.08737058
Cu	-2.62427917	-2.53314560	-1.33228170
H	-1.42579543	-4.26130415	0.10577810

O	2.91915232	-1.11862317	0.28822399
N	3.08228900	-3.41667942	0.48701050
H	2.53971173	-4.26623496	0.36199838
H	5.00655410	-1.55999588	1.03535208
F	-1.50698615	0.01925513	-5.02987370
F	-3.71222316	-0.01048768	-5.10781429
F	-2.55912527	-1.64694817	-6.01638053
H	-3.41572115	-0.81625909	1.12587055
O	-2.18628215	-2.73056057	-3.54774928
O	-3.01258263	-0.89059383	-2.57987462
C	-2.61219061	-1.54722055	-3.59210569
C	-2.60992757	-0.79544032	-4.95914268
C	4.41693676	-3.63107343	0.90762596
C	4.82915004	-4.96682307	1.07473059
C	6.12855264	-5.25625528	1.48960223
C	7.03562429	-4.21954724	1.74394426
C	6.62295977	-2.89353673	1.57816772
C	5.32301185	-2.58645027	1.16277259
H	4.12689373	-5.77477723	0.87599418
C	-4.81941703	0.96731431	3.10409416
C	-4.46684611	2.31076793	2.93720785
C	-4.98722048	3.01942672	1.85062810
C	-5.84521551	2.38712016	0.94374217
C	-6.20454728	1.04710068	1.13179147
C	-5.69766751	0.33021583	2.21826357
H	-3.80701831	2.79124339	3.65195127
H	-4.72151730	4.06460607	1.71480266
H	-6.24136315	2.94033293	0.09597394
H	0.58036395	-3.38003956	0.14025578

TS4_1

E = -12485.85

G = -12187.55

N_{imag} = 1, 214i cm^{-1}

C	2.21679112	-3.06198958	0.82082131
C	1.07427248	-3.82740668	0.09316514
H	2.04996602	-3.08149317	1.90547895
H	1.51775976	-4.47784937	-0.66870760
C	0.03894836	-2.95855997	-0.65379639
C	2.41767110	-1.61920274	0.40003193
C	1.69423711	-1.06790937	-0.62762765
C	0.76887745	-1.88854382	-1.48285302
H	-0.50905447	-3.60340091	-1.34235845
H	0.04225542	-1.24585341	-1.98601407
H	1.32265372	-2.41077972	-2.27953747
H	1.87865404	-0.04681632	-0.93864586
H	3.15844531	-3.60510397	0.66785992
H	0.56528038	-4.48715210	0.80314524
N	-1.01009492	-2.34260507	0.21764546
C	-0.62527239	-1.61932142	1.44033415
H	-1.51586220	-1.50323346	2.06163410
H	0.10711997	-2.19149275	2.01624114
C	-0.06404383	-0.24634943	1.09756230
C	-0.82812527	0.67655384	0.44567975
C	-1.67562268	0.73326208	-0.61070095
S	-2.54475477	-3.00575450	0.13111061
O	-3.41115184	-2.18838496	0.98102326
O	-2.86392291	-3.18798043	-1.28490129
H	-2.27202486	-5.65407962	-1.01931585
H	4.76991767	5.65539355	-3.56036274
H	6.71259311	2.00613127	-4.77282423
H	6.22950503	4.41888832	-5.16671410
N	3.27411380	-0.88011345	1.17060388
C	3.53398499	0.53734104	0.91843227
H	2.59254635	1.09610900	0.84904604
C	4.12654598	-1.42607980	2.25392520
H	3.51704650	-1.65487238	3.13960776
H	4.62225048	-2.34690666	1.93180553
C	4.34881078	0.98118097	2.15860454
C	5.12660495	-0.29290144	2.53959335
H	3.65351017	1.26931649	2.95515636
H	4.99287259	1.83750346	1.94457210
H	5.45847714	-0.29177021	3.58146335
H	6.00405052	-0.40266507	1.89445436
C	4.33799172	0.75350231	-0.39399224
H	-1.54703168	0.10355553	-1.49198312
Cu	-0.34291275	2.54240464	0.62596622
H	-2.49149716	1.45228758	-0.65639628
O	5.10192136	-0.10711693	-0.84154522
N	4.12376979	1.99057713	-0.93717973
H	3.48935594	2.60468233	-0.41708658
H	5.75646723	0.83766048	-2.80324913
F	2.91935771	6.21605953	1.87212171
F	2.52372665	6.48901568	-0.28116647
F	0.94876608	6.91934741	1.19591769
H	0.82058762	0.05347292	1.64636618
O	0.26193273	4.37734463	0.83047805
O	2.44008340	3.73850140	0.63277337
C	1.52702128	4.56507128	0.77713398
C	1.96745953	6.06737821	0.90161072
C	4.72338932	2.58502719	-2.07200656
C	4.44960216	3.94894829	-2.29496362
C	4.98920264	4.60187874	-3.40246586
C	5.80861611	3.90914683	-4.30351050
C	6.07878855	2.55518774	-4.07974985
C	5.54518895	1.88496129	-2.97375501
H	3.81819774	4.48783031	-1.59324288
C	-2.38715658	-4.63322140	0.87734098
C	-2.34204405	-4.73346780	2.27417734
C	-2.12162492	-5.98337324	2.85635479
C	-1.94764573	-7.11499534	2.04936008
C	-2.00272045	-7.00134297	0.65598660
C	-2.22180888	-5.75577420	0.05970283
H	-2.48966450	-3.85376739	2.89273866
H	-2.09065005	-6.07371378	3.93910255
H	-1.77653231	-8.08565988	2.50790848
H	-1.87801624	-7.88115822	0.03002285

TS4_2

E = -12484.83

G = -12185.32

Nimag = 1, 237i cm-1

C	3.25723199	-1.52364274	-2.03694597
C	2.66143691	-0.79852189	-3.26681777
H	2.98696138	-2.58939736	-2.04153951
H	3.35417327	-0.00434067	-3.56985102
C	1.30202820	-0.10069526	-3.04900486
C	2.85894885	-0.94542300	-0.69763529
C	1.91701240	0.04706042	-0.60031174
C	1.35400847	0.77797094	-1.78996817
H	1.11437914	0.55031252	-3.90401944
H	0.34712134	1.14877194	-1.56863862
H	1.96432543	1.66668784	-2.01971368
H	1.65370229	0.44437122	0.37388578
H	4.35005705	-1.50823267	-2.12257945
H	2.60303102	-1.49416708	-4.10920777
N	0.11157857	-1.01257464	-2.99600134
C	0.14527707	-2.20337792	-2.12667388
H	-0.74102702	-2.80473730	-2.37446893
H	1.01882515	-2.83079935	-2.33128944
C	0.02264728	-1.91123369	-0.65265091
C	0.36875833	-2.85780727	0.26829705
C	0.34287039	-4.21526376	0.33043563
S	-0.78085234	-1.14554982	-4.41398856
O	-1.93791119	-1.98896418	-4.10421809
O	-0.97675236	0.20931481	-4.92853998
H	0.90268009	-0.23945371	-6.59106080
H	2.81110366	4.97733443	5.28391983
H	6.37138819	4.88124066	2.85969473
H	4.92149650	6.06333318	4.50623261
N	3.41947785	-1.53334478	0.40519580
C	3.30156625	-0.94138645	1.74252422
H	2.25172565	-0.77251838	1.98858001
C	4.47264752	-2.57978004	0.35614196
H	4.02884149	-3.53755694	0.05956110
H	5.24887783	-2.32173226	-0.37091181
C	3.92767916	-2.01207397	2.66325997
C	5.04028462	-2.62477356	1.78960699
H	3.16290910	-2.75899832	2.90731549
H	4.29823825	-1.58866179	3.60056250

H	5.29862294	-3.64250665	2.09462587
H	5.94115922	-2.00733292	1.84834270
C	4.06601978	0.40454756	1.84353126
H	-0.39458827	-4.80193531	-0.22679604
Cu	0.45595865	-2.42890466	2.16008058
H	0.99540059	-4.78657857	0.98817766
O	5.11511355	0.60754382	1.22339347
N	3.47180175	1.27857429	2.71378715
H	2.57746659	0.97386960	3.10911984
H	5.72676581	2.64543398	1.99430731
F	2.20675197	-0.79786075	6.26227585
F	0.61838914	0.73073610	6.30332223
F	0.11403922	-1.37826947	6.65840080
H	-0.52700130	-1.01808100	-0.36982353
O	0.49189212	-1.95950419	4.04413164
O	0.89352883	0.24696564	3.64438322
C	0.72914617	-0.74496068	4.37246217
C	0.89738550	-0.54461168	5.92033657
C	3.90935542	2.54962618	3.15204072
C	3.08933656	3.21745919	4.08307985
C	3.45341283	4.47422639	4.56478482
C	4.63766584	5.08369705	4.12956696
C	5.44973857	4.41802742	3.20546413
C	5.09859917	3.15745353	2.71110280
H	2.17150603	2.74246989	4.42341466
C	0.26826361	-2.03186095	-5.57228924
C	0.39090617	-3.42217140	-5.44732653
C	1.29477674	-4.09878564	-6.26954246
C	2.06262044	-3.39167181	-7.20328509
C	1.92120314	-2.00469797	-7.32573007
C	1.02230270	-1.31459529	-6.50750449
H	-0.21809306	-3.96485091	-4.73135769
H	1.39520066	-5.17771990	-6.18379545
H	2.76572986	-3.92322667	-7.83949001
H	2.50926221	-1.45750523	-8.05794675

TS4_3

E = -12466.82

G = -12166.27

Nimag = 1, 289i cm-1

C	-3.47176145	-4.03080736	1.08729514
C	-4.67733559	-4.11858626	2.04732796
H	-3.73721462	-4.43978837	0.10222488
H	-4.30109524	-4.21763928	3.07275901
C	-5.60283354	-2.89068919	2.05328139
C	-2.93151141	-2.63086694	0.88936674
C	-3.62231256	-1.52178569	1.34003363
C	-4.78865619	-1.60450495	2.27833404
H	-6.29605318	-3.02016897	2.88593580
H	-5.43022430	-0.72577468	2.13841931
H	-4.45474758	-1.58175999	3.32669025
H	-3.19863244	-0.53830764	1.17765999
H	-2.67392883	-4.67994453	1.46667464
H	-5.25767863	-5.02095547	1.83019908
N	-6.47634758	-2.82095616	0.83814823
C	-5.89066661	-2.54984601	-0.50770786
H	-6.73379486	-2.42997189	-1.19695368
H	-5.38391051	-3.47056783	-0.80718738
C	-4.94855701	-1.37674655	-0.72442338
C	-5.34920718	-0.05278808	-0.73654584
C	-4.96167915	0.92102470	-1.61962297
S	-8.02940991	-2.27292362	1.19068439
O	-8.08186924	-0.81356514	1.42319450
O	-8.53393516	-3.11252132	2.28286459
H	-8.57962986	-4.76082880	-0.15461250
H	1.64229414	-9.93806893	0.39034734
H	2.62750522	-7.33255968	3.67687103
H	2.80150104	-9.55770190	2.56951328
N	-1.81962731	-2.50286059	0.11174674
C	-1.07601792	-3.62426712	-0.46956328
H	-1.75797756	-4.31332799	-0.97825106
C	-1.12923717	-1.20466831	-0.10183877
H	-1.75160292	-0.55460465	-0.72727607
H	-0.97046268	-0.70522611	0.85993653
C	-0.12561510	-2.92986061	-1.47833767
C	0.19017044	-1.58470829	-0.79527054
H	-0.66450895	-2.77452498	-2.41953103
H	0.76493497	-3.52854060	-1.68714057
H	0.51357390	-0.82016070	-1.50623236
H	0.97832250	-1.71820967	-0.04831866
C	-0.26784235	-4.39729289	0.60868840
H	-4.56825573	0.67657483	-2.61279464
Cu	-6.99890326	0.68667460	-0.07236486
H	-5.07013146	1.98353766	-1.41095910
O	0.12491135	-3.85583802	1.64365714
N	-0.02424218	-5.70000426	0.25698897
H	-0.43397751	-6.00449282	-0.62133228
H	1.31630695	-5.50548687	2.62962901
F	-10.85445592	3.61264127	2.00010932
F	-11.38735357	1.78514264	0.89597133
F	-10.75113244	3.59528070	-0.19675606
H	-4.00256566	-1.64878171	-1.19181809
O	-8.70627593	1.69181188	-0.07377992
O	-8.35043094	2.59321275	1.99176080
C	-9.02315883	2.33936624	0.98696325
C	-10.51278923	2.84473638	0.92835471
C	0.74255290	-6.69067177	0.92026774
C	0.83876401	-7.94730977	0.29431037
C	1.57615414	-8.97238415	0.88570559
C	2.22635046	-8.75915781	2.10787206
C	2.12753009	-7.50932858	2.72736304
C	1.39146586	-6.47074714	2.14742062
H	0.33490174	-8.11514914	-0.65601413
C	-8.93722717	-2.63391499	-0.31005304
C	-9.54838285	-1.58590088	-1.00536019
C	-10.28773595	-1.88757230	-2.15366959
C	-10.40727366	-3.21213506	-2.58681525
C	-9.79596724	-4.25065415	-1.87079329
C	-9.05764634	-3.96755906	-0.72134766
H	-9.45492513	-0.56267067	-0.65459545
H	-10.76875182	-1.08493814	-2.70622253
H	-10.98095188	-3.43893916	-3.48194672
H	-9.89671447	-5.27945793	-2.20636065

TS4_4

E = -12478.27

G = -12177.78

Nimag = 1, 123i cm-1

C	0.16793960	-1.34686056	2.00315352
C	-0.10214769	-0.45202455	3.23932911
H	-0.49289005	-2.22595981	1.99642590
H	0.82927728	0.07000446	3.48968795
C	-1.17111902	0.64845815	3.06651785
C	0.01143339	-0.63748733	0.67916155
C	-0.64041856	0.56634695	0.59601429
C	-0.92822983	1.44767146	1.77902573
H	-1.09398760	1.32970164	3.91459747
H	-1.79713967	2.08389383	1.57890950
H	-0.07914498	2.13059170	1.94099852
H	-0.79222514	1.01022494	-0.38329581
H	1.18181675	-1.74564124	2.09771718
H	-0.34951148	-1.08189507	4.10039975
N	-2.58657086	0.16818513	3.08887313
C	-2.94468046	-1.01997234	2.29849125
H	-4.00015083	-1.26094505	2.51672668
H	-2.37852619	-1.90285254	2.60987647
C	-2.90348503	-0.85105413	0.80485623
C	-2.88898277	-1.99569670	0.01697348
C	-3.52413274	-3.17849242	0.21725786
S	-3.41043932	0.27226719	4.55476511
O	-2.93556141	1.48694276	5.22549102
O	-3.37553576	-0.99390612	5.30067136
H	-5.86354211	-1.18171503	5.04022882
H	5.56992494	-6.75800540	2.83323568
H	7.16658906	-2.77943263	2.40627007
H	7.42855846	-5.12924476	3.19316042
N	0.41920426	-1.28249327	-0.46723942
C	1.12848039	-2.57363862	-0.44777756
H	-8.20330134	-0.80428102	4.25055519
C	0.80851157	-0.49689553	-1.68949531

H	1.41675410	0.35779172	-1.37656328
H	-0.08244972	-0.12195218	-2.19590293
C	1.31841023	-2.87868676	-1.95133344
C	1.60481328	-1.48991508	-2.56218773
H	2.12209136	-3.59859264	-2.12779133
H	0.38746503	-3.29336381	-2.35013465
H	2.67259416	-1.26398316	-2.50046917
H	1.30389694	-1.44108828	-3.61038598
C	2.51263755	-2.47264134	0.24631258
H	-4.37490268	-3.26127263	0.90013277
Cu	-2.03360331	-1.90641327	-1.70125872
H	-3.28527517	-4.07643819	-0.34692503
O	3.15853816	-1.42263724	0.27029298
N	2.92957770	-3.66696135	0.77717482
H	2.27385804	-4.43849047	0.69616431
H	5.08034790	-2.05762270	1.27374640
F	-0.02583004	-1.73872767	-5.97866110
F	-1.39350887	-0.12155231	-6.57754570
F	-2.16389709	-2.16586314	-6.32926970
H	-3.15794965	0.12076789	0.39287687
O	-1.59236824	-2.04220651	-3.59957911
O	-1.74542039	0.21001588	-3.92340393
C	-1.58595933	-0.95891471	-4.29123013
C	-1.29723588	-1.24101151	-5.81126762
C	4.15082764	-3.99949424	1.41428683
C	4.29719885	-5.32670861	1.85905017
C	5.47087223	-5.72927374	2.49511945
C	6.51354201	-4.81598253	2.69677290
C	6.36406775	-3.49764277	2.25455754
C	5.19319205	-3.07795477	1.61446771
H	3.48869652	-6.03874537	1.70279912
C	-5.09305784	0.52364502	3.97152595
C	-5.35898770	1.60696696	3.12493438
C	-6.66696200	1.81291185	2.68487854
C	-7.69031363	0.94471377	3.09002377
C	-7.40943947	-0.13070674	3.93874936
C	-6.10206783	-0.34919041	4.38655410
H	-4.55560877	2.26704693	2.81266110
H	-6.88758812	2.64744312	2.02443792
H	-8.70654905	1.10736181	2.73982646
H	0.51276561	-3.32838172	0.04931759

Int4_7

E = -12520.16

G = -12216.89

Nimag = 0

C	2.03681123	-2.92131409	0.85524139
C	1.12639792	-3.60221610	-0.19754548
H	1.54093956	-2.91611590	1.83821678
H	1.76424459	-4.02886711	-0.98033372
C	0.12681975	-2.66519795	-0.91274473
C	2.39234463	-1.48968176	0.56436100
C	1.45087114	-0.65337989	-0.24039731
C	0.87491516	-1.43541777	-1.43245779
H	-0.31952544	-3.20737727	-1.74735394
H	0.19823278	-0.77610419	-1.98283028
H	1.67892363	-1.74812188	-2.10732001
H	1.94805678	0.24380716	-0.61024607
H	2.94375360	-3.51545254	0.99512265
H	0.60915582	-4.43864213	0.27723235
N	-1.01065895	-2.17294867	-0.08399472
C	-0.69209106	-1.29626025	1.06823287
H	-1.62560072	-0.86204004	1.42636897
H	-0.26744883	-1.88650094	1.89267596
C	0.27652052	-0.14760052	0.69489621
C	-0.32369942	1.10261947	0.04083269
C	-1.52962482	1.05434960	-0.55553189
S	-2.39125740	-3.10693843	0.02067087
O	-3.42674294	-2.25708793	0.60854369
O	-2.59231792	-3.71861133	-1.29344135
H	-1.70594632	-5.89895243	-0.34238827
H	5.59430632	5.44536597	-3.58002840
H	5.95954950	1.54407071	-5.37109313
H	6.16904103	4.02052700	-5.54871354
N	3.44815097	-0.95325441	1.10917310
C	3.87707657	0.45586503	0.87435212
H	3.03440679	1.13716782	1.02313212
C	4.43688203	-1.67382901	1.97798029
H	3.96396719	-1.85021788	2.95011541
H	4.68904944	-2.63389455	1.52521428
C	4.98330044	0.67953062	1.92653031
C	5.62699435	-0.71100603	2.07278857
H	4.52315969	1.00150440	2.86663824
H	5.68566537	1.45280715	1.61127641
H	6.16393160	-0.83127848	3.01637453
H	6.32391445	-0.89895431	1.25011414
C	4.39554313	0.57237558	-0.59336778
H	-2.13473504	0.14700194	-0.61447509
Cu	0.71416014	2.69493111	0.16382526
H	-1.96995946	1.94010741	-1.01138563
O	4.68062036	-0.43178581	-1.25533301
N	4.48591375	1.86480365	-0.99542348
H	4.18872041	2.57351244	-0.30400128
H	5.18481931	0.49711579	-3.26069233
F	3.80583540	6.17483633	2.33364640
F	4.09062885	6.52155258	0.17258690
F	2.14126965	6.93030085	1.11275030
H	0.72937316	0.16571649	1.64376729
O	1.60365352	4.41817694	0.41275589
O	3.71944395	3.74675879	0.95535296
C	2.80213082	4.57901708	0.80349456
C	3.19472059	6.06974005	1.11387491
C	4.95271976	2.37953640	-2.23011554
C	5.07217951	3.77904297	-2.32860002
C	5.50692338	4.36330502	-3.51774825
C	5.82980633	3.56440254	-4.62199633
C	5.71180640	2.17443208	-4.51997497
C	5.27606603	1.57248037	-3.33511906
H	4.82880955	4.40006757	-1.47078016
C	-2.03492937	-4.42248038	1.19476810
C	-2.03571843	-4.12954702	2.56509755
C	-1.66379234	-5.12626388	3.47157569
C	-1.30447255	-6.39874520	3.01131260
C	-1.32374675	-6.68292316	1.64068162
C	-1.68630416	-5.69337501	0.72298560
H	-2.33938150	-3.14879018	2.91630441
H	-1.66356837	-4.90994896	4.53684006
H	-1.01920129	-7.17101183	3.72120214
H	-1.05926483	-7.67511052	1.28407621

Int4_8

E = -12522.53

G = -12219.64

Nimag = 0

C	3.21371232	-1.76904810	-2.25509914
C	2.85529451	-0.78617459	-3.40147390
H	2.61586791	-2.68820189	-2.34030570
H	3.70814137	-0.11452778	-3.55351618
C	1.62675964	0.11505890	-3.14113711
C	2.94975038	-1.23980018	-0.87511727
C	1.75364897	-0.35214173	-0.68342907
C	1.75796072	0.75872932	-1.75744935
H	1.59467941	0.89035870	-3.90799478
H	0.91884925	1.43473344	-1.56737171
H	2.68563820	1.33873224	-1.70186481
H	1.76952683	0.10157701	0.30683450
H	4.25280181	-2.08495657	-2.36134585
H	2.73460176	-1.35671295	-4.32462194
N	0.30242470	-0.57050634	-3.18579399
C	0.08197867	-1.65580208	-2.19805260
H	-0.97155872	-1.93587101	-2.23376097
H	0.66399036	-2.54256047	-2.47248822
C	0.40647276	-1.17419916	-0.76945171
C	0.37268145	-2.25608696	0.30994916
C	0.46745304	-3.56339593	-0.00462813
S	-0.47331165	-0.71276157	-4.66342646
O	-1.83334078	-1.16751798	-4.37331669
O	-0.24842464	0.54088301	-5.38377818
H	1.46506403	-0.65997862	-6.81375559
H	3.01821431	4.10761160	6.00406831

H	4.98821482	5.34281526	2.37733091
H	4.14352908	5.88463083	4.65787847
N	3.71068142	-1.58930406	0.12027110
C	3.53498898	-1.10947553	1.51836388
H	2.48223593	-1.23721106	1.80638632
C	4.91222258	-2.48750726	0.01706398
H	4.55128173	-3.50574431	-0.16181625
H	5.53291735	-2.17333676	-0.82284453
C	4.45335140	-2.03193400	2.34292880
C	5.60806357	-2.34536546	1.37559857
H	3.89997152	-2.94041361	2.60499156
H	4.77806260	-1.55406082	3.26844154
H	6.15100127	-3.25503988	1.64234033
H	6.31855403	-1.51310162	1.34559695
C	3.93093625	0.39299895	1.58667548
H	0.53642185	-3.94604058	-1.02687646
Cu	0.22189108	-1.68811645	2.12327873
H	0.46877087	-4.33273029	0.76582750
O	4.54932019	0.94326416	0.66800426
N	3.51277472	0.97027648	2.74313409
H	2.98702686	0.35973731	3.38781210
H	4.71633628	3.05951009	1.44653467
F	1.21398923	-1.34218694	7.13089486
F	0.71630073	0.73525572	6.57811421
F	-0.83078972	-0.82919488	6.50504088
H	-0.34889046	-0.41586671	-0.52514994
O	-0.03057530	-1.18424387	3.99213712
O	2.13704390	-0.71877107	4.54391617
C	0.92044980	-0.85939335	4.77291676
C	0.48364930	-0.58062393	6.25778709
C	3.71622827	2.29586426	3.20012336
C	3.23787288	2.60042211	4.48914979
C	3.39211159	3.88574925	5.00732586
C	4.02331054	4.88294072	4.25259706
C	4.49696828	4.57646912	2.97290100
C	4.34992271	3.29271136	2.43725179
H	2.75022592	1.82563831	5.07500393
C	0.36610895	-2.02662701	-5.55869305
C	0.12741904	-3.35858989	-5.19393505
C	0.85979962	-4.37313101	-5.81604047
C	1.80988274	-4.05702553	-6.79453720
C	2.02550503	-2.72358225	-7.16233887
C	1.30650808	-1.69845435	-6.54194266
H	-0.62900690	-3.59797003	-4.45365617
H	0.68129954	-5.40955940	-5.54152792
H	2.37528290	-4.85054301	-7.27657811
H	2.75260204	-2.47946182	-7.93254694

Int4_9

E = -12503.51

G = -12201.49

Nimag = 0

C	-3.62022707	-4.18736689	0.25710988
C	-4.59945150	-4.28573422	1.45737951
H	-4.15818578	-4.39871239	-0.67761632
H	-4.00689821	-4.40609990	2.37186997
C	-5.49547156	-3.05053351	1.65270080
C	-3.02182213	-2.81767237	0.10171216
C	-3.91879821	-1.64376244	0.32064395
C	-4.65645525	-1.76900885	1.66935366
H	-6.00741767	-3.17242392	2.61042210
H	-5.29731904	-0.89353320	1.80493941
H	-3.93582383	-1.79727424	2.49468556
H	-3.35301266	-0.71469722	0.29571699
H	-2.85358390	-4.95695789	0.35111746
H	-5.21414492	-5.18240299	1.34030430
N	-6.55983858	-2.95378428	0.61129209
C	-6.14665973	-2.54368059	-0.75813129
H	-6.99602457	-2.06845161	-1.24947695
H	-5.94840282	-3.46842314	-1.31284877
C	-4.92889803	-1.58411062	-0.90251875
C	-5.30316809	-0.12693871	-1.17255048
C	-4.63133783	0.47360143	-2.17787944
S	-8.02556509	-2.42445846	1.27934073
O	-7.93989666	-1.06847610	1.83467391
O	-8.44094003	-3.48965665	2.20534902
H	-9.02192296	-4.54589600	-0.41123742
H	2.59912010	-9.47983026	1.15269925
H	1.61936338	-7.10207443	4.60915490
H	2.69819964	-9.11826881	3.62127132
N	-1.78868513	-2.65509011	-0.29019402
C	-0.85860345	-3.76825343	-0.62868700
H	-1.37609468	-4.48900336	-1.26517183
C	-1.10446396	-1.32152840	-0.45229087
H	-1.55135837	-0.81467977	-1.31319172
H	-1.26722100	-0.72129775	0.44288647
C	0.29464294	-3.05804165	-1.37526553
C	0.36592317	-1.68349581	-0.68676978
H	0.02716677	-2.95315218	-2.43197073
H	1.22770487	-3.62187128	-1.31051232
H	0.86892840	-0.93164957	-1.29857973
H	0.89125791	-1.76062210	0.27014516
C	-0.37995721	-4.45939381	0.68249011
H	-3.87204423	-0.05387558	-2.77286686
Cu	-6.66672093	0.77088455	-0.21119883
H	-4.80593690	1.51101278	-2.45924702
O	-0.53942211	-3.93979222	1.78668688
N	0.23202085	-5.65522564	0.43845284
H	0.26156103	-5.95266453	-0.53277625
H	0.45631237	-5.46035256	3.15958388
F	-9.52399850	3.28421430	3.44032571
F	-10.43626124	1.64078391	2.29634865
F	-10.09769250	3.60205486	1.34107271
H	-4.37562050	-1.94991084	-1.78385542
O	-8.17794576	1.75280558	0.53568466
O	-7.18887432	2.27972789	2.52815592
C	-8.13470020	2.19730916	1.73728981
C	-9.55287863	2.69004171	2.21311027
C	0.87517912	-6.54460556	1.34017063
C	1.48128342	-7.68299037	0.77950714
C	2.13374538	-8.60411374	1.59809760
C	2.18923949	-8.40097597	2.98258082
C	1.58339642	-7.26823960	3.53514389
C	0.92432597	-6.33479363	2.72802222
H	1.44016973	-7.84141564	-0.29670006
C	-9.11911589	-2.40385566	-0.13769004
C	-9.64915934	-1.18029589	-0.55773169
C	-10.52562870	-1.17261439	-1.64798571
C	-10.85310330	-2.36737641	-2.29751556
C	-10.31441084	-3.58500597	-1.85863600
C	-9.44357809	-3.61106232	-0.76828048
H	-9.37883210	-0.26249457	-0.04469613
H	-10.94800083	-0.23090001	-1.98852740
H	-11.53206232	-2.35308799	-3.14666253
H	-10.57584743	-4.51201947	-2.36240348

Int4_10

E = -12511.80

G = -12209.35

Nimag = 0

C	-0.12903073	-1.65122247	2.13772238
C	-0.24182633	-0.74832771	3.39627180
H	-0.90945091	-2.42546453	2.15922374
H	0.74533180	-0.31612891	3.59788016
C	-1.23238747	0.42838165	3.26807070
C	-0.29429381	-0.92996860	0.82760498
C	-1.21545733	0.24656990	0.77156775
C	-0.96038402	1.18867610	1.96772856
H	-1.09501001	1.08993321	4.12463579
H	-1.62307751	2.05499170	1.88121070
H	0.07377338	1.55071365	1.96151432
H	-1.08970010	0.78602415	-0.16785400
H	0.82261787	-2.18451936	2.16933226
H	-0.50042385	-1.37392686	4.25544775
N	-2.66858919	0.04376474	3.26479741
C	-3.14738053	-0.82115871	2.15952477
H	-4.24099613	-0.84105511	2.18988883
H	-2.81253824	-1.85229163	2.30353840
C	-2.72748075	-0.24160978	0.79672052
C	-3.03284028	-1.12551914	-0.41343643

C	-3.07336689	-2.46830119	-0.29905233
S	-3.43856568	-0.19097702	4.73086864
O	-2.77509377	0.68479406	5.70446537
O	-3.57365941	-1.61784004	5.05774082
H	-6.07742500	-1.34515797	5.01217225
H	6.45320244	-6.38979994	1.90186652
H	7.27316294	-2.16903934	2.17503337
H	8.01337751	-4.52790185	2.47977381
N	0.28642791	-1.37474372	-0.24946127
C	1.08694874	-2.62918051	-0.30544661
H	-8.34936628	-0.43253264	4.51637053
C	0.22577484	-0.72234050	-1.60233558
H	0.50486923	0.32763439	-1.50435014
H	-0.81308021	-0.78781150	-1.95281152
C	1.15674922	-2.93728849	-1.81922310
C	1.19525304	-1.53964881	-2.46261525
H	2.02356433	-3.55359933	-2.06765103
H	0.25058281	-3.47704220	-2.11304873
H	2.20359981	-1.11814559	-2.40754364
H	0.88153161	-1.55211272	-3.50871807
C	2.49153879	-2.37817194	0.31389503
H	-2.93640513	-3.01027310	0.64172901
Cu	-3.29666528	-0.18313966	-2.04303680
H	-3.26061721	-3.10381057	-1.16331699
O	2.93443861	-1.24151202	0.48013315
N	3.14113200	-3.54250801	0.60988955
H	2.62569446	-4.40002522	0.43224436
H	5.00639656	-1.66491848	1.30487805
F	-2.77451738	2.63225745	-5.79414838
F	-4.27307763	4.03152111	-4.99205315
F	-4.91173014	2.07823866	-5.77159459
H	-3.27024623	0.70625114	0.68576803
O	-3.58327985	0.79635552	-3.70504267
O	-3.70014547	2.81987694	-2.64738225
C	-3.72527587	2.07139305	-3.63064402
C	-3.93239567	2.71381245	-5.05375261
C	4.45442622	-3.74309210	1.11195541
C	4.86908808	-5.07600025	1.28373349
C	6.14419340	-5.35532547	1.77380013
C	7.01920329	-4.31086799	2.09768371
C	6.60174075	-2.98735814	1.92576768
C	5.32585477	-2.68993658	1.43567339
H	4.19008697	-5.88880924	1.03211301
C	-5.07671217	0.44716312	4.35663743
C	-5.19149478	1.73878921	3.82823921
C	-6.46157078	2.24242851	3.54653994
C	-7.59813784	1.46083791	3.79602514
C	-7.46740296	0.17402734	4.32793756
C	-6.19904179	-0.34435058	4.61107740
H	-4.30228169	2.32891262	3.62921184
H	-6.56337312	3.23933165	3.12544355
H	-8.58543908	1.85569795	3.56977573
H	0.56216650	-3.41159101	0.24726207

CF_3COOH
E = -1442.28
G = -1439.08
Nimag = 0

O	-2.24015579	-1.97840415	0.00000000
C	-2.19913822	-3.18562112	0.00000000
C	-3.47982018	-4.08594897	0.00000000
F	-4.59450778	-3.32434788	0.00000000
F	-3.50536176	-4.88635597	-1.10364457
F	-3.50536176	-4.88635597	1.10364457
O	-1.10385078	-3.96446685	0.00000000
H	-0.30966103	-3.38590417	0.00000000

Int4_11
E = -13967.71
G = -13645.11
Nimag = 0

C	6.31226208	2.39459529	0.14493317
C	6.78402007	3.72346779	0.78729421
H	6.21983623	2.51304834	-0.94602385
H	7.33450778	3.48657930	1.70495809
C	5.65649452	4.69792599	1.19515085
C	4.97772027	1.88728396	0.61564030
C	3.96284324	2.85911313	1.13131654
C	4.61074003	3.93832869	2.01488090
H	6.09006998	5.49677203	1.79803807
H	3.82810670	4.61579231	2.36642856
H	5.08663414	3.47971985	2.88811734
H	3.19374316	2.34270719	1.70703596
H	7.07786265	1.62657539	0.28410550
H	7.49311471	4.20544700	0.11085265
N	4.93896144	5.37056381	0.07430198
C	4.14871936	4.51828408	-0.84472439
H	3.53816129	5.17408492	-1.46595813
H	4.81166845	3.95748216	-1.51851207
C	3.22181998	3.53532685	-0.09034492
C	1.88484334	4.07665444	0.43166149
C	1.68167002	5.40529119	0.55618878
S	5.56899249	6.78906838	-0.54963186
O	4.51301478	7.38323680	-1.36943866
O	6.14047441	7.52875664	0.57567667
H	8.44592913	6.80708641	-0.21122128
H	-1.28998063	-1.15300931	5.84137076
H	2.53397645	-0.07384440	7.50713087
H	0.15531354	-0.73891754	7.83500839
N	4.66625722	0.63148424	0.46547094
C	3.36248469	0.04101685	0.88582970
H	2.53514273	0.64933023	0.50980580
C	5.57977170	-0.42786707	-0.07926703
H	5.67896397	-0.26284831	-1.15753482
H	6.56178073	-0.33605516	0.38718314
C	3.37516194	-1.36185997	0.24346835
C	4.86578249	-1.74516476	0.24783969
H	2.98949984	-1.29093095	-0.77893010
H	2.74469886	-2.06075466	0.79538041
H	5.10486866	-2.52086639	-0.48298252
H	5.16836409	-2.09649979	1.23912162
C	3.31761312	0.00150440	2.44621151
H	2.43820783	6.15499049	0.31762100
Cu	0.55765898	2.77135016	0.85918933
H	0.73049659	5.79621871	0.91463092
O	4.34239903	0.14184451	3.12253692
N	2.05830118	-0.20456329	2.90568131
H	1.32421649	-0.28636612	2.18181653
H	3.46415828	0.17709904	5.22172407
F	-2.26266246	-1.41646381	-0.14477611
F	-2.63396092	-0.97042199	1.98503568
F	-3.28655441	0.44200049	0.42295935
H	2.99049333	2.74200590	-0.81218531
O	-0.93989559	1.54819259	1.05492116
O	0.10420859	-0.47643347	0.88923599
C	-0.88272814	0.28692031	0.90652435
C	-2.28693774	-0.40828151	0.77682682
C	1.61248092	-0.34589149	4.24337870
C	0.26862223	-0.72273611	4.42708658
C	-0.25018186	-0.86174748	5.71381404
C	0.56045052	-0.62992679	6.83206157
C	1.89562856	-0.25721639	6.64579693
C	2.43116484	-0.11210409	5.36200566
H	-0.36017478	-0.91137872	3.56163785
C	6.91289254	6.32065880	-1.64855178
C	6.60756755	5.81833729	-2.92051372
C	7.64802870	5.37481287	-3.74152009
C	8.97367855	5.44236862	-3.29648159
C	9.26588268	5.96058643	-2.02923688
C	8.23476755	6.40050643	-1.19500244
H	5.58044649	5.79444725	-3.26947190
H	7.42241615	4.98641240	-4.73130301
H	9.77945876	5.10019154	-3.94099403
H	10.29630663	6.02672464	-1.68964178
H	0.55870215	4.52224523	-1.14449860
O	-1.76219292	4.75999495	-0.56696858
C	-1.28680872	4.53096723	-1.65679472
C	-2.17882700	4.25420983	-2.91319491
F	-3.46791900	4.58189788	-2.67003610
F	-1.75728414	4.95508116	-4.00273085

F	-2.13144536	2.92251420	-3.22647538
O	0.00459626	4.43110845	-1.98148266

Int4_12

E = -13970.09

G = -13650.82

Nimag = 0

C	3.18573187	-1.72840578	-2.14549094
C	2.85050020	-0.69612084	-3.25605758
H	2.51634728	-2.59673932	-2.22273616
H	3.72811796	-0.05616888	-3.40372826
C	1.66352469	0.24186595	-2.94241395
C	3.01118897	-1.19905247	-0.75265893
C	1.84114827	-0.28955119	-0.50037621
C	1.85018970	0.84788033	-1.54836187
H	1.64088116	1.03617582	-3.68960796
H	1.03640913	1.54236690	-1.31887275
H	2.79634242	1.39753413	-1.50200853
H	1.90032374	0.14031519	0.49868123
H	4.19307752	-2.11647760	-2.30041680
H	2.68925848	-1.23430634	-4.19233098
N	0.31376149	-0.39111620	-2.96850238
C	0.06374300	-1.48209341	-1.99503312
H	-1.00827143	-1.68508237	-1.98829545
H	0.57403813	-2.39799118	-2.31433970
C	0.46900165	-1.06272685	-0.56769749
C	0.45249539	-2.18215600	0.47432138
C	0.47552964	-3.48438659	0.11111515
S	-0.49748316	-0.49656294	-4.43383351
O	-1.88858356	-0.81173028	-4.11286186
O	-0.16176741	0.70993909	-5.19054214
H	1.46039144	-0.71014198	-6.56164026
H	3.31741202	4.21046083	6.03715854
H	5.16784338	5.41969899	2.33930550
H	4.38352101	5.98150429	4.63641580
N	3.83050804	-1.54376299	0.19675087
C	3.73995722	-1.05492562	1.60096665
H	2.71156924	-1.19000893	1.95884730
C	5.02880611	-2.43851484	0.02642470
H	4.66283296	-3.46115707	-0.11178568
H	5.58993111	-2.13366510	-0.85732178
C	4.72120994	-1.95957524	2.37202333
C	5.81189222	-2.27171586	1.33335460
H	4.19711937	-2.87076158	2.68071732
H	5.10124848	-1.46762719	3.26862054
H	6.38185685	-3.17210711	1.57367414
H	6.50880751	-1.43214429	1.24589187
C	4.12408807	0.45262316	1.63538619
H	0.47781043	-3.83458377	-0.92401904
Cu	0.43891775	-1.66476698	2.31197556
H	0.49575048	-4.27802655	0.85645413
O	4.69886886	0.99602337	0.68521279
N	3.74960322	1.03794404	2.80220303
H	3.26079124	0.42677528	3.47399351
H	4.89373898	3.12166501	1.44519463
F	1.69172083	-1.43383904	7.25145837
F	1.18459701	0.66378275	6.78921784
F	-0.37722749	-0.88671973	6.74313627
H	-0.25822538	-0.30183532	-0.25910591
O	0.30218746	-1.21286875	4.19610056
O	2.48389742	-0.69978166	4.63538434
C	1.28694106	-0.87558264	4.92980827
C	0.92510659	-0.63893418	6.44091563
C	3.95333820	2.37084708	3.23688952
C	3.50971457	2.68608101	4.53563316
C	3.66470195	3.97953697	5.03291855
C	4.26285576	4.97345422	4.24747742
C	4.70256857	4.65582783	2.95837646
C	4.55403376	3.36383567	2.44335164
H	3.04772186	1.91376729	5.14549301
C	0.19111367	-1.91459140	-5.30012634
C	-0.21697141	-3.20227449	-4.92719071
C	0.38450981	-4.30735333	-5.53558377
C	1.37419677	-4.12327658	-6.50823729
C	1.76068191	-2.83107718	-6.88406178
C	1.17261255	-1.71744796	-6.27840795
H	-1.00431590	-3.33645652	-4.19280108
H	0.07280069	-5.31009103	-5.25498307
H	1.83665018	-4.98625939	-6.98041756
H	2.51785773	-2.68796793	-7.65070214
H	-1.53074528	-2.89224553	0.78671688
O	-2.84733626	-1.12521085	-0.20687268
C	-3.22724084	-2.03378141	0.49871976
C	-4.72703627	-2.20111381	0.91750057
F	-5.48795511	-1.22073155	0.38167108
F	-5.21794209	-3.40251686	0.49289625
F	-4.85858076	-2.15062259	2.27483569
O	-2.49848182	-3.01497671	1.03382529

TS4_5

E = -13955.88

G = -13637.03

Nimag = 1, 1269i cm-1

C	6.11787322	2.28376295	-0.10804361
C	6.63616954	3.54188829	0.64167986
H	5.97097582	2.51243843	-1.17394663
H	7.19220177	3.20636704	1.52440207
C	5.54544294	4.51154099	1.15247554
C	4.80208107	1.75920300	0.38977723
C	3.79427006	2.74787707	0.89642189
C	4.46136430	3.71984386	1.88838591
H	6.00777480	5.22567797	1.83516797
H	3.70090151	4.39048400	2.29699391
H	4.90232088	3.15969864	2.71961314
H	2.97341873	2.23650036	1.39949809
H	6.88043642	1.50292579	-0.08186929
H	7.34916396	4.06181534	-0.00211237
N	4.85784394	5.32140494	0.10734004
C	4.11776128	4.57644588	-0.93414967
H	3.52638882	5.29169928	-1.50646008
H	4.81157559	4.09193273	-1.63406187
C	3.15752024	3.52765659	-0.32118953
C	1.78900396	4.08116793	0.08585740
C	1.62775835	5.31234754	0.61839134
S	5.50516433	6.80703215	-0.32201417
O	4.47781468	7.48770577	-1.10854397
O	6.02279097	7.40803688	0.90678499
H	8.36117057	6.74133134	0.15050519
H	-1.00362805	-1.00167198	6.21602391
H	2.92393968	0.21128511	7.50632890
H	0.58824215	-0.45562220	8.06106252
N	4.51197028	0.49290099	0.31193114
C	3.25184100	-0.10338292	0.84680610
H	2.38195004	0.43822324	0.46891469
C	5.43159299	-0.58206977	-0.19582234
H	5.46402128	-0.50288825	-1.28734734
H	6.43343350	-0.42462524	0.20516518
C	3.28183664	-1.55491154	0.32547901
C	4.78338112	-1.88890974	0.27727103
H	2.83880860	-1.58510260	-0.67537752
H	2.70927730	-2.22330864	0.97099894
H	5.01076308	-2.71451257	-0.40071207
H	5.15119864	-2.14695911	1.27504568
C	3.30785519	-0.01347215	2.40589889
H	2.45983669	5.97862400	0.84467034
Cu	0.35900580	2.80988441	0.60207082
H	0.63130303	5.70538815	0.80955969
O	4.37225542	0.20137592	2.99574420
N	2.09116483	-0.20732293	2.97240015
H	1.30434092	-0.32430653	2.31638502
H	3.66741749	0.33420627	5.14378729
F	-2.46025003	-1.50084067	0.64939706
F	-2.51991218	-0.67201792	2.69320104
F	-3.43728044	0.43119633	1.02000736
H	2.97547371	2.79558306	-1.11708885
O	-1.05994580	1.63685004	1.14016676
O	0.00661894	-0.38034932	1.05981056
C	-0.98688858	0.36472457	1.15072749
C	-2.37538541	-0.34227475	1.36334336
C	1.75235397	-0.26556517	4.34852761

C	0.43310676	-0.64297417	4.65988527
C	0.01873888	-0.70898108	5.98968358
C	0.91147367	-0.40315363	7.02447446
C	2.22234549	-0.02971016	6.71090607
C	2.65314328	0.04364718	5.38228484
H	-0.26010255	-0.88834467	3.86050401
C	6.89486301	6.46356296	-1.40745908
C	6.64566613	6.12737415	-2.74473960
C	7.72023159	5.77326160	-3.56505707
C	9.02317153	5.76312851	-3.05329288
C	9.25907513	6.11447869	-1.71874089
C	8.19349119	6.46396007	-0.88510158
H	5.63600353	6.16235652	-3.14085120
H	7.53881195	5.51435697	-4.60494145
H	9.85558254	5.49063855	-3.69714489
H	10.27240041	6.12029653	-1.32563219
H	0.91063077	3.81016654	-0.96794291
O	-1.47870927	4.44598175	-1.24748524
C	-0.77660646	4.13738532	-2.21137749
C	-1.40212954	4.15210571	-3.65721516
F	-2.68681122	4.59386445	-3.66078357
F	-0.68795726	4.95949146	-4.50360880
F	-1.40004648	2.89131975	-4.20109836
O	0.46193662	3.76750987	-2.22890169

TS4_6

E = -13957.95

G = -13638.03

Nimag = 1, 1284i cm-1

C	3.18236363	-1.59583701	-2.27169138
C	2.64451483	-0.61583389	-3.34561611
H	2.69223550	-2.57373465	-2.38354668
H	3.39240955	0.17011936	-3.50090717
C	1.32499393	0.09258197	-2.97324007
C	2.94278566	-1.16156400	-0.85257571
C	1.68444044	-0.40387580	-0.54124244
C	1.47152274	0.71863897	-1.58285982
H	1.12864876	0.87452596	-3.70803232
H	0.57168800	1.27914955	-1.31325063
H	2.32144856	1.40893238	-1.57541426
H	1.74202071	0.03917522	0.45230221
H	4.24364210	-1.78123124	-2.44558172
H	2.55018331	-1.15477639	-4.29038373
N	0.10869557	-0.77130508	-2.95557961
C	0.05226736	-1.85940332	-1.95414488
H	-0.97115581	-2.23673994	-1.92191834
H	0.69831088	-2.69889241	-2.24280075
C	0.41307187	-1.33581671	-0.54866154
C	0.46749662	-2.45906027	0.48489753
C	1.15314896	-3.60575883	0.27845910
S	-0.72749434	-1.01647445	-4.39072628
O	-2.01414409	-1.60296180	-4.02027511
O	-0.66402789	0.24163143	-5.13357392
H	1.11134937	-0.80686100	-6.61900642
H	3.27307559	3.90524842	6.26715820
H	4.87949020	5.40254518	2.56042834
H	4.20143151	5.79515563	4.92516287
N	3.78018518	-1.49384679	0.08631650
C	3.65313022	-1.07820684	1.51021765
H	2.63683620	-1.27539442	1.86333061
C	5.04889337	-2.27459014	-0.12362142
H	4.76721043	-3.30884713	-0.34714594
H	5.59578669	-1.86096463	-0.97160361
C	4.67547118	-1.96795361	2.24315873
C	5.79887280	-2.14699658	1.20763386
H	4.20326704	-2.92654902	2.48443660
H	5.01074397	-1.51190197	3.17545437
H	6.41779467	-3.02570797	1.40151034
H	6.44619335	-1.26460000	1.18813236
C	3.96414440	0.44912957	1.60697698
H	1.74724286	-3.80558325	-0.61553968
Cu	0.26693157	-1.91686921	2.38176422
H	1.12810026	-4.41683637	1.00221199
O	4.44520389	1.07093712	0.65391911
N	3.64228596	0.94953068	2.82650048
H	3.21215721	0.28452961	3.48373065
H	4.63398441	3.15530111	1.53946796
F	2.04658715	-0.62505736	7.15841473
F	0.19594884	0.36852280	6.50153792
F	0.18904511	-1.78778499	6.97656996
H	-0.39154750	-0.65212430	-0.25332969
O	0.22051733	-1.42089541	4.23224072
O	2.43719538	-0.96747414	4.52681123
C	1.25957565	-1.09297348	4.89957676
C	0.92446282	-0.79030538	6.40560211
C	3.81808927	2.26359894	3.32822185
C	3.43555750	2.48301911	4.66501960
C	3.57270823	3.74847327	5.23380850
C	4.09380147	4.80872480	4.48119122
C	4.47400206	4.58614756	3.15381533
C	4.34092452	3.32332056	2.56720073
H	3.03783030	1.65773492	5.25036810
C	0.19463867	-2.25612513	-5.31053139
C	0.08583428	-3.60178054	-4.93481074
C	0.87150997	-4.55338979	-5.59099733
C	1.74550072	-4.16186154	-6.61221615
C	1.83175581	-2.81625698	-6.98885383
C	1.05712045	-1.85321841	-6.33665401
H	-0.61404959	-3.90140227	-4.16168271
H	0.79256523	-5.60029811	-5.30980617
H	2.35159768	-4.90693973	-7.12134909
H	2.49901072	-2.51468518	-7.79209622
H	-0.83201084	-2.65611877	0.96056512
O	-2.26327322	-0.65465956	1.48440123
C	-2.75937751	-1.75134995	1.21324103
C	-4.32525648	-1.91657452	1.24186708
F	-4.95549756	-0.77574092	1.62488026
F	-4.80255629	-2.25501583	0.00237108
F	-4.70205380	-2.90730238	2.10937653
O	-2.16104077	-2.85104071	0.89127176

Int4_13

E = -13999.34

G = -13676.48

Nimag = 0

C	5.43318100	2.42881196	-0.81132353
C	6.31963363	3.30264711	0.13271646
H	5.08081928	3.02737684	-1.66100772
H	6.94933471	2.62483755	0.72003511
C	5.55732483	4.18726294	1.15175461
C	4.21363051	1.90570410	-0.11726523
C	3.46364320	2.88806259	0.73930094
C	4.45133716	3.37728093	1.83323552
H	6.26654531	4.54172294	1.90125500
H	3.92331136	4.00132387	2.55777230
H	4.87457818	2.51678073	2.36186266
H	2.62219020	2.38718554	1.21161296
H	6.03510207	1.62569769	-1.23663332
H	6.99059472	3.90659931	-0.48226611
N	4.89793712	5.40088947	0.59151617
C	3.92814049	5.15885700	-0.49292419
H	3.40712557	6.09463347	-0.69808148
H	4.44296232	4.86815129	-1.41767483
C	2.88502835	4.07196001	-0.10535733
C	1.66407413	4.70489779	0.55363891
C	1.14669670	4.46202144	1.81766305
S	5.75752598	6.84094435	0.55552067
O	4.79741994	7.87885812	0.18158031
O	6.49084859	6.92165845	1.81803930
H	8.57656243	6.18318899	0.55536099
H	-0.53777743	0.14273040	6.65548412
H	3.73517177	-0.16645294	7.11046121
H	1.46742463	-0.03341196	8.13411459
N	3.84932520	0.66473472	-0.19953479
C	2.67689563	0.08717856	0.53298442
H	1.80192857	0.71080545	0.35205031
C	4.54687358	-0.39687403	-1.00291710
H	4.32909693	-0.20015076	-2.05754638
H	5.62234775	-0.33772675	-0.83421018
C	2.49695336	-1.30546037	-0.10491839

C	3.92395699	-1.71049743	-0.51661443
H	1.84855120	-1.20317991	-0.98072391
H	2.03204370	-2.00759417	0.59055458
H	3.93648744	-2.46969455	-1.30205552
H	4.47986588	-2.08963775	0.34598251
C	3.04352411	0.02089298	2.03890067
H	1.58996167	3.74826739	2.50732687
Cu	0.02934291	3.42098327	0.43057425
H	0.44215379	5.16435171	2.25747542
O	4.22069383	-0.08484942	2.40625029
N	1.95173104	0.09177915	2.84532161
H	1.04651880	0.21592211	2.36881944
H	4.00601815	-0.11741719	4.64568305
F	-3.02758871	-0.55008921	1.09836841
F	-2.53108837	-0.07127910	3.19463404
F	-3.83068132	1.27153647	2.03342140
H	2.54167241	3.65017569	-1.05515891
O	-1.58544207	2.47307693	1.24536006
O	-0.40894469	0.52972560	1.37353037
C	-1.43452118	1.23561037	1.47368749
C	-2.72852501	0.47911223	1.95049527
C	1.88825587	0.04041495	4.26046030
C	0.60606884	0.11249921	4.83761071
C	0.45867142	0.08641617	6.22379377
C	1.58294075	-0.01291900	7.05333355
C	2.85475729	-0.08780424	6.47653000
C	3.02053411	-0.06134479	5.08782683
H	-0.26777823	0.18191969	4.19623217
C	6.95243312	6.67947758	-0.77580184
C	6.52368393	6.85064780	-2.09889422
C	7.42846031	6.62096753	-3.13876548
C	8.74290432	6.23172606	-2.85484168
C	9.16178345	6.07833742	-1.52777682
C	8.26616936	6.29849021	-0.47800914
H	5.50928018	7.17323001	-2.30974675
H	7.10723261	6.75307395	-4.16864538
H	9.44304030	6.05647595	-3.66770706
H	10.18598391	5.78863292	-1.30771212
H	1.31188045	5.59497321	0.02967096
O	-0.36424407	2.94871194	-1.51529778
C	0.45069539	2.19585770	-2.14182933
C	0.03862121	1.87555824	-3.62754287
F	-1.18383576	2.35801122	-3.98512725
F	0.95545165	2.41422461	-4.50063837
F	0.02067771	0.52292582	-3.85022072
O	1.52391338	1.69421628	-1.76710679

Int4_14

E = -13998.12

G = -13677.37

Nimag = 0

C	2.99743123	-2.06590638	-2.07002399
C	2.65685919	-1.07483803	-3.22129518
H	2.36385882	-2.95805056	-2.15198796
H	3.49272447	-0.37393580	-3.32713120
C	1.38426816	-0.23266103	-2.98335936
C	2.73964716	-1.48202609	-0.71341730
C	1.44858708	-0.73303870	-0.51771683
C	1.43965762	0.40000916	-1.58889613
H	1.34094138	0.55602577	-3.73642753
H	0.56697191	1.03501010	-1.41143913
H	2.33835808	1.01568632	-1.48807433
H	1.41713909	-0.27529308	0.46978130
H	4.02474173	-2.41307845	-2.17426279
H	2.58932538	-1.63734864	-4.15467980
N	0.09869421	-0.97972063	-3.09099187
C	-0.14709361	-2.05515978	-2.10984398
H	-1.19652449	-2.34432481	-2.18363353
H	0.45298248	-2.95031763	-2.32220225
C	0.11736452	-1.53926707	-0.67365951
C	-0.14625280	-2.66440298	0.30882747
C	0.74722158	-3.60459980	0.80054633
S	-0.63812877	-1.10815024	-4.59220266
O	-1.97103834	-1.65723141	-4.34835260
O	-0.46955251	0.18463752	-5.25353565
H	1.34732817	-0.84497988	-6.68313622
H	1.64684220	4.22169015	5.69420357
H	3.23884225	5.64105415	1.95058780
H	2.28464079	6.11859132	4.20181711
N	3.63358673	-1.56015797	0.22995947
C	3.45915439	-1.01441554	1.60946394
H	2.49964086	-1.35386983	2.00827438
C	5.00634823	-2.16576846	0.07662532
H	4.88776067	-3.25253390	0.01772439
H	5.46237309	-1.79966176	-0.84325834
C	4.63615081	-1.62199135	2.39729589
C	5.75074976	-1.73270744	1.34389069
H	4.34610852	-2.61077925	2.76884217
H	4.90249873	-1.00282502	3.25470673
H	6.52206307	-2.45600009	1.61755475
H	6.22476327	-0.75968214	1.18388167
C	3.48582520	0.54015887	1.55884298
H	1.80756875	-3.58399551	0.56153234
Cu	0.37686816	-2.16449971	2.25454818
H	0.38207612	-4.53299640	1.23299157
O	3.98796561	1.13927827	0.59904831
N	2.91863177	1.08094590	2.66197217
H	2.54317137	0.40784508	3.34720442
H	3.55638697	3.29913573	1.19331364
F	2.47330394	-1.76353290	7.16811357
F	0.84361166	-3.17456974	6.74298401
F	2.91353897	-3.66989111	6.15503051
H	-0.65313785	-0.78351735	-0.48659022
O	1.10838638	-2.72518424	4.04746015
O	2.34087452	-0.88976307	4.62955061
C	1.79395807	-1.98620107	4.82818772
C	1.99935413	-2.64324219	6.24454816
C	2.78674751	2.44378560	3.01915428
C	2.24657126	2.71043163	4.29018020
C	2.06905231	4.02713415	4.71115599
C	2.42577018	5.09172678	3.87350128
C	2.96189790	4.82163423	2.61019320
C	3.14639421	3.50617919	2.17291915
H	1.96196090	1.88137235	4.93328479
C	0.30465410	-2.32868863	-5.51522711
C	0.13515298	-3.68691048	-5.21528427
C	0.93551991	-4.62867351	-5.86736291
C	1.88461845	-4.21446384	-6.80979192
C	2.03251098	-2.85555171	-7.11084988
C	1.24385654	-1.90204557	-6.46099549
H	-0.61988301	-4.00222168	-4.50241888
H	0.81049690	-5.68527859	-5.64523956
H	2.50197685	-4.95198585	-7.31636996
H	2.75973258	-2.53549165	-7.85243266
H	-1.20951070	-2.88681231	0.40957553
O	-0.10961064	-0.22740226	2.54966855
C	-1.17737044	0.25940376	2.03560328
C	-1.14724277	1.83315650	2.02445584
F	-0.84866975	2.36112834	3.24571405
F	-0.18082478	2.27004499	1.14132750
F	-2.32784889	2.38167350	1.62173436
O	-2.15014511	-0.31326773	1.52962296

H_2O

E = -421.49

G = -419.81

Nimag = 0

H	0.76870868	0.00000000	-0.54110322
O	0.00000000	0.00000000	0.05739252
H	-0.76870868	0.00000000	-0.54110322

prolinamide

E = -4770.81

G = -4650.91

Nimag = 0

H	8.10273013	-4.69708837	2.27087751
N	0.37998477	-1.20445832	0.00822436
C	1.17004012	-2.43852047	-0.22656400
C	6.75054090	-3.09082966	1.75242866
C	-0.25789296	-0.84458031	-1.28883402

H	-0.44837849	0.23244827	-1.32148201
H	-1.22260452	-1.36463560	-1.37396424
C	1.21739187	-2.67373313	-1.78831529
C	0.71222930	-1.34123975	-2.37878974
H	2.21972438	-2.94396363	-2.13438995
H	0.53998891	-3.49454472	-2.04787653
H	1.54193501	-0.63194883	-2.48756177
H	0.23699460	-1.47032303	-3.35745140
C	2.58643163	-2.27883676	0.34871233
C	5.46770861	-2.73105623	1.32598288
H	4.12909476	-5.86477132	1.07956910
H	0.68574247	-3.29647412	0.25763157
O	3.11827868	-1.16958572	0.48304246
N	3.19619442	-3.47119801	0.64299186
H	2.61895524	-4.29712128	0.51430925
H	5.19958710	-1.69285262	1.18423978
C	4.51565770	-3.73639688	1.08079743
C	4.86657789	-5.08681261	1.26965470
C	6.14961196	-5.42913348	1.69525878
C	7.10216370	-4.43148569	1.93903568
H	6.40455936	-6.47695653	1.83546614
H	7.48086738	-2.30681002	1.93991546
H	1.06280882	-0.47556895	0.23683444

Int4_15

E = -8178.62

G = -7999.33

Nimag = 0

C	1.69655107	14.23191562	2.99442480
C	0.56804498	14.67148875	2.02415436
H	2.63905516	14.09841063	2.44414659
H	-0.14678413	15.28987009	2.58023409
C	-0.25761157	13.51964544	1.40363029
C	1.47868878	12.91789159	3.73703052
C	0.58798632	11.86229728	3.07844567
C	-0.67674404	12.53051136	2.50060245
H	-1.14521916	13.94157556	0.93086734
H	-1.36097097	11.77798581	2.09696821
H	-1.21011497	13.07175972	3.29058238
H	0.33383503	11.13412409	3.85449403
H	1.89956629	15.00659988	3.74121807
H	0.98423859	15.30752947	1.23821069
N	0.43346613	12.72782295	0.34128549
C	1.66667172	12.01306813	0.73245237
H	1.98775324	11.40344214	-0.11398746
H	2.47941011	12.71239896	0.96064082
C	1.37757766	11.10284062	1.94836017
C	0.59055078	9.87877633	1.52023668
C	0.67669848	8.64192367	2.13931274
S	0.29346328	13.20375306	-1.25672160
O	0.74616906	12.07177613	-2.06381919
O	-1.05870128	13.73921755	-1.41915033
H	-0.04208248	16.08090546	-1.29522603
C	3.74221716	15.28914642	-1.74645732
C	1.46319971	14.54750501	-1.48822582
C	2.82001399	14.24287385	-1.65882536
O	2.02438313	12.69792937	4.81403057
H	1.61115763	17.94020448	-1.46231088
H	1.35049209	8.48222133	2.98088019
C	3.30908911	16.61818747	-1.66768477
H	-0.08293199	7.88130920	1.97041285
H	-0.23806277	10.06662247	0.83572980
C	1.94856932	16.90806929	-1.51030436
C	1.01592983	15.87172929	-1.41580121
H	3.14456980	13.21043695	-1.73966941
H	2.33796878	10.78523306	2.37131056
H	4.79705916	15.06463607	-1.88176902
H	4.03086778	17.42794913	-1.73823815
Cu	1.82763146	8.62632448	0.43591494
O	3.03962397	9.23769804	-1.27079569
O	3.08180846	7.13440548	-0.50807668
C	3.45200286	8.04346761	-1.30790582
C	4.49060598	7.69257528	-2.41806361
F	4.83354554	6.37793246	-2.41975708
F	3.99641962	7.99452861	-3.65493497
F	5.63684429	8.42011301	-2.24171270

Int4_16

E = -8178.29

G = -7996.29

Nimag = 0

C	0.97846123	14.40747426	2.99343139
C	-0.06106523	14.48923828	1.84651587
H	1.98886573	14.59188741	2.59968578
H	-1.03653776	14.74476625	2.27804159
C	-0.26946805	13.17403261	1.05939924
C	1.05593371	13.06785715	3.71443038
C	0.75861760	11.81134669	2.89696966
C	-0.50806983	12.01682851	2.03901678
H	-1.13829578	13.28908239	0.40985049
H	-0.74213819	11.09580696	1.49459528
H	-1.36367866	12.25811068	2.67999120
H	0.62323600	10.99015031	3.60756071
H	0.80414037	15.18607519	3.74296232
H	0.20345025	15.30509214	1.16966084
N	0.85505077	12.76564215	0.16221114
C	2.14901342	12.44086267	0.79624750
H	2.78613899	11.98625548	0.03320554
H	2.65159272	13.35110354	1.14744201
C	1.94784254	11.42927039	1.94071666
C	3.20086903	11.15874499	2.74682297
C	4.23947654	12.04602552	2.99019073
S	0.91529436	13.36758965	-1.40219932
O	1.89983708	12.55416913	-2.11565174
O	-0.46681710	13.45067501	-1.87207774
H	-0.37420075	15.96045215	-1.43211257
C	3.44567401	16.50903801	-0.92304693
C	1.56964903	15.03702258	-1.28191368
C	2.94882584	15.21648429	-1.11107974
O	1.37143675	12.99430945	4.89811404
H	0.52403007	18.26358830	-1.10901117
H	4.25529378	13.05042903	2.57281177
C	2.57332177	17.60389200	-0.91422824
H	4.93832039	11.85631280	3.80222767
H	3.13524804	10.27203491	3.37956781
C	1.19939458	17.41195853	-1.10239048
C	0.68829937	16.12437928	-1.28443957
H	3.62174088	14.36591651	-1.14826743
F	6.20054790	9.12302601	-2.62929587
H	4.51413202	16.65968562	-0.79250675
H	2.96536075	18.60739468	-0.76926974
Cu	4.81830890	10.76448846	1.50474770
O	4.95829065	9.28665641	-0.04826304
O	6.65625506	10.69512695	0.31446939
C	6.11636199	9.73507199	-0.30352062
C	6.89991001	9.03776617	-1.45870886
F	8.12360971	9.58906515	-1.66505434
F	7.08258213	7.71207509	-1.17952079
H	1.63376157	10.48399416	1.48036250

P4_1

E = -6753.93

G = -6584.27

Nimag = 0

C	5.65685028	2.39323399	-0.69776966
C	6.44546948	3.28717410	0.29443662
H	5.46853033	2.93960651	-1.63318855
H	7.04764611	2.63958638	0.94328849
C	5.57542369	4.14753311	1.24159837
C	4.28570146	1.91334160	-0.22928478
C	3.52711016	2.78392633	0.76935899
C	4.48334520	3.27489408	1.87642725
H	6.21489689	4.56168548	2.02225970
H	3.93237086	3.84057741	2.63370329
H	4.95415268	2.42118242	2.37786500
H	2.72521720	2.16608919	1.18425167
H	6.23942898	1.51085959	-0.98273929
H	7.14940221	3.91682709	-0.25598510
N	4.89393630	5.31923868	0.60891823
C	3.90628343	5.02802984	-0.45595381

H	3.40525267	5.96152363	-0.71472642
H	4.40166480	4.65392853	-1.36039850
C	2.85545333	4.00951675	0.04715453
C	1.85779109	4.67917976	0.96286645
C	0.53458534	4.54671971	0.84852570
S	5.70110856	6.77986554	0.53402941
O	4.70471230	7.78885183	0.17092226
O	6.46401225	6.90929021	1.77619798
H	8.55429779	6.28569357	0.46891654
C	7.29215585	6.58906748	-3.20008997
C	6.87031864	6.65557593	-0.82649501
C	6.39999557	6.77623124	-2.14098206
O	3.79453832	0.87703853	-0.67018457
H	10.14108431	5.96546263	-1.42788841
H	0.08845524	3.93216575	0.06691825
C	8.63585204	6.29073685	-2.94460934
H	-0.14790110	5.04767357	1.53135250
H	2.27381130	5.30529571	1.75249447
C	9.09526828	6.18543555	-1.62641003
C	8.21248144	6.36452987	-0.55793919
H	5.36198840	7.02855026	-2.33148388
H	2.32033608	3.63059349	-0.83219137
H	6.93755685	6.68249535	-4.22336772
H	9.32575364	6.14725530	-3.77243760

P4_2

E = -6754.16

G = -6584.05

Nimag = 0

C	3.02394284	-2.12441832	-2.17311514
C	2.66503781	-1.07874419	-3.26310408
H	2.44178974	-3.04328529	-2.32630652
H	3.48941714	-0.35842977	-3.33543302
C	1.38937384	-0.25305069	-2.97281973
C	2.73668980	-1.65851981	-0.75463284
C	1.44603714	-0.86541003	-0.53186817
C	1.44328890	0.30969973	-1.54466449
H	1.33524323	0.57000682	-3.68734501
H	0.57997782	0.95732980	-1.35672224
H	2.35028856	0.91469035	-1.43159460
H	1.48378603	-0.48091040	0.49222311
H	4.07907984	-2.40840801	-2.23476707
H	2.59338897	-1.57163425	-4.23558409
N	0.09916404	-0.99632528	-3.10832832
C	-0.13839749	-2.11307963	-2.16651980
H	-1.18295902	-2.41375637	-2.26071101
H	0.48086880	-2.98506454	-2.41450982
C	0.11796529	-1.65719389	-0.71016257
C	-0.09887281	-2.82812088	0.22012715
C	0.67228210	-3.20823653	1.24233696
S	-0.62523149	-1.08505035	-4.61160977
O	-1.97030122	-1.62070450	-4.39388412
O	-0.44335445	0.21989158	-5.24858098
H	1.35222410	-0.80171540	-6.70858040
C	0.29769948	-2.29722830	-5.56769964
H	-0.67300669	-0.92134415	-0.49233070
C	0.11554213	-3.65963311	-5.29591185
O	3.53133656	-1.86017998	0.15987543
H	0.39096810	-4.05994828	1.85759236
H	-1.01268587	-3.39104679	0.01528383
C	1.84936975	-4.17345893	-6.91179165
H	1.59421912	-2.69778290	1.50461684
C	2.01018911	-2.81011180	-7.18504735
C	1.23598953	-1.86219695	-6.51040357
H	-0.63631547	-3.98196162	-4.58301087
H	0.76784751	-5.65589639	-5.76918257
C	0.90130967	-4.59647842	-5.97241666
H	2.45722187	-4.90683412	-7.43570621
H	2.73801932	-2.48229106	-7.92274028

Table 7.4. Cartesian coordinates (in Å), energies (in kcal mol^{-1}), and number of imaginary frequencies computed at COSMO(MeOH)-ZORA-M06/TZ2P//COSMO(MeOH)-ZORA-BLYP-D3(BJ)/TZ2P.

$Pd(PPh_3)_2$
E = -12037.45
G = -11746.64
G = -9606.72
Nimag = 0

Pd	-0.00123873	0.11419815	-0.03829563
P	2.30589796	0.06101763	-0.01832795
P	-2.30801368	0.09329306	0.03314191
C	-3.16284259	-0.21670624	-1.57375437
C	-4.36087606	0.41182925	-1.94754582
C	-2.57298978	-1.14657876	-2.44864678
C	-4.96344942	0.10904663	-3.17438525
H	-4.82514266	1.13590284	-1.28413071
C	-3.18143343	-1.45729495	-3.66723879
H	-1.63172089	-1.61687176	-2.16922522
C	-4.37876409	-0.82792316	-4.03359726
H	-5.89042424	0.60363160	-3.45609499
H	-2.71855035	-2.18080507	-4.33469553
H	-4.84845934	-1.06230338	-4.98613014
C	-3.11312739	1.64064210	0.63696436
C	-4.25552187	1.65058801	1.45250460
C	-2.54182954	2.86300631	0.24011218
C	-4.82147781	2.86465474	1.85914018
H	-4.70431851	0.71438774	1.77164549
C	-3.11486093	4.07418964	0.63589919
H	-1.64194539	2.85588531	-0.37252982
C	-4.25585273	4.07724545	1.44943358
H	-5.70455993	2.86161086	2.49429743
H	-2.66667216	5.01372156	0.32045096
H	-4.69676629	5.01949236	1.76650919
C	-3.02379941	-1.20672499	1.13197275
C	-4.21303191	-1.89389759	0.84182266
C	-2.33092620	-1.50440874	2.31905729
C	-4.70331366	-2.86037600	1.72763342
H	-4.75581086	-1.67920864	-0.07421055
C	-2.82733080	-2.46078578	3.20849438
H	-1.39572332	-0.98889075	2.53069551
C	-4.01508613	-3.14303228	2.91300026
H	-5.62337166	-3.39045205	1.49156070
H	-2.28421359	-2.68193715	4.12457153
H	-4.39723333	-3.89498476	3.59950262
C	3.08761236	-1.20475063	-1.11125867
C	2.43902950	-2.44750841	-1.22594498
C	4.28751277	-0.99064428	-1.80714578
C	2.99150813	-3.46520549	-2.00773443
H	1.49625470	-2.60494579	-0.70479152
C	4.83384636	-2.00680133	-2.60010259
H	4.79641267	-0.03393679	-1.73241332
C	4.19082052	-3.24578981	-2.69855388
H	2.48364872	-4.42390850	-2.08629316
H	5.76271247	-1.83020181	-3.13779545
H	4.61712091	-4.03421776	-3.31462175
C	3.16231202	1.61894868	-0.51498324
C	4.32863632	2.09299228	0.10540422
C	2.60545504	2.34979020	-1.57989592
C	4.93159494	3.27657688	-0.33648539
H	4.76728537	1.54217119	0.93239262
C	3.21528906	3.52380570	-2.02879999
H	1.68792831	1.99537177	-2.04644945
C	4.38002222	3.99138603	-1.40553963
H	5.83319096	3.63750742	0.15357342
H	2.77805640	4.07883135	-2.85580889
H	4.85006300	4.91050223	-1.74779156
C	3.04400108	-0.31145301	1.63277695
C	4.20612959	-1.07956567	1.80465846
C	2.39933857	0.22103224	2.76370485
C	4.71876390	-1.30583286	3.08729560
H	4.71129232	-1.50261470	0.94107989
C	2.91865131	0.00488465	4.04257200
H	1.48403432	0.79535568	2.63164248
C	4.07982837	-0.76164179	4.20726555
H	5.61779563	-1.90572576	3.21020296
H	2.41345846	0.42402831	4.90993733
H	4.47976645	-0.93864441	5.20309088

$Pd(PPh_3)$
E = -6021.88
G = -5886.69
Nimag = 0

H	0.72661939	-0.29288399	2.77586313
H	0.44522062	4.76298000	4.90808055
Pd	0.96245009	2.19164259	0.72555334
H	2.94210984	4.00360339	2.48006542
P	0.45475747	2.58229698	2.82645047
C	-0.58959775	4.07628722	3.13668697
C	-1.66009464	4.32626012	2.25954158
C	-2.51226716	5.41208430	2.47281353
C	-2.29310912	6.27404139	3.55604619
C	-1.22290794	6.03829369	4.42562160
C	-0.37628246	4.94213729	4.22117554
H	-1.81441151	3.66709996	1.40721716
H	-3.33966187	5.59293700	1.79026052
H	-2.95033371	7.12540077	3.71738220
H	-1.04569857	6.70543020	5.26635596
C	1.88569881	2.84726455	3.96465149
C	1.92201920	2.33903530	5.27275273
C	3.01651698	2.60738142	6.10360800
C	4.07662055	3.39334526	5.63961592
C	4.04509473	3.90469535	4.33524374
C	2.96075195	3.62558914	3.50051804
H	1.09887597	1.73734933	5.64647667
H	3.03636731	2.20496943	7.11396998
H	4.92494527	3.60270705	6.28713440
H	4.86885963	4.51228520	3.96707180
C	-0.49821548	1.24175917	3.67355395
C	-1.57898775	1.50027211	4.53111180
C	-2.24823175	0.44362846	5.16064347
C	-1.83872157	-0.87662087	4.94795754
C	-0.75779143	-1.14076733	4.09522406
C	-0.09884047	-0.08907863	3.45543862
H	-1.89956203	2.52161899	4.71229176
H	-3.08731907	0.65557960	5.81970897
H	-2.35973660	-1.69580171	5.43807377
H	-0.43667928	-2.16554250	3.92241644

$Pd(PPh_3)(MeOH)$
E = -6890.86
G = -6726.81
Nimag = 0

Pd	-0.09280297	0.10238154	0.01245623
O	2.17920760	0.14913078	-0.01952530
P	-2.28741556	0.07293604	0.05418278
C	-3.14059664	-0.22217411	-1.56204609
C	-4.29836773	0.46577998	-1.95760581
C	-2.60825141	-1.20932245	-2.41065305
C	-4.91510632	0.16873906	-3.17919864
H	-4.72310117	1.23074061	-1.31437555
C	-3.23135492	-1.51488113	-3.62285677
H	-1.70013769	-1.73147193	-2.11475804
C	-4.38738949	-0.82413816	-4.01149007
H	-5.80998074	0.71123950	-3.47653105
H	-2.81272934	-2.28450502	-4.26768622
H	-4.86858350	-1.05529502	-4.95908458
C	-3.10334833	1.62314307	0.65260384
C	-4.21880929	1.62741439	1.50481508
C	-2.57700642	2.84981946	0.20963734
C	-4.79863262	2.83765655	1.90485934
H	-4.63829021	0.68985897	1.85716339
C	-3.16438472	4.05641878	0.59724383
H	-1.70016289	2.84973060	-0.43528285

C	-4.27665610	4.05323958	1.45022485
H	-5.65963803	2.82820553	2.56973138
H	-2.75038126	4.99806079	0.24339276
H	-4.72838729	4.99233182	1.76143944
C	-3.05324443	-1.22253169	1.13382769
C	-4.24251604	-1.89169750	0.80296863
C	-2.41424777	-1.52526578	2.34907514
C	-4.78318220	-2.84557640	1.67324992
H	-4.74893703	-1.67117966	-0.13212255
C	-2.96057394	-2.46831823	3.22338177
H	-1.48158369	-1.02159287	2.59671081
C	-4.14663795	-3.13376554	2.88558242
H	-5.70258236	-3.36087878	1.40379077
H	-2.45792413	-2.69134860	4.16195233
H	-4.56766422	-3.87544429	3.56051962
C	2.88367811	-0.10261277	1.24178019
H	2.49374609	-0.50075430	-0.67400501
H	3.96318964	-0.02180642	1.08038005
H	2.62751626	-1.09083247	1.63582484
H	2.55147700	0.67010953	1.93627656

4_38

E = -6475.16

G = -6318.52

Nimag = 0

C	1.47666040	0.37465119	-0.04882294
C	0.78657378	-1.01262070	-0.10541361
H	0.88669803	1.07172137	0.56289326
H	1.52063469	-1.73782959	-0.47664104
C	-0.44385309	-1.11962846	-1.04146465
C	1.63853378	1.02417739	-1.41180283
C	0.42237575	0.97681364	-2.31793649
C	-0.17502407	-0.44877674	-2.40492022
H	-0.59214240	-2.18086382	-1.25146826
H	-1.09084955	-0.43430576	-3.00174573
H	0.54280771	-1.08770831	-2.93398332
H	-2.45283180	-0.99543849	2.90377917
H	2.45955203	0.29581271	0.42551197
H	0.51827345	-1.33044831	0.90588435
N	-1.74207665	-0.69553456	-0.42695172
C	-1.98365809	0.68042249	0.03026106
H	-2.49442460	0.67753895	0.99832691
H	-1.02760545	1.17793850	0.19812201
C	-2.80980926	1.48758721	-0.94629794
C	-3.43681328	1.08237681	-2.04147206
C	-1.85288550	-1.89242178	2.78815086
S	-2.72806338	-1.90405553	0.17383113
O	-3.94273436	-1.24453485	0.65979807
O	-2.82884271	-2.94943619	-0.84845030
H	-1.10981907	-4.29145231	0.46321088
H	-1.08066766	-1.83690537	4.79537285
H	0.28124910	-3.90201321	4.52513048
H	0.25767683	-5.13833066	2.36504594
O	2.69064780	1.56399034	-1.75514427
C	-1.09497661	-3.76276205	1.41040622
Br	-2.90342223	3.37658270	-0.39005995
C	-1.08225896	-2.37162059	3.84930017
H	-3.38050387	0.03535718	-2.32686837
C	-0.31851416	-3.53574200	3.69592986
H	-0.32141293	1.67715721	-1.91442403
H	0.70117992	1.34028489	-3.31131789
C	-1.84634543	-2.59468516	1.57540410
H	-4.01353126	1.75452991	-2.66678525
C	-0.32938206	-4.23136552	2.48180751

Int4_17

E = -18526.95

G = -18060.96

Nimag = 0

C	0.71919726	-1.64663127	-1.17189288
C	0.13601042	-1.22734348	-2.54100341
H	-0.07021292	-2.12339718	-0.57502635
H	0.93874366	-0.81759069	-3.16642018
C	-0.93995559	-0.12726227	-2.43727609
C	1.21066710	-0.45738185	-0.37443469
C	0.25285670	0.71722460	-0.30671634
C	-0.33302679	1.07726531	-1.69341608
H	-1.18999722	0.19730622	-3.45299833
H	-1.05030338	1.89536768	-1.59633184
H	0.47459673	1.45284429	-2.33310897
C	-5.57681014	1.11391968	1.55388412
H	1.53237979	-2.36864293	-1.29136209
H	-0.23859189	-2.10633453	-3.06682733
N	-2.20068792	-0.60843983	-1.76278180
C	-3.06257316	0.36522502	-1.05474388
H	-3.82993373	-0.20075051	-0.53078871
H	-2.45692451	0.84606251	-0.28564611
C	-3.70026615	1.43639902	-1.94493359
C	-3.66581945	1.46472824	-3.33966395
C	-2.32895787	-3.43937715	-0.23679704
S	-2.98357766	-1.93957859	-2.45210005
O	-4.37885462	-1.90521636	-2.00865882
O	-2.67662148	-2.02017452	-3.88106670
H	-1.55239348	-4.26025360	-3.46280451
H	-1.83733676	-4.61658835	1.49675514
H	-0.70118389	-6.40146871	0.18476464
H	-0.56038209	-6.23036743	-2.29325075
O	2.30533466	-0.44580821	0.19116749
H	-6.23547797	-1.88270005	0.06953344
Pd	-5.74220352	0.87330353	-2.68993593
H	-4.71252871	-2.66002230	1.84883873
H	-3.66773025	-1.01998497	3.41130429
H	-4.22458702	1.40127945	3.20583874
C	-7.77434758	2.42303493	-0.26474839
C	-8.66325782	2.56154583	0.81505241
C	-9.13733379	3.82386181	1.17956332
C	-8.73263890	4.96034023	0.46460936
C	-7.85212991	4.82845380	-0.61430291
C	-7.37550232	3.56329142	-0.97688447
H	-9.82382827	3.92337799	2.01762283
C	-1.77574710	-4.54229259	0.41418733
H	-3.25112056	0.62866451	-3.89567900
C	-1.13645001	-5.54660519	-0.32637182
H	-9.10574341	5.94208066	0.74760796
H	-7.53644846	5.70675260	-1.17302714
C	-2.23483546	-3.35493543	-1.63125589
H	-3.74490604	2.40398494	-3.87716037
C	-1.05511135	-5.45113597	-1.71934277
H	-2.82029288	-2.65184654	0.32603427
C	-1.60890800	-4.35006942	-2.38282193
H	-5.80498385	2.17163058	1.46848985
H	-8.98566917	1.68264054	1.36776526
Br	-3.63307206	3.24641015	-0.99921094
P	-7.12809657	0.77512385	-0.79216245
H	-8.40860458	-1.19022480	1.16552121
H	-6.68575825	3.45098434	-1.80993543
C	-8.68305360	-0.22313604	-0.74951140
C	-9.54597444	-0.08517719	-1.85051266
C	-10.75079371	-0.78493104	-1.90420834
C	-11.10719255	-1.64766617	-0.86025602
C	-10.25656328	-1.79030539	0.24017306
C	-9.05327002	-1.07686502	0.29980355
H	-9.26335908	0.56216896	-2.67552918
H	-11.39901849	-0.67712200	-2.76994390
H	-12.03730301	-2.20910139	-0.90902315
H	-10.52756752	-2.45581931	1.05721653
C	-6.16475229	0.19781590	0.66486940
C	-5.82644666	-1.16485242	0.77375304
C	-4.94721486	-1.60133430	1.76733713
C	-4.36307644	-0.68121337	2.64704622
C	-4.67840294	0.67752008	2.53232538
H	0.75989076	1.57625127	0.14237685
H	-0.55673287	0.41540326	0.37444549
C	-5.44851405	-2.01017942	-6.16334786
H	-4.75704234	1.32527057	-6.17423875
H	-3.01205287	0.56280232	-7.75697397
H	-2.79514161	-1.86055003	-8.30487343
H	-4.35894419	-3.50277959	-7.27408755
C	-7.86043946	-1.47084665	-4.28778398
C	-9.02518582	-1.74099999	-5.02064957

C	-9.82900649	-2.83620218	-4.68724349
C	-9.47254449	-3.67343558	-3.62468093
H	-10.73875622	-3.02889796	-5.25173788
H	-6.12530550	-2.73414101	-5.71971317
H	-9.31831627	-1.09096051	-5.83972072
P	-6.77194723	-0.01505820	-4.59885833
H	-7.58188937	0.16367313	-7.49924442
C	-7.82884509	1.13172755	-5.58204799
C	-8.43069031	2.20546978	-4.90358337
C	-9.26099093	3.10073929	-5.58465833
C	-9.48552588	2.93988161	-6.95741679
C	-8.87782360	1.88105287	-7.64404611
C	-8.05432827	0.98065392	-6.96053139
H	-9.72184468	3.92751571	-5.04884191
H	-10.12421344	3.63992847	-7.49112936
H	-9.04543342	1.75653811	-8.71167141
C	-5.57373262	-0.64994479	-5.84771520
C	-4.67983274	0.27019341	-6.42621412
C	-3.69284299	-0.16048650	-7.31292239
C	-3.57156734	-1.52281480	-7.62202738
C	-4.44910971	-2.44341533	-7.04272773
C	-8.30563893	-3.41396984	-2.89653488
C	-7.50725881	-2.31604387	-3.22128399
H	-10.10640575	-4.51595974	-3.35801498
H	-8.02948923	-4.05489790	-2.06226522
H	-6.61215026	-2.09790101	-2.64607624
H	-8.23067244	2.34221950	-3.84291991

Int4_18

E = -12519.65

G = -12208.72

Nimag = 0

C	0.50104609	-1.51770925	-0.65890040
C	0.00390861	-1.44525941	-2.12104735
H	-0.32461919	-1.84332716	-0.01178283
H	0.84504399	-1.18922043	-2.77692575
C	-1.07026164	-0.36225968	-2.35321205
C	0.95271408	-0.16774478	-0.14393702
C	-0.00243890	0.98018372	-0.41519506
C	-0.50901663	0.99116905	-1.87743135
H	-1.25041284	-0.28952466	-3.43084913
H	-1.22827080	1.80121449	-2.01875719
H	0.33395692	1.21549797	-2.54172443
C	-6.06290555	1.48094059	1.06814628
H	1.31463012	-2.24126128	-0.55367310
H	-0.34082878	-2.42886061	-2.44231015
N	-2.38238164	-0.68518171	-1.67517616
C	-3.26569530	0.40868200	-1.23014486
H	-4.07406319	-0.02348523	-0.64315746
H	-2.69541830	1.04460901	-0.55230309
C	-3.84453074	1.27819314	-2.35510001
C	-3.76004161	1.05599216	-3.72393307
C	-2.61253172	-3.00572637	0.50504333
S	-3.11909770	-2.15324214	-2.05738118
O	-4.54844925	-2.02201867	-1.76684771
O	-2.69832364	-2.58419766	-3.39650816
H	-1.67705666	-4.67156646	-2.33179639
H	-2.23407796	-3.67040450	2.51615938
H	-1.05963900	-5.74598939	1.79967962
H	-0.78424465	-6.25097220	-0.62034235
O	2.01308751	-0.01023657	0.46273852
H	-6.61152107	-1.76899222	0.19417558
Pd	-5.82674803	0.74349023	-2.87753734
H	-5.19285959	-2.13515194	2.18140927
H	-4.26429325	-0.19084257	3.43658909
H	-4.82904892	2.12662274	2.71149176
C	-8.35936853	2.25933359	-0.93721639
C	-9.44505831	2.35796365	-0.05086030
C	-10.06317232	3.59138862	0.17104237
C	-9.59985817	4.73961700	-0.48563866
C	-8.51906297	4.64841203	-1.36902103
C	-7.90421802	3.41214380	-1.59679415
H	-10.90495615	3.65791005	0.85670822
C	-2.11399614	-3.89247376	1.45906785
H	-3.35395318	0.11533135	-4.08809157
C	-1.45316150	-5.06052044	1.05363396
H	-10.08191476	5.69861092	-0.31007007
H	-8.15561475	5.53596266	-1.88208619
C	-2.44396305	-3.30277353	-0.85283293
H	-3.80319925	1.87895386	-4.42970925
C	-1.29649831	-5.34528424	-0.30651079
H	-3.11905611	-2.09529038	0.80874525
C	-1.79546478	-4.46468077	-1.27328127
H	-6.29540827	2.49437394	0.75475512
H	-9.81339426	1.47572363	0.46424980
Br	-3.88094968	3.22715319	-1.73894246
P	-7.46018099	0.67474895	-1.24473931
H	-9.08762407	-0.79020593	0.85848737
H	-7.06143410	3.33125094	-2.27994993
C	-8.79383317	-0.59488243	-1.27772669
C	-9.21667793	-1.04064797	-2.54144678
C	-10.25421040	-1.97103099	-2.65617371
C	-10.87098128	-2.47522295	-1.50528966
C	-10.44737555	-2.04526220	-0.24133311
C	-9.41510842	-1.10942560	-0.12666593
H	-8.72588866	-0.65889829	-3.43498972
H	-10.57313069	-2.30790812	-3.63978086
H	-11.67266869	-3.20485398	-1.59173872
H	-10.91966476	-2.43962521	0.65550497
C	-6.57964245	0.38903613	0.34934509
C	-6.24659702	-0.91499850	0.75579621
C	-5.42903126	-1.12056043	1.86990240
C	-4.91043745	-0.02879381	2.57712240
C	-5.22930426	1.27216937	2.17054268
H	0.48316106	1.92700670	-0.16132409
H	-0.84738378	0.84723227	0.27707240

Int4_19

E = -13383.26

G = -13043.13

Nimag = 0

C	-1.21955963	-2.82258701	-2.52562118
C	-2.66919438	-2.36891679	-2.82460361
H	-1.03738270	-2.77674530	-1.44418696
H	-2.88850136	-2.55858862	-3.88234001
C	-2.92618755	-0.86320426	-2.61755215
C	-0.17260093	-1.93298818	-3.16311611
C	-0.42289101	-0.44451192	-3.02645530
C	-1.87190724	-0.09312997	-3.43207569
H	-3.91294334	-0.61478940	-3.03320818
H	-2.01707517	0.98511225	-3.38250285
H	-2.03779551	-0.36574742	-4.47988495
H	-2.51453252	2.41401407	-6.94113882
H	-1.06237834	-3.85747831	-2.84359462
H	-3.36952873	-2.98476042	-2.26004429
N	-2.93396088	-0.41759698	-1.17018255
C	-2.89645432	1.05368637	-0.89536897
H	-2.73230938	1.16963398	0.17269069
H	-1.99963082	1.42274039	-1.39709644
C	-4.09739831	1.90825884	-1.32896682
C	-4.15497145	2.58574917	-2.56240053
C	-1.50246951	-2.22233800	1.05466282
S	-3.83958311	-1.31537901	-0.07154283
O	-4.11447644	-0.44898398	1.07802236
O	-4.98317693	-1.98530978	-0.72541288
H	-4.03423385	-4.21366379	-0.09886874
H	0.32273837	-2.93172590	1.94501515
H	-0.28396320	-5.33460145	1.70974845
H	-2.46297255	-5.97869686	0.69707882
O	0.81316086	-2.38681030	-3.74626154
H	-1.57488054	0.28829647	-7.84467346
Pd	-5.64599495	1.04683913	-2.54458075
H	-2.75038272	-1.86425740	-7.40625320
C	-6.95537254	-1.44796939	-4.70786837
C	-7.97028336	-1.87962402	-5.57559971
C	-8.39122551	-3.21453835	-5.56020810
C	-7.79716054	-4.13241590	-4.68697145
H	-9.18274777	-3.53655491	-6.23323920
H	-4.84030332	-1.89453174	-6.08611872
H	-8.43680972	-1.17774377	-6.26025320

P	-6.34675215	0.29443827	-4.64114157
H	-6.71661978	0.82457833	-7.58673434
C	-0.62824784	-3.21358001	1.50144887
H	-3.37147557	2.42340827	-3.30037930
C	-0.97258114	-4.56600120	1.36881419
C	-7.57856000	1.22442250	-5.64407824
C	-8.62369181	1.86285197	-4.95556828
C	-2.71999918	-2.60457478	0.47744317
H	-4.68013605	3.53298814	-2.65629252
C	-2.19612025	-4.93021195	0.79800618
H	-1.23840983	-1.17252209	1.13878909
C	-3.08376474	-3.94619355	0.34981928
C	-9.60871127	2.56402498	-5.65717838
C	-9.54797208	2.64618920	-7.05384676
Br	-4.87477914	2.93960532	0.27042872
O	-7.10547749	-0.21411413	-1.06466483
C	-8.50277021	2.02149269	-7.74537521
C	-7.52348213	1.31015222	-7.04494549
H	-10.41478206	3.05371872	-5.11569445
H	-10.30829125	3.19935258	-7.60033866
H	-8.45132236	2.08582653	-8.82991773
C	-4.86266677	0.23987061	-5.74276798
C	-4.19009496	1.45091252	-5.99224423
C	-3.02144303	1.47019956	-6.75391937
C	-2.49366046	0.27536329	-7.26331514
C	-3.15241420	-0.93231927	-7.01519695
C	-6.78282289	-3.70839983	-3.81894423
C	-6.37139948	-2.37454570	-3.82465322
C	-8.42309800	-0.65792537	-1.47854003
H	-8.12597456	-5.16888609	-4.67783865
H	-6.32127299	-4.41282992	-3.13075852
H	-5.60884126	-2.04815368	-3.12506426
H	-8.65544583	1.81492289	-3.86886607
H	0.30539170	0.10684719	-3.62818862
H	-0.26460497	-0.18086622	-1.97006699
C	-4.33555663	-0.95047404	-6.26483423
H	-4.58297782	2.37762768	-5.58125285
H	-6.52684679	-0.99208335	-0.90267154
H	-9.01348224	0.24185549	-1.66708169
H	-8.89807329	-1.24145929	-0.68071865
H	-8.37254296	-1.25449343	-2.39466226

TS4_7

E = -18508.39

G = -18041.72

Nimag = 1, 162i cm-1

C	-0.54018028	-0.26122878	-1.79366754
C	-1.55905414	-1.37165400	-2.14301144
H	-3.51311225	8.31345919	-7.24578927
H	-1.09236853	-2.34122389	-1.93114004
C	-1.97245717	-1.43706638	-3.62513753
C	0.62516997	-0.20680548	-2.76500711
C	0.25750265	-0.29470072	-4.22911692
C	-0.72636490	-1.44468964	-4.52966877
H	-2.46102130	-2.40819983	-3.74280607
H	-1.02965630	-1.40773765	-5.57783682
H	-0.22188771	-2.40739845	-4.37185836
Br	-1.12541211	3.02187351	-3.64143364
H	-5.35632290	6.68055087	-6.85256763
H	-2.43103285	-1.31286421	-1.48587069
N	-2.99355695	-0.39032010	-4.06615705
C	-3.52101599	0.61400667	-3.09500744
H	-4.56181340	0.38421006	-2.83036293
H	-2.97253698	0.49930126	-2.16739335
C	-3.52306038	2.05812538	-3.48859919
C	-4.13011698	2.72929608	-4.50108357
C	-6.09011307	-2.01163398	-3.43782350
S	-4.13735965	-1.03538137	-5.13132636
O	-5.11023234	0.02021604	-5.41889107
O	-3.39524148	-1.65658712	-6.23106631
H	-3.72725289	-3.91285972	-5.02221669
H	-7.58428072	-2.77518874	-2.09079214
H	-6.78997332	-5.12569604	-2.24450438
H	-4.86152935	-5.69662721	-3.71203160
O	1.78676265	-0.06118898	-2.37927451
H	-4.47797006	8.38028339	-0.15288942
Pd	-3.92952224	3.67298477	-2.23126124
H	-2.80243157	9.27421210	1.43420832
H	-0.54225678	8.24198702	1.58236894
H	0.04391036	6.32329663	0.09987005
C	-4.07598660	6.82065867	-3.68862376
C	-3.04424744	7.74334262	-3.91347760
C	-2.84183166	8.27597002	-5.19313802
C	-3.67128278	7.89835344	-6.25316435
C	-4.70742966	6.97933749	-6.03245877
C	-4.90296132	6.43857777	-4.76132791
H	-2.39899750	8.04883011	-3.09552792
C	-6.73204688	-3.02144019	-2.71804662
H	-4.94722459	2.26429996	-5.04887295
C	-6.28618314	-4.34480193	-2.80823353
H	-2.03678338	8.98890000	-5.35687979
C	-1.88092508	6.28428535	-0.86339653
C	-4.99941066	-2.34474875	-4.25091985
H	-3.79258625	3.70388835	-4.83865632
C	-5.20111702	-4.66749739	-3.63132212
H	-6.44364921	-0.98769348	-3.38633253
C	-4.55244083	-3.66861487	-4.36169588
H	-1.63512501	5.42970094	-1.48912694
H	-1.00604784	0.73243222	-1.85138559
H	-0.16076268	-0.38556099	-0.77523363
P	-4.37406276	6.02524754	-2.05121305
H	-5.81017143	8.60775703	-2.55089923
H	-5.69868661	5.71474418	-4.59840471
C	-6.01424526	6.69199710	-1.56381292
C	-6.85159366	5.88100336	-0.78340563
C	-8.09735298	6.35235914	-0.36039859
C	-8.52046261	7.63515691	-0.72552183
C	-7.69425553	8.44564457	-1.51564205
C	-6.44578835	7.97774737	-1.93454745
H	-6.52444603	4.88516065	-0.50408252
H	-8.73362323	5.71840459	0.25192490
H	-9.49148538	8.00201633	-0.40099444
H	-8.02288524	9.44127603	-1.80489588
C	-3.16468008	6.85373517	-0.94020996
C	-3.48571958	7.94172433	-0.11593046
C	-2.54051726	8.44080397	0.78635749
C	-1.26898590	7.86144623	0.86861547
C	-0.93780463	6.78559699	0.03491368
H	1.16851210	-0.38145348	-4.82936187
H	-0.22698897	0.66176774	-4.47577554
H	-6.94488222	6.05775043	3.50508358
H	-4.71176231	6.87659301	2.74896107
H	1.49661055	2.96410695	2.49482962
H	-0.55658369	2.85931220	3.90152572
C	-4.71253940	3.83369911	1.20159046
C	-5.96227639	3.37105826	1.64493896
C	-6.75852747	4.16822159	2.47406089
C	-6.31933590	5.43532647	2.87008238
C	-5.06764998	5.89534209	2.44533519
C	-4.27017456	5.10198372	1.62071823
H	-6.32166614	2.39071183	1.35214210
C	-1.90090520	2.88863387	2.21892267
H	-2.79158057	2.84536132	2.83910275
P	-3.66343906	2.91115680	-0.00742797
H	-2.47405773	0.41883206	1.20398047
C	-4.22469606	1.16617236	0.17842560
C	-5.47131784	0.81438097	-0.37482947
C	-5.93215134	-0.49907836	-0.30474348
C	-5.13919031	-1.49264159	0.28476565
C	-3.89506043	-1.15476635	0.82332116
C	-3.44151175	0.17003487	0.77999683
H	-6.06847773	1.56895192	-0.88227487
H	-6.90135704	-0.75108969	-0.72487129
H	-5.48679865	-2.52187911	0.31272304
H	-3.27004055	-1.92058289	1.27642169
C	-2.01882088	2.94164168	0.81805198
C	-0.86079187	2.99990590	0.03207893
C	0.40182357	3.00240573	0.63291806
C	0.51551666	2.95419383	2.02556911
C	-0.63932642	2.89745712	2.81776630

H	-0.94450692	3.05339925	-1.04915584
H	1.29309487	3.04908405	0.01142522
H	-7.72447135	3.79560958	2.80705971
H	-3.29987288	5.46702586	1.30588485

TS4_8

E = -12508.62

G = -12199.33

Nimag = 1, 162i cm-1

C	1.40279019	-0.90270472	-1.88525271
C	0.03543920	-1.63753528	-1.83502214
H	-8.41330585	7.79867673	0.00697569
H	0.15178500	-2.58909324	-2.36731790
C	-1.16037651	-0.91400598	-2.50419924
C	1.68011802	-0.19253656	-3.20040311
C	0.52031677	0.57796221	-3.80204530
C	-0.76013723	-0.28927420	-3.85610106
H	-1.91157868	-1.67295989	-2.72230562
H	-1.59447320	0.29625389	-4.25391662
H	-0.58734008	-1.11739702	-4.55532909
Br	-0.03472127	3.89105873	-0.20024254
H	-6.16903496	7.84733758	-1.07424199
H	-0.20890233	-1.88855576	-0.79786388
N	-1.88762153	0.06466052	-1.63537181
C	-1.16033644	1.12182893	-0.90250470
H	-1.28858520	1.00569013	0.17966166
H	-0.09545029	0.99081505	-1.08262514
C	-1.55472798	2.52000136	-1.31596796
C	-2.06461525	2.98067557	-2.46924859
C	-3.03650852	-0.08581354	1.77090355
S	-3.36335283	-0.37416642	-0.95545745
O	-4.15226165	0.84716331	-0.79967962
O	-3.89685594	-1.48024054	-1.75721222
H	-2.54509714	-2.98008256	0.00586672
H	-2.71124664	0.14156819	3.88387645
H	-1.96640690	-2.21312541	4.20741220
H	-1.89436400	-3.77523344	2.27206623
O	2.78675744	-0.23562779	-3.73849936
H	-1.53594462	4.35280808	2.64748954
Pd	-2.73782245	3.50642030	0.06538934
H	-0.43408809	5.42954217	4.60103333
H	-1.77280524	6.83048514	6.16685890
H	-4.21243284	7.14132288	5.77564796
C	-5.63161151	5.33254687	1.17412734
C	-6.90010728	5.30629067	1.77671962
C	-7.89726367	6.19260241	1.35658054
C	-7.63578667	7.11225018	0.33393158
C	-6.37416453	7.14058838	-0.27342920
C	-5.37890606	6.25060596	0.14088503
H	-7.11218770	4.59145982	2.56675202
C	-2.66568076	-0.53955654	3.03943656
H	-2.45587614	2.28371015	-3.20903407
C	-2.25095120	-1.86332228	3.21834952
H	-8.87753983	6.16366860	1.82698279
C	-4.24633796	5.91100521	4.00627268
C	-2.98128476	-0.97455596	0.69143836
H	-2.11683003	4.04045460	-2.69827734
C	-2.20750675	-2.74440772	2.12916742
H	-3.37737311	0.93215945	1.62095744
C	-2.56971657	-2.30377177	0.85460279
H	-5.31100981	6.05253195	3.84379907
H	1.45764692	-0.13201713	-1.10297853
H	2.22025914	-1.60203294	-1.68459725
P	-4.25153822	4.22744851	1.69296762
H	-4.28813564	3.04426276	4.46310299
H	-4.40308052	6.25804812	-0.34120744
C	-5.12041941	2.80558188	2.48141185
C	-5.94127791	2.00578590	1.66526713
C	-6.55983039	0.86854581	2.18437933
C	-6.35864306	0.50781690	3.52312091
C	-5.53958919	1.29445355	4.33795570
C	-4.92284788	2.44042954	3.82182805
H	-6.07733542	2.26341597	0.61861668
H	-7.18769800	0.25574443	1.54195299
H	-6.83148016	-0.38548422	3.92409925
H	-5.37461511	1.01721649	5.37658636
C	-3.49742645	5.11592743	3.12304660
C	-2.12012639	4.95272807	3.34279095
C	-1.50123294	5.56295622	4.43878778
C	-2.25332966	6.35052554	5.31756752
C	-3.62583957	6.52569677	5.09753269
H	0.80120214	0.92471802	-4.80085617
H	0.34747705	1.47139665	-3.18507499

TS4_9

E = -13367.21

G = -13029.25

Nimag = 1, 175i cm-1

C	-6.19836634	1.59349622	-7.51798120
C	-7.41066956	1.64799348	-6.56020336
H	-5.93592735	10.22169907	3.41006919
H	-8.32022015	1.88113477	-7.12692948
C	-7.27117416	2.74914497	-5.48903709
C	-5.88434437	2.94474692	-8.12698355
C	-5.87364579	4.11645856	-7.16038885
C	-7.08937398	4.10142034	-6.20381230
H	-8.20130167	2.78758870	-4.91026577
H	-7.02498641	4.93115512	-5.49525246
H	-8.00612703	4.26518824	-6.78223866
Br	-6.24460323	6.64479994	-2.94266017
H	-7.16884739	9.53221819	1.35775828
H	-7.56592855	0.66438492	-6.11287957
N	-6.11421045	2.48681728	-4.55202391
C	-5.60275334	3.63115536	-3.76276462
H	-4.70771317	3.32040611	-3.22486824
H	-5.26611378	4.38935061	-4.47067732
C	-6.57815956	4.26652480	-2.79895328
C	-7.84389832	3.95206205	-2.45381113
C	-5.66340575	1.32667361	-1.09383008
S	-6.18104469	0.95911714	-3.77411559
O	-7.55317411	0.69285116	-3.30757324
O	-5.59187390	-0.02463707	-4.69182908
H	-3.30887994	0.76097211	-3.51565839
H	-5.24412580	1.54664113	1.00215251
H	-2.78978030	1.29659719	0.73065884
H	-1.81633526	0.89515564	-1.52741158
O	-5.63727921	3.08634642	-9.32601471
H	-4.75917370	2.60625787	3.29673877
Pd	-5.96482735	4.64323855	-0.86467841
H	-2.52345222	1.72636085	3.87265792
H	-0.47388479	2.81028468	2.96268494
H	-0.68622242	4.81270576	1.49092424
C	-5.66790126	6.55763693	2.11231353
C	-4.96720342	6.95460712	3.26325047
C	-5.06502427	8.27002029	3.72778472
C	-5.86297144	9.19881009	3.04805558
C	-6.55730992	8.81128450	1.89553137
C	-6.45533377	7.49817837	1.42647504
H	-4.33773233	6.24294836	3.79037909
C	-4.81943426	1.38458828	0.01764037
H	-8.26481930	2.97798137	-2.70017042
C	-3.43832217	1.23680711	-0.13858470
H	-4.51748560	8.56965776	4.61857585
C	-2.83952281	4.82137181	1.55658883
C	-5.09958297	1.10520460	-2.35365942
H	-8.48901117	4.65504575	-1.93515651
C	-2.88982445	1.01286893	-1.40808937
H	-6.73631479	1.42946237	-0.98742162
C	-3.71969865	0.94059748	-2.52744252
H	-2.92475400	5.70473165	0.92810774
H	-5.31351803	1.28559447	-6.94298654
H	-6.35434215	0.86292937	-8.31739651
P	-5.62701673	4.83938612	1.44432435
H	-6.35172315	4.86210635	4.37329125
H	-6.97511235	7.19825660	0.51826284
C	-6.85894261	3.93731853	2.48198867
C	-7.69106051	3.00137735	1.84768414
C	-8.61792367	2.25796448	2.58560004
C	-8.72676096	2.45327808	3.96664851
C	-7.90993022	3.39607845	4.60517069

C	-6.98017359	4.13434241	3.86794194
H	-7.61323975	2.87159507	0.77048409
H	-9.25506907	1.53408529	2.08290784
H	-9.44810264	1.87911655	4.54333787
H	-7.99718315	3.55510818	5.67751738
C	-4.00444930	4.20585501	2.05448577
C	-3.87516529	3.09195621	2.89584613
C	-2.60754944	2.59374177	3.22206266
C	-1.45658999	3.20261835	2.71333513
C	-1.57576731	4.32486346	1.88220106
H	-5.82461636	5.05225302	-7.72473073
H	-4.94292810	4.02714840	-6.58012973
O	-3.38569358	4.29247909	-1.60597675
H	-3.02427695	3.97699851	-0.75746763
C	-2.69382256	5.50886509	-1.97894683
H	-1.61836248	5.32816380	-2.09687583
H	-2.85764618	6.30485634	-1.24201226
H	-3.12101876	5.82665254	-2.93174557

Int4_20

E = -18536.74

G = -18067.71

Nimag = 0

C	3.22458601	2.23642266	-1.14130930
C	3.11988849	0.70393763	-0.97188295
H	2.39448373	2.71501937	-0.60504917
H	3.99300971	0.22790102	-1.43531114
C	1.87996977	0.09244733	-1.65501762
C	3.08940182	2.68868048	-2.57839133
C	1.96622091	2.04358611	-3.35230462
C	1.89825467	0.51732315	-3.13695382
H	1.97281764	-1.00107063	-1.62161450
H	1.04992925	0.11120319	-3.68973726
H	2.79205169	0.04702053	-3.56629815
C	-3.57648130	6.87706324	0.10242278
H	4.15929225	2.61927105	-0.72018279
H	3.16802461	0.45064908	0.08871238
N	0.58014554	0.46554954	-0.95935144
C	-0.67731659	0.14899178	-1.73195290
H	-0.41736872	-0.53245195	-2.54982681
H	-1.34300478	-0.40769193	-1.07719077
C	-1.40723029	1.35514229	-2.26675071
C	-1.53632402	1.56438573	-3.57585596
C	1.01619138	2.54431105	1.36267855
S	0.48504207	-0.07429087	0.65126656
O	-0.93764500	-0.07713242	1.02768304
O	1.23264769	-1.32922783	0.85043210
H	2.26653818	-0.23735311	2.90809349
H	1.36596222	4.57066243	1.98575831
H	2.77070425	3.92013601	3.93679389
H	3.21506759	1.51627188	4.40146422
O	3.81754090	3.55920666	-3.06478577
H	-0.60273657	5.77482441	1.33992355
Pd	-2.27639918	2.60977247	-0.84833106
H	0.01508356	8.12135307	0.89443252
H	-1.65783957	9.69336406	-0.07943582
H	-3.96080125	8.88192499	-0.58616350
C	-4.84019398	4.26756617	1.36011531
C	-5.30957401	4.18976397	2.68087772
C	-6.68174771	4.18590009	2.94286229
C	-7.60199658	4.26816417	1.89194375
C	-7.14176636	4.35611450	0.57428148
C	-5.76999245	4.34910787	0.31074212
H	-4.61040474	4.10931086	3.50602955
C	1.56336768	3.52269370	2.19361126
H	-1.07222327	0.89021143	-4.30079386
C	2.35196189	3.15571323	3.28733008
H	-7.03088625	4.11005175	3.97006039
H	-8.66970416	4.25775063	2.09795306
C	1.28465630	1.20154734	1.62988453
H	-2.09987244	2.39216369	-3.99563091
C	2.60268976	1.80318832	3.55064819
H	0.40081874	2.82725871	0.51608455
C	2.07123177	0.81319884	2.71964375
H	-4.58830618	6.54801400	-0.10937114
H	-7.84564094	4.41336466	-0.25134373
Br	-0.38693358	4.30259388	-1.48006883
P	-3.04393396	4.20626722	0.92836625
H	-2.50028024	5.80960661	3.40485724
H	-5.42637826	4.39277899	-0.71616758
C	-2.22211326	3.84427297	2.53762976
C	-1.72244739	2.55349093	2.76226505
C	-1.15629367	2.21341295	3.99351927
C	-1.06136320	3.16906878	5.00667727
C	-1.54124579	4.46733584	4.78645409
C	-2.12417178	4.80334529	3.56275880
H	-1.75038798	1.81273030	1.97093616
H	-0.76422017	1.21128576	4.14387090
H	-0.60655551	2.91183213	5.96027274
H	-1.46538771	5.21723636	5.57039526
C	-2.64056876	5.98769880	0.65255140
C	-1.34046483	6.45000921	0.92271509
C	-0.99212739	7.77796241	0.66970464
C	-1.93065739	8.65995153	0.12137459
C	-3.22206072	8.20440684	-0.16405300
H	2.06193602	2.28927034	-4.41486112
H	1.03723174	2.50051649	-2.97999443
H	-7.14082183	1.13178005	-1.26521291
P	-4.13166874	1.18869376	-0.98520968
H	-4.52649962	0.33751020	-3.81260837
H	-3.84917871	1.75186200	1.89071657
C	-3.93485517	-0.41251426	-1.87445998
C	-3.47252212	-1.53312068	-1.16283397
C	-3.25042765	-2.74440793	-1.82210114
C	-3.48844031	-2.84792507	-3.19762380
C	-3.95546154	-1.73601198	-3.90830532
C	-4.17400729	-0.52197295	-3.25162958
H	-3.28377628	-1.45986462	-0.09548382
H	-2.88981414	-3.60391635	-1.26212975
H	-3.31529643	-3.79048768	-3.71140238
H	-4.14721327	-1.81169594	-4.97606674
C	-5.03040080	0.60350964	0.51437525
C	-6.06199396	-0.35147986	0.40289809
C	-6.73220576	-0.79989930	1.54169522
C	-6.37039334	-0.32127422	2.80840171
C	-5.32909705	0.60163054	2.92751596
C	-4.66560820	1.05593667	1.78474227
H	-6.32494159	-0.76450736	-0.56545811
H	-7.52956657	-1.53237434	1.44161702
H	-6.89102008	-0.67745149	3.69409735
H	-5.02775105	0.97009035	3.90475505
C	-5.35799073	2.10009430	-2.02412400
C	-4.87621412	3.07970242	-2.90956126
C	-5.75671169	3.80171748	-3.71874291
C	-7.13259151	3.55778458	-3.64686575
C	-7.61893533	2.58623649	-2.76546202
C	-6.73858593	1.86009682	-1.95899351
H	-3.81242020	3.29530640	-2.94094074
H	-5.36854821	4.56074767	-4.39332600
H	-7.82130318	4.12602409	-4.26719248
H	-8.68768104	2.39893391	-2.69482322

Int4_21

E = -12525.50

G = -12213.04

Nimag = 0

C	0.36188196	-1.64298025	-0.29396172
C	-0.93391510	-1.98174956	-1.06741930
H	0.21155761	-0.71995257	0.28093790
H	-0.83915890	-2.98652999	-1.49619148
C	-1.22916631	-1.05125214	-2.26272665
C	1.55859811	-1.38265561	-1.18575753
C	1.28408120	-0.53085323	-2.40995057
C	0.02601899	-1.02726753	-3.15750703
H	-2.05354934	-1.48516818	-2.84154412
H	-0.12477263	-0.45208123	-4.07209768
H	0.18241251	-2.06468576	-3.47709004
C	-1.93691871	5.79606600	3.44476052
H	0.60666630	-2.43508936	0.42005441
H	-1.77088513	-2.03565978	-0.37032660

N	-1.65900120	0.36317085	-1.86124627
C	-1.61154063	1.32334488	-3.02505999
H	-0.54672914	1.38726746	-3.26141619
H	-2.12232838	0.86991586	-3.88782880
C	-2.09681050	2.74095963	-2.85749117
C	-2.53234767	3.44072225	-3.90698348
C	-1.17999027	1.07877232	1.11747872
S	-3.00079940	0.38694305	-0.84613134
O	-3.66557917	1.71829752	-0.96707598
O	-3.90060614	-0.75147421	-1.04425350
H	-3.76184452	-1.13921393	1.46986773
H	0.20004912	1.62512723	2.67207548
H	-0.83025138	0.12301096	4.36457607
H	-2.81782074	-1.24783905	3.76985389
O	2.68074893	-1.81723548	-0.92398188
H	-0.09034786	3.86754950	1.32888789
Pd	-2.28427580	3.50088582	-0.97894853
H	1.70117477	4.53601973	2.90970481
H	1.17004454	6.03205595	4.82942200
H	-1.16084036	6.84604456	5.15903248
C	-4.08659020	5.79423753	1.05546680
C	-5.15865390	6.01161821	1.93741971
C	-5.98132981	7.13185345	1.78325714
C	-5.74185258	8.04382020	0.74862736
C	-4.67530527	7.83181118	-0.13351485
C	-3.85298991	6.71149861	0.01575614
H	-5.35628489	5.30577856	2.73852072
C	-0.66105952	1.01849673	2.41064496
H	-2.65906431	2.97488530	-4.88937481
C	-1.24311419	0.17267866	3.36065890
H	-6.80908145	7.29051051	2.47071272
H	-6.38502519	8.91240743	0.62810697
C	-2.29161955	0.29107413	0.79822425
H	-2.77612612	4.49745771	-3.83788693
C	-2.35868603	-0.60123114	3.02780190
H	-0.72786087	1.71266093	0.36055794
C	-2.89750216	-0.54284591	1.74038232
H	-2.95075295	6.15601156	3.59491625
H	-4.48738864	8.53450758	-0.94209849
Br	-0.53927578	5.24099851	-1.43584382
P	-2.94872834	4.35260943	1.21514991
H	-2.68521519	3.15827560	3.96772867
H	-3.02905635	6.54536730	-0.67330698
C	-3.93990726	3.16379255	2.20858861
C	-5.09705525	2.62346995	1.61646428
C	-5.88660391	1.70992215	2.31507191
C	-5.52818588	1.31925940	3.61171316
C	-4.37531273	1.84472175	4.20029964
C	-3.58120845	2.76126375	3.50253463
H	-5.37986267	2.91960449	0.61081626
H	-6.77889375	1.30037960	1.84744004
H	-6.14075640	0.60317406	4.15438124
H	-4.08421204	1.53653976	5.20153373
C	-1.64481017	4.94122350	2.36836468
C	-0.32679693	4.49844105	2.17882925
C	0.68318056	4.88561901	3.06490338
C	0.38468404	5.72771094	4.14163248
C	-0.92615323	6.18591238	4.32729152
H	2.16236537	-0.53178362	-3.06160014
H	1.12490568	0.49954146	-2.05758526

Int4_22
E = -13391.40
G = -13050.54
Nimag = 0

C	-4.96671818	-2.17550619	-3.64026859
C	-5.59992412	-2.67533067	-2.32235609
H	-4.23449126	9.99917102	0.17169504
H	-6.43366640	-3.35056811	-2.55061067
C	-6.18162453	-1.53669146	-1.45934920
C	-5.92919157	-1.32041495	-4.43798819
C	-6.64696801	-0.24090730	-3.64819327
C	-7.20909859	-0.75882416	-2.30183474
H	-6.70554298	-1.99063124	-0.61122947
H	-7.65068734	0.06518483	-1.73523484
H	-8.02530860	-1.46203672	-2.50507060
Br	-6.87373801	4.16805746	-0.19656811
H	-6.18820254	8.84260238	1.19680769
H	-4.87395769	-3.26970542	-1.76556756
N	-5.10821023	-0.61922490	-0.92466817
C	-5.39035095	0.82183081	-0.64543454
H	-4.42376552	1.32524819	-0.59677496
H	-5.88863335	1.24013815	-1.52331813
C	-6.20709651	1.14112517	0.58837110
C	-7.15238692	0.39424690	1.15375005
C	-2.01606101	-0.74786449	-1.86501732
S	-3.91744020	-1.30613269	0.03400091
O	-3.34166675	-0.23182676	0.86652443
O	-4.41617357	-2.51835266	0.68948090
H	-2.68921157	-3.86380232	-0.62193765
H	-0.53140658	-0.30324289	-3.35675658
H	0.19238426	-2.67254733	-3.60139097
H	-0.87678162	-4.45213905	-2.23075906
O	-6.10718645	-1.47641900	-5.64666103
H	-1.43387806	3.00628016	2.80379579
Pd	-5.45385872	2.85176932	1.40786969
H	0.19079141	1.67246544	1.49770143
H	0.09196090	1.66333252	-0.98830903
H	-1.64824823	3.00978139	-2.16368125
C	-3.91893721	6.29499200	1.32919597
C	-2.82174341	6.94834647	0.74461895
C	-2.93754059	8.27859835	0.32938301
C	-4.14686363	8.96480318	0.49597185
C	-5.24476286	8.31578437	1.07377272
C	-5.13380580	6.98391414	1.48322188
H	-1.88148176	6.42127498	0.61048140
C	-1.00150244	-1.08160264	-2.76168589
H	-7.41645506	-0.59904550	0.78622057
C	-0.59444311	-2.41620717	-2.89679825
H	-2.08383010	8.77887448	-0.12200846
C	-2.51518456	3.76228881	-0.34298024
C	-2.61298970	-1.76434966	-1.10902510
H	-7.70339785	0.73088691	2.02962180
C	-1.19571434	-3.41834965	-2.12856344
H	-2.33545392	0.28256913	-1.75094961
C	-2.21345469	-3.09664460	-1.22380668
H	-3.28704219	4.32682675	-0.86016942
H	-4.09781699	-1.54465943	-3.40696747
H	-4.62079985	-3.01044926	-4.25641448
P	-3.84205076	4.57882998	1.97463120
H	-1.43615750	5.89582937	3.18090887
H	-5.99061705	6.47190965	1.91347306
C	-3.23657646	4.80754956	3.69456606
C	-4.01506795	4.29900675	4.74471680
C	-3.60233491	4.45737644	6.07231241
C	-2.40760476	5.12711263	6.35594421
C	-1.62936942	5.64497009	5.31111305
C	-2.04254093	5.48949174	3.98605520
H	-4.94576318	3.78550852	4.51943547
H	-4.21162372	4.05907660	6.88021733
H	-2.08337463	5.24978811	7.38670045
H	-0.70252699	6.16993892	5.53043329
C	-2.45688346	3.78159020	1.06521564
C	-1.47616656	3.02011342	1.71939888
C	-0.56119217	2.26282126	0.97941220
C	-0.61685202	2.25716050	-0.41696454
C	-1.59604833	3.01175694	-1.07725112
H	-7.44071135	0.19292884	-4.26318292
H	-5.90147361	0.54756191	-3.46646968
O	-4.22976550	1.52201327	2.73954684
H	-3.88798063	0.85574293	2.08986303
C	-4.88554599	0.78783948	3.81438415
H	-5.27999391	1.52620604	4.51309533
H	-4.14287623	0.16011863	4.31758784
H	-5.70002522	0.17264965	3.42143466

K_2HPO_4
E = -1368.55
G = -1374.87
Nimag = 0

P	-0.78832194	1.37332753	1.84659948
O	-0.81482457	2.18250343	0.52376084
O	-1.85627504	1.85236013	2.85450321
O	-1.25025996	-0.17000687	1.33459566
O	0.63319214	1.24101005	2.43713979
K	1.82662339	2.59094488	0.43636155
K	-2.82841343	3.77893058	1.25537963
H	-1.21473938	-0.79203780	2.08487390

proline
E = -2802.96
G = -2735.76
Nimag = 0

C	4.04855338	0.13226173	0.00228855
H	3.74488897	-0.29272610	0.96366001
H	4.27745325	-0.69001607	-0.68868900
C	5.09847479	1.96705297	-1.14855375
C	5.24292136	1.09243212	0.11366816
H	5.62121577	2.92455662	-1.08428600
H	5.47247773	1.43040871	-2.02709221
H	5.15273732	1.70648389	1.01838049
H	6.19814832	0.56202735	0.15537487
C	3.06701231	3.44734686	-0.60938787
O	2.26050416	3.21285459	0.43794559
H	3.24627401	2.18439192	-2.32673190
O	3.37290736	4.57500749	-0.98095974
N	2.95253394	0.99486461	-0.54589091
C	3.56289067	2.14697062	-1.28011356
H	2.23555647	2.17643245	0.42856452
H	2.31519726	0.46827734	-1.13983767

PPh_3
E = -5979.33
G = -5842.60
Nimag = 0

H	2.59925892	0.61851463	4.88522017
P	2.24920570	0.04639969	-0.01608954
H	4.52444575	-0.93806576	5.18105312
C	3.07785620	-1.20102770	-1.11191132
C	2.46350955	-2.46178161	-1.22499530
C	4.26783689	-0.95924488	-1.81794502
C	3.03647256	-3.46568884	-2.01173081
H	1.53439290	-2.65843474	-0.69271143
C	4.83562999	-1.96073170	-2.61424679
H	4.75515281	0.00861716	-1.74427271
C	4.22445241	-3.21614083	-2.71043538
H	2.55314818	-4.43740767	-2.08537859
H	5.75792371	-1.76047881	-3.15542338
H	4.66769279	-3.99352484	-3.32858289
C	3.13014871	1.60585715	-0.50156419
C	4.25641562	2.11535274	0.16501574
C	2.62024708	2.30765289	-1.60961513
C	4.86388770	3.29885857	-0.27147022
H	4.66327189	1.58822142	1.02305612
C	3.23440162	3.48242303	-2.05314323
H	1.74057311	1.93048093	-2.12862903
C	4.35773563	3.98287938	-1.38233184
H	5.73572848	3.68248774	0.25426441
H	2.83259100	4.01079058	-2.91495093
H	4.83185870	4.90118247	-1.72124091
C	3.03174093	-0.32330322	1.62571156
C	4.11566336	-1.19873150	1.80219511
C	2.48663634	0.31963866	2.75290101
C	4.64740826	-1.42102992	3.07815037
H	4.54930806	-1.70521698	0.94500527
C	3.02666840	0.10853928	4.02464618
H	1.63877968	0.99222181	2.63293356
C	4.10828011	-0.76620802	4.19099978
H	5.48694767	-2.10228767	3.20037590

KH_2PO_4
E = -1392.87
G = -1391.79
Nimag = 0

P	-1.17018412	1.53914952	1.53940621
O	-0.29917623	1.79724296	0.16587955
O	-2.59377724	1.94051362	1.22083329
O	-1.17454468	-0.09902494	1.70485156
O	-0.48050225	2.18510716	2.72839478
H	0.65888338	1.83492009	0.34983295
K	-2.72111122	3.73132324	3.32021927
H	-0.38608559	-0.41231507	2.18776992

KBr
E = -160.37
G = -175.95
Nimag = 0

Br	0.00000000	0.00000000	1.19226772
K	0.00000000	0.00000000	4.35236362

Int4_23
E = -15162.76
G = -14773.49
Nimag = 0

C	-4.21491261	-0.07294687	1.95749754
C	-5.25380268	0.68479485	1.09447736
H	-3.49167425	0.63504521	2.38007354
H	-6.07672514	-0.00568788	0.87247074
C	-4.77157205	1.17509039	-0.29124733
C	-3.39740094	-1.07979587	1.17858822
C	-2.90714050	-0.59375303	-0.16723672
C	-4.06020114	0.00535791	-1.00426557
H	-5.67156246	1.43645958	-0.86439404
H	-3.67764765	0.29956884	-1.98511046
H	-4.81715559	-0.76638722	-1.19055875
C	-3.10117627	4.96173049	-7.18315241
H	-4.70827028	-0.57400304	2.79586009
H	-5.69208659	1.49614368	1.67619522
N	-3.86561351	2.39556758	-0.30831443
C	-3.63842565	2.93121090	-1.70109518
H	-4.01644065	2.16549572	-2.37677850
H	-4.27024093	3.80502214	-1.85680426
C	-2.18652588	3.23360961	-2.05516137
C	-1.21981819	2.32098343	-1.92448213
C	-2.00299362	2.69668946	2.12203486
S	-4.19799130	3.65605937	0.76974198
O	-3.52791665	4.84988194	0.23604715
O	-5.63040389	3.78098918	1.08456455
H	-4.96370568	3.63178982	3.56131379
H	-0.27290992	1.99413783	3.19120035
H	-1.34661053	2.20462071	5.42707072
H	-3.68854354	3.02003970	5.61649883
O	-3.13435501	-2.20143519	1.61615024
H	-1.34848841	7.07227750	-5.15245615
Pd	-1.74480652	5.11722794	-2.66775495
H	-0.51242569	7.85417781	-7.35665522
H	-1.32717160	6.78539240	-9.45404471
H	-2.98814256	4.93205756	-9.33414658
C	-4.13602347	3.46092056	-4.69999284
C	-5.52298265	3.30045582	-4.57407229
C	-6.09790550	2.03334875	-4.72183398
C	-5.29279806	0.92510401	-5.00300973
C	-3.90787556	1.08602039	-5.15001304
C	-3.33056605	2.34627688	-4.99549356
H	-6.15243247	4.15341682	-4.34160249
C	-1.29290685	2.35964657	3.27445392
H	-1.41958014	1.32741768	-1.52211130
C	-1.90013585	2.47729713	4.53235434
H	-7.17294822	1.91408905	-4.61093347
H	-5.73940040	-0.06058564	-5.10754243
C	-3.31978455	3.15571028	2.24846634
H	-0.18734986	2.51167250	-2.20743332
C	-3.21761891	2.93516603	4.64095413
H	-1.56236268	2.58353532	1.13748815
C	-3.93876200	3.28232480	3.49350943
H	-3.82591097	4.15504427	-7.14315731
H	-3.27884799	0.22710619	-5.37048597
O	0.24687527	8.85096207	-2.48083543
P	-3.29784339	5.05504189	-4.35607542
H	-5.19849816	6.57775606	-6.07158533

H	-2.25330216	2.46240133	-5.07488262
C	-4.65326730	6.24026522	-4.00404459
C	-4.94299131	6.55221448	-2.66487314
C	-6.00418508	7.40934068	-2.35950418
C	-6.77383209	7.96646135	-3.38738332
C	-6.47974753	7.66688362	-4.72338079
C	-5.42305873	6.80621090	-5.03350928
H	-4.33532035	6.13220199	-1.86670668
H	-6.22444433	7.64658889	-1.32143876
H	-7.59583456	8.63737813	-3.14920824
H	-7.07236411	8.10342885	-5.52376961
C	-2.64241095	5.56199535	-5.99817566
C	-1.70435483	6.60749647	-6.06772683
C	-1.23759722	7.04495597	-7.31001223
C	-1.69548846	6.44434051	-8.48933958
C	-2.62690640	5.40269780	-8.42275723
H	-2.41051989	-1.41033400	-0.69882343
H	-2.16439202	0.19250253	0.02982170
O	-1.22446976	7.23437941	-3.00634567
C	-0.20971737	7.68944951	-2.35156114
H	1.54465458	6.74428521	-1.57423850
C	0.47890979	6.77580170	-1.32207396
N	-0.04320625	5.35042115	-1.29293962
C	-0.21006434	4.94721820	0.15885478
C	0.53861976	6.01501402	0.96699154
C	0.31069009	7.28398505	0.12846213
H	0.66467863	4.74942428	-1.71443609
H	-0.71032447	7.65889994	0.27590780
H	0.17232718	3.93470770	0.29329280
H	-1.27382366	4.95599532	0.39184157
H	1.60978142	5.78407792	1.02325035
H	0.14969246	6.10116979	1.98656720
H	1.00962947	8.09353463	0.34953402

Int4_24

E = -15151.80

G = -14758.60

Nimag = 0

C	1.60009369	-0.72788715	-0.62848995
C	0.72963161	-1.66895932	-1.47589482
H	1.21400994	-0.65501019	0.38792010
H	1.29184507	-1.96970150	-2.36851860
C	-0.58521403	-1.05643119	-1.98525451
C	1.77230810	0.71078688	-1.17533468
C	0.53136057	1.29471753	-1.87945852
C	-0.29285696	0.28272148	-2.69153047
H	-0.98153277	-1.72105714	-2.75349639
H	-1.23534061	0.75022452	-2.99546741
H	0.25190269	0.02609939	-3.60957081
H	3.52120930	0.11059118	-1.91123116
H	2.59148694	-1.18569545	-0.53787138
H	0.53473159	-2.58589540	-0.90870766
N	-1.68705492	-0.97323510	-0.95918115
C	-1.39053769	-0.61457484	0.45805737
H	-2.21744439	-0.98259449	1.06747995
H	-0.49915334	-1.13706622	0.80091094
C	-1.31303596	0.88836895	0.66995206
C	-2.29956429	1.68615746	0.25041761
C	-2.45063644	-3.93029215	0.78498901
S	-2.96338739	-2.03476702	-1.15607690
O	-4.03290146	-1.59743048	-0.25352860
O	-3.23789729	-2.13508607	-2.59427601
H	-1.67378710	-4.23968447	-2.53440265
H	-1.93289615	-5.35610934	2.31173828
H	-0.76717413	-6.89337220	0.73860297
H	-0.64758523	-6.34049132	-1.68492339
N	2.10463412	1.59597006	0.02493229
C	2.45987202	3.02837284	-0.28735507
Pd	0.31516049	1.78105646	1.51789853
C	3.33056868	1.13598575	0.79049818
H	3.20603266	1.48500275	1.81574171
H	3.39540036	0.05158351	0.81197876
C	3.96665145	3.02468666	-0.66028928
C	4.55515026	1.82650907	0.13614261
H	4.42697439	3.97840161	-0.39442209
H	4.08160770	2.86926235	-1.73404291
H	5.25757774	2.15462703	0.90810097
H	5.09316185	1.14139829	-0.52613242
C	2.22524043	3.94827987	0.95552480
C	-1.87110989	-5.11138959	1.25451163
H	-3.13547828	1.27863041	-0.32189113
C	-1.21731339	-5.97590319	0.36824350
O	1.74660492	3.42682332	2.03527293
O	2.54689635	5.15398222	0.83445909
C	-2.36671063	-3.62772708	-0.58023416
H	-2.31082379	2.75722968	0.42997591
C	-1.14715333	-5.66516197	-0.99518430
H	-2.96315042	-3.25824395	1.46437416
C	-1.72048965	-4.48605678	-1.47869483
H	-3.45400723	2.38344128	4.93804901
H	1.74261152	0.84817768	3.81306975
H	1.82892383	3.40323386	-1.09441951
P	-0.95746830	1.82686760	3.38000282
H	-0.30351002	-0.70607803	4.69751076
C	-1.94233092	0.31616763	3.71827607
C	-3.25711638	0.18875608	3.23714489
C	-3.93625393	-1.02436373	3.36537577
C	-3.31000430	-2.12380223	3.96504809
C	-2.00120934	-2.00233936	4.44370335
C	-1.31972234	-0.78774481	4.32404420
H	-3.73928407	1.02364091	2.74111252
H	-4.94995131	-1.11388724	2.98400392
H	-3.83944938	-3.06895993	4.05695703
H	-1.50774807	-2.85125165	4.91012181
C	-2.09294384	3.25053784	3.49254036
C	-1.78733522	4.39229133	2.73202955
C	-2.59502909	5.52837469	2.81828168
C	-3.71191176	5.53140438	3.66255738
C	-4.01686059	4.39778307	4.42499187
C	-3.21079021	3.25892798	4.34387519
H	-0.91809188	4.38396461	2.07889816
H	-2.35550874	6.40711191	2.22474656
H	-4.34387159	6.41396320	3.72497767
H	-4.88188070	4.39842701	5.08354814
C	0.18755557	1.97107417	4.80899448
C	-0.17915229	2.64896917	5.98248481
C	0.70678874	2.70468032	7.06267229
C	1.95894350	2.08429991	6.98062820
C	2.32925901	1.41062812	5.81098521
C	1.44979259	1.35866744	4.72718743
H	-1.14560202	3.13771228	6.05500315
H	0.41852300	3.23520144	7.96694687
H	2.64574046	2.13162030	7.82222971
H	3.30300692	0.93249522	5.73908132
O	2.80788061	0.71291254	-2.19024739
H	0.87267555	2.08865536	-2.55204248
H	-0.11045837	1.75792542	-1.13378650

Int4_25

E = -15158.42

G = -14765.05

Nimag = 0

C	1.06092326	-1.31354520	0.18696102
C	0.25435118	-2.01866890	1.29828695
H	0.44999611	-0.53178357	-0.26980176
H	0.66782458	-3.02036849	1.46468512
C	0.28257856	-1.33251668	2.67923420
C	2.40149885	-0.66033624	0.61483371
C	2.45215439	-0.14291073	2.06504336
C	1.73539686	-1.04099565	3.07435080
H	-0.10936546	-2.05296282	3.39863491
H	1.76081639	-0.57069086	4.06286887
H	2.25043642	-2.00728844	3.15670613
H	-3.36745795	-1.10132705	-2.08774523
H	1.26050720	-2.03242386	-0.61765084
H	-0.77658888	-2.16610597	0.95666066
N	-0.59580390	-0.10530106	2.82738376
C	-0.90568819	0.75145394	1.64788988
H	-1.86546977	1.23349743	1.84628724
H	-1.06876777	0.12047320	0.77471924

C	0.09870251	1.86540320	1.36650356
C	0.47572873	2.74215074	2.29632803
C	-3.84245432	-1.03824187	2.12330029
S	-1.86490240	-0.29211401	3.90730460
O	-2.54906760	1.00241619	3.99982763
O	-1.31914367	-0.89970673	5.12517646
H	-2.20270772	-3.14786215	4.26196642
H	-5.29016216	-1.65075804	0.65795158
H	-5.11645463	-4.06801165	1.22208028
H	-3.57688545	-4.81690911	3.02937371
N	2.65173918	0.51751012	-0.33272205
C	3.01086048	0.06165411	-1.74872058
Pd	0.73932913	1.84167808	-0.55739927
C	3.78295452	1.41872935	0.12290042
H	4.55016972	0.81792649	0.62543907
H	3.40293224	2.16708353	0.81931965
C	4.36053363	0.75892048	-2.08015625
C	4.35331244	1.99481683	-1.16803764
H	5.19093843	0.09754410	-1.80883985
H	4.44304711	0.99331830	-3.14409667
H	5.34844733	2.42380823	-1.01819484
H	3.69397298	2.77245418	-1.57103101
C	1.98120320	0.42618093	-2.83892208
C	-4.61329310	-1.98062746	1.43999778
H	0.14843180	2.63961461	3.33371989
C	-4.51491683	-3.33998760	1.76022446
O	1.20851834	1.43878449	-2.64865652
O	2.01577891	-0.24416883	-3.90007580
C	-2.97540669	-1.47504328	3.13525449
H	1.12968990	3.58125528	2.07317380
C	-3.64888124	-3.76278318	2.77474771
H	-3.92319868	0.01568624	1.87838381
C	-2.87198315	-2.83114725	3.46917766
H	-2.43029384	3.29349786	1.60979300
H	3.13009382	-1.02116648	-1.77093166
H	1.22601896	4.21113363	-2.43148521
P	-1.07594098	3.13124751	-1.01980211
H	-1.41328894	0.41239520	-1.87114014
C	-1.50298169	4.52846184	0.08848042
C	-1.12695853	5.83811191	-0.25236329
C	-1.38137582	6.89646584	0.62622592
C	-2.01935788	6.65898740	1.84771302
C	-2.40034669	5.35597662	2.19089586
C	-2.13505383	4.29609311	1.32316776
H	-0.63985528	6.03798672	-1.20109164
H	-1.08424780	7.90535523	0.35065681
H	-2.22044626	7.48275755	2.52837703
H	-2.89715943	5.16246027	3.13836099
C	-0.89904358	3.90731722	-2.67161031
C	-2.00778544	4.08736872	-3.51297974
C	-1.85135263	4.73034674	-4.74479719
C	-0.59261963	5.19975023	-5.13823183
C	0.51425357	5.02112377	-4.29972626
C	0.36428062	4.37049612	-3.07312297
H	-2.98707301	3.72558040	-3.21412063
H	-2.71225926	4.86340658	-5.39554027
H	-0.47389341	5.69844050	-6.09722129
H	1.49495957	5.37806887	-4.60548193
C	-2.57325693	2.07805565	-1.12949232
C	-3.85736780	2.53300028	-0.79226896
C	-4.95722918	1.67638590	-0.91146468
C	-4.78441544	0.36920521	-1.37722687
C	-3.50703160	-0.08561769	-1.72685721
C	-2.40669698	0.76288248	-1.60173999
H	-4.00323295	3.54770516	-0.43672583
H	-5.94781498	2.03418386	-0.64228442
H	-5.64166570	-0.29285606	-1.46913814
H	2.01757593	0.85154628	2.10784662
H	3.50553758	-0.05263947	2.34649738
O	3.47628821	-1.62851244	0.54757976
H	3.29537925	-2.25797603	-0.17335055

H_2O
E = -423.00
G = -421.36
Nimag = 0

H	0.76839599	0.00000000	0.29009758
O	0.00000000	0.00000000	0.89004694
H	-0.76839599	0.00000000	0.29009758

Int4_26
E = -14733.59
G = -14356.46
Nimag = 0

C	1.53342269	-0.86831283	-0.78942849
C	0.47674789	-1.50151034	-1.71308341
H	1.23392111	-0.94177167	0.26235611
H	0.93198929	-1.64303647	-2.70194763
C	-0.79899649	-0.66681994	-1.94042097
C	1.80607231	0.58616441	-1.12901258
C	0.76259445	1.40349530	-1.62623355
C	-0.44029237	0.78496224	-2.33502956
H	-1.31990227	-1.09945597	-2.79463745
H	-1.32251285	1.41895774	-2.21868463
H	-0.21324475	0.76110721	-3.41184824
H	1.05644747	2.35946169	-2.05729750
H	2.45689785	-1.44550948	-0.87829312
H	0.22544888	-2.49808961	-1.34170310
N	-1.82173336	-0.72675813	-0.84348764
C	-1.52727484	-0.17505496	0.51004220
H	-2.36659304	-0.44722877	1.15137572
H	-0.63347936	-0.64550180	0.93104050
C	-1.40919776	1.33373293	0.49929982
C	-2.48654169	2.11994616	0.44114317
C	-1.90282180	-3.43897188	1.28713089
S	-2.89864408	-2.00668249	-0.85863118
O	-4.01491182	-1.63666849	0.01963458
O	-3.17433266	-2.33518886	-2.26144822
H	-1.69174897	-4.38931239	-1.99205365
H	-1.03720823	-4.50659405	2.94161279
H	-0.07568464	-6.30671565	1.51578882
H	-0.41769712	-6.25859982	-0.94934072
N	3.06211620	1.03512609	-0.94485743
C	3.54632805	2.36011064	-1.38511147
Pd	0.44277452	2.10535628	0.54569197
C	4.11579640	0.28739560	-0.20008472
H	3.72989494	-0.06566543	0.76050508
H	4.43365363	-0.58431551	-0.78427249
C	5.08160913	2.19697578	-1.30317963
C	5.25839377	1.30413933	-0.06109612
H	5.58268011	3.16271199	-1.22561999
H	5.44477485	1.68208760	-2.20014771
H	5.12892928	1.89907275	0.84982726
H	6.23371331	0.81308156	-0.01638730
C	3.07295743	3.57616756	-0.51974080
C	-1.17721490	-4.48320120	1.86424659
H	-3.48805722	1.68722168	0.36780178
C	-0.63843244	-5.49560111	1.06100259
O	2.31485102	3.38520527	0.48985042
O	3.52241099	4.69504818	-0.88378236
C	-2.07328846	-3.41637463	-0.10367155
H	-2.42699604	3.20487437	0.45832279
C	-0.82782010	-5.46853941	-0.32572294
H	-2.33079326	-2.66271728	1.91136561
C	-1.54385560	-4.42428140	-0.91773750
H	-1.44863074	3.07841059	5.29191332
H	2.77613497	1.36765640	2.22519610
H	3.20915481	2.54426598	-2.41023191
P	0.14595522	2.38154823	2.83536334
H	1.23714349	-0.14688146	3.85236023
C	-0.63920305	0.90525234	3.60230099
C	-2.03741557	0.80053690	3.70219261
C	-2.62655338	-0.39465765	4.12276120
C	-1.82989046	-1.50172194	4.43835091
C	-0.43776371	-1.40418239	4.33963048
C	0.15535645	-0.20807657	3.92589264
H	-2.66601006	1.64227993	3.43290259
H	-3.70927610	-0.46250422	4.19594364
H	-2.29171908	-2.43236778	4.75893512
H	0.18956145	-2.25820500	4.58275392

C	-0.85413116	3.82321766	3.34696709
C	-0.93617834	4.90052503	2.44885203
C	-1.64920590	6.05177604	2.79354359
C	-2.29030416	6.13151890	4.03532197
C	-2.21469652	5.05920927	4.93276099
C	-1.49906470	3.90787562	4.59271440
H	-0.44236607	4.82904832	1.48222897
H	-1.70922237	6.88070037	2.09253675
H	-2.85061510	7.02443392	4.30197399
H	-2.71343167	5.11816786	5.89714378
C	1.75099012	2.53192420	3.72132159
C	1.88181406	3.23333739	4.93021469
C	3.11458622	3.26819277	5.58965347
C	4.22185453	2.60117796	5.05180185
C	4.09724702	1.90572623	3.84363317
C	2.86996795	1.87912591	3.17757741
H	1.03102689	3.75538963	5.35691129
H	3.20880181	3.81635894	6.52406601
H	5.17833223	2.62933534	5.56818666
H	4.95594791	1.39255049	3.41756166

Int4_27

E = -14722.92

G = -14347.92

Nimag = 0

C	1.36320120	-1.57266344	0.82760405
C	0.97788289	-1.74735807	2.30786282
H	0.52418261	-1.14561426	0.26661875
H	1.74933449	-2.35911660	2.79425682
C	0.88936554	-0.44395296	3.12721977
C	2.59889282	-0.69179524	0.68052713
C	2.79174878	0.38036607	1.56539875
C	2.18123930	0.38166387	2.95833873
H	0.83745952	-0.73501592	4.17659210
H	2.02533629	1.40052707	3.31655765
H	2.92399607	-0.07377559	3.63164213
H	3.73806473	0.91142173	1.50820725
H	1.55900845	-2.55780718	0.39576100
H	0.04718527	-2.31294106	2.37625311
N	-0.34713337	0.39760672	2.95043696
C	-0.60202563	1.27674890	1.76711677
H	-1.46966521	1.88568639	2.03552102
H	-0.88420746	0.66503789	0.90092156
C	0.52158757	2.21460176	1.38720287
C	0.70750582	3.39738524	1.96931386
C	-3.36981091	-0.30242407	1.35072094
S	-1.77872883	-0.18363319	3.61571728
O	-2.59846743	0.98320521	3.96585363
O	-1.42509897	-1.14580190	4.66404253
H	-1.98820570	-3.00448560	2.92755269
H	-4.47734375	-0.37938146	-0.49155287
H	-4.22764288	-2.84140449	-0.75036619
H	-3.01115815	-4.15776159	0.97672650
N	3.52019779	-1.02124695	-0.25655041
C	3.18426260	-1.59084184	-1.57412683
Pd	1.57024756	1.51231829	-0.16498274
C	4.84480331	-0.35566136	-0.33907301
H	5.38939225	-0.54159603	0.59183499
H	4.72108018	0.72754349	-0.46100072
C	4.55792187	-2.10314956	-2.04824868
C	5.52256742	-0.98335425	-1.58463206
H	4.78333092	-3.04759868	-1.54069371
H	4.57955321	-2.26917793	-3.12663240
H	6.51961361	-1.36655380	-1.35249129
H	5.62848393	-0.22738100	-2.36894664
C	2.62235299	-0.50180948	-2.55251233
C	-3.93434778	-0.95435834	0.25297419
H	0.06817701	3.71933006	2.79559679
C	-3.79398930	-2.33896227	0.11008876
O	2.47023562	0.69485106	-2.12765177
O	2.40781874	-0.88872100	-3.73028480
C	-2.64873646	-1.04833502	2.29421361
H	1.48100430	4.09234319	1.65364596
C	-3.10231217	-3.07924543	1.07544162
H	-3.49529515	0.76705875	1.47812064
C	-2.52147701	-2.43660758	2.17249275
H	-2.47975040	2.56011326	-0.22341077
H	2.44805786	-2.39257455	-1.48436592
H	2.69723840	3.78004613	-1.84438397
P	0.09723805	2.57719948	-1.63668245
H	0.05535386	-0.32538286	-1.72443385
C	-0.95215690	3.91167011	-0.94268701
C	-0.51187648	5.24347068	-0.96207248
C	-1.23453818	6.23306962	-0.28825075
C	-2.40103236	5.90274590	0.41016068
C	-2.84807117	4.57569930	0.42651500
C	-2.12709650	3.58687468	-0.24321802
H	0.39500696	5.51075597	-1.49667196
H	-0.88492800	7.26257351	-0.31042683
H	-2.96028654	6.67345677	0.93502595
H	-3.75664496	4.31143962	0.96245481
C	0.96092214	3.35368571	-3.05497369
C	0.38559229	3.45505718	-4.32987154
C	1.08228236	4.09147248	-5.36194527
C	2.35095935	4.63413073	-5.12602061
C	2.92899532	4.53078471	-3.85509172
C	2.24007858	3.88553526	-2.82532047
H	-0.59519301	3.03347804	-4.52636034
H	0.63335988	4.16244483	-6.34990673
H	2.88976048	5.12848128	-5.93090599
H	3.91820421	4.94224373	-3.66859981
C	-1.11845055	1.37797522	-2.31686992
C	-2.30952093	1.80183748	-2.93408865
C	-3.22134613	0.86222004	-3.42230708
C	-2.95729725	-0.50681186	-3.29716676
C	-1.77565736	-0.93492191	-2.68390914
C	-0.86233420	0.00280335	-2.19846670
H	-2.53372748	2.86092927	-3.01810626
H	-4.14080610	1.20044911	-3.89393924
H	-3.67415082	-1.23511617	-3.66818444
H	-1.56933025	-1.99643963	-2.57421868

TS4_8

E = -14705.00

G = -14331.25

Nimag = 1, 300i cm-1

C	0.91284420	-0.84120697	-0.77183880
C	-0.03181860	-1.23145719	-1.93998041
H	0.34870893	-0.76577652	0.16202814
H	0.58182461	-1.61116931	-2.76582544
C	-0.88513827	-0.08149535	-2.52376902
C	1.62564410	0.47820640	-1.01989129
C	0.83646356	1.56747565	-1.60981342
C	-0.00139291	1.13471711	-2.82094021
H	-1.31589670	-0.42573122	-3.46655350
H	-0.60994373	1.97421874	-3.16414256
H	0.69393155	0.86398394	-3.62833478
H	1.39337323	2.47493597	-1.83471901
H	1.63551642	-1.64503281	-0.62803331
H	-0.66787406	-2.05788556	-1.61328766
N	-2.03990084	0.35274196	-1.68937922
C	-1.76131122	0.93587022	-0.34805071
H	-2.70395612	1.32171860	0.04432410
H	-1.40914558	0.16487418	0.34315397
C	-0.78141657	2.08828164	-0.45200282
C	-1.19649906	3.33898689	-0.73977309
C	-3.31031528	-2.42979378	-0.19064958
S	-3.51549460	-0.35398705	-1.98414588
O	-4.47440029	0.27338605	-1.06871309
O	-3.75210962	-0.28945765	-3.43050842
H	-3.23437605	-2.75322984	-3.59561271
H	-3.05503239	-4.04256335	1.20957219
H	-2.75228844	-5.77103868	-0.55296935
H	-2.85130133	-5.13224038	-2.95625052
N	2.95308199	0.53428949	-0.90360734
C	3.79964548	1.66501640	-1.36291005
Pd	0.93658261	2.00543980	0.74445907
C	3.76742091	-0.49831134	-0.18556900
H	3.32208946	-0.70777301	0.78976485
H	3.78068448	-1.41850031	-0.77880763

C	5.21695977	1.04708372	-1.33436830
C	5.16554874	0.12805694	-0.09963030
H	5.98660853	1.81839937	-1.27426035
H	5.38133750	0.45926949	-2.24454578
H	5.26039460	0.71964275	0.81670594
H	5.94708535	-0.63544926	-0.10091634
C	3.75479366	2.95716732	-0.46794579
C	-3.09211208	-3.76252846	0.16100203
H	-2.26141243	3.57243110	-0.77737059
C	-2.92356573	-4.73494745	-0.83302987
O	3.20963089	2.90180048	0.67940984
O	4.32249679	3.95822324	-0.98410981
C	-3.35926717	-2.08658113	-1.54692393
H	-0.50516179	4.15807069	-0.91874415
C	-2.97823638	-4.37724675	-2.18484745
H	-3.44195515	-1.67280372	0.57486601
C	-3.19503539	-3.04572737	-2.55180831
H	0.76308304	4.29661173	2.61113225
H	3.25256229	1.31187400	2.37259553
H	3.49322891	1.94979754	-2.37174238
P	0.43303781	1.45919924	2.94504025
H	0.23840956	-1.48727573	2.98501078
C	1.82268713	0.63268802	3.84041752
C	1.64574420	-0.07395788	5.04252443
C	2.74227878	-0.65447126	5.68472436
C	4.02603068	-0.53310739	5.13549659
C	4.20891084	0.17367911	3.94255283
C	3.11193750	0.75423000	3.29601585
H	0.65467791	-0.18265884	5.47327168
H	2.59580833	-1.20295708	6.61238735
H	4.87689464	-0.98899492	5.63625282
H	5.20348770	0.27144436	3.51317964
C	-0.97602439	0.29910297	3.14081273
C	-2.29167733	0.78978881	3.21606341
C	-3.37535317	-0.09191215	3.24422931
C	-3.16078978	-1.47439826	3.19609233
C	-1.85499495	-1.96926168	3.09849870
C	-0.77017804	-1.09021109	3.06078862
H	-2.46995396	1.86076586	3.25722685
H	-4.38717941	0.30132215	3.30773413
H	-4.00471110	-2.15907616	3.22720289
H	-1.67736491	-3.04068872	3.05317584
C	0.00736563	2.87549944	4.04627356
C	-0.56764307	2.70858682	5.31796694
C	-0.81757939	3.81891088	6.12774890
C	-0.49407203	5.10623081	5.67708317
C	0.07668797	5.27954970	4.41189781
C	0.32348511	4.16797667	3.59838071
H	-0.82714389	1.71601078	5.67467202
H	-1.26398676	3.68131084	7.10991929
H	-0.68992766	5.96880657	6.30972124
H	0.32556447	6.27646289	4.05566112

TS4_9

E = -14711.96

G = -14336.10

Nimag = 1, 411i cm-1

C	0.82606848	-1.09223960	1.59493203
C	-0.22342428	-1.59934410	2.60622788
H	0.64237887	-1.55295019	0.61982023
H	0.15360342	-1.47802340	3.62857368
C	-1.55356850	-0.82917197	2.53333028
C	0.85595187	0.43126327	1.44834257
C	-0.32395320	1.22377397	1.77232256
C	-1.25005301	0.64259754	2.83504802
H	-2.24705688	-1.22257987	3.28383611
H	-2.15709184	1.24684746	2.91137286
H	-0.74893920	0.68144187	3.81064396
H	-0.12067133	2.27692489	1.91821949
H	1.81549606	-1.43596739	1.90766908
H	-0.37448917	-2.67053089	2.45609356
N	-2.18968168	-0.91783198	1.17656014
C	-2.73952368	0.30941988	0.55061310
H	-3.60127189	0.67696231	1.12638822
H	-3.10671203	0.03341072	-0.43809469
C	-1.69567590	1.40856789	0.39605576
C	-2.09994700	2.69174189	0.26820744
C	-0.87758717	-2.56115608	-1.36095878
S	-2.74266272	-2.39860151	0.66105785
O	-3.78664861	-2.15917912	-0.34287402
O	-3.04596202	-3.22711493	1.83552075
H	-1.13922425	-4.75149931	1.24960360
H	0.61358083	-2.63993755	-2.90118741
H	1.71978882	-4.67230604	-1.97779468
H	0.83935133	-5.73394370	0.09408937
N	2.06986745	1.03482423	1.32212461
C	3.26062116	0.35614192	0.75435072
Pd	-0.00920096	0.69298834	-0.68583907
C	2.29027947	2.49375137	1.47694492
H	1.83015754	2.84915397	2.40257516
H	1.84501048	3.04166914	0.63451562
C	4.24946863	1.52196588	0.48735142
C	3.81755825	2.61737309	1.47567554
H	5.28545899	1.20084270	0.61223306
H	4.12134311	1.87680354	-0.54280946
H	4.20904756	2.40802511	2.47799417
H	4.14656923	3.61636053	1.17631697
C	3.05602071	-0.46463961	-0.55829964
C	0.22925389	-3.11259400	-2.00443942
H	-3.15766263	2.94926921	0.23868977
C	0.85020051	-4.25197965	-1.47931646
O	2.03859797	-0.27358562	-1.29483108
O	4.01434432	-1.24323188	-0.82171595
C	-1.35381551	-3.15975060	-0.18852411
H	-1.39363346	3.51146002	0.17404019
C	0.35924536	-4.84782574	-0.31277469
H	-1.34777951	-1.66519872	-1.74942653
C	-0.75096911	-4.30309093	0.34138389
H	0.80608994	3.16559464	-1.49497172
H	1.55717867	-0.34108746	-3.37970310
H	3.67622341	-0.33098561	1.50089030
P	-0.82026565	1.18799950	-2.84091599
H	-2.88081473	-0.87324305	-3.16946144
C	-2.64971145	1.26981783	-2.93405197
C	-3.33347313	2.48043370	-2.73671000
C	-4.72891875	2.49643674	-2.63834755
C	-5.45615943	1.30581482	-2.73337439
C	-4.78185513	0.09394887	-2.93187308
C	-3.38976869	0.07547689	-3.02513333
H	-2.77858466	3.40942729	-2.65891856
H	-5.24535834	3.44084127	-2.48273950
H	-6.54052783	1.31984735	-2.65360194
H	-5.33760877	-0.83753788	-3.00214186
C	-0.26537400	2.87568825	-3.33681133
C	-0.61448038	3.43678873	-4.57673280
C	-0.17094853	4.71669203	-4.91817454
C	0.62782658	5.44613132	-4.02669692
C	0.98359591	4.89075951	-2.79320391
C	0.53751127	3.60989719	-2.45141031
H	-1.23148035	2.87718332	-5.27444373
H	-0.44620370	5.14533203	-5.87901504
H	0.97232713	6.44187518	-4.29559675
H	1.60527954	5.45185361	-2.09943312
C	-0.33881462	0.15830710	-4.29202950
C	-1.15725851	-0.00788412	-5.42289930
C	-0.70899531	-0.76343924	-6.51034103
C	0.56064749	-1.35344228	-6.48275816
C	1.38032007	-1.18660866	-5.36065814
C	0.93399491	-0.43920618	-4.26589165
H	-2.14370013	0.44422569	-5.45565606
H	-1.35142342	-0.89004349	-7.37886500
H	0.90592105	-1.94250950	-7.32928436
H	2.36427531	-1.64975217	-5.33077022

Int4_28

E = -14748.35

G = -14370.77

Nimag = 0

C	1.11915039	-0.64990211	-0.29975217
C	0.86482644	-1.42410548	-1.61651520

H	0.21843363	-0.67006624	0.31047816
H	1.81635580	-1.58010697	-2.14007276
C	-0.07031705	-0.67388688	-2.58516727
C	1.50906843	0.79602225	-0.58040916
C	0.53788969	1.53054845	-1.53316542
C	0.49048148	0.72514370	-2.86659968
H	-0.14356578	-1.23284023	-3.51893095
H	-0.13755097	1.25628686	-3.58874140
H	1.49502176	0.62455033	-3.28959437
H	0.91402158	2.53269976	-1.72995161
H	1.88659567	-1.15817958	0.28114451
H	0.46820577	-2.41354013	-1.37428114
N	-1.48199436	-0.49708029	-2.10640667
C	-1.74819183	0.44220888	-0.97710187
H	-2.80248338	0.72087580	-1.01400993
H	-1.57847903	-0.06170835	-0.01559154
C	-0.89098829	1.68478665	-1.05264214
C	-1.40485120	2.88407907	-0.76340213
C	-2.97367675	-2.37339233	0.44211828
S	-2.55034023	-1.77352214	-2.22753705
O	-3.89733026	-1.19455511	-2.17981372
O	-2.14145424	-2.56670294	-3.38932985
H	-1.15306043	-4.26777126	-1.74954294
H	-3.26454680	-2.83063617	2.52094953
H	-1.91349012	-4.91951182	2.44222968
H	-0.85815514	-5.63906860	0.30490815
N	2.83317057	1.01055270	-0.85965233
C	3.36733530	2.21236238	-1.52720079
Pd	1.43567363	1.95985947	1.33213645
C	3.92240472	0.20627799	-0.23160430
H	3.65672882	-0.03957437	0.79850164
H	4.05764511	-0.72487381	-0.79576878
C	4.88391493	1.92423495	-1.61190816
C	5.15491310	1.11199835	-0.33349697
H	5.45942312	2.84838460	-1.67878442
H	5.09241227	1.31870861	-2.50135507
H	5.20155689	1.77825470	0.53610051
H	6.08276369	0.53599292	-0.37766448
C	3.07477669	3.59067370	-0.81779422
C	-2.80126173	-3.14728907	1.59210535
H	-2.45156312	3.00770244	-0.49553100
C	-2.04033182	-4.32017004	1.54456277
O	2.35948405	3.62871005	0.24263677
O	3.56877593	4.59225911	-1.38939819
C	-2.36784374	-2.78716560	-0.75230721
H	-0.78501089	3.77705594	-0.77081427
C	-1.44333647	-4.72423627	0.34481245
H	-3.58499830	-1.47831099	0.47324229
C	-1.60142815	-3.95721305	-0.81164378
H	-0.95377784	-1.11157683	4.81937089
H	0.91823621	3.30783109	3.91002359
H	2.93399113	2.30903262	-2.52698070
P	0.68834226	0.58845600	2.96472848
H	3.41152082	-0.27112418	3.39045805
C	1.14683995	1.27812400	4.61630266
C	1.44380623	0.46717042	5.72384254
C	1.73264643	1.04828017	6.96236617
C	1.72303581	2.44095416	7.10742975
C	1.42643019	3.25437438	6.00723221
C	1.14297137	2.67515719	4.76713217
H	1.45919373	-0.61383331	5.62105529
H	1.96561011	0.41282340	7.81369174
H	1.94979871	2.88967901	8.07168455
H	1.42154497	4.33672202	6.11201012
C	-1.11914735	0.29222463	3.17443176
C	-2.00853514	1.00598076	2.35958822
C	-3.39075970	0.84920748	2.51052825
C	-3.89162976	-0.01470767	3.48870800
C	-3.00747469	-0.71523553	4.32122290
C	-1.62818185	-0.56380664	4.16736628
H	-1.60884020	1.69037860	1.61700860
H	-4.07198636	1.40265703	1.86853224
H	-4.96496497	-0.14139668	3.60743610
H	-3.39452351	-1.38173308	5.08827758
C	1.45095059	-1.08591799	2.96942972
C	0.73629630	-2.24749290	2.64333906
C	1.40272874	-3.46882485	2.49657456
C	2.78659244	-3.54359332	2.67845698
C	3.50661698	-2.38772796	3.01092824
C	2.84458554	-1.16739663	3.14954573
H	-0.33574190	-2.20415951	2.48591127
H	0.83826283	-4.35878862	2.23328754
H	3.30294349	-4.49295300	2.55987992
H	4.58349903	-2.43592220	3.15368216

Int4_29

E = -14738.68

G = -14362.16

Nimag = 0

C	0.93308307	-0.83604001	0.20518151
C	0.40120958	-1.31132430	1.58502266
H	0.24214676	-1.12224556	-0.58584327
H	1.20329901	-1.22850431	2.32836592
C	-0.78773895	-0.48586230	2.11590749
C	1.11651621	0.68394060	0.19172993
C	-0.16025348	1.44952721	0.62155082
C	-0.44401235	1.01233339	2.09842768
H	-1.00594671	-0.79533074	3.13902725
H	-1.27621828	1.59949097	2.49787208
H	0.43553499	1.18095175	2.72721858
H	0.03482620	2.52038375	0.58133790
H	1.86359523	-1.35689225	-0.01668340
H	0.14349988	-2.37087190	1.51875984
N	-2.06923164	-0.65898448	1.35646024
C	-2.10744000	-0.14910740	-0.04637341
H	-3.15217350	-0.07383073	-0.34960505
H	-1.62133769	-0.86486154	-0.71959129
C	-1.46446105	1.21836099	-0.12043331
C	-2.15185806	2.24028404	-0.63668121
C	-2.75561271	-3.39407282	-0.69942559
S	-3.03594540	-1.98617743	1.66376212
O	-4.37202732	-1.64948461	1.16075725
O	-2.85667261	-2.32864182	3.07695982
H	-1.32987468	-4.24422574	2.29268516
H	-2.46245086	-4.45402557	-2.55122232
H	-0.91565449	-6.13000587	-1.56127478
H	-0.36444195	-6.03953961	0.86417851
N	2.26608257	1.13050828	0.80507360
C	3.47903871	0.30404376	1.01907349
Pd	1.84907059	1.06006104	-1.87966502
C	2.51448365	2.54417374	1.19703088
H	1.62252615	2.99616124	1.62847605
H	2.80639962	3.12191148	0.30856353
C	4.51718852	1.29513177	1.61321277
C	3.66654073	2.43284675	2.19770485
H	5.15578925	0.80163766	2.34803035
H	5.15561101	1.68163230	0.81024569
H	3.27656806	2.15749305	3.18471280
H	4.21869788	3.37182391	2.29243845
C	4.09809595	-0.39828199	-0.22884868
C	-2.20591399	-4.40190294	-1.49657672
H	-3.14113836	2.10058892	-1.06513897
C	-1.33971611	-5.34799905	-0.93682524
O	3.70470134	-0.06109964	-1.39859116
O	4.99907085	-1.23518357	0.02337369
C	-2.41987906	-3.34413438	0.66055429
H	-1.74786310	3.24477824	-0.64875240
C	-1.02579616	-5.29652715	0.42650981
H	-3.44977994	-2.67440016	-1.12030862
C	-1.56303433	-4.29089482	1.23404627
H	-2.08121709	3.74542338	-3.91034349
H	1.80201075	0.46831445	-5.16526992
H	3.24699201	-0.48624561	1.74066472
P	0.40505727	2.11681944	-3.24298985
H	-0.76398474	-0.40786569	-2.54775144
C	1.41154611	2.55333292	-4.73256963
C	1.65761483	3.87664900	-5.12844620
C	2.45952429	4.13993207	-6.24584833
C	3.01903635	3.08692382	-6.97649479
C	2.77656692	1.76259476	-6.58533355

C	1.98271911	1.49743719	-5.46867676
H	1.22433399	4.70197006	-4.57244421
H	2.64167434	5.16949050	-6.54533264
H	3.64080257	3.29385836	-7.84414426
H	3.20912919	0.93888182	-7.14835326
C	-0.27205641	3.74470937	-2.72160395
C	0.48351031	4.46186647	-1.77823067
C	0.04472620	5.70360151	-1.31323925
C	-1.16207997	6.23751190	-1.78145322
C	-1.91732646	5.52922578	-2.72315729
C	-1.47379051	4.29023240	-3.19593762
H	1.40869850	4.03032671	-1.40250597
H	0.63579948	6.24681359	-0.57995315
H	-1.51396561	7.19699247	-1.41062317
H	-2.85716549	5.93768490	-3.08665788
C	-0.96840749	1.15572342	-4.00089748
C	-1.62795409	1.56924211	-5.17159966
C	-2.65338837	0.78831503	-5.71225362
C	-3.01852712	-0.41863716	-5.10071560
C	-2.34191667	-0.85128662	-3.95528118
C	-1.31902990	-0.06806064	-3.41520001
H	-1.33144226	2.48717216	-5.67139522
H	-3.16177366	1.11679651	-6.61558891
H	-3.81498680	-1.02469269	-5.52541290
H	-2.60148668	-1.79814838	-3.48914047

TS4_10

E = -14717.40

G = -14345.01

Nimag = 1, 806i cm-1

C	1.64586244	-0.94222877	-1.31362273
C	0.65647133	-1.81494491	-2.09786208
H	0.92792050	-1.01549556	0.06861213
H	1.25169363	-2.52412280	-2.68980901
C	-0.23943504	-1.06232637	-3.10517658
C	1.94843074	0.39146137	-1.75881103
C	1.06879335	1.05409165	-2.83771546
C	0.60711245	-0.02637260	-3.84712853
H	-0.62164395	-1.79463416	-3.82020176
H	0.02960630	0.45025523	-4.64513643
H	1.47233053	-0.52677980	-4.29524370
H	1.68427660	1.78348608	-3.36472468
H	2.49999661	-1.50956862	-0.95256191
H	0.04193665	-2.41034135	-1.42027086
N	-1.44815210	-0.36085948	-2.56243324
C	-1.23400255	0.86490402	-1.73122566
H	-2.18545239	1.39095318	-1.64922011
H	-0.91561743	0.57931211	-0.70979607
C	-0.18134621	1.75710243	-2.33579288
C	-0.35619167	3.07558139	-2.44809538
C	-2.85324362	-3.72883060	-3.36603933
S	-2.70735902	-1.32774341	-2.01042785
O	-2.31463647	-2.20622139	-0.89511695
O	-3.84362477	-0.42647172	-1.77394420
H	-3.60972668	-0.65049016	-4.66150189
H	-2.99756805	-5.58992393	-4.44096882
H	-3.79206408	-4.52434167	-6.54369810
H	-4.10085140	-2.05807839	-6.65757766
N	3.12550587	1.00324835	-1.45652241
C	3.31483972	2.47142943	-1.50526342
Pd	0.99188355	0.49925414	0.53570025
C	4.15189661	0.36167199	-0.58370354
H	3.67364949	-0.13948586	0.26488973
H	4.69502228	-0.38841784	-1.17134485
C	4.81639726	2.61843147	-1.18002171
C	5.05085046	1.52254888	-0.12316274
H	5.05353115	3.62301412	-0.82603931
H	5.40463579	2.41710961	-2.08282340
H	4.72287511	1.87465032	0.86107865
H	6.09835353	1.22001648	-0.04597563
C	2.42794572	3.30543143	-0.50915822
C	-3.13289479	-4.51281449	-4.49016992
H	-1.28129728	3.55373176	-2.13417402
C	-3.57970761	-3.91144784	-5.67141217
O	2.55430855	4.55464997	-0.64769500
O	1.68007194	2.74095231	0.35213888
C	-3.03283656	-2.34576986	-3.44922726
H	0.42877202	3.72073786	-2.83455895
C	-3.75406056	-2.52211157	-5.73809330
H	-2.50070256	-4.17660919	-2.44294563
C	-3.48251853	-1.72799317	-4.62312842
H	-2.35104946	-0.45163366	1.05482693
H	1.70658169	2.64434276	2.63586049
H	-4.57987548	0.53793445	0.69498136
P	-0.02608560	0.34137526	2.58434777
H	1.49413901	-2.10898426	2.34703045
C	0.76388689	1.23909283	3.98309337
C	0.58634153	0.86217204	5.32434375
C	1.18936563	1.60171770	6.34639050
C	1.97028049	2.72238807	6.03793474
C	2.15162751	3.09954921	4.70195491
C	1.55771751	2.35847436	3.67516472
H	-0.01681065	-0.00593935	5.57330325
H	1.04982857	1.30232062	7.38268638
H	2.43865040	3.29527078	6.83493636
H	2.76139949	3.96663528	4.45790857
C	-0.32206767	-1.35346711	3.23364250
C	-1.45078786	-1.67148634	4.00661672
C	-1.62240029	-2.96894989	4.49968833
C	-0.66605485	-3.95524746	4.23178778
C	0.46237802	-3.64258671	3.46351888
C	0.62972345	-2.34900733	2.96186177
H	-2.19879165	-0.91187475	4.21516217
H	-2.50264142	-3.20843990	5.09186686
H	-0.80256207	-4.96427224	4.61381240
H	1.20479679	-4.40716367	3.24669980
C	-1.71220743	1.06510248	2.46554930
C	-2.07826469	2.24233123	3.13473073
C	-3.34506262	2.80239634	2.92813824
C	-4.25196000	2.19129295	2.05610717
C	-3.88977867	1.01387313	1.38657563
C	-2.62763652	0.45556905	1.58666387
H	-1.37994044	2.72357291	3.81308734
H	-3.62019383	3.71608591	3.45033476
H	-5.23376006	2.63034578	1.89444761
H	3.09217013	2.85254072	-2.50434127

TS4_11

E = -14710.63

G = -14339.46

Nimag = 1, 823i cm-1

C	0.81055257	-0.87107507	0.93059190
C	-0.24544528	-1.54992300	1.84251142
H	-0.15841633	-0.94476309	-0.33511371
H	0.31645182	-2.13431214	2.58379208
C	-1.16185352	-0.59988388	2.64894329
C	1.21955886	0.47513920	1.27108922
C	0.17500314	1.37734858	1.93281717
C	-0.37421374	0.60732876	3.15987637
H	-1.55606805	-1.16189214	3.49938428
H	-1.02318423	1.26292141	3.74835125
H	0.45402382	0.27586813	3.79574675
H	0.65078983	2.29171602	2.27744239
H	1.62764531	-1.55725594	0.71512115
H	-0.85497363	-2.26117590	1.28054219
N	-2.34404243	-0.05088231	1.92697171
C	-2.07084855	0.78607845	0.72834249
H	-2.99053809	1.30335849	0.45289902
H	-1.77936113	0.15491040	-0.11988189
C	-0.96802147	1.78818914	1.00346024
C	-0.99116660	2.99733506	0.43444500
C	-4.13915475	-2.42833526	4.22474259
S	-3.71523018	-1.00098051	1.88978332
O	-3.46767966	-2.34915759	1.35263195
O	-4.76281066	-0.19669761	1.24935760
H	-4.23314187	0.97891487	3.91515025
H	-4.50209737	-3.51277296	6.05055716
H	-4.91610543	-1.46433233	7.40035180
H	-4.78578454	0.78144386	6.33549862
N	2.48152462	0.90796312	1.16666180

C	3.59824940	0.07786244	0.64965673
Pd	0.71508721	-0.03102631	-1.27375600
C	2.98012086	2.29304179	1.36963767
H	2.34940759	2.86075688	2.04871045
H	2.99775235	2.79296126	0.39270134
C	4.88861173	0.80731253	1.15109254
C	4.39067672	2.05599797	1.91738631
H	5.48610946	0.14735333	1.78380212
H	5.50566118	1.09540383	0.29601295
H	4.33202000	1.85325861	2.99217415
H	5.03559683	2.92563380	1.76574787
C	3.64871132	-0.03081324	-0.91470202
C	-4.44811259	-2.53202035	5.58547938
H	-1.80932980	3.30382096	-0.21249763
C	-4.68030566	-1.37919587	6.34256544
O	4.46462265	-0.88684969	-1.34991037
O	2.95353269	0.78568439	-1.60731362
C	-4.06959375	-1.15969458	3.64418791
H	-0.18398383	3.71054951	0.58376524
C	-4.60702731	-0.11314753	5.74483205
H	-3.95032971	-3.31169046	3.62387041
C	-4.30061370	0.00413897	4.38854861
H	-2.46664615	-1.52402407	-2.37057029
H	0.63685957	2.79701598	-1.95394375
H	3.51707827	-0.92750068	1.06875061
P	-0.49721871	0.44514825	-3.16022325
H	1.66149885	-1.19414832	-4.10417833
C	-0.05275566	2.08620938	-3.87037486
C	-0.23892526	2.40769657	-5.22443615
C	0.09223830	3.68229222	-5.69521207
C	0.60608558	4.64611771	-4.81877359
C	0.79702314	4.32962121	-3.46843212
C	0.47634144	3.05314108	-2.99851174
H	-0.63924054	1.66728810	-5.91111131
H	-0.05242665	3.92317339	-6.74594006
H	0.86172623	5.63658235	-5.18791532
H	1.20183530	5.07261644	-2.78505646
C	-0.38658423	-0.70794939	-4.58620190
C	-1.45339516	-0.93619503	-5.47036332
C	-1.29215418	-1.80436484	-6.55522320
C	-0.06546045	-2.44457134	-6.76768741
C	1.00191443	-2.21947262	-5.88887200
C	0.84018597	-1.35999517	-4.79898294
H	-2.40762772	-0.44247336	-5.31015162
H	-2.12377875	-1.97925789	-7.23402203
H	0.05684190	-3.12046705	-7.61084020
H	1.95445895	-2.71972812	-6.04694805
C	-2.29988239	0.58548291	-2.82659379
C	-2.97366357	1.81440927	-2.84602639
C	-4.31761489	1.88675533	-2.45657164
C	-4.99673131	0.73404551	-2.05442383
C	-4.32900589	-0.49794230	-2.03969627
C	-2.98917416	-0.57090582	-2.41527743
H	-2.45378540	2.71612170	-3.15481396
H	-4.82853140	2.84697200	-2.46646806
H	-6.03568475	0.79310134	-1.74032186
H	-4.84625387	-1.39443361	-1.70885265

Int4_30

E = -14735.62

G = -14360.89

Nimag = 0

C	1.61416238	-0.59618358	-0.35450428
C	0.95883272	-1.79167404	-1.03200356
H	0.35606863	-1.07900702	1.94076735
H	1.75481636	-2.45548256	-1.40337045
C	0.07774303	-1.45155437	-2.25305676
C	1.67076616	0.66080669	-0.96773901
C	0.83946730	0.93715170	-2.22965680
C	0.76805321	-0.35936315	-3.07668059
H	-0.04600385	-2.35040892	-2.85714785
H	0.21628600	-0.15992003	-4.00048812
H	1.77670993	-0.69729180	-3.33921274
H	1.35186010	1.71072646	-2.80571393
H	2.42853324	-0.86559714	0.31173094
H	0.39542146	-2.37921020	-0.30560129
N	-1.31530076	-0.97692989	-1.95577865
C	-1.47221486	0.36076357	-1.31051506
H	-2.51960800	0.65627671	-1.38307656
H	-1.20265863	0.28886098	-0.23965446
C	-0.59239546	1.38275624	-1.98099032
C	-1.06385467	2.56524708	-2.38058018
C	-3.13532259	-1.50023252	1.04946096
S	-2.49447277	-2.09621199	-1.57089568
O	-3.78302452	-1.45711416	-1.86307048
O	-2.13671653	-3.34459464	-2.25165948
H	-1.16308024	-4.10752893	0.04520475
H	-3.57447226	-1.00092139	3.09447743
H	-2.21315186	-2.85638806	4.03094704
H	-1.00599140	-4.40935872	2.51006799
N	2.49416661	1.64940431	-0.53312547
C	2.14075185	3.08065412	-0.64633976
Pd	0.41117908	0.37707865	1.44765770
C	3.41964686	1.44248583	0.61263906
H	2.89669535	0.91870209	1.42721302
H	4.25664842	0.81546765	0.28664265
C	3.40259353	3.77821954	-0.10703272
C	3.84325970	2.85974993	1.05264411
H	3.18991941	4.80105861	0.20951982
H	4.16550842	3.80601480	-0.89326495
H	3.31172049	3.13197665	1.96969212
H	4.91607573	2.92066959	1.25312519
C	0.85625822	3.46718014	0.16257196
C	-3.04840012	-1.68068577	2.43110436
H	-2.10911316	2.83420940	-2.24764919
C	-2.28214278	-2.72440591	2.95637386
O	0.22699507	2.58708789	0.83511579
O	0.51862129	4.67785351	0.07030006
C	-2.44428072	-2.37557025	0.20319697
H	-0.41519938	3.31083447	-2.83389282
C	-1.59876063	-3.59550644	2.10119414
H	-3.74346502	-0.70470049	0.63306163
C	-1.67645303	-3.42734624	0.71671883
H	-2.44013385	1.21721632	1.51812176
H	0.36047948	3.72252589	2.95827359
H	1.94873125	3.35005858	-1.68760801
P	-0.36287762	0.97281547	3.51328071
H	1.13597117	-1.43648472	4.09100513
C	0.86355202	2.09766735	4.29393472
C	1.71654266	1.67163942	5.32399509
C	2.69543215	2.53572209	5.82708091
C	2.82818372	3.82804637	5.30892088
C	1.97619287	4.25657091	4.28248658
C	1.00116780	3.39843372	3.77197311
H	1.61915987	0.67371896	5.73964563
H	3.34936751	2.19727764	6.62741561
H	3.58918868	4.49800774	5.70190654
H	2.07524517	5.25980426	3.87443787
C	-0.62563828	-0.36613077	4.74116741
C	-1.71983296	-0.37335901	5.61887870
C	-1.88107349	-1.42235363	6.53073609
C	-0.94509955	-2.46036412	6.58476091
C	0.15253194	-2.45309971	5.71504518
C	0.30466782	-1.41831729	4.79062287
H	-2.45524609	0.42343362	5.58544906
H	-2.74123274	-1.42763495	7.19576439
H	-1.07448209	-3.27528070	7.29271002
H	0.87943504	-3.26095105	5.74432182
C	-1.90776437	1.95287091	3.46763600
C	-2.27080406	2.80274092	4.52651247
C	-3.47126200	3.51568210	4.47025460
C	-4.31211160	3.39038574	3.35706169
C	-3.94566092	2.55745877	2.29369469
C	-2.74443062	1.84638396	2.34732360
H	-1.61720475	2.91068736	5.38763118
H	-3.74871019	4.16952247	5.29348986
H	-5.24480328	3.94765970	3.31552009
H	-4.58865915	2.47037017	1.42114636

Int4_31

E = -14732.35
G = -14358.19
Nimag = 0

C	1.51340723	-0.91217200	0.90272213
C	0.74043857	-2.01337968	1.62919772
H	-0.59488037	-0.98867033	-1.00037022
H	1.47390100	-2.62856817	2.17089902
C	-0.29138203	-1.54560796	2.69091806
C	1.43250745	0.43097716	1.31969562
C	0.31289728	0.84479301	2.28718586
C	0.19455908	-0.26187863	3.36242755
H	-0.40048806	-2.33548664	3.43401899
H	-0.50756877	0.05249687	4.14123730
H	1.17159359	-0.43747644	3.82615078
H	0.61492010	1.76661736	2.78278687
H	2.47227300	-1.25232978	0.51522422
H	0.26446288	-2.68356135	0.91265479
N	-1.68157807	-1.26486304	2.20892925
C	-1.87634698	-0.12194898	1.27483603
H	-2.93389255	0.14306743	1.27347443
H	-1.59492090	-0.43031095	0.25745125
C	-1.04506883	1.08720022	1.64398942
C	-1.49413939	2.31802648	1.38143244
C	-3.07487613	-2.66734496	-0.73889273
S	-2.74205820	-2.53927395	2.00172137
O	-4.08948225	-1.95901577	1.98220669
O	-2.40101936	-3.54764006	3.00948004
H	-1.05800268	-4.72611005	1.10278049
H	-3.22425701	-2.68445810	-2.88856237
H	-1.56843671	-4.51063303	-3.17062558
H	-0.50310891	-5.55308908	-1.17701558
N	2.38070522	1.35168512	1.02669427
C	3.72807532	1.00520903	0.50837486
Pd	0.74086491	-0.24354111	-1.18245995
C	2.22316793	2.82235004	1.10288123
H	1.50289501	3.11523073	1.86388737
H	1.86350124	3.19643477	0.13285346
C	4.50999554	2.35671707	0.54101080
C	3.64638536	3.30144287	1.39656625
H	5.51903432	2.21693124	0.93374676
H	4.59831416	2.75189625	-0.47697556
H	3.86308198	3.17126024	2.46316131
H	3.79128135	4.35401014	1.13760692
C	3.82419418	0.41206545	-0.92356424
C	-2.75317810	-3.13026442	-2.01722090
H	-2.47035437	2.48345428	0.93347488
C	-1.82090751	-4.16061061	-2.17464060
O	4.96292777	-0.02098068	-1.24273286
O	2.81135445	0.45081755	-1.70217768
C	-2.44402333	-3.23847579	0.37300301
H	-0.89105735	3.19875854	1.58622711
C	-1.21587651	-4.74193043	-1.05444760
H	-3.81317280	-1.88556372	-0.59869646
C	-1.52170767	-4.28165164	0.22842452
H	-2.86748264	-0.28319461	-1.87857570
H	1.52744536	2.63952132	-2.23438579
H	4.16924666	0.27282592	1.19386256
P	-0.36408143	0.59405222	-3.00187170
H	0.70406019	-1.94572358	-3.81990670
C	0.59829545	1.79877128	-3.99366591
C	0.50618654	1.85781331	-5.39317546
C	1.23272726	2.82006788	-6.10190988
C	2.04881163	3.73010404	-5.41997605
C	2.14588235	3.67139062	-4.02413374
C	1.43061251	2.70543290	-3.31361410
H	-0.12703592	1.15752261	-5.92943643
H	1.15857182	2.85896357	-7.18608039
H	2.61144780	4.47795467	-5.97362500
H	2.78428705	4.37196096	-3.49120911
C	-0.98136106	-0.64957399	-4.19486555
C	-2.17693342	-0.48131555	-4.91093357
C	-2.59871253	-1.46681379	-5.80868331
C	-1.82327259	-2.61507615	-6.00724102
C	-0.62378950	-2.77914046	-5.30434003
C	-0.20900484	-1.80524935	-4.39362689
H	-2.78173409	0.40814106	-4.76232240
H	-3.53127023	-1.33646585	-6.35220329
H	-2.15489487	-3.38154325	-6.70338048
H	-0.02180222	-3.67232436	-5.45190970
C	-1.85674815	1.52474256	-2.46800210
C	-1.93321287	2.92421079	-2.51978736
C	-3.06387379	3.58328084	-2.02264989
C	-4.12587185	2.85405485	-1.47922282
C	-4.05654880	1.45518354	-1.43340759
C	-2.92745711	0.79836907	-1.91948011
H	-1.11874279	3.50260942	-2.94368211
H	-3.11238057	4.66873445	-2.06390839
H	-5.00162148	3.36954120	-1.09299770
H	-4.87921375	0.88042707	-1.01464987

Int4_32

E = -14742.41
G = -14368.08
Nimag = 0

C	1.52922759	-0.47003890	-0.50593690
C	0.63064190	-1.46328712	-1.23602602
H	1.04510296	2.25613164	1.27799496
H	1.27181898	-2.17557076	-1.77762534
C	-0.32148740	-0.84610717	-2.28856157
C	1.64284238	0.85980462	-0.90113226
C	0.70197124	1.41874588	-1.97873633
C	0.39506585	0.30081939	-3.00723758
H	-0.60270423	-1.61829091	-3.00533074
H	-0.23008801	0.70324742	-3.81052199
H	1.32757259	-0.07426003	-3.44325626
H	1.20722510	2.23721064	-2.49452217
H	2.37612412	-0.92653259	0.00437992
H	0.06171717	-2.06564503	-0.52226402
N	-1.61613682	-0.29504812	-1.76473199
C	-1.52864657	0.88016892	-0.85016876
H	-2.53232407	1.27390834	-0.69592189
H	-1.11964388	0.56449732	0.13385817
C	-0.62791666	1.93132232	-1.44336515
C	-0.99873797	3.21127174	-1.52931256
C	-2.78468496	-1.58795519	1.24874455
S	-2.88863710	-1.34009294	-1.50368707
O	-4.07414514	-0.50267722	-1.28821498
O	-2.87776549	-2.30665302	-2.60646060
H	-1.92550820	-4.01610789	-1.00377794
H	-2.63923380	-1.78499273	3.38148086
H	-1.74806838	-4.09966388	3.30254908
H	-1.39509806	-5.22627996	1.10850601
N	2.65674556	1.67848214	-0.46100762
C	2.67258720	3.14226169	-0.56818901
Pd	0.60524236	0.13029383	1.53962466
C	3.63672930	1.20291304	0.54284446
H	3.09512347	0.71516100	1.37450551
H	4.29565070	0.45503521	0.08598027
C	4.11537456	3.49049470	-0.12226167
C	4.38275297	2.46989637	1.00085900
H	4.20676411	4.53064487	0.19697681
H	4.78681364	3.32384161	-0.97089403
H	3.96097305	2.83099556	1.94564427
H	5.44851627	2.28565542	1.15653942
C	1.65744028	3.91045881	0.31048955
C	-2.48526653	-2.27412546	2.42665394
H	-1.97653547	3.54361858	-1.18833705
C	-1.98367651	-3.57849162	2.37871167
O	0.98196611	3.27297386	1.27680226
O	1.50741179	5.11796515	0.15850053
C	-2.57857522	-2.23371745	0.02228533
H	-0.33299813	3.97139579	-1.93080734
C	-1.78117543	-4.21111854	1.14725169
H	-3.17912557	-0.57851847	1.28838381
C	-2.07681676	-3.53894645	-0.04134097
H	-2.86783659	0.07570002	4.92492237
H	2.49932401	1.42439028	3.90717690
H	2.49172582	3.47176622	-1.59339498
P	-0.26704498	0.77130918	3.51363833
H	0.32320265	-2.05287715	3.59263447

C	0.53837493	2.23447736	4.30310982
C	-0.17630951	3.31325160	4.84217952
C	0.50538419	4.39669050	5.40976960
C	1.90357472	4.40627716	5.45022804
C	2.62253126	3.32662004	4.91888090
C	1.94324088	2.25173079	4.34360334
H	-1.26208059	3.31630787	4.81270745
H	-0.05784043	5.23226534	5.81970820
H	2.43138864	5.25029592	5.88822231
H	3.71000586	3.32995379	4.94364008
C	-0.26092763	-0.44617238	4.89990282
C	-0.56058377	-0.08031092	6.22353804
C	-0.54261190	-1.03899668	7.24002312
C	-0.21807593	-2.37009573	6.94542586
C	0.09467909	-2.73794025	5.63208231
C	0.07621766	-1.77811022	4.61515443
H	-0.80341250	0.95213673	6.46093375
H	-0.77825249	-0.74860389	8.26132848
H	-0.20208359	-3.11415314	7.73838878
H	0.35659673	-3.76778136	5.40039586
C	-2.03114434	1.29081949	3.34433652
C	-2.33349116	2.19362139	2.30599069
C	-3.65412215	2.55725803	2.04358871
C	-4.69819593	2.01273045	2.80481064
C	-4.40618779	1.12104527	3.84085958
C	-3.07880116	0.76743815	4.11539829
H	-1.53010211	2.60117794	1.69782491
H	-3.87288167	3.25512876	1.23850834
H	-5.72923351	2.28215959	2.58905311
H	-5.20953215	0.69534458	4.43781817

Int4_33

E = -14734.57

G = -14361.17

Nimag = 0

C	1.40673622	-0.99313721	1.06823754
C	0.59975013	-1.82832729	2.04762054
H	2.11707102	-0.34863669	-1.57798004
H	1.30096966	-2.37496087	2.69751182
C	-0.32514220	-1.02265977	2.98813874
C	1.48724230	0.39202169	1.14214792
C	0.60350992	1.15673710	2.15982333
C	0.39483635	0.26195352	3.40971390
H	-0.54380208	-1.63227376	3.86544366
H	-0.18982218	0.80802210	4.15710381
H	1.36167346	-0.00402015	3.85088699
H	1.15637206	2.05064092	2.45772231
H	2.20217850	-1.54140079	0.56807657
H	0.03513805	-2.59828172	1.51639243
N	-1.66852743	-0.62564231	2.44114222
C	-1.72971461	0.44324486	1.40391002
H	-2.75546778	0.80762890	1.34991536
H	-1.46414479	0.01868183	0.41266399
C	-0.77735263	1.57265213	1.69153823
C	-1.15598973	2.84917210	1.57712250
C	-2.98630797	-2.04900132	-0.46453901
S	-2.85769297	-1.79332802	2.29240936
O	-4.13071113	-1.07258158	2.17645943
O	-2.66132495	-2.74373728	3.39102370
H	-1.68283349	-4.36483861	1.69003888
H	-3.00067361	-2.23104798	-2.60428925
H	-1.85935399	-4.43883290	-2.61512309
H	-1.20732473	-5.51458114	-0.46571555
N	2.49027644	1.13847212	0.54614207
C	3.82060204	0.63484226	0.17505327
Pd	0.22124527	-0.44254813	-0.90885242
C	2.26764226	2.50556062	0.03366078
H	1.57606579	3.05283638	0.67440356
H	1.82802707	2.46380414	-0.97463906
C	4.55468087	1.90003844	-0.39927856
C	3.67834398	3.09687144	0.01907068
H	5.57939775	1.95455117	-0.02691576
H	4.59468598	1.83485430	-1.49198485
H	3.94796477	3.44172061	1.02361968
H	3.77254930	3.93621211	-0.67589562
C	3.99489987	-0.47841168	-0.87594148
C	-2.71325798	-2.70021582	-1.66965891
H	-2.17574302	3.12068998	1.31524143
C	-2.07024264	-3.94141233	-1.67230163
O	5.03924690	-1.12489350	-0.90224596
O	3.06885847	-0.67239960	-1.83141443
C	-2.60132594	-2.65978391	0.73680479
H	-0.45665464	3.66581567	1.74039889
C	-1.69933491	-4.54559511	-0.46554407
H	-3.49693049	-1.09244543	-0.46458161
C	-1.96123405	-3.90511890	0.74767683
H	-3.09194404	-0.32594193	-4.40481361
H	2.12163636	0.87199289	-3.69559794
H	4.31850838	0.25754853	1.07590101
P	-0.58812683	0.36497041	-2.85316402
H	-0.08994406	-2.45040759	-3.22197699
C	0.25558463	1.92402320	-3.37744263
C	-0.36631612	3.18060270	-3.38439248
C	0.37133563	4.33302505	-3.68504795
C	1.73186911	4.24117498	-3.99232351
C	2.35527824	2.98573106	-4.00573598
C	1.62441662	1.83826392	-3.69707127
H	-1.42274979	3.26974228	-3.15283799
H	-0.12312963	5.30193149	-3.68067818
H	2.30328439	5.13753575	-4.22117905
H	3.41224801	2.90273107	-4.24825560
C	-0.49152174	-0.67327988	-4.36729880
C	-0.66948344	-0.13710396	-5.65401947
C	-0.61699591	-0.97034905	-6.77444426
C	-0.38637918	-2.34411279	-6.61894512
C	-0.19951300	-2.88156534	-5.34048284
C	-0.24652448	-2.04674266	-4.21924735
H	-0.84738634	0.92818202	-5.77814033
H	-0.75567903	-0.55026149	-7.76803988
H	-0.34558641	-2.99035312	-7.49265559
H	-0.01012555	-3.94541180	-5.21704125
C	-2.36974414	0.81879268	-2.71788834
C	-2.75152982	1.62652537	-1.62974024
C	-4.09592490	1.91136491	-1.39191567
C	-5.08505379	1.37624536	-2.22851700
C	-4.71470955	0.57289498	-3.31133717
C	-3.36383928	0.30054637	-3.56090553
H	-1.98928934	2.02129401	-0.96359141
H	-4.37548201	2.53896943	-0.54882000
H	-6.13474422	1.58249293	-2.03422590
H	-5.47613925	0.15287812	-3.96453338

Int4_34

E = -8688.97

G = -8466.90

Nimag = 0

C	1.58846642	-0.59848575	-0.50240697
C	0.71154577	-1.69013628	-1.07164786
C	-2.11788133	-3.60346790	0.20618797
H	1.33578325	-2.52403826	-1.43187018
C	-0.18061761	-1.24314256	-2.25365887
C	1.68829403	0.64719573	-1.02424896
C	0.85759893	1.03857302	-2.25025808
C	0.57773794	-0.21998431	-3.10918627
H	-0.45234434	-2.10957933	-2.85732856
H	-0.01299597	0.05345656	-3.98966344
H	1.52298966	-0.66226114	-3.44318200
H	1.41142887	1.76299069	-2.85456881
H	2.17878229	-0.87452370	0.36662979
H	0.08852629	-2.12083165	-0.27891304
N	-1.47938982	-0.60066917	-1.85587658
C	-1.37536667	0.67972658	-1.08817013
H	-2.37671229	1.09471356	-0.97689769
H	-0.95088068	0.48747032	-0.09220853
C	-0.48484888	1.63245422	-1.85183691
C	-0.88033762	2.86540526	-2.17740597
C	-2.81721038	-1.49198644	1.21597837
S	-2.79744314	-1.56885672	-1.54489800
O	-3.96340314	-0.67928527	-1.48416673
O	-2.77192739	-2.65661331	-2.52776885

H	-1.94743184	-4.20227420	-0.68229376
H	-2.74327779	-1.41416550	3.36556962
H	-1.90261511	-3.74439998	3.60475305
H	-1.51993746	-5.14563623	1.58358389
N	2.56567883	1.61276105	-0.52843047
C	2.35568819	3.05281847	-0.64303659
H	2.15302764	3.35420973	-1.67332531
C	3.44928294	1.30580773	0.61439212
H	2.87529073	0.89844037	1.45964841
H	4.17839188	0.54396767	0.30998503
C	3.71351726	3.62078116	-0.15546498
C	4.10538683	2.65837139	0.98833824
H	3.64182544	4.66463205	0.15927180
H	4.42278022	3.55548522	-0.98657004
H	3.70317320	3.01908733	1.94065164
H	5.18987729	2.57192465	1.09687035
C	1.20892360	3.64239757	0.20069503
C	-2.56602856	-2.02366126	2.48336701
H	-1.86478553	3.23915877	-1.90433637
C	-2.09527307	-3.33571247	2.61603234
O	0.71776824	2.77902118	1.12521698
O	0.80621148	4.78999868	0.07629770
C	-2.58498500	-2.28930027	0.08729775
H	-0.22553255	3.54696563	-2.71583882
C	-1.87765073	-4.12451711	1.48024891
H	-3.19848263	-0.48185536	1.10860223
H	0.01631226	3.24833083	1.62730412

Int4_35
E = -8687.32
G = -8464.66
Nimag = 0

C	1.56292950	-1.33012231	1.77176654
C	0.58166314	-2.26682503	2.43353504
H	3.80735463	-0.31844827	0.26234077
H	1.09151128	-2.95886368	3.12427604
C	-0.49337817	-1.53029734	3.25373836
C	1.64457757	-0.00470790	2.05060603
C	0.78113384	0.62454276	3.14838613
C	0.20673603	-0.45532632	4.09422744
H	-1.00899894	-2.23956644	3.90185939
H	-0.48810751	0.01008311	4.80073164
H	1.01033554	-0.93465287	4.66420636
H	1.36958387	1.33964793	3.73083815
H	2.17596990	-1.76416568	0.98713030
H	0.11573914	-2.90674047	1.67804710
N	-1.58392916	-0.85675381	2.45466722
C	-1.27881726	0.41287644	1.70949528
H	-2.22752065	0.89597568	1.47126570
H	-0.75285822	0.17755962	0.77497373
C	-0.40788168	1.33114951	2.52630460
C	-0.67977681	2.62957146	2.67920185
C	-2.28010705	-1.23545030	-0.95220275
S	-2.74321020	-1.80795798	1.71857398
O	-3.93676648	-0.96927105	1.55143552
O	-2.84155399	-3.05224696	2.48763319
H	-1.44499152	-4.16073475	0.60774556
H	-1.83154908	-0.75818875	-3.00384428
H	-0.62969284	-2.89696774	-3.43053789
H	-0.46442575	-4.61075296	-1.63216093
N	2.36338537	0.89028667	1.26750913
C	3.04475519	0.44916623	0.05478435
H	0.38708163	-0.05016981	-1.76328898
C	2.83928410	2.21893179	1.72132882
H	3.11876408	2.19832564	2.77949194
H	2.05285810	2.97445296	1.58944679
C	3.72170235	1.73933128	-0.48036664
C	4.05093869	2.50228631	0.81610506
H	4.59757426	1.51059569	-1.09186930
H	3.00762402	2.30697496	-1.08773520
H	4.96139093	2.09300652	1.26937379
H	4.20133245	3.57249800	0.64699028
C	2.12320577	-0.16516445	-1.00254381
C	-1.72794876	-1.49493076	-2.21083235
H	-1.57291076	3.08003863	2.25105821
C	-1.06162004	-2.70245123	-2.45243691
O	2.47364182	-1.05567496	-1.76373536
O	0.89846596	0.41659731	-1.06521205
C	-2.15235695	-2.19619254	0.05962104
H	-0.00931082	3.28355018	3.23269821
C	-0.96354810	-3.66471746	-1.44063150
H	-2.80992853	-0.30773439	-0.76665180
C	-1.50895491	-3.41627655	-0.17872458

P4_3
E = -6314.25
G = -6159.61
Nimag = 0

C	2.12729925	0.35809781	0.52960907
C	1.56665950	-0.82625642	-0.30036139
H	-2.59332909	0.29024574	1.58284282
H	2.41061455	-1.40756902	-0.69074040
C	0.72042162	-0.41977643	-1.52887031
C	2.53474085	1.57047841	-0.29021673
C	1.67368744	1.90448516	-1.51763252
C	1.47881952	0.61950597	-2.36464001
H	0.53598942	-1.30895447	-2.13320399
H	0.92234050	0.86254905	-3.27554208
H	2.45111113	0.20674227	-2.65588326
H	2.20777825	2.67116375	-2.08566765
C	-1.40733190	-2.40331306	3.30583185
H	1.00283671	-1.49454544	0.35442199
N	-0.63013025	0.15711408	-1.23180355
C	-0.67103345	1.45927209	-0.50618635
H	-1.68255750	1.85821259	-0.58152296
H	-0.45108610	1.30839748	0.56099165
C	0.31220587	2.44455280	-1.10632434
C	-0.01495303	3.73139378	-1.26498087
C	-2.14774823	-0.68161012	1.76729000
S	-1.91257294	-0.88146124	-0.97739838
O	-3.12748730	-0.06269188	-1.04602981
O	-1.74072213	-2.00407040	-1.90312451
H	-0.95753621	-3.40707434	0.07419237
H	-2.24177791	-0.50268159	3.91003398
H	-1.26171783	-2.75236593	4.32486235
H	-0.63711375	-4.21333059	2.40931622
O	3.50291179	2.26469325	0.01094222
C	-1.23161938	-2.78104320	0.91684459
C	-1.77564370	-1.50974317	0.69949014
H	0.69960437	4.45107572	-1.65759964
C	-1.05322997	-3.22555636	2.22953125
C	-1.95658105	-1.13665691	3.07471307
H	-1.00389805	4.10200895	-1.00418691
H	2.98485825	0.04443022	1.13286605
H	1.36619064	0.71428146	1.23813615

Table 7.5. Cartesian coordinates (in Å), energies (in kcal mol^{-1}), and number of imaginary frequencies computed at COSMO(DCM)-ZORA-M06-2X/TZ2P//COSMO(DCM)-ZORA-BLYP-D3(BJ)/DZP.

4_56
E = -11782.94
G = -11467.79
Nimag = 0

C	1.48522540	1.04786766	-1.66441363
C	2.92999694	1.37868394	-1.25869748
H	0.81694758	1.88028906	-1.39611972
H	3.62139918	0.68669519	-1.77036073
C	3.10279128	1.23902952	0.26090736
C	0.95933750	-0.21671078	-1.00826804
C	1.57904495	-0.78016015	0.05238379
C	2.82831131	-0.21247825	0.69225368
H	4.11555167	1.54324332	0.56872713
H	2.73661619	-0.25916642	1.79115464

H	3.70485923	-0.84125828	0.43876408
H	1.19680535	-1.70807217	0.47988440
H	1.41134131	0.93846641	-2.75914965
H	3.18325801	2.39422025	-1.59627054
H	-3.76585172	5.77576748	0.36556457
H	-3.57247438	4.00720089	0.24799172
C	-1.81392861	5.04196251	2.13246199
H	-0.83305240	5.15628803	2.60963287
H	-2.47337603	5.84832988	2.48540961
O	0.87078529	3.55809555	1.68455730
N	1.58961327	4.57940897	-0.23409300
C	1.43229294	5.01881844	-1.62532112
C	2.92533347	4.82158014	0.33161536
H	2.92345176	4.53121915	1.38348151
H	3.17212980	5.88868531	0.23396704
S	-2.23609711	2.06525409	-2.08217640
H	-2.24660845	4.08496022	2.45668637
H	-0.88164511	3.98047127	-1.06517415
C	0.63032513	4.01043410	0.54427155
N	-0.18553080	-0.72971913	-1.64905977
H	-0.64241254	-0.01761563	-2.22753161
C	-1.16993856	-1.54605507	-0.92196598
C	-1.53979225	-2.82582859	-1.69483046
C	-2.45070433	-0.73076472	-0.60314461
C	-2.55813135	-3.67779945	-0.91673933
H	-1.96216799	-2.53717485	-2.67300157
H	-0.61903350	-3.39515416	-1.89342789
C	-3.46162701	-1.57428323	0.19088889
H	-2.90902802	-0.40883037	-1.54811861
N	-2.11981420	0.49635657	0.12755521
C	-3.81801860	-2.86337651	-0.57148108
H	-2.82995093	-4.56977032	-1.50234320
H	-2.09075488	-4.03582438	0.01748610
H	-4.36153645	-0.97032406	0.38237186
H	-3.02354530	-1.83419171	1.17084195
H	-1.75718981	0.35069410	1.07289637
C	-1.86182348	1.70540176	-0.44306902
H	-4.34357856	-2.59490803	-1.50424531
H	-4.51483810	-3.46885679	0.02828896
N	-1.31986254	2.61861981	0.40535814
H	-0.93517885	2.28891396	1.29568529
C	-0.81847218	3.93735020	0.02340847
H	-0.72273000	-1.84142484	0.03747224
H	3.67653207	4.23306222	-0.21133389
H	1.40154345	6.11645448	-1.68601903
H	0.52889484	4.60852251	-2.07630307
H	2.29516834	4.66038506	-2.20299969
C	-1.70874974	5.10749791	0.59486389
C	-1.09812654	6.46010484	0.17046304
H	-1.73996946	7.28072700	0.52202324
H	-0.09737146	6.60654794	0.59971803
H	-1.02319433	6.53624901	-0.92344137
C	-3.11996750	4.97190092	-0.01712492
H	-3.08359755	5.03985322	-1.11261575
H	2.38948634	1.90420978	0.76774616

4_57

E = -11779.25

G = -11464.31

Nimag = 0

C	-3.13637077	1.36351142	1.12252195
C	-1.69807630	0.90873511	1.19566156
H	-3.49955021	0.61005888	-1.88474596
H	-1.60072788	0.15988148	2.00523461
C	-1.20725220	0.28594623	-0.12289912
C	-4.00738463	0.94921831	0.18118824
C	-3.58357438	0.02596445	-0.94984211
C	-2.25921130	-0.69723759	-0.65558567
H	-0.24392087	-0.22452576	0.03325798
H	-1.90518230	-1.20417685	-1.56371327
H	-2.43993483	-1.46438422	0.11115296
H	-1.04163352	1.08305713	-0.86849560
H	-4.37359943	-0.72146619	-1.12258155
H	-1.05037872	1.75621004	1.47768452
H	-6.52110315	-6.60901185	0.06078146
H	-5.89511803	-5.57723676	-1.25298349
C	-3.78585258	-6.44615747	0.33299972
H	-2.87523214	-6.30890803	0.93284374
H	-4.19273861	-7.44169972	0.56247576
O	-4.72308634	-3.34191805	-1.88568380
N	-2.57150933	-3.99815788	-1.46781872
C	-1.42756075	-4.23879254	-0.58202305
C	-2.22055270	-3.89805439	-2.89086868
H	-3.13591235	-3.86771392	-3.48483562
H	-1.61405046	-4.76937158	-3.17214185
S	-3.77601282	-1.97322238	2.81738507
H	-3.50910371	-6.43040741	-0.72991064
H	-3.41042804	-3.78513247	1.07949326
C	-3.84572678	-3.72537068	-1.08033072
N	-5.36961634	1.33560209	0.11773718
H	-5.85441115	0.79238978	-0.59737367
C	-6.21498718	1.43589112	1.33362762
C	-6.14912282	2.81391056	2.02175152
C	-5.95975364	0.30223626	2.36465196
C	-7.14517726	2.89596583	3.19273525
H	-5.13305420	2.99357270	2.40142285
H	-6.35746419	3.59016277	1.26965976
C	-6.95503307	0.38770168	3.53528490
H	-4.93852982	0.38295058	2.75283319
N	-6.02792080	-0.99348311	1.68671990
C	-6.89591745	1.76867514	4.21147602
H	-7.06678475	3.87918547	3.68208515
H	-8.17464082	2.81066087	2.80225808
H	-6.72276681	-0.41361062	4.25311136
H	-7.97489175	0.20418534	3.15394075
H	-6.76755692	-1.09123438	0.98769512
C	-5.05051852	-1.94008727	1.67946968
H	-5.89985184	1.90543466	4.66758870
H	-7.63317850	1.81805687	5.02777298
N	-5.21203091	-2.88485826	0.70722874
H	-5.79765036	-2.64427858	-0.09753185
C	-4.24726203	-3.93504416	0.39449395
H	-7.24845303	1.31457055	0.96405119
H	-1.63483134	-2.98498127	-3.07605921
H	-0.64359309	-3.50068538	-0.80620761
H	-1.02208669	-5.24663646	-0.74960273
H	-1.70267256	-4.13688612	0.46653079
C	-4.84171149	-5.37043038	0.66389895
C	-5.19543605	-5.45260630	2.16537385
H	-5.61857862	-6.44185392	2.39338135
H	-4.30281861	-5.30016513	2.78776524
H	-5.93416009	-4.68693194	2.43684401
C	-6.11125663	-5.61654748	-0.17749513
H	-6.88464179	-4.86828617	0.04646990
H	-3.47309693	2.01928035	1.92233816

4_58

E = -11778.91

G = -11463.71

Nimag = 0

C	-3.07752615	1.63398070	1.04828266
C	-1.70370457	0.95929548	1.21721484
H	-2.96905316	2.64454083	0.61410985
H	-1.81441000	0.11724385	1.91895587
C	-1.18392799	0.41746084	-0.12224540
C	-4.01867216	0.83463949	0.16956329
C	-3.59078683	-0.19763205	-0.58212938
C	-2.15437630	-0.65111905	-0.65317343
H	-0.17538142	-0.00886338	-0.00485735
H	-1.89328421	-0.92801651	-1.68745852
H	-2.03969710	-1.56708028	-0.04878773
H	-4.31714922	-0.77286177	-1.16101421
H	-3.52108339	1.78108332	2.04093290
H	-0.99424440	1.67579102	1.65949936
H	-6.55443271	-6.65752561	0.05322430
H	-5.96329662	-5.58201295	-1.24171134
C	-3.82095208	-6.48738825	0.27982377
H	-2.90069344	-6.36704924	0.86804698
H	-4.22331537	-7.48966506	0.48705263
O	-4.77699173	-3.35268734	-1.85711552

N	-2.60835281	-3.95584723	-1.44484108
C	-1.47466048	-4.26777437	-0.56828524
C	-2.24599611	-3.79449552	-2.85935576
H	-3.15443527	-3.64703105	-3.44612744
H	-1.71423533	-4.69250012	-3.20349311
S	-3.78788422	-1.99353746	2.80628461
H	-3.56230064	-6.44117397	-0.78696844
H	-3.45457821	-3.82897694	1.09726116
C	-3.89278842	-3.73405677	-1.05804237
N	-5.36453683	1.29956609	0.08862151
H	-5.86330490	0.75040551	-0.61704649
C	-6.20999104	1.39982602	1.31449149
C	-6.13983857	2.78682453	1.98493053
C	-5.96247748	0.27608308	2.35493995
C	-7.12269743	2.88778043	3.16521089
H	-5.11949298	2.97592954	2.34786293
H	-6.35776912	3.54991221	1.22229810
C	-6.94010380	0.38590920	3.53911481
H	-4.93698034	0.34468487	2.73604651
N	-6.05783279	-1.03177252	1.70123654
C	-6.86445789	1.77444035	4.19658413
H	-7.03686879	3.87782911	3.63940786
H	-8.15685688	2.79882046	2.78814690
H	-6.70408787	-0.40918212	4.26278346
H	-7.96525273	0.20419890	3.17179302
H	-6.80138781	-1.12723666	1.00662501
C	-5.08383810	-1.98107678	1.69156081
H	-5.86177093	1.91262535	4.63769785
H	-7.59042202	1.83794359	5.02196689
N	-5.27024122	-2.94733040	0.74608041
H	-5.85593597	-2.70432881	-0.05848598
C	-4.29151077	-3.97928746	0.41238030
H	-7.24451463	1.27973700	0.94735692
H	-1.58442339	-2.92417184	-2.97855665
H	-0.66702505	-3.54844369	-0.76545518
H	-1.10134428	-5.28141912	-0.77382184
H	-1.74741586	-4.19684657	0.48361646
C	-4.87221412	-5.42317567	0.65829113
C	-5.19494676	-5.54111106	2.16431528
H	-5.61582590	-6.53439544	2.37868085
H	-4.28865176	-5.40582016	2.77116725
H	-5.92529422	-4.77975040	2.46873475
C	-6.15744078	-5.65499045	-0.16378479
H	-6.93180813	-4.92035022	0.09809757
H	-1.11119878	1.24426434	-0.85031151

4_59

E = -11782.04

G = -11467.19

Nimag = 0

C	1.45517700	0.78688835	-1.71337234
C	2.64841047	1.55576729	-1.19876414
C	-3.08642838	4.87055668	-0.13025920
H	3.53683428	1.35490283	-1.83088845
C	2.97645213	1.21212661	0.26514538
C	0.94758761	-0.31236004	-1.11842076
C	1.51342328	-0.85143615	0.18129142
C	2.92503211	-0.30875645	0.47369676
H	3.96702873	1.60881977	0.53797017
H	3.21612397	-0.57553726	1.50150466
H	3.64502042	-0.79445069	-0.20753753
H	-3.01766044	4.93364614	-1.22443011
H	2.23849740	1.69670350	0.92178316
H	2.45389246	2.63261707	-1.29174197
H	-3.78355803	5.64333877	0.22604730
H	-3.49756309	3.88534255	0.12606246
C	-1.85522974	5.00936463	2.05938412
H	-0.89841872	5.18111429	2.56821386
H	-2.57100053	5.77645901	2.38956242
O	0.90232029	3.59547122	1.71023538
N	1.64239411	4.74918644	-0.12138449
C	1.52313287	5.26055148	-1.49131240
C	2.96455560	4.95384961	0.48753620
H	2.92723473	4.64105940	1.53238198
H	3.23565984	6.01649541	0.41794488
S	-2.00759991	1.99895430	-2.14684709
H	-2.24132674	4.02883401	2.37165290
H	-0.74492042	3.98828161	-1.09905399
C	0.68438154	4.08767440	0.58167726
N	-0.07141059	-1.08430950	-1.72901179
H	-0.48227930	-0.57390929	-2.51933451
C	-1.13200092	-1.71913029	-0.92650571
C	-1.67498985	-2.96314549	-1.65414426
C	-2.30487657	-0.75658995	-0.60391653
C	-2.76321373	-3.67284785	-0.82935010
H	-2.09210895	-2.64986294	-2.62770503
H	-0.83422303	-3.64126434	-1.86363074
C	-3.38727121	-1.45449693	0.23871980
H	-2.74332541	-0.42176264	-1.55431072
N	-1.83738012	0.45310486	0.06917567
C	-3.91231427	-2.71259396	-0.47496274
H	-3.15049212	-4.54101161	-1.38488691
H	-2.31434619	-4.06025651	0.10218826
H	-4.20514307	-0.74364888	0.43232460
H	-2.95670984	-1.73679678	1.21626458
H	-1.59237672	0.35274627	1.05532577
C	-1.65225832	1.67200984	-0.50181822
H	-4.43081102	-2.40933837	-1.40089019
H	-4.65516408	-3.21973330	0.15999335
N	-1.19445398	2.61891753	0.36169186
H	-0.80969720	2.30990509	1.25941701
C	-0.73453671	3.95464176	-0.00774169
H	-0.68679744	-2.04825237	0.02316318
H	3.71944684	4.35879344	-0.04636820
H	1.52579548	6.36003018	-1.49229714
H	0.61419962	4.90501607	-1.97480247
H	2.38465348	4.90782819	-2.07614360
C	-1.70420540	5.08024729	0.52530851
C	-1.16006247	6.46733649	0.12253563
H	-1.85658716	7.24737552	0.46257429
H	-0.18040286	6.66790159	0.57757872
H	-1.06320527	6.55577555	-0.96846029
H	0.99140928	1.14478418	-2.63525601
H	1.53601389	-1.95221384	0.14299168
H	0.84167660	-0.58277354	1.01505663

TS4_12

E = -17406.24

G = -16977.39

Nimag = 1, 133i cm-1

C	2.18920497	0.95817769	-1.24194667
C	3.71807223	0.78681279	-1.10242441
H	1.85078885	1.88614103	-0.75665832
H	4.09074741	0.20572944	-1.95975810
C	4.18052068	0.02640772	0.15814502
C	1.36597436	-0.15917546	-0.64169063
C	1.91232970	-1.03945440	0.29037794
C	3.40036808	-1.28803235	0.29531325
H	5.24375805	-0.19575616	0.03040113
H	3.69994618	-1.81764484	1.20637827
H	3.67978880	-1.94530800	-0.54760931
H	1.28316544	-1.83412946	0.68230853
H	1.92620774	1.06349532	-2.30547445
H	4.20806944	1.76942074	-1.13832345
N	4.09082687	0.85258154	1.39462520
C	2.79006372	1.34510830	1.89194277
H	2.98436127	1.86470328	2.84045786
H	2.41769029	2.10803073	1.20186466
C	1.69411847	0.30911230	2.15784820
C	2.03114704	-0.79118773	3.13743236
C	0.42627870	0.90982174	2.10648344
H	0.30870053	1.90126867	1.68381310
N	-0.74587341	0.35338803	2.52984562
O	-0.86292823	-0.88559881	2.81417460
O	-1.80531709	1.12825804	2.58308873
S	-1.89909282	2.20743288	-2.34119352
H	-1.53129524	3.87891785	2.78274970
H	-2.00908215	4.60602053	-0.94972481
C	0.06290186	4.16481683	-0.39435493
N	0.05933529	-0.12036098	-0.93621833

H	-0.26129167	0.62422179	-1.57110959
C	-0.95573143	-1.11385065	-0.55065271
C	-0.79418902	-2.43950355	-1.32360799
C	-2.36756903	-0.52815317	-0.80588412
C	-1.86489451	-3.45155225	-0.88157619
H	-0.89222839	-2.22710210	-2.40158011
H	0.21532831	-2.84202567	-1.16059542
C	-3.44010480	-1.52708139	-0.34539400
H	-2.48141566	-0.33812228	-1.88196929
N	-2.54322879	0.76009112	-0.12863936
C	-3.28179760	-2.87840717	-1.06559459
H	-1.75297799	-4.38511806	-1.45375921
H	-1.70731133	-3.70275749	0.18150227
H	-4.43181062	-1.09287820	-0.54001469
H	-3.34953249	-1.67239224	0.74458910
H	-2.53346864	0.71774297	0.90443685
C	-2.14217257	1.95297614	-0.65345886
H	-3.47793999	-2.73674294	-2.14237903
H	-4.03387816	-3.58908686	-0.69090695
N	-1.96268794	2.93863937	0.26037605
H	-1.85756317	2.62108601	1.23263402
C	-1.44840577	4.26461870	-0.07790535
H	-0.85885057	-1.30886371	0.52938687
S	5.45470885	1.06099878	2.33595125
O	5.24737760	2.26226330	3.15531315
H	6.27897084	-1.68876199	1.94670766
O	6.61797937	0.94783895	1.44551971
C	-1.74288750	5.27750408	1.08510535
C	-1.17422196	6.65841017	0.69015386
H	-1.43502282	7.39775527	1.46062473
H	-0.07967930	6.63423452	0.59950985
H	-1.59490535	7.00166976	-0.26554670
C	-3.27725588	5.38878314	1.23687540
H	-3.73767180	5.73725306	0.30041990
H	-3.52148694	6.10950314	2.03051629
H	-3.72441609	4.42101807	1.50041252
C	-1.11837357	4.83347806	2.42716540
H	-0.03138668	4.72101765	2.34128298
H	-1.33814030	5.59147909	3.19334173
O	0.79394346	3.50639092	0.37731224
N	0.57174157	4.83875531	-1.45714027
C	-0.20148515	5.52442556	-2.49941805
C	2.02826008	4.83471221	-1.66391485
H	2.52512742	4.58691880	-0.72338234
H	2.34271198	5.82980942	-2.00338905
H	2.30521208	4.09300548	-2.42820045
H	-0.18098249	6.61344554	-2.34817707
H	-1.23092109	5.16761371	-2.52221299
H	0.25072284	5.29498310	-3.47350382
C	5.49522385	-0.34913600	3.45620453
C	5.03349365	-0.20207805	4.76733921
C	4.95879756	-1.32876817	5.59061209
C	5.33925337	-2.58315817	5.10323274
C	5.81541760	-2.71404042	3.79237263
C	5.90328431	-1.59513608	2.96266607
H	4.72925530	0.77641613	5.12989280
H	4.59619177	-1.22531699	6.61245550
H	5.26993317	-3.46027842	5.74541266
H	6.12226070	-3.68901699	3.41586246
H	3.05077422	-1.15182887	2.99724658
H	1.32767642	-1.62332675	3.07910820
H	1.97303149	-0.37031404	4.15538145

TS4_13

E = -17398.38

G = -16969.49

Nimag = 1, 397i cm-1

C	2.07014260	1.62731605	-0.19376629
C	3.03227511	2.01643379	0.94539108
H	1.02431922	1.80791791	0.10495276
H	4.00897632	2.24741964	0.50075403
C	3.29133955	0.89973253	1.97748986
C	2.17767431	0.18765022	-0.63252185
C	2.62714243	-0.81301212	0.28340297
C	3.71902814	-0.37778134	1.25328610
H	4.09883882	1.21963365	2.64489275
H	3.93059586	-1.17179787	1.97633178
H	4.64130044	-0.17814432	0.69049384
H	2.79093279	-1.79653463	-0.15086803
H	2.23975036	2.27645840	-1.06243546
H	2.66505453	2.92283592	1.43641219
N	2.13741242	0.55812140	2.86502898
C	0.88730132	0.06327349	2.24322790
H	0.21071959	-0.21339759	3.05955451
H	0.39013838	0.84863188	1.65915195
C	1.09096827	-1.20496363	1.38811986
C	1.60534741	-2.36488901	2.24939619
C	-0.08029836	-1.41656730	0.57453774
H	-0.67067604	-0.57218150	0.23471522
N	-0.55479447	-2.61019946	0.12902996
O	-1.66006308	-2.61528264	-0.55810288
O	0.06173322	-3.71738897	0.35187537
S	5.51360393	0.72017866	-1.63920193
H	4.36730247	3.94835976	-5.53671232
H	5.44258242	3.22742526	-1.97388447
C	3.49807918	4.23822871	-2.14271945
N	1.61308044	-0.08745274	-1.80875089
H	1.19810328	0.72206447	-2.27612101
C	1.90314512	-1.20664795	-2.75858206
C	1.38251561	-2.58456411	-2.33630044
C	3.41350470	-1.20072330	-3.11655600
C	1.72461052	-3.63509772	-3.40692612
H	1.81851917	-2.89564572	-1.38081114
H	0.29731244	-2.52300466	-2.18816367
C	3.73754994	-2.29181936	-4.14942185
H	4.01085300	-1.35836462	-2.21027993
N	3.77714138	0.12824850	-3.62465786
C	3.23595715	-3.67049347	-3.68817407
H	1.36888503	-4.61947798	-3.06819919
H	1.18541940	-3.39969390	-4.34093391
H	4.82455112	-2.29614753	-4.31874121
H	3.25707659	-2.02878382	-5.10771098
H	3.22547869	0.44991494	-4.42427171
C	4.46293596	1.08516003	-2.93475455
H	3.77289629	-3.96763246	-2.77075443
H	3.46814711	-4.42361040	-4.45613704
N	4.27174965	2.34766913	-3.41087302
H	3.40985215	2.51226677	-3.93903257
C	4.74939170	3.56320620	-2.74754898
H	1.35280590	-0.91629098	-3.66715470
S	1.99973504	1.40699154	4.30423397
O	3.34254631	1.48669492	4.89109532
H	-0.51810802	2.49524745	3.37529029
O	0.88738526	0.80394137	5.04871233
C	5.53646398	4.47917471	-3.75414182
C	5.98883040	5.77140444	-3.04340533
H	6.56496862	6.39156915	-3.74490887
H	5.13145354	6.36451741	-2.69608146
H	6.63457667	5.55023842	-2.18294347
C	6.77977574	3.68760033	-4.21627986
H	7.43007667	3.44794327	-3.36252308
H	7.35771817	4.28503277	-4.93593320
H	6.48761569	2.74640645	-4.70086145
C	4.66749151	4.84489285	-4.97624175
H	3.76093121	5.38643319	-4.67637558
H	5.24736014	5.48539804	-5.65643349
O	2.42606271	4.17692034	-2.78621604
N	3.58266864	4.84718124	-0.92941552
C	4.77097666	4.93127972	-0.07175444
C	2.39851925	5.53051696	-0.38670174
H	2.09886410	5.05744579	0.55591894
H	1.58383276	5.46225432	-1.10965536
H	2.63943158	6.58462746	-0.18802968
H	5.18007416	5.95163111	-0.08028972
H	5.54534553	4.23320811	-0.38839715
H	4.47990304	4.68018324	0.95647497
C	1.51570991	3.07936626	3.83692601
C	2.46211824	4.10941589	3.86819498
C	2.09372018	5.38182035	3.42371711
C	0.79870911	5.61339721	2.94775055

C	-0.13875115	4.57434303	2.92198020
C	0.21279689	3.30002873	3.37300813
H	3.46699675	3.91134734	4.23277142
H	2.82165505	6.19179081	3.44626134
H	0.51850707	6.60513067	2.59538492
H	-1.14879945	4.75641381	2.55744950
H	2.27592608	-1.98440708	3.02648840
H	2.11422414	-3.13000005	1.65810670
H	0.74407970	-2.84455775	2.73424930

TS4_14

E = -17401.14

G = -16972.55

Nimag = 1, 166i cm-1

C	1.45430843	1.37579955	0.13530378
C	2.33274308	1.94405780	1.27509578
H	0.38937811	1.50213592	0.38831278
H	3.26837625	2.32808740	0.84111185
C	2.77496475	0.93515489	2.36092245
C	1.66635571	-0.08373605	-0.16804250
C	2.37941476	-0.89806869	0.71220725
C	3.37167757	-0.30044411	1.67724817
H	3.55260913	1.40809081	2.97018605
H	3.67467358	-1.03713170	2.43013049
H	4.28850738	0.00318272	1.14302674
H	2.54578213	-1.93080713	0.40224124
H	1.60881297	1.97972306	-0.76816050
H	1.81844125	2.80384593	1.71742309
N	1.73281409	0.48150267	3.34206334
C	0.47157100	-0.09176592	2.83045495
H	-0.17264698	-0.30688770	3.69179909
H	-0.06365074	0.63333329	2.20308992
C	0.64195562	-1.40133189	2.06109454
C	1.32744684	-2.52887975	2.79683166
C	-0.45984004	-1.60025017	1.22009904
H	-1.20488935	-0.83004553	1.16508316
N	-0.70766120	-2.64507276	0.38497859
O	0.13671759	-3.59011901	0.20125485
O	-1.83700644	-2.63375769	-0.28049765
S	-2.34875951	2.50295009	0.25811983
H	-4.89940287	-2.16930014	0.86500798
H	-4.29278288	1.50154495	1.67314346
C	-3.28449814	0.19960683	3.11395565
N	0.95204158	-0.68015808	-1.14576293
H	1.12743848	-1.68399716	-1.23952462
C	0.25589530	-0.10235874	-2.31822690
C	1.24231471	0.56173571	-3.30374817
C	-0.91713274	0.84479806	-1.98570129
C	0.52603814	1.01104293	-4.58896352
H	1.70904624	1.43267107	-2.81895813
H	2.04462897	-0.15545206	-3.53114119
C	-1.63144643	1.26208512	-3.28857934
H	-0.55453111	1.75477861	-1.49685678
N	-1.84092250	0.19608338	-1.05924557
C	-0.65866289	1.93805747	-4.26801766
H	1.24492493	1.51528922	-5.25244823
H	0.15701019	0.12114823	-5.12724410
H	-2.45604780	1.93764142	-3.01891252
H	-2.07418997	0.36463480	-3.75282078
H	-1.91446576	-0.83220803	-1.09095404
C	-2.52371917	0.82816916	-0.07372973
H	-0.28146322	2.87317933	-3.81881704
H	-1.18942664	2.21533671	-5.19141523
N	-3.33294488	0.00995349	0.65695882
H	-3.20049378	-0.99838885	0.53065476
C	-4.09896454	0.43907106	1.82183789
H	-0.17704376	-0.98322494	-2.81831516
S	1.59315999	1.41097201	4.74410078
O	2.94975386	1.61601199	5.26596769
H	-0.96383863	2.22432072	3.60329029
O	0.56257871	0.77644910	5.57413575
C	-5.49046403	-0.29347730	1.85992808
C	-6.23950603	0.10511715	3.14955281
H	-7.23681703	-0.35753542	3.15342293
H	-5.70686253	-0.23335490	4.04902363
H	-6.37322220	1.19374418	3.21085438
C	-6.29719393	0.18552361	0.63235271
H	-6.47666021	1.26978166	0.68232670
H	-7.27068107	-0.32473353	0.59963807
H	-5.75958782	-0.03276847	-0.30031989
C	-5.33679144	-1.82983671	1.81483514
H	-4.70279991	-2.18859593	2.63442543
H	-6.32923448	-2.29574575	1.90127883
O	-2.71625283	-0.89640526	3.27923878
N	-3.24939808	1.19283315	4.05491948
C	-3.84755441	2.52786603	3.91173005
C	-2.75606670	0.88059616	5.40578355
H	-1.94330749	1.56355836	5.68095416
H	-2.38321752	-0.14494933	5.41701779
H	-3.57811428	0.99084166	6.12945415
H	-4.88538213	2.54733746	4.27554251
H	-3.80669316	2.86231096	2.87276383
H	-3.25758197	3.22910322	4.51443602
C	0.97903590	3.00728968	4.17621583
C	1.83904284	4.11037148	4.18058772
C	1.40650733	5.30990330	3.60905208
C	0.13535909	5.39481745	3.03049255
C	-0.71607605	4.28405970	3.03616399
C	-0.30307628	3.08422160	3.61569085
H	2.83288370	4.02051120	4.61169918
H	2.06928142	6.17424709	3.60591531
H	-0.19165684	6.32655403	2.57051447
H	-1.69878676	4.34278056	2.57541766
H	2.19872379	-2.17053054	3.35263805
H	1.60932169	-3.34109962	2.12255199
H	0.60832245	-2.92970088	3.53153367

TS4_15

E = -17401.14

G = -16972.69

Nimag = 1, 186i cm-1

C	2.03199191	0.98389975	-1.49723126
C	3.52640425	0.61834661	-1.33194888
H	1.83921187	1.99946863	-1.10961544
H	3.81062524	-0.05529214	-2.15237269
C	3.88484648	-0.13144970	-0.03513163
C	1.07080185	0.06852899	-0.78326365
C	1.51444169	-0.84023456	0.20207283
C	2.94198443	-1.32642047	0.14030271
H	4.91469372	-0.48049204	-0.15250678
H	3.20223047	-1.89487827	1.04017800
H	3.06698468	-2.00769474	-0.71087245
H	0.76705637	-1.55687142	0.54478227
H	1.79165737	1.03153830	-2.56672017
H	4.13849435	1.52566124	-1.42107804
N	3.87970887	0.72570792	1.18580991
C	2.63016550	1.34197535	1.67896835
H	2.86564729	1.82379836	2.63579942
H	2.36202923	2.14598170	0.98047163
C	1.42383827	0.40969390	1.87163715
C	1.59447417	-0.65237683	2.94968315
C	0.21014112	1.15871345	1.84083646
H	0.21052593	2.22646540	1.64616960
N	-1.04617033	0.64106069	1.99268159
O	-1.24533027	-0.63645787	1.91314215
O	-2.04225016	1.44255269	2.15451596
S	-0.67996849	-2.75872472	-2.31369886
H	2.21718464	-2.38494831	-6.40506943
H	1.54292419	-3.79513177	-2.96257666
C	3.50650956	-2.83139319	-3.20583730
N	-0.23825711	0.30350391	-0.85932364
H	-0.83295335	-0.33132858	-0.31090183
C	-0.94438372	1.13417404	-1.83664131
C	-2.14447349	1.82996585	-1.17714660
C	-1.41066886	0.25170371	-3.03229123
C	-2.91201407	2.67666540	-2.20611980
H	-2.81057226	1.06247640	-0.74887263
H	-1.79099818	2.44403051	-0.33810186
C	-2.16194852	1.10735638	-4.06340067
H	-2.07532054	-0.52967592	-2.63916499

N	-0.28208221	-0.43641253	-3.65281986
C	-3.35542908	1.82978372	-3.41248165
H	-3.78592644	3.13862322	-1.72285244
H	-2.26381143	3.49905255	-2.55487956
H	-2.49745043	0.45786833	-4.88541467
H	-1.46664974	1.85111056	-4.49118552
H	0.26476532	0.10766709	-4.32238657
C	0.17751429	-1.68041085	-3.32613569
H	-4.09083799	1.07825433	-3.07866763
H	-3.85625139	2.46239188	-4.16059618
N	1.37082002	-1.98789755	-3.90249207
H	1.93592787	-1.23478015	-4.30149475
C	2.10747608	-3.23392051	-3.70973156
H	-0.24679281	1.89562023	-2.20829107
S	5.25343619	0.68126921	2.13863394
O	5.01679208	1.56463469	3.28737404
H	6.52759709	-1.68222010	1.03705740
O	6.40837802	0.88951690	1.25326667
C	2.15949880	-4.09348635	-5.02984517
C	2.97903589	-5.37633364	-4.77661970
H	2.98492365	-5.99348745	-5.68641004
H	4.02261794	-5.14731051	-4.51896818
H	2.54193511	-5.97662518	-3.96699382
C	0.70944151	-4.47874829	-5.39589699
H	0.24051201	-5.05912040	-4.58956190
H	0.70830093	-5.08606479	-6.31261597
H	0.09668858	-3.58467483	-5.57255013
C	2.78877506	-3.29961039	-6.19360698
H	3.82604945	-3.01656963	-5.97459506
H	2.77911464	-3.91888354	-7.10225139
O	4.05917301	-1.83268260	-3.71619057
N	4.09159323	-3.55666983	-2.21231849
C	3.51710723	-4.71624475	-1.51863237
C	5.45497869	-3.21021231	-1.78267891
H	5.72634966	-2.23765875	-2.19732471
H	6.16915845	-3.97169079	-2.12997688
H	5.48328087	-3.17623062	-0.68707749
H	4.06004585	-5.63219402	-1.79160007
H	2.46199523	-4.84434689	-1.75536985
H	3.61138701	-4.56100095	-0.43480004
C	5.37545166	-1.01485290	2.73861076
C	4.76257136	-1.36029018	3.94735935
C	4.76628833	-2.69674605	4.35307515
C	5.37437628	-3.67330802	3.55614919
C	6.00569533	-3.31163241	2.36053491
C	6.01825568	-1.97718333	1.94996467
H	4.29021264	-0.59461680	4.55648656
H	4.28956303	-2.97496659	5.29192867
H	5.36488372	-4.71567392	3.87201281
H	6.49919339	-4.06809604	1.75194091
H	2.45378095	-1.29890548	2.76416258
H	0.69271015	-1.26539289	3.03462675
H	1.76862646	-0.14083866	3.90988794

TS4_16
E = -17402.15
G = -16974.21
Nimag = 1, 369i cm-1

C	1.85333379	0.96934828	-1.46700174
C	3.39208633	0.85361739	-1.46440176
H	1.53818239	1.87559080	-0.92742654
H	3.70433958	0.26042017	-2.33731308
C	3.97117047	0.15225931	-0.22058162
C	1.13180186	-0.19332823	-0.81705542
C	1.77450841	-1.00313664	0.15512182
C	3.27269825	-1.19601837	-0.00980658
H	5.03762850	-0.00658066	-0.40373937
H	3.66853588	-1.70154346	0.88074382
H	3.48537403	-1.84398346	-0.87532416
H	1.23250706	-1.89465276	0.47038345
H	1.48647711	1.09396641	-2.49569229
H	3.84082017	1.85026753	-1.56884150
N	3.88260490	1.01154305	0.99554183
C	2.58057431	1.22025848	1.66538659
H	2.76735930	1.73340026	2.61635910
H	1.99296952	1.91910266	1.06587789
C	1.71794340	-0.02096538	1.92876622
C	0.27164361	0.40747360	2.12312820
C	2.28866254	-0.97028604	2.83133323
H	3.31112272	-0.89822047	3.17153148
N	1.68574795	-2.14089656	3.19969664
O	0.54669626	-2.49431945	2.69605820
O	2.28921274	-2.90978185	4.04375633
S	-1.98150826	2.16041644	-2.10408696
H	-2.96632963	4.55956447	2.30455309
H	-1.08050148	4.17317572	-0.94103655
C	0.21851711	4.11614991	0.82738931
N	-0.15619034	-0.30580074	-1.13807764
H	-0.54807186	0.40119536	-1.78359724
C	-1.14301138	-1.23195877	-0.55895627
C	-1.20866671	-2.56130905	-1.33357139
C	-2.53434543	-0.54231655	-0.54882733
C	-2.25237293	-3.49492108	-0.69669025
H	-1.47319687	-2.34773650	-2.38254568
H	-0.21187087	-3.02605198	-1.33306090
C	-3.57254007	-1.46907107	0.10025169
H	-2.82971840	-0.32671167	-1.58457792
N	-2.49330326	0.74825499	0.15260253
C	-3.63520126	-2.82222743	-0.63178858
H	-2.31059721	-4.43219387	-1.26997576
H	-1.92412628	-3.75879856	0.32312881
H	-4.55203411	-0.96928017	0.08462180
H	-3.29984539	-1.63205103	1.15754790
H	-2.49313441	0.68939584	1.17284198
C	-2.11010369	1.93207481	-0.40092019
H	-4.00900217	-2.65817018	-1.65674070
H	-4.35692062	-3.48037291	-0.12568187
N	-1.85459224	2.92678544	0.48832962
H	-1.76264798	2.67341036	1.47565600
C	-1.16335307	4.17459725	0.14512540
H	-0.84786861	-1.43965768	0.47708542
S	5.28487108	1.43780216	1.79661223
O	4.97811067	2.62078515	2.60956217
H	6.29022643	-1.24386000	1.34575018
O	6.35344140	1.47229249	0.78825341
C	-1.99507054	5.44219359	0.54591938
C	-1.16529441	6.70032744	0.21312191
H	-1.74363530	7.60210677	0.45977629
H	-0.23006574	6.73168752	0.78992573
H	-0.91755745	6.74031166	-0.85706204
C	-3.28368676	5.43239238	-0.30553526
H	-3.04614389	5.45394102	-1.37862223
H	-3.89635613	6.31340352	-0.06588510
H	-3.87903770	4.53114982	-0.10465124
C	-2.36663247	5.44319859	2.04328198
H	-1.47253025	5.45556730	2.67786698
H	-2.97132831	6.33436839	2.26619151
O	0.28014240	3.80397580	2.03334251
N	1.32619687	4.38649273	0.07626182
C	1.32383104	4.72140841	-1.35768029
C	2.63127547	4.53488176	0.74418473
H	2.51005374	4.34115823	1.81062789
H	3.00873893	5.55611288	0.58854727
H	3.35313925	3.82286761	0.32487504
H	1.20009332	5.80198039	-1.51786626
H	0.54154233	4.17733483	-1.89238636
H	2.29103874	4.41757192	-1.77549914
C	5.63528097	0.08242935	2.92844427
C	5.36878988	0.23834355	4.29227499
C	5.52172607	-0.86068254	5.14248453
C	5.92932954	-2.09505361	4.62921211
C	6.20972148	-2.23286011	3.26429375
C	6.06908011	-1.14260027	2.40523074
H	5.03414755	1.19973918	4.67336217
H	5.30902133	-0.75193985	6.20504501
H	6.02896988	-2.95316077	5.29223877
H	6.53503808	-3.19311880	2.86642397
H	0.23489636	1.14793926	2.93752389
H	-0.36028940	-0.44354271	2.38383368
H	-0.10566600	0.90262517	1.22548671

TS4_17
E = -17395.48
G = -16965.96
Nimag = 1, 433i cm-1

C	1.99013386	0.37463373	-1.68729410
C	3.50411258	0.08300925	-1.68302032
H	1.79864485	1.39920427	-1.33095950
H	3.69471279	-0.74650564	-2.37656423
C	4.04544720	-0.35665993	-0.31290048
C	1.18402795	-0.58385079	-0.83440718
C	1.77307944	-1.22539959	0.28981418
C	3.25105901	-1.56642045	0.18333083
H	5.09624055	-0.63013710	-0.44490310
H	3.61525150	-1.89668725	1.16455708
H	3.38710362	-2.39341842	-0.52729231
H	1.17183960	-1.99063597	0.77514298
H	1.61184642	0.34113648	-2.71863034
H	4.05292633	0.96490295	-2.03538072
N	4.02550041	0.76074826	0.67819198
C	2.74853389	1.19428314	1.29137505
H	2.98768659	1.85395285	2.13463067
H	2.20588617	1.81358309	0.56798425
C	1.81477863	0.08102826	1.79602410
C	0.39904179	0.61802524	1.94714604
C	2.38159926	-0.66807977	2.88033154
H	3.41237402	-0.54405991	3.17715537
N	1.77186170	-1.70681926	3.52229156
O	0.62144071	-2.15339845	3.13329464
O	2.37941800	-2.26054473	4.51902476
S	2.32243649	-3.55007218	-2.67787024
H	-0.06128228	-2.01760315	-7.06097607
H	2.99288167	-2.46172660	-4.85864329
C	2.41548954	-0.37226119	-5.21697124
N	-0.11193808	-0.66732714	-1.16723483
H	-0.39098572	-0.06401020	-1.94249537
C	-1.10223889	-1.73758440	-0.86796309
C	-1.55964114	-1.82826844	0.59647636
C	-0.60017531	-3.09494989	-1.43216584
C	-2.61105583	-2.94020349	0.75915888
H	-0.71441567	-2.03806777	1.25932258
H	-1.97488788	-0.85551453	0.89428030
C	-1.64516628	-4.20010306	-1.21232563
H	0.34319894	-3.37436122	-0.94835886
N	-0.30144840	-2.93228268	-2.85981843
C	-2.06717629	-4.29063948	0.26330183
H	-2.90144909	-3.00813252	1.81823859
H	-3.52032498	-2.68101028	0.18923196
H	-1.22319380	-5.15164968	-1.56825043
H	-2.53043049	-3.98056307	-1.83426957
H	-1.06713178	-2.54640238	-3.41850424
C	0.94736105	-2.84813873	-3.40492172
H	-1.19733692	-4.58139814	0.87688858
H	-2.82571342	-5.07867504	0.38333238
N	0.97670853	-2.20728281	-4.60767127
H	0.22432369	-1.53839220	-4.79155273
C	2.19872259	-1.89489951	-5.34727813
H	-1.98037491	-1.44680572	-1.46606054
S	5.46405127	1.28099343	1.34390351
O	5.23983127	2.63396919	1.87034444
H	6.34311633	-1.47365886	1.50182810
O	6.51055244	1.02414230	0.34445598
C	2.09334238	-2.38410381	-6.83888076
C	3.38641732	-2.02451321	-7.59971597
H	3.32148064	-2.40219673	-8.63021964
H	3.53991585	-0.93772305	-7.64817329
H	4.26707345	-2.48240267	-7.12915047
C	1.93215307	-3.92025017	-6.80590990
H	2.80022013	-4.39412676	-6.32505520
H	1.84785759	-4.30948697	-7.83074361
H	1.03040139	-4.20864451	-6.24924348
C	0.88294869	-1.74926908	-7.55542358
H	0.96137186	-0.65471347	-7.58216989
H	0.83530858	-2.12122075	-8.58920613
O	1.40909530	0.37220304	-5.22765539
N	3.68005940	0.11291715	-5.09942551
C	4.90850826	-0.67826493	-4.95981819
C	3.89553347	1.56762826	-5.10040604
H	2.94090967	2.06937650	-5.26720781
H	4.60502645	1.83004000	-5.89784328
H	4.31746068	1.88390635	-4.13666939
H	5.51431058	-0.61461441	-5.87483290
H	4.69057973	-1.72423815	-4.74622450
H	5.49353749	-0.27098325	-4.12395983
C	5.77388912	0.20196290	2.75100380
C	5.53649317	0.67033888	4.04719200
C	5.65724963	-0.21670636	5.12073893
C	6.00475357	-1.55132302	4.89488599
C	6.25533929	-2.00344916	3.59375421
C	6.14638246	-1.12759810	2.51337553
H	5.25064805	1.70694798	4.20610831
H	5.46721889	0.13635532	6.13337389
H	6.08012606	-2.24248006	5.73296410
H	6.53378360	-3.04174167	3.41880993
H	0.44190177	1.52065139	2.57864550
H	-0.24814388	-0.11428510	2.43164695
H	-0.03497426	0.90721030	0.98253431

TS4_18
E = -17396.58
G = -16968.24
Nimag = 1, 369i cm-1

C	1.63379431	3.89338557	-1.31105280
C	1.53646352	5.26126941	-0.60227614
H	0.88098336	3.20902551	-0.88411759
H	1.88483393	6.05073338	-1.28555841
C	2.39100106	5.36229931	0.67149695
C	2.97245082	3.21442840	-1.20615295
C	3.90735201	3.58468951	-0.19983948
C	3.84204430	5.00434434	0.32686838
H	2.34084165	6.39251321	1.03481985
H	4.48650577	5.09358541	1.21129867
H	4.21021666	5.72138112	-0.42410035
H	4.91281195	3.17000858	-0.31665912
H	1.35516519	4.00902852	-2.36453563
H	0.48416425	5.46896332	-0.36603320
N	1.86199038	4.51019491	1.77736064
C	2.02056366	3.03416807	1.76883402
H	1.71228371	2.65994232	2.75098186
H	1.31834999	2.59543885	1.05036263
C	3.44560256	2.54279194	1.47953192
C	3.47835300	1.10103870	1.01329443
C	4.39835892	2.98721477	2.44705920
H	4.13970285	3.70649126	3.20896544
N	5.73596620	2.70688910	2.42133470
O	6.26551541	2.05272628	1.44024516
O	6.47529447	3.13669227	3.38983878
S	-0.95294096	1.47206056	-0.26820780
H	0.02821269	-3.38615342	0.77982130
H	-0.86427518	0.12531440	1.85478415
C	0.94973262	-0.63395584	2.83186160
N	3.24660175	2.15642264	-1.98562159
H	4.16544999	1.73692400	-1.83262924
C	2.46994394	1.51029701	-3.06948953
C	2.41049067	2.37204853	-4.35025046
C	1.05632614	1.02142938	-2.66297048
C	1.76444984	1.58576013	-5.50422522
H	1.82469964	3.28287960	-4.16042905
H	3.43223942	2.68593377	-4.60832649
C	0.42045145	0.23883818	-3.83027413
H	0.41047381	1.87018338	-2.42415867
N	1.12097260	0.20144143	-1.45250159
C	0.36399096	1.08463303	-5.11323307
H	1.71029627	2.22544905	-6.39783482
H	2.40400497	0.72366876	-5.76019335
H	-0.58668658	-0.07568671	-3.51919000
H	1.01203269	-0.67517048	-4.01081588
H	1.71753884	-0.62714455	-1.51426743
C	0.23386517	0.24780112	-0.41720716
H	-0.30203893	1.94909764	-4.94929349

H	-0.07317754	0.49083401	-5.93003296
N	0.38948235	-0.74955799	0.49587029
H	1.24594816	-1.30905704	0.44850877
C	-0.21715202	-0.75209916	1.83109941
H	3.06348463	0.61383826	-3.30741606
S	1.16231085	5.22120845	3.11161427
O	0.05466758	4.36742215	3.56362576
H	3.54939528	6.79334644	3.53788284
O	0.93051530	6.63380992	2.78139217
C	-1.11241022	-2.02029156	2.06265163
C	-1.64753612	-2.00133501	3.51038970
H	-2.30540382	-2.86724186	3.67209379
H	-0.83057487	-2.05607568	4.24386363
H	-2.23289096	-1.09271006	3.70846275
C	-2.29613352	-1.93989900	1.07410941
H	-2.90901314	-1.04802318	1.26701529
H	-2.93248963	-2.83069172	1.17883082
H	-1.93654726	-1.88976836	0.03733150
C	-0.32442874	-3.32467788	1.81925473
H	0.54444168	-3.39753575	2.48490973
H	-0.98242355	-4.18667440	2.00220179
O	1.96922772	-1.33498195	2.64852009
N	0.86607933	0.25206449	3.85820038
C	-0.28925269	1.09675760	4.19426428
C	2.02230992	0.36285910	4.76913471
H	2.77853437	1.04864113	4.35911127
H	2.48218442	-0.62072658	4.90493910
H	1.67319162	0.74913051	5.73175210
H	-0.71670156	0.77761044	5.15545051
H	-1.06121495	1.03814507	3.42868342
H	0.02481965	2.14305422	4.26909302
C	2.44113810	5.13257059	4.37453924
C	2.39631175	4.11733132	5.33393723
C	3.47740444	3.95752191	6.20541938
C	4.58142064	4.80963980	6.11665550
C	4.60347482	5.83885633	5.16706257
C	3.53319159	6.00649756	4.28875111
H	1.53161519	3.46477466	5.39323359
H	3.45787053	3.16095260	6.94795381
H	5.42914851	4.67222363	6.78614308
H	5.46283086	6.50446808	5.10219638
H	3.20870983	0.43856242	1.84629086
H	4.48137506	0.82517515	0.67455796
H	2.75814281	0.93157821	0.21069165

TS4_19

E = -17398.20

G = -16971.95

Nimag = 1, 279i cm-1

C	1.56765281	0.47348188	0.40120588
C	1.84586461	0.77111668	1.89284757
H	1.29971735	-0.58745495	0.26305168
H	1.58599751	1.81932507	2.09602923
C	3.31196371	0.60446111	2.32451815
C	2.71805918	0.77758534	-0.52701217
C	4.04146759	0.90505336	-0.04309919
C	4.22523277	1.39283925	1.37777110
H	3.39232901	1.01024080	3.33642812
H	5.27670586	1.27956052	1.67453801
H	3.97302983	2.45761776	1.44624066
H	4.77024501	1.27397641	-0.76962106
H	0.68228225	1.04003465	0.08868748
H	1.20095981	0.14078271	2.51927588
N	3.73722033	-0.82174185	2.41258418
C	3.91374219	-1.62682406	1.18577793
H	4.33691085	-2.59421060	1.48273223
H	2.92247643	-1.83696474	0.76558631
C	4.79674735	-1.00112694	0.09706268
C	4.51581934	-1.60790028	-1.26578099
C	6.13941670	-0.77418590	0.51766622
H	6.43060314	-0.87588297	1.55274150
N	7.12666692	-0.22252454	-0.25253953
O	6.88787579	0.19250842	-1.45088475
O	8.30813726	-0.09962805	0.25669081
S	3.18903492	4.06735715	-2.18628115
H	-0.25617154	6.22609076	0.82638543
H	3.31919889	5.28242745	0.02390053
C	2.59985876	4.62696991	1.99614825
N	2.50326782	0.80369198	-1.84781442
H	3.29283087	1.11826043	-2.41880024
C	1.22371423	0.74036443	-2.55457569
C	1.33316293	-0.14898111	-3.80480804
C	0.76886800	2.17573582	-2.94950678
C	-0.01328372	-0.19686935	-4.54895999
H	2.11459286	0.26158726	-4.46682031
H	1.65146770	-1.15764127	-3.50443674
C	-0.58747979	2.12264517	-3.66797506
H	1.52731947	2.60013733	-3.62184510
N	0.71023344	3.05207047	-1.78305439
C	-0.50947617	1.21490846	-4.90941346
H	0.08960236	-0.80829199	-5.45774418
H	-0.76071959	-0.69458859	-3.90760326
H	-0.88112832	3.14476535	-3.94923613
H	-1.35256259	1.73642758	-2.97170416
H	-0.15836290	3.03984443	-1.24597857
C	1.73251859	3.82914820	-1.31921914
H	0.18089658	1.66782510	-5.64109622
H	-1.49811005	1.15964033	-5.38908945
N	1.47509657	4.41477881	-0.11899177
H	0.71091991	4.04939020	0.45419368
C	2.40073167	5.27574747	0.61330709
H	0.47962162	0.30615797	-1.87619388
S	4.21390623	-1.39370484	3.90421234
O	4.43356983	-2.83904968	3.76643294
H	4.91773517	1.17026298	5.06768739
O	3.27289850	-0.86145703	4.90005288
C	1.86973622	6.75661894	0.70531695
C	2.87413359	7.61409310	1.50381565
H	2.52132032	8.65478839	1.53835092
H	2.97810294	7.25924359	2.53858692
H	3.86616248	7.61118766	1.03156907
C	1.76178308	7.30422416	-0.73482992
H	2.73853854	7.28498960	-1.23755625
H	1.40016364	8.34241083	-0.71001787
H	1.05878565	6.70796074	-1.33179244
C	0.48510987	6.81627044	1.38348526
H	0.52387828	6.43931413	2.41325748
H	0.13592797	7.85888398	1.40524999
O	1.60888965	4.11726821	2.56304123
N	3.84300116	4.61831046	2.55194943
C	5.08293400	5.10745259	1.93593307
C	4.02642119	4.05476718	3.89707587
H	4.78184774	3.25972757	3.85340869
H	3.07576739	3.65057170	4.24936892
H	4.37967152	4.83588029	4.58573186
H	5.45234647	5.99125133	2.47476794
H	4.93943350	5.36400171	0.88766562
H	5.84302795	4.31560782	1.99638835
C	5.80518955	-0.61251294	4.22854042
C	6.98226066	-1.27824425	3.86995790
C	8.20472058	-0.61677010	4.00482715
C	8.24648613	0.69237089	4.49554620
C	7.06472831	1.33855038	4.87650304
C	5.83671876	0.68627869	4.75097866
H	6.93826287	-2.29427007	3.48543517
H	9.12376235	-1.12342680	3.71583071
H	9.20152717	1.20754348	4.58908889
H	7.09962935	2.34983207	5.27934711
H	4.88156909	-2.64767881	-1.26789564
H	5.03578874	-1.06196612	-2.05744097
H	3.44137198	-1.63200212	-1.47901557

TS4_20

E = -17403.47

G = -16974.37

Nimag = 1, 359i cm-1

C	-3.28102627	1.55877090	0.97202027
C	-1.74836289	1.42430874	1.04122166
H	-3.56925582	2.58724037	0.69799044
H	-1.50747907	0.58642717	1.70675679

C	-1.08753841	1.10322730	-0.31102270
C	-3.94155799	0.63006538	-0.01635967
C	-3.22056928	0.09072010	-1.11462080
C	-1.73597187	-0.14574822	-0.91311357
H	-0.02750229	0.91691282	-0.12514947
H	-1.25853817	-0.41176672	-1.86166607
H	-1.56255942	-0.99316102	-0.23695423
H	-3.73278463	-0.66781049	-1.70262230
H	-3.71450994	1.36777885	1.96471860
H	-1.31016113	2.33403666	1.47198664
N	-1.14160369	2.25526800	-1.25776331
C	-2.41925546	2.68690793	-1.87682827
H	-2.17014798	3.38805112	-2.68293403
H	-2.98370957	3.26501171	-1.13450975
C	-3.31102356	1.57960932	-2.46743393
C	-2.68576503	0.87679004	-3.67354101
C	-4.65916535	2.05407278	-2.58270527
H	-4.97210713	2.97483336	-2.10138966
N	-5.67044227	1.41591537	-3.23344921
O	-5.53166135	0.20405738	-3.66060605
O	-6.80125491	2.03005750	-3.38898012
S	-4.69866727	-1.15635996	3.06904715
H	0.44002065	-3.39654494	4.14420073
H	-2.25708127	-1.78106101	3.47935369
C	-0.59023457	-2.02929599	2.05867850
N	-5.26402326	0.53855347	0.08617251
H	-5.68701406	1.01600452	0.88759446
C	-6.12932481	-0.46765128	-0.54384972
C	-7.55098487	0.08592645	-0.72176175
C	-6.16489228	-1.75511347	0.33066830
C	-8.44657199	-0.96995876	-1.39260264
H	-7.95925628	0.35259845	0.26914235
H	-7.50986302	0.99453452	-1.33594637
C	-7.03624305	-2.82029040	-0.35596625
H	-6.59781899	-1.49259043	1.30538643
N	-4.82795268	-2.27350762	0.60480662
C	-8.46102345	-2.28794628	-0.59808955
H	-9.46886298	-0.57569573	-1.49406593
H	-8.06634879	-1.15231961	-2.41136222
H	-7.05731357	-3.72083209	0.27549807
H	-6.57383596	-3.09923287	-1.31891450
H	-4.40711547	-2.84967916	-0.12620338
C	-4.10792677	-2.06776278	1.74440110
H	-8.94889492	-2.12058936	0.37742397
H	-9.05314147	-3.04860127	-1.12896116
N	-2.88523933	-2.66421870	1.74266717
H	-2.52685059	-3.05180775	0.86663870
C	-1.86338947	-2.51979612	2.77855702
H	-5.72355507	-0.69751344	-1.53602697
S	0.29477649	2.85702182	-1.86156611
O	0.02898494	4.21119842	-2.36305477
H	1.48414092	0.22465733	-2.05693793
O	1.32113139	2.61590754	-0.83792032
C	-1.63168799	-3.86433395	3.56731385
C	-2.94960741	-4.22399632	4.28678577
H	-2.82079886	-5.16297459	4.84475658
H	-3.24289615	-3.43374308	4.99110187
H	-3.76773738	-4.35850869	3.56689092
C	-1.23788096	-5.01390513	2.61602590
H	-2.01970397	-5.19217756	1.86423143
H	-1.11430148	-5.93897473	3.19777221
H	-0.29728801	-4.80103877	2.09309390
C	-0.51815683	-3.65653573	4.61552083
H	-0.78374136	-2.86444663	5.32915721
H	-0.37150581	-4.58604734	5.18421610
O	-0.30562335	-2.53153146	0.94965696
N	0.16330302	-1.04746436	2.62601351
C	-0.08286535	-0.39084916	3.91595856
C	1.39981005	-0.61724849	1.95448751
H	2.27370384	-0.88849789	2.56482743
H	1.38476941	0.47354951	1.82773498
H	1.46328337	-1.10824681	0.98201698
H	0.03474302	0.69337420	3.78542315
H	0.64313694	-0.73514262	4.66639000
H	-1.09078430	-0.58589811	4.28069538
C	0.68959902	1.82307440	-3.28089886
C	0.36494927	2.26488473	-4.56688915
C	0.54883282	1.39850172	-5.64757974
C	1.04826458	0.10903393	-5.43920727
C	1.38802205	-0.31461660	-4.14792115
C	1.21490196	0.54311497	-3.06074420
H	-0.03507430	3.26485650	-4.71354764
H	0.29393770	1.73122780	-6.65291209
H	1.18017751	-0.56606225	-6.28371036
H	1.79002107	-1.31408654	-3.98723932
H	-1.63742895	0.63166750	-3.49914506
H	-3.24027235	-0.02478217	-3.94185428
H	-2.72283466	1.57052240	-4.52731519

TS4_21

E = -17390.22

G = -16963.33

Nimag = 1, 115i cm-1

C	-4.64671863	1.62656614	1.10500226
C	-3.15447564	1.76807234	1.46555854
H	-4.96514599	2.46738641	0.47186189
H	-2.95832257	1.20232239	2.38932898
C	-2.20185231	1.20792946	0.39516936
C	-4.99491643	0.34060874	0.37614538
C	-4.02083935	-0.34788456	-0.35683572
C	-2.57481293	-0.24675733	0.08211456
H	-1.18784967	1.24258998	0.80333209
H	-1.90646561	-0.66244529	-0.67903467
H	-2.41333509	-0.84484877	0.99588207
H	-4.31525877	-1.26656970	-0.85360389
H	-5.25350143	1.69388161	2.01942046
H	-2.91659404	2.82134899	1.66528775
N	-2.17188361	2.05187526	-0.83338614
C	-3.32075186	2.14382334	-1.75432331
H	-2.98513259	2.71337615	-2.63195336
H	-4.11035246	2.74950731	-1.29336282
C	-3.90203451	0.82970001	-2.27702679
C	-2.92144565	-0.08065494	-2.98811800
C	-5.21263588	1.00549560	-2.75289019
H	-5.80291281	1.86212457	-2.45661973
N	-5.86726641	0.18456046	-3.62790106
O	-5.39433996	-0.94018487	-4.00001205
O	-7.03670026	0.57990107	-4.06643194
S	-9.49636243	0.84533103	0.61292505
H	-9.52699621	6.10867650	-1.62859032
H	-9.97354953	3.18677888	-0.35531228
C	-10.83686498	3.81656837	-2.27768072
N	-6.30105955	0.03787423	0.39586729
H	-6.92334691	0.73087537	0.83084317
C	-7.03437220	-1.22625111	0.18038133
C	-6.26332075	-2.52447275	0.45518078
C	-7.74099016	-1.31266120	-1.19693866
C	-7.27066519	-3.69136064	0.51121815
H	-5.52932414	-2.72956696	-0.33639108
H	-5.71428336	-2.43010953	1.40372258
C	-8.76666599	-2.46287422	-1.15705509
H	-6.97682064	-1.55947807	-1.94858439
N	-8.30698057	-0.04858745	-1.68043478
C	-8.07754611	-3.79322512	-0.79722040
H	-6.73309624	-4.63311613	0.69885331
H	-7.95879434	-3.53440696	1.35882967
H	-9.25596017	-2.53499664	-2.13955607
H	-9.54131783	-2.21254027	-0.41501444
H	-7.98854315	0.19958134	-2.63492980
C	-9.03304378	0.89515133	-1.04751034
H	-7.39492410	-4.07384834	-1.61807433
H	-8.83002645	-4.59256015	-0.71879883
N	-9.38899621	1.93492595	-1.85977524
H	-9.16574112	1.86083570	-2.85394130
C	-9.68496007	3.28867334	-1.40225401
H	-7.83611718	-1.15859418	0.92706572
S	-0.74223360	2.80385826	-1.27186331
O	-1.08843957	3.97958719	-2.08066883
H	0.80828042	0.42634793	-0.70998016
O	0.06709138	2.93528979	-0.05385464

C	-8.40836008	4.22177862	-1.46706266
C	-7.33065002	3.63399876	-0.52836039
H	-6.43160914	4.26658840	-0.56031388
H	-7.68550164	3.58327006	0.50988066
H	-7.04679669	2.62181374	-0.83803279
C	-7.83548380	4.30429785	-2.89849376
H	-7.52501346	3.31749538	-3.26975402
H	-6.94795530	4.95386789	-2.89664383
H	-8.56940613	4.71637604	-3.60205553
C	-8.78082639	5.63664316	-0.97524998
H	-9.17970506	5.60951299	0.04831355
H	-7.88367471	6.27233766	-0.97110003
O	-10.82114139	3.56236844	-3.50116558
N	-11.80987392	4.57499763	-1.70032203
C	-11.98964156	4.82426642	-0.26474588
C	-12.84072972	5.18731537	-2.55157570
H	-12.55337277	5.07248857	-3.59842629
H	-12.92888385	6.25293823	-2.29932173
H	-13.81215039	4.70038703	-2.38027105
H	-13.03442786	4.61127176	0.00207159
H	-11.77399903	5.87622895	-0.02873825
H	-11.34721912	4.18458923	0.33943585
C	0.07974469	1.62728661	-2.35751284
C	-0.03209074	1.77432490	-3.74332511
C	0.48566802	0.77664356	-4.57381684
C	1.10470415	-0.34850907	-4.02059206
C	1.22623295	-0.47402778	-2.63063274
C	0.71695193	0.51644269	-1.78957587
H	-0.52581479	2.64834372	-4.16024980
H	0.39839092	0.87791830	-5.65462499
H	1.49793353	-1.12802548	-4.67187457
H	1.71925147	-1.34477187	-2.20038845
H	-1.91055426	0.06599492	-2.60831165
H	-3.19573940	-1.13538003	-2.91115607
H	-2.92146766	0.17630270	-4.05843616

TS4_22

E = -17398.11

G = -16969.06

Nimag = 1, 122i cm-1

C	-3.03382072	1.28056387	1.32309852
C	-1.51942960	0.97484066	1.30753025
H	-3.20970300	2.32746615	1.02694702
H	-1.32143578	0.18650939	2.04820420
C	-0.95951427	0.44343827	-0.02655439
C	-3.85965300	0.44909439	0.37857655
C	-3.25534909	-0.24790756	-0.68399939
C	-1.83313553	-0.71266443	-0.51843758
H	0.05520145	0.08822526	0.17651777
H	-1.44303742	-1.11175687	-1.45862452
H	-1.79646816	-1.52543583	0.22410053
H	-3.91908155	-0.89014798	-1.26184948
H	-3.40781095	1.18867293	2.34829384
H	-0.96249344	1.86908506	1.61766311
N	-0.82097554	1.48668520	-1.08611964
C	-2.00576968	2.19468315	-1.61718842
H	-1.65995195	2.81733455	-2.45158300
H	-2.35074352	2.88424282	-0.83578279
C	-3.18346287	1.33375070	-2.09853696
C	-2.90135162	0.46979877	-3.31814448
C	-4.39787949	2.07207424	-2.03088427
H	-4.42449775	3.07123233	-1.60806979
N	-5.64014981	1.60142519	-2.35713055
O	-5.82721000	0.33972678	-2.58680205
O	-6.63878285	2.41670000	-2.36811846
S	-3.61642718	-1.87884757	2.77728374
H	-3.66074058	-6.27550679	-0.94929256
H	-3.40138844	-3.73665017	1.03888212
C	-4.07607251	-3.56893579	-1.04878805
N	-5.18748904	0.60314276	0.32187749
H	-5.63009313	0.10824573	-0.46275713
C	-6.13143582	1.07927899	1.35021406
C	-6.01389134	2.56549407	1.72659950
C	-6.10172581	0.15944443	2.60414345
C	-7.16320597	2.93918127	2.68249410
H	-5.05606347	2.76331049	2.22469269
H	-6.04790367	3.16932903	0.80800939
C	-7.24299257	0.54393192	3.55605993
H	-5.14255395	0.26521204	3.12348678
N	-6.18821900	-1.24965454	2.19213192
C	-7.16527995	2.03652465	3.93082576
H	-7.06800243	3.99511120	2.97633438
H	-8.12562496	2.83548350	2.15307887
H	-7.18771913	-0.09086676	4.45266627
H	-8.20815488	0.33548818	3.06263840
H	-7.02449532	-1.47167542	1.64297074
C	-5.08252599	-2.01908837	1.91109060
H	-6.24223656	2.21482950	4.50900642
H	-8.01014451	2.29637768	4.58613319
N	-5.28172546	-2.92349461	0.92197806
H	-6.02538098	-2.74003581	0.24314445
C	-4.30212906	-3.89857725	0.44298348
H	-7.11632751	0.94456813	0.87621435
S	0.64188859	1.55255128	-1.89562278
O	0.56376723	2.67084430	-2.84390696
H	1.59234981	-1.10616091	-1.19632042
O	1.70298012	1.49690028	-0.88039065
C	-4.81059605	-5.36905258	0.69180342
C	-4.94036885	-5.56062384	2.21913979
H	-5.30020308	-6.57643922	2.43755944
H	-3.96997292	-5.42027511	2.71608440
H	-5.65239268	-4.84290422	2.64817580
C	-6.18113732	-5.60589834	0.02241878
H	-6.94511518	-4.92609669	0.42470930
H	-6.51008870	-6.63567744	0.22335397
H	-6.12788017	-5.46249408	-1.06441779
C	-3.78958599	-6.38323094	0.13654013
H	-2.80970242	-6.27251511	0.61970946
H	-4.14691916	-7.40437659	0.33256507
O	-5.05622636	-3.18753057	-1.72346293
N	-2.82566816	-3.67423752	-1.57842942
C	-1.61767658	-4.13330341	-0.88422934
C	-2.63746427	-3.40871453	-3.01327068
H	-3.53427775	-2.92810758	-3.40754628
H	-2.45156760	-4.34953250	-3.55358656
H	-1.76942279	-2.75377581	-3.14843773
H	-0.79180809	-3.45415383	-1.12826772
H	-1.34522715	-5.14679001	-1.21288058
H	-1.75249304	-4.13545606	0.19694235
C	0.77038032	0.02398391	-2.84841731
C	0.34827458	0.00938048	-4.18176299
C	0.37384862	-1.19442348	-4.89026027
C	0.81853498	-2.36701503	-4.27043642
C	1.25556819	-2.33658408	-2.94124510
C	1.23937570	-1.13888095	-2.22360019
H	0.00277983	0.92555787	-4.65289578
H	0.04272504	-1.21451160	-5.92771257
H	0.82906606	-3.30453426	-4.82471347
H	1.61513888	-3.24592155	-2.46181521
H	-2.05575262	-0.20096920	-3.15902470
H	-3.78332668	-0.11599394	-3.58990543
H	-2.64044492	1.13367525	-4.15823304

TS4_23

E = -17396.47

G = -16966.65

Nimag = 1, 396i cm-1

C	-2.98822512	0.88328656	1.30532664
C	-1.44378645	0.81583724	1.17972887
H	-3.33126547	1.93095729	1.35426945
H	-1.10260078	-0.10431611	1.67614196
C	-0.87948008	0.75895950	-0.25394584
C	-3.73896423	0.22822587	0.18541643
C	-3.10232757	0.00297909	-1.07496329
C	-1.62209332	-0.31185929	-1.06342604
H	0.18072414	0.50260739	-0.17388970
H	-1.23293362	-0.35505673	-2.08386938
H	-1.44478792	-1.30072688	-0.60942742
H	-3.70069184	-0.56189476	-1.79454383
H	-3.28732838	0.43074313	2.25690299

H	-0.99861530	1.66127769	1.71970653
N	-0.93394361	2.07680180	-0.94337851
C	-2.24441081	2.69451775	-1.22676530
H	-2.06885452	3.57741165	-1.85353856
H	-2.64714175	3.07099055	-0.27773767
C	-3.29473246	1.81215507	-1.93114466
C	-2.93860832	1.45331727	-3.36816032
C	-4.61037914	2.31903731	-1.62553575
H	-4.75914843	2.93125115	-0.74213992
N	-5.77412403	1.97420385	-2.21420045
O	-5.81282498	1.21313690	-3.26655722
O	-6.89898104	2.38147423	-1.68837992
S	-7.31204264	-3.02931227	-0.73402071
H	-6.32410581	-3.05178013	-6.46828638
H	-6.46809077	-3.23223230	-3.20457123
C	-5.14148695	-1.89914897	-4.32335101
N	-5.05188101	0.04309750	0.22595979
H	-5.41993500	-0.39373967	-0.62213403
C	-6.15918741	0.59551008	1.05155295
C	-5.95874933	0.57819127	2.57339826
C	-7.43846001	-0.21493817	0.67987890
C	-7.20449046	1.16606487	3.26960010
H	-5.78555082	-0.45937551	2.90186141
H	-5.08616985	1.17341845	2.86031798
C	-8.67118568	0.41390568	1.33974462
H	-7.31322432	-1.24005739	1.05330615
N	-7.57816104	-0.33046442	-0.77490139
C	-8.49831194	0.43899606	2.86849426
H	-7.05912171	1.11959984	4.35912902
H	-7.28815807	2.23294696	3.00103748
H	-9.55550987	-0.17303188	1.05220367
H	-8.81173408	1.43773738	0.95420803
H	-7.55223257	0.57135386	-1.28367386
C	-7.25910879	-1.47950982	-1.46774805
H	-8.46540657	-0.59876641	3.24223664
H	-9.36692306	0.92457500	3.33807665
N	-6.88868554	-1.26156760	-2.75166923
H	-6.68012710	-0.27882929	-3.02357782
C	-6.53587182	-2.28217220	-3.74235853
H	-6.30538179	1.63345179	0.70462224
S	0.44031743	2.65399419	-1.70874383
O	0.22428952	4.08460197	-1.95531951
H	1.27697116	-0.01455807	-2.47818706
O	1.58655079	2.18172383	-0.92124465
C	-7.65539619	-2.46732784	-4.82392624
C	-8.88917807	-3.06748440	-4.10959164
H	-9.70419810	-3.20392164	-4.83554788
H	-8.65362904	-4.04228963	-3.66007027
H	-9.24701534	-2.40321840	-3.31156223
C	-8.06812449	-1.13340467	-5.48259794
H	-8.45905178	-0.43295841	-4.73062291
H	-8.86764322	-1.32103299	-6.21483252
H	-7.21801244	-0.66488392	-5.98818982
C	-7.15497321	-3.46976319	-5.88688375
H	-6.81706086	-4.40495720	-5.41339139
H	-7.97298326	-3.71931821	-6.57824597
O	-5.03848261	-1.19105881	-5.33911555
N	-4.03151301	-2.33979962	-3.64439639
C	-4.04036385	-3.29402421	-2.52556196
C	-2.71072851	-2.11255258	-4.25470498
H	-2.76038825	-1.24453861	-4.91380526
H	-2.39801881	-2.99379985	-4.83800959
H	-1.97440329	-1.93953948	-3.46342524
H	-3.18012188	-3.07772019	-1.87985319
H	-3.94726160	-4.33090521	-2.88758632
H	-4.94714107	-3.20302430	-1.92309601
C	0.51280572	1.83301485	-3.31058548
C	0.07584046	2.51135065	-4.45201327
C	0.00269831	1.82116985	-5.66460423
C	0.35764994	0.47005220	-5.72806999
C	0.81974410	-0.19078976	-4.58311336
C	0.90905364	0.49014042	-3.36805896
H	-0.21792580	3.55556024	-4.38401353
H	-0.34338228	2.33907558	-6.55798202
H	0.28434819	-0.06757185	-6.67246425
H	1.11361146	-1.23819607	-4.63585713
H	-1.94021714	1.01949541	-3.43194573
H	-3.67147752	0.77320133	-3.80298039
H	-2.93638934	2.37857690	-3.96510391

TS4_24

E = -17401.71

G = -16972.26

Nimag = 1, 361i cm-1

C	-2.47575453	-1.04048245	-3.40070693
C	-1.16558868	-1.85369437	-3.38830070
H	-3.20392254	-1.46983220	-2.69376696
H	-0.67536803	-1.72747587	-4.36081755
C	-0.14603852	-1.39824391	-2.32843912
C	-2.30449326	0.41980403	-3.05299139
C	-1.18159688	0.87586777	-2.32307283
C	0.11278065	0.10299088	-2.47212873
H	0.77921343	-1.95165288	-2.50400248
H	0.82453975	0.44634489	-1.70934767
H	0.57698907	0.29201747	-3.44895969
H	-1.05747625	1.95302646	-2.23582126
H	-2.93817055	-1.10184270	-4.39738147
H	-1.38887407	-2.92128298	-3.26204505
N	-0.57495926	-1.74648020	-0.94226598
C	-1.66941145	-0.99676685	-0.28045608
H	-1.68551904	-1.29301587	0.77614724
H	-2.62195125	-1.33530066	-0.70543192
C	-1.60976427	0.53705896	-0.36554735
C	-2.98843476	1.14069666	-0.14539063
C	-0.48161743	1.11849758	0.29411770
H	0.32436806	0.51574060	0.68605266
N	-0.20508798	2.45634701	0.32197955
O	-0.94850020	3.30879091	-0.30992520
O	0.83695794	2.86095926	0.96967356
S	-2.68501372	0.76872385	-6.67860218
H	1.94136429	2.58997492	-7.35901117
H	-0.44817927	-0.34059330	-7.18309080
C	1.35191415	-0.52835392	-5.92937724
N	-3.33850067	1.20422162	-3.37155249
H	-4.08214674	0.77268326	-3.92592258
C	-3.36951929	2.66932884	-3.32816784
C	-4.76404961	3.17592220	-2.93039473
C	-2.95481926	3.24299419	-4.71426355
C	-4.78529302	4.71435511	-2.89749948
H	-5.50287512	2.80589362	-3.66196489
H	-5.03339687	2.76022753	-1.94922019
C	-2.95734109	4.77949378	-4.66814256
H	-3.67882318	2.89071723	-5.46148383
N	-1.64974292	2.73984749	-5.13285627
C	-4.33814284	5.31190225	-4.24350745
H	-5.79665855	5.06390665	-2.64189939
H	-4.11065618	5.06627341	-2.09854184
H	-2.67712490	5.16460162	-5.65960048
H	-2.19060615	5.12068774	-3.95073716
H	-0.83588195	3.21882561	-4.74312642
C	-1.42361078	1.66180417	-5.93688300
H	-5.07698647	5.05270092	-5.02083587
H	-4.30647295	6.40987189	-4.18075534
N	-0.10822007	1.37034626	-6.11379782
H	0.58653714	1.83602732	-5.52577243
C	0.42157981	0.24609001	-6.88296985
H	-2.64626171	3.00103877	-2.57406424
S	0.39395684	-2.75573776	-0.03334807
O	-0.43810587	-3.31635025	1.03918045
H	2.74522651	-1.43916501	-1.09456605
O	1.09970493	-3.63081474	-0.98009760
C	1.15492661	0.71944272	-8.19441670
C	1.70776660	-0.51602909	-8.93558484
H	2.18896967	-0.19910424	-9.87185838
H	2.45905511	-1.04681934	-8.33414213
H	0.90325406	-1.21938450	-9.19169990
C	0.11408105	1.42875226	-9.08765285
H	-0.71053533	0.75109618	-9.34720818
H	0.59544204	1.76912011	-10.01595612
H	-0.31160570	2.30362845	-8.57841270

C	2.30848516	1.69461118	-7.88053752
H	3.07763142	1.22266254	-7.25706524
H	2.77167397	2.02209406	-8.82264765
O	2.11915866	0.12301964	-5.18853658
N	1.28879226	-1.88836334	-5.89960822
C	0.41187662	-2.73618852	-6.71931680
C	2.21618244	-2.62933786	-5.03048138
H	2.85042461	-1.91674603	-4.50062871
H	2.83669680	-3.30371457	-5.63791519
H	1.64541914	-3.23267408	-4.31101761
H	0.95539771	-3.14029480	-7.58493995
H	-0.46486899	-2.18854635	-7.06785575
H	0.06686448	-3.57391752	-6.09960724
C	1.61749938	-1.68396678	0.73784243
C	1.47259277	-1.32511198	2.08171845
C	2.34901342	-0.38451738	2.63050627
C	3.34926841	0.18916999	1.84093365
C	3.49563559	-0.19275668	0.50179365
C	2.63302296	-1.13617880	-0.05687770
H	0.67897507	-1.76654772	2.67906898
H	2.23924785	-0.09244797	3.67387130
H	4.01806472	0.93494372	2.26804449
H	4.28170549	0.24708683	-0.11032650
H	-3.32277433	0.87712636	0.87164651
H	-2.95533594	2.22942451	-0.22596334
H	-3.72480611	0.73810179	-0.85008332

TS4_25

E = -17390.08

G = -16962.46

Nimag = 1, 417i cm-1

C	-2.26109754	-0.48886382	-2.50324586
C	-1.12740203	-1.52101585	-2.30336375
H	-3.01155227	-0.59021068	-1.70364153
H	-0.63960262	-1.69599538	-3.27451035
C	-0.02557347	-1.06772069	-1.32716969
C	-1.78576965	0.94940333	-2.51561573
C	-0.64363963	1.32614414	-1.76657186
C	0.49467406	0.31523862	-1.73504984
H	0.78402056	-1.80122375	-1.38324845
H	1.26241157	0.66377187	-1.03202795
H	0.96644917	0.23985782	-2.72783425
H	-0.33455311	2.36424924	-1.85101975
H	-2.78949309	-0.70520728	-3.44313116
H	-1.55282158	-2.47594470	-1.96768989
N	-0.49593780	-1.07963593	0.08745413
C	-1.44617089	-0.04916955	0.55966644
H	-1.50456443	-0.12181957	1.65291301
H	-2.44689363	-0.29971735	0.18872420
C	-1.12161590	1.40396317	0.18149778
C	-2.36987820	2.26097247	0.24932024
C	0.08327700	1.89267071	0.77811299
H	0.75741087	1.24606624	1.31997852
N	0.59897665	3.14489613	0.57898651
O	0.05196762	3.97008884	-0.24972435
O	1.67053074	3.47740024	1.21844716
S	-3.56476996	5.68896127	-0.02061232
H	-8.21020828	3.50472524	-0.93088488
H	-5.42448264	4.67210946	1.33813907
C	-5.67787146	2.49060210	1.29733428
N	-2.56706190	1.79764948	-3.20107021
H	-3.38050032	1.36172071	-3.63835798
C	-2.29346322	3.17071133	-3.71204890
C	-0.89064392	3.32672458	-4.33174793
C	-2.59941726	4.30783004	-2.70781878
C	-0.76904352	4.68919881	-5.03672797
H	-0.11902539	3.26348560	-3.55504083
H	-0.72448775	2.49769358	-5.03523745
C	-2.47199851	5.66306858	-3.43370285
H	-1.88627326	4.27503250	-1.87324076
N	-3.94797873	4.09978408	-2.16388991
C	-1.07932461	5.83632177	-4.06011661
H	0.24568205	4.79438537	-5.44917992
H	-1.47196376	4.72843981	-5.88647555
H	-2.68173949	6.45885734	-2.70736016
H	-3.24775222	5.71005607	-4.21707561
H	-4.53178793	3.42057470	-2.65240179
C	-4.39977164	4.53757277	-0.95900676
H	-0.31954772	5.85038240	-3.26002770
H	-1.02229042	6.80622174	-4.57686042
N	-5.60127854	3.98319400	-0.58711048
H	-5.84893767	3.11506259	-1.07378638
C	-6.01849595	3.91903899	0.81943861
H	-3.02165941	3.27324564	-4.53255875
S	0.28387247	-2.04452814	1.20469178
O	-0.64751493	-2.25720284	2.32034307
H	2.82458982	-1.30638775	0.02694444
O	0.85072545	-3.17985616	0.46424920
C	-7.52756145	4.29951099	0.99646556
C	-7.91153143	4.15974869	2.48476010
H	-8.96133807	4.45418841	2.62657728
H	-7.80145890	3.12357905	2.83513187
H	-7.29048422	4.80974216	3.11689888
C	-7.68103925	5.77410910	0.56258562
H	-7.05857384	6.43203795	1.18638756
H	-8.72975681	6.08902745	0.66328505
H	-7.37523235	5.90459373	-0.48431730
C	-8.45005689	3.40923746	0.13768562
H	-8.36214713	2.35263754	0.41947180
H	-9.49439516	3.72517046	0.27678673
O	-5.96099031	1.52887751	0.54863484
N	-5.04845052	2.32692006	2.49244036
C	-4.65719949	3.41169738	3.40605699
C	-4.77087068	0.96374112	2.97001294
H	-4.94458697	0.26138757	2.15246804
H	-5.42591161	0.71327115	3.81806676
H	-3.72684700	0.90191451	3.30321435
H	-3.76948388	3.08485469	3.96039861
H	-5.45528447	3.63680015	4.12736942
H	-4.39436528	4.31663019	2.85347968
C	1.65325998	-1.05858319	1.83195193
C	1.55319106	-0.46003462	3.09181161
C	2.56380665	0.41014511	3.51057468
C	3.65309488	0.67566812	2.67649312
C	3.75071730	0.05457101	1.42554776
C	2.75240069	-0.82033800	0.99665673
H	0.69211748	-0.66371719	3.72312533
H	2.49061835	0.88901533	4.48594842
H	4.42905887	1.36787728	2.99985801
H	4.60425814	0.25548231	0.77963591
H	-2.75660963	2.23144590	1.27808275
H	-2.15140374	3.30094103	0.01181123
H	-3.16196538	1.88525922	-0.40813316

TS4_26

E = -17397.02

G = -16967.70

Nimag = 1, 351i cm-1

C	-1.97442071	-0.93571664	-3.70415383
C	-0.64330681	-1.66723953	-3.41348019
H	-2.79206440	-1.38366668	-3.11729310
H	-0.02729168	-1.60892149	-4.32164227
C	0.21315992	-1.07635060	-2.27930002
C	-1.97156953	0.53767180	-3.39200533
C	-1.03529862	1.07995278	-2.47690167
C	0.33640645	0.44057345	-2.44706702
H	1.20034244	-1.54090337	-2.35805152
H	0.91689439	0.86598043	-1.62046574
H	0.86513222	0.65181646	-3.38699113
H	-1.04634373	2.17031698	-2.39726460
H	-2.23605084	-1.09503764	-4.75458930
H	-0.84371773	-2.72790214	-3.21211275
N	-0.29744443	-1.41059883	-0.92036211
C	-1.58589784	-0.83870469	-0.48066328
H	-1.74070662	-1.12959273	0.56537164
H	-2.37570203	-1.33071614	-1.06100229
C	-1.74597505	0.68588047	-0.60944788
C	-3.21233255	1.07957944	-0.67659663
C	-0.86023164	1.41488652	0.23926863
H	-0.05352506	0.92419654	0.75923140

N	-0.83689105	2.77214694	0.39240194
O	-1.57793798	3.54056031	-0.32930613
O	-0.02446097	3.27776860	1.26136079
S	-0.09273797	0.56943859	-6.31692045
H	-0.14314485	5.65358252	-6.56508434
H	1.43003121	2.41316960	-5.38101133
C	0.84082945	3.79084963	-3.76536174
N	-2.95178285	1.33323374	-3.84643830
H	-2.86997170	2.30687454	-3.54778387
C	-3.95072346	1.11969807	-4.91609639
C	-4.94772569	-0.02767562	-4.67743593
C	-3.27124093	1.01192371	-6.31237574
C	-6.01681208	-0.01358610	-5.78719054
H	-4.43270751	-0.99648434	-4.69170217
H	-5.40706763	0.09260509	-3.68538413
C	-4.34357448	1.01416844	-7.41142930
H	-2.68566935	0.08800924	-6.37588455
N	-2.31372726	2.11185356	-6.48746245
C	-5.37185522	-0.10950170	-7.18236202
H	-6.71560040	-0.84905891	-5.63182606
H	-6.60396457	0.91795562	-5.71693288
H	-3.84920576	0.90330197	-8.38759729
H	-4.85644188	1.99171187	-7.41044209
H	-2.72452518	3.04519757	-6.38828427
C	-0.98675568	2.01278902	-6.13465203
H	-4.86800123	-1.08612559	-7.28284037
H	-6.14615840	-0.06548451	-7.96289825
N	-0.45492069	3.17197006	-5.68090434
H	-1.09054850	3.87608804	-5.29558796
C	0.92911823	3.37503839	-5.25244416
H	-4.52921515	2.05661174	-4.91484385
S	0.78579861	-2.08658237	0.15810136
O	0.06232519	-2.29672424	1.41872961
H	3.21367340	-1.41729091	-1.30580738
O	1.44203084	-3.20583125	-0.53320134
C	1.64401669	4.43999400	-6.16696477
C	3.08486982	4.68210251	-5.67244063
H	3.58054384	5.40580557	-6.33537750
H	3.09968453	5.09423640	-4.65397358
H	3.67518953	3.75642239	-5.68597142
C	1.68719993	3.86425910	-7.59966531
H	2.26902107	2.93204429	-7.63021709
H	2.15692485	4.59032311	-8.27893925
H	0.67577854	3.64983909	-7.96999332
C	0.87447940	5.77829695	-6.16936160
H	0.80359363	6.20275667	-5.15971707
H	1.39900433	6.49737774	-6.81496055
O	-0.12077711	4.50891650	-3.41430173
N	1.78163080	3.35006553	-2.88836032
C	2.95326135	2.52880587	-3.20939191
C	1.69781756	3.76801504	-1.47878269
H	0.72680129	4.23022487	-1.29772981
H	2.50585030	4.47819420	-1.24596189
H	1.80812664	2.88950421	-0.83213367
H	3.86937256	3.13689211	-3.19029118
H	2.86102910	2.05864222	-4.18827769
H	3.04400619	1.74030917	-2.45371042
C	2.07068556	-0.84803261	0.44181270
C	1.96136704	0.01660380	1.53585645
C	2.88219839	1.05655464	1.67902209
C	3.91087830	1.21753101	0.74583172
C	4.03494751	0.32296553	-0.32307071
C	3.11615810	-0.71660906	-0.48134480
H	1.16368675	-0.12107191	2.26132772
H	2.78628916	1.74544968	2.51618007
H	4.62030844	2.03672207	0.85435101
H	4.84850001	0.43376603	-1.03846791
H	-3.66871305	0.89782866	0.30997333
H	-3.32825737	2.14058532	-0.91284839
H	-3.75589174	0.47646960	-1.41259764

TS4_27
E = -17401.71
G = -16972.76
Nimag = 1, 287i cm-1

C	-4.86812132	-1.08056192	-2.19343599
C	-4.13965385	-2.15787927	-3.03055755
H	-4.68601358	-1.24424359	-1.11810574
H	-4.68986148	-2.29502476	-3.97397615
C	-2.68995905	-1.81132457	-3.41685052
C	-4.46224830	0.34006261	-2.50799402
C	-3.21899738	0.61701719	-3.13116274
C	-2.64882643	-0.42490123	-4.07294313
H	-2.35069077	-2.56978407	-4.12801526
H	-1.61678710	-0.15130982	-4.33070410
H	-3.22414608	-0.46089863	-5.01250463
H	-3.05818601	1.65965855	-3.41686940
H	-5.94979937	-1.20094071	-2.32558879
H	-4.16284466	-3.11565283	-2.49419038
N	-1.76322698	-1.89856017	-2.25156484
C	-1.81245242	-0.87690957	-1.18126754
H	-0.95466526	-1.04332662	-0.51702101
H	-2.70614058	-1.05533785	-0.57110856
C	-1.80738905	0.58526246	-1.64501142
C	-2.38460138	1.49961421	-0.58673487
C	-0.60821162	0.97578866	-2.31567234
H	0.17187099	0.26978931	-2.55665593
N	-0.38493847	2.21714350	-2.84285638
O	-1.32121793	3.10146002	-2.87979845
O	0.78401441	2.48310089	-3.32715188
S	-4.60840856	4.62115503	-1.49420002
H	-3.56515699	5.35600058	3.39193717
H	-2.46672521	5.24015033	-0.23169232
C	-1.29969374	4.00550182	1.16408792
N	-5.23421119	1.34177405	-2.07017646
H	-4.92176984	2.31134466	-2.25096036
C	-6.44613960	1.21302651	-1.24091045
C	-7.70512432	0.94757899	-2.09589452
C	-6.65753001	2.50647419	-0.41619933
C	-8.94700387	0.79379237	-1.20184505
H	-7.83441937	1.79557637	-2.78886740
H	-7.55813868	0.04947929	-2.71071788
C	-7.88476998	2.35520103	0.49896107
H	-6.82635126	3.33436475	-1.11855861
N	-5.47774186	2.87195320	0.36941053
C	-9.15010212	2.03509012	-0.31646778
H	-9.83485671	0.62144306	-1.82854895
H	-8.82398333	-0.09778165	-0.56297982
H	-8.01374912	3.28826624	1.06709181
H	-7.69490352	1.54657266	1.22632127
H	-5.40825355	2.46030616	1.30195992
C	-4.58934203	3.85238437	0.03934653
H	-9.39244752	2.90096273	-0.95560444
H	-10.00159914	1.88655728	0.36427663
N	-3.69252444	4.15295333	1.01252008
H	-3.60164425	3.49948958	1.79773834
C	-2.47498190	4.94772116	0.82018321
H	-6.29274983	0.37798269	-0.54029819
S	-0.49449966	-2.97953830	-2.28539875
O	-0.12855104	-3.27471963	-0.89331359
H	0.05276002	-2.19319778	-5.01570873
O	-0.87596492	-4.05790364	-3.20832290
C	-2.50292819	6.25510667	1.69540360
C	-1.20434552	7.05627945	1.46624431
H	-1.24089460	7.98827769	2.04854875
H	-0.31887609	6.49104048	1.78830053
H	-1.08205169	7.32401328	0.40798958
C	-3.71105990	7.10270841	1.24077859
H	-3.62636603	7.36890737	0.17808035
H	-3.75770645	8.02889289	1.83196144
H	-4.65186944	6.55379314	1.38071068
C	-2.64290287	5.92093879	3.19561933
H	-1.79236164	5.32870707	3.55637827
H	-2.69014488	6.85519711	3.77403582
O	-1.44600711	3.19857634	2.11191366
N	-0.16457427	4.05795913	0.42604984
C	0.09004488	4.92001542	-0.73805002
C	0.92380699	3.11711744	0.74100088
H	0.86203054	2.82348675	1.79143267
H	1.88383834	3.60803473	0.54314923

H	0.84153649	2.22364625	0.10319160
H	0.78058149	5.73029641	-0.46367043
H	-0.83342897	5.34487422	-1.12814047
H	0.53546380	4.31238604	-1.53401134
C	0.88778091	-2.09086991	-3.02031067
C	1.91526487	-1.61153166	-2.20199598
C	2.91415996	-0.81305525	-2.76647950
C	2.87719533	-0.49861664	-4.12756322
C	1.85192944	-0.99954117	-4.93908251
C	0.85179769	-1.80240450	-4.39055092
H	1.92106668	-1.85069090	-1.14158910
H	3.71405461	-0.42714909	-2.13614724
H	3.64813439	0.13767483	-4.55949581
H	1.82834280	-0.76044063	-6.00145725
H	-1.73268718	1.47948182	0.29799580
H	-2.43881839	2.52416898	-0.95743296
H	-3.38110293	1.17684755	-0.26741476

4_60
E = -2494.50
G = -2445.34
Nimag = 0

H	-1.29840416	2.60553986	1.38386617
C	-1.00440510	4.16360933	-0.03417530
N	-1.28990718	2.79141034	0.38021423
H	-0.23957514	4.17614788	-0.82000229
H	-1.83056821	0.52147254	1.13152415
C	-1.74322331	1.81747963	-0.45214533
S	-1.92360906	2.06693813	-2.13902144
H	-3.39130091	-0.36945765	-1.14190619
N	-2.04134382	0.63106215	0.13886860
C	-2.46777898	-0.56586660	-0.58371388
H	-1.90656254	4.66247370	-0.41460500
H	-0.63226094	4.70276901	0.84323888
H	-1.69594077	-0.90079995	-1.29008631
H	-2.65092509	-1.35117231	0.15698618

4_61
E = -2414.85
G = -2357.29
Nimag = 0

C	0.45869183	0.64532042	0.61146429
C	0.18397641	-0.70820309	1.22699344
C	-0.25796532	-1.75900443	0.49384032
N	0.38414484	-0.74664208	2.60320976
C	0.39326492	-2.01958742	3.32164940
H	1.51338360	0.92855619	0.75548732
H	-0.16052635	1.42012134	1.08828912
H	0.24696788	0.63779032	-0.46358073
H	-0.45448832	-1.63157542	-0.56799432
H	-0.44827074	-2.73818729	0.92702894
H	1.04971144	-0.05636863	2.95201914
H	1.11956678	-2.73582162	2.89770231
H	-0.60405870	-2.48058187	3.28406945
H	0.64615661	-1.83035995	4.37079453

4_62
E = -1383.14
G = -1369.87
Nimag = 0

N	-0.02712591	-0.77332776	1.57667624
O	-0.20698283	0.41947012	1.88903879
O	-0.55345990	-1.74019476	2.16019806
C	0.91218697	-1.07422538	0.44756776
H	1.02873626	-0.17174506	-0.15201661
H	0.49558042	-1.90821424	-0.11948209
H	1.86107334	-1.36722744	0.90786592

4_63
E = -4912.82
G = -4793.73
Nimag = 0

C	4.36071095	1.18833588	2.99649657
C	3.92241991	0.22518470	1.91390845
C	4.80445107	-0.32335065	1.03804071
N	2.56076377	0.00091610	1.89255335
C	1.96123574	-1.02561574	1.05207686
H	4.10080803	0.79471153	3.99129580
H	3.85149148	2.15717637	2.88571222
H	5.44327911	1.35434309	2.95828430
H	5.85648649	-0.05286542	1.08979724
H	4.50039900	-1.02250294	0.26197314
H	2.04534415	0.22944050	2.74788208
H	2.40450289	-2.02286258	1.22668037
H	2.09186471	-0.77780044	-0.01276968
H	0.88880793	-1.07149287	1.26770337
H	-0.89905493	1.62434080	0.87346927
C	0.52158960	2.82123388	1.90585369
N	-0.45972613	1.74244994	1.78759599
H	0.41922993	3.31601710	2.87753971
H	-2.03910934	-0.10514477	1.48600912
C	-0.64877436	0.76511417	2.70922252
S	0.17130483	0.75386091	4.21908857
H	-1.04098168	-1.87710286	3.56832149
N	-1.51795710	-0.21648863	2.35695982
C	-1.92083961	-1.31678024	3.23066891
H	1.54329705	2.43206734	1.80507776
H	0.32126437	3.54083300	1.10477461
H	-2.46263680	-0.94987060	4.11345114
H	-2.57315126	-1.97748750	2.65030556

4_64
E = -3800.58
G = -3718.15
Nimag = 0

C	2.91911475	1.52304041	0.79245291
C	3.25837975	0.04861071	0.81836397
C	4.31011542	-0.43674982	1.52282202
N	2.43168762	-0.73305386	0.02005100
C	2.54078880	-2.18883515	0.02325678
H	1.87171948	1.70096575	1.07529759
H	3.05298718	1.92660760	-0.22270611
H	3.56089096	2.08229577	1.48205307
H	4.95137465	0.24609723	2.07482233
H	4.56704783	-1.49328024	1.53993360
H	1.48517879	-0.37300332	-0.09812341
H	2.46097155	-2.61950953	1.03712340
H	3.50979085	-2.49544268	-0.39691118
H	1.74309627	-2.60319512	-0.60293091
N	0.08838723	0.21598094	2.42039051
O	-0.39794282	0.19229789	1.27175396
O	0.11792502	1.22704776	3.14551289
C	0.72286820	-1.03228536	2.94905053
H	0.38203124	-1.87298248	2.34573561
H	0.44314922	-1.12789465	4.00061946
H	1.80558124	-0.88734440	2.85681295

4_65
E = -3880.87
G = -3806.41
Nimag = 0

H	-2.24039212	2.50673829	2.44438110
C	-0.29976829	3.17717716	3.02272247
N	-1.33933925	2.17682979	2.79419810
H	0.15982699	3.03511970	4.00816969
H	-3.08578595	0.55948072	2.28418096
C	-1.13393996	0.83206503	2.82010318
S	0.36216689	0.14206465	3.28950316
H	-1.49250316	-1.81130863	1.82879165
N	-2.20518222	0.07528068	2.46917523
C	-2.23470117	-1.38436365	2.51533100
H	0.48787711	3.11827167	2.25843350
H	-0.77513854	4.16288199	2.98153654
H	-2.02307735	-1.75350978	3.52817084
H	-3.23671338	-1.70398922	2.21045635
N	-4.69181348	2.22711461	4.19728610
O	-4.46026235	2.18113850	2.96699802
O	-5.66928224	2.80898959	4.69336314
C	-3.72539195	1.53903925	5.10839691
H	-3.73499479	0.47817366	4.84488490

H	-4.04309642	1.70725776	6.13725171
H	-2.73676183	1.95935028	4.90320097

4_66

E = -8696.53

G = -8516.52

Nimag = 0

C	0.74906254	1.04678290	-0.23499446
C	1.87004437	1.16444391	-1.29118282
H	1.10163547	1.46019886	0.72451045
H	1.49822323	0.77396109	-2.25286322
C	3.13234739	0.35850102	-0.92165594
C	0.37001557	-0.40409808	-0.02248305
C	1.52836858	-1.33900733	0.27492272
C	2.76163405	-1.11300163	-0.63595927
H	3.79403446	0.35480852	-1.79665734
H	3.62182153	-1.67300364	-0.24960779
H	2.53068459	-1.54892618	-1.61983907
H	6.42423922	2.82653658	2.19344307
H	-0.14332244	1.61208877	-0.53506257
H	2.12690175	2.21807439	-1.45121208
N	3.93903413	0.99160859	0.17499688
C	3.81027365	0.64201982	1.59285054
H	4.30184893	1.43381364	2.17626700
H	2.76151644	0.66332283	1.91155913
C	4.46693810	-0.67270838	2.01423252
C	5.74139488	-1.07681051	1.34728165
C	3.83707466	-1.32557487	3.01010580
H	2.88337157	-1.00849555	3.41890542
N	4.29119414	-2.53564805	3.64534061
O	5.47618047	-2.91888921	3.51583897
O	3.43205814	-3.15329317	4.32779601
H	8.71600818	2.03544316	2.77395286
H	10.04593145	0.75063603	1.10646405
H	9.10183312	0.28081936	-1.14946649
H	5.76393816	-0.69010798	0.32572123
O	-0.79505705	-0.80304798	-0.08758072
H	5.87837475	-2.16137884	1.34768406
H	6.59582450	-0.63792038	1.88658141
C	6.48770267	1.96691596	0.21254112
C	7.01180524	2.26129544	1.47451816
C	8.29911882	1.81837423	1.79151722
C	9.04577723	1.09941863	0.85259978
S	4.78855276	2.40973301	-0.17095304
O	4.39001415	3.46208718	0.77594283
H	6.80496955	1.05496427	-1.72322216
O	4.67325311	2.61953770	-1.61849144
C	8.51522525	0.83169319	-0.41567396
C	7.23000506	1.26469575	-0.74400786
H	1.17910653	-2.37720489	0.19337373
H	1.78974565	-1.17618850	1.33042805

4_67

E = -9211.56

G = -8971.07

Nimag = 0

H	-1.21569178	2.58070509	1.36238269
C	-1.06503237	4.17890106	0.03426255
H	-0.83106878	-1.80799501	0.41185366
H	3.37375705	4.74136729	0.12962976
H	1.16039199	6.59243126	-1.47949984
H	0.30692876	5.09270811	-1.92820139
H	2.07910445	5.14408877	-1.97829443
C	-2.08450635	5.28981106	0.49444019
C	-1.56203989	6.68124207	0.07794274
H	-2.29613550	7.44867606	0.36317552
H	-0.61093246	6.92317576	0.57183523
H	-1.41638261	6.74326032	-1.00944455
C	-3.42611691	5.01719486	-0.22131026
H	-3.30514685	5.05816529	-1.31253721
H	-4.16648056	5.77292896	0.07948795
H	-3.81589385	4.02464207	0.04046155
C	-2.30258609	5.25521005	2.02140927
H	-1.37015358	5.45001762	2.56630814
H	-3.03916071	6.02253317	2.30160206
O	0.54117724	3.90247183	1.80098048
N	1.28428680	5.04349765	-0.04024916
C	1.19061024	5.49446580	-1.43424306
C	2.57536662	5.33219075	0.60206880
H	2.51118443	5.07975590	1.66214977
H	2.80565315	6.39965864	0.48186879
S	-1.96172394	2.09197557	-2.14692845
H	-2.69313472	4.27925413	2.34237978
H	-1.03888192	4.18014712	-1.05670909
C	0.33384168	4.36347129	0.65591975
N	0.02940460	-0.79309250	-1.21323748
H	-0.30653140	-0.23349249	-2.00833955
C	-1.11467885	-1.53281635	-0.62220607
C	-1.49212543	-2.82775715	-1.37123527
C	-2.35514065	-0.61748207	-0.54245615
C	-2.66441887	-3.56182285	-0.69517771
H	-1.76314973	-2.56455747	-2.40937895
H	-0.60671463	-3.48214827	-1.42156531
C	-3.53302178	-1.32823278	0.14810630
H	-2.64758460	-0.34259224	-1.56552094
N	-2.06241291	0.64478429	0.14063729
C	-3.89070736	-2.64011544	-0.57281650
H	-2.92331269	-4.46861966	-1.26374127
H	-2.35362996	-3.89005068	0.31214513
H	-4.39594748	-0.64560137	0.16824440
H	-3.25839869	-1.54482481	1.19564798
H	-1.92396971	0.58361618	1.15136260
C	-1.82660043	1.84190072	-0.45157275
H	-4.26816801	-2.40308386	-1.58263828
H	-4.70527002	-3.14979189	-0.03529018
N	-1.51613496	2.84345116	0.41919356
H	0.69839412	-1.47061571	-1.60005373

Int4_36

E = -17920.62

G = -17478.19

Nimag = 0

C	1.72262743	0.67326079	-1.39382055
C	3.20823818	0.74657179	-1.76397458
H	1.51339408	1.30498832	-0.52278545
H	3.38448145	0.14607614	-2.66908246
C	4.12089409	0.18766182	-0.65532295
C	1.26639903	-0.76294418	-1.08542049
C	2.15143436	-1.40235191	0.00302986
C	3.66242186	-1.23110570	-0.24677319
H	5.13678825	0.09722835	-1.05882180
H	4.23540711	-1.58863940	0.62005446
H	3.93974525	-1.87363424	-1.09584605
H	5.57026677	0.46048731	3.71186895
H	1.11701848	1.06319608	-2.22370123
H	3.49279606	1.77963391	-2.00152925
N	4.26806379	1.12109180	0.51961802
C	3.36742846	1.10478275	1.67875861
H	3.43251856	2.08307274	2.17511903
H	2.32075294	1.00813787	1.37263589
C	3.71254951	0.06423409	2.74341940
C	5.15403091	-0.24848979	2.97784975
C	2.65585024	-0.43666455	3.41207028
H	1.62728636	-0.20892993	3.15326161
N	2.71431732	-1.36484568	4.51045202
O	3.78677884	-1.56006473	5.12755069
O	1.63309495	-1.94266421	4.79948003
S	-0.57801729	-0.00377933	-4.92792906
H	-4.42715150	1.23494195	-1.65607706
H	-1.43272753	2.09348849	-3.81483557
C	-1.11918345	2.40973454	-1.66454064
N	1.35466509	-1.52287321	-2.32356583
H	1.07252362	-0.93784516	-3.11580647
C	0.66208390	-2.82318572	-2.38630751
C	1.62049034	-3.95964397	-2.79321493
C	-0.53967803	-2.77786967	-3.37024666
C	0.90028110	-5.31779735	-2.85394229
H	2.05110201	-3.71448676	-3.77951112
H	2.45511473	-3.98913400	-2.07665328
C	-1.27368132	-4.12759565	-3.41860591

H	-0.16576614	-2.53137622	-4.37325567
N	-1.46794831	-1.69937183	-2.99598640
C	-0.30913897	-5.26351869	-3.80493065
H	1.60095359	-6.10526343	-3.17292943
H	0.55180607	-5.58793878	-1.84131443
H	-2.10542267	-4.05850736	-4.13614998
H	-1.71131468	-4.33486700	-2.42628110
H	-1.74116679	-1.75030908	-2.00946525
C	-1.40647496	-0.42841894	-3.48543623
H	0.04748747	-5.09665643	-4.83624229
H	-0.84570451	-6.22484566	-3.80111588
N	-2.10305802	0.48328144	-2.74771099
H	-2.38767186	0.18647853	-1.81199200
C	-1.95642657	1.93251387	-2.87115102
H	0.25512766	-3.05404506	-1.38846443
S	5.05385447	2.59235878	0.24843319
O	4.10617526	3.71260744	0.37600744
H	7.67127393	1.46651765	0.66099288
O	5.84042953	2.42784321	-0.98032322
C	-3.35931351	2.63777378	-2.96737727
C	-3.16939466	4.16508599	-3.07577666
H	-4.15071976	4.64874913	-3.18348057
H	-2.68629113	4.57943083	-2.18025882
H	-2.56556949	4.43055542	-3.95431651
C	-4.04526850	2.11697881	-4.24963177
H	-3.45099755	2.36797781	-5.14005745
H	-5.03904927	2.57575549	-4.35381097
H	-4.16626860	1.02614364	-4.21408160
C	-4.23692625	2.31430716	-1.73965014
H	-3.76751222	2.65652743	-0.80834690
H	-5.20968716	2.81613985	-1.84493864
O	-1.29902846	1.84752116	-0.55414504
N	-0.21799561	3.40756332	-1.82486708
C	0.18002773	4.02237087	-3.09867621
C	0.49560650	3.93859651	-0.65058507
H	0.08522342	3.48302548	0.25210949
H	0.36499213	5.02915948	-0.61457249
H	1.56863692	3.71539850	-0.72524974
H	-0.19801854	5.05184062	-3.16352112
H	-0.18305525	3.44917255	-3.95101471
H	1.27742835	4.04702412	-3.14183877
C	6.17765898	2.67359164	1.65229409
C	5.79656683	3.35816718	2.80974596
C	6.64035056	3.32461847	3.92383834
C	7.85071193	2.62622043	3.86742261
C	8.23074937	1.96714988	2.69142089
C	7.39340718	1.98503551	1.57568917
H	4.85888813	3.90757418	2.83823683
H	6.34928080	3.84537113	4.83493596
H	8.50251814	2.59855613	4.73963104
H	9.17814381	1.43195412	2.64548861
H	5.71184101	-0.12262988	2.04614155
H	5.29619974	-1.25511676	3.37913049
H	1.91991934	-2.47600237	0.07310805
H	1.85138680	-0.97006714	0.96057191
O	-0.10039704	-0.73988958	-0.51044527
H	-0.44641393	0.18655388	-0.55216535

H_2O

E = -503.11

G = -501.69

Nimag = 0

H	0.77466463	0.00000000	1.50030076
O	0.00000000	0.00000000	2.10752715
H	-0.77466463	0.00000000	1.50030076

Int4_37

E = -17406.22

G = -16981.23

Nimag = 0

C	2.29207992	0.33542453	-2.15862393
C	3.77644948	-0.03996845	-1.93236158
H	2.07739935	1.31321907	-1.70896741
H	3.97136560	-0.98513065	-2.46636647
C	4.16588966	-0.27281964	-0.45003698
C	1.41490110	-0.71002065	-1.50808391
C	1.62375445	-0.74516831	-0.00622603
C	3.10169556	-1.10792330	0.30013277
H	5.08753271	-0.86623060	-0.45006358
H	3.28544443	-1.08644848	1.38131681
H	3.25363506	-2.15082282	-0.01878615
H	4.64084612	1.53721322	3.78439188
H	2.07248094	0.38992537	-3.23310905
H	4.43787824	0.71670010	-2.37377925
N	4.54202154	0.97414242	0.29661852
C	3.55595690	1.84137595	0.96125601
H	4.02738095	2.82117093	1.12476501
H	2.69747052	2.03881753	0.31516255
C	3.09292115	1.35166098	2.33250238
C	4.10686555	0.73898382	3.24347723
C	1.78776603	1.56418306	2.59623138
H	1.10031577	1.96969479	1.86333121
N	1.10793209	1.21196722	3.81332951
O	1.73804152	1.05836795	4.88620080
O	-0.14165775	1.07843510	3.71803598
S	-2.30987800	0.67470385	-3.07288273
H	-1.93533527	2.61171046	1.84397342
H	-1.95894963	2.88558353	-1.93959733
C	0.02076352	3.10776358	-1.03357431
N	0.70631442	-1.48339568	-2.24622547
H	1.38073173	0.25099773	0.38031536
C	-0.11915083	-2.54006678	-1.65714455
C	0.03553526	-3.83671254	-2.47556807
C	-1.60401068	-2.08712886	-1.67065173
C	-0.88524476	-4.94857581	-1.94547336
H	-0.20559451	-3.61313882	-3.52827613
H	1.08963703	-4.15309783	-2.44278981
C	-2.52705979	-3.18862437	-1.12811696
H	-1.88149854	-1.84031793	-2.70293268
N	-1.76053106	-0.84644265	-0.90609670
C	-2.35544317	-4.49212546	-1.92881186
H	-0.77418898	-5.85212172	-2.56494567
H	-0.57754425	-5.22087134	-0.92075573
H	-3.56763418	-2.83323462	-1.17441719
H	-2.28846766	-3.37199688	-0.06571588
H	-1.51523454	-0.90453990	0.08443837
C	-1.85847691	0.39737189	-1.44685565
H	-2.69433352	-4.32336647	-2.96558711
H	-2.99780193	-5.27811082	-1.50297693
N	-1.63387105	1.41294620	-0.55509231
H	-1.08016365	1.17639914	0.27071912
C	-1.48504664	2.81199422	-0.96103824
H	0.14796010	-2.76898056	-0.60985882
S	6.00733102	1.70672630	-0.09071165
O	5.77888659	3.06913374	-0.59904341
H	7.48317006	-0.18101520	1.51293445
O	6.76861598	0.73677836	-0.88914813
C	-2.24834049	3.78275360	0.00688272
C	-2.01507292	5.23371469	-0.46617486
H	-2.58837877	5.92729183	0.16538636
H	-0.95445061	5.51447295	-0.39993752
H	-2.34641911	5.36921437	-1.50563310
C	-3.75131970	3.44148564	-0.09857792
H	-4.11216787	3.57618517	-1.12877921
H	-4.33294776	4.10063598	0.56183611
H	-3.93620171	2.39999503	0.19749712
C	-1.78601184	3.63480580	1.47218961
H	-0.72579782	3.88915577	1.58602387
H	-2.37867127	4.30877979	2.10842573
O	0.73908954	2.74764377	-0.07184727
N	0.52896767	3.75160886	-2.11076788
C	-0.22131877	4.09163906	-3.33076513
C	1.94329841	4.16172690	-2.10227068
H	2.33521697	4.07779753	-1.08709205
H	2.01502160	5.20226305	-2.44551510
H	2.53117357	3.52297510	-2.77651815
H	-0.62291933	5.11312455	-3.27657255
H	-1.02827813	3.37590409	-3.50330275
H	0.46911683	4.03016365	-4.18060121
C	6.78836429	1.86650641	1.52353295

C	6.69472068	3.07269188	2.22248857
C	7.22095536	3.14802007	3.51575642
C	7.83781096	2.03182223	4.08905494
C	7.94262120	0.83548669	3.36767439
C	7.41630109	0.74559920	2.07873455
H	6.21753309	3.93490274	1.76345927
H	7.14710186	4.08072420	4.07332439
H	8.24198451	2.09324566	5.09871975
H	8.43123075	-0.03062347	3.81201712
H	4.85090006	0.19499518	2.65509366
H	3.65305518	0.08119295	3.98924363
H	0.97594803	-1.46236981	0.50833456

Int4_38

E = -17405.86

G = -16978.14

Nimag = 0

C	2.16316606	0.99591676	-1.22333471
C	3.69555718	0.86509229	-1.09590629
H	1.79965501	1.89455399	-0.70408389
H	4.07982160	0.32824828	-1.97692655
C	4.19172165	0.06689705	0.12772265
C	1.37911544	-0.17416363	-0.66748859
C	1.96435592	-1.11885285	0.14138800
C	3.45863065	-1.28083379	0.21167406
H	5.25883545	-0.11766920	-0.02422592
H	3.74673720	-1.81301306	1.12607285
H	3.81611276	-1.90929806	-0.62569300
H	1.35777887	-1.92201539	0.55116696
H	1.89704873	1.13410436	-2.28305259
H	4.15950449	1.86136621	-1.09661907
N	4.11340886	0.84229266	1.40002305
C	2.83817269	1.37334465	1.91744937
H	3.07278771	1.91159798	2.84713062
H	2.45954913	2.13026385	1.22362661
C	1.73248479	0.37340857	2.24708459
C	2.08041187	-0.79628605	3.12396947
C	0.47595460	0.93596669	2.14693015
H	0.34144170	1.91832393	1.70692814
N	-0.70955312	0.36923781	2.57821761
O	-0.81615084	-0.86105749	2.86641415
O	-1.75397701	1.14463007	2.62798789
S	-1.95843046	2.19486468	-2.32910190
H	-1.71329594	3.98612043	2.76961443
H	-1.96326822	4.56062362	-1.00509417
C	0.07658436	4.17889862	-0.31139594
N	0.04979152	-0.11429615	-0.92150629
H	-0.27539593	0.64412706	-1.53096068
C	-0.95245825	-1.11585980	-0.54762244
C	-0.81456512	-2.43235436	-1.34320275
C	-2.37303079	-0.53364894	-0.77129777
C	-1.86973001	-3.45249254	-0.88282478
H	-0.94611523	-2.20435196	-2.41453297
H	0.19930959	-2.83636500	-1.21828282
C	-3.43501328	-1.53458798	-0.29133687
H	-2.50832826	-0.34407823	-1.84484024
N	-2.54402356	0.75805750	-0.09724374
C	-3.29271960	-2.88218490	-1.02235814
H	-1.77219575	-4.38079762	-1.46640058
H	-1.68249986	-3.71389739	0.17315447
H	-4.43139811	-1.10092782	-0.46228141
H	-3.32082336	-1.68555550	0.79579803
H	-2.53318612	0.71930193	0.93279164
C	-2.15938335	1.95056518	-0.63513283
H	-3.51935448	-2.73453952	-2.09236332
H	-4.03282906	-3.59665956	-0.63099157
N	-1.96384365	2.94405794	0.26857247
H	-1.83718815	2.63906980	1.24053000
C	-1.45151746	4.26640599	-0.08790782
H	-0.83769378	-1.33489539	0.52786365
S	5.49460948	1.01794134	2.32791289
O	5.31727987	2.21094830	3.16692319
H	6.28165723	-1.73669411	1.89869285
O	6.64737208	0.89923783	1.42478545
C	-1.83115663	5.31882103	1.01311028
C	-1.25360474	6.69080627	0.60146081
H	-1.56272558	7.45433048	1.32928780
H	-0.15542323	6.67522585	0.57197182
H	-1.62409704	6.99547408	-0.38748895
C	-3.37326247	5.41263878	1.06225990
H	-3.77724839	5.71794147	0.08556277
H	-3.67750224	6.15901786	1.81009398
H	-3.82231525	4.44795603	1.33390732
C	-1.28980736	4.93377819	2.40798680
H	-0.19792457	4.83576228	2.39773800
H	-1.57060180	5.71402406	3.13052836
O	0.77424708	3.57448678	0.53243316
N	0.63068712	4.79799895	-1.38486978
C	-0.10242587	5.42862902	-2.49055266
C	2.09651773	4.82257405	-1.51112835
H	2.54444931	4.58923844	-0.54291469
H	2.41042246	5.82217755	-1.83854018
H	2.42908510	4.08324439	-2.25471204
H	-0.16740967	6.51717825	-2.34994848
H	-1.09964606	4.99855058	-2.59103970
H	0.44157735	5.22611206	-3.42205957
C	5.52621826	-0.40647766	3.43028693
C	5.07705907	-0.26903388	4.74683537
C	4.99624027	-1.40415713	5.55783239
C	5.35964517	-2.65681249	5.05332899
C	5.82442896	-2.77787868	3.73744905
C	5.91579337	-1.65094517	2.91892168
H	4.78666578	0.70854887	5.12297536
H	4.64315196	-1.30835344	6.58374727
H	5.28639322	-3.54030543	5.68629675
H	6.11828346	-3.75169000	3.34787524
H	3.09099096	-1.15462153	2.92542302
H	1.36461170	-1.61335770	3.02551222
H	2.06057906	-0.45550202	4.17373980

Int4_39

E = -17428.96

G = -16997.55

Nimag = 0

C	1.81697693	1.15843482	-1.20818664
C	3.33394816	0.89289770	-1.37819361
H	1.65381235	2.01748400	-0.54138032
H	3.48042049	0.28848934	-2.28568022
C	3.95856678	0.11836177	-0.20172167
C	1.08314269	0.01312147	-0.57822021
C	1.71542233	-0.71069060	0.57337314
C	3.13176407	-1.13543380	0.10129981
H	4.97725658	-0.15880218	-0.48934284
H	3.60579460	-1.74783264	0.87554094
H	3.05771787	-1.75296845	-0.80619236
H	1.12310520	-1.59357823	0.82741566
H	1.35571936	1.42332670	-2.16710877
H	3.86103328	1.84425790	-1.52193713
N	4.07184981	0.97394431	1.01015356
C	2.84060366	1.32177510	1.74939574
H	3.11953084	1.67737860	2.74646757
H	2.37008235	2.17417393	1.25222302
C	1.81070954	0.16313593	1.90265437
C	2.24750008	-0.78329185	3.05023012
C	0.50419121	0.85248013	2.20986923
H	0.45278736	1.93355744	2.24182415
N	-0.62367434	0.22829807	2.50328833
O	-0.74307465	-1.06830760	2.53028005
O	-1.73283727	0.96148781	2.72597191
S	-1.80837959	2.09061914	-2.17397447
H	-2.97069347	4.22325599	2.32085839
H	-1.12499160	4.16213560	-0.95647772
C	0.26771106	4.22931283	0.72452222
N	-0.05965609	-0.32412302	-1.08957515
H	-0.41629665	0.27760815	-1.86635581
C	-1.06336661	-1.28040799	-0.56728529
C	-1.04307244	-2.59470407	-1.36225607
C	-2.45532012	-0.59510503	-0.64790531
C	-2.12147970	-3.54565618	-0.81023934
H	-1.23230265	-2.37900905	-2.42714929

H	-0.04425862	-3.05017638	-1.28825248
C	-3.51056700	-1.54557587	-0.06361310
H	-2.69162686	-0.38421073	-1.70019141
N	-2.44943780	0.68106213	0.06715214
C	-3.51309185	-2.88654199	-0.82025039
H	-2.13159278	-4.47119495	-1.40482323
H	-1.85679560	-3.82495655	0.22347530
H	-4.49446860	-1.05811820	-0.12609361
H	-3.28547625	-1.71286178	1.00264149
H	-2.39971266	0.62633866	1.11203836
C	-1.98587931	1.84409065	-0.46274016
H	-3.82504533	-2.71157214	-1.86416135
H	-4.25456814	-3.56383479	-0.37081953
N	-1.67658604	2.79216677	0.45303966
H	-1.65613649	2.47375569	1.43879603
C	-1.14978203	4.11625190	0.13130872
H	-0.83921849	-1.45893919	0.49225606
S	5.55328732	1.16910738	1.75319267
O	5.46069964	2.37553426	2.58312856
H	6.33021122	-1.57755869	1.26882650
O	6.56955972	1.04556187	0.69961428
C	-2.09759966	5.27358702	0.60652763
C	-1.39704560	6.61957269	0.32088634
H	-2.06983496	7.45235669	0.57101576
H	-0.48265823	6.73215548	0.92071614
H	-1.12978137	6.70873875	-0.74239420
C	-3.39202466	5.17504004	-0.23077705
H	-3.17894279	5.29899068	-1.30223588
H	-4.09839049	5.95938898	0.07758439
H	-3.87643878	4.19914894	-0.08848535
C	-2.44645790	5.16504515	2.10498859
H	-1.54516269	5.20941302	2.72688892
H	-3.11470300	5.99296050	2.38406758
O	0.43786641	4.07714155	1.95046091
N	1.30918564	4.47202330	-0.12935288
C	1.19050159	4.68852075	-1.58176201
C	2.64346683	4.74969450	0.43058396
H	2.60349734	4.63750484	1.51542776
H	2.94732838	5.77464576	0.17199317
H	3.38042311	4.05016983	0.01293477
H	0.98810354	5.74516743	-1.81192629
H	0.41076572	4.05750042	-2.01509032
H	2.14542989	4.41034295	-2.04351766
C	5.73573460	-0.23714318	2.86195478
C	5.43779519	-0.08786937	4.21952954
C	5.46299616	-1.21389383	5.04640461
C	5.78038895	-2.46863980	4.51696991
C	6.09474824	-2.60113128	3.15834720
C	6.07907590	-1.48353625	2.32254623
H	5.18269966	0.89143235	4.61602219
H	5.22686788	-1.10950316	6.10452799
H	5.78943054	-3.34525148	5.16332774
H	6.35462633	-3.57641158	2.74882166
H	3.22575268	-1.23423331	2.85986391
H	1.50014253	-1.57318945	3.18096539
H	2.31632015	-0.20626120	3.98156490

$PhCO_2H$
E = -3168.54
G = -3119.32
Nimag = 0

O	-0.00210683	0.12479766	0.00000000
C	0.02202758	-1.10188738	0.00000000
H	-0.12264488	-3.85558121	0.00000000
H	1.92186487	-1.14174323	0.00000000
O	1.19098365	-1.81179849	0.00000000
C	-1.18490189	-1.97047812	0.00000000
C	-2.44666296	-1.35205928	0.00000000
C	-3.60610680	-2.12665900	0.00000000
C	-3.51467733	-3.52432039	0.00000000
C	-2.25995441	-4.14483624	0.00000000
C	-1.09657774	-3.37311805	0.00000000
H	-2.50224871	-0.26561325	0.00000000
H	-4.58197328	-1.64275320	0.00000000
H	-4.42077632	-4.12939160	0.00000000
H	-2.18803807	-5.23179559	0.00000000

Int4_41
E = -17412.45
G = -16984.08
Nimag = 0

C	-0.23200261	2.45481402	0.26420244
C	0.76114520	3.59450947	-0.06486977
H	-0.17511979	2.21450260	1.33465482
H	0.47479979	4.04776737	-1.02582991
C	2.21226015	3.10114874	-0.19410915
C	0.06211062	1.18317036	-0.47111502
C	1.49228460	0.72445529	-0.60845116
C	2.27819080	1.93483682	-1.18539354
H	2.82318310	3.93531958	-0.55164120
H	3.31237095	1.63751500	-1.38870474
H	1.83180267	2.24537126	-2.14090458
H	1.54528258	-0.10595750	-1.31623008
H	-1.26647776	2.76438230	0.07888864
H	0.69571045	4.37324925	0.70482885
N	2.76589491	2.69451218	1.12618151
C	2.33319546	1.42113264	1.73894162
H	3.06861347	1.13501807	2.49831763
H	1.40218521	1.57957864	2.28457182
C	2.18141469	0.24304280	0.72927064
C	3.58346668	-0.31816825	0.39109050
C	1.35543966	-0.79890615	1.51308855
H	1.77825553	-0.95278683	2.51198416
N	1.26162895	-2.17750707	0.92592829
O	1.48746638	-2.36191859	-0.28893926
O	0.87968348	-3.07712799	1.70104015
S	4.11058027	3.46845468	1.74168636
O	4.10972366	3.24795866	3.19160920
H	5.36007367	3.54955746	-0.87104147
O	4.10994212	4.82328330	1.17517477
N	-0.93891204	0.55831598	-1.00849446
H	-1.90473814	0.92317716	-0.76208041
C	-0.96149503	-0.77830081	-1.63605606
C	-1.10590100	-0.67309850	-3.16272811
C	-2.13803621	-1.58347817	-1.01183326
C	-1.13249448	-2.08799808	-3.77048276
H	-2.03857255	-0.13543838	-3.40049923
H	-0.27009714	-0.08604734	-3.57206918
C	-2.12847708	-2.99904457	-1.60712013
H	-3.07668125	-1.08101201	-1.28534633
N	-2.08892252	-1.62732123	0.44736593
C	-2.24118748	-2.95285850	-3.14252029
H	-1.27315532	-2.01664860	-4.85929016
H	-0.15373711	-2.56834378	-3.60094922
H	-2.96309371	-3.56685875	-1.17048891
H	-1.19351923	-3.50841583	-1.31528799
H	-1.38273742	-2.25071035	0.84898177
C	-2.33666003	-0.51585002	1.27389952
H	-3.22527208	-2.53644720	-3.41685949
H	-2.19766131	-3.97424046	-3.54954832
S	-3.52808187	0.68592266	0.68372925
N	-1.65641796	-0.50352927	2.38416472
H	0.29335857	-0.52709721	1.70269473
C	-1.99342050	0.45858713	3.42754973
H	-1.86591105	1.23295006	6.13867370
H	-2.77857711	1.13241512	3.07329469
C	-0.72657997	1.25781503	3.78310154
H	-0.02536914	-1.28609810	-1.38867229
H	4.26686413	0.47835367	0.08862832
H	3.53418709	-1.06046070	-0.41274770
H	4.00939335	-0.79550295	1.28403949
C	5.51836400	2.57887564	1.05874042
C	6.17134167	1.62079587	1.83960949
C	7.17452429	0.84130000	1.25700837
C	7.51413399	1.02125652	-0.08731704
C	6.86390488	1.99726011	-0.85384224
C	5.86408932	2.78611850	-0.28337022
H	5.89109196	1.48511567	2.88095868
H	7.68655763	0.08900310	1.85542689
H	8.29054372	0.40545631	-0.53935415

H	7.13719847	2.14569411	-1.89770455
C	-2.59430448	-0.25642422	4.69652476
C	-3.95476009	-0.85518909	4.27577380
H	-4.42738507	-1.35733552	5.13343719
H	-4.63373599	-0.07114078	3.91037491
H	-3.82044663	-1.59084250	3.47113832
C	-1.68275393	-1.38696611	5.21375243
H	-1.47734000	-2.10152575	4.40586155
H	-2.18090481	-1.91332838	6.04267780
H	-0.72371149	-0.98887936	5.56432310
C	-2.81825694	0.79862778	5.80137560
H	-3.46293283	1.61511647	5.44215574
H	-3.30773888	0.33856101	6.67288703
O	0.30504816	0.68338853	4.18210692
N	-0.75622807	2.62285633	3.60702078
C	-1.92717025	3.40380919	3.17302564
C	0.38356980	3.43047995	4.07150772
H	0.05820679	4.10916461	4.87440158
H	0.78267615	4.03191806	3.24362184
H	1.16334192	2.76398979	4.44382096
H	-2.56215781	3.68154022	4.02848064
H	-2.51967847	2.85386116	2.43726835
H	-1.56285225	4.32471185	2.70024701

Int4_42

E = -20599.00

G = -20104.96

Nimag = 0

C	-1.02548005	3.00546993	-0.64988233
C	0.30821892	2.82841485	-1.42208574
H	-0.87091512	3.60202163	0.26567535
H	0.07745568	2.60179438	-2.47383538
C	1.18860738	1.68168490	-0.88708318
C	-1.63442456	1.71945964	-0.19548298
C	-0.74874629	0.61887941	0.31259173
C	0.35309633	0.40345075	-0.76241096
H	2.01048575	1.52629714	-1.59282665
H	0.97337843	-0.45405301	-0.47990916
H	-0.11110882	0.17239960	-1.73211690
H	-1.32624190	-0.30287689	0.42155053
H	-1.75081521	3.56892719	-1.25178516
H	0.86799877	3.77201524	-1.39814192
N	1.80284105	2.01630759	0.41947178
C	0.95295253	2.08248051	1.62354174
H	1.57848476	2.04135760	2.52107920
H	0.44303372	3.04998492	1.65724212
C	-0.07287910	0.90856645	1.71629431
C	0.66131852	-0.37922951	2.16137430
C	-1.05627215	1.41363752	2.78923514
H	-1.56103083	2.34401956	2.49862938
N	-2.11552276	0.50265477	3.25909854
O	-2.20274674	-0.66840472	2.84234151
O	-2.92698981	0.98256156	4.09892466
S	-4.72527685	4.14299445	0.48939904
H	-2.19371361	3.32952821	5.14494479
H	-4.21863886	5.72089894	2.89896412
C	-2.20595564	5.29868888	2.14448224
N	-2.92638427	1.59373077	-0.27883741
H	-3.46002761	2.43403678	-0.58427128
C	-3.78404978	0.45492503	0.12641179
C	-4.12467736	-0.41513569	-1.09582155
C	-5.06519155	1.00862190	0.79978381
C	-5.04093590	-1.57644443	-0.67156017
H	-4.62541466	0.21196569	-1.85141401
H	-3.19226331	-0.79072475	-1.54219892
C	-5.96118550	-0.16204198	1.23159882
H	-5.60329480	1.63934745	0.07881416
N	-4.73611805	1.85198490	1.94808454
C	-6.30877314	-1.06116229	0.03201884
H	-5.30801359	-2.17081952	-1.55753945
H	-4.48673982	-2.24226502	0.01130794
H	-6.87056155	0.24750203	1.69409826
H	-5.43516152	-0.75326720	2.00077707
H	-4.48649347	1.35822024	2.81051466
C	-4.42161191	3.17760593	1.88086915
H	-6.91709459	-0.48593842	-0.68608666
H	-6.92341538	-1.90707326	0.37286924
N	-3.85267064	3.68455585	2.99883182
H	-3.50894804	3.01248454	3.68881353
C	-3.37638866	5.06316396	3.12573091
H	-3.23548577	-0.13970643	0.86359821
S	3.45219072	2.12868256	0.60672058
O	3.72212428	3.17456497	1.60153381
H	4.00223348	-0.46078206	-0.55656035
O	4.03036156	2.20113000	-0.74287496
C	-2.95328280	5.34341257	4.61521276
C	-2.43278687	6.79452525	4.71396959
H	-2.20398627	7.02805225	5.76317709
H	-1.51552293	6.93698633	4.12721225
H	-3.18725457	7.51283195	4.36361042
C	-4.21335744	5.20387991	5.50090690
H	-4.99694323	5.90612863	5.17985320
H	-3.95621693	5.42717406	6.54614546
H	-4.62720348	4.18709095	5.46366306
C	-1.85558738	4.37382535	5.10865438
H	-0.96444944	4.40621106	4.47347816
H	-1.56944821	4.65170982	6.13335930
O	-1.31165748	4.42774679	2.06447721
N	-2.12404032	6.47042857	1.47078635
C	-3.19600993	7.46687106	1.34779436
C	-0.91757795	6.73848153	0.67241778
H	-0.08228209	6.15935386	1.07292638
H	-0.68878881	7.80969663	0.72673722
H	-1.08181658	6.46070469	-0.37988944
H	-3.02156938	8.31817542	2.02075741
H	-4.16920381	7.02023908	1.55408177
H	-3.20941937	7.83178110	0.31272964
C	3.92605346	0.56070335	1.35004444
C	4.01759310	0.46025835	2.74142700
C	4.23808178	-0.79270283	3.31856399
C	4.37009469	-1.92409150	2.50787055
C	4.29360476	-1.80737532	1.11316565
C	4.07002089	-0.56192471	0.52434080
H	3.89825890	1.34179767	3.36292938
H	4.29629417	-0.88110397	4.40007249
H	4.53455912	-2.90106211	2.96114022
H	4.40578130	-2.68880505	0.48279066
H	1.57527357	-0.52431660	1.58117805
H	0.02509095	-1.26209052	2.04058484
H	0.93594763	-0.29784843	3.21677796
H	-0.47151890	1.67556604	3.71096766
O	-0.03073018	0.11636418	5.56217361
O	0.94919920	2.03240271	4.84027373
C	0.95029094	0.90923345	5.45474273
H	1.55215642	-1.46066758	6.62143882
C	2.28353762	0.47712506	6.07004851
C	3.39371570	1.33437302	6.06355127
C	4.61927705	0.91910008	6.59216604
C	4.74897769	-0.36567128	7.13589491
C	3.64453582	-1.22732323	7.15100042
C	2.42081095	-0.80449976	6.62358205
H	3.27973140	2.32417527	5.62518357
H	5.47739309	1.59146079	6.57427282
H	5.70556782	-0.69428165	7.54263789
H	3.74075089	-2.22932296	7.57061115

Int4_43

E = -17412.45

G = -16984.08

Nimag = 0

C	-0.23200261	2.45481402	0.26420244
C	0.76114520	3.59450947	-0.06486977
H	-0.17511979	2.21450260	1.33465482
H	0.47479979	4.04776737	-1.02582991
C	2.21226015	3.10114874	-0.19410915
C	0.06211062	1.18317036	-0.47111502
C	1.49228460	0.72445529	-0.60845116
C	2.27819080	1.93483682	-1.18539354
H	2.82318310	3.93531958	-0.55164120
H	3.31237095	1.63751500	-1.38870474

H	1.83180267	2.24537126	-2.14090458
H	1.54528258	-0.10595750	-1.31623008
H	-1.26647776	2.76438230	0.07888864
H	0.69571045	4.37324925	0.70482885
N	2.76589491	2.69451218	1.12618151
C	2.33319546	1.42113264	1.73894162
H	3.06861347	1.13501807	2.49831763
H	1.40218521	1.57957864	2.28457182
C	2.18141469	0.24304280	0.72927064
C	3.58346668	-0.31816825	0.39109050
C	1.35543966	-0.79890615	1.51308855
H	1.77825553	-0.95278683	2.51198416
N	1.26162895	-2.17750707	0.92592829
O	1.48746638	-2.36191859	-0.28893926
O	0.87968348	-3.07712799	1.70104015
S	4.11058027	3.46845468	1.74168636
O	4.10972366	3.24795866	3.19160920
H	5.36007367	3.54955746	-0.87104147
O	4.10994212	4.82328330	1.17517477
N	-0.93891204	0.55831598	-1.00849446
H	-1.90473814	0.92317716	-0.76208041
C	-0.96149503	-0.77830081	-1.63605606
C	-1.10590100	-0.67309850	-3.16272811
C	-2.13803621	-1.58347817	-1.01183326
C	-1.13249448	-2.08799808	-3.77048276
H	-2.03857255	-0.13543838	-3.40049923
H	-0.27009714	-0.08604734	-3.57206918
C	-2.12847708	-2.99904457	-1.60712013
H	-3.07668125	-1.08101201	-1.28534633
N	-2.08892252	-1.62732123	0.44736593
C	-2.24118748	-2.95285850	-3.14252029
H	-1.27315532	-2.01664860	-4.85929016
H	-0.15373711	-2.56834378	-3.60094922
H	-2.96309371	-3.56685875	-1.17048891
H	-1.19351923	-3.50841583	-1.31528799
H	-1.38273742	-2.25071035	0.84898177
C	-2.33666003	-0.51585002	1.27389952
H	-3.22527208	-2.53644720	-3.41685949
H	-2.19766131	-3.97424046	-3.54954832
S	-3.52808187	0.68592266	0.68372925
N	-1.65641796	-0.50352927	2.38416472
H	0.29335857	-0.52709721	1.70269473
C	-1.99342050	0.45858713	3.42754973
H	-1.86591105	1.23295006	6.13867370
H	-2.77857711	1.13241512	3.07329469
C	-0.72657997	1.25781503	3.78310154
H	-0.02536914	-1.28609810	-1.38867229
H	4.26686413	0.47835367	0.08862832
H	3.53418709	-1.06046070	-0.41274770
H	4.00939335	-0.79550295	1.28403949
C	5.51836400	2.57887564	1.05874042
C	6.17134167	1.62079587	1.83960949
C	7.17452429	0.84130000	1.25700837
C	7.51413399	1.02125652	-0.08731704
C	6.86390488	1.99726011	-0.85384224
C	5.86408932	2.78611850	-0.28337022
H	5.89109196	1.48511567	2.88095868
H	7.68655763	0.08900310	1.85542689
H	8.29054372	0.40545631	-0.53935415
H	7.13719847	2.14569411	-1.89770455
C	-2.59430448	-0.25642422	4.69652476
C	-3.95476009	-0.85518909	4.27577380
H	-4.42738507	-1.35733552	5.13343719
H	-4.63373599	-0.07114078	3.91037491
H	-3.82044663	-1.59084250	3.47113832
C	-1.68275393	-1.38696611	5.21375243
H	-1.47734000	-2.10152575	4.40586155
H	-2.18090481	-1.91332838	6.04267780
H	-0.72371149	-0.98887936	5.56432310
C	-2.81825694	0.79862778	5.80137560
H	-3.46293283	1.61511647	5.44215574
H	-3.30773888	0.33856101	6.67288703
O	0.30504816	0.68338853	4.18210692
N	-0.75622807	2.62285633	3.60702078
C	-1.92717025	3.40380919	3.17302564
C	0.38356980	3.43047995	4.07150772
H	0.05820679	4.10916461	4.87440158
H	0.78267615	4.03191806	3.24362184
H	1.16334192	2.76398979	4.44382096
H	-2.56215781	3.68154022	4.02848064
H	-2.51967847	2.85386116	2.43726835
H	-1.56285225	4.32471185	2.70024701

Int4_44

E = -17427.76

G = -16997.89

Nimag = 0

C	-1.43523191	2.23160921	-1.69138959
C	-0.05168292	2.08898753	-2.27132861
H	0.68206448	-0.72679241	2.52110307
H	-0.11544233	1.94044061	-3.36496906
C	0.73187241	0.90084102	-1.67439318
C	-1.98009062	1.38521962	-0.79111563
C	-1.23338762	0.13525256	-0.32602333
C	-0.22548263	-0.27151058	-1.41936770
H	1.52963135	0.59840743	-2.36078652
H	0.33019582	-1.17161009	-1.13267636
H	-0.76398757	-0.48863427	-2.35295697
H	-1.93822911	-0.68909265	-0.16296830
H	-0.80682984	1.34560671	2.97814506
H	0.52422960	3.01851188	-2.13135550
N	1.41388008	1.20996390	-0.37262767
C	0.54195958	1.54596902	0.77757617
H	1.17739820	1.66294221	1.66378234
H	0.00273349	2.49024739	0.61256276
C	-0.45259605	0.38055050	1.02438019
C	0.34393352	-0.86374632	1.48339158
C	-1.36341197	0.89288123	2.14977631
H	-2.06607455	1.64253719	1.75362859
N	-2.26842045	-0.11282418	2.80436894
O	-2.49801086	-1.20571250	2.26557041
O	-2.81469792	0.25477978	3.87539747
S	-4.56321867	4.44726505	1.25775540
H	-3.62770878	3.28668847	6.11156363
H	-2.87654287	5.17622215	2.94297270
C	-1.14067155	4.02528994	3.61811565
N	-3.17064230	1.71995191	-0.11767739
H	-3.52400204	2.64437175	-0.38783844
C	-4.26890968	0.75425241	0.05805476
C	-4.88623786	0.26050592	-1.26487040
C	-5.37148753	1.39372651	0.94361107
C	-6.01336919	-0.75396681	-1.00280275
H	-5.27877992	1.13197377	-1.81724342
H	-4.09314651	-0.18488396	-1.88499773
C	-6.48803419	0.37796456	1.22810390
H	-5.79053975	2.25637422	0.40758846
N	-4.82813770	1.92025208	2.20246053
C	-7.09391810	-0.15720419	-0.08274001
H	-6.46045579	-1.07849035	-1.95508800
H	-5.58498293	-1.65258815	-0.52541640
H	-7.25989269	0.85920372	1.84687663
H	-6.07197202	-0.46143303	1.81298724
H	-4.57697607	1.21623481	2.90117428
C	-4.24787164	3.14861713	2.33845588
H	-7.59950182	0.67173630	-0.60736249
H	-7.86275799	-0.91099918	0.14566676
N	-3.43751599	3.27211683	3.42561013
H	-3.15037630	2.41363359	3.90606876
C	-2.61892424	4.45048141	3.71328608
H	-3.87234247	-0.11812771	0.59665921
S	2.82248539	2.13098462	-0.45044245
O	2.57418921	3.57310325	-0.25528399
H	3.62944634	-0.52356303	0.33630202
O	3.54704604	1.69482920	-1.65529386
C	-2.97221888	5.11187404	5.09132254
C	-1.98265393	6.27117363	5.33752167
H	-2.25622317	6.80830434	6.25705367
H	-0.95337074	5.90296759	5.45391732
H	-2.00258795	6.99129493	4.50643185
C	-4.40774464	5.67058630	4.97560372

H	-4.47245621	6.43092139	4.18448856
H	-4.70810061	6.13002986	5.92855408
H	-5.12050374	4.86903458	4.73746708
C	-2.90926372	4.10596641	6.25897116
H	-1.90689973	3.67464640	6.36003232
H	-3.17427410	4.61857167	7.19552764
O	-0.72745434	3.08820723	4.33572668
N	-0.33401982	4.68858199	2.74494507
C	-0.76589835	5.75802636	1.82848800
C	1.11811568	4.45103727	2.78424770
H	1.32167569	3.60984143	3.44941930
H	1.63066803	5.35012696	3.16042660
H	1.48224551	4.23306958	1.77485429
H	-0.71395769	6.74480473	2.31174061
H	-1.77848510	5.57589591	1.45964967
H	-0.08703984	5.75624797	0.96779793
C	3.66339451	1.52446328	1.02462658
C	4.02738826	2.42205072	2.03024721
C	4.65557379	1.93091559	3.17913802
C	4.91016392	0.56202896	3.30842177
C	4.54924648	-0.32435603	2.28477106
C	3.92364678	0.15385653	1.13382413
H	3.81813725	3.48136682	1.91458802
H	4.93939637	2.61918898	3.97397427
H	5.39212055	0.18238328	4.20847285
H	4.75078020	-1.38975316	2.38662605
H	1.23245597	-0.99843351	0.86064771
H	-0.26587924	-1.77199307	1.43355218
H	-2.01142717	3.10633238	-2.00513294

Int4_45

E = -17428.37

G = -16999.42

Nimag = 0

C	3.14727685	0.46907650	-2.02115856
C	4.02553312	1.63269169	-2.54284385
H	2.09984380	0.64706022	-2.31137744
H	5.05451804	1.26862416	-2.68843615
C	4.12121014	2.83557689	-1.59034761
C	3.17273671	0.23683911	-0.51518031
C	3.44200440	1.45508163	0.37733828
C	4.55135011	2.34804444	-0.20397013
H	4.85214411	3.53859022	-2.00087943
H	4.76623093	3.18968537	0.46477490
H	5.47942788	1.76573318	-0.30550236
H	3.74334578	1.06583397	1.35709205
H	3.43720743	-0.44753549	-2.54387641
H	3.65216216	1.96291783	-3.52210947
N	2.82365113	3.57609675	-1.50561065
C	1.70465782	2.97617930	-0.74935721
H	0.97097073	3.75767089	-0.54147426
H	1.20279898	2.24838739	-1.40080834
C	2.13786320	2.30510385	0.59417228
C	2.35888147	3.38367295	1.67584753
C	0.93297571	1.41458530	0.93957826
H	2.70435006	2.92877907	2.61053632
N	1.06718026	0.43159921	2.07605840
O	0.28150063	-0.54401655	2.04138090
O	1.86399953	0.64412977	2.99856797
S	-0.37278510	-0.05577337	-3.25517274
H	-3.91878527	-0.62245005	0.40443471
H	-2.18705879	1.34041275	-2.30971548
C	-2.08878365	2.36253866	-0.37766903
N	2.90410999	-0.84629774	0.11783574
H	1.41679187	3.91407107	1.87322336
C	2.51911846	-2.11922597	-0.52207329
C	3.72629277	-2.86461071	-1.13581173
C	1.34547426	-2.06713319	-1.53581854
C	3.32878767	-4.28245129	-1.58290860
H	4.11162340	-2.30032764	-1.99851484
H	4.53007838	-2.90040921	-0.38530792
C	0.94079389	-3.49645313	-1.94576366
H	1.62874578	-1.52151636	-2.43888389
N	0.21319373	-1.33842868	-0.95097551
C	2.13670048	-4.24802572	-2.55650812
H	4.19189285	-4.77987318	-2.05176746
H	3.05497935	-4.87744723	-0.69458601
H	0.10883683	-3.43000418	-2.66274862
H	0.57176833	-4.03381917	-1.05552655
H	0.04176365	-1.48861385	0.04712581
C	-0.60781561	-0.48519270	-1.61099203
H	2.44196810	-3.74205913	-3.48904137
H	1.83559618	-5.27105476	-2.82949522
N	-1.62675486	0.02561384	-0.85477279
H	-1.59919422	-0.13940076	0.15469770
C	-2.45240021	1.16172919	-1.26887955
H	2.16230813	-2.74505043	0.31685910
S	2.75587421	5.19180221	-1.89857199
O	1.34932418	5.51471408	-2.17583484
H	5.32309471	5.64908181	-0.63701433
O	3.80181877	5.43194079	-2.90078376
C	-3.98489965	0.82559260	-1.24122277
C	-4.77207501	2.10185455	-1.60885677
H	-5.84612975	1.87384691	-1.66515033
H	-4.63330133	2.89187579	-0.85713696
H	-4.45782724	2.49312865	-2.58702126
C	-4.23233221	-0.26135812	-2.31039960
H	-3.96488767	0.10516059	-3.31174943
H	-5.29388968	-0.54813526	-2.31520730
H	-3.63083963	-1.15673288	-2.10210713
C	-4.44279067	0.30655221	0.13728193
H	-4.25940906	1.04781338	0.92416232
H	-5.51946892	0.08396695	0.10313247
O	-2.09475269	2.21697213	0.86557034
N	-1.75291749	3.53929865	-0.97439501
C	-1.67809492	3.77920953	-2.42606144
C	-1.57452515	4.74018085	-0.14239639
H	-2.39402860	5.45033314	-0.33095743
H	-0.62886037	5.22736794	-0.40620416
H	-1.57422697	4.44992838	0.90998448
H	-0.89027105	4.51957821	-2.60307729
H	-2.63148963	4.16908402	-2.81133400
H	-1.40537441	2.86832244	-2.96276490
C	3.21421037	6.07977010	-0.39937348
C	2.21890851	6.65693937	0.39414267
C	2.57189622	7.22716070	1.62026442
C	3.90496687	7.21631193	2.04218131
C	4.89652199	6.65284612	1.22855826
C	4.55727309	6.08493130	-0.00019082
H	1.18691617	6.65636746	0.05622859
H	1.80207591	7.67506518	2.24730310
H	4.17491370	7.65272109	3.00297565
H	5.93661417	6.65527741	1.55211630
H	3.09378560	4.12579578	1.35594545
H	0.65964367	0.79103463	0.09301333
H	0.05061475	2.00836996	1.21626601

Int4_46

E = -17409.53

G = -16980.34

Nimag = 0

C	2.81092479	0.46070285	0.11164401
C	3.68572732	-0.33542139	1.09422622
H	2.96965808	1.52089568	0.32327310
H	3.79822197	-1.38020922	0.76745880
C	3.03967832	-0.33548699	2.49019776
C	1.29527310	0.11794497	0.19979873
C	0.75260650	-0.49098455	1.53763584
C	1.76957475	-1.19380207	2.43073119
H	3.73142632	-0.74600952	3.23736732
H	1.33567096	-1.34927980	3.42982351
H	2.04312743	-2.18218552	2.03726373
H	-0.10704639	-1.13782858	1.33795704
H	3.14836042	0.28575797	-0.91862712
H	4.68443920	0.11781360	1.13211223
N	2.66811825	1.08794903	2.86262313
C	1.24901799	1.35912352	3.21330098
H	0.98149683	0.85733955	4.15766545
H	1.13885870	2.43928436	3.35392357
C	0.27139184	0.87038117	2.11580466

C	-1.13887437	0.86844792	2.71433494
C	0.51813689	1.62818283	0.78462511
H	1.24407265	2.43665362	0.83529392
N	-0.55322867	2.08819502	-0.05032354
O	-1.65675441	1.47254476	-0.08243908
O	-0.29933121	3.04484277	-0.83486198
S	1.41401212	0.51655197	-4.19507047
H	-1.92276356	3.84303883	-5.55958613
H	1.58076286	3.07062559	-4.46889487
C	0.74709192	4.64837636	-3.19949790
N	0.90354520	-0.54387752	-0.96249998
H	1.35848215	-0.22783957	-1.82795655
C	-0.41130974	-1.17395396	-1.17863625
C	-0.35111446	-2.70570462	-1.01164232
C	-0.93858353	-0.84077505	-2.59634356
C	-1.74227329	-3.33309757	-1.20889206
H	0.36158729	-3.11117328	-1.75037773
H	0.04764718	-2.94796719	-0.01574842
C	-2.34378405	-1.43513039	-2.79511600
H	-0.25075610	-1.28065249	-3.33094006
N	-0.94596039	0.59864838	-2.86780948
C	-2.33003046	-2.96018286	-2.58184650
H	-1.68274650	-4.42723659	-1.10337417
H	-2.41664894	-2.96923795	-0.41379574
H	-2.69490623	-1.18667102	-3.80781083
H	-3.03911922	-0.96321090	-2.07914299
H	-1.61380337	1.15330549	-2.32423997
C	-0.01747886	1.26663437	-3.60074108
H	-1.71981225	-3.42586132	-3.37475911
H	-3.35089025	-3.35878704	-2.68431074
N	-0.31428071	2.57127438	-3.84257138
H	-1.13687207	2.94916158	-3.36661989
C	0.63246643	3.58771291	-4.31775186
H	-1.12634740	-0.76517834	-0.45500493
S	3.81063139	1.92143728	3.77005108
O	3.34824481	3.31102522	3.87139461
H	5.34962334	-0.19134703	5.02859489
O	5.12277651	1.60247333	3.19659102
C	0.23603394	4.17732650	-5.71526774
C	1.20253413	5.33751693	-6.03753130
H	1.02890495	5.69641713	-7.06225835
H	1.05557204	6.17992843	-5.34844381
H	2.25022417	5.00693960	-5.96639771
C	0.42019688	3.05248651	-6.75944770
H	1.46463832	2.71231240	-6.79612255
H	0.13590993	3.42109362	-7.75612500
H	-0.20907012	2.18550008	-6.51638401
C	-1.22634392	4.66845602	-5.76766350
H	-1.40037797	5.46779247	-5.04005510
H	-1.44668015	5.04481260	-6.77787513
O	-0.15399495	5.49714564	-3.04766405
N	1.85769985	4.62707667	-2.40733370
C	2.77751056	3.49361107	-2.24704933
C	1.94252411	5.61934816	-1.32546375
H	1.47468155	6.55338777	-1.64590449
H	2.99947915	5.78936702	-1.08947968
H	1.42359862	5.24748628	-0.42793903
H	3.81679626	3.83896754	-2.33758731
H	2.59061506	2.70512558	-2.97633251
H	2.63348576	3.06033468	-1.24831963
C	3.71722300	1.17384143	5.40379098
C	2.72146280	1.60128685	6.29199411
C	2.57530542	0.94140588	7.51449277
C	3.41450070	-0.13038518	7.84099779
C	4.41155801	-0.54144339	6.94937155
C	4.56862313	0.10854150	5.72242772
H	2.08420517	2.44411791	6.03742892
H	1.80763328	1.26887578	8.21424326
H	3.29608532	-0.64089013	8.79588142
H	5.07253058	-1.36720064	7.20905794
H	-1.14458101	0.24252615	3.61805808
H	-1.87032882	0.47131783	2.00580315
H	-1.44833755	1.88564117	2.99627810

TS4_13

E = -20590.91
G = -20097.61
Nimag = 1, 1345i cm-1

C	-1.04722105	3.02829881	-0.64585216
C	0.26971387	2.86489362	-1.45043350
H	-0.86471460	3.57519423	0.29532039
H	0.01522791	2.71072240	-2.50983950
C	1.13064913	1.66284886	-1.00911195
C	-1.67537823	1.73493838	-0.23927683
C	-0.80416391	0.59355948	0.18691277
C	0.25947200	0.40468704	-0.93016256
H	1.92991752	1.52322060	-1.74386314
H	0.86291545	-0.48368243	-0.71471937
H	-0.23874868	0.24169363	-1.89716239
H	-1.39972651	-0.31838689	0.27997235
H	-1.77137907	3.63502249	-1.20576021
H	0.85449540	3.79123198	-1.38023094
N	1.78673369	1.88637603	0.29971898
C	0.95868358	1.96067726	1.51637593
H	1.60450542	1.87472890	2.39521807
H	0.48059155	2.94194206	1.58510801
C	-0.09268571	0.81195743	1.59497575
C	0.63593277	-0.50945065	1.94735875
C	-1.04970687	1.27086550	2.69921209
H	-1.38002458	2.31084733	2.63251358
N	-2.09388764	0.45379218	3.12594972
O	-2.20623898	-0.75278238	2.75990171
O	-2.94494855	0.95449500	3.96750954
S	-4.73672854	4.20459012	0.57182248
H	-2.08801002	3.21515612	5.15201271
H	-4.08497111	5.67178775	2.96621533
C	-2.07076754	5.25153439	2.22039970
N	-2.97118344	1.64264968	-0.28307842
H	-3.49712603	2.50589188	-0.53446044
C	-3.83436692	0.50202989	0.10850899
C	-4.19548147	-0.34258783	-1.12549501
C	-5.10094815	1.05923070	0.80451848
C	-5.12178523	-1.50040854	-0.71309536
H	-4.69578131	0.30274193	-1.86610598
H	-3.27228868	-0.72236009	-1.58760597
C	-6.00790446	-0.10853645	1.22218947
H	-5.63817219	1.71297791	0.10367975
N	-4.74345477	1.86865120	1.96870221
C	-6.37733507	-0.98196509	0.01029575
H	-5.40353375	-2.07722094	-1.60633945
H	-4.56959805	-2.18340917	-0.04572929
H	-6.90780193	0.30329947	1.70115156
H	-5.48123629	-0.71867498	1.97566545
H	-4.37195226	1.34124789	2.77412620
C	-4.38692282	3.18436403	1.91716641
H	-6.98420629	-0.38681191	-0.69296647
H	-6.99986396	-1.82646366	0.34077806
N	-3.74139875	3.63306501	3.01781080
H	-3.36635661	2.91089359	3.64440252
C	-3.25152317	5.00047301	3.18422008
H	-3.28426717	-0.10889342	0.83306049
S	3.43127749	2.05615866	0.46062023
O	3.70382941	3.16971293	1.38052769
H	4.02429067	-0.60025163	-0.51744871
O	3.99956615	2.04623321	-0.89509475
C	-2.84258927	5.24376454	4.68384680
C	-2.32133572	6.69147763	4.82077516
H	-2.09597084	6.90052231	5.87600468
H	-1.40180140	6.84741487	4.24056066
H	-3.07390552	7.41856827	4.48432855
C	-4.11203807	5.08342432	5.55220861
H	-4.89289859	5.79207472	5.23844708
H	-3.86732752	5.28318468	6.60527924
H	-4.52279767	4.06716016	5.48470034
C	-1.75243309	4.26085382	5.16736502
H	-0.84749551	4.32554671	4.55401863
H	-1.49204951	4.50173123	6.20847835
O	-1.16965212	4.38672031	2.14244798
N	-1.99442591	6.42516435	1.54753191
C	-3.06569778	7.42509008	1.44275244

C	-0.78779549	6.70554068	0.75382547
H	0.04138846	6.10338181	1.13209661
H	-0.54562536	7.77187661	0.84076490
H	-0.95966136	6.46379264	-0.30610021
H	-2.90549269	8.25102820	2.15010716
H	-4.04141212	6.96754254	1.61107912
H	-3.05969238	7.82841476	0.42218427
C	3.92141220	0.54762327	1.31313182
C	4.00736639	0.54310326	2.70896662
C	4.24082999	-0.66412391	3.37245785
C	4.39824405	-1.84550630	2.64165316
C	4.33293215	-1.82397478	1.24182000
C	4.08993951	-0.62604290	0.56824890
H	3.88396353	1.46631066	3.26603507
H	4.29302297	-0.67771165	4.45861282
H	4.57537939	-2.78644788	3.16129056
H	4.46577858	-2.74380936	0.67344821
H	1.51765398	-0.64579600	1.31617102
H	-0.02839256	-1.37061847	1.82672123
H	0.97068232	-0.48125080	2.98822755
H	-0.25958812	1.43451212	3.81819584
O	-0.02816183	-0.36452255	5.46826870
O	0.65201591	1.64743194	4.66382985
C	0.80334752	0.55796714	5.38653645
H	1.67056668	-1.45996199	6.92706763
C	2.13250462	0.46694437	6.09879189
C	3.09668306	1.48001068	5.98535501
C	4.34501582	1.33714586	6.59550233
C	4.63769775	0.18261382	7.33202176
C	3.67380436	-0.82535803	7.46112719
C	2.42800597	-0.68235149	6.84712274
H	2.86157047	2.36849449	5.40426806
H	5.09457166	2.12135891	6.49112440
H	5.61368755	0.06798754	7.80336867
H	3.89679996	-1.72369264	8.03680684

TS4_14

E = -17401.60

G = -16974.18

Nimag = 1, 1608i cm-1

C	-0.26799336	2.50835067	0.15283642
C	0.77442523	3.61481746	-0.14563408
H	-0.27340496	2.28791071	1.22812819
H	0.54460152	4.05781699	-1.12617338
C	2.21830513	3.08369678	-0.20041818
C	0.03467790	1.21305088	-0.53273307
C	1.45140406	0.70976963	-0.55728380
C	2.29307248	1.88033469	-1.14505126
H	2.85952706	3.89210549	-0.56441576
H	3.32599979	1.54830574	-1.29209450
H	1.89658420	2.16528948	-2.13043217
H	1.52477505	-0.15442743	-1.21983660
H	-1.28091843	2.84377894	-0.09831817
H	0.69321939	4.40830605	0.60710475
N	2.71274465	2.71123505	1.15119477
C	2.19020003	1.48662106	1.79446650
H	2.85730338	1.21700742	2.61888621
H	1.23429657	1.71876072	2.25833256
C	2.04851797	0.26760676	0.84138593
C	3.45419007	-0.33933141	0.59005893
C	1.16803888	-0.73716751	1.61438323
H	1.46662344	-0.82294902	2.66462356
N	1.04008879	-2.04960476	1.08724084
O	1.26557109	-2.29246923	-0.14134037
O	0.55187767	-2.94615741	1.85079865
S	4.06492343	3.45503625	1.78038923
O	4.02812554	3.26321388	3.23411197
H	5.37204456	3.46008538	-0.80417724
O	4.11919059	4.79896504	1.18928142
N	-0.94436769	0.61932759	-1.14766148
H	-1.88500520	1.04686830	-1.01769019
C	-0.98570058	-0.73612597	-1.73383351
C	-1.20017113	-0.68724681	-3.25279884
C	-2.13114446	-1.51834403	-1.02956508
C	-1.25777938	-2.12501663	-3.80415829
H	-2.14292260	-0.15780086	-3.46946300
H	-0.38308268	-0.11955992	-3.72210968
C	-2.15042881	-2.95647065	-1.56341720
H	-3.08597900	-1.02670298	-1.26359623
N	-1.97503234	-1.48652225	0.42087544
C	-2.33531323	-2.96519279	-3.09261933
H	-1.45206058	-2.09320255	-4.88649811
H	-0.27220340	-2.60078925	-3.66542885
H	-2.96540123	-3.50402040	-1.06749403
H	-1.20255128	-3.45220641	-1.29430576
H	-1.29061424	-2.13420493	0.82113789
C	-2.25689937	-0.38309299	1.20660160
H	-3.33202696	-2.55959855	-3.33608440
H	-2.30898571	-4.00097089	-3.46262167
S	-3.55249072	0.70320732	0.74320928
N	-1.44496390	-0.25396980	2.25262203
H	-0.14777079	-0.44862145	1.92290881
C	-1.82982253	0.54181862	3.42139689
H	-1.67709614	0.98709396	6.20244575
H	-2.69215849	1.15383439	3.14551162
C	-0.64775752	1.43803153	3.83217749
H	-0.04151004	-1.23255651	-1.49329185
H	4.16040591	0.40687740	0.21678316
H	3.39946827	-1.16450982	-0.12828828
H	3.85028888	-0.72453219	1.53909001
C	5.46200658	2.51607409	1.14291653
C	6.07189617	1.55327462	1.95203940
C	7.06767539	0.73995602	1.40423544
C	7.44203912	0.89031353	0.06536082
C	6.83412656	1.87024971	-0.73010122
C	5.84233700	2.69280522	-0.19409796
H	5.76295587	1.43900318	2.98779235
H	7.54641601	-0.01608883	2.02512890
H	8.21298573	0.24865288	-0.35926812
H	7.13416947	1.99571128	-1.76960777
C	-2.32107042	-0.37381156	4.60388301
C	-3.63936763	-1.04160363	4.15044436
H	-4.04555331	-1.65430872	4.96888278
H	-4.39051714	-0.28955342	3.86963725
H	-3.47109313	-1.69519524	3.28380266
C	-1.30262039	-1.47580953	4.96141947
H	-1.04511390	-2.06183171	4.06905879
H	-1.74244229	-2.15033608	5.71208066
H	-0.37972925	-1.04394020	5.36252095
C	-2.60148206	0.52692170	5.82636790
H	-3.31042956	1.32941479	5.56924084
H	-3.04298855	-0.06616329	6.64076269
O	0.37624117	0.94633505	4.34234704
N	-0.73948450	2.78162729	3.55902165
C	-1.93873241	3.47138463	3.05106046
C	0.34176243	3.67593642	4.00641332
H	-0.03023800	4.35221618	4.79072935
H	0.69722899	4.27828457	3.16035103
H	1.16454531	3.07441309	4.39567549
H	-2.59893719	3.77669973	3.87769197
H	-2.49391494	2.84554160	2.34771960
H	-1.61067980	4.37356229	2.52001992

TS4_15

E = -20584.81

G = -20094.20

Nimag = 1, 1414i cm-1

C	2.39622631	-1.48832843	-1.30837674
C	3.78815221	-2.15571839	-1.41143695
H	2.47901121	-0.49179599	-0.85907996
H	3.74884265	-2.95528667	-2.16647116
C	4.22808252	-2.78719270	-0.08119438
C	1.43349596	-2.26769944	-0.45833943
C	1.88061379	-2.86346345	0.85836371
C	3.12158898	-3.71709624	0.43586482
H	5.14032662	-3.36248672	-0.26529833
H	3.45760914	-4.32188464	1.28286581
H	2.84154892	-4.41306973	-0.36818800
H	1.10411972	-3.52992784	1.24825287
H	1.96477406	-1.33524782	-2.30658088

H	4.52960119	-1.41685799	-1.73829732
N	4.57200251	-1.73805801	0.92132329
C	3.48669434	-1.00664093	1.62691291
H	3.91241856	-0.54437978	2.52344877
H	3.13330157	-0.18802352	0.98777792
C	2.30326723	-1.91945834	2.04617955
C	2.72919823	-2.82465620	3.23557721
C	1.17583020	-1.05794104	2.62976960
H	1.42300973	-0.63673201	3.60804582
N	0.57196230	-0.06176778	1.85567397
O	0.48633447	-0.23955938	0.58757129
O	0.00018010	0.92546464	2.40403370
S	-1.23573720	-1.03501539	-3.55641362
H	-1.02621085	3.26213050	-0.55205494
H	-0.23731263	1.26514032	-3.65615088
C	1.51978731	1.59498127	-2.39362434
N	0.32406608	-2.65159544	-1.02944228
H	0.16886413	-2.35001247	-2.00849262
C	-0.88211578	-3.18066136	-0.36401210
C	-1.09328886	-4.68174220	-0.60502371
C	-2.11389691	-2.39170459	-0.88401449
C	-2.34785774	-5.15014949	0.15633984
H	-1.19946146	-4.85301735	-1.68882202
H	-0.21002943	-5.24046667	-0.26267916
C	-3.32217068	-2.77125824	-0.02065320
H	-2.30306316	-2.68502910	-1.92411699
N	-1.86383296	-0.94494891	-0.91629294
C	-3.59361586	-4.28753365	-0.13565491
H	-2.55664276	-6.20177123	-0.09194880
H	-2.12419405	-5.11765890	1.22725625
H	-4.19869613	-2.19782814	-0.35610665
H	-3.12540751	-2.49467856	1.02571391
H	-1.64972932	-0.52522604	-0.00529080
C	-1.26385850	-0.32541325	-1.98408845
H	-3.95330342	-4.49894932	-1.15678837
H	-4.39997284	-4.56710115	0.55855035
N	-0.69032982	0.86798700	-1.69870671
H	-0.37196007	0.98785355	-0.72691695
C	0.00927895	1.69304952	-2.68611883
H	-0.76599388	-2.98062107	0.70557069
S	6.13079029	-1.64731627	1.50419941
O	6.30759269	-0.30289933	2.06622531
H	6.41023288	-4.53029391	1.56502572
O	7.01213660	-2.15031477	0.44174295
C	-0.51909882	3.16972151	-2.68445681
C	0.31181819	3.98626508	-3.69748418
H	-0.07327095	5.01461286	-3.75212108
H	1.36958947	4.03685604	-3.40245574
H	0.25196876	3.54808346	-4.70413303
C	-1.99444462	3.12793304	-3.14093207
H	-2.08172999	2.69657056	-4.14899988
H	-2.41006476	4.14576513	-3.16243904
H	-2.59947925	2.52152159	-2.45291377
C	-0.42880509	3.81860013	-1.28788223
H	0.60736491	3.85493447	-0.93157568
H	-0.82556631	4.84339215	-1.33661846
O	1.92284037	1.78862985	-1.22908588
N	2.36512201	1.27368871	-3.41623814
C	1.98258015	1.03014057	-4.81449009
C	3.81546858	1.30207523	-3.17504257
H	3.99540104	1.48194316	-2.11366758
H	4.27911230	2.10328818	-3.77021770
H	4.25783551	0.34270333	-3.47463072
H	2.09905318	1.94136926	-5.41981975
H	0.95819311	0.66256789	-4.88830121
H	2.64622194	0.25575005	-5.22060798
C	6.19617866	-2.81648725	2.87140909
C	6.05136570	-2.35259685	4.18215577
C	5.96317159	-3.27960690	5.22402704
C	6.01817321	-4.65028096	4.95288438
C	6.18126666	-5.10155612	3.63685598
C	6.27712307	-4.18622438	2.58764592
H	5.99888992	-1.28473078	4.37828857
H	5.84522396	-2.92811893	6.24816400
H	5.93944135	-5.36950053	5.76711457
H	6.23629450	-6.16900950	3.42693518
H	3.63565191	-3.39284147	3.02189650
H	1.91682672	-3.51958159	3.48210101
H	2.93926595	-2.19856660	4.11205264
H	-0.00805773	-1.81184734	2.94410135
O	-0.32558604	-4.32126381	3.01682097
O	-1.13985757	-2.20692560	3.21667697
C	-1.24892358	-3.52010047	3.25236808
H	-2.03193146	-6.06893382	3.60599480
C	-2.64713169	-4.00995267	3.53559430
C	-3.73345140	-3.12277559	3.58942489
C	-5.03467667	-3.60905848	3.73389699
C	-5.26057234	-4.98636727	3.83798571
C	-4.17854111	-5.87517564	3.80720912
C	-2.87961641	-5.38869212	3.65678451
H	-3.55168047	-2.05480209	3.49759199
H	-5.87397589	-2.91449125	3.75808562
H	-6.27674972	-5.36679111	3.94043388
H	-4.35141400	-6.94793512	3.88993078

TS4_16

E = -17424.09

G = -16996.88

Nimag = 1, 700i cm-1

C	2.46387647	-0.28022707	-2.36595629
C	3.93749214	-0.16555289	-1.91052704
H	2.04327648	0.73365235	-2.49071090
H	4.48569986	-1.06234082	-2.23710155
C	4.12225740	-0.06797747	-0.38740385
C	1.53215232	-1.00616946	-1.43031261
C	1.85980557	-1.03199178	0.06562692
C	3.37136473	-1.21777741	0.28424958
H	5.19301963	-0.12532765	-0.17203082
H	3.60025631	-1.27326430	1.35431073
H	3.69205048	-2.16812380	-0.16740516
H	1.32249219	-1.87450540	0.51204102
H	2.42361065	-0.72865505	-3.36362698
H	4.40050523	0.70128821	-2.40066565
N	3.65133602	1.24324530	0.15053609
C	2.19975187	1.49988577	0.26535675
H	2.04741634	2.35071364	0.93576677
H	1.82283936	1.81485375	-0.71737216
C	1.36552364	0.27851623	0.78409814
C	1.50792075	0.11161797	2.32045038
C	-0.06309685	0.68816835	0.49694888
H	-0.28989852	1.74774499	0.55203555
N	-1.12260763	-0.03590410	0.26203957
O	-2.28056545	0.45707042	-0.06719509
O	-1.04761874	-1.43755293	0.28028714
S	0.72890521	2.76398717	-3.56211925
H	-3.68430183	3.63140670	-1.00242858
H	-0.17026516	4.51206324	-2.05966858
C	-0.33904439	4.25104417	0.10177120
N	0.40553438	-1.54178276	-1.75269145
H	-0.42072885	-1.65358623	-0.67162080
C	-0.25081073	-1.54643578	-3.07506869
C	0.38822463	-2.53345322	-4.07467708
C	-0.41678053	-0.14632144	-3.71761784
C	-0.47246326	-2.63198505	-5.34763960
H	1.40079830	-2.19579674	-4.34048487
H	0.48538545	-3.51526028	-3.58881083
C	-1.30681632	-0.25981504	-4.97015674
H	0.55411420	0.24770814	-4.03062803
N	-0.95255555	0.80782731	-2.74676297
C	-0.69798198	-1.24728724	-5.98191233
H	0.01175794	-3.30934322	-6.06735941
H	-1.44803265	-3.07772755	-5.08848149
H	-1.40802191	0.74291678	-5.41081670
H	-2.31338895	-0.59544139	-4.66821528
H	-1.70685384	0.49185453	-2.12316372
C	-0.54466624	2.09506659	-2.61405529
H	0.26769737	-0.84752920	-6.33708343
H	-1.35353902	-1.33358442	-6.86174329
N	-1.20864978	2.80518301	-1.66339707
H	-1.81090474	2.27639510	-1.01727774

C	-0.90908659	4.19415429	-1.32568656
H	-1.26581717	-1.92152517	-2.85984742
S	4.71067345	2.22786401	0.97798413
O	4.18954095	3.59824070	0.89784599
H	5.86748879	-0.01098373	2.39474694
O	6.05916434	1.90234910	0.49659996
C	-2.16011812	5.12622536	-1.50849252
C	-1.77347227	6.55616798	-1.07313531
H	-2.61154328	7.24247034	-1.26140014
H	-1.53424268	6.60037168	-0.00120794
H	-0.90349139	6.92042130	-1.63844710
C	-2.51658987	5.12291328	-3.01173694
H	-1.67835110	5.49983211	-3.61526870
H	-3.39170055	5.76430021	-3.19087286
H	-2.75567632	4.10688002	-3.35438360
C	-3.37418787	4.63911800	-0.69109154
H	-3.14868972	4.61474219	0.38154377
H	-4.22361680	5.31699151	-0.86162946
O	-0.96575636	3.68742780	1.02675859
N	0.82917888	4.91574923	0.31527897
C	1.68035788	5.52825431	-0.71629611
C	1.28291432	5.13933067	1.69716655
H	1.27670090	6.21760233	1.91812363
H	2.30594169	4.76358507	1.80622980
H	0.60880735	4.61854065	2.38008996
H	2.72586393	5.37194632	-0.42512608
H	1.48756499	6.60844413	-0.79515090
H	1.53040908	5.05165668	-1.68656517
C	4.59610604	1.71428563	2.69978363
C	3.79676356	2.43876607	3.58837237
C	3.61591609	1.95679883	4.88761296
C	4.22975925	0.76585529	5.28693071
C	5.04357455	0.05856978	4.39239208
C	5.23409986	0.53068577	3.09311473
H	3.32399174	3.36157101	3.26713943
H	2.99091416	2.51244182	5.58550415
H	4.08052154	0.38959762	6.29811961
H	5.53144736	-0.86281393	4.70748634
H	2.54801444	-0.03451196	2.62432973
H	0.91496504	-0.75105459	2.65248665
H	1.13156147	1.00954764	2.82674680

TS4_17

E = -20581.89

G = -20090.25

Nimag = 1, 1033i cm-1

C	0.44679892	-3.67692543	-0.48476314
C	0.26026765	-5.12049022	0.06340587
H	0.81851915	-3.00764791	0.31250219
H	0.39196595	-5.81731333	-0.77688659
C	-1.11977641	-5.42739650	0.68144194
C	-0.80245974	-3.04083155	-0.99324915
C	-2.11545934	-3.38097199	-0.35228796
C	-2.22338540	-4.91891891	-0.24642095
H	-1.18950909	-6.51195867	0.80787110
H	-3.21591010	-5.19301796	0.12592277
H	-2.11054509	-5.36793447	-1.24441090
H	-2.91906859	-2.99791733	-0.99028044
H	1.22639733	-3.67722892	-1.25012721
H	1.05317582	-5.32900822	0.79217275
N	-1.27387680	-4.82797567	2.02981139
C	-1.36003334	-3.35704705	2.12347346
H	-1.70200154	-3.08164194	3.12574853
H	-0.34587443	-2.95415747	2.05179294
C	-2.28891666	-2.68772451	1.06378555
C	-3.78062915	-2.82609857	1.45127795
C	-1.85157654	-1.20846616	1.07988358
H	-0.82394199	-1.03242492	1.40121482
N	-2.16843404	-0.35919262	0.01879445
O	-1.49763069	0.73397103	-0.11303615
O	-3.12080714	-0.62216311	-0.78323728
S	3.27627649	-1.09388964	0.48053456
H	-0.80884672	1.89666751	2.32804267
H	2.91696022	0.93386532	2.41672121
C	1.62215799	-0.60754716	3.27445073
N	-0.83168909	-2.17021019	-1.95909908
H	-1.76174545	-1.76392280	-2.13937437
C	0.24196413	-1.59926342	-2.82199006
C	0.63568605	-2.57124987	-3.95076908
C	1.48651836	-1.10177320	-2.06094928
C	1.59006876	-1.86427910	-4.93214916
H	1.12628085	-3.45535621	-3.51489907
H	-0.27293217	-2.91331174	-4.46611244
C	2.38817521	-0.34328103	-3.05642389
H	2.06978431	-1.94557008	-1.67618724
N	1.09529634	-0.30439655	-0.90781228
C	2.81253675	-1.27103711	-4.20872819
H	1.90780671	-2.57965883	-5.70496026
H	1.03936666	-1.05690386	-5.44350390
H	3.26404298	0.02333605	-2.50330765
H	1.84149923	0.53258559	-3.44363490
H	0.22457305	0.23921401	-0.95180504
C	1.82620607	-0.21577536	0.23802837
H	3.42936434	-2.09000649	-3.80039836
H	3.44224522	-0.71911262	-4.92222607
N	1.30255687	0.61523241	1.17633734
H	0.32484148	0.89005793	1.03983000
C	1.84805074	0.73292900	2.52963283
H	-0.24906989	-0.72505920	-3.27452129
S	-1.72992587	-5.76368077	3.33034866
O	-1.27600485	-5.07080935	4.54141507
H	-3.69170588	-7.23485678	1.79125403
O	-1.29878683	-7.13656108	3.03160862
C	1.19484377	1.96152155	3.26076070
C	1.74607781	2.04655223	4.70156176
H	1.30457949	2.91657627	5.20779296
H	1.49617949	1.14997199	5.28442115
H	2.83766882	2.17359121	4.70791976
C	1.59667318	3.24356999	2.49597684
H	2.69063927	3.36130606	2.47610264
H	1.16367341	4.12377597	2.99308323
H	1.23448524	3.22296071	1.45923901
C	-0.34277861	1.84389528	3.32220517
H	-0.65621900	0.90225204	3.78158734
H	-0.75207254	2.67534840	3.91288419
O	0.52185365	-1.17777487	3.15524713
N	2.61222805	-1.09757599	4.07408247
C	3.99436364	-0.60273474	4.09886068
C	2.42201011	-2.42272901	4.68262765
H	1.36899072	-2.70015849	4.60282356
H	2.72782043	-2.38960026	5.73651421
H	3.03642904	-3.17059879	4.15646051
H	4.44053112	-0.87680687	5.06258394
H	4.03382356	0.48295355	4.01100417
H	4.58111385	-1.05390286	3.28401096
C	-3.53034857	-5.73930502	3.34748265
C	-4.19926743	-4.85492159	4.19853676
C	-5.58998733	-4.75126602	4.11107544
C	-6.29602344	-5.52341115	3.18358382
C	-5.61535410	-6.42042254	2.35000082
C	-4.22697582	-6.53694693	2.43069848
H	-3.63711059	-4.25213996	4.90700330
H	-6.11993440	-4.05951234	4.76447150
H	-7.37895464	-5.43144357	3.11171916
H	-6.16701939	-7.03107716	1.63646669
H	-4.10138125	-3.87092735	1.47906227
H	-4.40082645	-2.28157331	0.72904569
H	-3.94103529	-2.38986519	2.44292398
H	-2.45824563	-0.67993415	2.15384673
O	-4.02831451	1.20101533	1.95806031
O	-2.89873670	-0.25320637	3.28897756
C	-3.57890419	0.84612299	3.06535478
H	-2.63385037	0.44575325	5.60285533
C	-3.75776055	1.72205920	4.28617775
C	-4.46318596	2.92907194	4.16909340
C	-4.59500026	3.78237730	5.26728913
C	-4.02151743	3.43409480	6.49712865
C	-3.32015629	2.22828554	6.62168234
C	-3.18909967	1.37699559	5.52169774
H	-4.89498124	3.18783657	3.20392111

H	-5.14145942	4.72013073	5.16589823
H	-4.11991928	4.10052052	7.35406425
H	-2.87005159	1.95609647	7.57644263

TS4_19

E = -17409.13

G = -16979.26

Nimag = 1, 152i cm-1

C	2.78917925	0.49138083	0.07559651
C	3.67859764	-0.29333689	1.05549336
H	2.92694882	1.55300976	0.29064614
H	3.80247741	-1.33735274	0.73082386
C	3.03842583	-0.29391092	2.45325065
C	1.28578140	0.11762896	0.16510783
C	0.74381596	-0.46161498	1.51159148
C	1.77146689	-1.15844216	2.39961056
H	3.73363081	-0.70066942	3.19947531
H	1.34297355	-1.31637749	3.40040589
H	2.04831280	-2.14541449	2.00478334
H	-0.11415857	-1.11437902	1.32308639
H	3.13050952	0.32507528	-0.95467386
H	4.67109501	0.17348612	1.08629351
N	2.66332815	1.12897230	2.82136212
C	1.24671909	1.39144477	3.18317822
H	0.99082271	0.88919858	4.13058837
H	1.12994459	2.47080904	3.32364674
C	0.26139640	0.89662594	2.09481194
C	-1.13667417	0.87423652	2.72238028
C	0.46657751	1.68075184	0.77425894
H	1.19091569	2.49084079	0.80750308
N	-0.61819415	2.09994951	-0.03936143
O	-1.69308211	1.42831312	-0.08376623
O	-0.42240363	3.08215570	-0.81739280
S	1.38483670	0.49541451	-4.22309440
H	-1.88075854	3.86393685	-5.47929946
H	1.62838340	3.06885906	-4.42022958
C	0.82593553	4.67218652	-3.16619396
N	0.88445724	-0.52939015	-0.98443284
H	1.37174543	-0.27091979	-1.85137501
C	-0.41825827	-1.17893389	-1.20113610
C	-0.34029412	-2.71172193	-1.05998063
C	-0.96057112	-0.82622799	-2.60944950
C	-1.73220697	-3.34180702	-1.24996054
H	0.36519325	-3.10186439	-1.81352590
H	0.06997619	-2.96634095	-0.07166596
C	-2.37001627	-1.41434435	-2.79127470
H	-0.28619580	-1.26587786	-3.35642690
N	-0.95600254	0.61411326	-2.86801212
C	-2.34823740	-2.94342057	-2.60381591
H	-1.66442571	-4.43756087	-1.17022061
H	-2.39379075	-2.99989813	-0.43480142
H	-2.74013253	-1.15077670	-3.79324592
H	-3.05177069	-0.95474813	-2.05478904
H	-1.59820484	1.17114274	-2.29618861
C	-0.01006119	1.27562801	-3.58763749
H	-1.75402936	-3.39299717	-3.41782094
H	-3.36993851	-3.34328001	-2.69151017
N	-0.26407706	2.59934302	-3.77276875
H	-1.06389690	2.98407305	-3.26515678
C	0.68534865	3.60055559	-4.27670449
H	-1.12747419	-0.78802198	-0.46341056
S	3.80859679	1.97538730	3.71402748
O	3.33636169	3.36167303	3.81232633
H	5.37515697	-0.11996770	4.96670775
O	5.11745325	1.66320648	3.12952506
C	0.27796335	4.17075053	-5.67762141
C	1.25558311	5.31149954	-6.03606027
H	1.07738678	5.64677614	-7.06804505
H	1.12637115	6.17143832	-5.36616549
H	2.29969470	4.96832170	-5.96757238
C	0.43082924	3.02939015	-6.70863546
H	1.46806611	2.66903057	-6.75149830
H	0.14324122	3.39240432	-7.70651554
H	-0.21158569	2.17687373	-6.45002235
C	-1.17971415	4.67785482	-5.71527787
H	-1.33209878	5.49287250	-5.00050041
H	-1.41355833	5.03724915	-6.72864208
O	-0.00054599	5.59907982	-3.06491406
N	1.87515326	4.53376420	-2.30157037
C	2.64514543	3.28473547	-2.17217663
C	1.92931685	5.43787063	-1.14134819
H	1.49707986	6.40260798	-1.41720833
H	2.97530592	5.56732605	-0.84239900
H	1.35404989	5.01612233	-0.30288383
H	3.44823397	3.45435108	-1.44861205
H	3.10013304	2.98803603	-3.12149932
H	2.00609411	2.47037339	-1.81458077
C	3.73636396	1.23490895	5.35182359
C	2.74618761	1.65907094	6.24773751
C	2.61745190	1.00408272	7.47481321
C	3.46764010	-0.06002998	7.79783716
C	4.45882027	-0.46795448	6.89825241
C	4.59895442	0.17753409	5.66694479
H	2.09959197	2.49533281	5.99504283
H	1.85415708	1.32891571	8.18056222
H	3.36247206	-0.56689814	8.75616523
H	5.12823810	-1.28778288	7.15509798
H	-1.12486537	0.21160554	3.59954871
H	-1.88421834	0.51003027	2.01353302
H	-1.43397345	1.88033266	3.05336591

TS4_20

E = -17352.11

G = -16926.89

Nimag = 1, 1908i cm-1

C	2.27706739	-0.57836644	-2.30016491
C	3.73297526	-0.79133654	-1.80591984
H	2.04192193	0.49726715	-2.30513794
H	4.12539138	-1.71608331	-2.25763038
C	3.89798222	-0.96266252	-0.28344518
C	1.19445540	-1.28585784	-1.49284913
C	1.46663913	-1.46506787	0.00327240
C	2.89400850	-2.00033801	0.22683661
H	4.92049697	-1.29406126	-0.07088009
H	3.07634302	-2.23025277	1.28323372
H	3.02837059	-2.93174819	-0.34390759
H	0.71969299	-2.18094134	0.37253359
H	2.22163620	-0.88750499	-3.34808226
H	4.36308655	0.03243198	-2.16888887
N	3.69887146	0.28195931	0.53458185
C	2.35888323	0.91105774	0.45462599
H	2.31819723	1.72107339	1.18792098
H	2.18184479	1.36006246	-0.53056566
C	1.25583127	-0.12039520	0.81634644
C	1.30082806	-0.41920022	2.32571280
C	-0.04556517	0.57089526	0.34709245
H	-0.00978502	0.77088355	-0.71840938
N	-1.30294415	0.06245479	0.69721117
O	-2.19318466	-0.41395455	-0.01032005
O	-1.54582265	0.41975985	1.99878912
S	0.83284891	2.75537281	-3.38734006
H	-3.66786816	4.05429432	-1.24655999
H	0.07596419	4.34844771	-1.64647391
C	-0.46583273	3.75379530	0.38756705
N	0.04418241	-1.68940718	-1.89109644
H	-0.56546709	1.24345168	1.62393051
C	-0.47559602	-1.51817257	-3.26163945
C	0.14823141	-2.50873759	-4.27188564
C	-0.45094938	-0.07724878	-3.83702211
C	-0.58119234	-2.44947513	-5.62556236
H	1.21280814	-2.27180587	-4.41746531
H	0.09658751	-3.52024985	-3.84191719
C	-1.21013668	-0.02978056	-5.17679024
H	0.57480746	0.25554691	-4.01300182
N	-1.02318458	0.86740000	-2.86674348
C	-0.59890011	-1.01621556	-6.18766182
H	-0.09756210	-3.13473506	-6.33885905
H	-1.61921693	-2.80000838	-5.49223778
H	-1.17430988	1.00087468	-5.56034657
H	-2.26928331	-0.28209933	-4.99734378

H	-1.83831919	0.53862736	-2.34388165
C	-0.56867161	2.12352845	-2.62852390
H	0.43389579	-0.70196101	-6.41846353
H	-1.16414271	-0.98182462	-7.13161009
N	-1.29522329	2.83897250	-1.71640094
H	-2.02234425	2.34809446	-1.19201485
C	-0.81106423	4.06734977	-1.08068715
H	-1.54408451	-1.79089395	-3.18115300
S	4.96284639	1.39890892	0.50660533
O	4.80516259	2.41320330	-0.55294416
H	4.26438804	0.42085753	3.16045927
O	6.21502201	0.62569354	0.56256632
C	-1.83032363	5.25112155	-1.22318143
C	-1.26907638	6.46938560	-0.45865540
H	-1.91773033	7.34224756	-0.62019899
H	-1.22060618	6.27911832	0.62298634
H	-0.26023213	6.72762776	-0.81195071
C	-1.93247804	5.58645508	-2.72773387
H	-0.96218093	5.92003869	-3.12272770
H	-2.66770825	6.38907509	-2.88383981
H	-2.25123246	4.70591440	-3.30219516
C	-3.22814333	4.88855523	-0.68085785
H	-3.18425525	4.60650592	0.37765695
H	-3.89735728	5.75451913	-0.79130287
O	-1.33333650	3.21645555	1.11232123
N	0.77381847	4.07617851	0.84616610
C	1.87140183	4.62408209	0.03198782
C	1.05544111	3.98548942	2.28718459
H	0.15749968	3.64580648	2.80674422
H	1.35554599	4.97417445	2.66346889
H	1.87972033	3.28643417	2.47523583
H	1.87048095	5.72394790	0.05084884
H	1.81808547	4.26469298	-0.99802068
H	2.81563815	4.26783151	0.45413162
C	4.68704763	2.24145485	2.08105281
C	4.82236873	3.63206149	2.12657662
C	4.61370270	4.29353494	3.33961684
C	4.26559592	3.56855901	4.48328724
C	4.14378300	2.17448309	4.42487968
C	4.36464051	1.50033156	3.22263939
H	5.07571636	4.18321801	1.22487248
H	4.70986239	5.37735518	3.38507617
H	4.08628696	4.08933200	5.42308164
H	3.87208352	1.61067523	5.31623290
H	2.28027095	-0.81835209	2.60482511
H	0.53225286	-1.14947264	2.60752756
H	1.13645005	0.49812537	2.90604843

7.4. Computational Details for Chapter 5

Table 7.6. Cartesian coordinates (in Å), energies (in kcal mol^{-1}), and number of imaginary frequencies computed at COSMO(Et_2O)-ZORA-M06/TZ2P//COSMO(Et_2O)-ZORA-BLYP-D3(BJ)/TZ2P.

5_34
E = -8181.81
G = -7993.69
Nimag = 0

C	1.02607602	-1.13652637	-3.87229419
C	1.39718648	-2.41751193	-4.64555062
C	2.02945575	-1.53659228	-2.85133557
C	2.36533902	-2.71726597	-3.55134596
O	0.24783170	-0.18895296	-4.00108868
O	1.06328527	-2.98106841	-5.68848355
N	3.22911281	-3.71392999	-3.33394415
N	2.46461092	-0.97453309	-1.71839814
C	1.88655118	0.26517389	-1.18035373
C	1.64678561	0.00087021	0.31850215
H	0.93359059	0.43783135	-1.69745046
C	2.81489056	1.50945330	-1.45487963
H	3.00170107	-1.51114453	-1.03090726
C	3.33221004	-4.88972107	-4.21110093
H	2.69271425	-4.72278369	-5.08273315
N	0.59871935	0.65550588	0.86610582
C	0.22340231	0.53747097	2.28947152
H	3.80536446	-3.69536965	-2.49184665
H	-0.01713655	1.18771940	0.25292513
C	-0.68342719	-0.68388387	2.50910210
C	-0.42810043	1.84740760	2.74469786
H	1.16690251	0.38302114	2.83252270
H	-0.91471489	-0.79967360	3.57749589
H	-0.18334476	-1.59577344	2.15799215
H	-1.62835884	-0.56336613	1.95875400
H	1.98576099	2.79873559	0.12551727
H	1.11780837	2.90046667	-1.43153966
H	2.70729696	3.67130483	-1.24383258
H	4.05686602	1.30233674	0.34742859
H	4.81956830	2.20536830	-0.98701297
H	4.68549215	0.43518750	-1.07383776
H	3.63255604	2.50322331	-3.20950373
H	2.07611352	1.68132796	-3.51466607
H	3.57294777	0.73273914	-3.36393368
H	-0.68858167	1.78728594	3.80989747
H	-1.35478643	2.03790968	2.18112215
H	0.25257451	2.69719139	2.59878377
C	2.10922651	2.79202893	-0.96489317
C	3.03407000	1.60964678	-2.98157324
C	4.17345177	1.34977493	-0.74347047
O	2.40148023	-0.75313359	0.95849775
H	2.99812958	-5.79252481	-3.68240766
H	4.37036914	-5.02378058	-4.53974572

5_35
E = -8181.27
G = -7992.14
Nimag = 0

C	-0.36202093	-3.08228059	-6.47323294
C	-0.76346998	-1.60961205	-6.64442330
C	-0.24157402	-2.82526116	-5.01778024
C	-0.61001022	-1.46661403	-5.16392401
O	-0.16285345	-4.05537305	-7.21153535
O	-1.05033054	-0.84853706	-7.56618259
N	-0.73610707	-0.44085470	-4.32271948
N	0.07487736	-3.59751318	-3.96215530
C	0.67442124	-4.93900665	-4.16741756
C	2.16559800	-4.71219423	-4.52710930
H	0.16282085	-5.36286920	-5.04045263
C	0.40110780	-5.88708632	-2.96599264
H	0.33529984	-3.13396732	-3.08994120
C	-1.14139754	0.90727146	-4.75152550
H	-0.36683685	1.63583641	-4.48059702
N	2.39603500	-4.75649864	-5.86306552
C	3.63393161	-4.22528066	-6.46562735
H	-0.56930030	-0.59121760	-3.32684324
H	1.57204333	-4.79443907	-6.47610558
C	3.52431217	-2.69646135	-6.61037500
C	3.88221550	-4.92794383	-7.80412763
H	4.44256376	-4.46374630	-5.76068575
H	4.45589675	-2.27973627	-7.01963733
H	3.33595352	-2.23606045	-5.63115734
H	2.69762753	-2.43609465	-7.28748868
H	2.25719559	-7.03419250	-3.19733453
H	0.90677665	-7.62688045	-4.20178593
H	0.91838968	-7.94005407	-2.44940874
H	1.90306783	-4.99402306	-1.64577288
H	0.68720470	-6.01098445	-0.81581608
H	0.24493632	-4.38903170	-1.35872176
H	-1.35431489	-6.83004698	-2.07575438
H	-1.44411685	-6.68006645	-3.84905727
H	-1.69250658	-5.24660735	-2.82108788
H	4.81249849	-4.56069821	-8.25842628
H	3.05779258	-4.72735475	-8.50528301
H	3.96458350	-6.01441054	-7.66356613
C	1.17220922	-7.20102267	-3.22246262
C	-1.11653116	-6.17660197	-2.92732561
C	0.84458766	-5.27524441	-1.61797648
O	3.02746982	-4.44399501	-3.67369062
H	-2.08955077	1.18625838	-4.27414936
H	-1.26941333	0.89777168	-5.83751105

5_36
E = -13314.81
G = -13038.16
Nimag = 0

C	0.60966236	-1.07340398	-3.49640520
C	0.80404882	-2.31481986	-4.39044765
C	1.64563579	-1.64510748	-2.59236819
C	1.81989967	-2.78457399	-3.40917300
O	-0.08787320	-0.05690963	-3.48873922
O	0.33746442	-2.76394626	-5.43862031
N	2.60722107	-3.86002603	-3.34159721
N	2.18760916	-1.24053763	-1.43590581
C	1.87440685	0.05649510	-0.81866019
H	0.06790440	-10.62712603	-1.69383175
H	1.03433742	0.49879816	-1.36208214
H	-0.00040749	-10.86994733	0.78540196
H	2.94353785	-1.79026997	-1.02705798
C	2.49372868	-5.00149945	-4.26005661
H	1.60566421	-4.84166250	-4.88576363
C	2.31271073	-6.26928681	-3.37674939
H	4.97680172	-3.77746941	-4.07083309
H	3.10504963	-4.10912911	-2.47786814
H	1.29307482	-6.24817702	-2.95058847
N	3.32874256	-6.22000684	-2.32204955
H	2.38043441	-7.14987081	-4.03722875
P	3.94119128	-7.54215526	-1.70992554
H	4.40451173	-10.51086843	-1.87191815
H	3.45163628	-8.31821800	1.13462294
H	4.02882207	-5.27397327	0.07378064
H	1.69829949	-9.71472439	2.19358554
C	4.84055635	-8.64062893	-2.87602770
C	5.49385269	-8.03345014	-3.96086643
C	6.21275959	-8.81370600	-4.86879451
C	5.97499541	-5.60114472	-6.77348115
C	6.28917387	-10.20017716	-4.69558798
C	5.64149858	-10.80910697	-3.61381475
C	4.91441370	-10.03349362	-2.70677047
H	5.42836015	-6.95708312	-4.09146286
C	6.04400224	-4.70784431	-5.70071812
C	4.91817185	-4.47744396	-4.90099904

H	2.71831881	-6.55189169	-6.45929869
H	6.70651120	-8.33691798	-5.71349511
H	6.85011026	-10.80791924	-5.40527439
H	5.69856433	-11.88903851	-3.47985297
C	5.13672205	-7.05166061	-0.43001784
C	6.25549155	-7.84724957	-0.14223713
C	7.12880563	-7.47630994	0.88475399
C	4.77010717	-6.25811667	-7.04746197
C	6.88837067	-6.31424025	1.62499388
C	5.77493498	-5.51640884	1.33505545
C	4.89946905	-5.88196875	0.31035564
H	6.45114695	-8.74708707	-0.72176731
H	7.99911055	-8.09412335	1.10359219
H	7.56961224	-6.02821494	2.42591062
H	5.58829430	-4.61024220	1.91086051
C	3.71573662	-5.14413827	-5.15852377
C	3.65141490	-6.03003746	-6.24427344
H	4.70350549	-6.95244939	-7.88464898
H	6.85182644	-5.78078996	-7.39516677
H	6.97723517	-4.18914870	-5.48089414
C	2.75686054	-8.68023878	-0.88371975
C	1.79514175	-9.33714300	-1.67401195
C	0.80752015	-10.12047642	-1.07462840
C	0.76971367	-10.25671636	0.31865243
C	1.72248429	-9.60676446	1.10946646
C	2.71191760	-8.81842617	0.51278924
H	1.82454225	-9.24646132	-2.75887361
H	2.73873457	0.73233620	-0.87818614
H	1.59506307	-0.08562585	0.23300825

5_37

E = -13312.34

G = -13038.05

Nimag = 0

C	1.89201250	-1.89111939	-6.54789592
C	2.31968966	-3.29998463	-6.11599639
C	1.44206741	-1.66012139	-5.15344933
C	1.83345782	-2.95821982	-4.73836699
O	1.88982050	-1.23093237	-7.58904733
O	2.80929618	-4.28454742	-6.66867168
N	1.74839172	-3.53906862	-3.53068297
N	0.86787263	-0.62756066	-4.52886212
C	0.57649048	0.65125475	-5.19438249
H	2.11800998	-7.32952391	-8.39831848
H	0.82816591	0.55035109	-6.25401561
H	0.53413843	-9.24097443	-8.14282410
H	0.67677053	-0.69424061	-3.52849940
C	2.10794029	-4.92919980	-3.15843844
H	2.20162434	-4.90936711	-2.06336966
C	3.50152321	-5.33032037	-3.70539095
H	0.96073965	-6.74315588	-1.51703203
H	1.20641256	-3.04239100	-2.82232972
H	3.45059436	-5.34852111	-4.80158624
N	3.89784575	-6.58691015	-3.07312119
H	4.20351312	-4.52236364	-3.43041428
P	4.16708215	-7.89474436	-3.91865071
H	5.23440268	-9.40886971	-6.30293959
H	2.06246612	-9.97817688	-4.18684961
H	2.74699371	-8.32031529	-1.46149775
H	0.50322788	-10.54827722	-6.02356119
C	5.79784877	-7.97936739	-4.77699980
C	6.83382805	-7.18142362	-4.26744068
C	8.09941421	-7.21076848	-4.85970461
C	-0.89912622	-7.88943053	-4.13001148
C	8.33647436	-8.03761067	-5.96384454
C	7.30507845	-8.83165675	-6.47866728
C	6.03784107	-8.80170955	-5.88999890
H	6.63218262	-6.53635591	-3.41284893
C	-0.38859756	-7.79619008	-2.83298597
C	0.56442924	-6.81936744	-2.52898428
H	0.91028952	-5.41786847	-5.61031584
H	8.89975778	-6.58636469	-4.46337886
H	9.32245941	-8.05827598	-6.42740244
H	7.48634979	-9.46931961	-7.34361084
C	4.14556238	-9.30513445	-2.76213302
C	4.88236094	-10.47268370	-3.01049099
C	4.77020886	-11.56619869	-2.14670424
C	-0.44003585	-7.01365572	-5.11885007
C	3.92369269	-11.49860483	-1.03455151
C	3.19502197	-10.33069519	-0.78020388
C	3.30404368	-9.23560760	-1.64052477
H	5.54806431	-10.52861143	-3.86889497
H	5.34620693	-12.47045733	-2.34153338
H	3.83646578	-12.35313778	-0.36387667
H	2.53977638	-10.27444087	0.08889214
C	1.02909735	-5.93908598	-3.51365275
C	0.52655246	-6.05311220	-4.81756580
H	-0.81232562	-7.09883152	-6.13810646
H	-1.63912122	-8.65111803	-4.37451145
H	-0.72893753	-8.48324677	-2.05825675
C	3.00117965	-8.35261628	-5.26440706
C	3.00467467	-7.60750291	-6.45730501
C	2.11489805	-7.92227109	-7.48410595
C	1.22358550	-8.99050637	-7.33660186
C	1.20801383	-9.72667234	-6.14871129
C	2.08625236	-9.40541464	-5.11114503
H	3.69692481	-6.77972745	-6.58973893
H	1.17775119	1.45741470	-4.75322401
H	-0.48903281	0.89412328	-5.09331999

TS5_1

E = -25764.79

G = -25188.12

Nimag = 1, 192i cm-1

C	-5.28606512	0.37238647	1.71949568
C	-6.44543735	-0.20000749	0.89280764
C	-5.24995212	1.51154386	0.76299450
C	-6.28973872	0.95183230	-0.02445461
O	-4.64017010	0.05690606	2.72546697
O	-7.20622404	-1.17944415	0.95225978
N	-6.86465886	1.36578164	-1.15236374
N	-4.56373818	2.64511679	0.67655121
C	-3.56771740	3.02490673	1.68353141
C	-2.26331508	3.37680353	0.94578947
H	-3.41377027	2.13956911	2.31346093
C	-4.08770016	4.18024870	2.60997326
H	-4.75623549	3.27836041	-0.11879789
C	-8.05138752	0.72283845	-1.71502246
H	-8.38133804	-0.02598696	-0.98460794
C	-7.69308691	-0.01537307	-3.02704503
H	-7.99116761	3.50365645	-1.99743303
H	-6.44245830	2.19905061	-1.60648275
H	-8.61800812	-0.29666961	-3.54447525
N	-6.88464745	-1.21561193	-2.77838586
H	-7.14717685	0.66325163	-3.69243797
P	-7.50103613	-2.70793345	-3.00006962
H	-8.61833912	-2.56274726	-0.30838026
H	-6.42916654	-2.70258731	-0.28301476
H	-8.75478151	-4.97122032	-4.46998620
H	-3.64447087	5.81216443	1.21236668
H	-4.85598892	6.20715058	2.46778996
H	-5.30085210	5.18557577	1.08265456
H	-5.05473520	2.74761853	3.96378808
H	-6.12808859	3.37770294	2.69330740
H	-5.68882695	4.41402377	4.07092866
H	-2.64722743	3.66888434	4.18514180
H	-3.33649244	5.30411105	4.31804440
H	-2.09204328	4.96372435	3.09301787
H	-3.44385512	-1.49090027	-6.78014919
H	-4.94662699	0.09695790	-7.99316669
H	-6.04820705	1.94653972	-6.73583668
C	-2.96917040	4.54923610	3.60792914
C	-5.31423210	3.64356263	3.38146845
C	-4.49229463	5.42237211	1.78817347
O	-2.24638062	4.16531445	-0.00772925
N	-1.15713767	2.74971718	1.42193445
C	0.19255459	2.98087912	0.86965233
H	-1.25450540	2.11587860	2.21250224
C	1.12016031	1.86614309	1.35904399
C	0.70998751	4.37746971	1.25048195

H	0.09220188	2.92699924	-0.22214155
H	2.11137497	1.97468458	0.89944054
H	0.72321851	0.88006089	1.08678949
H	1.24212257	1.91387958	2.45289430
H	1.69435516	4.55207956	0.79216505
H	0.81148924	4.46453346	2.34244667
H	0.01628977	5.14786982	0.89248247
C	-1.73507688	1.86829136	-2.38753926
C	-0.66962966	2.55615826	-2.97154005
C	0.64413002	2.09892719	-2.81555850
C	0.89717581	0.94346555	-2.06741162
C	-0.15912549	0.23098288	-1.49298360
C	-1.46784838	0.69131665	-1.65942404
H	-0.87027011	3.47963369	-3.51075124
H	1.46948022	2.65264406	-3.26172680
H	1.91911044	0.59119520	-1.93151616
H	0.02918258	-0.68157870	-0.92751943
N	-2.58101741	-0.01953760	-1.14947597
C	-4.78456336	4.06747913	-2.77554922
C	-3.15423474	2.31129804	-2.39497202
H	-3.53200719	2.31662794	-1.37673642
C	-3.60123494	3.42780233	-3.15405657
H	-3.10731793	3.72906895	-4.07296598
O	-5.55871359	3.76067677	-1.81101272
O	-5.12806190	5.14383278	-3.60020233
C	-6.35681170	5.82774582	-3.24815638
H	-6.39054482	6.71124991	-3.89357280
H	-7.22846007	5.19063868	-3.44354082
H	-6.35633411	6.12262622	-2.19260463
C	-3.70174698	-0.23284783	-1.96033844
H	-2.39380292	-0.80298647	-0.52115707
O	-4.37181916	-1.28945115	-1.81414465
N	-3.98266469	0.77773976	-2.81966443
H	-3.00827575	-1.18663332	-4.35908476
H	-5.88521455	-1.14076717	-2.42776347
C	-4.29527404	0.53805458	-4.16165185
C	-5.15605765	1.41630460	-4.84903715
C	-5.38041859	1.25612373	-6.22025879
C	-4.76804471	0.21672010	-6.92521356
C	-3.92184940	-0.67074221	-6.24421494
C	-3.67966558	-0.50770066	-4.88208304
H	-5.64478677	2.21667102	-4.30678052
C	-9.18991126	1.69959741	-1.96750259
C	-10.48712528	1.18105577	-2.10840581
C	-11.56258660	2.02377386	-2.39569071
C	-11.35232298	3.39988017	-2.55060319
C	-10.06270432	3.92104576	-2.40991025
C	-8.98435124	3.07713840	-2.11796611
H	-10.65690309	0.11283899	-1.98547981
H	-12.56554505	1.60865524	-2.49335629
H	-12.18957468	4.06043108	-2.77385417
H	-9.89236563	4.99146701	-2.52282551
C	-6.43855193	-3.87308947	-2.11759960
C	-5.94649986	-5.02043195	-2.76434871
C	-5.12386203	-5.90588639	-2.06545271
C	-4.78905845	-5.64941904	-0.73152985
C	-5.26843224	-4.49942746	-0.09601044
C	-6.08924532	-3.60517866	-0.78219143
H	-6.18484230	-5.21512972	-3.80608799
H	-4.73891068	-6.79240253	-2.56758064
H	-4.14585595	-6.34269669	-0.19040351
H	-4.99775180	-4.28632960	0.93729732
C	-7.55973265	-3.17933011	-4.75030831
C	-6.88452977	-2.36521135	-5.67147018
C	-6.87890657	-2.71075297	-7.02429957
C	-7.54022660	-3.86317017	-7.45743414
C	-8.21260819	-4.67873987	-6.53692045
C	-8.22784276	-4.33935285	-5.18354926
H	-6.36174007	-1.47629206	-5.33169062
H	-6.35375725	-2.07626073	-7.73470981
H	-7.53274282	-4.13013491	-8.51387880
H	-8.72701649	-5.57715137	-6.87554511
C	-9.22064481	-2.70257885	-2.39497654
C	-10.30394181	-2.65513280	-3.28900447
C	-11.60506590	-2.51687369	-2.79833685
C	-11.82921365	-2.42091859	-1.42202197
C	-10.74972858	-2.45402533	-0.53184735
C	-9.44646627	-2.59127568	-1.01029666
H	-10.13733909	-2.70764258	-4.36188304
H	-12.44089313	-2.47375744	-3.49538822
H	-12.84399415	-2.30714290	-1.04220056
H	-10.91821914	-2.35800682	0.53993926

TS5_2

E = -25761.27

G = -25185.17

Nimag = 1, 142i cm-1

C	-5.56800433	0.76642829	1.81987460
C	-6.98616839	0.70466091	1.24406686
C	-5.28826423	1.87728608	0.86953695
C	-6.58339214	1.78232525	0.29418627
O	-4.91459625	0.15975640	2.67549989
O	-8.02004741	0.06141774	1.47171449
N	-7.13131115	2.47215749	-0.70695689
N	-4.24498009	2.67396595	0.64251008
C	-2.99287337	2.51388383	1.39593716
C	-1.83443763	2.55755124	0.38513336
H	-3.03614466	1.52394354	1.86774408
C	-2.84036994	3.57580190	2.55171562
H	-4.28573835	3.36947073	-0.11899592
C	-8.41889543	2.15117797	-1.33695084
H	-8.60626155	2.99668223	-1.99968019
C	-9.56580951	2.17788517	-0.30399455
H	-8.72574845	-0.48776435	-0.55076914
H	-6.51765696	3.16424005	-1.20105872
H	-9.55321894	1.28393704	0.32316677
N	-10.86017897	2.33711792	-0.98447247
H	-9.41753049	3.04798710	0.35145779
P	-12.08434705	1.28426333	-1.24841585
H	-12.01622739	-1.46156659	-2.34846650
H	-10.47746625	0.18553318	-3.40220201
H	-14.48224409	-0.05642873	-0.23220443
H	-2.02047989	5.15974893	1.26850219
H	-2.71313889	5.72851447	2.81247173
H	-3.78207329	5.23031908	1.48458152
H	-4.07664076	2.39222278	3.92837600
H	-4.98462707	3.62230018	3.02090255
H	-3.92452648	4.12075913	4.35720042
H	-1.49479964	2.26604296	3.68995734
H	-1.45877147	3.97276091	4.18420578
H	-0.64548026	3.47186811	2.68554539
H	-10.11505349	9.20854151	-0.99154552
H	-8.54030923	8.88104610	0.91737693
H	-7.15819987	6.80734595	1.03213519
C	-1.52729053	3.30121000	3.31629682
C	-4.03096505	3.41190500	3.52323067
C	-2.83375207	5.00921326	1.98928202
O	-1.82241762	3.36166956	-0.55875301
N	-0.83919395	1.66381195	0.61501461
C	0.40917522	1.64195700	-0.17219775
H	-0.90460587	1.05470437	1.42874685
C	1.02311218	0.24079300	-0.09790450
C	1.37459137	2.73761758	0.30923232
H	0.11269930	1.86277392	-1.20805181
H	1.93455033	0.19690031	-0.70895440
H	0.31711025	-0.51609727	-0.46650690
H	1.29893176	-0.00911701	0.93870424
H	2.27851626	2.75039809	-0.31666611
H	1.67474456	2.55434665	1.35167704
H	0.89345425	3.72209040	0.24534147
C	-7.91896392	4.50412026	-5.11483960
C	-7.05471817	4.70673645	-6.19650035
C	-7.41993749	4.34046591	-7.49651912
C	-8.66920639	3.75309912	-7.72544517
C	-9.55709567	3.56320421	-6.66534980
C	-9.19000302	3.94847092	-5.36826627
H	-6.06968702	5.12260219	-5.99358632
H	-6.72731453	4.49998538	-8.32176832
H	-8.95932869	3.45022775	-8.73120180
H	-10.53928930	3.12612612	-6.83660743

N	-10.08719921	3.77278432	-4.30227987
C	-5.40498196	5.31105813	-2.44727947
C	-7.46125617	4.71599443	-3.69425462
H	-7.29970333	3.74605212	-3.21765436
C	-6.35811132	5.58579370	-3.43472814
H	-6.28341169	6.53340892	-3.96342428
O	-5.34048859	4.31425149	-1.65558825
O	-4.42325822	6.30038394	-2.37764710
C	-3.51533085	6.20439842	-1.25184899
H	-2.79972101	7.02219559	-1.39027294
H	-4.06282662	6.34955734	-0.31235364
H	-2.99432911	5.24346923	-1.22582115
C	-10.09630499	4.58578901	-3.16623570
H	-11.00764219	3.39299474	-4.52023099
O	-11.14873800	4.62412151	-2.46191759
N	-8.92851960	5.19368276	-2.88671035
H	-10.28585997	7.47585073	-2.77297749
H	-10.98238251	3.22615226	-1.53320748
C	-8.85468645	6.15659000	-1.85111365
C	-7.96932551	5.97493375	-0.78133111
C	-7.85574191	6.95587426	0.20808208
C	-8.62927002	8.11838413	0.14421682
C	-9.51252677	8.30238105	-0.92881274
C	-9.61615555	7.33300432	-1.92674896
H	-7.35610176	5.08277881	-0.72525832
C	-8.34352684	0.88221673	-2.18113298
C	-8.05016491	0.97752873	-3.55117358
C	-7.95405439	-0.16731470	-4.34419663
C	-8.15998200	-1.42980321	-3.77670644
C	-8.43855060	-1.53397402	-2.40987308
C	-8.52019345	-0.38740251	-1.61375174
H	-7.91461249	1.94803171	-4.01553171
H	-7.73004351	-0.06952598	-5.40615137
H	-8.09868560	-2.32582358	-4.39411470
H	-8.59961895	-2.51142300	-1.95738590
C	-12.37618157	1.15940505	-3.03588500
C	-13.51878383	1.72933117	-3.62048242
C	-13.64162617	1.75531017	-5.01303015
C	-12.63564136	1.21090207	-5.81811164
C	-11.50190969	0.63310340	-5.23429395
C	-11.36690245	0.61116129	-3.84824484
H	-14.29888966	2.16106389	-2.99831948
H	-14.52216974	2.20757010	-5.46730625
H	-12.73218208	1.24380984	-6.90291026
H	-10.70854762	0.22144501	-5.85516469
C	-13.61527966	1.91083054	-0.50825391
C	-13.79081468	3.29705183	-0.35994821
C	-14.98982333	3.78281651	0.16620255
C	-16.00206618	2.89455996	0.54652706
C	-15.82143690	1.51425124	0.40311642
C	-14.62883351	1.01715102	-0.12699285
H	-13.00321617	3.98808206	-0.65546207
H	-15.13077729	4.85639307	0.28274777
H	-16.93357794	3.27901659	0.96058965
H	-16.60705000	0.82424781	0.70799301
C	-11.70928785	-0.32253770	-0.52861976
C	-11.35670263	-0.37478339	0.83247511
C	-10.97354578	-1.58851019	1.39874569
C	-10.97629067	-2.75363265	0.62432202
C	-11.37075746	-2.70857200	-0.71572686
C	-11.72966142	-1.49418520	-1.30136040
H	-11.36147916	0.52772045	1.44010628
H	-10.65959507	-1.62047369	2.44023106
H	-10.67044959	-3.69976034	1.06935169
H	-11.38288455	-3.61799495	-1.31462288

TS5_3

E = -25763.76

G = -25186.60

Nimag = 1, 193i cm-1

C	-5.71978838	0.43427722	1.95762335
C	-6.92503284	0.01272879	1.12946840
C	-5.44170170	1.47827576	0.93541745
C	-6.56180210	1.06687253	0.15530322
O	-5.16961001	0.05780519	3.00727570
O	-7.81685433	-0.84789745	1.20312862
N	-7.04561187	1.49574121	-1.00394571
N	-4.54340381	2.44046475	0.75247113
C	-3.41345890	2.68512220	1.67487231
C	-2.27945782	1.64760234	1.38254874
H	-3.78454928	2.47552389	2.68934472
C	-2.97969285	4.17826164	1.64361664
H	-4.68998563	3.05464356	-0.06917407
C	-8.17302739	0.83669237	-1.66598129
H	-8.57740585	0.11398025	-0.94621330
C	-7.65887198	0.04968740	-2.89729543
H	-8.12916220	3.61236519	-1.88435055
H	-6.53725937	2.28091144	-1.45865651
H	-8.51606215	-0.26688403	-3.50295940
N	-6.87145435	-1.11994186	-2.49589404
H	-7.04343622	0.70433891	-3.52372994
P	-7.39618289	-2.65216551	-2.69799253
H	-8.87044557	-2.42699723	-0.17016622
H	-6.74533389	-2.41443440	0.13165741
H	-8.32722339	-5.10630220	-4.05796779
H	-1.78387860	3.98114773	-0.18435140
H	-2.14233257	5.66326637	0.29926852
H	-3.39938057	4.68058262	-0.46053504
H	-4.49590460	4.73817594	3.13258835
H	-5.03781681	4.93085362	1.44498533
H	-3.88947450	6.09382750	2.14670604
H	-2.08523802	3.99522677	3.63989674
H	-1.54549867	5.41709287	2.71491038
H	-0.92256358	3.79958120	2.29801259
H	-3.21920661	-1.27280555	-6.88184056
H	-4.85094400	0.16595419	-8.11391963
H	-6.12646695	1.91291285	-6.87287581
C	-1.80742570	4.35229611	2.63602980
C	-4.17798611	5.03298011	2.12082623
C	-2.54973030	4.64325958	0.23153554
O	-1.28049451	1.89131309	0.69193364
N	-2.54247295	0.43874988	1.93771918
C	-1.72042464	-0.75674564	1.70837668
H	-3.39477627	0.31937315	2.50553330
C	-2.63987669	-1.94684557	1.38724960
C	-0.80917447	-1.02938014	2.91701375
H	-1.07874175	-0.51379201	0.84959425
H	-2.04657251	-2.85001475	1.18537309
H	-3.28016746	-1.74538937	0.51823924
H	-3.29826599	-2.15417434	2.24338538
H	-0.16924843	-1.90360384	2.72816465
H	-1.41445659	-1.22873716	3.81379026
H	-0.16853477	-0.15897180	3.11250287
C	-1.82830955	2.07584516	-2.78001774
C	-0.90967972	2.88650993	-3.45124163
C	0.44060839	2.52523768	-3.52041340
C	0.88034857	1.34475291	-2.90931340
C	-0.02993822	0.50930282	-2.25704009
C	-1.37677637	0.87318223	-2.20877383
H	-1.24876180	3.82623733	-3.88179237
H	1.15089479	3.17139893	-4.03470781
H	1.93335458	1.06755726	-2.94713984
H	0.30135967	-0.41948045	-1.79367254
N	-2.33836505	0.03611287	-1.60633425
C	-4.97041818	4.15439000	-2.60604563
C	-3.25564722	2.41764314	-2.53860203
H	-3.46837916	2.35767361	-1.47136627
C	-3.85416513	3.54632110	-3.17613234
H	-3.50707650	3.88997069	-4.14584175
O	-5.57646236	3.81824260	-1.53369239
O	-5.43599910	5.25651952	-3.33156953
C	-6.52006691	6.00077015	-2.72240936
H	-6.57965844	6.93846773	-3.28441451
H	-7.46661295	5.45640636	-2.81348793
H	-6.31820284	6.19811349	-1.66376598
C	-3.60456586	-0.14379271	-2.12168679
H	-2.00990776	-0.72163926	-1.01104945
O	-4.25144172	-1.18102604	-1.82872673
N	-4.08917250	0.88410624	-2.90445818
H	-2.86413988	-0.95338904	-4.45445260

H	-5.86737916	-1.02153743	-2.17813514
C	-4.31584269	0.63996034	-4.26795889
C	-5.23013141	1.44994003	-4.97128447
C	-5.41309666	1.27901122	-6.34597796
C	-4.69916522	0.29913140	-7.04330855
C	-3.78624308	-0.50794729	-6.35093535
C	-3.58850476	-0.33511913	-4.98216890
H	-5.78308398	2.21378707	-4.43491640
C	-9.27957609	1.79336703	-2.07235606
C	-10.53179375	1.25312312	-2.40745448
C	-11.57114539	2.08230310	-2.83287111
C	-11.36965157	3.46505443	-2.93083634
C	-10.12674440	4.00750113	-2.59191612
C	-9.08516962	3.17635746	-2.16264632
H	-10.69658428	0.17982369	-2.32645764
H	-12.54045190	1.65151814	-3.08278462
H	-12.17928434	4.11447785	-3.26217913
H	-9.96653042	5.08322236	-2.65712337
C	-6.37245670	-3.66682693	-1.60722021
C	-5.65961409	-4.76712181	-2.11137544
C	-4.81172400	-5.48386131	-1.26376520
C	-4.67316211	-5.10711656	0.07599981
C	-5.38175627	-4.00949126	0.57392581
C	-6.22751345	-3.28297631	-0.26173519
H	-5.74225790	-5.04875745	-3.15745512
H	-4.25098033	-6.33104271	-1.65630616
H	-4.00458065	-5.66537270	0.73050558
H	-5.26837786	-3.70322540	1.61179040
C	-7.23211514	-3.26174516	-4.39679611
C	-6.53684411	-2.47378234	-5.32635809
C	-6.39942546	-2.92409389	-6.64228477
C	-6.94535990	-4.15258974	-7.02461212
C	-7.63394479	-4.94151498	-6.09336917
C	-7.78289892	-4.49852250	-4.77966904
H	-6.10435909	-1.52320369	-5.02561495
H	-5.86496062	-2.30960836	-7.36261763
H	-6.83611081	-4.49904789	-8.05180583
H	-8.05748321	-5.89914017	-6.39347282
C	-9.17573189	-2.67232155	-2.31120451
C	-10.12727654	-2.69280145	-3.34625783
C	-11.48449549	-2.55306756	-3.04523113
C	-11.89619392	-2.39256612	-1.71919048
C	-10.94926703	-2.36428460	-0.68928608
C	-9.59107240	-2.50083853	-0.97808283
H	-9.81454532	-2.79944647	-4.38174626
H	-12.21727509	-2.56071080	-3.85111151
H	-12.95460903	-2.27732213	-1.48796941
H	-11.26382951	-2.22036237	0.34340491

TS5_4

E = -25752.29

G = -25173.96

Nimag = 1, 165i cm-1

C	-6.51228658	1.54644070	2.36444076
C	-7.66147578	1.44494875	1.35932180
C	-5.77177487	2.35963000	1.37194298
C	-6.80841634	2.22804300	0.40744521
O	-6.23844667	1.05280920	3.47187051
O	-8.76614058	0.89700801	1.30298241
N	-6.86068892	2.59753305	-0.86581917
N	-4.57268715	2.95661740	1.36389048
C	-3.60886705	2.64812983	2.45365866
C	-2.85888426	1.38362343	1.97016379
H	-4.22427705	2.36968457	3.31718832
C	-2.75800951	3.86461714	2.89826197
H	-4.20572694	3.27757299	0.45538895
C	-7.95638766	2.28593411	-1.78156959
H	-7.79802091	2.96692832	-2.61618858
C	-9.32344302	2.68037513	-1.17463595
H	-8.86338913	1.43310768	-4.18533728
H	-5.97526992	2.96772299	-1.30583433
H	-9.67204195	1.91630693	-0.47367753
N	-10.31806378	2.90235600	-2.24211113
H	-9.19608767	3.61730994	-0.61367010
P	-11.66009420	1.98617730	-2.51735114
H	-11.48506913	3.32922260	-5.05225666
H	-12.15641367	4.42356543	-1.02862159
H	-13.31966118	1.60495423	-0.16445695
H	-1.42321374	3.76359078	1.17400805
H	-1.28343890	5.26429810	2.13269557
H	-2.67039536	5.03515839	1.05275285
H	-4.24910325	4.48198035	4.38793467
H	-4.47160796	5.22534239	2.78362075
H	-3.15898525	5.78691486	3.85200130
H	-2.29963146	2.84566541	4.78801661
H	-1.22499609	4.21396451	4.40838060
H	-1.03587963	2.66920362	3.54041284
H	-3.97728026	7.47561374	-3.02443231
H	-5.14725473	7.87577425	-0.85668824
H	-7.28008902	6.67247467	-0.37212094
C	-1.76883515	3.36301547	3.97421163
C	-3.72124949	4.90249898	3.51869349
C	-1.98530304	4.51583600	1.73551200
O	-1.88239381	1.41869722	1.20567526
N	-3.46607443	0.23830741	2.38738222
C	-3.27476301	-1.04806617	1.69348903
H	-4.32332518	0.33614736	2.94462102
C	-4.21548065	-1.11597930	0.47463745
C	-3.50723435	-2.19922837	2.67739816
H	-2.23241991	-1.05575691	1.34621038
H	-4.02919092	-2.02630076	-0.11335136
H	-4.06609420	-0.24417812	-0.17636799
H	-5.26268746	-1.12797646	0.81023351
H	-3.36330801	-3.16502679	2.17384886
H	-4.53502616	-2.16938784	3.07104793
H	-2.80884300	-2.13488643	3.52298553
C	-6.10840767	2.05646261	-5.52494903
C	-5.24995636	1.02470075	-5.92563242
C	-5.58768329	0.14645445	-6.95880737
C	-6.80968111	0.29972122	-7.62138441
C	-7.67809751	1.32207040	-7.24489723
C	-7.33744167	2.19280280	-6.19701477
H	-4.30865509	0.91179265	-5.39104512
H	-4.90292137	-0.65222739	-7.24053771
H	-7.08919107	-0.37574825	-8.42960608
H	-8.63740088	1.44324754	-7.74639010
N	-8.28719023	3.13227280	-5.77939625
C	-3.84471226	3.45873482	-2.85680987
C	-5.75375756	2.87357613	-4.30808872
H	-6.10102212	2.35048838	-3.41496852
C	-4.39622684	3.27367007	-4.13300785
H	-3.77700107	3.49203268	-4.99995304
O	-4.39413282	3.31444456	-1.72107322
O	-2.49616424	3.81966910	-2.91798219
C	-1.85987465	4.02543787	-1.63544808
H	-0.81499267	4.26309920	-1.86176445
H	-2.32984908	4.86154618	-1.10647644
H	-1.91661240	3.12487161	-1.01354267
C	-8.15679955	4.05574991	-4.74640620
H	-9.23937719	3.02384586	-6.11735071
O	-9.19930919	4.65431765	-4.35150478
N	-6.89734938	4.21130759	-4.28279189
H	-4.90121539	5.83671328	-4.64990832
H	-10.02140087	3.55625189	-2.99798765
C	-6.54788621	5.25700985	-3.39056137
C	-7.23311248	5.53105104	-2.19567561
C	-6.73710001	6.47508446	-1.29628119
C	-5.54534083	7.15587992	-1.57139374
C	-4.88729010	6.92679064	-2.78291666
C	-5.39250190	5.99795308	-3.69606153
H	-8.16676948	5.02941699	-1.98107766
C	-7.89752543	0.86937992	-2.34581327
C	-7.31183516	-0.19249161	-1.64464542
C	-7.26516843	-1.47114535	-2.20357240
C	-7.78827006	-1.70551688	-3.48092763
C	-8.35961312	-0.64874482	-4.19436783
C	-8.41731166	0.62309749	-3.62367921
H	-6.88193468	-0.03122788	-0.66374203
H	-6.80509510	-2.28460347	-1.64335812
H	-7.73283594	-2.70053387	-3.92188235

H	-8.74676334	-0.80349541	-5.19903859
C	-13.13505072	3.01965308	-2.35057822
C	-14.32652862	2.66267925	-3.00397840
C	-15.47455425	3.43120762	-2.80705754
C	-15.43336540	4.55115283	-1.96773951
C	-14.24327632	4.91083903	-1.32652766
C	-13.08933260	4.14748514	-1.51598154
H	-14.35320626	1.79776050	-3.66417254
H	-16.40027855	3.16035797	-3.31263165
H	-16.33127986	5.15009353	-1.81956660
H	-14.21142726	5.78801094	-0.68196543
C	-11.71124097	0.67277966	-1.28527878
C	-10.78982648	-0.39082156	-1.33411740
C	-10.75656364	-1.31962078	-0.29778422
C	-11.63713673	-1.20167395	0.78151863
C	-12.56393404	-0.15600572	0.82343893
C	-12.60635649	0.78552761	-0.20614033
H	-10.08818731	-0.47745892	-2.15413708
H	-10.02446037	-2.12424306	-0.32734566
H	-11.59477159	-1.92138956	1.59791672
H	-13.24926266	-0.06383130	1.66451870
C	-11.69479555	1.33504289	-4.20894002
C	-11.82098859	-0.03322068	-4.48487185
C	-11.79489995	-0.47461282	-5.81045541
C	-11.65479482	0.44212258	-6.85461868
C	-11.55863916	1.81182111	-6.57957121
C	-11.58062052	2.26410247	-5.26079171
H	-11.93298558	-0.75172902	-3.67770203
H	-11.88037305	-1.53916477	-6.02366358
H	-11.62881498	0.09230239	-7.88581307
H	-11.47082023	2.52900347	-7.39508018

TS5_5
E = -25763.59
G = -25187.82
Nimag = 1, 182i cm-1

C	-4.70211551	2.77787646	1.87918228
C	-4.03546889	2.18130916	3.13403761
C	-5.29999248	1.43473015	1.63389618
C	-4.66372941	0.88566964	2.77203608
O	-4.72234149	3.86012682	1.28613560
O	-3.29416588	2.57638339	4.04082438
N	-4.61942388	-0.36716385	3.24115528
N	-6.11314871	0.92946404	0.70573448
C	-6.87649318	1.82036321	-0.18164144
C	-6.82140762	1.26212566	-1.61419885
H	-6.35694702	2.78609824	-0.15000033
C	-8.33898807	2.07022362	0.33089011
H	-6.39686807	-0.05611205	0.79451878
C	-4.17948522	-0.65849492	4.60430964
H	-3.54571375	0.17982095	4.90875187
C	-3.35755684	-1.96424760	4.65478551
H	-4.04962107	-0.18084727	7.25909174
H	-5.27679790	-1.01777108	2.78055382
H	-3.11750606	-2.17075749	5.70836646
N	-2.13630220	-1.94963299	3.82473480
H	-3.97266501	-2.79616045	4.28672623
P	-0.86137976	-0.95116763	4.10898185
H	0.57182644	1.64396502	4.20370834
H	1.62461936	-0.34893240	2.65057323
H	0.06579529	-2.12362887	6.64093678
H	-8.51907373	3.86364771	-0.92131710
H	-10.06978680	3.20764246	-0.34494672
H	-9.19901312	2.39084631	-1.66396589
H	-7.77032189	2.21699947	2.43436674
H	-9.25921178	3.08842415	2.02122834
H	-7.67627843	3.77521118	1.55619436
H	-9.16142746	0.16224418	-0.36305566
H	-10.11992269	0.97336649	0.91160964
H	-8.60995481	0.13190880	1.32642665
H	-1.29301158	-1.25769024	-0.73601851
H	-2.63146007	-0.43161010	-2.66938791
H	-5.10202626	-0.84944048	-2.71776389
C	-9.07226697	2.93406854	-0.71750423
C	-8.24773723	2.84181075	1.66567738
C	-9.10156138	0.74805134	0.56128842
O	-7.35701029	0.19136301	-1.93409704
N	-6.13286180	2.05152462	-2.48126345
C	-5.96050534	1.74314799	-3.90995750
H	-5.71534616	2.91123224	-2.12713797
C	-4.49119978	1.93554273	-4.30622176
C	-6.91981763	2.59235826	-4.76010337
H	-6.24024698	0.68632381	-4.01156862
H	-4.33763940	1.64550453	-5.35471344
H	-3.83730785	1.32506508	-3.67158671
H	-4.19451739	2.99067917	-4.19839621
H	-6.82039312	2.33403617	-5.82401960
H	-6.69485939	3.66305506	-4.64156447
H	-7.95910747	2.41736913	-4.45184918
C	-5.49976652	-5.69016229	1.23773253
C	-5.40401637	-6.93779311	0.61072799
C	-6.52344984	-7.76658156	0.48042617
C	-7.75908101	-7.35162268	0.99070518
C	-7.88176263	-6.10029377	1.59909353
C	-6.75962169	-5.26953057	1.70662386
H	-4.42937983	-7.27309955	0.26297642
H	-6.42718572	-8.73925803	-0.00013616
H	-8.63293261	-7.99706437	0.90795636
H	-8.84587385	-5.76040775	1.97754900
N	-6.86450707	-3.97949485	2.27167188
C	-1.85326427	-4.79757000	1.50766168
C	-4.30926349	-4.83646019	1.54835707
H	-4.19433114	-4.70942956	2.63162793
C	-3.07159524	-5.09438571	0.89084474
H	-3.05982219	-5.44439401	-0.13801471
O	-1.66270487	-4.32352691	2.67157922
O	-0.74899814	-5.06365668	0.69106708
C	0.53888146	-4.76204417	1.27916365
H	1.27477579	-5.01035894	0.50747357
H	0.61411428	-3.70233849	1.54640440
H	0.71216002	-5.36585702	2.17710284
C	-6.15401689	-2.89647119	1.73971134
H	-7.79026468	-3.69936496	2.60037073
O	-6.65644058	-1.73594490	1.84852315
N	-4.94777321	-3.19217049	1.22748700
H	-2.41081448	-2.46977706	1.11481910
H	-1.94948890	-2.85810338	3.30942526
C	-4.36218855	-2.40776551	0.21626461
C	-5.11300725	-1.94049189	-0.87714748
C	-4.49485300	-1.22117594	-1.89783099
C	-3.11501826	-0.98325851	-1.86435383
C	-2.36338780	-1.45523974	-0.78624240
C	-2.98219487	-2.15403420	0.25333206
H	-6.18491986	-2.12092980	-0.91646885
C	-5.32275013	-0.75115845	5.60943708
C	-6.61523389	-1.13698088	5.23232181
C	-7.62028492	-1.25395031	6.19798438
C	-7.34490690	-0.99972039	7.54441281
C	-6.05493899	-0.61314298	7.92461715
C	-5.05104029	-0.48897302	6.96080273
H	-6.85222068	-1.32705520	4.18740390
H	-8.63208103	-1.50851914	5.89453032
H	-8.13292185	-1.09010028	8.29138534
H	-5.83267168	-0.40046386	8.97007936
C	-0.90080814	-0.35619829	5.82886316
C	-1.50374397	0.87830319	6.13032022
C	-1.63318548	1.27459392	7.46356569
C	-1.16780914	0.45183766	8.49317663
C	-0.55896707	-0.77214795	8.19210257
C	-0.42066944	-1.17793651	6.86406204
H	-1.89967990	1.51760905	5.34270112
H	-2.11064362	2.22664925	7.69212937
H	-1.27655893	0.76306371	9.53152916
H	-0.18834663	-1.41196009	8.99184370
C	-0.86396616	0.50338245	3.03658810
C	-1.67726999	0.48440806	1.89691272
C	-1.69440836	1.58201869	1.03640594
C	-0.91169089	2.70219700	1.32099310
C	-0.09097570	2.71906634	2.45675744
C	-0.05725564	1.62205931	3.31553734

H	-2.32029470	-0.36531606	1.70828127
H	-2.34273313	1.56255051	0.16235569
H	-0.94994208	3.57292358	0.66787407
H	0.51346655	3.59712994	2.67964541
C	0.65392177	-1.89718771	3.81661747
C	0.77188001	-3.18572002	4.36815088
C	1.97355506	-3.88033675	4.24452440
C	3.04494114	-3.31295714	3.54685734
C	2.91508237	-2.04772964	2.96586571
C	1.72381573	-1.33180400	3.10450441
H	-0.07925836	-3.65451285	4.85526077
H	2.06471033	-4.87811612	4.67136573
H	3.97795174	-3.86567811	3.44136771
H	3.74058549	-1.61561746	2.40188664

TS5_6

E = -25759.27

G = -25179.24

Nimag = 1, 157i cm-1

C	-4.72709814	1.25802609	1.14109975
C	-5.03666983	1.93496221	2.48526990
C	-5.20965296	-0.01594464	1.74255124
C	-5.40633946	0.58931505	3.01180192
O	-4.27183763	1.59882730	0.04694507
O	-5.02078336	3.08518769	2.93722564
N	-5.83204584	0.04172125	4.15489464
N	-5.45762023	-1.25901561	1.32590082
C	-5.34746096	-1.69599510	-0.07325064
C	-4.97117729	-3.18370778	-0.01581732
H	-4.53834949	-1.11556090	-0.53774387
C	-6.64814258	-1.44383984	-0.93876688
H	-5.66170711	-1.97207786	2.04499393
C	-6.24326200	0.75916933	5.37269931
H	-6.84070962	0.02226807	5.92337753
C	-7.20651601	1.93504579	5.01889584
H	-4.16314082	2.50837554	4.83600672
H	-5.86854462	-0.99386595	4.18423255
H	-6.68486798	2.89701578	5.01252382
N	-8.37878590	1.99235434	5.90955849
H	-7.60313847	1.77088208	4.00873605
P	-8.43507059	2.74672089	7.37397707
H	-7.01546559	3.45326089	9.89612108
H	-10.01326890	3.05455456	9.81615995
H	-9.20000174	5.49290324	6.78189000
H	-5.44552947	-1.49733390	-2.77815855
H	-7.19586704	-1.67951633	-3.03242150
H	-6.24767787	-3.04379080	-2.39734980
H	-7.25861465	0.44477053	-0.00490310
H	-7.74375024	0.26606753	-1.70271343
H	-6.04750862	0.64436803	-1.29016528
H	-7.72023360	-3.24379915	-0.29027597
H	-8.73956523	-2.00036607	-1.04147054
H	-8.15007073	-1.77968108	0.62196170
H	-4.84978165	-2.27865337	8.33778605
H	-6.22968717	-3.52826282	10.00170374
H	-8.40271513	-4.53195051	9.27318306
C	-6.36186446	-1.95110639	-2.37037215
C	-6.93269582	0.07251536	-0.98570260
C	-7.88397592	-2.16506268	-0.37020924
O	-5.61762139	-3.99070151	0.68136980
N	-3.91368048	-3.54997340	-0.76978811
C	-3.39959024	-4.93469816	-0.81229774
H	-3.39590128	-2.82737047	-1.26768923
C	-2.50776190	-5.21198024	0.40814366
C	-2.67248021	-5.15538877	-2.14203584
H	-4.28540792	-5.58457573	-0.75977915
H	-2.18006242	-6.26116993	0.40795431
H	-3.06228945	-5.01799755	1.33514367
H	-1.61677978	-4.56720905	0.38511857
H	-2.31645953	-6.19208660	-2.20688993
H	-1.79691446	-4.49224194	-2.22125225
H	-3.33988125	-4.96115440	-2.99294865
C	-9.96394327	-3.70158532	3.60281560
C	-11.22914924	-4.29241839	3.52988635
C	-11.54858957	-5.18908276	2.50293677
C	-10.59240739	-5.49942917	1.52917562
C	-9.32010491	-4.92727031	1.58840586
C	-9.00762909	-4.03410321	2.62204519
H	-11.97987042	-4.02048740	4.26846737
H	-12.54188237	-5.63414992	2.45950150
H	-10.83409309	-6.19141065	0.72287222
H	-8.56482208	-5.17374789	0.84434573
N	-7.74396024	-3.43481362	2.69102147
C	-10.53529953	-1.26324732	6.43026673
C	-9.58907181	-2.65980656	4.61877178
H	-9.33085351	-1.70560061	4.13901634
C	-10.44521048	-2.47698361	5.74460382
H	-11.00711112	-3.31659690	6.14311681
O	-9.92423867	-0.18013806	6.20389460
O	-11.45053369	-1.31689461	7.49705946
C	-11.67513262	-0.06530820	8.19107926
H	-12.49052476	-0.26714363	8.89347848
H	-10.78431364	0.25076445	8.74445078
H	-11.96108405	0.73021312	7.49492247
C	-7.13026388	-3.06758925	3.88216307
H	-7.07500721	-3.61745705	1.92828088
O	-5.90948528	-2.72338374	3.83058660
N	-7.93117481	-3.11458514	4.97476947
H	-5.60192144	-2.04453420	6.01556880
H	-8.95184068	1.11223223	5.89968257
C	-7.45151768	-3.13712997	6.29565802
C	-8.22136218	-3.84533664	7.24512949
C	-7.79281451	-3.96909402	8.56614939
C	-6.57529946	-3.41185997	8.97503337
C	-5.80505488	-2.71226792	8.04333590
C	-6.23772408	-2.55862679	6.72336673
H	-9.13129783	-4.33695728	6.92154769
C	-5.08387826	1.17465725	6.27120279
C	-5.02069260	0.68433714	7.58122843
C	-4.02392661	1.11615576	8.46081690
C	-3.05869111	2.02960615	8.02631333
C	-3.10162638	2.50597330	6.70988848
C	-4.11133621	2.09057799	5.83911923
H	-5.76979027	-0.01821857	7.92691309
H	-4.00995946	0.74305639	9.48409799
H	-2.27834640	2.36931850	8.70721750
H	-2.35236863	3.21727776	6.36207013
C	-7.47701488	4.27222585	7.27644825
C	-6.08494707	4.24372168	7.46984714
C	-5.34144396	5.40965317	7.29034866
C	-5.97983284	6.60117434	6.93134616
C	-7.36750508	6.63227879	6.75167620
C	-8.12122764	5.46968247	6.92043675
H	-5.58534291	3.32319326	7.74891879
H	-4.26181142	5.38096170	7.42527305
H	-5.39486296	7.50940319	6.79029753
H	-7.86391343	7.56201557	6.47762709
C	-7.86670511	1.78314357	8.80224236
C	-8.14491516	0.40445770	8.81262848
C	-7.77580116	-0.36396224	9.91488963
C	-7.11793004	0.23059383	10.99689917
C	-6.84332607	1.60192999	10.98684595
C	-7.22552502	2.38611036	9.89614004
H	-8.63508447	-0.06123829	7.95973804
H	-7.98502903	-1.43016954	9.91267870
H	-6.81709625	-0.37680411	11.85030252
H	-6.33035276	2.06467519	11.82921709
C	-10.18478475	3.11307622	7.65572191
C	-11.04311944	3.29578890	6.55974783
C	-12.38893173	3.59196384	6.78168714
C	-12.87699445	3.70365082	8.08772116
C	-12.02002126	3.51939258	9.17841173
C	-10.67294112	3.22264262	8.96749118
H	-10.65888917	3.18720560	5.54817562
H	-13.05930183	3.72278393	5.93325616
H	-13.93062066	3.92363886	8.25686886
H	-12.40361241	3.59497845	10.19499574

TS5_7

E = -25763.31

G = -25186.50
Nimag = 1, 159i cm-1

C	-4.86516574	2.77886326	1.97242848
C	-4.23235466	2.19576134	3.24087508
C	-5.40989005	1.42715689	1.68015786
C	-4.78831484	0.88025400	2.83310610
O	-4.85840677	3.85964489	1.36447055
O	-3.53068937	2.60315364	4.17234626
N	-4.67010519	-0.37244793	3.28582747
N	-6.15622346	0.91330149	0.70740248
C	-6.91559858	1.76310576	-0.23551363
C	-6.10462284	1.92153323	-1.56186613
H	-6.96529027	2.75983196	0.22382276
C	-8.38315744	1.26335695	-0.37471113
H	-6.33133966	-0.10109458	0.73922019
C	-4.25312057	-0.63012994	4.66545185
H	-3.64666638	0.22930205	4.96663193
C	-3.39628405	-1.91275455	4.75302917
H	-4.18533862	-0.19541260	7.33160755
H	-5.27754391	-1.06391644	2.81460312
H	-3.17739548	-2.10017630	5.81404889
N	-2.15093797	-1.88225933	3.96791653
H	-3.97915852	-2.76694033	4.38233410
P	-0.92860108	-0.80365501	4.17259033
H	0.26983236	1.92742524	4.26675808
H	1.53927625	-0.00459155	2.79635727
H	0.12961187	-1.95175483	6.63891317
H	-9.05337534	3.25907119	-0.98768012
H	-10.19267199	1.94794604	-1.37412594
H	-8.71320676	2.15573276	-2.34952419
H	-8.53940746	0.67636425	1.74017478
H	-10.09562796	1.03869522	0.95628563
H	-9.00315509	2.36737151	1.42154110
H	-7.95818184	-0.28566649	-1.85899094
H	-9.52414216	-0.46945004	-1.01685234
H	-8.02458283	-0.89807290	-0.18040914
H	-1.39794808	-0.89725670	-0.92614340
H	-2.79032791	-0.09389319	-2.83819671
H	-5.21009935	-0.69560502	-2.93223482
C	-9.12721741	2.21729350	-1.33629270
C	-9.04075123	1.34149639	1.02446609
C	-8.46679682	-0.19035096	-0.89445133
O	-6.38486175	1.32530191	-2.60917537
N	-5.05898993	2.77373143	-1.39471916
C	-3.94996262	3.02525114	-2.34084163
H	-4.96428609	3.22006247	-0.47259506
C	-3.17525449	4.24761660	-1.82430350
C	-4.42256217	3.23782792	-3.78690554
H	-3.28023546	2.14725151	-2.31182373
H	-2.26198712	4.39165146	-2.41726727
H	-2.89285348	4.12349815	-0.77046988
H	-3.79533679	5.15414234	-1.90352292
H	-3.55406230	3.48797147	-4.41356505
H	-5.13773447	4.07435201	-3.82985008
H	-4.91334752	2.34266668	-4.18041653
C	-5.29996900	-5.67367182	1.11734866
C	-5.17314648	-6.93878819	0.53514753
C	-6.25541510	-7.82537972	0.50010623
C	-7.48068970	-7.45123301	1.06377961
C	-7.63419064	-6.18414835	1.63212260
C	-6.55143150	-5.29691239	1.64428519
H	-4.20412494	-7.23822183	0.14175636
H	-6.13755199	-8.80984651	0.04921725
H	-8.32414127	-8.14065575	1.05221181
H	-8.59232566	-5.87694558	2.05145632
N	-6.68586767	-3.99153530	2.16623886
C	-1.70643164	-4.55211142	1.16862316
C	-4.15177814	-4.72557033	1.30587086
H	-3.99030770	-4.52881391	2.37425322
C	-2.92324770	-4.96269078	0.61615926
H	-2.92505525	-5.38408363	-0.38557796
O	-1.50645221	-3.93209004	2.25533029
O	-0.60002267	-4.86657183	0.36670596
C	0.67666198	-4.44568772	0.90663512
H	1.40739712	-4.64912159	0.11701555
H	0.67202729	-3.37943371	1.16060383
H	0.92615790	-5.01733276	1.80847949
C	-6.05654598	-2.89644235	1.56249755
H	-7.58826537	-3.74313814	2.57399125
O	-6.56196445	-1.74255957	1.73663027
N	-4.92296758	-3.18204827	0.91042465
H	-2.42736471	-2.27424115	0.86125433
H	-2.00284178	-2.65512674	3.27418232
C	-4.37117123	-2.31772650	-0.05538406
C	-5.14543036	-1.88097047	-1.14385366
C	-4.58478614	-1.06809596	-2.12642979
C	-3.23058326	-0.71588091	-2.06008431
C	-2.45159353	-1.16690183	-0.99243826
C	-3.01954986	-1.95467692	0.01330201
H	-6.18880059	-2.18118462	-1.20809149
C	-5.41978565	-0.73291518	5.64129195
C	-6.70549120	-1.10153738	5.22497710
C	-7.73763629	-1.22894325	6.16112661
C	-7.49475330	-0.99081881	7.51749869
C	-6.21195152	-0.61923394	7.93675390
C	-5.18089564	-0.49205700	7.00270455
H	-6.91405482	-1.27787326	4.17151347
H	-8.73603110	-1.51065901	5.82715965
H	-8.30128977	-1.08721975	8.24354795
H	-6.01652984	-0.42235818	8.99057307
C	-0.95377437	-0.22419488	5.89287169
C	-1.61329621	0.97042791	6.23183989
C	-1.72195110	1.33808757	7.57502466
C	-1.17880233	0.52633534	8.57498328
C	-0.51428446	-0.65819620	8.23536886
C	-0.39682964	-1.03591387	6.89719426
H	-2.06565141	1.59937090	5.46698183
H	-2.24180423	2.25926024	7.83520870
H	-1.27027017	0.81589954	9.62129145
H	-0.08429796	-1.28791531	9.01297259
C	-1.03649058	0.64505815	3.09501965
C	-1.81801406	0.53177334	1.93825238
C	-1.91315246	1.60595129	1.05334826
C	-1.23149656	2.79322484	1.32955703
C	-0.44153279	2.90406343	2.48117653
C	-0.33517451	1.83296672	3.36688684
H	-2.37208813	-0.37976541	1.75563131
H	-2.54076710	1.51270875	0.16958592
H	-1.31901392	3.64233645	0.65574659
H	0.08174697	3.83490984	2.69480545
C	0.61037582	-1.68157375	3.81090271
C	0.75846844	-3.01383421	4.23414930
C	1.96792210	-3.67276161	4.01980476
C	3.01980651	-3.01843543	3.37090906
C	2.86420273	-1.70034296	2.92989952
C	1.66194789	-1.02534382	3.15032027
H	-0.07537096	-3.53728722	4.69460780
H	2.08142794	-4.70709534	4.34072941
H	3.95847072	-3.54252999	3.19387619
H	3.67644141	-1.19729620	2.40683402

TS5_8
E = -25755.00
G = -25176.00
Nimag = 1, 180i cm-1

C	-5.34526207	2.94987146	1.87595971
C	-5.24532850	2.83667746	3.40772240
C	-6.25846612	1.78547229	1.89192973
C	-6.12381497	1.62740544	3.29670474
O	-4.83611586	3.65059147	0.98657715
O	-4.69428929	3.46113617	4.30976085
N	-6.65560982	0.68195215	4.08986119
N	-6.93643109	1.08894848	0.97418789
C	-6.74138216	1.28891804	-0.47531121
C	-5.44053023	0.52732785	-0.86704703
H	-6.55761408	2.36296708	-0.61683613
C	-8.01909912	0.92768314	-1.28292656
H	-7.40198119	0.23014275	1.29462434
C	-5.99847745	0.08091596	5.27172605
H	-5.95255302	-0.99238319	5.03759328

C	-6.90763774	0.17945375	6.51835085
H	-4.84059538	1.76712149	7.17153621
H	-7.28909861	0.03002694	3.58205969
H	-6.79468986	1.13291774	7.04707164
N	-6.70150773	-0.94177221	7.45972794
H	-7.95041746	0.12146656	6.17902853
P	-5.74836672	-0.97125925	8.79547969
H	-3.28250287	-0.55589487	10.42489163
H	-4.51008934	-2.63663870	10.86524005
H	-7.97341803	0.07832583	10.25415714
H	-7.31504767	2.11526048	-2.98728453
H	-8.60850863	0.95759060	-3.38092031
H	-6.94612229	0.37313602	-3.11267483
H	-9.34447144	1.85612743	0.19956111
H	-10.05435412	1.70042093	-1.42853828
H	-8.83423764	2.95842768	-1.10394439
H	-7.71323478	-1.23912701	-1.24166700
H	-9.37672575	-0.72848546	-1.64981192
H	-8.81982684	-0.64983210	0.02994606
H	-3.16457739	-3.38138723	4.21446007
H	-2.55453345	-2.81739222	1.86405703
H	-4.37207962	-2.15075750	0.25434588
C	-7.69678580	1.10294953	-2.78379208
C	-9.13013857	1.92322162	-0.87588093
C	-8.50420680	-0.51671612	-1.01363517
O	-5.42544750	-0.65551513	-1.24400594
N	-4.33088377	1.27975395	-0.66342517
C	-2.97561954	0.71276578	-0.57141582
H	-4.45590814	2.22551293	-0.27683358
C	-2.56177981	0.63034387	0.90862792
C	-1.99810643	1.54702898	-1.41073740
H	-3.04873282	-0.29992909	-0.99014982
H	-1.56695194	0.17217095	1.00738758
H	-3.28244131	0.02505419	1.46890958
H	-2.52977031	1.63314073	1.35924225
H	-0.98804626	1.11627818	-1.36106296
H	-1.94939792	2.57922811	-1.03197440
H	-2.31859035	1.57554909	-2.46109861
C	-9.22685594	-4.79646053	3.33391627
C	-9.37306418	-6.17165138	3.12249608
C	-10.36389309	-6.66366528	2.26574516
C	-11.22952650	-5.77509461	1.61654035
C	-11.08598002	-4.39713885	1.79619053
C	-10.07903627	-3.91463705	2.64023106
H	-8.73110222	-6.85934606	3.66812238
H	-10.47151256	-7.73755807	2.11959020
H	-12.01065299	-6.15253631	0.95746897
H	-11.73839655	-3.69805165	1.27326787
N	-9.86458269	-2.53048891	2.80427808
C	-6.83856531	-4.63871866	6.24326638
C	-8.29239810	-4.19089099	4.33300256
H	-8.84298579	-3.56722599	5.04816888
C	-7.31707367	-5.00492724	4.97794255
H	-6.87392949	-5.86004327	4.47589052
O	-7.12104779	-3.59687155	6.89961733
O	-5.92239953	-5.55633744	6.77767139
C	-5.37427744	-5.18789256	8.06826482
H	-4.73591647	-6.02748612	8.36192754
H	-4.77500285	-4.27224435	7.99656199
H	-6.16876900	-5.03642904	8.80461624
C	-8.58187117	-1.98965056	2.90021979
H	-10.53169730	-1.88959390	2.37212180
O	-8.41474040	-0.78644415	2.53699344
N	-7.64105228	-2.81492245	3.39934799
H	-5.51859845	-3.23657498	4.95810068
H	-6.99425574	-1.89303182	7.13595407
C	-6.29517293	-2.74615718	3.00534782
C	-5.93932884	-2.43478229	1.67636449
C	-4.60491505	-2.43522329	1.27821679
C	-3.59669122	-2.80094906	2.18131215
C	-3.94005773	-3.11572304	3.49745125
C	-5.27139184	-3.05751052	3.92183234
H	-6.71087582	-2.19024439	0.95186237
C	-4.56346282	0.54535623	5.42031324
C	-3.63613394	0.11854300	4.45942525
C	-2.29253922	0.46807180	4.56567386
C	-1.85441180	1.24223408	5.64581283
C	-2.77854576	1.69692367	6.58806743
C	-4.12886298	1.36660802	6.45923113
H	-3.97082178	-0.50021415	3.63269213
H	-1.58449356	0.12867328	3.81097591
H	-0.80015738	1.49872480	5.74481631
H	-2.44940866	2.32476353	7.41544101
C	-5.94789888	0.60230270	9.67785851
C	-4.94278490	1.58060653	9.73708780
C	-5.18988334	2.79018705	10.38998319
C	-6.43218004	3.02643298	10.98536452
C	-7.43382547	2.04962875	10.93366928
C	-7.19540164	0.83839911	10.28547392
H	-3.97869565	1.40846656	9.27176291
H	-4.41044581	3.54986969	10.42764526
H	-6.62165671	3.97249122	11.49097827
H	-8.40069973	2.23062659	11.40091472
C	-3.98610150	-1.27213979	8.49767422
C	-3.61506597	-1.81895893	7.25875782
C	-2.26893656	-2.02997402	6.97057008
C	-1.29124073	-1.71369284	7.91812891
C	-1.65945937	-1.19739729	9.16447597
C	-3.00530874	-0.97372264	9.45936384
H	-4.37300966	-2.05569809	6.52042189
H	-1.98233057	-2.42168052	5.99788848
H	-0.23845850	-1.86491234	7.68273644
H	-0.89790989	-0.95582259	9.90479657
C	-6.38914323	-2.31645624	9.82708177
C	-7.72385169	-2.72840631	9.69030613
C	-8.22055547	-3.73885721	10.51444254
C	-7.39446491	-4.33783631	11.47019607
C	-6.06206231	-3.93123377	11.60086653
C	-5.55467007	-2.92396916	10.77919304
H	-8.36223893	-2.28246375	8.93414465
H	-9.25180427	-4.06864144	10.39717198
H	-7.78502429	-5.13195525	12.10561657
H	-5.41238091	-4.40714923	12.33404292

TS5_9

E = -25753.73

G = -25175.52

Nimag = 1, 245i cm-1

C	0.91830663	0.86669541	-1.19143806
C	0.20032329	-0.48067464	-1.34606921
C	2.17856304	0.10118397	-0.95648277
C	1.51613929	-1.13985840	-1.13051694
O	0.63645341	2.06591258	-1.27573306
O	-0.94740527	-0.88276816	-1.56928672
N	1.90119899	-2.42610018	-1.20541986
N	3.43672101	0.46928853	-0.73927371
C	3.84735455	1.86776258	-0.89684729
C	4.63592176	2.28355325	0.35526107
H	2.92085030	2.45216417	-0.96202171
C	4.63976982	2.10017647	-2.24377112
H	4.12122825	-0.25923769	-0.48951225
C	0.95626571	-3.39217422	-1.79506870
H	-0.04041259	-2.97354249	-1.57480378
C	0.95318458	-4.74204706	-1.07357161
H	1.80915787	-1.45658465	-3.56005891
H	2.90332525	-2.63418108	-1.06634680
H	0.87317541	-4.53495339	0.00108639
N	2.14212749	-5.59934815	-1.31092251
H	0.02997798	-5.26499503	-1.35851905
P	2.45344500	-6.87167843	-0.30875927
H	5.28152015	-7.48199610	-0.73169274
H	-0.05793260	-7.55724919	-1.60645513
H	4.07010451	-8.40740467	1.60672979
H	5.30880346	4.12704886	-1.71602404
H	3.72760172	4.07446993	-2.54291957
H	5.22799918	3.80617232	-3.46246992
H	6.66557335	1.96130707	-1.40362749
H	6.55439484	1.65163642	-3.15623620
H	6.02315369	0.41501678	-2.00065002
H	4.31380251	1.67517941	-4.35424064

H	2.80213936	1.79517022	-3.41316908
H	3.83672776	0.34417520	-3.28978200
H	6.83069427	-5.41616507	1.09202157
H	8.46955186	-7.00820199	0.07963868
H	8.40112279	-7.44454739	-2.37605647
C	4.72988345	3.62077187	-2.49975332
C	3.84180430	1.43629352	-3.39070097
C	6.05582954	1.49458112	-2.18802791
O	5.43893628	1.51776039	0.90626509
N	4.40876595	3.55588177	0.77596752
C	5.07373937	4.13452294	1.95751125
H	3.65749674	4.08872570	0.34037855
C	4.35941947	3.70449850	3.24920341
C	5.14412427	5.65693971	1.79873506
H	6.09035490	3.71427796	1.96093797
H	4.89464298	4.08978447	4.12907592
H	4.32307590	2.60917593	3.31129561
H	3.33102843	4.09546338	3.26648640
H	5.66365307	6.10266695	2.65764601
H	4.13285878	6.09081927	1.75360760
H	5.68436619	5.93155525	0.88217579
C	5.34151887	-2.34237460	-4.44369235
C	6.13995688	-1.29553233	-4.91880722
C	6.14790974	-0.94853218	-6.27337579
C	5.34130425	-1.65604407	-7.17233356
C	4.56042628	-2.72304363	-6.72423125
C	4.56983032	-3.08094534	-5.36821026
H	6.71826016	-0.71861524	-4.20182665
H	6.76282950	-0.11921033	-6.62068561
H	5.32435744	-1.38356821	-8.22747633
H	3.94513003	-3.28934571	-7.42252503
N	3.80074353	-4.16186627	-4.92382648
C	5.75231704	-1.98548320	-0.69706928
C	5.15753342	-2.59843572	-2.98626069
H	4.12247278	-2.42158678	-2.68669888
C	6.11347322	-2.16311207	-2.04071634
H	7.16863152	-2.12952836	-2.30195395
O	4.58720439	-2.07328258	-0.19725793
O	6.82964968	-1.68352147	0.12441439
C	6.51054188	-1.52008821	1.53212742
H	7.47397353	-1.34597227	2.02233740
H	6.04617632	-2.43123924	1.92409116
H	5.84924357	-0.66111946	1.67900835
C	4.09126705	-4.96685657	-3.82833119
H	3.06566980	-4.51798429	-5.53194852
O	3.46086782	-6.05869768	-3.68229710
N	4.98455928	-4.44458968	-2.97540560
H	5.16102351	-4.27995757	-0.35087741
H	2.55506116	-5.71093816	-2.27772990
C	5.83736437	-5.19496848	-2.16767284
C	6.75841051	-6.09986772	-2.73178488
C	7.69348622	-6.74703118	-1.92674258
C	7.73409776	-6.50202882	-0.54524258
C	6.82321894	-5.60385332	0.01964975
C	5.88461393	-4.95503429	-0.78522598
H	6.72761188	-6.28164224	-3.80530451
C	1.02098766	-3.45754807	-3.32573442
C	0.54312103	-4.57752996	-4.02028578
C	0.45434654	-4.57138445	-5.41585900
C	0.83593167	-3.43783864	-6.14060532
C	1.32678897	-2.32059048	-5.45831238
C	1.42178941	-2.33499017	-4.06661184
H	0.23947622	-5.47267588	-3.48426554
H	0.08677189	-5.45623750	-5.93505320
H	0.76017407	-3.42979021	-7.22771576
H	1.65097787	-1.44050663	-6.01114377
C	0.87557521	-7.49038766	0.35197102
C	0.68838093	-7.68795644	1.72895809
C	-0.54474537	-8.14293772	2.20378556
C	-1.59227230	-8.39498859	1.31355603
C	-1.41216495	-8.19020952	-0.05955995
C	-0.18555814	-7.73553367	-0.54101794
H	1.49179948	-7.47454914	2.42883736
H	-0.68762880	-8.29054623	3.27324187
H	-2.55388509	-8.74258843	1.68900034
H	-2.23107764	-8.37230600	-0.75383222
C	3.29394906	-8.18532327	-1.22290998
C	2.54073278	-9.14409434	-1.92490287
C	3.19239905	-10.10584583	-2.69444460
C	4.59065189	-10.12179938	-2.76061609
C	5.33662176	-9.17981996	-2.04896543
C	4.69520753	-8.20854661	-1.27988746
H	1.45727461	-9.15570946	-1.86592091
H	2.60789377	-10.84629261	-3.23861498
H	5.09699465	-10.87406328	-3.36456509
H	6.42241227	-9.18884118	-2.09573611
C	3.46214586	-6.38474205	1.11061883
C	3.53707578	-5.02834396	1.46126780
C	4.26447553	-4.64671216	2.58858572
C	4.92242543	-5.61044693	3.35837552
C	4.85497323	-6.96262510	3.00318821
C	4.12105699	-7.35562617	1.88337857
H	3.06889444	-4.26700876	0.84443228
H	4.32796027	-3.59252046	2.84877516
H	5.49966879	-5.30701802	4.23137343
H	5.37862637	-7.71155305	3.59576233

TS5_10

E = -25763.58

G = -25185.65

Nimag = 1, 201i cm-1

C	0.87724262	1.03533219	-1.89128395
C	0.26437012	-0.34176357	-2.13110841
C	2.09873650	0.34966786	-1.39329557
C	1.53475289	-0.94003297	-1.61728522
O	0.53818825	2.21355836	-2.04891234
O	-0.81131921	-0.77422654	-2.57333982
N	2.06867658	-2.15288452	-1.41144698
N	3.27660189	0.76310199	-0.94578057
C	3.64077585	2.18448095	-0.93822615
C	4.28177738	2.47927866	0.43033207
H	2.70459479	2.74750984	-1.04663001
C	4.56449532	2.57056077	-2.15660135
H	3.97963130	0.05838955	-0.66398821
C	1.54831338	-3.41672744	-1.95461165
H	2.42651048	-4.05772571	-2.10013498
C	0.90977703	-3.14813795	-3.32782652
H	-0.59972699	-2.39761278	-0.55411415
H	3.06463361	-2.15510160	-1.09620731
H	-0.06036253	-2.66788243	-3.16566820
N	0.72144840	-4.41179342	-4.08869580
H	1.54351514	-2.44951414	-3.89017986
P	-0.44848230	-4.27986590	-5.27463003
H	0.43614092	-4.00577037	-8.07968541
H	-1.40385356	-5.31739578	-2.74969952
H	1.69914102	-5.79740211	-6.59439498
H	5.28837287	4.45130187	-1.27273943
H	3.77789265	4.61999779	-2.20802172
H	5.32961534	4.40050847	-3.05037172
H	6.46314587	2.15913658	-1.13586844
H	6.55465387	2.17854681	-2.91751024
H	5.84481382	0.78922382	-2.08246005
H	4.47556501	2.40382520	-4.32696360
H	2.87714095	2.64432818	-3.55730521
H	3.69033889	1.06146893	-3.49807623
H	5.56675601	-6.01534660	-0.70179742
H	6.46790525	-7.77858300	-2.22237956
H	6.38272238	-7.43085041	-4.69346023
C	4.74960526	4.10396396	-2.16441251
C	3.85147660	2.14422083	-3.46168415
C	5.93807916	1.88056387	-2.05855027
O	5.06048703	1.68031102	0.97054563
N	3.94677315	3.67983739	0.97042143
C	4.44736983	4.13149115	2.28176080
H	3.22695989	4.23817869	0.51411588
C	3.59462902	3.54562237	3.41882563
C	4.49172275	5.66302665	2.30394304
H	5.46773811	3.72932482	2.36287852
H	4.00779150	3.83559204	4.39561676
H	3.58199818	2.44988261	3.35388377

H	2.56092091	3.91700679	3.35287207
H	4.89205534	6.01480849	3.26438576
H	3.48083038	6.08374982	2.18546288
H	5.12895290	6.04908232	1.49646564
C	5.22052244	-0.92869828	-4.76900005
C	6.26677437	-0.00608129	-4.87672313
C	6.33463570	0.88757804	-5.94867379
C	5.34035222	0.86621859	-6.93266897
C	4.31635512	-0.08093241	-6.87300772
C	4.27168932	-0.99048757	-5.80841423
H	6.99795404	0.04634485	-4.07608872
H	7.14403067	1.61463859	-6.00158381
H	5.36738468	1.57676232	-7.75854937
H	3.55743070	-0.12762951	-7.65287980
N	3.28652797	-1.99366987	-5.76403616
C	5.77422599	-1.78080375	-1.19172959
C	4.97357810	-1.72248123	-3.52266552
H	4.00930420	-1.44771692	-3.08445035
C	6.01930111	-1.84116165	-2.56665775
H	7.05019454	-1.92984194	-2.90028729
O	4.64799048	-1.71244739	-0.60080058
O	6.93094848	-1.76443882	-0.42284640
C	6.71723781	-1.52359442	0.99777419
H	7.71894874	-1.53368788	1.43853926
H	6.09844412	-2.31469624	1.43779544
H	6.23552263	-0.55133619	1.15129889
C	3.55381440	-3.27725164	-5.24382874
H	2.67264065	-2.05080219	-6.57744097
O	2.92974038	-4.25446029	-5.74806170
N	4.40135067	-3.30575536	-4.20501748
H	4.58006357	-3.95579061	-1.63420159
H	1.63482827	-4.68327571	-4.51720474
C	4.91995026	-4.50953633	-3.69702382
C	5.44538603	-5.49893070	-4.54928832
C	5.98718083	-6.66970171	-4.02059009
C	6.03622349	-6.86613067	-2.63265894
C	5.53152325	-5.87894045	-1.78253110
C	4.97453033	-4.70818787	-2.30665848
H	5.41398926	-5.34215732	-5.62506699
C	0.57674980	-4.14514387	-1.04211391
C	0.68565686	-5.53374518	-0.89711715
C	-0.26044106	-6.24592812	-0.15215658
C	-1.31928380	-5.56830613	0.46134291
C	-1.42553762	-4.17949286	0.32625131
C	-0.48697692	-3.47121944	-0.42728763
H	1.50840481	-6.06082544	-1.38038999
H	-0.16853731	-7.32691448	-0.04955914
H	-2.05626263	-6.11995382	1.04478879
H	-2.25197346	-3.64627457	0.79565601
C	-2.01953343	-4.07916291	-4.41884424
C	-3.04953452	-3.31248885	-4.98800530
C	-4.27063587	-3.20227664	-4.32167725
C	-4.46112849	-3.85153766	-3.09693160
C	-3.43325188	-4.61530690	-2.53385748
C	-2.20961827	-4.73667579	-3.19045133
H	-2.89644151	-2.80124280	-5.93593477
H	-5.06998156	-2.60324997	-4.75504536
H	-5.41348233	-3.75629351	-2.57649368
H	-3.57653665	-5.11010145	-1.57597170
C	-0.18479525	-2.84473341	-6.35606971
C	-0.32549992	-1.55176036	-5.81178668
C	0.06904259	-0.44221652	-6.56033730
C	0.58615108	-0.60948088	-7.84899226
C	0.70469123	-1.89115641	-8.39841230
C	0.32519390	-3.01151241	-7.65475048
H	-0.72231293	-1.39808931	-4.81036173
H	-0.02371943	0.55306594	-6.12813566
H	0.89474071	0.26057118	-8.42743732
H	1.10088370	-2.02215341	-9.40460009
C	-0.44117821	-5.81555164	-6.22315833
C	-1.65415167	-6.49628430	-6.42544546
C	-1.65970353	-7.69588478	-7.14030056
C	-0.46418548	-8.21789341	-7.64397819
C	0.74238759	-7.53932658	-7.43867309
C	0.76412499	-6.33556226	-6.73253271
H	-2.58224625	-6.09909153	-6.02105430
H	-2.59879250	-8.22469604	-7.29701632
H	-0.47188735	-9.15737646	-8.19547066
H	1.67305639	-7.94586782	-7.83240174

TS5_11

E = -25757.84

G = -25178.21

Nimag = 1, 286i cm-1

C	1.06033987	0.19822919	-2.76828955
C	0.96446695	-1.15037975	-3.48869373
C	2.24495609	-0.32826193	-2.03960365
C	2.08387927	-1.61668854	-2.61699699
O	0.39803209	1.24701581	-2.70898271
O	0.28652069	-1.65186371	-4.38726309
N	2.64266095	-2.80465722	-2.38882219
N	3.12270857	0.21144375	-1.19581763
C	3.00519922	1.63729097	-0.82616370
C	2.19348199	1.69710168	0.49077625
H	2.38535512	2.09372332	-1.60654307
C	4.36201015	2.39508587	-0.86472645
H	3.79177704	-0.42380150	-0.72043608
C	2.28028779	-3.94938887	-3.25204606
H	1.28559319	-3.70712845	-3.63927120
C	2.19973765	-5.27712811	-2.45550963
H	4.80471422	-5.11811288	-3.42554136
H	3.45889703	-2.83955241	-1.75121617
H	1.46085644	-5.92566670	-2.94736081
N	1.94973087	-5.12219784	-0.99694478
H	3.15211332	-5.80380327	-2.50667961
P	0.49148002	-4.73042332	-0.31510804
H	-0.89310380	-5.65177488	-2.69683701
H	-0.57904106	-4.76136730	2.43279359
H	1.32254725	-7.50866262	0.24050336
H	3.75124398	3.91697420	0.59122717
H	3.30920766	4.30819680	-1.09405334
H	5.00015579	4.45660405	-0.55807964
H	6.36299647	2.36772772	-0.03198930
H	5.66875019	0.74954120	-0.20714507
H	5.10284792	1.81484088	1.10450368
H	5.81604597	2.89986771	-2.41084220
H	4.13856001	2.82075543	-3.00847159
H	5.03174265	1.31988427	-2.65767081
H	2.89740198	-3.48812278	3.31398525
H	3.59235170	-5.06910649	5.10423297
H	5.06140245	-7.00728650	4.53510701
C	4.08353843	3.85857468	-0.45390701
C	4.86549930	2.35415967	-2.32654321
C	5.43282612	1.78749713	0.06184761
O	2.70689816	1.62115980	1.62107005
N	0.85705631	1.73980674	0.26045064
C	-0.15888565	1.67228965	1.32270123
H	0.53677191	1.75731458	-0.71733467
C	-1.21243935	0.61718455	0.95825498
C	-0.77432787	3.06064087	1.56233736
H	0.38095579	1.36141455	2.22722935
H	-1.99059002	0.56733499	1.73261644
H	-0.74875739	-0.37103488	0.87450217
H	-1.69520392	0.86531113	0.00124069
H	-1.50138215	3.02133990	2.38611622
H	-1.29275454	3.41333391	0.65822936
H	0.01053133	3.78451134	1.81971648
C	6.97964783	-5.30847436	-1.66547088
C	8.25907700	-4.85250468	-1.99962041
C	9.07682339	-5.57347716	-2.87643110
C	8.60739342	-6.76604632	-3.43725426
C	7.34134659	-7.25023024	-3.10047273
C	6.53269656	-6.53393818	-2.20875730
H	8.59095778	-3.89787876	-1.59528631
H	10.06626945	-5.19717935	-3.13250046
H	9.22901640	-7.32747836	-4.13411533
H	6.97653640	-8.18535982	-3.52557564
N	5.24233956	-6.98895749	-1.88987350
C	5.58000798	-2.34479303	0.23340103
C	6.02035935	-4.47565313	-0.88392526

H	5.12924176	-4.23055777	-1.46700867
C	6.43587612	-3.41855709	-0.04773923
H	7.34437694	-3.51460919	0.54234707
O	4.45822199	-2.08589598	-0.30570220
O	6.08345919	-1.49544249	1.21946998
C	5.08374868	-0.90257794	2.09215705
H	5.63412006	-0.22313181	2.74976705
H	4.60219451	-1.69330257	2.68223578
H	4.33124322	-0.33871093	1.54195545
C	4.61055608	-6.75867467	-0.65242468
H	4.89162060	-7.81240655	-2.37962578
O	3.52240679	-7.36141659	-0.41111552
N	5.21368166	-5.84335389	0.10985310
H	3.65188838	-3.83991205	0.97517958
H	2.46877073	-5.86961567	-0.48248216
C	4.76720679	-5.61909900	1.42722671
C	5.17467500	-6.50226320	2.44338604
C	4.74835170	-6.31054532	3.75740997
C	3.92405936	-5.22215714	4.07751814
C	3.53642180	-4.33274357	3.07285953
C	3.95703874	-4.52528814	1.75424317
H	5.81871708	-7.34022533	2.18017511
C	3.23415098	-4.03226746	-4.44246815
C	2.87377328	-3.40477826	-5.64431803
C	3.76598325	-3.37774778	-6.72124480
C	5.03066505	-3.96686318	-6.60589741
C	5.39782657	-4.58934218	-5.40771988
C	4.50095979	-4.62264296	-4.33743508
H	1.90122535	-2.91937622	-5.72019273
H	3.47479993	-2.88848649	-7.65057721
H	5.72659375	-3.93782382	-7.44389762
H	6.38022545	-5.04708713	-5.29538243
C	0.71172908	-3.63053526	1.10634693
C	1.49022873	-2.46859077	0.95394722
C	1.52988684	-1.52247488	1.97566523
C	0.80492022	-1.73407982	3.15323994
C	0.05591630	-2.90218272	3.31958584
C	0.00363184	-3.85386366	2.29767592
H	2.07120676	-2.31538528	0.05341584
H	2.11777904	-0.61632205	1.85807715
H	0.83572299	-0.98858545	3.94758351
H	-0.48853628	-3.07909941	4.24632488
C	-0.58306696	-3.87318870	-1.48831101
C	-0.94740105	-2.53109595	-1.28692298
C	-1.84889794	-1.91877160	-2.15605414
C	-2.38276668	-2.63507162	-3.22837202
C	-2.02838528	-3.97402898	-3.42778973
C	-1.13877805	-4.60073850	-2.55740778
H	-0.53393309	-1.96852767	-0.45896186
H	-2.10828847	-0.87202082	-2.01110731
H	-3.07005396	-2.14746308	-3.91782296
H	-2.44730331	-4.53235228	-4.26359762
C	-0.41958363	-6.20093932	0.23389824
C	-1.80393454	-6.10766669	0.46607896
C	-2.50029698	-7.21793142	0.94346961
C	-1.82184564	-8.41858540	1.18596061
C	-0.44912349	-8.51403887	0.93882018
C	0.26123561	-7.40865918	0.46048774
H	-2.33175721	-5.17631067	0.26778952
H	-3.57250409	-7.14806846	1.12171654
H	-2.36812602	-9.28430009	1.55875861
H	0.07511184	-9.45307835	1.11134543

TS5_12

E = -25764.36

G = -25186.88

Nimag = 1, 199i cm-1

C	0.92748103	1.24572494	-2.08221080
C	0.28032966	-0.11091810	-2.31340263
C	2.12768689	0.54308476	-1.56775454
C	1.53062704	-0.73816719	-1.77798029
O	0.59183704	2.43401547	-2.21379022
O	-0.80928468	-0.51547951	-2.74282008
N	2.01583732	-1.95485136	-1.51172393
N	3.31865715	0.92145930	-1.11420606
C	3.63320661	2.34697792	-0.86861831
C	3.02074057	2.70050905	0.51342249
H	3.08912117	2.91425614	-1.63551064
C	5.14084192	2.66278062	-1.06313064
H	3.93813671	0.17723763	-0.74513371
C	1.46087070	-3.22522190	-2.00247867
H	2.32143242	-3.89291860	-2.13078071
C	0.82292930	-2.99256886	-3.38232264
H	-0.62777409	-2.07553302	-0.61787076
H	3.00018078	-1.97120088	-1.15524738
H	-0.12802844	-2.46995340	-3.23755302
N	0.58206108	-4.28054337	-4.08100291
H	1.47917705	-2.34400072	-3.97830370
P	-0.55933328	-4.15821650	-5.29234036
H	0.42245275	-4.06254081	-8.07272170
H	-1.57999405	-5.01505203	-2.73193072
H	1.57519956	-5.83616655	-6.41243195
H	5.12653414	4.38851206	0.29081427
H	4.67848152	4.78352765	-1.39182586
H	6.37785713	4.45435605	-0.97494948
H	5.83613645	2.01492325	0.91158109
H	7.11192562	2.08276835	-0.35807456
H	5.94937115	0.74704573	-0.34586600
H	6.54781062	2.60042219	-2.73040455
H	4.87665704	2.98074870	-3.22241237
H	5.32418075	1.31578209	-2.78135124
H	5.47435456	-5.76943808	-0.30596894
H	6.63389702	-7.50267583	-1.67750757
H	6.71551646	-7.25481737	-4.16038119
C	5.33824169	4.16560528	-0.76364868
C	5.48933508	2.37180287	-2.54015471
C	6.05838117	1.82325023	-0.14807809
O	3.59871201	2.48924603	1.59025865
N	1.75314286	3.18067362	0.40577948
C	0.81900446	3.17587263	1.54661099
H	1.32335939	3.17203951	-0.52917086
C	0.19519963	1.77508405	1.69319150
C	-0.23475292	4.26995141	1.34414106
H	1.42289077	3.39633688	2.43785158
H	-0.47241797	1.73558254	2.56615144
H	0.98321010	1.02053385	1.82046282
H	-0.38859084	1.52462033	0.79492470
H	-0.92927745	4.29075198	2.19519690
H	-0.81896081	4.07914684	0.43089136
H	0.24153512	5.25587461	1.25356770
C	5.18307189	-1.00435764	-4.82360344
C	6.22133982	-0.08188708	-4.99701688
C	6.35384781	0.64437215	-6.18415986
C	5.43401478	0.45188321	-7.22091062
C	4.41105813	-0.48861223	-7.08300786
C	4.29555579	-1.22415161	-5.89603938
H	6.90238899	0.09391581	-4.16869700
H	7.15900255	1.36975292	-6.29107458
H	5.51803727	1.02380945	-8.14469571
H	3.70916859	-0.66634825	-7.89593153
N	3.30523662	-2.21827844	-5.76638747
C	5.68408214	-1.68119971	-1.15612339
C	4.90805242	-1.65841784	-3.50291162
H	3.94311815	-1.32935542	-3.10816322
C	5.94445168	-1.70470334	-2.52537362
H	6.97319900	-1.85605758	-2.84394877
O	4.55554189	-1.57019932	-0.56692430
O	6.82999788	-1.77057592	-0.37149004
C	6.59781044	-1.81542747	1.06139467
H	7.59318863	-1.90308499	1.50706846
H	5.98138023	-2.68286632	1.32752253
H	6.10390932	-0.90191853	1.41144724
C	3.55611472	-3.41918610	-5.07678220
H	2.72117353	-2.37672301	-6.58847154
O	2.96239460	-4.46812439	-5.46095109
N	4.36738916	-3.30522658	-4.01399791
H	4.39973004	-3.83671428	-1.39706127
H	1.48863776	-4.63762148	-4.46244388
C	4.93533661	-4.44069708	-3.40290298
C	5.60818314	-5.40884578	-4.16979433

C	6.20430814	-6.50782509	-3.55313650
C	6.15996371	-6.64738477	-2.15825010
C	5.51023793	-5.67730458	-1.39122118
C	4.89941317	-4.58029810	-2.00683031
H	5.64924753	-5.29181152	-5.25078822
C	0.47167846	-3.88504585	-1.05752696
C	0.52495666	-5.27145407	-0.86939612
C	-0.44500276	-5.91959106	-0.09713703
C	-1.47179931	-5.17997512	0.49893421
C	-1.52281439	-3.79304041	0.31975158
C	-0.55929087	-3.14868089	-0.45895232
H	1.32284602	-5.84691551	-1.33853650
H	-0.39648164	-6.99959878	0.04028998
H	-2.22700436	-5.68194801	1.10342170
H	-2.32281382	-3.21162583	0.77730740
C	-2.13263191	-3.84979731	-4.47449832
C	-3.12089894	-3.06529705	-5.09107827
C	-4.33471297	-2.85333388	-4.43566268
C	-4.55765668	-3.41736435	-3.17467087
C	-3.57128632	-4.19971631	-2.56451547
C	-2.35641041	-4.42392363	-3.21010026
H	-2.93997756	-2.61634793	-6.06538338
H	-5.10157425	-2.23902888	-4.90483996
H	-5.50246147	-3.23952772	-2.66210642
H	-3.73906955	-4.62707174	-1.57843607
C	-0.20247151	-2.78897742	-6.43083007
C	-0.29888810	-1.46468569	-5.95640167
C	0.18111589	-0.41516913	-6.74036371
C	0.74187539	-0.67161786	-7.99569031
C	0.81727720	-1.98308752	-8.47728968
C	0.35030197	-3.04464805	-7.69811698
H	-0.72566257	-1.24321685	-4.98041874
H	0.12199798	0.60408489	-6.36152049
H	1.11958474	0.15236773	-8.59955712
H	1.24453431	-2.18394392	-9.45898596
C	-0.58437750	-5.72220527	-6.18805367
C	-1.81983072	-6.33334370	-6.46126345
C	-1.84983491	-7.53608033	-7.17028700
C	-0.65735524	-8.12644961	-7.60056388
C	0.57152811	-7.51668812	-7.32362735
C	0.61891409	-6.31255209	-6.61939604
H	-2.74612848	-5.88032632	-6.11496813
H	-2.80571948	-8.01355391	-7.38063549
H	-0.68507644	-9.06636549	-8.15065550
H	1.49976940	-7.97925049	-7.65623172

TS5_13
E = -25763.33
G = -25185.03
Nimag = 1, 166i cm-1

C	3.22167447	-0.25309816	1.88681090
C	1.97746800	-0.56721679	1.02921899
C	3.75185865	0.51049916	0.72026869
C	2.61627638	0.20171114	-0.06720085
O	3.65454119	-0.54997394	3.00460057
O	0.94121674	-1.23052537	1.13715647
N	2.28771039	0.41741876	-1.35403491
N	4.86244942	1.20913902	0.48974636
C	6.02458005	1.04949681	1.37469113
C	6.66165818	-0.32635658	1.08225467
H	5.65017938	1.04273361	2.40721758
C	7.02443048	2.24136990	1.26034864
H	4.99893884	1.54007396	-0.49428234
C	0.87133986	0.31458216	-1.74839896
H	0.49192083	-0.61988248	-1.31425578
C	0.68271922	0.27497949	-3.27414681
H	-1.56148614	0.09597497	-0.58162613
H	2.90842578	1.04873057	-1.87285714
H	-0.40424967	0.23940522	-3.43626988
N	1.36729188	-0.81049775	-4.00280350
H	1.03843793	1.20782004	-3.72908724
P	1.28255069	-2.41666133	-3.66488297
H	-0.25249784	-4.67806267	-4.65618807
H	0.48959962	-4.24231476	-1.42569470
H	1.72098267	-2.36355670	-0.74194663
H	8.28330140	3.27003047	-0.17272697
H	6.78803086	2.64535397	-0.89481207
H	8.11139341	1.52470160	-0.50576441
H	6.89669858	4.40683885	1.48535197
H	6.05542930	3.50309761	2.77151702
H	5.32795731	3.63293138	1.15074941
H	8.74261136	2.89723873	2.43656634
H	8.89856623	1.23651103	1.81736790
H	7.82803594	1.57633081	3.19993584
H	1.51873637	4.28183449	-4.56359205
H	2.20894953	4.94218363	-6.87221641
H	4.24005794	3.90713767	-7.88818758
C	8.19270561	1.96647320	2.23827403
C	6.27629875	3.52394640	1.69355969
C	7.58173101	2.42273116	-0.16964771
O	7.13006366	-0.61464212	-0.03754004
N	6.63765373	-1.18023942	2.12818239
C	7.11242136	-2.57408716	2.05750091
H	6.06652304	-0.91497904	2.93359062
C	6.02614282	-3.51847200	2.58640372
C	8.43715613	-2.72130283	2.82329371
H	7.29663976	-2.76138552	0.99116238
H	6.33651473	-4.56438916	2.45817542
H	5.07934797	-3.36301781	2.05955168
H	5.84819962	-3.34306784	3.65838007
H	8.83176610	-3.74106684	2.70953709
H	8.28619513	-2.52544270	3.89519751
H	9.18202338	-2.01157757	2.43915295
C	5.86622383	-1.18210618	-4.76282677
C	6.43921354	-2.13925294	-5.60615939
C	7.51483186	-2.92784284	-5.18079403
C	8.03064222	-2.75439817	-3.89149012
C	7.47399844	-1.80594515	-3.03273206
C	6.39061023	-1.02625599	-3.46447674
H	6.01499689	-2.28028464	-6.59806375
H	7.94449624	-3.67081359	-5.85178629
H	8.86626893	-3.36448210	-3.54809271
H	7.85268661	-1.67271607	-2.02202786
N	5.80198185	-0.10302076	-2.58850971
C	3.06175167	0.11240795	-6.98079118
C	4.65051117	-0.38908431	-5.14105825
H	3.79450347	-0.67436503	-4.51910687
C	4.33632358	-0.25762890	-6.53048378
H	5.14362630	-0.25265747	-7.25905988
O	1.99980871	0.26920653	-6.30899781
O	3.01190610	0.32331139	-8.35981562
C	1.72648366	0.77956000	-8.85265555
H	1.87011486	0.93723763	-9.92616371
H	1.43854852	1.71670636	-8.36162547
H	0.94925574	0.02505402	-8.67761696
C	5.13823969	1.04447914	-2.99969409
H	6.15477913	-0.10941399	-1.61973758
O	4.78275641	1.89786707	-2.12985838
N	4.92829519	1.15217442	-4.33064873
H	2.80332086	2.57539833	-3.33105989
H	1.66031439	-0.49451442	-4.98877336
C	4.23928082	2.24498233	-4.90362184
C	4.65078405	2.65856469	-6.18246234
C	3.91808721	3.61591672	-6.88863225
C	2.78037718	4.19596569	-6.32086779
C	2.39094991	3.82150049	-5.02830132
C	3.10758378	2.85116406	-4.33066460
H	5.54481067	2.21640082	-6.61281890
C	0.01649395	1.43849642	-1.17772470
C	0.44613052	2.77081098	-1.21702253
C	-0.37366000	3.79059608	-0.72612572
C	-1.63057672	3.48416871	-0.19185990
C	-2.06065420	2.15368461	-0.14466943
C	-1.23766923	1.13529034	-0.63466127
H	1.42761059	3.01978731	-1.61582465
H	-0.02891237	4.82377643	-0.75636019
H	-2.26784892	4.27883905	0.19463352
H	-3.03189061	1.90787825	0.28379383
C	-0.28874748	-2.80989251	-2.85552550
C	-1.44530827	-2.18725249	-3.36263061

C	-2.68525515	-2.44913855	-2.78243622
C	-2.78037477	-3.33682609	-1.70429172
C	-1.63782221	-3.98065670	-1.22089065
C	-0.39116247	-3.72596913	-1.79647205
H	-1.37269974	-1.50963444	-4.21028799
H	-3.57740384	-1.96069955	-3.17162873
H	-3.74890751	-3.53177023	-1.24524095
H	-1.71333208	-4.68226646	-0.39161095
C	1.36347712	-3.34256816	-5.22158531
C	2.29698738	-3.00690339	-6.21590514
C	2.32780290	-3.73216764	-7.40668136
C	1.44212418	-4.79562485	-7.60946556
C	0.51968687	-5.13691887	-6.61473215
C	0.47369646	-4.41325489	-5.42087741
H	3.00379861	-2.19138779	-6.09302108
H	3.04771965	-3.45512271	-8.17581510
H	1.46832792	-5.35767480	-8.54242826
H	-0.17325165	-5.96298995	-6.76870102
C	2.66357527	-2.94399396	-2.61361216
C	3.83236434	-3.45595899	-3.20583103
C	4.93888434	-3.75326624	-2.41103309
C	4.88527505	-3.55584318	-1.02863082
C	3.71662236	-3.06882847	-0.43684348
C	2.60787473	-2.76096169	-1.22255354
H	3.89288310	-3.61354564	-4.27797725
H	5.84553574	-4.12564733	-2.87986755
H	5.75230476	-3.78811705	-0.41489832
H	3.65262054	-2.93283061	0.63932811

TS5_14

E = -25758.09

G = -25183.49

Nimag = 1, 236i cm-1

C	4.04079035	0.43295258	2.32144831
C	2.74329820	0.68697904	1.52875779
C	4.50345868	-0.39605945	1.17824776
C	3.32912616	-0.13412486	0.43278707
O	4.51588856	0.74806260	3.41744840
O	1.66664906	1.26761743	1.70875197
N	3.03074467	-0.53650164	-0.80211470
N	5.58548992	-1.12441447	0.91546774
C	6.72957251	-1.15712091	1.83351352
C	6.96366977	-2.61811096	2.25726553
H	6.42966336	-0.56374242	2.70685216
C	7.99402681	-0.47165709	1.20624974
H	5.62943025	-1.67888138	0.05251160
C	1.79276754	-0.29340619	-1.55120455
H	2.07957576	-0.41047620	-2.60227700
C	1.29275471	1.17086121	-1.38430029
H	0.52068346	-0.72154161	0.83637688
H	3.67382140	-1.24465294	-1.20025756
H	0.55161493	1.25807432	-0.58440072
N	0.77537540	1.74089235	-2.63820390
H	2.14241498	1.80348479	-1.09823994
P	-0.71435592	1.52599364	-3.31152404
H	0.94322342	0.33037869	-5.29162153
H	-2.03136234	1.78191096	-5.91279683
H	-2.39451886	3.69395311	-2.33234466
H	9.29295872	-0.65078709	-0.52321544
H	7.63871154	-1.19006905	-0.83680303
H	8.73257538	-2.22483826	0.11206868
H	8.48596106	1.51925017	0.47044526
H	7.29168048	1.52115348	1.79816086
H	6.81014626	1.04466393	0.14793755
H	10.01216743	0.03299517	1.84527710
H	9.44095065	-1.52719944	2.48183459
H	8.83437531	-0.00275084	3.17887885
H	5.49640669	3.23510346	-2.21594723
H	7.96917388	2.91807947	-2.22995273
H	8.92945779	0.73188870	-2.94504142
C	9.13635801	-0.49905326	2.24390661
C	7.61668626	0.99312835	0.88905627
C	8.43835328	-1.18671070	-0.08623965
O	6.98419835	-3.54300688	1.43198399
N	7.16017791	-2.79137716	3.59057311
C	7.38617128	-4.11174969	4.20473853
H	7.02700636	-1.99343578	4.21043808
C	6.04751172	-4.78351612	4.55219021
C	8.30221719	-3.95190788	5.42338946
H	7.89299963	-4.71048188	3.43434251
H	6.21824542	-5.79081853	4.95850045
H	5.42305072	-4.86828498	3.65315146
H	5.50517702	-4.19134327	5.30447985
H	8.50679577	-4.93262729	5.87390165
H	7.82416424	-3.32152774	6.18954458
H	9.25746605	-3.49099345	5.13708432
C	3.54636725	-1.92173451	-5.85418329
C	3.41824972	-2.02569970	-7.24423469
C	3.13521291	-3.25083421	-7.85703972
C	2.96627804	-4.39378034	-7.06665722
C	3.12441331	-4.31907872	-5.68163091
C	3.43281963	-3.09308567	-5.07428228
H	3.48737176	-1.11569826	-7.83772684
H	3.02608787	-3.30826772	-8.93920679
H	2.72306024	-5.35051305	-7.52818164
H	3.01960543	-5.21227814	-5.06518297
N	3.60442882	-3.01057276	-3.68458593
C	3.30514683	1.79267508	-5.58639155
C	3.60269319	-0.60020548	-5.16484601
H	2.73448761	-0.46360997	-4.51601524
C	3.95979691	0.58032903	-5.85592485
H	4.74592951	0.56539082	-6.60725049
O	2.34047204	1.98526520	-4.79413243
O	3.76745868	2.86383624	-6.35001658
C	3.03508766	4.10157719	-6.14520091
H	3.46963568	4.81297738	-6.85433301
H	3.16069858	4.46201466	-5.11656514
H	1.96596643	3.96161123	-6.34099783
C	4.48725542	-2.10218280	-3.06122387
H	3.51446486	-3.87817416	-3.15371867
O	4.86033207	-2.36507700	-1.87715987
N	4.76599858	-1.01444853	-3.77890737
H	4.00482688	1.38055403	-2.91903372
H	1.50934390	1.88504650	-3.37369452
C	5.61646736	0.00641334	-3.31248544
C	7.00914730	-0.16212496	-3.33508117
C	7.85007169	0.87995923	-2.94280437
C	7.31142968	2.10624745	-2.53824280
C	5.92436629	2.28242428	-2.52766797
C	5.08008772	1.24015850	-2.91510875
H	7.41698027	-1.11988088	-3.65506512
C	0.74525943	-1.34611462	-1.22502802
C	0.33673739	-2.26176769	-2.20067217
C	-0.62897917	-3.22832685	-1.90234037
C	-1.17441852	-3.29932387	-0.61709869
C	-0.74423728	-2.40445669	0.37214423
C	0.20891099	-1.43108013	0.07071602
H	0.76871395	-2.21767835	-3.19744974
H	-0.95629914	-3.92097014	-2.67623873
H	-1.92657201	-4.05245736	-0.38265981
H	-1.15854088	-2.46161643	1.37852768
C	-0.88079180	2.90982066	-4.46397575
C	-0.28232268	4.14287500	-4.15466002
C	-0.40198678	5.20813445	-5.04654281
C	-1.10860116	5.04623193	-6.24313083
C	-1.70157191	3.81707595	-6.55089818
C	-1.59020824	2.74454230	-5.66370645
H	0.28741672	4.25282853	-3.23495578
H	0.06926979	6.16205949	-4.81371486
H	-1.18987996	5.87773278	-6.94243213
H	-2.24194247	3.68851138	-7.48771727
C	-0.93973122	0.00135264	-4.27607174
C	-2.06715682	-0.82500070	-4.15253613
C	-2.12988777	-2.01724809	-4.87748414
C	-1.08011177	-2.38184165	-5.72510934
C	0.02483609	-1.53642597	-5.88308650
C	0.09369938	-0.33944343	-5.17101489
H	-2.88453778	-0.55426455	-3.48988391
H	-2.99651166	-2.66782782	-4.76681892
H	-1.12238196	-3.32435274	-6.27025423

H	0.83702828	-1.81574024	-6.55038255
C	-1.94862303	1.59776719	-1.99538157
C	-2.20311242	0.46800607	-1.19835022
C	-3.07351740	0.56925779	-0.11354303
C	-3.69992360	1.78651387	0.17264996
C	-3.45739542	2.90830525	-0.62807440
C	-2.58067813	2.82105389	-1.71078718
H	-1.72087110	-0.47818021	-1.41090514
H	-3.25406023	-0.30475960	0.50976954
H	-4.37873016	1.86227711	1.02126328
H	-3.94810052	3.85515912	-0.40749152

TS5_15

E = -25760.33

G = -25182.47

Nimag = 1, 59i cm-1

C	3.01097843	-0.15029601	2.37038138
C	1.71259336	-0.15696659	1.53859642
C	3.76613556	-0.14796331	1.09118092
C	2.57639352	-0.15975239	0.32668310
O	3.32088279	-0.24499751	3.56684634
O	0.49843473	-0.23165985	1.73943590
N	2.35408454	-0.25996016	-0.98070465
N	5.05925903	-0.18338656	0.73589030
C	6.08614375	-0.53355930	1.74527584
C	5.98542316	-2.06793017	1.88735368
H	5.76799219	-0.07047816	2.68829429
C	7.48485657	0.03840655	1.38995018
H	5.24537555	-0.47308002	-0.24556139
C	0.98465222	-0.36308873	-1.53454030
H	0.36147909	-0.79846810	-0.74668263
C	1.07446388	-1.32931188	-2.72434783
H	-1.12296262	0.97324515	-0.42246413
H	3.17020677	-0.41957896	-1.58776761
H	1.44677108	-0.80074635	-3.60859087
N	-0.16498341	-2.08590714	-3.04974862
H	1.80717857	-2.10528290	-2.48653380
P	-1.48619493	-1.34015099	-3.75136758
H	-1.53131828	-1.85675408	-0.90311696
H	-2.30258580	-1.45771077	-6.58899806
H	0.48313873	-1.23800224	-5.77140104
H	8.94717114	0.07244843	-0.21237361
H	7.27510150	0.03183441	-0.80279938
H	8.00526116	-1.44524020	-0.13737022
H	8.36606030	2.02891038	1.23986017
H	7.12089183	1.89250155	2.50807056
H	6.64111755	1.97164391	0.79330654
H	9.47388692	-0.04084638	2.27947955
H	8.59087900	-1.58355132	2.36929562
H	8.15665996	-0.23930339	3.46061645
H	3.40341914	1.17217860	-5.77631894
H	4.09097072	0.13231862	-7.95043081
H	5.00220745	-2.19106697	-7.95367770
C	8.48483158	-0.49247760	2.44091862
C	7.39476571	1.57837068	1.48953603
C	7.95123408	-0.35709268	-0.02937792
O	6.48735111	-2.84387207	1.04549094
N	5.19244038	-2.46764355	2.90391191
C	4.60412062	-3.82178085	2.96571201
H	4.69884508	-1.73296625	3.42911526
C	3.32000544	-3.86910063	2.11588893
C	4.35320821	-4.19827392	4.42955060
H	5.35241636	-4.49781747	2.53195564
H	2.90880287	-4.88846771	2.10251465
H	3.52226354	-3.56898161	1.08064745
H	2.56220877	-3.19058099	2.53438418
H	3.93306275	-5.21121272	4.49166103
H	3.63561320	-3.50213249	4.88954800
H	5.28859619	-4.16837224	5.00464114
C	4.23285205	-5.13225670	-2.66306904
C	4.30404355	-6.50818114	-2.90667005
C	4.93877495	-7.36831655	-2.00376565
C	5.49720861	-6.85067327	-0.82916550
C	5.44553527	-5.48047066	-0.57119379
C	4.83101206	-4.62376596	-1.49660892
H	3.82508929	-6.90543911	-3.79869980
H	4.97980534	-8.43751124	-2.20836909
H	5.97552224	-7.51462697	-0.10927736
H	5.87065944	-5.05780352	0.33534617
N	4.78228478	-3.23790973	-1.24384496
C	1.96239602	-4.14009880	-5.51349460
C	3.43473323	-4.18962151	-3.52317818
H	2.53114130	-3.89012671	-2.97247103
C	3.07512132	-4.64206485	-4.84590395
H	3.74134275	-5.30808279	-5.38675540
O	1.09675666	-3.31419511	-5.09759504
O	1.81908187	-4.63936489	-6.82216631
C	0.63326835	-4.16988755	-7.50700660
H	0.62476872	-4.69671301	-8.46724340
H	0.67754249	-3.08546790	-7.67473707
H	-0.27439177	-4.39852246	-6.93640698
C	4.72946637	-2.28028761	-2.24970762
H	5.29708926	-2.93767859	-0.40348581
O	5.02399823	-1.07839135	-1.97453333
N	4.32979183	-2.72884234	-3.46829818
H	3.57877106	-0.11028246	-3.68693591
H	0.15489604	-2.80200311	-3.75931263
C	4.33646893	-1.89756138	-4.61718054
C	4.77275195	-2.45795790	-5.83069852
C	4.67111722	-1.73392601	-7.02161979
C	4.16338694	-0.43099659	-7.02021615
C	3.77797167	0.15034997	-5.80738772
C	3.85389202	-0.57813522	-4.62091911
H	5.19868864	-3.45474001	-5.83058448
C	0.45028195	1.01775116	-1.89191809
C	1.09333220	1.79430765	-2.86816962
C	0.63929069	3.07802946	-3.16254113
C	-0.47543580	3.59835489	-2.49365132
C	-1.11955828	2.83162076	-1.51959852
C	-0.64804156	1.55129297	-1.21014583
H	1.95249325	1.39865495	-3.40406171
H	1.14370865	3.66849000	-3.92589739
H	-0.83700949	4.59860863	-2.73103538
H	-1.98157839	3.23210413	-0.98679375
C	-2.25653577	-2.62692855	-4.76575015
C	-2.55400026	-3.86215718	-4.16351812
C	-3.10372669	-4.88647592	-4.93337895
C	-3.37436436	-4.67712578	-6.29075447
C	-3.09668955	-3.44131145	-6.88116692
C	-2.53491558	-2.41168543	-6.12313283
H	-2.34442916	-4.02493405	-3.10805366
H	-3.31984570	-5.84985103	-4.47383028
H	-3.80161778	-5.48138647	-6.88852793
H	-3.30591869	-3.27892197	-7.93757478
C	-2.65059809	-0.85818481	-2.45807824
C	-3.82057460	-0.14755068	-2.77826632
C	-4.70923454	0.20806376	-1.76388221
C	-4.44995892	-0.16398058	-0.43923896
C	-3.31272550	-0.91517707	-0.13000628
C	-2.41415441	-1.26928648	-1.13716882
H	-4.04354985	0.11919579	-3.80889522
H	-5.60918110	0.77056251	-2.00821499
H	-5.14442067	0.12120346	0.35010205
H	-3.11508439	-1.21903431	0.89687101
C	-1.02422712	0.02853081	-4.83737201
C	-1.61062589	1.30059087	-4.79219324
C	-1.18880022	2.28148480	-5.69032789
C	-0.17527831	2.00402176	-6.61163325
C	0.43027967	0.74241638	-6.63528882
C	0.01055155	-0.25381595	-5.75573660
H	-2.35556465	1.54441292	-4.04186428
H	-1.63640177	3.27320290	-5.64990729
H	0.15579923	2.77812889	-7.30351127
H	1.23584499	0.52811889	-7.33488172

TS5_16

E = -25758.72

G = -25181.93

Nimag = 1, 227i cm-1

C	4.49017228	1.21906898	1.54995455

C	3.14350482	1.48699443	0.85238389
C	4.76310108	0.19440620	0.51385166
C	3.51694840	0.42100578	-0.12073406
O	5.04085439	1.55985907	2.60689206
O	2.13728655	2.17123130	1.05821241
N	2.97961002	-0.26299514	-1.12575262
N	5.73013833	-0.69900573	0.27449379
C	6.65633819	-1.09396278	1.36599376
C	5.83793170	-2.08904168	2.23099664
H	6.83075411	-0.18645060	1.95926424
C	8.02553708	-1.58035246	0.82758741
H	5.53598116	-1.40637182	-0.45025431
C	1.64700934	-0.10410478	-1.71713258
H	1.75097794	-0.50000988	-2.73326650
C	1.23955533	1.39052395	-1.86497231
H	0.72708125	0.16807422	0.85022211
H	3.46856112	-1.14611731	-1.35504911
H	0.55202569	1.69657938	-1.07082362
N	0.65881147	1.67143397	-3.18619078
H	2.12913702	2.02667202	-1.78390893
P	-0.89046335	1.42136427	-3.66320790
H	0.54878057	-0.31902323	-5.42019103
H	-2.57611390	1.21366870	-6.04316932
H	-2.46521924	3.81551251	-3.15225318
H	8.87100481	-3.01842565	-0.56320176
H	7.34346380	-2.32403791	-1.12735457
H	7.32547670	-3.54756300	0.16969421
H	9.69977350	-0.66378969	-0.23175796
H	8.92890161	0.41387733	0.96209551
H	8.12540985	0.08061096	-0.59429348
H	9.86460869	-2.35879367	1.69898447
H	8.38554883	-3.00255413	2.45738430
H	8.92422650	-1.33829700	2.81366882
H	6.06366619	2.65748054	-2.68494600
H	8.42629166	1.86782583	-2.77123224
H	8.91873442	-0.49678370	-3.38885239
C	8.84633689	-2.10391560	2.02635543
C	8.73617880	-0.35916849	0.20223235
C	7.87265620	-2.69009045	-0.23744534
O	5.74405835	-3.29814864	1.97431054
N	5.13665001	-1.46026805	3.21642115
C	3.92562042	-2.05555446	3.81384528
H	5.21337911	-0.43855431	3.27203139
C	2.69981067	-1.72255656	2.93983409
C	3.76918157	-1.56196506	5.25592264
H	4.09021864	-3.14164771	3.80370295
H	1.79686620	-2.21156658	3.33275772
H	2.85405081	-2.06401913	1.90770752
H	2.52442753	-0.63727726	2.92507791
H	2.88221338	-2.01555622	5.71958111
H	3.64398160	-0.46839150	5.27878739
H	4.65275082	-1.82388633	5.85387784
C	2.92640669	-2.39121284	-5.71637546
C	2.68859646	-2.64124940	-7.07227504
C	2.19315174	-3.87682510	-7.50438143
C	1.92247810	-4.87901626	-6.56496923
C	2.18429235	-4.66131875	-5.21065603
C	2.70277727	-3.43000644	-4.78604294
H	2.84862266	-1.83184966	-7.78244479
H	2.00104287	-4.04794636	-8.56298502
H	1.51992148	-5.83935212	-6.88655957
H	2.00011726	-5.44869476	-4.47921705
N	2.99229178	-3.20639902	-3.43031247
C	3.33672840	1.32028034	-5.90295041
C	3.26967355	-1.02925627	-5.20673061
H	2.49794902	-0.65405243	-4.52841633
C	3.74494404	-0.01264405	-6.07148329
H	4.44506380	-0.24760571	-6.86983548
O	2.53839866	1.79829568	-5.04611586
O	3.89415875	2.18954791	-6.84334367
C	3.39975498	3.55315262	-6.76946437
H	3.93416776	4.09482222	-7.55618163
H	3.61277210	3.99381889	-5.78799263
H	2.31692232	3.58435668	-6.94679287
C	4.06146703	-2.39654995	-2.99419960
H	2.80375712	-3.97134896	-2.78052899
O	4.47681153	-2.55525679	-1.80521345
N	4.46354783	-1.48012721	-3.87510993
H	4.21027987	1.09016652	-3.21129991
H	1.37055652	1.62402917	-3.96986700
C	5.51454275	-0.58496024	-3.57902765
C	6.84550634	-1.02220283	-3.64935147
C	7.88837829	-0.14394930	-3.35426663
C	7.61163142	1.18339764	-3.00541535
C	6.28604990	1.62565324	-2.95624359
C	5.23909169	0.74776528	-3.24500114
H	7.04416561	-2.05836759	-3.91978007
C	0.61901600	-0.95810526	-0.99428329
C	0.02287654	-2.04107001	-1.65015896
C	-0.93804622	-2.81946521	-0.99641498
C	-1.28949082	-2.53116452	0.32596860
C	-0.67540906	-1.46269370	0.99340149
C	0.27020658	-0.67638306	0.33615004
H	0.29844868	-2.26586232	-2.67824572
H	-1.41290102	-3.64693417	-1.52234049
H	-2.03684281	-3.13784555	0.83734140
H	-0.94150750	-1.23789262	2.02597350
C	-1.10992894	2.50168130	-5.09486736
C	-0.37186698	3.69486414	-5.18310393
C	-0.55824506	4.53631341	-6.28020049
C	-1.47355697	4.19252799	-7.28217420
C	-2.20487065	3.00163142	-7.19421892
C	-2.02423635	2.15013554	-6.10294548
H	0.35189013	3.94350103	-4.40990872
H	0.01847404	5.45762257	-6.35680290
H	-1.61198502	4.85020588	-8.13970251
H	-2.90910949	2.73079805	-7.98070135
C	-1.26396166	-0.26754029	-4.22104124
C	-2.40556629	-0.97475112	-3.81529720
C	-2.58361090	-2.29645931	-4.23188056
C	-1.63632638	-2.90531752	-5.05910204
C	-0.51577971	-2.18863631	-5.49711745
C	-0.32707302	-0.87127293	-5.08274162
H	-3.14408674	-0.50889025	-3.16832792
H	-3.46085309	-2.85115853	-3.90075130
H	-1.76900739	-3.94071445	-5.37137594
H	0.20956132	-2.65816216	-6.15415374
C	-2.00663229	1.86629105	-2.31629389
C	-2.21158335	0.98254173	-1.24101213
C	-3.00779186	1.37696931	-0.16605778
C	-3.61030443	2.64026176	-0.16410140
C	-3.41715086	3.51508244	-1.23932652
C	-2.61471222	3.13479258	-2.31687795
H	-1.75118912	0.00118553	-1.23541973
H	-3.15141356	0.69467098	0.66999670
H	-4.23222525	2.94477524	0.67715862
H	-3.88943784	4.49710297	-1.23896706

5_41

E = -2611.87

G = -2560.35

Nimag = 0

H	-2.39494922	4.07472871	1.46055424
H	-3.53028941	4.10369821	2.83595810
H	-8.18693387	2.64151680	0.40100115
O	-6.07456986	3.50564238	2.41039408
H	-8.64399288	4.20144142	-0.35407480
H	-8.40874579	4.09286492	1.41096509
N	-6.65153089	4.13004659	0.26847060
N	-4.41344163	4.10055345	0.93048157
C	-3.34471452	3.68326694	1.84150181
C	-5.73409113	3.86267650	1.27051371
H	-3.27665161	2.58800075	1.93412520
H	-6.30694474	4.18604347	-0.68914602
H	-4.17681822	4.15009869	-0.05959171
C	-8.05109603	3.73401249	0.44006351

5_52

E = -2490.26

G = -2440.24

Nimag = 0

H	-3.24717177	2.72216835	2.20891024
H	-2.40106957	4.04174258	1.33491922
H	-8.34538542	2.76594387	0.85994935
S	-6.21492079	3.27294068	2.84881364
H	-8.53696022	3.81553297	-0.57627668
H	-8.45327358	4.53120525	1.06775542
N	-6.62728437	3.81647752	0.24073928
N	-4.43710574	3.94426701	0.93931198
C	-3.31920055	3.76344246	1.86420476
C	-5.73820026	3.69762475	1.27199541
H	-3.44478864	4.40981216	2.74101716
H	-6.29886308	4.26413766	-0.61578294
H	-4.20415148	4.00996765	-0.05212681
C	-8.07690490	3.73062044	0.41458232

5_43

E = -3662.31

G = -3600.64

Nimag = 0

C	-6.21359213	2.22551465	1.77085581
C	-7.56216265	2.61096089	1.13426919
C	-5.57210941	3.20812307	0.85343125
C	-6.80953323	3.56010768	0.26794292
O	-5.80759578	1.45748048	2.64451497
O	-8.74767879	2.29997284	1.25992843
N	-7.18065978	4.42710372	-0.68299212
N	-4.30634620	3.60319652	0.67059086
C	-3.17288807	3.03130696	1.41326670
H	-8.88130136	5.58229190	-1.17118730
H	-3.56665890	2.31639872	2.14152158
H	-2.48949017	2.51245417	0.72779487
H	-4.09959428	4.29651469	-0.04894201
C	-8.56496845	4.53176279	-1.17005826
H	-9.20896835	3.95764266	-0.49769023
H	-2.62713837	3.82479429	1.94025058
H	-8.64947800	4.12411925	-2.18694295
H	-6.46264513	4.94849925	-1.18698445

5_44

E = -2315.25

G = -2276.98

Nimag = 0

C	-1.68675780	-1.52956762	-0.72924969
H	-2.42263683	-0.73326906	-0.83765877
C	-0.44975131	-1.25859780	-0.30110715
H	0.30310469	-2.03834585	-0.18371502
O	1.27183302	0.13826572	0.44820056
H	1.73861637	2.12732644	-0.05896330
C	-0.03496535	0.12605865	0.04206534
O	-0.73964068	1.12520083	-0.02092880
C	1.78910291	1.45998877	0.80782783
H	1.20089688	1.87893360	1.63092568
H	2.82356433	1.28611574	1.11113113
H	-1.99080570	-2.54435770	-0.97956684

5_45

E = -4933.27

G = -4830.72

Nimag = 0

H	-3.05210047	5.87650815	1.75104718
H	-3.71921997	4.77779827	2.98875390
C	-5.44338408	3.57424823	1.32655691
O	-5.40957201	2.90002699	2.37206355
H	-7.13541810	1.50889820	1.00814917
H	-7.90431665	2.16805180	-0.46118027
N	-6.31194037	3.29475894	0.28231448
N	-4.60889827	4.64902138	1.09487800
C	-3.43305082	4.86520733	1.93492560
O	-5.27994060	5.37715995	-1.77069268
H	-2.63113132	4.13604436	1.73275730
O	-4.29008699	6.04223893	-3.71363895
H	-4.59990748	5.02991811	0.14664162
C	-7.46651875	2.42635421	0.50999049
H	-8.23658354	2.90307256	1.13831898
C	-4.48746701	5.16834224	-2.68961912
H	-2.91236626	4.00972956	-3.67691498
H	-6.40124320	4.01118328	-0.44003941
C	-3.70911934	2.91657431	-2.03933660
H	-4.43428835	2.87256953	-1.22807070
C	-3.62358207	3.97723119	-2.85109183
C	-5.09727906	7.26475810	-3.65273680
H	-4.80108389	7.84065989	-4.53171369
H	-6.16087163	7.00802548	-3.68775178
H	-4.87538663	7.80882244	-2.72913623
H	-3.05895443	2.05466722	-2.18210702

5_46

E = -4812.66

G = -4711.00

Nimag = 0

H	-2.83414956	5.66831451	1.71782333
H	-3.79042291	5.04945513	3.09985037
C	-5.42940228	3.58359366	1.32381163
S	-5.43533646	2.52803001	2.66402122
H	-7.03480183	1.49531296	0.33778551
H	-7.95757109	2.65092774	-0.67326859
N	-6.33994254	3.49223375	0.31337522
N	-4.50569408	4.57211507	1.16784037
C	-3.40853631	4.81562158	2.09732451
O	-5.08728812	5.48956848	-1.62230315
H	-2.75201655	3.93787605	2.17837423
O	-4.49769665	5.90594603	-3.78187516
H	-4.53566521	5.11344346	0.30018626
C	-7.42511094	2.51967850	0.27554953
H	-8.12403361	2.67010668	1.11013020
C	-4.50784959	5.14759022	-2.65546793
H	-3.30081192	3.76909538	-3.85232548
H	-6.26157405	4.16090486	-0.45546415
C	-3.60682037	2.96789245	-1.91158359
H	-4.04883010	3.08597591	-0.92640644
C	-3.74627890	3.89636411	-2.86545324
C	-5.22887146	7.17362137	-3.68847820
H	-5.11290681	7.63737844	-4.66987166
H	-6.28237961	6.97679981	-3.46563336
H	-4.79082854	7.79557234	-2.90159560
H	-3.04058231	2.05774959	-2.10218799

5_47

E = -5985.24

G = -5872.93

Nimag = 0

C	-6.24251953	2.01194292	1.16696903
C	-7.57537390	2.68344253	0.78342691
C	-5.55154407	3.20158224	0.59968979
C	-6.77702882	3.81915724	0.24667323
O	-5.87319534	0.96059687	1.69718220
O	-8.77951869	2.42520894	0.86102803
N	-7.08581542	4.97453536	-0.35114108
N	-4.26998639	3.55766343	0.46112889
C	-3.15292861	2.70868732	0.89118800
O	-4.43157573	6.01863974	-1.20168467
H	-3.56004895	1.81023766	1.36421148
O	-3.39924256	7.02992694	-2.95960853
H	-4.06957404	4.43949541	-0.01995361
C	-8.46624699	5.38770663	-0.63032885
H	-9.14418697	4.62613011	-0.23386182
C	-4.07777977	6.00785241	-2.38514374
H	-8.67987104	6.35091536	-0.14767062
H	-6.31425593	5.57448486	-0.65741920
C	-4.97495987	3.80109941	-3.05933034
H	-5.37923970	3.61440383	-2.06930474
C	-4.31534017	4.92496394	-3.36328427
C	-3.10812652	8.16735280	-2.07710028
H	-2.55396840	8.86964550	-2.70217425
H	-4.04616963	8.60578650	-1.72269376
H	-2.50710743	7.82963166	-1.22738626
H	-3.91928634	5.09408362	-4.36475395
H	-2.54020809	2.41560267	0.02715768
H	-2.52262193	3.24538398	1.61295972

H	-8.62467002	5.48474846	-1.71330263
H	-5.13045965	3.02746754	-3.80942558

TS5_17
E = -5967.72
G = -5858.40
Nimag = 1, 253i cm-1

H	-0.00670841	2.46707357	-3.02674704
H	-2.51676693	5.87447976	-4.15730365
C	-1.95297309	3.11061328	-2.33334748
N	-0.20719095	2.80765902	-0.10094907
C	-3.34326968	2.91985896	-2.48259302
C	-3.83646793	1.92465656	-3.33007394
H	-0.88778312	0.65418634	-4.47518274
H	-3.35416094	0.31368953	-4.69744280
H	-4.91471167	1.79600896	-3.43132938
O	-4.96915002	5.75997028	-1.91257686
C	-2.96430152	1.09295767	-4.04248906
O	-4.99437111	5.89779508	-4.22289183
C	-1.58010604	1.28268903	-3.91309255
C	-1.08121507	2.29300313	-3.08911115
H	-4.02222944	3.55436642	-1.91755318
C	-4.30953319	5.85008920	-2.96949509
H	-1.01216589	6.24633653	-2.18401860
H	-0.43977264	2.00322229	-0.68342389
C	-2.02358376	5.86807694	-2.03605579
H	-2.44505542	6.15267488	-1.07101344
C	-2.90781094	5.91318997	-3.14143431
C	-6.42636020	5.76987140	-4.11232460
H	-6.80765061	5.81378281	-5.13916928
H	-6.70594352	4.81357305	-3.64820862
H	-6.85915160	6.58432771	-3.51470593
C	-0.49939521	4.09033278	-0.63270243
H	0.73234694	2.76452232	0.29559093
O	0.08339375	5.09051997	-0.15248043
N	-1.49278687	4.16798386	-1.55375965

TS5_18
E = -8593.17
G = -8416.41
Nimag = 1, 292i cm-1

H	-2.57864623	3.15167138	1.29449440
H	-3.88702599	2.14447598	1.98485773
C	-5.63686649	2.92697210	-0.04108698
N	-0.64585685	1.10105860	-0.78645701
H	-7.07821727	2.63062004	-2.46782661
H	-7.98946022	4.12841045	-2.10406680
N	-6.37376611	3.80924840	-0.82178457
N	-4.44831265	3.44707260	0.42118498
C	-3.47175293	2.56380769	1.05854479
O	-4.33184873	5.76010801	-1.40765735
H	-3.17354871	1.73582604	0.40024520
O	-4.27830152	6.36994674	-3.62913645
H	-4.09038620	4.26669850	-0.08298303
C	-7.44872391	3.28420996	-1.65876162
H	-8.14611866	2.69992076	-1.04637191
C	-3.65672746	5.88230554	-2.46391711
O	-6.04197080	1.78171152	0.24776440
H	-5.84622331	4.61398317	-1.18604295
C	-1.50036707	5.04043139	-1.63495034
H	-1.83853424	5.16739825	-0.60787246
C	-2.28996697	5.59643151	-2.65846357
C	-5.70425121	6.57856923	-3.51428212
H	-6.00747477	7.05655634	-4.45183255
H	-6.23087887	5.62114239	-3.40184689
H	-5.94764251	7.22195936	-2.65995863
C	-0.66122981	2.51564423	-0.80605576
H	0.22809474	0.72654129	-0.41624328
O	0.05835563	3.14103955	0.00886995
N	-1.56717504	3.11538745	-1.61715079
H	-0.29014563	1.81825770	-3.62103675
H	-1.89866702	5.67870425	-3.67111107
C	-2.13431179	2.54386728	-2.75020565
C	-3.51495816	2.71814880	-2.98242607
C	-4.11043384	2.25234628	-4.15577244
H	-1.36014210	0.93772074	-5.67935456
H	-3.81499532	1.22858528	-6.04249571
H	-5.18012204	2.39672785	-4.30786446
C	-3.34770232	1.59753778	-5.12958368
C	-1.97016731	1.43060658	-4.92089800
C	-1.36738217	1.91365534	-3.75845699
H	-4.10932602	3.20451916	-2.21965853
H	-0.41691819	5.07503716	-1.73939650
H	-0.98424612	0.61819589	-1.61841052

TS5_19
E = -8473.82
G = -8297.56
Nimag = 1, 278i cm-1

H	-2.55370399	3.10352255	1.16749165
H	-3.87466633	2.21538107	1.99906769
C	-5.65573685	2.89553385	-0.07814446
N	-0.60910399	1.09705758	-0.79697005
H	-7.65871795	2.54130745	-2.03929006
H	-7.92197364	4.31275344	-2.09740636
N	-6.32473584	3.73972289	-0.91169318
N	-4.42061048	3.32372357	0.28876375
C	-3.46117389	2.50822789	1.02506689
O	-4.35746789	5.70704621	-1.41013811
H	-3.19821569	1.59938216	0.46720598
O	-4.30972100	6.31546445	-3.63236407
H	-4.07266774	4.16981768	-0.18193931
C	-7.64744927	3.47055154	-1.45088697
H	-8.39463859	3.37107373	-0.65024795
C	-3.68425777	5.83916411	-2.46895480
S	-6.33018249	1.41018761	0.45665427
H	-5.82118821	4.58660790	-1.21553772
C	-1.51888952	5.03829640	-1.63065838
H	-1.85651598	5.16145432	-0.60331773
C	-2.31243929	5.57632130	-2.65750069
C	-5.74113100	6.49187603	-3.53035555
H	-6.04448489	6.97789116	-4.46349279
H	-6.24562055	5.52032969	-3.44103174
H	-6.00755769	7.11609846	-2.66891072
C	-0.67705549	2.50913652	-0.78215212
H	0.26323504	0.74284952	-0.40408259
O	-0.00617191	3.13992650	0.07034141
N	-1.58148412	3.09645544	-1.60326047
H	-0.18990934	1.92642877	-3.60752444
H	-1.92058855	5.65929595	-3.66970284
C	-2.09048821	2.53416813	-2.76882978
C	-3.47095196	2.64971358	-3.03520107
C	-4.00940587	2.20060441	-4.24227896
H	-1.15697327	1.07600439	-5.72918344
H	-3.61112823	1.26580762	-6.15605962
H	-5.08115181	2.29726096	-4.41850699
C	-3.18854153	1.62150478	-5.21644111
C	-1.81120222	1.51110357	-4.97220129
C	-1.26610221	1.97725365	-3.77496937
H	-4.11453420	3.07113726	-2.27336740
H	-0.43587113	5.07058654	-1.73845598
H	-0.90550987	0.62229640	-1.64934887

TS5_20
E = -9649.45
G = -9461.74
Nimag = 1, 225i cm-1

H	-0.03335930	2.51928968	-2.96272124
H	-2.51066918	5.78422768	-4.23885191
C	-2.00649658	3.09012106	-2.27678276
N	-0.21432063	2.79487538	-0.06261326
C	-3.38838482	2.87070238	-2.46619148
C	-3.84427824	1.90731659	-3.36849417
H	-0.84586159	0.76822685	-4.51898792
H	-3.29738481	0.37884726	-4.80406114
H	-4.91707967	1.75705323	-3.49496723
O	-4.87684994	5.78231881	-1.91324166
C	-2.93915883	1.13349017	-4.10413568
O	-5.00827199	5.87880575	-4.20413228
C	-1.56293915	1.35087439	-3.93887480

C	-1.10244149	2.32710628	-3.05492421
H	-4.09344772	3.46243705	-1.88872081
C	-4.27091567	5.85375472	-3.01780104
H	-0.93737702	6.14973575	-2.33144133
H	-0.43484421	1.98283674	-0.63875010
C	-1.98419384	5.92297843	-2.13854970
H	-2.34044191	6.29701889	-1.18136381
C	-2.87709210	5.89778293	-3.22040325
C	-6.44143686	5.75591573	-4.03537325
H	-6.84821788	5.67651900	-5.04851196
H	-6.69224663	4.86235105	-3.45088063
H	-6.85682657	6.64153722	-3.53622204
C	-0.55969661	4.06677034	-0.57460431
H	0.72423682	2.77643543	0.33739111
O	0.00153229	5.08337417	-0.10203788
N	-1.60026461	4.12412797	-1.44443742
C	-5.86217340	5.52963339	2.80162803
C	-5.37197858	5.54911086	1.39441120
O	-5.39397991	5.16405824	3.88891846
N	-4.24854427	5.18647043	0.78087140
C	-3.10829650	4.58390411	1.48382441
H	-3.33132558	4.55905046	2.55502878
H	-4.20381836	5.32195205	-0.24367387
H	-2.93348551	3.56476521	1.11602149
H	-2.19911635	5.17036406	1.30296601
C	-7.16879758	6.15019013	2.29578388
C	-6.59099812	6.12466857	0.93218198
O	-8.24968052	6.52108807	2.78321856
N	-7.02035425	6.49165885	-0.27831116
C	-8.35009331	7.05856344	-0.51063903
H	-8.86404661	7.16142174	0.45038826
H	-6.38226232	6.32995092	-1.07612325
H	-8.94140426	6.40154285	-1.16568636
H	-8.26687820	8.04781515	-0.98343770

Table 7.7. Cartesian coordinates (in Å), energies (in kcal mol^{-1}), and number of imaginary frequencies computed at COSMO(EtOAc)-ZORA-M06-2X/TZ2P//COSMO(EtOAc)-ZORA-BLYP-D3(BJ)/DZP.

5_51
E = -8776.64
G = -8590.81
Nimag = 0

C	-0.86388037	-1.04515747	3.15244577
C	-0.42411296	-2.23569846	4.01243136
C	0.21164014	-1.40907861	2.19912771
C	0.61886823	-2.51508208	2.98650331
O	-1.72804880	-0.16120202	3.20112806
O	-0.76657722	-2.75841635	5.07841118
N	1.57377180	-3.43544297	2.86198461
N	0.64345459	-0.88386779	1.05063212
C	0.03944723	0.30868450	0.44703390
C	-0.09995024	0.01191977	-1.05681273
H	-0.94782097	0.44383724	0.90707642
C	0.88902309	1.61096638	0.73166086
H	1.30672183	-1.38391806	0.45412669
C	1.76879302	-4.53315802	3.82121295
H	1.06818401	-4.39590438	4.64911104
N	-1.17459687	0.61761781	-1.64415388
H	0.13234757	-0.44381389	-3.79406791
H	2.18150103	-3.41040431	2.04186208
H	-1.80061035	1.11852804	-1.01408327
H	1.57628516	-5.49870637	3.33583904
C	2.29498867	1.49806137	0.10882338
O	0.73065295	-0.69209154	-1.64750938
H	2.79658318	-4.51615758	4.20429640
C	0.15266858	2.83901597	0.15381625
C	1.00891242	1.77147812	2.26372344
H	0.10368689	2.81231293	-0.94261910
H	-0.87160458	2.91073041	0.55112092
H	0.68652471	3.75518304	0.44320429
H	2.24961390	1.41722908	-0.98525694
H	2.88078766	2.39245463	0.36462178
H	2.83154847	0.62140938	0.49816217
H	1.54740736	2.70201411	2.49250809
H	0.01760627	1.81346495	2.73556350
H	1.56753699	0.93819492	2.70998571
C	-1.52923146	0.68995112	-3.01155623
C	-2.70053505	1.40179907	-3.32728995
C	-3.10608708	1.53205062	-4.65469559
C	-2.34991227	0.95721696	-5.68371808
C	-1.18635633	0.25036682	-5.36525383
C	-0.76729045	0.10828172	-4.03845711
H	-3.29034442	1.85188840	-2.52862869
H	-4.01554907	2.08607291	-4.88441168
H	-2.66617259	1.05941748	-6.72078531
H	-0.58987457	-0.20204779	-6.15711337

5_52
E = -8776.08
G = -8591.34
Nimag = 0

C	-1.59428239	0.74764847	1.63238830
C	-2.22116572	2.12632814	1.82922550
C	-1.55791882	1.01908074	0.18239914
C	-2.12277074	2.31119462	0.34958002
O	-1.21953969	-0.19115157	2.35830500
O	-2.62112246	2.81180892	2.77213641
N	-2.42637422	3.30142561	-0.47958310
N	-1.17051366	0.30272033	-0.88158615
C	-0.55276806	-1.03342092	-0.72958998
C	0.96498443	-0.83037983	-0.46676528
H	-1.00108345	-1.46785277	0.17236492
C	-0.91761790	-1.97514563	-1.91330243
H	-1.03042267	0.77463273	-1.77556330
C	-3.01377508	4.57745592	-0.04038590
H	-2.34886121	5.40623230	-0.31245663
N	1.23073615	-0.72735059	0.87303657
H	1.41142903	-0.01792207	3.36947909
H	-2.24917236	3.18336921	-1.47862905
H	0.40953141	-0.74680255	1.49895644
H	-3.99157110	4.72042075	-0.51643495
H	-3.13557725	4.54624381	1.04535663
O	1.80178798	-0.71861213	-1.37148526
C	-0.16333347	-3.30811326	-1.71000076
C	-2.44082308	-2.23392037	-1.84874816
C	-0.55705312	-1.36726074	-3.28731747
H	0.92089240	-3.17152022	-1.80972720
H	-0.37398777	-3.72964231	-0.71544258
H	-0.49069565	-4.03776867	-2.46391634
H	0.50926279	-1.12372037	-3.34274637
H	-0.80080086	-2.09200713	-4.07757612
H	-1.14276467	-0.45930401	-3.49679447
H	-2.74388228	-2.88879115	-2.67795006
H	-2.71589687	-2.72575724	-0.90385386
H	-3.00666649	-1.29510852	-1.92572585
C	2.44575835	-0.37656723	1.50403501
C	3.68795436	-0.37999374	0.84635879
C	4.84157680	-0.03081449	1.55599989
C	4.77798951	0.31831170	2.90876501
C	3.53737363	0.31731889	3.55978430
C	2.37767329	-0.02564028	2.86582736
H	3.73870709	-0.64920645	-0.20219834
H	5.80125987	-0.03605496	1.03936591
H	5.68335576	0.58728345	3.45140405
H	3.47016814	0.58835358	4.61301121

5_53
E = -13235.54
G = -12940.88
Nimag = 0

C	0.09433698	-1.40730543	-4.41756375
C	0.68550171	-2.66039749	-5.07122032
C	0.82518830	-1.77664150	-3.18033003
C	1.37999487	-2.93613608	-3.78477602
O	-0.66779602	-0.48768026	-4.74759056
O	0.61902314	-3.22049608	-6.17198927

N	2.20666490	-3.88172433	-3.35299086
N	0.92828716	-1.23811053	-1.96309029
C	0.24778881	0.00340622	-1.56707187
H	-1.39061218	-9.41265091	-1.50018123
H	-0.35662864	0.34744990	-2.41085615
H	-2.49587079	-8.44637516	0.51296284
H	1.53132322	-1.68649146	-1.27254787
C	2.63026341	-5.05220388	-4.14462108
H	1.94303205	-5.13505633	-4.99754304
C	2.41440874	-6.27843575	-3.22558444
H	-0.40273739	-0.18259707	-0.70309710
H	2.43198699	-3.98740801	-2.35655952
H	1.32087172	-6.44181553	-3.16774101
N	2.99080306	-6.00173881	-1.90570860
H	2.84319921	-7.17201512	-3.70741290
P	2.91168402	-7.08482240	-0.75620476
H	2.57300156	-9.95448962	0.13461470
H	1.15278644	-6.40034857	1.54222781
H	3.95932169	-4.44728116	-0.17888022
H	-1.21709431	-6.94297781	2.03274644
C	3.78564644	-8.66359595	-1.11362847
C	4.88146884	-8.60083724	-1.99083461
C	5.60878095	-9.75498144	-2.29044954
C	1.23253178	-7.61503542	-0.24938749
C	5.24955938	-10.97776182	-1.71059392
C	4.16094409	-11.04477385	-0.83333050
C	3.42698269	-9.89234863	-0.53712173
H	5.15520778	-7.64545050	-2.43286443
C	0.50384439	-8.45989001	-1.10767355
C	-0.83345065	-8.75534508	-0.83330937
C	-1.45398255	-8.21136998	0.29746556
H	6.45429641	-9.70213806	-2.97567594
H	5.81642317	-11.87846876	-1.94427046
H	3.88010602	-11.99632626	-0.38293510
C	3.71947499	-6.38777400	0.71535071
C	3.95029279	-7.19066402	1.84326314
C	4.57050906	-6.64627167	2.97052799
C	-0.73614797	-7.36545024	1.15096362
C	4.96862211	-5.30387315	2.97163152
C	4.74900010	-4.50601554	1.84263702
C	4.12596193	-5.04524336	0.71369584
H	3.64912360	-8.23677318	1.84530362
H	4.74667742	-7.27021065	3.84603749
H	5.45490176	-4.88182091	3.85064812
H	5.06641899	-3.46355132	1.84056506
H	3.27648898	-3.76866152	-6.47226744
C	0.60049074	-7.06172452	0.87682977
H	0.98361692	-8.89727815	-1.98214827
H	0.98512895	0.77445714	-1.30841265
C	4.07045080	-4.85280558	-4.73309208
C	5.12846725	-4.59667789	-3.63783732
H	6.11268507	-4.44634715	-4.10707400
H	4.88558000	-3.69188828	-3.06238651
H	5.18731774	-5.43148494	-2.93206751
C	4.45512021	-6.10857798	-5.54657356
H	4.59603584	-6.98605597	-4.90189569
H	5.39947881	-5.93079365	-6.08169618
H	3.68191404	-6.34939434	-6.29237491
C	4.03358210	-3.63517185	-5.68691987
H	3.79445054	-2.71201910	-5.14092150
H	5.01645141	-3.50242474	-6.16230849

5_54

E = -13231.97

G = -12938.75

Nimag = 0

C	2.70122056	-1.03814464	-5.00044586
C	3.30610450	-2.41205654	-4.71248969
C	1.44609183	-1.50945833	-4.38008380
C	1.98324899	-2.79919068	-4.11322436
O	3.08310312	0.01444025	-5.53175140
O	4.39824977	-2.94871125	-4.90793099
N	1.40758359	-3.85567780	-3.52935748
N	0.25077309	-0.95657611	-4.16278338
C	-0.07293817	0.43285011	-4.51954528
H	6.77357041	-4.75975322	-6.60465551
H	0.78441831	0.86052147	-5.04639928
H	6.50270174	-6.82168683	-7.97997262
H	-0.46571656	-1.49526087	-3.67426162
C	1.95223376	-5.22901335	-3.36988658
H	1.34904522	-5.67153483	-2.56200989
C	3.40560101	-5.13093718	-2.84721374
H	-0.95339302	0.45637465	-5.17372842
H	0.42976478	-3.74809313	-3.26034650
H	4.05076548	-4.81254976	-3.67541111
N	3.81978714	-6.37883975	-2.19909683
H	3.41628035	-4.29739051	-2.11977359
P	5.29649727	-6.91152573	-2.39905500
H	8.26262910	-6.56092611	-2.83810540
H	5.41439289	-9.03591908	-4.44998285
H	3.19436762	-8.81176688	-1.88418208
H	5.83328730	-8.96086110	-6.89205834
C	6.64341659	-6.03945272	-1.49704385
C	6.28882837	-5.35680250	-0.32232082
C	7.26587156	-4.69876115	0.42950909
C	5.88028292	-6.94350960	-4.13682450
C	8.60155741	-4.71763670	0.00984070
C	8.95832329	-5.39086302	-1.16463779
C	7.98270598	-6.04890413	-1.91916759
H	5.24493159	-5.34462740	-0.00978160
C	6.27186122	-5.74218380	-4.75449514
C	6.49193765	-5.70037416	-6.13298683
C	6.33366515	-6.85645727	-6.90389876
H	6.98664511	-4.16923033	1.33999466
H	9.36345723	-4.20330828	0.59489378
H	9.99661094	-5.39945264	-1.49542394
C	5.33572379	-8.63509667	-1.80981530
C	6.55184748	-9.28518568	-1.54763720
C	6.55626271	-10.63101062	-1.17023897
C	5.95416452	-8.05798725	-6.29355999
C	5.34896846	-11.32917371	-1.04748267
C	4.13500804	-10.67900044	-1.29908736
C	4.12549207	-9.33494633	-1.68211786
H	7.49322919	-8.74616617	-1.63219543
H	7.50177187	-11.13375246	-0.96919889
H	5.35470285	-12.37825461	-0.75245307
H	3.19442198	-11.22047804	-1.19956349
H	2.99478250	-7.78256326	-4.14247089
C	5.72266050	-8.10212804	-4.91723953
H	6.38604322	-4.83287471	-4.16821925
H	-0.27555614	1.02111032	-3.61497689
C	1.69378547	-6.09433882	-4.65996866
C	0.20919421	-5.93277346	-5.07050918
H	-0.02199913	-6.61482705	-5.90150555
H	-0.46247921	-6.18014618	-4.23306575
H	-0.01125134	-4.90949857	-5.40411729
C	2.59252863	-5.65991631	-5.83544300
H	2.43521193	-4.60562219	-6.09809238
H	2.35221561	-6.26681799	-6.72124577
H	3.65413903	-5.79990775	-5.60991187
C	1.94190713	-7.58853391	-4.35294500
H	1.35527348	-7.91621242	-3.48195430
H	1.63750646	-8.19258505	-5.22154781

TS5_21

E = -22707.23

G = -22160.97

Nimag = 1, 146i cm-1

C	-5.88234781	-1.98647795	0.42529019
N	-4.85157154	-0.97964694	0.72694420
H	-3.85435673	-1.13158999	0.47845882
H	-0.23352138	-4.31636521	-0.60766183
H	0.84146712	-2.99963760	-1.15484367
N	-3.14230241	1.50311874	2.00922891
H	-2.49689818	0.89443028	1.45387194
C	-2.69089973	2.76059089	2.62175013
H	-3.58856906	3.38271650	2.72560531
H	-0.91848761	2.70050844	-0.16466648
C	-1.68986963	3.49674327	1.67495086
N	-1.80491286	3.10070891	0.25984189

H	-0.66305117	3.26021790	1.96160242
P	-2.84570696	3.77620943	-0.80964677
C	-2.39778299	5.47868346	-1.25588511
C	-1.04357131	5.84425992	-1.18238436
C	-3.35443251	6.39726270	-1.72060332
C	-0.64819859	7.12516319	-1.57159749
H	-0.30978197	5.13186450	-0.81555953
C	-2.95016622	7.67464547	-2.11355363
H	-4.40519480	6.11931346	-1.77189105
C	-1.60059250	8.03855467	-2.03828413
H	0.40068124	7.41148008	-1.50757552
H	-3.68993689	8.38792906	-2.47438157
H	-1.29082863	9.03816300	-2.34060367
C	-4.53185639	3.86099244	-0.17413420
C	-4.88205263	4.87360640	0.73983075
C	-5.49458430	2.93758482	-0.60844878
C	-6.18967651	4.95326157	1.21063240
H	-4.14220355	5.60134018	1.06822570
C	-6.80240637	3.02742583	-0.12915531
H	-5.22346894	2.16159878	-1.31949217
C	-7.14961947	4.03326734	0.77579996
H	-6.45878471	5.72649469	1.92808931
H	-7.54758387	2.30564231	-0.45465247
H	-8.16806143	4.09111541	1.15645940
C	-2.77578272	2.73929610	-2.28351643
C	-2.52870436	1.36007506	-2.15649025
C	-3.01555002	3.31671365	-3.54279339
C	-2.52699636	0.56884777	-3.30771959
H	-2.33400960	0.89978873	-1.18544538
C	-3.02099202	2.50778566	-4.67991829
H	-3.18506505	4.38678412	-3.63829756
C	-2.77780313	1.13419119	-4.56186742
H	-3.20641593	2.95127800	-5.65711861
H	-2.77672197	0.50537968	-5.45174167
H	-1.81105104	4.58105675	1.79935010
H	-2.32383058	-0.49561946	-3.22203349
C	0.37489581	-0.64854214	0.53383351
C	0.67749670	0.63125351	1.10360251
H	-0.18043754	1.11973963	1.55862271
S	1.02532362	1.97979121	-0.50271363
C	1.78358041	3.52513803	0.21288900
H	1.22306268	3.87130318	1.09452941
H	1.75019183	4.31058302	-0.56100304
H	2.83272195	3.34587536	0.49026073
C	1.92772367	0.71386667	1.96591064
H	2.18513688	1.74384710	2.24614236
H	2.78751335	0.27095043	1.44348227
H	1.75784373	0.14372762	2.89343550
H	1.23050471	-1.25906529	0.25893189
C	-6.06616499	-8.32933007	2.26495913
C	-6.45294973	-1.87922127	-1.04279988
C	-7.07092351	-0.47385796	-1.19914678
C	-5.35314939	-2.06608887	-2.10189691
C	-7.55593767	-2.94281078	-1.23672243
H	-7.84928400	-0.29477196	-0.44535069
H	-7.50948583	-0.36743046	-2.20166288
H	-4.84597573	-3.03240540	-1.99558140
H	-5.79760201	-2.01206791	-3.10653879
H	-4.60486454	-1.26823106	-2.02699850
H	-8.02673713	-2.80663591	-2.22069168
H	-7.15462283	-3.96418545	-1.19331496
H	-8.34319262	-2.84386702	-0.47373422
C	-5.31684528	-3.37635897	0.75848007
O	-4.14804406	-3.68580673	0.51591904
N	-6.24567486	-4.21764457	1.32560337
H	-7.16685795	-3.81678455	1.49710779
H	-4.03581455	-5.80293814	1.16783953
H	-4.11678211	2.53649121	4.97025235
N	-1.04288692	-2.42143550	-0.29270813
O	-2.00958002	-0.42592384	0.36633409
C	0.11947592	-3.30349154	-0.37084480
H	-0.93981929	4.44340577	4.08801745
H	-2.82469077	1.84678017	5.99689923
C	-6.13182577	-5.59192396	1.62895735
H	-1.45702197	-2.55853098	-2.37396117
H	-2.47486811	-3.59368599	-1.31355689
H	-2.73987661	-1.84530949	-1.35441104
H	-6.29887403	0.29324918	-1.08125326
H	-6.72351410	-1.76955639	1.09537972
H	-3.45853569	0.92495619	4.61433476
C	-1.97967561	-2.61996342	-1.39769605
C	-4.91227633	-7.67366587	1.82445088
C	-4.93058349	-6.31195349	1.50591484
H	-8.22676423	-5.69017214	2.16578389
H	-8.16879572	-8.10045439	2.72817784
C	-7.29524824	-6.24889641	2.07155302
C	-0.91097650	-1.10417309	0.21512692
H	-6.03816958	-9.39000248	2.51114009
H	-3.97686415	-8.22453126	1.72696897
C	-7.25966710	-7.60644186	2.38694470
C	-2.11572308	2.57329127	4.07408469
C	-0.86785353	1.66894814	4.09654231
C	-1.76578854	3.97030595	4.63731821
C	-3.20075188	1.93299487	4.96711583
H	-1.08025569	0.68717837	3.65141925
H	-0.01687372	2.11353931	3.56745328
H	-0.55206789	1.50720665	5.13757872
H	-2.63887024	4.63918045	4.59488999
H	-1.45716941	3.88180581	5.68897425
H	0.64028427	-3.33557841	0.59328628
C	-6.42579716	0.53748388	2.11605590
C	-4.42222388	1.14824299	2.05590502
C	-5.65256190	1.71989230	2.68305890
C	-5.15862904	0.05592502	1.51232424
O	-5.92123920	2.72356602	3.35207568
O	-7.60160162	0.13671274	2.13424875

TS5_22

E = -22711.12

G = -22167.21

Nimag = 1, 145i cm-1

C	-5.41869375	-1.33626916	1.02451914
N	-4.51849084	-0.20506366	1.23227811
H	-3.69151775	-0.05092157	0.60382929
H	-0.44261507	0.38125324	-4.03541894
H	0.59875302	0.92601670	-2.68952331
N	-2.92114561	2.38079461	1.95250584
H	-2.59697950	1.83897146	1.10574016
C	-2.26682033	3.66877103	2.22180449
H	-1.22739049	3.53071492	1.88372799
H	-0.72544708	2.38811626	3.74401599
C	-2.23115906	3.93395875	3.73432983
N	-1.31188698	2.96231735	4.39651055
H	-3.24462756	3.84875929	4.13621398
P	-1.72382467	2.09630655	5.74602690
C	-2.84757411	0.70787339	5.43472506
C	-2.48373514	-0.15420423	4.38275483
C	-3.96693368	0.42152412	6.23010504
C	-3.22263772	-1.31079556	4.14671867
H	-1.63659010	0.09832014	3.74739722
C	-4.71853736	-0.72682299	5.96559464
H	-4.25216931	1.08291824	7.04440811
C	-4.33952723	-1.59737776	4.93927590
H	-2.93454054	-1.97490068	3.33629138
H	-5.60126890	-0.94197633	6.56562366
H	-4.91600635	-2.50165653	4.75520554
C	-2.40531069	3.17778689	7.02789239
C	-3.69178819	3.73095048	6.88957291
C	-1.63140199	3.46433158	8.16798455
C	-4.18736666	4.57557476	7.88501514
H	-4.30648193	3.50342554	6.02158716
C	-2.14086016	4.30943932	9.15562820
H	-0.64498731	3.02643346	8.29174659
C	-3.41543166	4.86783098	9.01440533
H	-5.18369227	5.00244155	7.77614874
H	-1.54016315	4.52722110	10.03759560
H	-3.80921005	5.52608310	9.78807387
C	-0.17187857	1.40657576	6.36138868
C	0.99018868	2.19700220	6.32596897
C	-0.15016782	0.13660001	6.95744685

C	2.17217500	1.70745459	6.88208717
H	0.96445598	3.18085421	5.86183029
C	1.03995004	-0.34579932	7.50597257
H	-1.04924839	-0.47530256	6.98066581
C	2.19782274	0.43757013	7.47030972
H	1.06236913	-1.33651172	7.95771347
H	3.12461902	0.05602877	7.89745627
H	-1.86534488	4.94478894	3.94511807
H	3.07579959	2.31474781	6.84985663
C	-0.55408175	-0.19982653	-0.15717687
C	-0.67911354	-0.55077201	1.23065642
H	-1.67399049	-0.34888141	1.62754367
S	0.43712713	0.84087257	2.41421604
C	1.34015644	-0.15559846	3.69599467
H	0.64653465	-0.76273182	4.28710897
H	1.84927953	0.54666114	4.36310366
H	2.08566945	-0.80218809	3.21845093
C	-0.17880089	-1.92751204	1.64434119
H	-0.34812801	-2.13458947	2.70895660
H	0.89161244	-2.05363665	1.42888606
H	-0.74196919	-2.67175649	1.06297322
H	0.35576841	-0.50451457	-0.66649359
C	-3.88351900	-6.94377234	4.15211587
C	-6.08627085	-1.31324784	-0.39232466
C	-6.82028927	0.03920477	-0.53525817
C	-5.03359938	-1.45488186	-1.51311840
C	-7.10640672	-2.46943412	-0.46555993
H	-7.50513416	0.20873504	0.30903162
H	-7.40636631	0.04717593	-1.46537641
H	-4.50908517	-2.41678641	-1.44932316
H	-5.53555613	-1.39508859	-2.49033171
H	-4.28408453	-0.65393515	-1.46296341
H	-7.63430373	-2.44259604	-1.42944026
H	-6.61407593	-3.44849775	-0.37786680
H	-7.85843544	-2.38529565	0.33429575
C	-4.59911295	-2.60791179	1.31928557
O	-3.45284240	-2.76711751	0.89361791
N	-5.25136381	-3.49242511	2.14780901
H	-6.20195519	-3.23605510	2.41244144
H	-2.75292133	-4.56214561	1.97279555
H	-1.67236729	4.26987116	-0.40604017
N	-1.48052215	0.64666852	-2.24180927
O	-2.64484447	0.94030806	-0.28786050
C	-0.26067665	0.28238663	-2.95798275
H	-2.17719003	6.54506985	2.58847325
H	-3.12538049	5.23514909	-0.77190914
C	-4.75495075	-4.65915574	2.76839173
H	-1.70651072	2.67313141	-2.88951024
H	-2.53229274	1.43534971	-3.88523524
H	-3.17593866	1.86865049	-2.27167561
H	-6.10472727	0.87099551	-0.57026863
H	-6.21453317	-1.24261969	1.77537439
H	-3.27067702	3.50897025	-0.34542603
C	-2.26676954	1.71884910	-2.85705741
C	-3.00926025	-6.24275383	3.31572195
C	-3.42990113	-5.10475356	2.62074513
H	-6.66515721	-5.01551068	3.72163170
H	-5.89830563	-7.03020208	4.93981367
C	-5.63822180	-5.36325165	3.60713367
C	-1.56436863	0.47387088	-0.85120349
H	-3.54328390	-7.82903630	4.68762930
H	-1.98022661	-6.58152520	3.19751802
C	-5.20319801	-6.49643410	4.29269170
C	-2.85017762	4.84116256	1.35497061
C	-4.33000340	5.11534938	1.69011843
C	-2.00871089	6.11651892	1.59147211
C	-2.72529516	4.43529943	-0.13173543
H	-4.96194184	4.25817925	1.42269737
H	-4.47954346	5.32248098	2.75775704
H	-4.68234156	5.98545796	1.11673592
H	-0.93380322	5.90652498	1.48029769
H	-2.28225402	6.88147295	0.85022136
H	0.00822213	-0.76104569	-2.75139697
C	-5.86219311	1.02598916	3.08059878
C	-4.08411003	1.94923213	2.44619063
C	-5.11661403	2.29435161	3.46761477
C	-4.79694617	0.75902665	2.09415638
O	-5.29182185	3.20722516	4.29480198
O	-6.90811846	0.44973154	3.42387023

TS5_23

E = -22710.37

G = -22165.63

Nimag = 1, 51i cm-1

C	-3.56114721	0.85204311	-3.32000240
N	-3.50352063	0.71573581	-1.84297445
H	-4.33879811	0.83658166	-1.22998541
H	-8.93833085	-0.45590433	-1.20230656
H	-9.10176543	-0.13165600	0.54603415
N	-2.57033243	1.67223656	1.13946632
H	-3.60824641	1.55044673	1.13211683
C	-1.82691352	2.21748732	2.28312542
H	-0.82036282	1.78455382	2.21779486
H	-4.43057132	1.04218967	3.79292970
C	-2.45889187	1.78784946	3.64247628
N	-3.44945118	0.70290121	3.58236867
H	-3.00806240	2.62794131	4.07679913
P	-3.16649015	-0.91113719	3.52955272
C	-2.16736496	-1.45385564	4.93950608
C	-2.24165911	-0.70964451	6.12920677
C	-1.41330031	-2.63911476	4.89290368
C	-1.55434999	-1.14508120	7.26327498
H	-2.83913804	0.19920296	6.16399920
C	-0.73438352	-3.07057670	6.03413204
H	-1.36263518	-3.22397952	3.97728816
C	-0.80151945	-2.32391190	7.21572635
H	-1.60769001	-0.56568282	8.18380680
H	-0.15213451	-3.99024841	6.00006425
H	-0.26662795	-2.66224797	8.10235803
C	-2.32914311	-1.49103945	2.03081108
C	-0.92922800	-1.42183938	1.92578870
C	-3.09598635	-1.95349058	0.94690831
C	-0.30397873	-1.83256860	0.74846422
H	-0.32851758	-1.04513456	2.75116129
C	-2.46068964	-2.35323789	-0.22812677
H	-4.17699290	-1.99547597	1.01911916
C	-1.06705042	-2.29856074	-0.32644397
H	0.77774192	-1.75734323	0.66046119
H	-3.05457213	-2.69981647	-1.07143144
H	-0.57502084	-2.59537361	-1.25156072
C	-4.80326788	-1.66217201	3.65617735
C	-5.84860839	-1.14003312	2.87667546
C	-5.02599717	-2.74747812	4.52028787
C	-7.12032573	-1.70381255	2.96942754
H	-5.65273805	-0.32138374	2.19369785
C	-6.30361942	-3.30662823	4.59859058
H	-4.22032839	-3.14306369	5.13402618
C	-7.34921287	-2.78529945	3.82599374
H	-6.48343805	-4.14582235	5.26899645
H	-8.34439428	-3.22339120	3.89544730
H	-1.64959203	1.54233050	4.34266638
H	-7.92927176	-1.29456499	2.36825812
C	-7.04368059	1.97908062	1.21500979
C	-6.31520166	2.89274035	2.07360508
H	-5.25437440	2.91295201	1.82105629
S	-6.26333288	2.04920912	3.94547108
C	-5.75544965	3.38764005	5.13899642
H	-4.98622831	4.02795242	4.69299088
H	-5.34052368	2.90266087	6.03280198
H	-6.62114575	3.99783199	5.42204800
C	-6.88896677	4.29397469	2.24246711
H	-6.32876804	4.89697201	2.96785748
H	-7.94052415	4.25095547	2.56143626
H	-6.84635166	4.80908060	1.26954539
H	-8.12886404	2.00396889	1.26306162
C	-0.29284953	6.52549111	-3.29061742
C	-4.76309676	0.14273098	-3.99114567
C	-4.62391456	-1.37063423	-3.70469014
C	-6.13246062	0.65832360	-3.49751218
C	-4.63903887	0.37810444	-5.51499163

H	-3.66639619	-1.75383028	-4.08895236
H	-5.43912239	-1.92403665	-4.19272290
H	-6.30131537	1.68706083	-3.83323336
H	-6.92703193	0.01432270	-3.90350351
H	-6.22212671	0.63984910	-2.40546102
H	-5.44576181	-0.15320811	-6.04013770
H	-4.71907770	1.44614444	-5.75937691
H	-3.67748939	0.00265841	-5.89681785
C	-3.42966753	2.37690644	-3.58961501
O	-4.38111183	3.16441069	-3.54995935
N	-2.11350398	2.74404260	-3.74002045
H	-1.42877353	1.97807243	-3.68378250
H	-3.35886472	5.16156675	-3.95354149
H	0.07029799	3.66929965	0.82509287
N	-7.13623570	0.07982393	-0.29753802
O	-5.09346650	0.83324153	0.44305360
C	-8.58729760	0.18383390	-0.38247296
H	-1.31654753	4.11055202	4.34264950
H	-0.77108150	5.24239574	0.83478614
C	-1.55253155	4.03424652	-3.61075738
H	-6.81783223	-1.97853740	0.20961528
H	-6.98517388	-1.61481049	-1.53112717
H	-5.49719514	-1.15894834	-0.66297831
H	-4.66591802	-1.57482527	-2.63027097
H	-2.65632514	0.35866903	-3.69919819
H	-1.48568630	3.86222741	-0.01440317
C	-6.58100969	-1.24189488	-0.58099126
C	-1.65997687	6.45209947	-3.57573153
C	-2.29789628	5.21806851	-3.73898298
H	0.39287637	3.18209820	-3.20609405
H	1.51019283	5.38011728	-2.93767834
C	-0.17624648	4.10406569	-3.32297010
C	-6.38800681	0.99001585	0.47659329
H	0.19304929	7.49256871	-3.16672398
H	-2.24506938	7.36651759	-3.67569625
C	0.44522680	5.34140822	-3.16554715
C	-1.65330825	3.78217137	2.18180817
C	-3.02002926	4.49703891	2.17962368
C	-0.80076505	4.25316907	3.38295607
C	-0.91310184	4.15289049	0.87598267
H	-3.61039182	4.20891256	1.29963596
H	-3.61340842	4.27737886	3.07471180
H	-2.86967158	5.58572721	2.14398065
H	0.15513630	3.70902375	3.41961448
H	-0.57810553	5.32514130	3.28256661
H	-8.87959659	1.21780780	-0.60390134
C	-0.91595692	0.75112931	-1.69603876
C	-1.91270137	1.25827840	0.06676059
C	-0.46687665	1.11137477	-0.29420251
C	-2.31757299	0.87134415	-1.24397300
O	0.61089917	1.22864513	0.30057886
O	-0.36100558	0.51502759	-2.79077537

TS5_24
E = -22707.75
G = -22163.58
Nimag = 1, 153i cm-1

C	-5.29533481	-0.66407600	0.84364018
N	-4.42990861	0.52020870	0.97218696
H	-3.57556481	0.64069327	0.37163245
H	0.31341400	-1.16324667	-2.85156707
H	1.31659533	-0.48471683	-1.53826594
N	-2.84822364	3.16363562	1.58742922
H	-2.43200354	2.53272375	0.84947705
C	-2.22747687	4.49097358	1.73591650
H	-1.17115905	4.30893035	1.48804933
H	-0.84154391	3.38961612	3.59056476
C	-2.29205824	4.95698777	3.19216347
N	-1.19513358	4.30608174	3.98094860
H	-3.27782972	4.70951100	3.59732396
P	-1.46925125	4.13094250	5.61097640
C	-2.67749468	2.84162806	6.00588549
C	-2.81090106	1.76576606	5.11110470
C	-3.44598171	2.88870715	7.18103329
C	-3.70376748	0.73605732	5.39911076
H	-2.21394048	1.73578825	4.20314830
C	-4.33550621	1.84958109	7.46022030
H	-3.35461812	3.72798730	7.86786863
C	-4.46328555	0.77532257	6.57187245
H	-3.81194857	-0.09343714	4.70741523
H	-4.93324961	1.87999925	8.37017839
H	-5.15726575	-0.03183986	6.78924926
C	-2.07871399	5.69499415	6.27651912
C	-3.42840821	6.05074156	6.09195239
C	-1.19605233	6.56269340	6.94105484
C	-3.88052735	7.28329092	6.56466682
H	-4.11514279	5.37607976	5.58423995
C	-1.66296125	7.79205713	7.41157236
H	-0.15823337	6.27779314	7.09820972
C	-3.00124939	8.15240574	7.22204737
H	-4.92311596	7.56401872	6.42174427
H	-0.98174139	8.46467341	7.93066500
H	-3.36215152	9.11147572	7.59190511
C	0.11674023	3.71057113	6.35656877
C	1.30337736	4.20357433	5.78771185
C	0.15453633	2.91773753	7.51428189
C	2.52771848	3.89059861	6.38017381
H	1.26250729	4.80430125	4.88186108
C	1.38427665	2.61678621	8.10161494
H	-0.76355148	2.51865151	7.93993895
C	2.56845123	3.10046660	7.53472811
H	1.41813174	1.99284852	8.99351001
H	3.52730939	2.85443677	7.98969159
H	-2.16387770	6.03763195	3.27885691
H	3.45148871	4.25829548	5.93549614
C	-0.61699983	-0.20444011	0.83131067
C	-1.09407980	0.01407982	2.16131767
H	-2.00976637	0.60218363	2.20046173
S	0.20257111	1.47073249	3.13723045
C	0.62297369	0.78155805	4.80883292
H	-0.25046802	0.76298529	5.47088953
H	1.39478992	1.42121952	5.25086867
H	1.02330643	-0.23315580	4.69914439
C	-1.14597871	-1.18120549	3.09541492
H	-1.39733649	-0.90860816	4.12786709
H	-0.19493541	-1.73319104	3.09962549
H	-1.93051254	-1.85525703	2.72093709
H	0.22422600	-0.88132851	0.71096474
C	-5.25277471	-3.32505972	6.88649465
C	-5.32929594	-1.19785015	-0.61813531
C	-5.92959795	-0.08319672	-1.50744436
C	-3.93246911	-1.57949518	-1.15717998
C	-6.26724377	-2.42653452	-0.64821931
H	-6.92971065	0.21053101	-1.15376203
H	-6.02275100	-0.44449869	-2.54174409
H	-3.43974690	-2.30073396	-0.49775549
H	-4.04661368	-2.02440446	-2.15720283
H	-3.28142063	-0.70457543	-1.26270564
H	-6.39072584	-2.77255699	-1.68426221
H	-5.85700477	-3.25438688	-0.05581031
H	-7.26303992	-2.17226566	-0.25350816
C	-4.89597693	-1.70382591	1.93019211
O	-4.08184353	-2.61639678	1.75377058
N	-5.54507619	-1.45645760	3.11433664
H	-6.18243529	-0.63943819	3.13515557
H	-3.60686507	-3.21644046	3.89225905
H	-0.88671966	5.48003755	-0.48761340
N	-0.74640667	0.10322437	-1.57562901
O	-2.12789355	1.31974306	-0.21276640
C	0.31331661	-0.87646293	-1.79198302
H	-3.24059540	7.24464846	1.93634392
H	-2.32009371	5.90011993	-1.46836635
C	-5.41675692	-2.13380157	4.34525212
H	-0.01319253	1.67322451	-2.81962808
H	-1.17370900	0.55045656	-3.59051951
H	-1.74981546	1.74326238	-2.38711166
H	-5.28840287	0.80849211	-1.51264071
H	-6.31996905	-0.33959821	1.07449376
H	-2.04574266	4.20621433	-0.97894349
C	-0.92923002	1.07427700	-2.65515289

C	-4.28507986	-3.59181324	5.91219334
C	-4.35800686	-3.00845387	4.64404349
H	-7.20914255	-1.18283017	5.08917032
H	-7.07508346	-2.24322194	7.32724734
C	-6.39493513	-1.86780459	5.32223008
C	-1.16235724	0.44305843	-0.28401358
H	-5.18435168	-3.78480309	7.87162550
H	-3.45553667	-4.26171792	6.13819707
C	-6.31180279	-2.46178081	6.58056444
C	-2.77866609	5.50831391	0.64225966
C	-4.28424551	5.26483313	0.35254959
C	-2.59097802	6.98401084	1.08374229
C	-1.95658601	5.25789590	-0.65288632
H	-4.47322166	4.24214227	-0.01111148
H	-4.90065782	5.43413129	1.25479378
H	-4.62091541	5.96629113	-0.42442482
H	-1.54105296	7.19799015	1.35477667
H	-2.86028904	7.64932470	0.24918306
H	0.12539433	-1.77596257	-1.19442187
C	-5.70244234	1.77380753	2.85732671
C	-3.98379928	2.72194015	2.12029813
C	-5.01348008	3.09196365	3.14918358
C	-4.67820401	1.49712759	1.83701379
O	-5.21373222	4.04380372	3.91856759
O	-6.69333550	1.15532439	3.30421490

TS5_25
E = -22710.90
G = -22168.18
Nimag = 1, 93i cm-1

C	-5.04145021	-2.50314433	2.15725956
N	-4.00612371	-1.47938265	2.31570333
H	-3.37006270	-1.32113016	1.51965654
H	3.37016958	1.14268692	-1.09004095
H	4.32173637	2.14105123	0.02908698
N	-1.59560178	0.41528350	3.35145150
H	-1.46106406	0.22805239	2.33771478
C	-0.69855392	1.37194041	4.00184097
H	-1.17497537	1.64160553	4.95256599
H	-0.91852813	2.78457110	1.01612080
C	-0.55985011	2.65760433	3.11652595
N	-1.47772809	2.69071058	1.95961903
H	0.44204137	2.70751717	2.68417724
P	-2.87658967	3.53019677	2.01709409
C	-2.61789783	5.31682032	2.19865892
C	-1.46727000	5.86210185	1.59965582
C	-3.53056116	6.14387106	2.87241885
C	-1.23662679	7.23648442	1.68029132
H	-0.76680177	5.21238619	1.07557693
C	-3.28968160	7.51786443	2.94750192
H	-4.41897017	5.71912745	3.33553856
C	-2.14521922	8.06226872	2.35371867
H	-0.34689754	7.66388984	1.21966627
H	-3.99369754	8.16273101	3.47156442
H	-1.95856587	9.13368671	2.41872021
C	-3.91705028	2.98581942	3.39445896
C	-3.56393577	3.34060573	4.71030014
C	-5.03162079	2.16419172	3.16422826
C	-4.31416275	2.85821786	5.78050466
H	-2.71156911	3.99038493	4.89797708
C	-5.77147617	1.68037480	4.24448875
H	-5.32058156	1.90186473	2.15207047
C	-5.41429957	2.02578557	5.54976550
H	-4.02683608	3.11397370	6.79863446
H	-6.61958989	1.02286697	4.06580200
H	-5.97866009	1.62628460	6.39086269
C	-3.71820053	3.22559686	0.45053896
C	-3.83796264	1.90587057	-0.01778148
C	-4.27531284	4.28775348	-0.27941607
C	-4.51164286	1.65194973	-1.21124816
H	-3.39806570	1.08133583	0.53233800
C	-4.94668217	4.02345926	-1.47586737
H	-4.17711101	5.31083854	0.07571013
C	-5.06760405	2.70908560	-1.93999998
H	-5.37147362	4.84740999	-2.04733947
H	-5.59051181	2.50931712	-2.87460827
H	-0.66314284	3.54660302	3.75441247
H	-4.59764923	0.62899195	-1.57096000
C	0.68783081	0.91722915	-0.81381399
C	-0.63717568	0.51991025	-1.21062443
H	-1.34632823	1.35388159	-1.20895364
S	-1.61156216	-0.64841183	0.24465145
C	-0.45177112	-2.07079456	0.34448628
H	-0.86719501	-2.77511480	1.07508444
H	0.53765482	-1.72333635	0.66671998
H	-0.37735439	-2.57209955	-0.62792691
C	-0.75013314	-0.32931717	-2.47378856
H	-1.77201743	-0.70054239	-2.62741979
H	-0.06646057	-1.18905677	-2.44007695
H	-0.46065477	0.28728499	-3.34009356
H	1.48191721	0.18412911	-0.91566708
C	-4.45402105	-9.07945921	2.47186010
C	-6.00145598	-2.16734290	0.95888493
C	-6.59129424	-0.76275120	1.21320714
C	-5.24693067	-2.17956834	-0.38849130
C	-7.14949055	-3.19929047	0.92087147
H	-7.09518035	-0.71820023	2.18962824
H	-7.32419079	-0.51681804	0.43191141
H	-4.88218222	-3.18565402	-0.63348860
H	-5.92641245	-1.85144830	-1.18846653
H	-4.37792718	-1.50925528	-0.38110847
H	-7.86248845	-2.92758154	0.12955186
H	-6.78194637	-4.21183304	0.70840658
H	-7.69730583	-3.21894309	1.87552618
C	-4.34780625	-3.87453520	2.00144677
O	-3.29487988	-4.00510476	1.37129842
N	-5.03078638	-4.90092562	2.60691089
H	-5.86009672	-4.63410613	3.13654920
H	-2.98507752	-6.19407784	1.36551962
H	-0.08103118	-0.13397517	6.20579053
N	2.27456619	2.56231094	0.02645936
O	0.03032920	3.08548327	-0.07213456
C	3.37279537	1.60444892	-0.09487195
H	1.81890671	2.61730474	4.38110636
H	1.41383998	-0.90339194	5.59661659
C	-4.78824500	-6.29069610	2.54413869
H	2.67428315	3.26998450	2.00379671
H	3.38427414	4.23360596	0.68108395
H	1.62353043	4.29976372	0.98622898
H	-5.80476814	-0.00184663	1.19685355
H	-5.63289424	-2.49031730	3.08275676
H	-0.15142573	-1.24756321	4.82378001
C	2.50092445	3.64994275	0.97898674
C	-3.54080771	-8.23713233	1.82988127
C	-3.69527076	-6.84753449	1.85867684
H	-6.55584944	-6.70114977	3.72466272
H	-6.26161538	-9.15881909	3.66097679
C	-5.70809297	-7.13460334	3.19362951
C	0.95129088	2.17969370	-0.27198210
H	-4.32246483	-10.16012928	2.44223470
H	-2.69009187	-8.66147899	1.29698684
C	-5.54079287	-8.51807628	3.15426378
C	0.68606569	0.72068694	4.33750112
C	1.37297730	0.20167097	3.05629712
C	1.57286473	1.77373474	5.03997118
C	0.45036468	-0.46261772	5.30181529
H	0.78134080	-0.59783579	2.59388006
H	1.51085748	0.98516600	2.30228215
H	2.36357739	-0.20721114	3.30255441
H	1.07180959	2.17127954	5.93591671
H	2.51985019	1.31283304	5.35583258
H	3.32410252	0.80242398	0.66391737
C	-4.22815311	-1.15084841	4.87618051
C	-2.59623061	-0.18896028	3.97771188
C	-3.09210050	-0.25660954	5.38520840
C	-3.64491239	-1.03306950	3.52222864
O	-2.73851917	0.22255508	6.46709504
O	-5.22776626	-1.71334499	5.35092763

TS5_26
E = -22707.65
G = -22164.03
Nimag = 1, 118i cm-1

C	-3.91335589	-3.51377409	3.78677740
N	-3.74043848	-2.06952508	4.07557442
H	-4.17894778	-1.37814028	3.45387169
H	-0.37852097	-0.54197904	-0.27416820
H	0.58821613	-1.73417403	0.63498988
N	-2.98837962	0.86257680	5.21993040
H	-3.46813953	0.93388270	4.29747443
C	-2.44283367	2.13785815	5.72792007
H	-2.40141804	2.76996497	4.82874530
H	-0.55266750	1.37818000	4.17711095
C	-0.99907020	1.99300172	6.24279185
N	-0.12937212	1.41845697	5.18706495
H	-0.97101566	1.35481949	7.13492539
P	1.47137754	1.20677718	5.43274033
C	2.29159496	2.71427904	6.03385097
C	1.97974045	3.20650855	7.31591693
C	3.17410959	3.42578079	5.20475682
C	2.54307433	4.40506615	7.75560278
H	1.31795342	2.64883250	7.97572055
C	3.73799354	4.62223848	5.65580479
H	3.42760720	3.04272136	4.21889382
C	3.42087228	5.11341871	6.92639435
H	2.30162406	4.78302508	8.74814173
H	4.42872385	5.16794396	5.01435653
H	3.86219336	6.04665618	7.27431133
C	2.22694375	0.68526800	3.87987538
C	1.85588885	1.28795164	2.66670638
C	3.19257289	-0.33964791	3.90018192
C	2.45950507	0.86670324	1.48039922
H	1.07904468	2.04795933	2.64303063
C	3.78039999	-0.75479340	2.70797493
H	3.46065873	-0.82463575	4.83529409
C	3.41492057	-0.15072015	1.49761337
H	2.15587683	1.31835030	0.53746483
H	4.51440035	-1.55830706	2.72004698
H	3.86950536	-0.48528646	0.56554347
C	1.79651584	-0.07588425	6.67383648
C	0.99187335	-1.22514833	6.66138945
C	2.85894629	0.03024546	7.58861038
C	1.22070998	-2.24580132	7.58138299
H	0.18863164	-1.31285636	5.93919010
C	3.09725377	-1.00734057	8.49237906
H	3.49580137	0.91172440	7.59387325
C	2.27345021	-2.13943371	8.49494942
H	3.92073068	-0.92741993	9.20073309
H	2.45117692	-2.93858402	9.21387103
H	-0.64735906	2.99645190	6.51430109
H	0.56437303	-3.11265562	7.59717336
C	-2.44177106	0.72825089	0.93117127
C	-3.52704962	1.66328812	1.07167150
H	-3.27334832	2.56278006	1.64088357
S	-4.81417798	0.74596066	2.46383594
C	-6.29560703	1.83089805	2.78481012
H	-6.23073909	2.30829619	3.77393294
H	-7.21450659	1.22246001	2.71549317
H	-6.32466452	2.61077799	2.00386853
C	-4.37590083	1.93387454	-0.15806953
H	-5.28300862	2.50614005	0.07654493
H	-4.67265797	0.99102960	-0.63803194
H	-3.78601185	2.52081659	-0.88171057
H	-2.56392386	-0.07184746	0.20511872
C	2.50668621	-4.15926185	3.15572214
C	-5.28385497	-3.82682022	3.12541812
C	-6.39109316	-3.42774242	4.12895535
C	-5.50005298	-3.07208246	1.79417630
C	-5.34121577	-5.35192874	2.88112318
H	-6.27788339	-3.97190898	5.07873839
H	-7.37803800	-3.66881842	3.70911402
H	-4.71521475	-3.32129368	1.07267770
H	-6.47823286	-3.35679794	1.37846662
H	-5.50525732	-1.98220066	1.93237789
H	-6.33202468	-5.62857270	2.49397841
H	-4.58659417	-5.66393671	2.14711663
H	-5.17265810	-5.90826414	3.81578662
C	-2.65326728	-3.98230450	3.00161313
O	-2.54764227	-3.92954324	1.77338623
N	-1.64741697	-4.36741787	3.85971553
H	-1.86438476	-4.27201946	4.86689525
H	-0.40457788	-4.70460334	1.44655924
H	-4.64203956	3.63401911	5.09507153
N	-0.46677697	-0.38733771	1.82185839
O	-1.36565153	1.45605326	2.90559241
C	-0.36877332	-1.19440199	0.60669311
H	-1.95989224	4.14809392	7.75686965
H	-5.47069678	3.57710109	6.67301086
C	-0.25996152	-4.39392131	3.57568858
H	-1.01107525	-1.99461150	3.08331551
H	0.73449340	-1.63232713	3.03227492
H	-0.38656811	-0.57032447	3.91695133
H	-6.36579291	-2.35075676	4.34484354
H	-3.90550912	-4.02224953	4.75935912
H	-5.21633131	2.07945403	5.74739697
C	-0.26739918	-1.18938827	3.03178174
C	1.64399778	-4.41700495	2.08601859
C	0.26520477	-4.54225702	2.28266087
H	0.18982308	-4.05564049	5.65343806
H	2.63391945	-3.83839051	5.29460692
C	0.60967628	-4.17114940	4.65832156
C	-1.44498201	0.62969066	1.90805934
H	3.57568618	-4.04568997	2.98495510
H	2.04394831	-4.50983429	1.07627448
C	1.98070807	-4.04654994	4.44826078
C	-3.41703721	2.84336268	6.73535324
C	-3.64535187	2.00286987	8.00708992
C	-2.84673509	4.22938302	7.11429735
C	-4.76883329	3.04465482	6.01528494
H	-4.09198679	1.02960468	7.76447305
H	-2.71116150	1.81588718	8.55023159
H	-4.33645249	2.53429075	8.67780568
H	-2.57493696	4.80543558	6.21646845
H	-3.60538260	4.80138901	7.66777314
H	-1.17956322	-1.94070498	0.52227215
C	-2.46481688	-2.33053213	6.30568364
C	-2.81157064	-0.34950895	5.71830542
C	-2.19282025	-0.97869928	6.93728967
C	-3.12433248	-1.64447788	5.18226299
O	-1.67205459	-0.58203395	7.98214087
O	-2.18163387	-3.51910203	6.57643471

TS5_27
E = -22711.48
G = -22168.98
Nimag = 1, 139i cm-1

C	-5.31995586	-2.87857734	2.65561698
N	-4.21885730	-1.91574924	2.88996692
H	-3.38162255	-1.97801861	2.27877316
H	3.83452190	-0.03139029	0.54162009
H	4.61553294	0.87720999	1.85044155
N	-1.96071393	0.06273443	4.17743664
H	-1.63767613	-0.23838316	3.22705990
C	-1.19877863	1.11024798	4.86305169
H	-1.83033154	1.46699481	5.68574480
H	-0.73104157	2.11376960	1.75509105
C	-0.91506018	2.29957262	3.87513233
N	-1.51404573	2.13957028	2.53403744
H	0.16036258	2.36825107	3.69147513
P	-2.91441867	2.86480241	2.10203045
C	-2.77884396	4.67481484	2.10946396
C	-1.52060715	5.23523020	1.82630639
C	-3.88869117	5.50148478	2.34644990
C	-1.38050877	6.62351455	1.77443163
H	-0.66447257	4.58668073	1.64353584
C	-3.73822536	6.88911620	2.29373104
H	-4.85978424	5.06494083	2.57216154
C	-2.48727909	7.44859987	2.00760929
H	-0.40797839	7.06182090	1.55423471

H	-4.59645364	7.53375551	2.47848627
H	-2.37394801	8.53145770	1.96907969
C	-4.30241199	2.44650367	3.19112260
C	-4.27464442	2.89013483	4.52622354
C	-5.37539154	1.66318402	2.73676827
C	-5.29858541	2.52709234	5.39903248
H	-3.46026893	3.51592814	4.88500629
C	-6.39196242	1.29890382	3.62069436
H	-5.42488643	1.34348688	1.70208945
C	-6.35232049	1.72422490	4.95036866
H	-5.25998292	2.84885390	6.43766700
H	-7.21046750	0.67344609	3.27003892
H	-7.13374696	1.41621233	5.64324453
C	-3.26552091	2.31833942	0.41716529
C	-3.44278561	0.94658081	0.16923795
C	-3.34250747	3.24219952	-0.63718266
C	-3.68929439	0.50065837	-1.12683804
H	-3.37727480	0.23336695	0.98304731
C	-3.58182714	2.78492303	-1.93586729
H	-3.20857197	4.30482071	-0.44948306
C	-3.75403736	1.41814098	-2.18082796
H	-3.63140434	3.49875765	-2.75683726
H	-3.93813594	1.06769271	-3.19582007
H	-1.21403046	3.24581685	4.34652886
H	-3.82118620	-0.56258171	-1.31207435
C	1.10856214	-0.00301423	0.32481040
C	-0.17601798	-0.32157484	-0.17332095
H	-0.84540306	0.53492709	-0.27142385
S	-1.39366732	-1.30899069	1.38679873
C	-0.20289537	-2.63834066	1.82852157
H	-0.25204627	-3.46509931	1.10858742
H	-0.44398399	-3.01694582	2.82965161
H	0.80989667	-2.20854105	1.84116380
C	-0.29015300	-1.31326873	-1.31637704
H	-1.33013018	-1.61271241	-1.49234605
H	0.30412808	-2.21755120	-1.12190891
H	0.10296920	-0.84825757	-2.23621957
H	1.87720739	-0.76880599	0.28745241
C	-3.97342488	-7.12496224	7.50129749
C	-5.78515484	-2.89571328	1.17176333
C	-6.36580708	-1.50097620	0.84672462
C	-4.63882639	-3.21467301	0.18560713
C	-6.90393549	-3.95372563	1.04016233
H	-7.21104754	-1.25981380	1.50814084
H	-6.72238089	-1.47267918	-0.19275340
H	-4.22006103	-4.20719971	0.38347153
H	-5.03027746	-3.18698610	-0.84237201
H	-3.82096462	-2.48547472	0.25514416
H	-7.32366058	-3.92632521	0.02445655
H	-6.51752345	-4.96422623	1.22581130
H	-7.72013288	-3.75437316	1.75126831
C	-4.87465239	-4.24723143	3.23884053
O	-4.24618805	-5.09499273	2.59490941
N	-5.20333790	-4.35021170	4.56760188
H	-5.67481882	-3.52832091	4.98081036
H	-4.00554981	-6.75710920	4.10020259
H	-0.97387644	-0.16014863	7.27336839
N	2.66286084	1.49445100	1.43437360
O	0.52053605	2.20664115	1.02712053
C	3.66904319	0.43372801	1.52156991
H	1.19964873	2.44986927	5.55384960
H	0.61207805	-0.94557703	7.02430360
C	-4.77427529	-5.31308379	5.50584431
H	2.89687319	2.42228248	3.33902465
H	3.87859071	3.11550376	2.01853560
H	2.11315939	3.40795712	2.07016864
H	-5.60429445	-0.72445573	0.96608826
H	-6.16832502	-2.51825819	3.25129680
H	-0.78335935	-1.40594359	6.02068090
C	2.90091796	2.67713319	2.26427086
C	-3.77027269	-7.42108189	6.14957929
C	-4.16625959	-6.52912189	5.14750016
H	-5.44401250	-4.06410410	7.13887693
H	-4.74805424	-5.66605217	8.90123092
C	-4.98146695	-5.01233688	6.86635968
C	1.38684699	1.24446169	0.93355323
H	-3.66144069	-7.82803650	8.27261953
H	-3.29779167	-8.36074268	5.86334210
C	-4.58406364	-5.91374823	7.85276108
C	0.11103738	0.52772967	5.49573167
C	1.02076812	-0.09206450	4.41295593
C	0.85304491	1.66280986	6.23705345
C	-0.28502143	-0.56210432	6.51690477
H	0.52310494	-0.93062666	3.91227200
H	1.30478456	0.63107524	3.63990474
H	1.94435673	-0.46987371	4.87510043
H	0.20237307	2.12638715	6.99429197
H	1.73662561	1.25655582	6.75007713
H	3.37988867	-0.35080847	2.24154686
C	-4.90185435	-1.25120443	5.30236519
C	-3.09723404	-0.43061150	4.63280751
C	-3.86779731	-0.31271931	5.91029320
C	-4.07618864	-1.31377102	4.08104930
O	-3.71051138	0.28683515	6.97772424
O	-5.97297124	-1.78095598	5.66621230

TS5_28

E = -22701.37

G = -22157.88

Nimag = 1, 142i cm-1

C	-2.30864633	-2.24720941	4.38135662
N	-2.39443735	-0.79010094	4.14370959
H	-2.29009437	-0.42134597	3.18148086
H	1.70539855	3.14904160	-0.78500643
H	3.16004265	3.24622204	0.22202643
N	-2.72430967	2.38264666	4.17020187
H	-2.54382479	1.97795318	3.22584464
C	-2.96616349	3.83529234	4.24855644
H	-2.56705992	4.23507161	3.30824903
H	-0.43819177	4.28125987	4.06262406
C	-2.15150741	4.47465093	5.37386952
N	-0.69297068	4.32108944	5.09388748
H	-2.40503318	4.02941894	6.34190543
P	0.39343445	4.56668847	6.29077658
C	1.96812456	5.22260842	5.66504619
C	2.12729729	6.59756737	5.41464089
C	3.04049773	4.34189928	5.43733953
C	3.33859753	7.07765400	4.91749435
H	1.32062930	7.29675508	5.61005542
C	4.24954260	4.83272154	4.94179663
H	2.93391315	3.27947772	5.63744025
C	4.39873220	6.19606374	4.67676086
H	3.45495017	8.14260318	4.72146857
H	5.07245535	4.14391389	4.75676379
H	5.34288528	6.57504210	4.28718720
C	0.84776268	3.00182576	7.08076404
C	0.49909453	1.82097270	6.40781635
C	1.68877695	2.95615542	8.20623185
C	0.98066227	0.59454750	6.86621195
H	-0.11430360	1.87642193	5.51296378
C	2.15338122	1.72411887	8.66624509
H	2.00613601	3.87298839	8.69916565
C	1.80431462	0.54593425	7.99386424
H	0.73810213	-0.31608650	6.32609737
H	2.80693916	1.68325337	9.53648090
H	2.18651168	-0.41021557	8.34132550
C	-0.34735282	5.71054866	7.48952217
C	-0.52522975	5.35880426	8.83628876
C	-0.84502591	6.93996264	7.01427423
C	-1.15646773	6.24986329	9.70830850
H	-0.20101219	4.38999133	9.20322637
C	-1.47042062	7.82373752	7.89174398
H	-0.77612084	7.19033937	5.95808801
C	-1.61987414	7.48285131	9.24149341
H	-1.85380443	8.77241794	7.51918211
H	-2.11333446	8.17301937	9.92447691
H	-2.39504068	5.54123973	5.41249512
H	-1.29376562	5.97197609	10.75218961
C	-0.75193454	3.12496975	0.38608160
C	-2.16252835	2.93228464	0.50861655

H	-2.59882288	3.54240856	1.30140170
S	-2.43118514	0.96749913	1.26610872
C	-4.24530275	0.52163679	1.25142997
H	-4.66206361	0.53748180	2.26489964
H	-4.37075770	-0.47811111	0.81837038
H	-4.78681852	1.24680616	0.63382139
C	-2.98755266	2.95673653	-0.76814676
H	-4.03351726	2.66594007	-0.60670331
H	-2.55351605	2.29131074	-1.52772365
H	-2.98260502	3.98457370	-1.16587312
H	-0.26192804	2.64666129	-0.45699224
C	2.80154963	-3.63959370	8.32699628
C	-2.99121080	-3.06411427	3.24159370
C	-4.48893247	-2.67835458	3.22649930
C	-2.36439731	-2.81476023	1.85313783
C	-2.87298624	-4.56402771	3.60353486
H	-4.95609445	-2.89127979	4.19990366
H	-5.01513551	-3.26176764	2.45775498
H	-1.32523495	-3.15881708	1.82817437
H	-2.94348159	-3.36061049	1.09391439
H	-2.37750263	-1.75384371	1.57227590
H	-3.42026226	-5.16519700	2.86372139
H	-1.82655637	-4.89399694	3.60666764
H	-3.30895037	-4.76514356	4.59389531
C	-0.84600032	-2.67053707	4.70415318
O	-0.02291156	-3.01847162	3.84971513
N	-0.60609906	-2.62544147	6.05398563
H	-1.36655779	-2.23795175	6.64127569
H	1.62573393	-3.89801648	5.12549907
H	-4.71150845	4.01240346	2.11471265
N	1.41422569	3.87127080	1.18946630
O	-0.49603836	4.38720814	2.39084763
C	2.09285338	2.99476760	0.22895510
H	-4.38810694	6.18075168	5.22135239
H	-6.23450461	3.83652578	3.02060288
C	0.56688452	-2.96694587	6.75926757
H	2.41895784	3.38054616	3.00679899
H	3.18592592	4.64772862	2.01234405
H	1.69885174	5.00938751	2.92447435
H	-4.63186328	-1.61554496	3.00522520
H	-2.90231724	-2.45233806	5.28175365
H	-5.05978741	2.50614948	2.99199772
C	2.22156647	4.24525295	2.34766455
C	2.76196104	-3.96758588	6.96763705
C	1.65446507	-3.64199093	6.17839721
H	-0.20916767	-2.04933624	8.55509150
H	1.73405262	-2.69474278	9.95493928
C	0.60987943	-2.62337656	8.12402559
C	0.01749578	3.78979856	1.36665196
H	3.66825979	-3.90204660	8.93233172
H	3.60205171	-4.48903624	6.50895181
C	1.71572812	-2.96629380	8.89971062
C	-4.49915861	4.17803293	4.29444439
C	-5.18929834	3.59315269	5.54289688
C	-4.67663873	5.71559801	4.26964210
C	-5.16171699	3.59542198	3.02691548
H	-5.14717767	2.49563795	5.54576836
H	-4.72991760	3.95160453	6.47285682
H	-6.24948624	3.88574069	5.54740576
H	-4.07959024	6.16965217	3.46415194
H	-5.73305795	5.96099445	4.08812993
H	1.98403090	1.92598841	0.48851930
C	-2.56805717	-0.01229365	6.60970088
C	-2.70005314	1.51006405	5.17269750
C	-2.73923393	1.49657315	6.67795726
C	-2.53050493	0.08923898	5.14137020
O	-2.82979025	2.33669117	7.57705077
O	-2.43942552	-0.93861901	7.43712588

TS5_29

E = -22713.62

G = -22169.45

Nimag = 1, 100i cm-1

C	-2.29196018	-3.23034290	-0.40373618
N	-1.38473236	-2.14209887	0.00637519
H	-0.36220258	-2.22882821	-0.19145845
H	3.68544565	-4.75548236	1.63883514
H	3.32533962	-3.99983039	3.21774260
N	0.28694058	-0.00635218	1.71162276
H	0.88939201	-0.60447354	1.09375303
C	0.84748671	1.10641768	2.47518208
H	0.00028625	1.75360663	2.73822072
H	2.50248642	1.11865660	-0.30538292
C	1.83980921	1.91849135	1.57248666
N	1.70015595	1.66059004	0.13157307
H	2.87411803	1.64864693	1.80943409
P	0.68551413	2.45885144	-0.86657503
C	1.18896584	4.18249284	-1.12071809
C	2.54387613	4.50984763	-0.94731710
C	0.27171193	5.15857618	-1.54501859
C	2.97988654	5.81053581	-1.20679197
H	3.24624885	3.75219794	-0.60447799
C	0.71715085	6.45564561	-1.80675832
H	-0.77997201	4.90726364	-1.66914319
C	2.06852589	6.78056672	-1.63940590
H	4.02927954	6.06716138	-1.06893097
H	0.00911576	7.21376478	-2.13845162
H	2.41134771	7.79457742	-1.84191226
C	-1.00720588	2.50576289	-0.23879332
C	-1.33725856	3.40176474	0.79577401
C	-1.97938783	1.63693632	-0.75831651
C	-2.63196563	3.41449562	1.30900733
H	-0.59008622	4.08815996	1.19050069
C	-3.27464674	1.66196044	-0.23842738
H	-1.72468789	0.94544518	-1.55705331
C	-3.60033417	2.54699232	0.79241622
H	-2.88399709	4.09367187	2.12155065
H	-4.02579778	0.97777162	-0.62663107
H	-4.60658379	2.54720084	1.20830924
C	0.74923330	1.58594797	-2.44342791
C	0.81769924	0.18211198	-2.45060169
C	0.72733875	2.31040825	-3.64692679
C	0.87199137	-0.48574752	-3.67538413
H	0.88249346	-0.38655183	-1.52305931
C	0.76995339	1.62571443	-4.86234508
H	0.69811174	3.39749240	-3.63834318
C	0.84293484	0.22820892	-4.87678188
H	0.75945801	2.18474854	-5.79694689
H	0.88869460	-0.30333312	-5.82677706
H	1.73135340	2.98846909	1.79341036
H	0.94869281	-1.57112503	-3.68832100
C	3.61144182	-2.39393114	-0.33340419
C	3.76316188	-1.62350647	-1.53691170
H	2.82024170	-1.38601388	-2.02803912
S	4.30462344	0.36741838	-1.05479831
C	4.17176677	1.25032478	-2.68589408
H	3.44386449	0.72913285	-3.31860591
H	3.81642018	2.27466416	-2.52007233
H	5.14573579	1.28078407	-3.18957394
C	4.83983004	-2.08021159	-2.51042326
H	4.96599900	-1.38057702	-3.34690976
H	5.80749842	-2.19089054	-2.00094495
H	4.55651851	-3.06155928	-2.92597535
H	4.48889841	-2.91457678	0.03764947
C	-0.54700483	-8.50617420	3.16835282
C	-2.80052969	-3.09303372	-1.87224028
C	-3.65089019	-1.80495303	-1.94222070
C	-1.63905402	-2.98169364	-2.87834336
C	-3.68128739	-4.32039554	-2.18691646
H	-4.45868957	-1.81664635	-1.19663796
H	-4.09168915	-1.69803182	-2.94369662
H	-1.02227466	-3.88680379	-2.88252505
H	-2.04013937	-2.81018471	-3.88822130
H	-0.99993085	-2.12938813	-2.62400552
H	-4.11288299	-4.22674187	-3.19362009
H	-3.09555948	-5.24999268	-2.15325524
H	-4.51031809	-4.40584390	-1.46782215
C	-1.54369099	-4.54340350	-0.09775256
O	-0.57697536	-4.93178187	-0.75923593
N	-2.01851850	-5.17731305	1.02880738

H	-2.80732317	-4.72839970	1.49409735
H	0.02586978	-6.80640367	0.25674330
H	-0.44452230	0.46365840	4.79480827
N	2.33875693	-3.08541839	1.62101856
O	1.33360979	-1.80595144	-0.02384350
C	3.50041908	-3.79395575	2.15366067
H	2.71197648	2.48641334	4.07368995
H	0.89015287	-0.37605954	5.63886920
C	-1.49855856	-6.30846517	1.69812191
H	1.05890160	-3.58485326	3.20941282
H	0.87221994	-4.63100103	1.77361144
H	0.24305768	-2.96538390	1.76090631
H	-3.02435099	-0.92667826	-1.74881874
H	-3.17584196	-3.15646135	0.24176523
H	0.19260437	-1.06748207	4.15620494
C	1.05622126	-3.59704851	2.11031038
C	0.03559924	-8.16336150	1.94447800
C	-0.42998829	-7.07428760	1.20186305
H	-2.91967584	-6.05836660	3.31123765
H	-2.08321710	-7.99541070	4.60625254
C	-2.09028139	-6.65264856	2.92716829
C	2.40768021	-2.42351806	0.38379113
H	-0.17492889	-9.35695242	3.73766086
H	0.86767094	-8.74932292	1.55454150
C	-1.61598695	-7.74306209	3.65492716
C	1.51376447	0.65012718	3.82256347
C	2.73600576	-0.26205178	3.57903418
C	1.93575684	1.91605557	4.60310942
C	0.46983272	-0.12840725	4.65320249
H	2.47413782	-1.12991479	2.96048684
H	3.56665763	0.26719580	3.09192704
H	3.10933358	-0.63436886	4.54476118
H	1.07300534	2.57879739	4.77152302
H	2.34323954	1.63204227	5.58435283
H	4.39721822	-3.17032849	2.07103753
C	-2.99222916	-0.98220044	1.69232120
C	-0.99473197	-0.34165206	1.74032531
C	-2.22031559	0.07997752	2.48318247
C	-1.72910876	-1.31041258	0.99645507
O	-2.48508251	0.92702645	3.34266488
O	-4.16129226	-1.39932868	1.63633292

TS5_30

E = -22713.07

G = -22169.32

Nimag = 1, 142i cm-1

C	-1.70706145	-3.22781901	-0.02738794
N	-0.78647261	-2.21918194	0.52914116
H	0.14528706	-1.98889831	0.10985649
H	5.30453247	-3.00376062	-0.62135071
H	4.75365802	-4.16415466	0.61762765
N	0.41235754	0.36862214	1.88457548
H	0.97457014	-0.01076607	1.08202124
C	0.64299548	1.75912697	2.30242805
H	1.62112901	2.00665618	1.87325469
H	2.80000233	1.17356123	3.55925601
C	0.79706559	1.85637909	3.83106634
N	2.00498896	1.11234385	4.25102785
H	-0.09414636	1.46827340	4.33239733
P	2.08759099	-0.18655381	5.25120773
C	1.34538076	0.16339263	6.86683446
C	-0.03696611	0.40206130	6.98237246
C	2.16815649	0.20696040	8.00656830
C	-0.58205403	0.69537524	8.23388263
H	-0.68825223	0.33972960	6.11348306
C	1.60863039	0.49799541	9.25306393
H	3.23464168	0.01264622	7.92471349
C	0.23684143	0.74509055	9.36757589
H	-1.65243413	0.87774656	8.32218380
H	2.24715235	0.52827012	10.13486312
H	-0.19535697	0.97151274	10.34166360
C	3.86567439	-0.45697229	5.45048768
C	4.72639495	0.65004620	5.55041125
C	4.37660698	-1.76194285	5.53277468
C	6.09572597	0.44587490	5.71805368
H	4.32629930	1.65902684	5.49254182
C	5.74904623	-1.95531220	5.70426093
H	3.71221194	-2.61890779	5.45335970
C	6.60749111	-0.85432671	5.79273845
H	6.76455761	1.30274688	5.78378095
H	6.14731419	-2.96722943	5.76263821
H	7.67810978	-1.00973538	5.92060905
C	1.38875462	-1.72358388	4.60342159
C	1.85148512	-2.14856178	3.34284099
C	0.48458627	-2.51412167	5.33090821
C	1.43368247	-3.37537772	2.83669153
H	2.53683211	-1.53230441	2.76384169
C	0.05709575	-3.73480902	4.80128109
H	0.12824706	-2.19045499	6.30539031
C	0.54396277	-4.16996161	3.56635450
H	-0.64657767	-4.35071496	5.35782575
H	0.23380316	-5.13267172	3.17067891
H	0.92589970	2.90480707	4.12483662
H	1.80234366	-3.69926453	1.87102263
C	3.95318898	-0.41768578	-0.02573082
C	3.74276377	0.99294385	0.09216689
H	2.69274377	1.29612093	0.11017639
S	4.33979278	1.53841662	2.11376428
C	4.12372129	3.37948077	2.25185734
H	3.17104757	3.68580735	1.80320945
H	4.11191111	3.65172635	3.31653644
H	4.94522001	3.90795479	1.75271117
C	4.60711234	1.90925637	-0.76047074
H	4.48659163	2.96727621	-0.49377436
H	5.66856601	1.64193235	-0.66498368
H	4.31652241	1.78905899	-1.81762994
H	4.98510950	-0.73944547	-0.13630450
C	-1.77283050	-8.16950841	4.31696516
C	-1.85088475	-3.12059548	-1.57534351
C	-2.46387544	-1.73441578	-1.88428224
C	-0.50927915	-3.26108268	-2.32271712
C	-2.82687373	-4.22839056	-2.03088565
H	-3.45003786	-1.62388033	-1.40872018
H	-2.58940031	-1.61468689	-2.96979357
H	-0.03684759	-4.22386663	-2.10237224
H	-0.69256277	-3.19495586	-3.40558736
H	0.18786964	-2.45573369	-2.05455021
H	-3.03788887	-4.12039719	-3.10423321
H	-2.39961040	-5.22641510	-1.86429257
H	-3.78132441	-4.16190185	-1.48702677
C	-1.33252659	-4.62515334	0.52654580
O	-0.43505073	-5.33303774	0.05669924
N	-2.10386702	-4.94359829	1.61962693
H	-2.65308672	-4.15944813	2.01692284
H	-0.85719373	-7.31725767	1.13384631
H	-0.06842431	4.44745653	3.04897273
N	3.30684330	-2.74035372	0.13461879
O	1.66440204	-1.11153975	-0.03754162
C	4.71069408	-3.11235391	0.30635454
H	-2.21825021	1.57623788	1.80352464
H	-0.54985557	4.91906455	1.40812417
C	-1.97687236	-6.05474840	2.47792950
H	2.68359633	-4.73565486	-0.07268924
H	2.73499562	-3.83413212	-1.61544606
H	1.43952702	-3.53740093	-0.43002117
H	-1.81342457	-0.92671886	-1.52233526
H	-2.69640478	-2.97761165	0.37428692
H	1.11399140	4.37872959	1.71815411
C	2.49656492	-3.75873677	-0.53702801
C	-1.21060353	-8.28131372	3.04112144
C	-1.30809456	-7.23669147	2.11641304
H	-3.05945624	-5.01930988	4.03455842
H	-2.89079238	-6.88998216	5.65825446
C	-2.55250565	-5.94288457	3.75814824
C	2.93693301	-1.38620895	0.02073720
H	-1.68786477	-8.98849595	5.03009650
H	-0.68590926	-9.19313492	2.75580863
C	-2.44798623	-6.99301199	4.66776677
C	-0.37681748	2.76340563	1.65499283
C	-0.31939269	2.57023902	0.12164729

C	-1.82274394	2.54192461	2.14289169
C	0.06090837	4.20955181	1.98494692
H	0.69512710	2.75518793	-0.26253197
H	-0.61162383	1.55129332	-0.16355577
H	-1.00423844	3.27506559	-0.37128360
H	-1.89773437	2.57337394	3.23715955
H	-2.47079506	3.32939814	1.73093132
H	5.16852539	-2.49887350	1.09044576
C	-2.14902463	-1.74730131	2.68728697
C	-0.58215811	-0.41797643	2.28293944
C	-1.59089569	-0.51906723	3.38343103
C	-1.10040799	-1.59581659	1.66127239
O	-1.87328578	0.12554729	4.40379006
O	-3.09385231	-2.54188160	2.88105338

TS5_31

E = -22717.69

G = -22173.08

Nimag = 1, 108i cm-1

C	-2.54246104	-2.90448914	-0.39597347
N	-1.59024586	-1.89076610	0.10723467
H	-0.56485672	-2.07519258	0.00700572
H	3.04219990	-4.94268369	2.04426843
H	2.58881278	-4.22784744	3.61937791
N	0.17802794	0.15999287	1.78964993
H	0.74125167	-0.46317555	1.16121965
C	0.79577856	1.26070690	2.52716031
H	-0.02574132	1.92148078	2.83305287
H	2.47219100	1.00534043	-0.15376291
C	1.75482309	2.06389635	1.57330994
N	1.69413325	1.65588893	0.16233066
H	2.79677521	1.91779965	1.87534926
P	0.72259843	2.32881107	-0.96555885
C	1.17477447	4.05359759	-1.28262098
C	2.51262986	4.43598349	-1.08747887
C	0.23591656	4.97667126	-1.77238923
C	2.90965518	5.73966771	-1.38890429
H	3.23026509	3.71815376	-0.69453601
C	0.64263609	6.27806535	-2.07386469
H	-0.80171894	4.68159514	-1.91492973
C	1.97622426	6.65814067	-1.88373503
H	3.94511803	6.03972702	-1.23472230
H	-0.08228881	6.99647687	-2.45393349
H	2.28840937	7.67531936	-2.11738922
C	-1.02907997	2.33327139	-0.50682334
C	-1.47692330	3.18427632	0.51995351
C	-1.93169687	1.47796070	-1.15806837
C	-2.81813932	3.16246809	0.89797610
H	-0.78616578	3.86188868	1.01855705
C	-3.27208617	1.46318316	-0.77038916
H	-1.59285031	0.82898326	-1.95797025
C	-3.71502967	2.30249433	0.25480233
H	-3.16033664	3.80169958	1.70941677
H	-3.96729169	0.78522668	-1.26207175
H	-4.75702649	2.27160589	0.56969736
C	0.93757554	1.35864604	-2.46866485
C	0.92220265	-0.04452791	-2.38714069
C	1.06536249	2.00584288	-3.70831066
C	1.03174097	-0.79226041	-3.56021358
H	0.86753211	-0.55348349	-1.42536362
C	1.17486256	1.24245763	-4.87233641
H	1.09203114	3.09179596	-3.76484762
C	1.15384291	-0.15477852	-4.79865392
H	1.28161374	1.73969410	-5.83534080
H	1.24074444	-0.74730975	-5.70898062
H	1.54490033	3.13681644	1.67015921
H	1.02594274	-1.87863390	-3.50331478
C	3.36175891	-2.62393011	0.14018711
C	3.66555927	-1.92912686	-1.08264220
H	2.78461803	-1.67786582	-1.67220440
S	4.26662435	0.06026352	-0.65268816
C	4.35970279	0.85017251	-2.33260024
H	3.62281617	0.38189144	-2.99523677
H	4.11876015	1.91681791	-2.24173512
H	5.36473922	0.73980971	-2.75763045
C	4.79795337	-2.49511922	-1.92708680
H	5.01576074	-1.86683778	-2.80058240
H	5.71766587	-2.59657141	-1.33358596
H	4.51113069	-3.49613331	-2.28948124
H	4.16771953	-3.17657152	0.61292910
C	-2.54533406	-5.14816345	5.70668720
C	-2.23945749	-3.26571672	-1.87745549
C	-2.41643786	-1.98048367	-2.71880984
C	-0.80203622	-3.80486190	-2.07313335
C	-3.27072387	-4.31808790	-2.34131295
H	-3.42530250	-1.55949045	-2.59306386
H	-2.26582732	-2.20439030	-3.78454921
H	-0.66635956	-4.75292664	-1.54263950
H	-0.62131768	-3.96458490	-3.14643377
H	-0.04501940	-3.10064941	-1.70507964
H	-3.12738155	-4.53261329	-3.41013562
H	-3.15976147	-5.25485993	-1.78155005
H	-4.29768433	-3.94584820	-2.20431352
C	-2.52569714	-4.08927907	0.61394852
O	-1.90447463	-5.14248002	0.43747537
N	-3.18853325	-3.76060300	1.77245413
H	-3.73623542	-2.88600170	1.75145866
H	-2.00939998	-6.12073893	2.47234484
H	-0.41688619	0.63789473	4.88823172
N	1.86238839	-3.14953030	1.98380948
O	1.12649448	-1.84210701	0.22360983
C	2.89084573	-3.99358505	2.59169994
H	2.75115923	2.59100686	4.04372655
H	0.92693226	-0.23851608	5.67638947
C	-2.98453820	-4.29122195	3.06548847
H	0.45548093	-3.72844112	3.42784151
H	0.09031027	-4.34422342	1.79445729
H	-0.17596053	-2.63238653	2.19503440
H	-1.68506192	-1.22065602	-2.42689753
H	-3.54222821	-2.44816918	-0.36214565
H	0.15568154	-0.90743203	4.22169528
C	0.48320510	-3.48383142	2.35958328
C	-2.12231186	-5.92893461	4.62638671
C	-2.34101223	-5.51659270	3.30845436
H	-3.91148422	-2.55348749	3.95869790
H	-3.53640809	-3.31299865	6.28833446
C	-3.41928148	-3.50595645	4.15077197
C	2.10406795	-2.53403822	0.74798410
H	-2.36973009	-5.47994385	6.72939784
H	-1.61493460	-6.87703002	4.80571598
C	-3.20092597	-3.93504258	5.45882861
C	1.50634794	0.77881049	3.83911409
C	2.69134244	-0.16191052	3.53462648
C	1.99189399	2.02970743	4.60644832
C	0.47585937	0.02290558	4.70803852
H	2.36062773	-1.05565881	2.99173214
H	3.47992566	0.32876715	2.94781814
H	3.14425293	-0.49360549	4.48098221
H	1.15171990	2.70701021	4.82366922
H	2.44306162	1.72875315	5.56306456
H	3.84606365	-3.45693420	2.63220946
C	-3.13595283	-0.63460182	1.78987913
C	-1.11827165	-0.09356507	1.81455297
C	-2.31671817	0.39151871	2.56597391
C	-1.90817016	-1.03301649	1.08230023
O	-2.52942110	1.24401635	3.43413627
O	-4.31671578	-1.04604304	1.78513114

TS5_32

E = -22702.68

G = -22157.65

Nimag = 1, 177i cm-1

C	-2.41559699	-2.68184896	1.77689352
N	-1.42972400	-1.64670814	1.38292090
H	-0.57275840	-1.87772011	0.84049891
H	3.14878565	-4.26725675	-2.13196986
H	2.06187252	-5.40596105	-1.29003319
N	0.46885106	0.95380685	1.22067595
H	0.81797659	0.14328678	0.64966360
C	1.51294981	1.87977384	1.70851234

H	2.40891368	1.52052885	1.19139565
H	2.75692833	-0.17705936	2.68915424
C	1.76911647	1.61770593	3.21046536
N	1.99901214	0.16317011	3.34924369
H	0.91053746	1.92200774	3.81966739
P	2.21649860	-0.64208292	4.77509265
C	0.89919662	-0.18223550	5.90919534
C	-0.38616407	-0.00247386	5.37513701
C	1.11067992	-0.09502615	7.29504202
C	-1.45198580	0.30488376	6.21552753
H	-0.54438148	-0.12510630	4.31063346
C	0.03124532	0.18945549	8.13204872
H	2.10137178	-0.25125528	7.71584745
C	-1.24356699	0.39597035	7.59450316
H	-2.44291158	0.45180200	5.79199617
H	0.18553107	0.24537333	9.20857403
H	-2.08118311	0.61184762	8.25531976
C	3.81878475	-0.29088746	5.54228933
C	4.02564437	0.98682346	6.09662700
C	4.90008918	-1.17395363	5.38327515
C	5.30438293	1.36598316	6.50624107
H	3.19482142	1.68177245	6.20686330
C	6.17438873	-0.78698396	5.80204166
H	4.75176630	-2.14488257	4.91888890
C	6.37765642	0.47923590	6.36011421
H	5.46327937	2.35411387	6.93568729
H	7.01225372	-1.47185163	5.67814057
H	7.37596157	0.77938888	6.67659192
C	2.11859475	-2.39021097	4.33390151
C	1.77025808	-2.76968099	3.02701929
C	2.34514377	-3.36166914	5.32373956
C	1.66760315	-4.12349758	2.71073242
H	1.57213255	-2.02525340	2.26330255
C	2.23295248	-4.71294965	4.99583335
H	2.60004406	-3.06742914	6.34097550
C	1.89791162	-5.09248970	3.68992995
H	2.40127017	-5.46984061	5.76076702
H	1.80322494	-6.14927499	3.44231234
H	2.64482491	2.19964697	3.53345210
H	1.38865073	-4.40744465	1.69920328
C	3.29653421	-1.74862231	-0.65153308
C	3.84037145	-0.50835833	-0.23226647
H	3.10675068	0.25757341	0.01387026
S	4.60728764	-0.82305752	1.89059921
C	5.35037446	0.77191917	2.48253005
H	6.26475500	1.02459668	1.85819397
H	4.60276392	1.61956148	2.41988630
H	5.66214468	0.63243119	3.56345962
C	5.05827544	0.02397064	-0.96064442
H	5.68758707	0.66266076	-0.33013677
H	5.67386951	-0.80057644	-1.34493255
H	4.72646351	0.63317945	-1.81857931
H	3.98891242	-2.45763074	-1.09743707
C	-1.85312875	-2.87332470	8.33468182
C	-2.64960069	-3.75931323	0.68381285
C	-3.80535362	-4.66416590	1.17038604
C	-3.08975067	-3.03047149	-0.60709254
C	-1.39931047	-4.62225716	0.40710909
H	-3.53959654	-5.17983746	2.10320777
H	-4.02488666	-5.42713028	0.40980514
H	-2.29436614	-2.38252701	-0.99469052
H	-3.34096857	-3.76725286	-1.38314635
H	-3.97714204	-2.40609754	-0.42206571
H	-1.57308881	-5.22666182	-0.49498018
H	-0.50559333	-4.01407474	0.23354737
H	-1.19027088	-5.28534014	1.25146193
C	-2.01668879	-3.25143856	3.16773093
O	-1.25195385	-4.20673674	3.32470054
N	-2.59351622	-2.55295347	4.19770151
H	-3.21103049	-1.76548094	3.94521603
H	-0.30107855	-3.40043220	5.34157648
H	3.54534105	3.69077213	1.56186755
N	1.54554934	-3.40860086	-0.97122732
O	0.99548220	-1.35823951	-0.08982844
C	2.56632086	-4.43343055	-1.20472231
H	0.01693893	3.99942087	2.91305436
H	2.76592015	4.91325437	0.53120486
C	-2.33772350	-2.73624074	5.57797397
H	0.03235802	-4.36081785	-2.10292363
H	0.98625908	-3.15159173	-3.01786766
H	-0.22240291	-2.62365512	-1.80625182
H	-4.72139750	-4.07864734	1.34161723
H	-3.36958281	-2.15203911	1.89677435
H	3.06288444	3.27344392	-0.10210578
C	0.52578935	-3.38449561	-2.03754227
C	-0.84716469	-3.20944669	7.42138188
C	-1.08180017	-3.15096566	6.04836889
H	-4.32154808	-2.07741032	6.11528424
H	-3.89565668	-2.20025803	8.56171904
C	-3.35119948	-2.40397061	6.48851965
C	1.94722140	-2.11468054	-0.53095586
H	-1.65687912	-2.90952366	9.40558767
H	0.13855086	-3.50418087	7.77966500
C	-3.10651193	-2.47266005	7.86132449
C	1.38022684	3.40423065	1.30515649
C	0.34800377	3.56234546	0.16941499
C	0.97616642	4.31339835	2.48764058
C	2.77347771	3.84520453	0.79258554
H	0.58845856	2.90977365	-0.68183606
H	-0.66464717	3.31681301	0.51375429
H	0.34905267	4.60472918	-0.18076417
H	1.73937673	4.31318965	3.27902542
H	0.87780196	5.34802304	2.12680683
H	3.25550711	-4.47165620	-0.35386524
C	-2.55859353	0.29466945	2.67289999
C	-0.72386594	0.76742262	1.77842528
C	-1.67252549	1.52662068	2.65271584
C	-1.56506115	-0.39468895	1.81942852
O	-1.69311752	2.62835474	3.21101762
O	-3.61215127	-0.03634912	3.25510185

TS5_33

E = -22712.28

G = -22169.71

Nimag = 1, 135i cm-1

C	-2.82953330	-2.74936735	-0.31455162
N	-1.79350966	-1.77665786	0.07166519
H	-1.00612480	-1.63895869	-0.57631855
H	3.07849427	0.99232847	-5.24770501
H	2.26409594	2.44494413	-5.86396754
N	0.46668083	-0.05660213	1.67642132
H	0.81389602	-0.27260936	0.72147799
C	1.22004766	0.86330406	2.53671659
H	0.50405875	1.21729228	3.28894402
H	1.76571851	2.20539916	-0.45624576
C	1.71902377	2.08971224	1.69777596
N	1.06351135	2.22684072	0.38808553
H	2.78396783	1.98001702	1.47021108
P	-0.28132826	3.11194810	0.13868199
C	0.01360641	4.90318264	0.20057924
C	1.28620480	5.36134894	-0.18348748
C	-0.99304844	5.81542841	0.55702421
C	1.54443898	6.73277898	-0.21327903
H	2.05940237	4.64556997	-0.45835425
C	-0.72523222	7.18600777	0.52204696
H	-1.97483341	5.45968238	0.86344758
C	0.54030724	7.64335634	0.13719682
H	2.52976240	7.09148823	-0.50809725
H	-1.50303245	7.89644161	0.79889617
H	0.74587202	8.71303966	0.11380357
C	-1.56412687	2.74765163	1.35725622
C	-1.44962329	3.25559609	2.66524088
C	-2.65106751	1.93143914	1.01029046
C	-2.41450313	2.93221774	3.61669111
H	-0.61703906	3.90277011	2.93512303
C	-3.61544313	1.61861958	1.96994713
H	-2.73651948	1.54184350	-0.00078765
C	-3.49557117	2.11417048	3.27061859
H	-2.31806191	3.30981183	4.63327851
H	-4.44998300	0.97214469	1.70840432

H	-4.23842143	1.84969549	4.02149035
C	-0.86550302	2.69078220	-1.51798081
C	-0.51255091	1.45684402	-2.08337529
C	-1.68213671	3.59002938	-2.22432178
C	-0.96617338	1.12874362	-3.36000186
H	0.12234009	0.76552367	-1.54104597
C	-2.14917098	3.24102861	-3.49237535
H	-1.93681805	4.55888727	-1.79933266
C	-1.78906897	2.01312866	-4.06143904
H	-2.78170770	3.93553759	-4.04372406
H	-2.14590365	1.75210353	-5.05732666
H	1.62062880	2.99765306	2.30835450
H	-0.67180253	0.17794130	-3.79996921
C	2.87217172	0.27808496	-2.65610209
C	3.11918123	-0.52698027	-1.48136986
H	3.25430490	0.07999210	-0.58240311
S	1.31919685	-1.52449160	-1.11140358
C	1.55626181	-2.95299681	0.06070920
H	2.41611310	-3.55571067	-0.25331642
H	1.68996696	-2.61368785	1.09354224
H	0.65051841	-3.56714820	-0.01087810
C	4.15699974	-1.63554004	-1.58831371
H	4.22221093	-2.23678268	-0.67152845
H	3.93487724	-2.30348517	-2.43265410
H	5.14260913	-1.17489501	-1.76402845
H	2.76452626	-0.24994155	-3.59917422
C	-1.35467949	-9.16077151	-1.04298957
C	-3.87527206	-2.15664418	-1.32132726
C	-4.64276981	-1.03820765	-0.58512888
C	-3.18652035	-1.56819709	-2.56763392
C	-4.85409940	-3.27883770	-1.72786077
H	-5.12553331	-1.41799348	0.32623817
H	-5.41155166	-0.61108536	-1.24461250
H	-2.60471529	-2.32640910	-3.10567731
H	-3.94597436	-1.15478376	-3.24711197
H	-2.51295880	-0.74983917	-2.28980449
H	-5.64418322	-2.86769973	-2.37182602
H	-4.34526755	-4.07815418	-2.28490165
H	-5.33593046	-3.72506136	-0.84448319
C	-2.10356211	-3.98886525	-0.86625486
O	-1.21841925	-3.88847725	-1.72220807
N	-2.52411990	-5.17020069	-0.31001274
H	-3.25347491	-5.09771465	0.39896768
H	-0.51172952	-5.97586520	-1.96365829
H	1.01228890	-0.66347090	4.80274416
N	2.48236065	2.39773708	-3.78622777
O	2.78299519	2.37085431	-1.50461328
C	2.26627929	1.70360851	-5.05479872
H	3.49202728	2.02098379	3.72856643
H	2.60627860	-1.47126845	4.73838076
C	-2.09823496	-6.48862792	-0.59479926
H	0.73321894	3.62527018	-3.76890091
H	2.19069349	4.35919284	-4.49845070
H	2.07673511	4.15817641	-2.72670344
H	-3.95714077	-0.23465696	-0.29657776
H	-3.36983694	-3.00446542	0.60521795
H	1.38818991	-1.79026935	3.48309827
C	1.82998437	3.70837916	-3.68917283
C	-0.67805440	-8.11774427	-1.68282780
C	-1.03758103	-6.78329659	-1.46852783
H	-3.60466401	-7.30499992	0.72753560
H	-2.94899442	-9.65987484	0.33438601
C	-2.78203081	-7.53521173	0.05036817
C	2.69779648	1.66691648	-2.60129624
H	-1.06412489	-10.19577145	-1.21781073
H	0.14606174	-8.33822532	-2.36092503
C	-2.41048788	-8.86021021	-0.17319236
C	2.38903759	0.15619117	3.30685444
C	3.45979151	-0.39391400	2.33921272
C	3.02455795	1.18611158	4.26881334
C	1.81018811	-1.01278137	4.13415684
H	3.01732101	-1.07237457	1.60189590
H	3.98675719	0.40166790	1.79587748
H	4.21341009	-0.95983084	2.90587970
H	2.26872610	1.59678212	4.95539442
H	3.80503875	0.70112517	4.87278819
H	1.30603877	1.15805646	-5.07979142
C	-2.54950862	-1.44305528	2.52426416
C	-0.69955418	-0.58387539	2.03185274
C	-1.52671065	-0.58744764	3.27791584
C	-1.66702730	-1.36063918	1.33760965
O	-1.43114553	-0.08260011	4.39901888
O	-3.64718208	-1.96710109	2.76388500

TS5_34

E = -22706.41

G = -22162.72

Nimag = 1, 111i cm-1

C	-2.25476507	-2.76281288	1.03117549
N	-1.31227789	-1.64068285	1.04675923
H	-0.65347594	-1.56476181	0.25845210
H	5.77460684	3.05580213	-0.79414984
H	5.09443950	4.14250485	0.45076930
N	0.47408114	0.95075328	1.55834812
H	0.74402848	0.41958366	0.68822617
C	1.46177381	1.94665492	1.99938132
H	2.27807914	1.84621713	1.27572629
H	3.19836747	0.03725378	2.45302274
C	2.04954334	1.56828713	3.37122613
N	2.54137308	0.15948769	3.29724783
H	1.29203650	1.64521048	4.16169645
P	3.16848010	-0.50883941	4.66959189
C	1.87277703	-0.61345514	5.91911227
C	0.67431868	-1.23776378	5.53044179
C	2.04788019	-0.16960265	7.23842557
C	-0.35935592	-1.38521471	6.45135238
H	0.55450081	-1.58863657	4.50832862
C	1.00750063	-0.32873722	8.15805648
H	2.98394756	0.28726027	7.54943754
C	-0.19300685	-0.92885085	7.76404320
H	-1.30012448	-1.83092903	6.13433522
H	1.13612116	0.01865332	9.18216804
H	-1.00394250	-1.04063318	8.48287820
C	4.58468165	0.43045466	5.30746751
C	4.39214050	1.74810417	5.76822317
C	5.88742498	-0.07307031	5.15070650
C	5.49592989	2.55017017	6.05840331
H	3.38922730	2.14766641	5.89979052
C	6.98557643	0.73809656	5.44404492
H	6.04244278	-1.08749588	4.78979985
C	6.79178491	2.04914983	5.89044503
H	5.34381329	3.56914609	6.41182369
H	7.99377128	0.34571433	5.31814625
H	7.65104777	2.68148700	6.11057745
C	3.70388556	-2.19936373	4.31148339
C	4.13371353	-2.59491387	3.03326616
C	3.70124874	-3.11478081	5.37977142
C	4.55634554	-3.91306623	2.83690113
H	4.14409847	-1.89145579	2.20352755
C	4.13513376	-4.42417699	5.16977975
H	3.35159350	-2.81191932	6.36468174
C	4.56093974	-4.82394958	3.89830216
H	4.13104274	-5.13294478	5.99662219
H	4.89194222	-5.84874117	3.73505257
H	2.87476718	2.25554166	3.59298968
H	4.88367691	-4.22720911	1.84632722
C	3.86350309	0.67848054	-0.94400914
C	3.29043776	-0.56166887	-1.36044674
H	3.47067583	-1.37829351	-0.65672193
S	1.11195989	-0.63610748	-1.10565111
C	0.71015848	0.87647977	-2.07933386
H	1.34165617	1.70672977	-1.73710175
H	0.87424927	0.70411795	-3.15084596
H	-0.34328755	1.13371554	-1.91344151
C	3.46109827	-0.95735528	-2.81887721
H	2.87771572	-1.85203513	-3.06976917
H	3.15629505	-0.14217051	-3.49061946
H	4.52686813	-1.16315445	-3.01385580
H	3.93614646	1.48364275	-1.66897747
C	-0.73187458	-9.19995773	0.90288383

C	-3.46326946	-2.49362890	0.05728877
C	-4.19323032	-1.23041450	0.56652730
C	-2.97003490	-2.26718543	-1.38655221
C	-4.43183679	-3.69507247	0.10312541
H	-4.52302257	-1.35885046	1.60751186
H	-5.07547508	-1.03487746	-0.05948694
H	-2.46364247	-3.15638252	-1.78350462
H	-3.82789615	-2.03512747	-2.03400211
H	-2.26697700	-1.42444573	-1.44053752
H	-5.31978922	-3.47632041	-0.50682099
H	-3.96870883	-4.60951413	-0.29148058
H	-4.77213748	-3.89148263	1.13155872
C	-1.45577150	-4.02472209	0.66034279
O	-0.55256592	-3.99067350	-0.18045089
N	-1.86677833	-5.15456479	1.32408721
H	-2.60684622	-5.02468826	2.01335187
H	0.05673067	-6.11703187	-0.35157412
H	2.17143184	4.37032906	3.45307429
N	4.73612506	2.11727027	0.82958851
O	4.24762686	-0.09201051	1.26441178
C	4.91766244	3.21892604	-0.11449062
H	-1.16693460	3.12443640	2.21081158
H	1.86336003	5.40905120	2.04695361
C	-1.44596876	-6.49243143	1.14961286
H	5.31065026	3.07580367	2.62353437
H	6.64732244	2.24899694	1.77279100
H	5.40891188	1.29424317	2.63397079
H	-3.54013881	-0.34889579	0.52089440
H	-2.66083604	-2.85132939	2.04744034
H	3.05967557	4.09622979	1.93121998
C	5.57393875	2.18803367	2.03154083
C	-0.09488347	-8.22362930	0.13072059
C	-0.43994311	-6.87307367	0.24456075
H	-2.86946457	-7.17681209	2.62983315
H	-2.23978155	-9.56111562	2.41379292
C	-2.08886847	-7.47229322	1.92848098
C	4.28942298	0.85955479	0.38743038
H	-0.45374712	-10.24849555	0.80559077
H	0.68608938	-8.50941744	-0.57364838
C	-1.73228676	-8.81435270	1.80419128
C	0.97218065	3.42871684	1.86000732
C	0.73098496	3.69281068	0.35656731
C	-0.33134454	3.70003328	2.63334383
C	2.08770973	4.37806075	2.35739726
H	1.66067223	3.57201799	-0.21714860
H	-0.01325440	2.99454893	-0.04715007
H	0.36168228	4.71785010	0.20589380
H	-0.24445044	3.43002644	3.69184605
H	-0.58579115	4.76799700	2.55983125
H	4.01373991	3.35956369	-0.71797955
C	-1.93960640	-0.67996278	3.36418921
C	-0.45962552	0.37988020	2.31529703
C	-1.10111494	0.56138829	3.66240803
C	-1.25361898	-0.77709046	2.06046875
O	-0.96375038	1.32480986	4.62293174
O	-2.78638417	-1.36386221	3.96316356

TS5_35

E = -22712.92

G = -22170.04

Nimag = 1, 138i cm-1

C	-2.68650735	-2.73150539	0.08667190
N	-1.66285728	-1.71678741	0.43208659
H	-0.79389766	-1.73088177	-0.12095468
H	3.46533952	0.42485467	-4.98731528
H	2.47811520	1.69243932	-5.76597634
N	0.56831900	0.05032827	1.98863328
H	0.92793923	-0.23701460	1.05713821
C	1.26368892	1.11214513	2.72469341
H	0.53698241	1.49963072	3.44919383
H	1.84424071	2.05990879	-0.41991862
C	1.65314092	2.26781865	1.73268181
N	1.07652511	2.11917486	0.38345722
H	2.73803070	2.28490411	1.58596575
P	-0.29360524	2.87922867	-0.07642090
C	-0.14340925	4.68778949	-0.07037859
C	1.10616996	5.22888115	-0.42253741
C	-1.23199635	5.53124729	0.20279280
C	1.25859407	6.61340200	-0.50637992
H	1.94430170	4.56564070	-0.63121260
C	-1.06939290	6.91628909	0.11562308
H	-2.19763626	5.11131613	0.47695850
C	0.17203328	7.45569255	-0.23942580
H	2.22477402	7.03627924	-0.77859809
H	-1.91181466	7.57376355	0.32590895
H	0.29461900	8.53614569	-0.30551111
C	-1.71225955	2.46439632	0.97019137
C	-1.76989701	2.93774164	2.29355043
C	-2.74598616	1.65999289	0.46512034
C	-2.84797912	2.59020424	3.10580307
H	-0.98125112	3.57587052	2.68803504
C	-3.82003487	1.31653499	1.28687286
H	-2.71044694	1.30256617	-0.55829771
C	-3.87117545	1.77823745	2.60470986
H	-2.87897716	2.93485019	4.13765331
H	-4.61046107	0.67532215	0.90121990
H	-4.69918346	1.48850131	3.24988274
C	-0.64657253	2.34564587	-1.76339067
C	-0.38248020	1.01824836	-2.13917786
C	-1.26120297	3.23338557	-2.66382935
C	-0.72986240	0.58501066	-3.41734966
H	0.10610410	0.33960058	-1.44660834
C	-1.61706343	2.78357388	-3.93626926
H	-1.44813669	4.26745187	-2.37991806
C	-1.35296249	1.46073242	-4.31251025
H	-2.09023882	3.47039260	-4.63880965
H	-1.62744391	1.11615802	-5.30921697
H	1.38569851	3.23037974	2.19036976
H	-0.51072862	-0.43942289	-3.71146408
C	2.99786860	-0.05358168	-2.29168546
C	3.23016824	-0.69293740	-1.02060688
H	3.30024348	0.02937894	-0.20446163
S	1.46649158	-1.71775221	-0.59183582
C	1.66194751	-2.97547677	0.77385001
H	2.55354546	-3.58690921	0.59316208
H	1.72575937	-2.49692569	1.75743181
H	0.77518241	-3.62295724	0.73896442
C	4.31983725	-1.75366077	-0.93886481
H	4.37573086	-2.21727753	0.05538074
H	4.15960144	-2.54283495	-1.68709440
H	5.28972029	-1.27336992	-1.14660459
H	2.93144247	-0.69585215	-3.16547967
C	-1.21736072	-6.93047938	4.92462462
C	-3.03918345	-2.71464658	-1.42622552
C	-3.64206158	-1.32993530	-1.75708161
C	-1.81290661	-2.95868068	-2.33372587
C	-4.10058549	-3.81109935	-1.66744785
H	-4.51190656	-1.11093207	-1.12030674
H	-3.96753712	-1.30414711	-2.80676240
H	-1.36696684	-3.93925556	-2.13985068
H	-2.12793507	-2.90373203	-3.38611776
H	-1.03718655	-2.19821503	-2.18264796
H	-4.43395323	-3.78366705	-2.71447007
H	-3.69142777	-4.80958307	-1.46360335
H	-4.98047360	-3.65527028	-1.02495208
C	-2.17918278	-4.08413737	0.65738652
O	-1.41865453	-4.84199305	0.04315382
N	-2.58791125	-4.26300819	1.95360252
H	-3.16737228	-3.50753712	2.35197038
H	-1.05317270	-6.48352015	1.53737748
H	1.15657899	-0.13263391	5.15311828
N	2.62995120	1.88245327	-3.69194853
O	2.86969048	2.17570804	-1.42399927
C	2.55658375	1.04210968	-4.88321714
H	3.48251934	2.52370653	3.72349188
H	2.78648292	-0.86749709	5.16084135
C	-2.10675519	-5.19018585	2.90485465
H	1.16826335	3.33120990	-4.24261016
H	2.87455135	3.82721498	-4.52445801
H	2.21847080	3.74929682	-2.85773476

H	-2.89836609	-0.53823865	-1.61710515
H	-3.59385548	-2.44412032	0.63363865
H	1.57307187	-1.38912950	3.97049040
C	2.19774621	3.27731757	-3.84155981
C	-0.87933989	-7.16212906	3.58743394
C	-1.31738849	-6.30467984	2.57290614
H	-3.04948870	-4.08016781	4.50293183
H	-2.27705098	-5.62225654	6.28603689
C	-2.44925250	-4.95355371	4.25003933
C	2.82399363	1.33366169	-2.42556110
H	-0.87081465	-7.60598811	5.70573718
H	-0.26641773	-8.02365125	3.32240292
C	-2.00724715	-5.81964511	5.24887360
C	2.47782125	0.56615978	3.54785881
C	3.56085774	-0.04389333	2.63340356
C	3.06963248	1.73510741	4.36774711
C	1.96434340	-0.52129219	4.51813981
H	3.15772541	-0.87289884	2.04138926
H	3.99105801	0.69251675	1.94156370
H	4.38302500	-0.43966074	3.24710855
H	2.30266023	2.18441738	5.01664502
H	3.88422744	1.36702753	5.00792054
H	1.67750798	0.37035822	-4.86533988
C	-2.47654497	-1.23394824	2.85021256
C	-0.61959936	-0.41221345	2.34397793
C	-1.47510701	-0.33382126	3.57231182
C	-1.57714931	-1.22907269	1.68032604
O	-1.39557005	0.22639302	4.66651716
O	-3.56404483	-1.78065829	3.11733353

TS5_36

E = -22704.73

G = -22160.93

Nimag = 1, 96i cm-1

C	2.69785722	-3.28006340	1.10435906
N	1.51673447	-2.39518234	0.98514525
H	1.52339720	-1.66435660	0.24915747
H	-3.70132658	3.17852740	-3.38438167
H	-4.91773873	2.72782491	-2.15624289
N	-0.99463843	-0.51653409	1.35802001
H	-0.37421047	-0.32051443	0.52205163
C	-1.97459733	0.57962457	1.53046920
H	-1.96207594	1.03297879	0.52901373
H	-0.45415221	2.65100735	0.83848550
C	-1.38840902	1.64878371	2.48420562
N	-0.21062593	2.22270114	1.80573378
H	-1.10025543	1.20651639	3.44521989
P	1.21926572	2.72374699	2.40185560
C	2.44670163	2.44355495	1.09919973
C	2.57893071	3.39047241	0.06900777
C	3.16964008	1.24011067	1.04852383
C	3.43186800	3.12681599	-1.00449556
H	2.00646365	4.31518370	0.09554938
C	4.01347549	0.98310272	-0.03126060
H	3.07399675	0.50144408	1.83733205
C	4.14338304	1.92479065	-1.05711280
H	3.52505821	3.85547611	-1.80861969
H	4.55491030	0.04195890	-0.06005086
H	4.79786977	1.71842146	-1.90324509
C	1.61768461	1.82438059	3.91742465
C	1.46519529	0.42883647	3.94890857
C	2.02761836	2.51025023	5.07505763
C	1.68759914	-0.27280432	5.13103863
H	1.16083697	-0.09542519	3.05312418
C	2.27826327	1.79426229	6.24674524
H	2.13523022	3.59146110	5.06822023
C	2.09844716	0.40854010	6.27914267
H	1.54505003	-1.34879812	5.15942431
H	2.60546987	2.32470029	7.13987437
H	2.28855637	-0.14390139	7.19651919
C	1.27633905	4.49746518	2.78779346
C	0.06783543	5.17099639	3.02150221
C	2.49943150	5.18356140	2.87574007
C	0.08462135	6.52720969	3.35736242
H	-0.87654765	4.63967524	2.92775179
C	2.50833753	6.53826755	3.21186285
H	3.43631797	4.66403792	2.68089974
C	1.30272853	7.20841152	3.45435981
H	3.45478233	7.07290146	3.28012351
H	1.31342470	8.26659445	3.71345694
H	-2.13975301	2.42629312	2.67425003
H	-0.85253165	7.05249354	3.53684151
C	-1.06277638	2.03482943	-2.26237494
C	0.32455707	1.74241447	-2.23318089
H	0.89038944	2.36799078	-1.54454241
S	0.76576502	-0.10188798	-1.17316399
C	-0.49497109	-1.15597312	-2.00941115
H	-1.35884670	-0.52176310	-2.26201030
H	-0.08784330	-1.61791888	-2.91744579
H	-0.82731367	-1.93947092	-1.31690609
C	1.03060697	1.49564146	-3.55626844
H	1.99879959	1.00000932	-3.41374524
H	0.41460610	0.87869934	-4.22672501
H	1.20181261	2.46532785	-4.05250779
H	-1.64560391	1.65626518	-3.09615704
C	5.36341824	-0.40686550	6.39031306
C	3.12396942	-3.87923296	-0.26669837
C	1.93487840	-4.71588829	-0.79422315
C	3.49702446	-2.80901406	-1.31643130
C	4.33183603	-4.80951512	-0.01032400
H	1.65889794	-5.50650224	-0.08012360
H	2.20889506	-5.19205511	-1.74638033
H	4.33512317	-2.19714485	-0.97002988
H	3.78589985	-3.31368378	-2.25069265
H	2.65543697	-2.14047225	-1.54208566
H	4.61674454	-5.31335985	-0.94473490
H	5.19911108	-4.24213448	0.35205211
H	4.08355390	-5.58349951	0.73190008
C	3.79315217	-2.50036916	1.88159617
O	4.67339635	-1.81973405	1.34084370
N	3.61606089	-2.59480764	3.23680898
H	2.86476307	-3.22613783	3.56238929
H	4.92143966	-0.21248320	3.01229595
H	-3.60058829	-0.61378206	-0.29207575
N	-3.03570483	3.13072992	-1.34498729
O	-0.99211815	3.45370899	-0.34616494
C	-3.86243794	2.62632935	-2.43998019
H	-4.20820242	2.21773693	2.15583509
H	-4.87434246	-1.19976400	0.81024531
C	4.27779245	-1.86141624	4.24897651
H	-4.56516991	4.12631090	-0.29760954
H	-3.60126953	5.18953135	-1.36563339
H	-2.89307148	4.57190335	0.15902998
H	1.05290345	-4.08478816	-0.96716040
H	2.37974653	-4.12532973	1.72828031
H	-3.21940769	-1.84848834	0.93150270
C	-3.55331266	4.32614370	-0.67570186
C	5.40879334	0.10538694	5.08996626
C	4.88000480	-0.61381232	4.01705661
H	3.76402956	-3.34801087	5.72910563
H	4.73315842	-2.06978716	7.62250660
C	4.23844310	-2.38297460	5.55294692
C	-1.65529512	2.88577838	-1.29970888
H	5.77048307	0.16670497	7.22195291
H	5.84937768	1.08455272	4.90454810
C	4.77946932	-1.65840243	6.61449888
C	-3.46810121	0.17668350	1.74867450
C	-3.79576207	-0.28573294	3.17897111
C	-4.33216870	1.41861824	1.41203902
C	-3.80786193	-0.94212904	0.73741996
H	-3.31503952	-1.23478655	3.42919908
H	-3.46891402	0.45410046	3.92424685
H	-4.88498520	-0.40478443	3.28092149
H	-4.06944583	1.82319281	0.42637667
H	-5.39411644	1.13267836	1.40641446
H	-3.65940917	1.56379172	-2.61438960
C	0.42736033	-2.98480718	3.24814779
C	-0.55194410	-1.47888045	2.15559002
C	-0.76950768	-2.09187786	3.52184340
C	0.59019939	-2.32710239	1.94689061

O	-1.49012115	-1.88322269	4.49795383
O	1.09324533	-3.81173973	3.91009306

TS5_38

E = -21530.06

G = -20999.91

Nimag = 1, 75i cm-1

C	-5.40542705	-0.29740212	1.42279736
N	-4.28724346	0.61602631	1.37843219
H	-3.61185862	0.55319818	0.58813217
H	0.04779908	0.26272186	-3.98619313
H	1.05080421	0.66161165	-2.56119414
N	-2.89479952	2.27711732	1.98380516
H	-2.44147223	1.90828835	1.11342580
C	-2.45158974	3.62312520	2.35305484
H	-1.42354909	3.65945239	1.95451381
H	-0.88954529	2.20520501	3.66479558
C	-2.33569086	3.79544612	3.87180805
N	-1.36351546	2.79362681	4.38933624
H	-3.31770933	3.65393502	4.32646965
P	-1.52868668	1.99785061	5.81978319
C	-2.38175126	0.40256922	5.76025526
C	-2.37381628	-0.31964834	4.55679893
C	-2.95999484	-0.14676394	6.91675902
C	-2.90671477	-1.60653656	4.52246443
H	-1.94977475	0.12389368	3.66124972
C	-3.50256809	-1.43348563	6.86786002
H	-2.98237882	0.41882335	7.84658518
C	-3.46391098	-2.16668913	5.67688089
H	-2.89354164	-2.16376301	3.59037980
H	-3.95029916	-1.86469725	7.76255353
H	-3.88212726	-3.16978950	5.64553048
C	-2.38565380	3.06062847	6.99992248
C	-3.78938215	3.13850728	6.96269778
C	-1.65106543	3.82654918	7.91996793
C	-4.45107285	3.99434230	7.84366474
H	-4.34763159	2.54612779	6.23976342
C	-2.32552366	4.67709015	8.79910502
H	-0.56658482	3.75055920	7.95751487
C	-3.72158381	4.76249477	8.75939494
H	-5.53785087	4.06172391	7.81548816
H	-1.76000433	5.26943504	9.51698802
H	-4.24348523	5.42684538	9.44722693
C	0.15969111	1.68163349	6.39951889
C	1.19162046	2.54488294	5.99572334
C	0.43455083	0.59717613	7.24768465
C	2.49540536	2.31790872	6.43996375
H	0.97176983	3.37186326	5.32457823
C	1.74124989	0.37880841	7.68717188
H	-0.35678517	-0.08821013	7.54210419
C	2.77068936	1.23651826	7.28338223
H	1.95753570	-0.46866140	8.33613193
H	3.79092028	1.05624515	7.62066096
H	-1.95812961	4.79668554	4.11067246
H	3.29797588	2.98068308	6.11882520
C	-0.47129883	-0.28313381	-0.13647406
C	-0.71003042	-0.56085512	1.25839645
H	-1.70887071	-0.26671747	1.58226416
S	0.42595466	0.74791460	2.42629515
C	1.17980948	-0.23647572	3.81249613
H	0.43644577	-0.50974675	4.56935251
H	1.95220227	0.38716272	4.27851230
H	1.64805681	-1.14279233	3.41279994
C	-0.37824828	-1.97033213	1.72868822
H	-0.47683709	-2.09385927	2.81370261
H	0.63936193	-2.26314794	1.43164537
H	-1.09224689	-2.65638525	1.24800172
H	0.41765080	-0.72267514	-0.58033885
C	-5.39774165	-5.89849117	4.92835565
C	-6.17487776	-0.31773903	0.05388436
C	-6.69065549	1.11596598	-0.20506077
C	-5.25969126	-0.75689341	-1.11102350
C	-7.37307105	-1.28400970	0.17257908
H	-7.29891884	1.47377160	0.63866434
H	-7.30965857	1.13216818	-1.11396082
H	-4.88992520	-1.77890225	-0.96029043
H	-5.83170513	-0.72520476	-2.05082902
H	-4.39091218	-0.09295557	-1.21896898
H	-7.94963674	-1.28038795	-0.76356900
H	-7.04506994	-2.31539543	0.36339634
H	-8.04703937	-0.98099916	0.98858896
C	-4.92333927	-1.69453690	1.85198276
O	-3.94330713	-2.25173080	1.34842664
N	-5.70040338	-2.24190736	2.84944684
H	-6.40477572	-1.62007104	3.24548505
H	-3.97889104	-4.26788724	2.27660222
H	-2.32613965	4.22444764	-0.31619424
N	-1.07943951	0.71126995	-2.28283463
O	-2.31050048	1.21185171	-0.41085632
C	0.12531524	0.15342909	-2.89661078
H	-2.32579190	6.45240370	2.78141820
H	-3.77794833	5.25825935	-0.43148572
C	-5.58308241	-3.49061674	3.48849226
H	-0.74855001	2.76796703	-2.78275039
H	-1.72153573	1.82573380	-3.95272512
H	-2.42848123	2.30870369	-2.37726795
H	-5.85391769	1.81261392	-0.34219799
H	-6.08926035	0.09402396	2.18694626
H	-3.92405626	3.52691361	-0.02652291
C	-1.51921449	1.97740567	-2.88322679
C	-4.55586497	-5.65419950	3.83878147
C	-4.63974094	-4.46250443	3.11266758
H	-7.17292410	-2.98548018	4.86660604
H	-7.01453198	-5.10756178	6.13189131
C	-6.44282402	-3.74065478	4.57434615
C	-1.29384657	0.56117135	-0.88940680
H	-5.31755987	-6.82806849	5.49049148
H	-3.81454435	-6.39804033	3.54654869
C	-6.34794374	-4.93394346	5.28762976
C	-3.20277427	4.79298415	1.61743507
C	-4.61396228	5.05143138	2.18377709
C	-2.35228224	6.07940760	1.74842485
C	-3.31510891	4.42661413	0.12001396
H	-5.24962882	4.16484033	2.08427630
H	-4.58048100	5.32115115	3.24865684
H	-5.07946100	5.88567277	1.63631285
H	-1.31744201	5.90549335	1.41595936
H	-2.78139618	6.87312334	1.11938791
H	0.21153727	-0.91514880	-2.66687668
S	-5.03722060	1.85086536	3.66686248
C	-4.03501805	1.59842986	2.28679319

TS5_39

E = -21530.58

G = -20998.40

Nimag = 1, 145i cm-1

C	-2.50581909	1.31174208	-2.55722665
N	-2.77024688	1.19967818	-1.11852451
H	-3.75706746	1.20185632	-0.78199844
H	-8.39229888	-0.92801461	-1.40045635
H	-8.75807316	-0.60533129	0.31503498
N	-2.34050475	1.64087214	1.08033801
H	-3.36973049	1.57003437	1.16577528
C	-1.58074574	2.16079114	2.20717911
H	-0.52702192	1.95061543	1.98580782
H	-4.13615835	1.21417442	3.58153882
C	-1.94825540	1.38760511	3.51877013
N	-3.23743230	0.66916120	3.50204748
H	-1.96246939	2.07857918	4.36848961
P	-3.32769909	-0.97147235	3.49685210
C	-2.23495337	-1.62396427	4.78535666
C	-2.18901413	-0.96002446	6.02430319
C	-1.49366143	-2.79843096	4.58188557
C	-1.40398278	-1.47578288	7.05525801
H	-2.76758897	-0.04991061	6.17450063
C	-0.70724458	-3.30587205	5.61951451
H	-1.52524669	-3.30780671	3.62159922
C	-0.66235411	-2.64662586	6.85221038
H	-1.36647610	-0.96350516	8.01558427
H	-0.12653065	-4.21377999	5.46236778

H	-0.04643758	-3.04433792	7.65794222
C	-2.85047770	-1.79975410	1.95343432
C	-1.66474658	-1.43044068	1.29548831
C	-3.62984446	-2.85710777	1.45475885
C	-1.28452017	-2.09054993	0.12916073
H	-1.04327990	-0.62257765	1.66682641
C	-3.23423952	-3.52094655	0.29140880
H	-4.54939002	-3.14629804	1.95661043
C	-2.06656966	-3.13639784	-0.37226871
H	-0.38979068	-1.76312477	-0.39606128
H	-3.85176304	-4.32593662	-0.10499178
H	-1.77088982	-3.64378565	-1.28944280
C	-5.02754872	-1.44108668	3.86035747
C	-6.03107180	-1.01201497	2.97859094
C	-5.33885090	-2.25018902	4.96415837
C	-7.35170883	-1.39314802	3.20106696
H	-5.76573044	-0.38267956	2.13891278
C	-6.66753713	-2.62908602	5.17599298
H	-4.55939520	-2.58495465	5.64462962
C	-7.67009083	-2.20564256	4.29494814
H	-6.91789571	-3.25993096	6.02783944
H	-8.70294432	-2.50821626	4.46526642
H	-1.15785700	0.65796546	3.73323850
H	-8.12887649	-1.04552474	2.52425448
C	-7.13544382	1.83617929	1.09090749
C	-6.64163362	2.90026049	1.91301832
H	-5.63092638	3.21399184	1.65048111
S	-6.17119956	2.11517818	3.88061002
C	-5.92132933	3.60117895	4.96721162
H	-5.27828599	4.34117634	4.47809853
H	-5.43703415	3.27015397	5.89652293
H	-6.88709361	4.06061086	5.21198726
C	-7.58420911	4.05942724	2.18630016
H	-7.18066126	4.76885143	2.91890081
H	-8.55547174	3.69524930	2.55116930
H	-7.75714933	4.60816014	1.24539585
H	-8.20103004	1.62292262	1.12937216
C	-0.51456316	7.57429448	-2.17155204
C	-3.39910348	0.36955854	-3.41111368
C	-3.10392547	-1.07713063	-2.95640348
C	-4.90997568	0.66165610	-3.26524368
C	-2.97721689	0.53168818	-4.88947755
H	-2.03892918	-1.32047818	-3.08782137
H	-3.69858513	-1.78731685	-3.54937688
H	-5.15120850	1.65499834	-3.65677562
H	-5.47888243	-0.09431963	-3.82772944
H	-5.24434632	0.61465481	-2.22331381
H	-3.52115115	-0.19234697	-5.51355262
H	-3.20275019	1.54096321	-5.25838587
H	-1.89920312	0.34589565	-5.01368760
C	-2.57920320	2.82454604	-2.92404299
O	-3.57675634	3.38552348	-3.39208651
N	-1.40479187	3.46984063	-2.60587700
H	-0.70111936	2.87513620	-2.13600949
H	-3.04877594	5.55400067	-3.26738264
H	-0.42714741	4.12295029	0.60752215
N	-6.79007670	-0.08238019	-0.36499401
O	-4.97553984	1.02040405	0.51569719
C	-8.22506427	-0.22225506	-0.57609244
H	-0.81557717	3.80583640	4.37017965
H	-1.45657674	5.49127986	1.09304662
C	-1.15440635	4.85416256	-2.51134540
H	-6.39160373	-2.12163632	0.09605853
H	-6.04281157	-1.63889990	-1.59119192
H	-4.97336293	-1.10101990	-0.26918927
H	-3.35074178	-1.21716497	-1.90017205
H	-1.46707755	0.98587505	-2.70293259
H	-2.15711212	4.10966226	0.22805256
C	-6.00840152	-1.30532638	-0.54390441
C	-1.75722720	7.19441175	-2.68810594
C	-2.08512771	5.84626398	-2.86710006
H	0.81488522	4.46616406	-1.71094214
H	1.38231788	6.85838066	-1.41203682
C	0.09961539	5.23635563	-1.99645074
C	-6.26578644	0.95828811	0.42330102
H	-0.26967022	8.62769266	-2.04029264
H	-2.48697895	7.95559788	-2.96517493
C	0.41092602	6.58229602	-1.82187981
C	-1.70345040	3.72554852	2.34546021
C	-3.10897777	4.12870201	2.81759521
C	-0.64204751	4.20688641	3.36171493
C	-1.41780031	4.39782034	0.98563409
H	-3.87101927	3.79027090	2.10640204
H	-3.35077760	3.70262546	3.79794101
H	-3.18432325	5.22304321	2.89943725
H	0.36715128	3.90665256	3.04153934
H	-0.66583757	5.30407490	3.43400825
H	-8.66462643	0.74330097	-0.85447069
S	-0.13174200	1.36826955	-0.48025470
C	-1.83423254	1.42252800	-0.15857719

TS5_41

E = -21530.30

G = -21000.84

Nimag = 1, 126i cm-1

C	-4.52395043	-2.05728996	2.94727976
N	-3.55279906	-1.00489091	2.68689234
H	-2.98624574	-1.16265319	1.84107473
H	3.28644189	1.10813654	-1.29189165
H	4.30860778	1.63689881	0.05766880
N	-1.78683311	0.30522180	3.28018948
H	-1.53430779	0.18231377	2.28221779
C	-0.91303094	1.12994326	4.09878272
H	-1.46019690	1.30405922	5.03399264
H	-0.84301327	2.80208605	1.31070738
C	-0.64051322	2.50924503	3.40158925
N	-1.45994608	2.72154566	2.19899670
H	0.39420821	2.56262769	3.05134010
P	-2.82499783	3.60991125	2.13490784
C	-2.52792804	5.40249537	2.13627154
C	-1.33264060	5.87165419	1.56154067
C	-3.47724543	6.30359015	2.64503872
C	-1.09883733	7.24731048	1.49453651
H	-0.60443195	5.16570642	1.16188738
C	-3.23229902	7.67692082	2.57249812
H	-4.39681094	5.93541055	3.09631176
C	-2.04602353	8.14747937	1.99704246
H	-0.17619108	7.61736789	1.04870160
H	-3.96571066	8.37937846	2.96664706
H	-1.85821187	9.21942208	1.94298994
C	-3.94248624	3.26803935	3.51773437
C	-3.53185775	3.58691106	4.82481108
C	-5.22303003	2.73872099	3.29668100
C	-4.38819176	3.35002639	5.89759398
H	-2.55680977	4.03182882	5.00684268
C	-6.07399886	2.50648733	4.37785135
H	-5.55949855	2.51780007	2.28856801
C	-5.65816585	2.80776568	5.67589916
H	-4.06184523	3.58694346	6.90921633
H	-7.06331858	2.08856855	4.20080698
H	-6.32264116	2.61891934	6.51817341
C	-3.59815513	3.16485081	0.56491635
C	-3.95036099	1.81953467	0.35409636
C	-3.79016870	4.11707791	-0.44708126
C	-4.49538950	1.43429209	-0.86864927
H	-3.78099256	1.08265873	1.13297403
C	-4.32289848	3.71626707	-1.67563531
H	-3.51412069	5.15632159	-0.28445443
C	-4.67456208	2.37906223	-1.88513212
H	-4.45854201	4.44975879	-2.46923862
H	-5.08429947	2.07015639	-2.84624207
H	-0.75780994	3.31645279	4.13492801
H	-4.75872139	0.39297485	-1.03512939
C	0.56175243	1.28859423	-1.08079787
C	-0.82517640	1.07031984	-1.32910160
H	-1.46580154	1.88624730	-0.98721683
S	-1.64151131	-0.45244017	0.02193266
C	-0.19765793	-1.59136073	0.01425747
H	-0.37854760	-2.36367805	0.77244489
H	0.71248724	-1.02869861	0.26185019

H	-0.07685319	-2.06862075	-0.96792217
C	-1.23356619	0.51715365	-2.68621844
H	-2.30017421	0.26298047	-2.71412374
H	-0.65285197	-0.38167695	-2.94065082
H	-1.03208857	1.27665966	-3.46088125
H	1.26937198	0.57168893	-1.48640260
C	-3.47601914	-8.50662725	3.98520412
C	-5.77836411	-1.94124086	2.00808931
C	-6.40364888	-0.54972786	2.24214045
C	-5.37418438	-2.09774871	0.52644662
C	-6.81330936	-3.02551436	2.37995456
H	-6.74726301	-0.44445971	3.28051825
H	-7.26130808	-0.40463238	1.56911908
H	-5.00048009	-3.10969305	0.31940311
H	-6.24530340	-1.90957219	-0.11801011
H	-4.58105146	-1.39273203	0.24839467
H	-7.72824613	-2.88077633	1.78717969
H	-6.43921309	-4.03782689	2.17696291
H	-7.08975361	-2.96077414	3.44381769
C	-3.80178111	-3.41479321	2.81228850
O	-2.90151639	-3.60051918	1.98713820
N	-4.27104648	-4.37182690	3.68176751
H	-4.98700410	-4.06039466	4.33724352
H	-2.42238892	-5.75685077	2.24098032
H	-0.47762673	-0.66611850	6.15306808
N	2.36749987	2.41462276	0.10305947
O	0.21219237	3.20249421	0.29336607
C	3.29357900	1.32628184	-0.21653828
H	1.61454378	2.20538538	4.80999944
H	1.00993221	-1.42639607	5.51653668
C	-3.96206286	-5.74699907	3.74994887
H	2.84551501	2.72069997	2.16353525
H	3.75321566	3.72494914	1.00005740
H	2.02723972	4.07207860	1.33154435
H	-5.67222993	0.23941705	2.05054841
H	-4.85600425	-1.91823583	3.98470651
H	-0.53241004	-1.58446835	4.63583076
C	2.77054599	3.28076972	1.21288869
C	-2.75363346	-7.73208300	3.07201799
C	-2.98393310	-6.35828107	2.94612098
H	-5.44957811	-6.04952239	5.29298413
H	-5.01989391	-8.47850781	5.50307411
C	-4.69024849	-6.52370789	4.67071420
C	1.00320297	2.30259540	-0.20777187
H	-3.28614778	-9.57541635	4.07412980
H	-1.99412530	-8.19803309	2.44437046
C	-4.44686536	-7.89157899	4.78590668
C	0.41957809	0.38065512	4.44987624
C	1.18648380	-0.00881107	3.16645080
C	1.28891764	1.29925920	5.33864822
C	0.08261217	-0.90333778	5.23869270
H	0.60654926	-0.72134941	2.56824943
H	1.41034240	0.85567832	2.52923501
H	2.14154189	-0.48643373	3.43046749
H	0.73532758	1.60673715	6.23928993
H	2.19222792	0.76108507	5.66133592
H	3.04951945	0.39867137	0.33145951
S	-3.56306125	-0.17720497	5.27045083
C	-2.92172610	-0.30583092	3.69227433

TS5_42

E = -21527.22

G = -20996.32

Nimag = 1, 155i cm-1

C	-3.38112341	-2.85691648	4.74159563
N	-3.38370522	-1.40959573	4.52058327
H	-3.89653473	-1.04858079	3.70424831
H	-0.41328564	0.18910966	-0.83769768
H	0.68502000	-1.02983174	-0.14602948
N	-3.04095910	0.78984404	4.94573451
H	-3.46985051	0.86921969	4.00815842
C	-2.58136317	2.09153352	5.45627798
H	-2.58325688	2.70916423	4.54587263
H	-0.64200230	1.44672407	3.95298524
C	-1.12993864	2.10774597	5.96494275
N	-0.21380433	1.54083338	4.93994947
H	-1.03433361	1.53518766	6.89224970
P	1.39823778	1.82858842	5.02249247
C	1.82982630	3.58696315	5.24333569
C	1.57140781	4.18348533	6.49331596
C	2.34193491	4.36536346	4.19234076
C	1.80090767	5.54758703	6.67637424
H	1.21395104	3.58115120	7.32626365
C	2.57827497	5.72874006	4.38714146
H	2.57267336	3.91139506	3.23254283
C	2.30149973	6.32186932	5.62321428
H	1.59728000	6.00428525	7.64395555
H	2.98471091	6.32589468	3.57191801
H	2.48551825	7.38546638	5.77006046
C	2.17131995	1.20249962	3.51989229
C	1.75542700	1.68095898	2.26476201
C	3.20695201	0.25443487	3.61269719
C	2.39813791	1.22753551	1.11259415
H	0.91876187	2.37068284	2.18701374
C	3.82488306	-0.20581141	2.45261360
H	3.50958851	-0.13459931	4.57960482
C	3.42718456	0.28755532	1.20307257
H	2.06933520	1.58932333	0.14024195
H	4.60840283	-0.95806316	2.52191420
H	3.91375536	-0.07360716	0.29736724
C	2.11430789	1.00776574	6.46704222
C	1.39350325	-0.00559850	7.11124499
C	3.40200355	1.36016809	6.90966448
C	1.96447056	-0.67364102	8.19680749
H	0.39251926	-0.26112950	6.76934783
C	3.97153383	0.67431738	7.98258218
H	3.95406329	2.15998599	6.41835621
C	3.25308229	-0.34242957	8.62586099
H	4.97321183	0.93521639	8.32134045
H	3.69953213	-0.87214949	9.46680256
H	-0.87743809	3.15637256	6.16442105
H	1.40309133	-1.45749732	8.70433145
C	-2.50269819	1.14763183	0.54091881
C	-3.67029990	1.89053301	0.89901237
H	-3.50840327	2.61873162	1.69894991
S	-4.88666617	0.49522628	2.04946852
C	-6.36558288	1.43502380	2.67410104
H	-6.66288432	1.03967631	3.65394579
H	-7.20730646	1.34982099	1.97495209
H	-6.09695616	2.49229136	2.79579138
C	-4.59512529	2.37624446	-0.20044469
H	-5.53707277	2.77586702	0.19887828
H	-4.83270941	1.56357898	-0.90152694
H	-4.09531745	3.18133032	-0.76539886
H	-2.55430092	0.52436112	-0.34934004
C	3.09044043	-3.54144710	3.75023949
C	-4.75236940	-3.51145639	4.40532831
C	-5.81250069	-2.87775363	5.33725016
C	-5.17584363	-3.30024433	2.93465561
C	-4.64862342	-5.02283476	4.71315389
H	-5.56658447	-3.05740158	6.39453393
H	-6.79939879	-3.31666326	5.13128676
H	-4.41449051	-3.69058800	2.25043972
H	-6.12612714	-3.82440111	2.75167334
H	-5.33758379	-2.23784021	2.70528022
H	-5.63678420	-5.49248438	4.60355564
H	-3.95097542	-5.51926257	4.02731900
H	-4.30506885	-5.18997397	5.74554238
C	-2.13756679	-3.46343727	4.02399273
O	-2.16400337	-4.05802981	2.94098305
N	-0.99518352	-3.21498613	4.74831977
H	-1.14141686	-2.62795298	5.59019108
H	0.02877144	-4.48733322	2.54718890
H	-4.94070922	3.30313262	4.77869664
N	-0.47443029	-0.01373508	1.25557277
O	-1.51480481	1.49901585	2.65513677
C	-0.32079743	-0.59172342	-0.07402269
H	-2.26365168	4.31010203	7.28529580
H	-5.72347227	3.28465976	6.37928014
C	0.35135635	-3.39754351	4.37999860

H	-0.70011331	-1.87447214	2.23878239
H	0.95130643	-1.19968302	2.27234516
H	-0.32295136	-0.50157474	3.30311240
H	-5.88050542	-1.79256553	5.18190307
H	-3.21891892	-2.99209332	5.82015680
H	-5.33406166	1.75412739	5.55673921
C	-0.11428611	-0.94488045	2.32927146
C	2.13314573	-4.11645883	2.90801493
C	0.76947531	-4.05833998	3.21203983
H	0.99070625	-2.35195819	6.15005586
H	3.39749078	-2.46219103	5.60534655
C	1.31746641	-2.84414175	5.24084363
C	-1.51276068	0.90047937	1.51325228
H	4.14794849	-3.58599138	3.49391911
H	2.44699564	-4.61454900	1.99054856
C	2.67146025	-2.91122870	4.92805380
C	-3.60312421	2.77357436	6.43454333
C	-3.71494999	2.04004540	7.78509429
C	-3.17198081	4.24081958	6.67173730
C	-4.98445462	2.77658342	5.74311855
H	-4.03850565	1.00196176	7.64464139
H	-2.75514630	2.02183892	8.31840771
H	-4.45036481	2.55524630	8.42169390
H	-2.98802356	4.76036050	5.71883220
H	-3.97086836	4.77893282	7.20249649
H	-1.06036310	-1.38849791	-0.28589963
S	-2.09285262	-0.93317495	6.85114443
C	-2.87079446	-0.47501860	5.37556018

TS5_43

E = -21530.17

G = -21000.93

Nimag = 1, 58i cm-1

C	-5.11172711	-2.42521929	3.27461288
N	-4.12921131	-1.34115144	3.09708289
H	-3.41521444	-1.53574153	2.37237526
H	3.71908113	-0.32117304	0.88630589
H	4.47350209	0.46687999	2.28385359
N	-2.42442886	-0.11071368	3.98369408
H	-1.91283308	-0.47947459	3.15482698
C	-1.70017778	0.79641962	4.85835936
H	-2.40848774	1.08102791	5.64609407
H	-0.83229966	2.03115510	1.98184598
C	-1.26611583	2.08604208	4.06992472
N	-1.68469519	2.06461318	2.65587785
H	-0.17587220	2.17018341	4.04796907
P	-2.93489395	2.94142722	2.07578171
C	-2.55036725	4.71139524	1.93072600
C	-1.20367941	5.08046543	1.76449946
C	-3.56033899	5.68704410	1.94476093
C	-0.87538476	6.42975783	1.61053821
H	-0.42579352	4.31744013	1.74317357
C	-3.22104267	7.03274540	1.78946505
H	-4.60086838	5.39790854	2.08147173
C	-1.88101248	7.40322407	1.62346136
H	0.16616620	6.72118067	1.48064317
H	-4.00131553	7.79283382	1.80149637
H	-1.62016388	8.45447776	1.50564591
C	-4.40431805	2.81554542	3.12635604
C	-4.38322179	3.43961893	4.38792105
C	-5.55562901	2.13356211	2.70381427
C	-5.49691046	3.35824140	5.22126029
H	-3.51224487	4.00523261	4.71069054
C	-6.66591874	2.05908252	3.54492103
H	-5.59610226	1.67597423	1.72161120
C	-6.63814693	2.66757248	4.80110925
H	-5.47376430	3.83723172	6.19906481
H	-7.55245817	1.52125003	3.21490066
H	-7.50497497	2.60082082	5.45743775
C	-3.24840407	2.29518858	0.41818335
C	-3.63548198	0.95064839	0.27596488
C	-3.03329945	3.09307161	-0.71608694
C	-3.80226032	0.40975446	-0.99649901
H	-3.78787894	0.33267023	1.15419511
C	-3.18817472	2.53617648	-1.98852812
H	-2.72916221	4.13145518	-0.60898840
C	-3.57167237	1.19884258	-2.12850356
H	-3.00335168	3.14858783	-2.87002801
H	-3.68634311	0.76805931	-3.12253653
H	-1.63694933	2.97323772	4.59631111
H	-4.09097707	-0.63284549	-1.10373983
C	1.03992078	-0.04721416	0.44802478
C	-0.26775888	-0.27749951	-0.09871128
H	-0.88219685	0.62696655	-0.11605415
S	-1.49115195	-1.38768877	1.21454425
C	-0.33703071	-2.74795318	1.65489779
H	-0.34545368	-3.53881675	0.89430186
H	-0.65098666	-3.16873022	2.61816910
H	0.67385361	-2.32651018	1.75631017
C	-0.35112037	-1.06318857	-1.40285037
H	-1.39082659	-1.28089472	-1.67711832
H	0.19603498	-2.01441208	-1.32727584
H	0.11207706	-0.47201931	-2.20973873
H	1.77026043	-0.84610459	0.36700918
C	-0.85692770	-5.20804065	7.38433248
C	-5.98903204	-2.64502880	2.01228531
C	-6.78481346	-1.34271980	1.76618130
C	-5.15719496	-2.97557398	0.75314612
C	-6.97731247	-3.79483314	2.31068757
H	-7.38669248	-1.07538442	2.64669133
H	-7.45881894	-1.47026422	0.90681617
H	-4.61890382	-3.92118685	0.87625080
H	-5.82498666	-3.04838739	-0.11830477
H	-4.41477279	-2.19588676	0.54395846
H	-7.66736243	-3.92392236	1.46437234
H	-6.44604344	-4.74170090	2.47062208
H	-7.57622373	-3.57272355	3.20724999
C	-4.30367799	-3.64887629	3.78116527
O	-3.91298109	-4.57934362	3.06751345
N	-3.98019228	-3.50712213	5.11398702
H	-4.35206313	-2.65745181	5.56568175
H	-2.07820120	-5.23394291	4.19034336
H	-1.78340598	-0.88717909	7.02833162
N	2.62170186	1.27714740	1.74378436
O	0.52035479	2.11409399	1.31331823
C	3.51789053	0.12552307	1.86791108
H	0.59532860	1.92884988	6.04779449
H	-0.18654427	-1.66095527	6.83534309
C	-2.95430300	-4.15233164	5.83864647
H	2.64320292	1.93079257	3.78173990
H	3.83462286	2.70891881	2.70312336
H	2.09784297	3.12548667	2.57176539
H	-6.10770237	-0.50863675	1.55454275
H	-5.77644436	-2.09372845	4.08268979
H	-1.44662895	-1.89641043	5.61271718
C	2.80873835	2.31784733	2.75893866
C	-0.96115617	-5.51403955	6.02366667
C	-2.00144239	-4.99785620	5.24543153
H	-3.59205345	-3.18751556	7.66319303
H	-1.74871431	-4.12275893	9.03109301
C	-2.85884897	-3.85403613	7.21035216
C	1.34114412	1.11682428	1.17566755
H	-0.03973411	-5.61360066	7.97967559
H	-0.22104228	-6.16146178	5.55311067
C	-1.81637016	-4.37504588	7.97308283
C	-0.48720986	0.07123515	5.53882151
C	0.55148049	-0.38879762	4.49218300
C	0.16562263	1.04721791	6.54333533
C	-1.00924868	-1.16485235	6.30054917
H	0.11771860	-1.11078493	3.79169456
H	0.94760422	0.44243837	3.89944503
H	1.39852603	-0.87519685	4.99796239
H	-0.57065999	1.39412141	7.28454022
H	0.97930417	0.53977408	7.08200362
H	3.10372666	-0.65508306	2.53141465
S	-4.62891898	-0.28745218	5.55309353
C	-3.66985912	-0.58546797	4.16234825

TS5_44

E = -21523.20

G = -20993.17
Nimag = 1, 143i cm-1

C	-2.58326841	-1.41719263	4.86871945
N	-2.76531194	-0.13304822	4.18809070
H	-2.32106709	-0.03715064	3.26117321
H	1.89155841	4.32616649	-0.48318750
H	3.34736781	4.57676734	0.49902351
N	-2.88451625	2.12377102	4.03092913
H	-2.41882270	1.90355491	3.13451683
C	-3.15613177	3.55767261	4.21060665
H	-2.71095273	3.97391769	3.29894898
H	-0.55579433	3.72701546	4.36144603
C	-2.34392480	4.17112432	5.36980608
N	-0.97010293	3.60598882	5.33654827
H	-2.80858550	3.95524802	6.33114968
P	0.13938711	4.02188570	6.47696088
C	1.66529916	3.19581899	5.98530206
C	2.90751945	3.82089385	6.16389346
C	1.58343470	1.90495915	5.43557807
C	4.07422185	3.13815175	5.81353394
H	2.96426703	4.83266337	6.56127024
C	2.75374915	1.24276671	5.07140261
H	0.61459752	1.43649536	5.28699216
C	3.99609411	1.85279554	5.26858529
H	5.04250586	3.61656770	5.95463615
H	2.69432694	0.24926091	4.63437342
H	4.90767984	1.32842789	4.98394875
C	-0.26228714	3.47316318	8.15701037
C	-1.53579459	3.02360375	8.53328428
C	0.77993665	3.50796917	9.10304556
C	-1.76578589	2.62539661	9.85278439
H	-2.32079600	2.89212167	7.79702299
C	0.53525573	3.12516263	10.42112796
H	1.78643379	3.79730090	8.80715866
C	-0.73946195	2.68907422	10.79983257
H	-2.74845849	2.24521260	10.13056199
H	1.34716834	3.14435679	11.14709785
H	-0.92501992	2.37982351	11.82785143
C	0.42597636	5.81922200	6.52831507
C	0.69354391	6.53402877	7.70642549
C	0.35929372	6.49180130	5.29144765
C	0.92369815	7.91107936	7.64269319
H	0.70827351	6.03025738	8.66900157
C	0.58991645	7.86692918	5.24022055
H	0.12154272	5.94401150	4.37880002
C	0.87890659	8.57541328	6.41260790
H	0.53881006	8.38667283	4.28429256
H	1.05866511	9.64903906	6.36846541
H	-2.32160265	5.26225136	5.23213185
H	1.13366051	8.46491169	8.55679131
C	-0.34919929	3.34217981	0.55378157
C	-1.73305225	2.97701683	0.47891158
H	-2.35408630	3.45054650	1.24450333
S	-1.95205461	0.93932593	1.09166657
C	-3.77235517	0.59600922	0.88681243
H	-4.14448794	0.02870163	1.74877761
H	-3.96191965	0.03447028	-0.03654718
H	-4.31071675	1.54937151	0.85177357
C	-2.36830245	2.99962972	-0.90544228
H	-3.41770552	2.67930072	-0.89347452
H	-1.81498620	2.34800211	-1.59620924
H	-2.33041349	4.02883971	-1.29826092
H	0.26060411	3.09967213	-0.31102720
C	3.03186810	-0.41328628	8.18537796
C	-3.25808963	-2.58850356	4.09653528
C	-4.77497621	-2.29190174	4.04609603
C	-2.72058173	-2.74659176	2.65623233
C	-3.02361523	-3.89089540	4.89447836
H	-5.18921713	-2.18170835	5.05920392
H	-5.30068584	-3.11683308	3.54368193
H	-1.63494099	-2.88992532	2.65610573
H	-3.19650513	-3.61837127	2.18260028
H	-2.95691125	-1.86954184	2.04070662
H	-3.55830978	-4.72310980	4.41458178
H	-1.95677234	-4.14567550	4.93551797
H	-3.40073208	-3.79240801	5.92399065
C	-1.07885376	-1.59370683	5.19248632
O	-0.27871672	-2.21178939	4.48231390
N	-0.74146543	-0.95131251	6.36656312
H	-1.49060164	-0.37510433	6.77769862
H	1.55883774	-2.25223844	5.71197884
H	-4.90229560	3.23139682	2.13545638
N	1.58321280	4.38315482	1.60807047
O	-0.40122158	4.18679560	2.78296934
C	2.39858066	4.02868141	0.44133144
H	-4.22754254	6.15869811	4.48271547
H	-6.43402962	3.52596817	2.99567905
C	0.53428754	-0.82118064	6.95824428
H	2.54758744	3.39594209	3.24639775
H	3.29678979	4.91937285	2.69499930
H	1.78718339	4.95886358	3.62555562
H	-4.97746363	-1.36520617	3.49353282
H	-3.11259781	-1.31702379	5.82433840
H	-5.44188159	2.09730243	3.40217611
C	2.34097439	4.40876294	2.86572349
C	2.89364383	-1.33778140	7.14723890
C	1.65832149	-1.55018328	6.53056575
H	-0.20488749	0.64120021	8.36828480
H	1.99288477	1.00524337	9.43895700
C	0.66503706	0.08608613	8.02610749
C	0.23771607	3.93487145	1.68709792
H	4.00346754	-0.23976500	8.64581719
H	3.76145386	-1.89479734	6.79378247
C	1.90552585	0.28869049	8.62686001
C	-4.66402606	4.00685400	4.17757028
C	-5.39984474	3.88546019	5.53426060
C	-4.68691399	5.49506852	3.72839021
C	-5.40400302	3.15950760	3.11425314
H	-5.41320413	2.84607904	5.89323296
H	-4.92741012	4.51148722	6.31326103
H	-6.43642424	4.23693844	5.40820875
H	-4.15092881	5.63407607	2.77099603
H	-5.72927025	5.81959968	3.58733865
H	2.62305710	2.94604824	0.38704489
S	-3.52673983	1.09466710	6.47833177
C	-3.04599958	1.04996710	4.82856519

TS5_45
E = -21531.13
G = -20999.44
Nimag = 1, 86i cm-1

C	-2.71828584	-2.47371670	0.49816742
N	-1.43752316	-1.77696057	0.58841850
H	-0.61551196	-2.18767571	0.10063152
H	3.63880158	-5.19512359	0.73337156
H	3.40677792	-4.61285644	2.40666423
N	0.18492498	-0.47727196	1.48890150
H	0.76283764	-1.04362260	0.83202401
C	0.81560646	0.53513663	2.31842072
H	0.00145998	1.17125190	2.68672680
H	2.06574035	0.83042597	-0.58498569
C	1.78990926	1.40547468	1.46237635
N	1.47401700	1.44969878	0.02546604
H	2.80652756	1.00206635	1.51628515
P	0.65454831	2.60202123	-0.79393221
C	-0.18287005	3.67624835	0.37887397
C	-1.22905671	3.14772647	1.15436973
C	0.23535898	5.00695402	0.55120288
C	-1.84576500	3.95061182	2.11207774
H	-1.56536167	2.12030364	1.02862097
C	-0.39518771	5.80276958	1.50992489
H	1.04200082	5.41419967	-0.05387748
C	-1.43080396	5.27550996	2.29032290
H	-2.64956938	3.53478859	2.71787326
H	-0.07349081	6.83360009	1.65007831
H	-1.91631174	5.90069653	3.03890641
C	-0.51542226	1.86096218	-1.95685866
C	-1.82573785	2.33990792	-2.09231283
C	-0.04437708	0.82220264	-2.78203269
C	-2.66822346	1.77163797	-3.05266643

H	-2.18785765	3.14589455	-1.45825745
C	-0.88548151	0.28150041	-3.75153125
H	0.96294792	0.43286986	-2.65329438
C	-2.19662718	0.75440008	-3.88345705
H	-3.69166116	2.13047914	-3.15203125
H	-0.52464567	-0.52271906	-4.39115811
H	-2.86109639	0.30525869	-4.62086778
C	1.80555496	3.58112317	-1.79367847
C	1.42189622	4.10415998	-3.03885740
C	3.10095304	3.80115678	-1.29699229
C	2.33469283	4.85893885	-3.77856234
H	0.42175176	3.92148836	-3.42729770
C	4.00330732	4.56466227	-2.03856582
H	3.39964573	3.37100141	-0.34279886
C	3.62175829	5.08923707	-3.27888367
H	5.00885600	4.73653474	-1.65672812
H	4.33495900	5.66715549	-3.86580976
H	1.81875603	2.41981908	1.87630503
H	2.04299805	5.26420112	-4.74657417
C	3.25441429	-2.79604151	-1.05958021
C	3.21877678	-1.97410162	-2.24004914
H	2.20093549	-1.76364051	-2.58445347
S	3.74563160	0.00913340	-1.74329253
C	3.61999787	0.89889517	-3.37266247
H	2.78458190	0.48784841	-3.95598956
H	3.43315742	1.96150316	-3.19254229
H	4.54938034	0.78596524	-3.94419867
C	4.16935782	-2.36467638	-3.36288242
H	4.16794720	-1.63940844	-4.18640460
H	5.19774991	-2.46080132	-2.98612577
H	3.86177856	-3.34165493	-3.77093386
H	4.18431197	-3.30726056	-0.82801748
C	-1.04271109	-5.04777272	6.28387531
C	-3.05712632	-2.83739654	-0.97500956
C	-3.08676963	-1.52451082	-1.77731426
C	-1.99449768	-3.77105007	-1.60664148
C	-4.44985625	-3.50131526	-1.01496035
H	-3.87479738	-0.83908233	-1.42936280
H	-3.26465175	-1.73540490	-2.84128073
H	-1.92074805	-4.71260363	-1.05251670
H	-2.27974255	-3.98944706	-2.64695948
H	-1.00321364	-3.29545881	-1.62458244
H	-4.74794288	-3.68008455	-2.05859668
H	-4.44627566	-4.46176640	-0.48523749
H	-5.20616714	-2.84807516	-0.55280230
C	-2.65499514	-3.66968635	1.49981228
O	-2.60699657	-4.86113305	1.17521959
N	-2.56214547	-3.21710426	2.79769297
H	-2.66211411	-2.19347353	2.91307260
H	-1.66477748	-5.79191014	3.00450871
H	-0.36756975	-0.32328281	4.64903092
N	2.24185262	-3.58973575	1.00962443
O	1.04620405	-2.23377769	-0.44434224
C	3.47101160	-4.29701288	1.35746567
H	2.80415219	1.68762645	3.97141276
H	0.98138384	-1.30335714	5.29235597
C	-2.08943873	-3.89485510	3.93873342
H	1.09638918	-4.02461606	2.73245221
H	0.89851833	-5.20193779	1.40423872
H	0.16232211	-3.58785052	1.28979419
H	-2.13066311	-0.99816144	-1.69545749
H	-3.48731473	-1.77656397	0.86174888
H	0.16665261	-1.77611568	3.78840996
C	1.03625323	-4.13055666	1.63966776
C	-1.10130328	-5.78152877	5.09458911
C	-1.62281803	-5.22169573	3.92464920
H	-2.38830596	-2.12681138	5.14364268
H	-1.47592919	-3.14036671	7.21166392
C	-2.04014633	-3.15841730	5.13836251
C	2.14959511	-2.86798583	-0.19596536
H	-0.63379478	-5.49494275	7.18925422
H	-0.73408798	-6.80774087	5.07011185
C	-1.51798112	-3.73000812	6.29614292
C	1.53319054	-0.07424864	3.57978780
C	2.71715004	-0.98694160	3.19073689
C	2.02633267	1.09092493	4.46852441
C	0.51329589	-0.91741057	4.37482925
H	2.40319495	-1.78546795	2.50685283
H	3.53876971	-0.43411963	2.71457827
H	3.12618620	-1.45812953	4.09713946
H	1.19406341	1.76057053	4.73493460
H	2.45650806	0.69519260	5.40044457
H	4.33595808	-3.63076015	1.25445045
S	-2.34055913	0.04208968	2.39199109
C	-1.13342266	-0.77462058	1.45144083

TS5_46

E = -21526.55

G = -20994.00

Nimag = 1, 159i cm-1

C	-2.66369463	-0.64569974	2.11394690
N	-1.24578575	-0.30127554	2.04868803
H	-0.72663597	-0.46059265	1.16669191
H	3.15441994	-3.55201810	-0.69641849
H	2.70344807	-4.10479233	0.94144051
N	0.44527208	1.16416567	2.38393494
H	0.67013083	0.82700836	1.42360331
C	1.46803891	2.03698552	2.97073668
H	2.22378912	2.07852029	2.17302741
H	3.58150113	0.56004645	2.76162313
C	2.17892417	1.34469193	4.14586738
N	2.99024276	0.24564685	3.56250735
H	1.44330858	0.93058643	4.84450520
P	3.41902692	-1.08647415	4.41574204
C	4.23462513	-0.70998345	5.99562394
C	3.52589177	0.00635284	6.97903767
C	5.56767112	-1.08797616	6.22488211
C	4.15278017	0.34198898	8.17926194
H	2.48652885	0.28501475	6.81918746
C	6.18644357	-0.74917956	7.43144299
H	6.11650131	-1.64863722	5.47194562
C	5.48239080	-0.03451146	8.40547640
H	3.60201439	0.89329308	8.94011728
H	7.21859734	-1.04770168	7.60981463
H	5.96784922	0.22683560	9.34498038
C	4.55914398	-2.05927958	3.40489185
C	5.56012965	-1.43544034	2.64249731
C	4.46446573	-3.46115532	3.43974524
C	6.44750209	-2.21642376	1.90057178
H	5.64598688	-0.35280862	2.60826131
C	5.36814874	-4.23193829	2.70766743
H	3.68274045	-3.94610155	4.01944765
C	6.35522221	-3.61163716	1.93472587
H	7.20962991	-1.72979072	1.29343051
H	5.29054296	-5.31809405	2.72965417
H	7.05095100	-4.21653985	1.35407635
C	1.98648688	-2.11410396	4.76834883
C	1.08204244	-2.36022442	3.71853681
C	1.89629772	-2.82444107	5.97803163
C	0.10813228	-3.34361540	3.87964434
H	1.16915923	-1.81532705	2.78202730
C	0.91037245	-3.80078826	6.12582392
H	2.60167324	-2.63381945	6.78366677
C	0.03277662	-4.07120672	5.07270530
H	0.83147500	-4.35568943	7.05952813
H	-0.72013744	-4.84675978	5.18624193
H	2.82846365	2.04770061	4.68178080
H	-0.59662090	-3.54526259	3.07778690
C	3.00561572	-0.54049657	-0.59944232
C	3.27239038	0.85565052	-0.76031755
H	2.39532085	1.48382571	-0.57513039
S	4.51781379	1.45355333	0.91416383
C	4.80371833	3.28002853	0.73525549
H	3.85971655	3.83552030	0.79411197
H	5.46742289	3.61283014	1.54478309
H	5.28794488	3.48654195	-0.22743920
C	4.09286320	1.29955391	-1.95944188
H	4.36907863	2.36066280	-1.91128673
H	5.01039677	0.70095692	-2.04798496
H	3.49486071	1.14788661	-2.87404688

H	3.81201240	-1.23294038	-0.82562344
C	-3.09278956	-5.17378479	6.88133125
C	-3.38827200	-0.36347083	0.76056245
C	-3.26421299	1.15437296	0.48404532
C	-2.78217018	-1.14442630	-0.42672785
C	-4.88051021	-0.72851181	0.92813644
H	-3.68786484	1.74167913	1.31252925
H	-3.80860385	1.41210610	-0.43604404
H	-2.83642428	-2.22429439	-0.25136989
H	-3.34261431	-0.90253403	-1.34266326
H	-1.73369209	-0.86556077	-0.60070767
H	-5.43773158	-0.44523235	0.02341599
H	-5.00991063	-1.80632428	1.08892070
H	-5.32189105	-0.19130107	1.78166312
C	-2.85155096	-2.07581169	2.68455437
O	-2.95695783	-3.09898745	1.99607814
N	-2.85606609	-2.05155124	4.05876409
H	-2.50404658	-1.15925812	4.46079542
H	-3.58255885	-4.62601033	3.54055833
H	2.64736238	4.18017612	4.56747540
N	1.71791848	-2.35658749	0.36639538
O	0.73326637	-0.28367447	0.07774829
C	2.89845844	-3.21663231	0.32753519
H	-0.96539165	3.40283319	3.96854700
H	2.17170899	5.41168955	3.38066741
C	-2.97048346	-3.12196201	4.96058118
H	0.42759677	-3.89395761	0.97926976
H	0.30105148	-3.49865222	-0.75828672
H	-0.38475315	-2.40207959	0.46666909
H	-2.21453374	1.45028756	0.35609589
H	-3.10959863	0.03941563	2.84804626
H	3.19993536	4.04813212	2.87930367
C	0.44517572	-3.07174182	0.25351875
C	-3.41239926	-5.43171537	5.54392101
C	-3.35666852	-4.41993396	4.58043204
H	-2.34965079	-1.85513112	6.59646866
H	-2.46756902	-3.65770118	8.29428784
C	-2.66411847	-2.85771160	6.30931947
C	1.79776747	-1.01599511	-0.05289434
H	-3.13102342	-5.97237782	7.62144798
H	-3.70364847	-6.43691708	5.23841581
C	-2.72342448	-3.87582030	7.25760252
C	1.06935096	3.54304792	3.16032079
C	0.53816240	4.04301444	1.79546407
C	0.01159902	3.81178746	4.24813440
C	2.35355764	4.33536553	3.51855586
H	1.30176309	3.93213579	1.00952128
H	-0.35010329	3.47275121	1.49026523
H	0.26496012	5.10599200	1.86207772
H	0.29719344	3.35870324	5.20736689
H	-0.08544691	4.89950683	4.39316972
H	3.75655656	-2.68813455	0.74933133
S	-1.18207016	0.72047875	4.55166011
C	-0.62780446	0.54524365	2.92863562

TS5_47

E = -21536.10

G = -21004.77

Nimag = 1, 24i cm-1

C	-2.39255599	-2.27129655	0.30518664
N	-1.18074934	-1.48371489	0.53005619
H	-0.27389210	-1.93948804	0.30870827
H	3.55111367	-5.06287929	1.95058460
H	2.98799300	-4.52739667	3.56117213
N	0.20054328	-0.05394736	1.62368688
H	0.91209447	-0.68461399	1.20230546
C	0.63592449	1.06677322	2.43539291
H	-0.25334575	1.69392209	2.57881732
H	2.64514596	0.82357539	0.04790345
C	1.72709939	1.90777363	1.67324851
N	1.89364548	1.54198608	0.26122566
H	2.71028144	1.77020627	2.13449659
P	1.14765455	2.26928390	-0.99025330
C	1.90525253	3.86754465	-1.39582290
C	3.23194540	4.09910583	-0.99899208
C	1.20627798	4.83531101	-2.13713778
C	3.86256784	5.29251929	-1.35697436
H	3.75780169	3.35309868	-0.40603394
C	1.84651419	6.02247342	-2.49725035
H	0.17098622	4.66344472	-2.42643848
C	3.17300983	6.24916270	-2.11030428
H	4.89016952	5.47619685	-1.04632099
H	1.30950463	6.77308402	-3.07541183
H	3.66770652	7.17846003	-2.39028366
C	-0.59552628	2.62121801	-0.66327995
C	-0.94268370	3.65289876	0.22725763
C	-1.59491935	1.88354765	-1.31441890
C	-2.28718107	3.93209834	0.46670638
H	-0.17186154	4.24743398	0.71375952
C	-2.93679508	2.17442769	-1.07086031
H	-1.32722306	1.09536835	-2.00939139
C	-3.28313400	3.19697825	-0.18509677
H	-2.55761057	4.72707865	1.16038070
H	-3.71192520	1.59755825	-1.57144971
H	-4.33261351	3.41802241	0.00592234
C	1.30573366	1.15900548	-2.40274239
C	1.16545438	-0.22417547	-2.20114189
C	1.51636966	1.67753570	-3.69054377
C	1.22957250	-1.08243668	-3.29914275
H	1.05992833	-0.64400967	-1.20483436
C	1.58041424	0.80637577	-4.77906690
H	1.64803754	2.74617913	-3.84324063
C	1.43140092	-0.57213382	-4.58499918
H	1.75391475	1.20372011	-5.77824439
H	1.48433910	-1.24854708	-5.43763200
H	1.48942720	2.97421057	1.76478208
H	1.12798576	-2.15456979	-3.14207283
C	3.74032496	-2.67595183	0.17653571
C	3.95502324	-1.95011805	-1.05555560
H	3.02430776	-1.77874217	-1.59915925
S	4.41986538	0.01984231	-0.63682388
C	4.47034373	0.82501060	-2.31261694
H	3.86329888	0.23573023	-3.01146601
H	4.04522724	1.83259429	-2.25206038
H	5.50306866	0.88942550	-2.67642167
C	5.07450817	-2.45649582	-1.95664885
H	5.25983862	-1.78968242	-2.80889651
H	6.01163593	-2.56559423	-1.39164756
H	4.79563070	-3.44657124	-2.35299914
H	4.59671366	-3.14621610	0.65096928
C	-1.84956089	-4.31316728	6.52026521
C	-2.46112709	-2.79199264	-1.16122603
C	-2.46676175	-1.56186734	-2.09626171
C	-1.25318758	-3.68927402	-1.52150359
C	-3.78364858	-3.56783175	-1.35297051
H	-3.30013645	-0.88698542	-1.85401914
H	-2.57221207	-1.88535270	-3.14190606
H	-1.24640349	-4.59675834	-0.90811652
H	-1.31436706	-3.97446369	-2.58256407
H	-0.30019859	-3.16540073	-1.36841232
H	-3.89632449	-3.85423741	-2.40886614
H	-3.80293140	-4.47603736	-0.73985857
H	-4.64540227	-2.93976848	-1.07825184
C	-2.46327486	-3.36811871	1.41300234
O	-2.34097053	-4.58208361	1.21578184
N	-2.61358001	-2.79924023	2.65752576
H	-2.74233315	-1.77097482	2.65970285
H	-1.95741229	-5.38065646	3.27211985
H	-0.87638627	0.49936527	4.71219711
N	2.25702782	-3.35154434	1.99383920
O	1.45308400	-2.07452131	0.25596283
C	3.31157696	-4.18063040	2.57341831
H	2.38420884	2.39595879	4.26325218
H	0.35196997	-0.48053232	5.56450578
C	-2.39096166	-3.37105727	3.92405170
H	0.87328870	-4.08929468	3.38333493
H	0.39676285	-4.38961510	1.68903371
H	0.26377614	-2.76256636	2.38856600
H	-1.53146473	-1.00195338	-2.00520923
H	-3.24209193	-1.59044452	0.46219403

H	-0.30458298	-1.02380622	4.01016028
C	0.87501325	-3.66766718	2.37269883
C	-1.76177669	-5.17086900	5.41866027
C	-2.03181170	-4.71613086	4.12455376
H	-2.75691938	-1.46554395	4.87367012
H	-2.29210119	-2.29322648	7.16269119
C	-2.49182369	-2.50919467	5.03403335
C	2.47454189	-2.68903524	0.78020604
H	-1.63423762	-4.67908129	7.52360670
H	-1.47640237	-6.21322562	5.56248188
C	-2.22059378	-2.97732483	6.31738435
C	1.13959842	0.61562396	3.85279616
C	2.36524245	-0.32077597	3.74838018
C	1.50065846	1.88084992	4.66594501
C	0.00601209	-0.13997657	4.57722572
H	2.10403872	-1.28440209	3.29540096
H	3.18119107	0.11375378	3.15415680
H	2.76289501	-0.51812145	4.75527325
H	0.66068750	2.59262702	4.67542051
H	1.72397955	1.60477455	5.70694277
H	4.22903757	-3.59155696	2.70388164
S	-2.45320591	0.40878331	2.00749934
C	-1.08102294	-0.40277551	1.35819631

TS5_48

E = -21526.59

G = -20994.73

Nimag = 1, 27i cm-1

C	-2.21625667	-1.70740411	2.01611466
N	-1.00605796	-0.97826534	1.62693217
H	-0.30805875	-1.46407463	1.02549745
H	3.44365308	-4.73114869	-1.06573665
H	2.23302928	-5.66230696	-0.14124168
N	0.28203236	0.83748289	1.13181145
H	0.76282029	0.10991016	0.55944250
C	1.19213224	1.93881010	1.51662639
H	2.15602402	1.57623660	1.13606460
H	2.35174348	0.18657506	2.90928535
C	1.36393301	2.04667295	3.04875672
N	1.63658392	0.67990458	3.53968366
H	0.44430749	2.41787444	3.50016188
P	1.96096869	0.14734698	5.06271017
C	0.89377539	0.90901754	6.30583865
C	-0.26721577	1.60546996	5.94064278
C	1.28841084	0.85178664	7.65528608
C	-0.99327823	2.29411956	6.91381774
H	-0.62017051	1.59789027	4.91271205
C	0.53287127	1.51035387	8.62386445
H	2.19162667	0.31981480	7.94600594
C	-0.59461490	2.25107388	8.25140321
H	-1.88594014	2.84723829	6.62350425
H	0.83355066	1.45670161	9.66915897
H	-1.16910553	2.78293936	9.00913693
C	3.66018063	0.54653392	5.58431547
C	3.93511050	1.86559694	5.99405012
C	4.71272840	-0.36576593	5.40516385
C	5.25290257	2.26245244	6.22340580
H	3.12418792	2.57847205	6.13366536
C	6.02858438	0.04029934	5.63890428
H	4.51150700	-1.37784336	5.06642204
C	6.30005073	1.35038574	6.04436413
H	5.46266585	3.28383992	6.53825393
H	6.84316659	-0.66790936	5.49345995
H	7.32868844	1.66343454	6.22004058
C	1.84989407	-1.65579296	4.90765559
C	1.43182743	-2.22173428	3.69187292
C	2.26568711	-2.48035249	5.96574668
C	1.45120167	-3.60648872	3.52849080
H	1.08860534	-1.59124475	2.88200925
C	2.28782243	-3.86380525	5.79188270
H	2.57546363	-2.05075022	6.91653190
C	1.88725092	-4.42658778	4.57342877
H	2.61071892	-4.50479582	6.61105751
H	1.90674609	-5.50862407	4.44499982
H	2.18217694	2.74437231	3.27745986
H	1.12506934	-4.03109844	2.58041241
C	3.43969759	-1.93315575	-0.25622612
C	3.94403984	-0.59876427	-0.01919627
H	3.23371467	0.20300877	-0.25213701
S	4.12469453	-0.35821120	2.04661207
C	4.84961192	1.33388528	2.28524757
H	5.94237538	1.29991332	2.20454573
H	4.44621857	2.02407621	1.53463217
H	4.57660209	1.69410089	3.28365590
C	5.33643416	-0.31451917	-0.56954374
H	5.70083976	0.68104014	-0.28597611
H	6.05396487	-1.06508679	-0.21020295
H	5.30680871	-0.36483768	-1.67047876
H	4.18635139	-2.70789414	-0.40901330
C	-1.12240957	-2.06620171	8.51663932
C	-2.71575462	-2.64871061	0.87978223
C	-4.12597815	-3.15599888	1.25927101
C	-2.81932897	-1.80709484	-0.41582357
C	-1.76872853	-3.84458509	0.63836235
H	-4.09793291	-3.74602878	2.18384490
H	-4.52064832	-3.79295512	0.45397914
H	-1.83091194	-1.47839961	-0.76135967
H	-3.27838348	-2.41226618	-1.21087732
H	-3.44259128	-0.91372442	-0.25674053
H	-2.07499327	-4.37089604	-0.27746326
H	-0.73175728	-3.51888858	0.50319089
H	-1.79882139	-4.54050653	1.48151094
C	-1.99503547	-2.39564498	3.39968702
O	-1.97767704	-3.61599760	3.58679818
N	-1.84310222	-1.47053287	4.40319951
H	-1.97643254	-0.48058572	4.12532662
H	-0.56781048	-3.58707464	5.51178919
H	2.73891036	4.23122815	1.70415277
N	1.71089710	-3.65230032	-0.36521134
O	1.10766277	-1.44257316	-0.10532766
C	2.73434776	-4.68657175	-0.21409316
H	-1.01926491	3.68478743	1.66243115
H	2.18355765	5.02013451	0.21429682
C	-1.63469911	-1.73533038	5.77436223
H	0.27683380	-4.84994188	-1.36056548
H	1.40934301	-3.99292153	-2.45474442
H	0.10959814	-3.09327655	-1.60656357
H	-4.82101575	-2.31381354	1.39904075
H	-2.99383677	-0.94503283	2.17796973
H	3.03885419	3.46287610	0.12441392
C	0.82685957	-3.91229363	-1.51390352
C	-0.68005749	-3.01687766	7.59147574
C	-0.93069513	-2.86078582	6.22684036
H	-2.67441949	0.06266978	6.35266913
H	-2.19483584	-0.20529544	8.77009527
C	-2.10823240	-0.79614130	6.70554055
C	2.09150105	-2.27848913	-0.22239219
H	-0.90840579	-2.18770856	9.57795591
H	-0.11284770	-3.88387210	7.92907657
C	-1.84283273	-0.95507485	8.06406594
C	0.95184565	3.31159752	0.79175116
C	0.45255155	3.02901925	-0.64111006
C	-0.06803039	4.21115440	1.52096954
C	2.31161137	4.04610388	0.70857008
H	1.13848752	2.35260885	-1.17329062
H	-0.53927617	2.55972415	-0.62366060
H	0.39055553	3.97069514	-1.20585625
H	0.30114455	4.52356016	2.50865112
H	-0.24434670	5.12123941	0.92796130
H	3.30118175	-4.51463181	0.70835088
S	-1.88312595	1.33060410	2.73001918
C	-0.80321893	0.35548879	1.79188379

TS5_49

E = -21531.50

G = -20999.76

Nimag = 1, 66i cm-1

C	-2.76639819	-2.14528359	0.46047490
N	-1.67901778	-1.15410475	0.52263924
H	-1.00071593	-1.23272799	-0.24648903

H	2.72377558	1.07945893	-5.37469123
H	1.95803570	2.62389767	-5.80688328
N	0.15930366	-0.36692444	1.64537909
H	0.60473347	-0.52718521	0.72770445
C	0.86146251	0.53333300	2.55790474
H	0.08690977	0.99072649	3.18732237
H	1.66821908	1.90321902	-0.41709218
C	1.58993492	1.64068122	1.72894082
N	0.96335872	1.92840643	0.42631331
H	2.60572272	1.31408598	1.48313954
P	-0.22420934	3.02886138	0.22638430
C	0.37219684	4.74922522	0.25343343
C	1.71421809	4.99410577	-0.08308931
C	-0.48786832	5.81721631	0.56153183
C	2.18643363	6.30795588	-0.12117296
H	2.37259184	4.16281306	-0.32912011
C	-0.00767092	7.12773524	0.51540245
H	-1.52081111	5.62749033	0.84728331
C	1.32742972	7.37285362	0.17245144
H	3.22643891	6.50003013	-0.38258540
H	-0.67347208	7.95666351	0.75183366
H	1.69958059	8.39632421	0.13952041
C	-1.49026736	2.94698406	1.51136578
C	-1.19135607	3.42519348	2.80066970
C	-2.76165485	2.43226166	1.22534652
C	-2.16434372	3.37535738	3.79667447
H	-0.21238288	3.84704499	3.02009148
C	-3.73468082	2.40413165	2.22549836
H	-2.98745815	2.06059264	0.22965192
C	-3.43817256	2.87318160	3.50635252
H	-1.93223990	3.73728054	4.79739100
H	-4.72241300	2.00486904	2.00544239
H	-4.19950190	2.84311407	4.28510292
C	-0.95329441	2.68595433	-1.39128611
C	-0.69815743	1.45721137	-2.01765752
C	-1.77125965	3.64516716	-2.01247738
C	-1.25554953	1.19344882	-3.26842731
H	-0.05803683	0.72105839	-1.54461581
C	-2.34315795	3.36069607	-3.25276485
H	-1.95216750	4.60934893	-1.54123898
C	-2.08230095	2.13654931	-3.88249888
H	-2.98003464	4.10067631	-3.73586485
H	-2.52218127	1.92406762	-4.85657041
H	1.69210519	2.54128444	2.34910643
H	-1.04326138	0.24270896	-3.75402715
C	2.56206625	0.11704029	-2.87107328
C	2.90169118	-0.84232988	-1.83246286
H	3.24317986	-0.36369181	-0.90764980
S	1.13762382	-1.73416741	-1.26343515
C	1.55844186	-3.15734334	-0.14326636
H	1.78606836	-4.05603908	-0.72754064
H	2.41572268	-2.89526870	0.48578382
H	0.69368627	-3.35414984	0.50143748
C	3.81421122	-1.98878723	-2.26239557
H	3.88071740	-2.78532361	-1.50930726
H	3.45893427	-2.42872473	-3.20506692
H	4.82863571	-1.59076903	-2.42842337
H	2.34064053	-0.29740141	-3.85018690
C	0.01245682	-8.10192026	1.19180616
C	-3.97860165	-1.70188361	-0.41795881
C	-4.74888346	-0.62392310	0.37226670
C	-3.51310311	-1.11118559	-1.76442575
C	-4.89256574	-2.92437353	-0.65194808
H	-5.23535570	-1.05546909	1.25918654
H	-5.51913357	-0.16180823	-0.26282390
H	-2.88880004	-1.82452686	-2.31605871
H	-4.38816245	-0.85247742	-2.37904811
H	-2.93262382	-0.19557515	-1.60482658
H	-5.81964996	-2.60750443	-1.15112313
H	-4.40272004	-3.67656038	-1.28518340
H	-5.16782801	-3.39867437	0.30285756
C	-2.10726558	-3.45989618	0.00287791
O	-1.69333624	-3.63639200	-1.14801699
N	-1.94925077	-4.36459026	1.03055664
H	-2.33104429	-4.08000884	1.93317408
H	-0.56945277	-5.53583046	-1.00950657
H	0.29389199	-0.80115344	4.91478958
N	2.26258068	2.35909871	-3.75678698
O	2.67523915	2.07197639	-1.49994848
C	1.95784006	1.80536468	-5.07524181
H	3.10613375	1.56694225	3.94339966
H	1.80079148	-1.76055404	5.03219944
C	-1.29141527	-5.61605641	1.02683223
H	0.55992890	3.64413513	-3.62117668
H	2.05861718	4.40410797	-4.22910538
H	1.90021076	3.99530358	-2.50103762
H	-4.06004260	0.15090044	0.71935917
H	-3.12293592	-2.24846620	1.49268323
H	0.65532584	-2.02499074	3.68812579
C	1.65697904	3.67228925	-3.51223007
C	0.04648310	-7.35395697	0.00424915
C	-0.59792671	-6.11633254	-0.09121924
H	-1.86816463	-5.97826285	3.09060382
H	-0.71849116	-8.16749735	3.23652136
C	-1.32907663	-6.36617158	2.22347852
C	2.48395523	1.49308200	-2.65821873
H	0.51864670	-9.06507860	1.25353771
H	0.58463965	-7.73319098	-0.86658690
C	-0.68075963	-7.59869846	2.30271805
C	1.86665525	-0.20990973	3.50937111
C	2.97606366	-0.92826889	2.70999942
C	2.49251999	0.82527722	4.47251139
C	1.10474820	-1.26401561	4.33945180
H	2.53669802	-1.58306445	1.95009972
H	3.66317317	-0.23135884	2.21181820
H	3.57556690	-1.55422630	3.38706487
H	1.70977149	1.35872508	5.03344399
H	3.14156536	0.31413251	5.19875656
H	0.96955429	1.31050843	-5.10801010
S	-2.10141618	-0.56476626	3.12782207
C	-1.15474631	-0.70560478	1.72103076

TS5_50

E = -21527.43

G = -20995.37

Nimag = 1, 145i cm-1

C	-1.80728971	-1.71823308	1.41972721
N	-0.98198890	-0.59312043	1.00936092
H	-0.29257795	-0.77723170	0.26656979
H	5.86348082	3.14242694	-0.31438763
H	5.08433593	4.16215200	0.92776609
N	0.24769481	1.30123824	1.29657627
H	0.68954122	0.89117089	0.45278648
C	1.19726132	2.13795320	2.06545665
H	2.10407182	2.09708255	1.44863123
H	2.66064429	0.04220252	2.29807818
C	1.59439703	1.48768216	3.40938886
N	1.97499300	0.07613870	3.12561227
H	0.76268247	1.49626347	4.12082604
P	2.54860938	-0.91517565	4.31030672
C	1.40184569	-0.98968071	5.70226195
C	0.02838257	-1.04600004	5.42076126
C	1.85970476	-1.08604155	7.02727592
C	-0.88637419	-1.17786190	6.46389398
H	-0.32233374	-0.94275895	4.39905651
C	0.93619763	-1.24175923	8.06375305
H	2.92398670	-1.04914420	7.24836299
C	-0.43469809	-1.28619975	7.78380537
H	-1.95381228	-1.19348254	6.24504892
H	1.28812372	-1.32231028	9.09120486
H	-1.15095465	-1.40047388	8.59670064
C	4.16182824	-0.38231047	4.95133865
C	4.23748090	0.82393059	5.67420384
C	5.33786347	-1.05365498	4.57970611
C	5.48246534	1.35140145	6.01593130
H	3.33011813	1.34779126	5.96923803
C	6.58011929	-0.51839422	4.92818816
H	5.28213002	-1.97727074	4.00798030
C	6.65347696	0.68343810	5.63953293
H	5.53937105	2.28640061	6.57182468

H	7.49194615	-1.03759542	4.63579500
H	7.62476812	1.10139748	5.90189852
C	2.73645609	-2.56755849	3.61236945
C	2.80169061	-2.77884895	2.22713332
C	2.90010141	-3.63981128	4.50931028
C	3.05789376	-4.06497561	1.74854417
H	2.67601671	-1.95595819	1.53127266
C	3.17598795	-4.91232095	4.01659615
H	2.81417370	-3.48057699	5.58255670
C	3.25956610	-5.12319813	2.63632660
H	3.29541003	-5.74413990	4.70685287
H	3.45591711	-6.12393869	2.25346416
H	2.43949383	2.05262555	3.82291844
H	3.09147666	-4.23725917	0.67397669
C	3.93188611	0.90903675	-0.94591097
C	3.36341157	-0.23399518	-1.56959629
H	3.38485009	-1.13652590	-0.95537055
S	1.11352626	-0.15927580	-1.57700853
C	0.96293473	1.60259158	-2.10047303
H	1.80212320	2.16400109	-1.66107758
H	0.98707915	1.69669596	-3.19408040
H	0.02278092	2.01738884	-1.71771793
C	3.67355366	-0.46218337	-3.03926131
H	3.07983257	-1.28387168	-3.45817056
H	3.47457040	0.44449586	-3.62910783
H	4.74362502	-0.70593563	-3.15500660
H	4.19051578	1.76027243	-1.56844614
C	0.52237709	-6.87665859	4.81803239
C	-2.92818360	-2.06868806	0.38570051
C	-3.87378826	-0.85000920	0.30637919
C	-2.34903264	-2.36195014	-1.01408578
C	-3.70305784	-3.29777051	0.90730321
H	-4.30789093	-0.62358561	1.29071780
H	-4.69174425	-1.05537016	-0.39947692
H	-1.67860202	-3.22935351	-0.99311258
H	-3.17226114	-2.56529636	-1.71533347
H	-1.78050107	-1.50222947	-1.39549882
H	-4.54450421	-3.52398736	0.23679167
H	-3.06032681	-4.18858127	0.95519041
H	-4.10910777	-3.11183240	1.91339429
C	-0.87175783	-2.90625959	1.72112401
O	-0.08995466	-3.36921611	0.88769738
N	-1.00105410	-3.38305046	3.00791588
H	-1.60535582	-2.84489746	3.62604099
H	-0.04072726	-5.55915195	1.71626799
H	2.19515663	4.22827797	3.79660886
N	4.55854403	2.14400613	1.06558796
O	3.84548875	-0.04419378	1.22212999
C	4.93216239	3.30551063	0.25927690
H	-1.28355861	3.53525651	2.54177206
H	1.96226152	5.49404418	2.57528083
C	-0.42385714	-4.54284769	3.57838377
H	4.96221976	2.88142961	3.00631146
H	6.34799188	2.06809312	2.22437833
H	4.97403096	1.10467389	2.83061722
H	-3.32891375	0.03942063	-0.03836089
H	-2.30424040	-1.39659287	2.34309938
H	3.00937808	4.09994176	2.21653670
C	5.25019909	2.04477127	2.35512889
C	0.45353574	-6.79022162	3.42420853
C	-0.00900198	-5.63190965	2.79753537
H	-0.62911122	-3.76128961	5.58314506
H	0.19597622	-5.82099213	6.67887847
C	-0.33654711	-4.61667447	4.97847795
C	4.11034162	0.95865322	0.45425302
H	0.88949656	-7.78403375	5.29628336
H	0.77268186	-7.63216218	2.81013008
C	0.13130531	-5.77865753	5.59184122
C	0.85993494	3.66588228	2.13077622
C	0.64303260	4.15166643	0.67991134
C	-0.38752816	3.99921679	2.96838748
C	2.08437641	4.41034893	2.71869463
H	1.54036972	3.97675014	0.06879412
H	-0.19531998	3.61892557	0.21356722
H	0.42349653	5.22942591	0.67116841
H	-0.28937282	3.63794049	4.00071506
H	-0.52521207	5.09169340	2.99583189
H	4.12779934	3.55999108	-0.44075789
S	-1.67875528	0.84792818	3.18390692
C	-0.74845297	0.50674786	1.78618432

TS5_51

E = -21531.62

G = -21000.76

Nimag = 1, 147i cm-1

C	-2.38561288	-2.35708952	0.73128217
N	-1.34749694	-1.31060009	0.73164929
H	-0.54792238	-1.51579628	0.11089173
H	3.44203689	0.71452271	-4.82240464
H	2.56419050	2.15685250	-5.37409696
N	0.23307786	-0.05947380	1.79372785
H	0.78707007	-0.33030079	0.96481112
C	0.82738167	0.86354511	2.74788985
H	0.02374655	1.10873494	3.45263924
H	1.85165182	2.01578640	-0.07553775
C	1.27789036	2.19036878	2.02753485
N	1.00073850	2.19687593	0.58122800
H	2.35541988	2.34209921	2.14160076
P	-0.24661808	3.02310933	-0.06389892
C	0.07555722	4.80425657	-0.23464195
C	1.40940531	5.24222617	-0.22435378
C	-0.97189051	5.72733755	-0.39698538
C	1.69397455	6.59868641	-0.39494674
H	2.21361330	4.52285003	-0.08470665
C	-0.67869348	7.08103643	-0.57202486
H	-2.00789389	5.39416606	-0.37359301
C	0.65235971	7.51555154	-0.57422057
H	2.72841886	6.93972184	-0.38646815
H	-1.48860052	7.79792269	-0.69960566
H	0.87701154	8.57310399	-0.70841605
C	-1.74585579	2.89305280	0.94198553
C	-1.88423799	3.67093000	2.10573079
C	-2.77439485	2.02468472	0.54866380
C	-3.04527199	3.56601283	2.87122100
H	-1.10336724	4.36897907	2.40089285
C	-3.93542541	1.93447179	1.31532079
H	-2.66862347	1.42599481	-0.34829507
C	-4.07276472	2.70368216	2.47299836
H	-3.15126662	4.16527940	3.77464255
H	-4.72978468	1.25655133	1.01080043
H	-4.97956134	2.62746135	3.07203124
C	-0.58242862	2.30821655	-1.68900839
C	-0.22121847	0.97647331	-1.94119186
C	-1.28570983	3.04819409	-2.65513236
C	-0.56966056	0.38454267	-3.15474516
H	0.34181792	0.41153055	-1.20793615
C	-1.64218550	2.44165755	-3.85983819
H	-1.54564889	4.08909315	-2.47617277
C	-1.28885222	1.10955330	-4.10771761
H	-2.18802872	3.01241926	-4.61002001
H	-1.56570197	0.64220036	-5.05230354
H	0.79212372	3.03751899	2.52476092
H	-0.27043307	-0.64273671	-3.35055836
C	3.16991901	-0.12021689	-2.24671914
C	3.46323735	-0.95006323	-1.11725337
H	3.66392737	-0.38149348	-0.20674812
S	1.63418648	-1.92296526	-0.58362507
C	1.90093390	-3.22227875	0.72332339
H	2.65889011	-3.93940393	0.38509207
H	2.20695950	-2.78083202	1.67730043
H	0.95188649	-3.75329868	0.85891374
C	4.41853692	-2.11502192	-1.32150079
H	4.51766744	-2.73326533	-0.41914206
H	4.08527030	-2.75608891	-2.14972516
H	5.41550949	-1.71745092	-1.57432561
H	3.08092215	-0.60948292	-3.21241608
C	0.94207629	-5.67749729	5.32133577
C	-3.05202243	-2.51088967	-0.66603460
C	-3.68175046	-1.15230417	-1.04805458
C	-2.04752529	-2.91246585	-1.77020909

C	-4.16933321	-3.57163316	-0.54642211
H	-4.35401827	-0.78885450	-0.25812588
H	-4.26151237	-1.25794722	-1.97643270
H	-1.60539727	-3.89231561	-1.56602716
H	-2.56580536	-2.94192980	-2.74042222
H	-1.23492699	-2.18061013	-1.85359666
H	-4.71009644	-3.65284224	-1.50032343
H	-3.75567141	-4.55702655	-0.29838602
H	-4.89404228	-3.28886240	0.23262607
C	-1.74641808	-3.64944831	1.32110256
O	-1.37843903	-4.61995597	0.64908286
N	-1.55891601	-3.53676587	2.67937124
H	-1.87642993	-2.64271039	3.09150722
H	-0.23389509	-5.86426376	2.11521041
H	0.56817806	-0.88795977	4.84435491
N	2.76477136	2.02232721	-3.29967669
O	3.03355867	1.92064054	-1.01084658
C	2.59660246	1.37955109	-4.60111756
H	2.82198369	2.10514297	4.27579380
H	2.21885680	-1.56623928	4.84079794
C	-0.73378026	-4.30893522	3.52362663
H	1.26188180	3.52108618	-3.45492279
H	2.91302931	4.04007174	-3.90563248
H	2.49605767	3.76509114	-2.19265333
H	-2.90335169	-0.40127529	-1.21933782
H	-3.15696425	-2.01271465	1.43304659
H	1.13360522	-1.83513961	3.46193631
C	2.33093775	3.41449531	-3.21088483
C	0.74734488	-6.15884418	4.02275300
C	-0.08659358	-5.49027241	3.12106970
H	-1.04070048	-2.90744143	5.13801067
H	0.42708460	-4.11409473	6.72802786
C	-0.54700717	-3.82885219	4.83433155
C	2.97715537	1.27011324	-2.13651776
H	1.59590654	-6.20655420	6.01366845
H	1.24991651	-7.07049639	3.69944807
C	0.28521088	-4.50647891	5.72135344
C	1.98173264	0.19007839	3.56526986
C	3.18385684	-0.15500018	2.65988872
C	2.42014162	1.16568189	4.68080598
C	1.44217945	-1.10243148	4.21578420
H	2.87336541	-0.77410229	1.81193442
H	3.67479277	0.74143700	2.25723734
H	3.93539392	-0.71757608	3.23300921
H	1.57283328	1.40888701	5.33975107
H	3.20817571	0.70391515	5.29354773
H	1.66346792	0.79472151	-4.65718867
S	-2.09025998	-0.33979093	3.16224492
C	-1.01240488	-0.57686724	1.84795068

TS5_52

E = -21521.47

G = -20990.12

Nimag = 1,69 i cm-1

C	1.89083500	-2.32002780	2.01566439
N	0.96101522	-1.30100096	1.53659329
H	1.22284411	-0.75772694	0.69635630
H	-3.66344702	3.44037440	-3.39447022
H	-4.88469636	2.55288344	-2.43818135
N	-1.13018693	-0.56473454	1.02767436
H	-0.55448007	-0.17000788	0.24898774
C	-2.32201195	0.29510216	1.24687161
H	-2.31539951	0.91746567	0.34122180
H	-0.96619764	2.48703348	1.13015154
C	-2.07138518	1.24124252	2.43216097
N	-0.85053922	1.99734998	2.08308290
H	-1.89754681	0.63969020	3.32236558
P	0.25067216	2.83530399	2.94597323
C	1.76531517	2.77717429	1.95626375
C	2.02546386	3.75072103	0.98033587
C	2.58104543	1.63648988	2.06045319
C	3.10654576	3.57843752	0.11132090
H	1.37054225	4.61262851	0.87443505
C	3.64877030	1.46749568	1.18219469
H	2.36241286	0.87946574	2.80749521
C	3.91039065	2.43906145	0.20722700
H	3.30326454	4.32525011	-0.65699320
H	4.25940363	0.57100495	1.25846115
H	4.74085111	2.30162698	-0.48450254
C	0.64212038	2.18118024	4.59357693
C	-0.21543903	1.35255140	5.33737769
C	1.81532524	2.68446721	5.19236955
C	0.08935601	1.05445654	6.66638610
H	-1.11635368	0.93739990	4.90321954
C	2.10690783	2.38423773	6.52156385
H	2.50646277	3.30090772	4.62103017
C	1.23568703	1.58250633	7.26501711
H	-0.57658366	0.40301749	7.23284729
H	3.02098117	2.76766440	6.97153318
H	1.46551315	1.34757528	8.30146335
C	-0.21677922	4.58559425	3.14712510
C	-1.56573179	4.93277824	2.96011088
C	0.72408684	5.57322954	3.49094951
C	-1.97221525	6.25905086	3.12397585
H	-2.28663528	4.17538171	2.66406283
C	0.31222775	6.89773229	3.64772792
H	1.77481527	5.31923622	3.62070995
C	-1.03543008	7.24073256	3.46850052
H	1.04403739	7.66413725	3.90491040
H	-1.35252231	8.27595075	3.58960038
H	-2.93464729	1.89941141	2.60339096
H	-3.01895387	6.52625756	2.97489098
C	-0.96068060	2.55212938	-2.23779481
C	0.43381938	2.37673135	-2.02768480
H	0.80563177	2.89504452	-1.14517935
S	0.90128726	0.40773894	-1.22440994
C	-0.22491449	-0.59725724	-2.28408967
H	-1.00756070	0.07716812	-2.66943296
H	0.31530864	-1.06402875	-3.11745265
H	-0.70706047	-1.37610526	-1.67939463
C	1.35997411	2.46211227	-3.22969714
H	2.37136756	2.11484114	-2.98512687
H	0.97842806	1.86196141	-4.07000586
H	1.42080568	3.51147540	-3.56706154
H	-1.38533003	2.28179412	-3.20017899
C	4.21219673	-0.19844495	7.78865309
C	2.50049312	-3.16961068	0.85752945
C	1.31874787	-3.81204035	0.09134268
C	3.35166843	-2.34056975	-0.12926129
C	3.35976683	-4.28776980	1.49105856
H	0.68832648	-4.41086905	0.76592271
H	1.70435307	-4.47196907	-0.69908085
H	4.21511967	-1.89774557	0.37725842
H	3.70953980	-2.99889619	-0.93593851
H	2.76535280	-1.53626940	-0.59496435
H	3.73939748	-4.95547394	0.70409591
H	4.21789058	-3.86969041	2.03228598
H	2.76283928	-4.89215834	2.19130253
C	2.91023430	-1.66238556	2.98446475
O	4.08257064	-1.39162866	2.69805476
N	2.33925091	-1.41718681	4.20989920
H	1.33189541	-1.65164055	4.28702562
H	4.55064512	0.15220170	4.40647271
H	-3.33785944	-1.25976091	-0.75467788
N	-3.17622552	3.04963633	-1.34127676
O	-1.30751363	3.45684083	-0.06523669
C	-3.80693423	2.67744023	-2.60609331
H	-4.83888090	1.46998876	1.40700737
H	-4.65296905	-2.05978491	0.14622175
C	2.98809531	-0.97225164	5.38167922
H	-4.93829456	3.50084149	-0.27809520
H	-4.12467486	4.92999249	-0.98494666
H	-3.41383969	4.11253812	0.43793756
H	0.68731666	-3.04854490	-0.38027780
H	1.28392537	-3.00867689	2.62010188
H	-2.94710891	-2.36256802	0.58494399
C	-3.95986869	3.95124249	-0.49409914
C	4.74089940	0.21090596	6.56034735
C	4.13718089	-0.16469809	5.35740289
H	1.55070858	-1.99323398	6.63063859

H	2.62662526	-1.30866512	8.75841446
C	2.44775524	-1.37468808	6.61626232
C	-1.78177575	3.03319001	-1.18995589
H	4.68859068	0.10246295	8.72107611
H	5.62993223	0.84147129	6.53226732
C	3.05760346	-0.99034601	7.80886457
C	-3.71893518	-0.42023498	1.23422282
C	-4.17355200	-0.93314773	2.61721780
C	-4.75098174	0.61494005	0.72178984
C	-3.65787208	-1.60020191	0.24148647
H	-3.51695931	-1.73272290	2.97548979
H	-4.17306341	-0.13088929	3.36910864
H	-5.20290361	-1.31636458	2.54173234
H	-4.45914556	1.00280532	-0.26290756
H	-5.74306251	0.14719205	0.64003870
H	-3.40559627	1.72232389	-2.96473972
S	-0.86716422	-1.82066712	3.45238201
C	-0.33646057	-1.18071154	1.94376861

Table 7.8. Cartesian coordinates (in Å), energies (in kcal mol^{-1}), and number of imaginary frequencies computed at COSMO(Et_2O)-ZORA-M06-2X/TZ2P//COSMO(Et_2O)-ZORA-BLYP-D3(BJ)/DZP.

5_64
E = -19784.00
G = -19314.12
Nimag = 0

C	-6.14449954	-2.61422710	0.97532564
N	-4.88946181	-2.00739685	1.42166354
H	-4.13501896	-1.98512062	0.73505384
C	-5.45697443	-6.17622828	2.16273527
S	-5.56140268	-2.15029597	4.04613194
N	-3.31037795	-1.21709749	2.84776127
H	-2.92983236	-0.68723090	2.04344372
C	-2.66617057	-0.74663486	4.07389179
H	-3.40734057	-0.80115786	4.88087410
H	-2.85533406	-6.61037107	1.46076343
C	-2.29482245	0.75415529	3.82528116
N	-2.03400206	0.95453459	2.39732632
H	-1.43163953	1.01451361	4.45715221
P	-1.82293565	2.36352072	1.72280267
C	-0.10154263	3.00582333	1.72362072
C	0.94036915	2.06944039	1.81196639
C	0.19545624	4.37453547	1.62491420
C	2.27038261	2.49819005	1.79665885
H	0.69611547	1.01204291	1.89648668
C	1.52679046	4.79996075	1.60690172
H	-0.60966980	5.10541088	1.56656628
C	2.56380812	3.86318864	1.69285535
H	3.07754571	1.76958112	1.86815186
H	1.75579858	5.86257251	1.53029976
H	3.60082335	4.19786292	1.68270446
C	-2.79441037	3.75000279	2.42679423
C	-2.47948436	4.18590988	3.72719737
C	-3.89559747	4.30748224	1.75813628
C	-3.25704988	5.16551200	4.34745013
H	-1.61948651	3.76884882	4.24971812
C	-4.66926113	5.29207584	2.38136528
H	-4.14466551	3.98404878	0.74973977
C	-4.35308349	5.71978060	3.67510319
H	-3.00735200	5.49851873	5.35439922
H	-5.51744016	5.72708892	1.85352106
H	-4.95772764	6.48627627	4.15886009
C	-2.31056089	2.22415453	-0.02751222
C	-3.49143367	1.52089213	-0.32582934
C	-1.58448532	2.83683624	-1.05877952
C	-3.94626544	1.44513734	-1.64254183
H	-4.04559942	1.04644556	0.48075905
C	-2.03711343	2.74596049	-2.37951392
H	-0.66486231	3.37386574	-0.83665996
C	-3.21855559	2.05657853	-2.67111593
H	-1.46561598	3.21463934	-3.17995949
H	-3.57264316	1.99277320	-3.69959148
H	-3.14301170	1.37273433	4.16901628
H	-4.86642598	0.91190048	-1.86869952
H	-0.56635675	-0.22530483	5.88048515
H	-5.36297718	-8.79803425	2.84209469
H	-5.17050284	-6.49821520	1.15120298
H	-6.09681526	0.09157517	0.48616424
H	-6.84765807	-2.47219027	1.80713174
H	-2.29420171	-3.49780034	3.56819349
C	-1.46496949	-1.66841186	4.47138338
C	-0.31265303	-1.56324000	3.44976169
C	-0.96262832	-1.25018961	5.87181785
C	-1.95352767	-3.13083332	4.54445885
H	-0.65694305	-1.82679841	2.44005252
H	0.09698911	-0.54642993	3.41114290
H	0.49810277	-2.25328656	3.72877822
C	-4.53378684	-1.76834044	2.72458774
C	-6.72962215	-1.87416053	-0.26305166
C	-7.01371539	-0.41307070	0.15782868
C	-5.75750942	-1.88405681	-1.46413860
C	-8.06191353	-2.55175176	-0.65381666
H	-7.73475510	-0.37562572	0.98793337
H	-7.43353147	0.14762043	-0.68961694
H	-5.54223347	-2.91014868	-1.78155746
H	-6.20600791	-1.33569999	-2.30588405
H	-4.80873011	-1.38453171	-1.22224342
H	-8.54369400	-1.98657246	-1.46492768
H	-7.89714072	-3.58064701	-0.99482888
H	-8.75312271	-2.57067895	0.20271442
C	-5.92261124	-4.14604718	0.81971717
O	-5.80729392	-4.73354618	-0.26719845
N	-5.83960218	-4.76790721	2.02742808
H	-5.83728154	-4.17341038	2.87164550
H	-1.13586471	-3.78225373	4.88080844
H	-2.79060409	-3.23723322	5.24653691
H	-1.77574490	-1.31112794	6.61138117
H	-0.15547960	-1.92340627	6.19670808
C	-4.24610574	-6.30015953	3.07948431
C	-4.39181081	-6.18601426	4.46878939
C	-3.28270292	-6.30440167	5.30767275
C	-2.01572318	-6.54725232	4.76539880
C	-1.86212738	-6.65318920	3.38068322
C	-2.97411187	-6.52547261	2.54114638
H	-5.38056146	-6.01851618	4.89487994
H	-3.40575658	-6.20807840	6.38603278
H	-1.15045173	-6.64339374	5.42072970
H	-0.87671213	-6.83437030	2.95160848
C	-6.62227404	-7.05704278	2.61951505
C	-7.92560538	-6.56315363	2.73488173
C	-8.96995559	-7.40189384	3.14575765
C	-8.72019900	-8.74501785	3.43992182
C	-7.41729449	-9.24680845	3.32035714
C	-6.37763326	-8.40748195	2.91556930
H	-8.12535394	-5.51829650	2.50704766
H	-9.97939277	-7.00075930	3.23660729
H	-9.53171655	-9.39741334	3.76119358
H	-7.21145575	-10.29274372	3.54774838

5_65
E = -19780.50
G = -19308.68
Nimag = 0

C	-5.69984050	-1.75634595	1.37286629
N	-4.49678961	-0.99301364	1.71196474
H	-3.70593847	-1.11787909	1.07911946
C	-5.19448522	-4.88826521	3.49000649
S	-5.36500267	-0.52167245	4.22759591
N	-3.02657333	0.16363099	3.01296971
H	-2.52038856	0.23117847	2.12966011
C	-2.31855452	0.79514896	4.15489719
H	-1.30953715	0.94763184	3.74468645
H	-2.67842006	-4.50240897	4.45779607
C	-2.17205456	-0.22442897	5.30689989

N	-1.20680410	0.24708932	6.30796836
H	-1.85101994	-1.17902155	4.84776977
P	-1.36044755	-0.24892878	7.80468704
C	-0.80399643	-1.96181948	8.18970590
C	0.19397937	-2.51993134	7.37591338
C	-1.32179595	-2.70141667	9.26384725
C	0.67256209	-3.80657460	7.63727179
H	0.57844226	-1.94195398	6.53547537
C	-0.83920535	-3.98604584	9.52568067
H	-2.10827733	-2.27712590	9.88620943
C	0.15679904	-4.53952213	8.71315227
H	1.44178130	-4.24149793	6.99944047
H	-1.24661519	-4.56087672	10.35713285
H	0.52478801	-5.54570042	8.91266867
C	-3.07005404	-0.19644444	8.46639820
C	-4.02162052	-1.08322998	7.92978194
C	-3.49137951	0.82397436	9.33513136
C	-5.37333544	-0.94141420	8.24456614
H	-3.71405438	-1.88647053	7.26816827
C	-4.84462937	0.95536411	9.65741583
H	-2.76555709	1.51782547	9.75566564
C	-5.78814693	0.07947106	9.10612920
H	-6.09845297	-1.62934389	7.81207976
H	-5.16454955	1.74539247	10.33668386
H	-6.84408314	0.19233480	9.35120703
C	-0.35682523	0.83647059	8.86986915
C	-0.24081037	2.19286333	8.52245028
C	0.23836674	0.36666074	10.05076346
C	0.46128265	3.07018844	9.35177601
H	-0.70281159	2.54605386	7.60554861
C	0.93917308	1.24921015	10.87877474
H	0.16518720	-0.68443904	10.32079788
C	1.04988361	2.60007556	10.53190740
H	1.40265952	0.87980954	11.79304620
H	1.59678439	3.28545068	11.17892653
H	-3.17233674	-0.40305058	5.71681721
H	0.54848884	4.12137541	9.07797677
H	-0.95953560	2.64189631	5.56669099
H	-5.04684216	-7.54580071	3.93342574
H	-4.33396319	-5.24355702	2.90199432
H	-5.80831809	0.72620506	0.21572509
H	-6.46083375	-1.43136526	2.09416956
H	-4.57372698	2.31157085	3.19254640
C	-2.84643084	2.23935821	4.54904574
C	-3.73182046	2.24341002	5.81573503
C	-1.59986098	3.11886621	4.81659697
C	-3.63870897	2.85713063	3.37548285
H	-4.58411318	1.56439761	5.70930909
H	-3.15904662	1.93959873	6.69652631
H	-4.10926691	3.26341587	5.98836402
C	-4.23461153	-0.44577601	2.94319529
C	-6.23153595	-1.41131300	-0.04784368
C	-6.65679926	0.07536067	-0.03621161
C	-5.16855543	-1.63271984	-1.14708726
C	-7.47096527	-2.29230618	-0.32354127
H	-7.45329056	0.24989878	0.70235145
H	-7.03513398	0.36554056	-1.02702874
H	-4.81502901	-2.66986652	-1.14360989
H	-5.60481064	-1.40617128	-2.13127241
H	-4.30734647	-0.96032236	-1.01421446
H	-7.93535204	-1.99566404	-1.27507170
H	-7.19857387	-3.35300030	-0.38476252
H	-8.22107793	-2.16801801	0.47259032
C	-5.41104362	-3.25502022	1.64925540
O	-5.05935919	-4.07735673	0.78954397
N	-5.55513262	-3.56627469	2.96611498
H	-5.67972032	-2.78731867	3.63094755
H	-3.88969850	3.90145137	3.61504631
H	-3.04843727	2.85553185	2.44670869
H	-1.01104186	3.25359934	3.89527107
H	-1.90313543	4.11258952	5.17964853
C	-4.76670624	-4.74215524	4.94593353
C	-5.71113830	-4.77821525	5.98037594
C	-5.30753924	-4.63559371	7.31101608
C	-3.95415181	-4.46691184	7.61923996
C	-3.00750870	-4.41612618	6.59092747
C	-3.41502047	-4.54701087	5.26049960
H	-6.76250815	-4.93621601	5.74437594
H	-6.04979777	-4.66250958	8.10860482
H	-3.63864887	-4.35802536	8.65430995
H	-1.95654420	-4.26942358	6.82444815
C	-6.31641197	-5.91210300	3.31666229
C	-7.60299702	-5.54796499	2.91044052
C	-8.61095889	-6.51370807	2.79747089
C	-8.33757607	-7.85339652	3.08767419
C	-7.04761991	-8.22397588	3.49123256
C	-6.04616544	-7.25776502	3.60543338
H	-7.81876973	-4.50650600	2.68255798
H	-9.61067929	-6.21626555	2.48086767
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5_66

E = -19779.57

G = -19305.39

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C	-7.17219412	-1.94536437	4.90444307
S	-3.11044874	-2.89972515	5.64582049
N	-1.65744308	-1.35060808	3.99456377
H	-1.60386642	-0.94995036	3.05527771
C	-1.27908425	-0.35167746	5.01190559
H	-1.83795417	-0.62396691	5.91533069
H	-6.46058798	-4.34497447	6.01855175
C	-1.75809644	1.06833446	4.53003116
N	-2.88343174	0.93056719	3.61504369
H	-0.90513997	1.59701730	4.07194040
P	-3.13739198	1.88381790	2.38731918
C	-1.62456489	2.38098886	1.47198243
C	-0.74365621	1.35931610	1.07408949
C	-1.27044396	3.72028443	1.25104919
C	0.46818165	1.67022949	0.45835157
H	-1.01099234	0.31754177	1.24424770
C	-0.05198139	4.03162528	0.63668469
H	-1.94300863	4.51860461	1.55767256
C	0.81679462	3.00963975	0.24136912
H	1.14392121	0.87194306	0.15336536
H	0.21837938	5.07381017	0.46868697
H	1.76597349	3.25461679	-0.23430433
C	-4.01251744	3.46789051	2.70268725
C	-3.69391391	4.18039624	3.87024202
C	-5.01404344	3.95009955	1.84724082
C	-4.36667308	5.36526113	4.17550575
H	-2.92916515	3.80058800	4.54615225
C	-5.68605526	5.13687266	2.15410922
H	-5.28478144	3.38975189	0.95448969
C	-5.36431125	5.84451755	3.31712518
H	-4.12045222	5.91129975	5.08592353
H	-6.46986392	5.50286264	1.49114001
H	-5.89570487	6.76436213	3.56022590
C	-4.19817711	0.98937924	1.21223220
C	-5.25650671	0.21816846	1.72498712
C	-3.99700732	1.07344111	-0.17420024
C	-6.10196443	-0.46739603	0.85243205
H	-5.39932375	0.15039144	2.79841714
C	-4.84494113	0.37811838	-1.04285272
H	-3.18091436	1.67258837	-0.57403604
C	-5.89533407	-0.39082926	-0.53044538
H	-4.68221870	0.43630385	-2.11883563
H	-6.55293814	-0.93469321	-1.20844981
H	-2.03160805	1.63911837	5.43443349
H	-6.90364019	-1.08222074	1.25358006
H	0.46765340	1.67800342	5.94519990
H	-8.83312089	-0.19421015	3.60112166
H	-8.01627571	-2.27954380	4.28289674
H	-2.05581139	-4.63898704	3.38938789
H	-4.56677992	-3.05792441	1.47439993
H	0.25181983	-2.61847758	5.27639126

C	0.24081776	-0.43131816	5.34245846
C	1.09984986	-0.26038202	4.06845342
C	0.59152013	0.67115908	6.36690012
C	0.53485795	-1.81293883	5.96721036
H	0.88733692	-1.06030376	3.34470344
H	0.92473957	0.70530111	3.57567595
H	2.16751463	-0.31658769	4.32789565
C	-2.74213370	-2.17549326	4.14367209
C	-4.08596478	-4.84372164	2.57466683
C	-2.55393790	-4.99655940	2.48009145
C	-4.61960027	-5.56970919	3.82981528
C	-4.73566711	-5.49197283	1.32696601
H	-2.15364207	-4.43778779	1.62166056
H	-2.30441926	-6.05931440	2.34615279
H	-5.71776714	-5.53539812	3.86393145
H	-4.31763303	-6.62707572	3.79345214
H	-4.22535707	-5.11894301	4.74591691
H	-4.54631790	-6.57536642	1.32821212
H	-5.82042880	-5.32324688	1.32062797
H	-4.31387827	-5.06830227	0.40278473
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O	-6.88966647	-3.20937653	2.33358167
N	-5.97293309	-2.56480594	4.33437709
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H	1.60649662	-1.90553490	6.19926029
H	-0.03822951	-1.95079406	6.89505987
H	-0.04647552	0.59005272	7.26034965
H	1.63892767	0.56688971	6.68632017
C	-7.39601081	-2.42714069	6.33688601
C	-8.05446370	-1.61187307	7.26824486
C	-8.29465533	-2.06833255	8.56841461
C	-7.87529118	-3.34609091	8.95491951
C	-7.21763035	-4.16455550	8.02973340
C	-6.98170030	-3.70856836	6.72931925
H	-8.37009662	-0.61114547	6.97907875
H	-8.80433547	-1.42143049	9.28226149
H	-8.05545877	-3.69865343	9.97017710
H	-6.88243267	-5.16010354	8.32058917
C	-7.04367998	-0.43029407	4.78093850
C	-5.93576331	0.22300771	5.34119919
C	-5.76782787	1.59716056	5.17466253
C	-6.70679281	2.33690755	4.44726749
C	-7.81257618	1.69207743	3.88677073
C	-7.98020508	0.31168379	4.05441121
H	-5.18189788	-0.35155844	5.87840109
H	-4.88552920	2.08572644	5.58123821
H	-6.56288885	3.40444861	4.29920067
H	-8.53768194	2.25949115	3.30339001

5_67

E = -19765.09

G = -19293.47

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S	-5.31326354	0.33440262	5.10952669
N	-3.04099267	-0.13826487	3.73577496
H	-2.54695738	-0.75702009	3.09417993
C	-2.12672178	0.81754383	4.43493864
H	-1.13755046	0.36134530	4.28028496
H	-7.92681973	-4.86208210	6.88038018
C	-2.34123728	0.79040819	5.96688662
N	-1.05303805	0.77554186	6.68835543
H	-2.94282543	-0.10128051	6.17688344
P	-1.13459924	0.12116823	8.13326662
C	-1.39310929	-1.70560453	8.20909493
C	-0.70002869	-2.48439269	7.26766820
C	-2.18594820	-2.33573588	9.18011155
C	-0.78000230	-3.87674420	7.31286563
H	-0.10468615	-1.98822345	6.50140326
C	-2.27192357	-3.73068835	9.21715658
H	-2.73615301	-1.74116049	9.90613424
C	-1.56351428	-4.50176757	8.29062613
H	-0.23823761	-4.47660839	6.58231133
H	-2.89889932	-4.21523959	9.96422603
H	-1.63203462	-5.58904397	8.32081960
C	-2.45603181	0.77527107	9.23764568
C	-3.80402367	0.59553830	8.86869815
C	-2.15057318	1.55554518	10.36492341
C	-4.82126168	1.19313301	9.61415299
H	-4.06824244	-0.01107827	8.00587249
C	-3.17513944	2.14063243	11.11654557
H	-1.11350089	1.70389562	10.66017625
C	-4.51119610	1.96437851	10.74035153
H	-5.86016573	1.05864013	9.31649747
H	-2.92827271	2.73622411	11.99519178
H	-5.30855704	2.42555959	11.32236720
C	0.44756884	0.41128193	8.97833527
C	1.20368248	1.54235944	8.62992627
C	0.89330496	-0.44601811	9.99611635
C	2.39805221	1.81349896	9.30265231
H	0.84561373	2.18816453	7.83030969
C	2.08660869	-0.16676678	10.66858389
H	0.31604263	-1.33087876	10.25777415
C	2.83759321	0.96298453	10.32449419
H	2.43200830	-0.83353854	11.45803988
H	3.76779569	1.17843120	10.84973978
H	-2.96205108	1.64318238	6.27855857
H	2.98593930	2.69002859	9.03125971
H	-1.28103383	3.23506088	5.53925193
H	-10.29609376	-2.02475823	7.68351379
H	-8.87237245	-3.22139555	5.48589976
H	-2.36843302	-2.62963838	4.03928678
H	-5.19400525	-3.52093310	2.78019121
H	-2.38403029	1.45514808	1.71968409
C	-2.07119357	2.22149768	3.75497894
C	-3.43166924	2.94597775	3.79393093
C	-1.00866978	3.07083249	4.48920309
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H	-3.33602337	3.92996214	3.30997685
C	-4.31894498	-0.50048424	4.00820119
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C	-4.15407760	-2.94291649	6.08387065
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H	-2.83086786	-4.04338832	3.04577114
H	-2.13643459	-4.25725547	4.67175139
H	-5.14047772	-2.86564758	6.54638581
H	-3.51780064	-3.53270951	6.75149264
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H	-3.88004581	-5.60982761	5.51755848
H	-5.60312232	-5.17610021	5.44051737
H	-4.74314785	-5.63247935	3.95414213
C	-6.69072577	-3.08584069	4.16736105
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H	-1.53638617	3.01656415	1.79170308
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H	-0.91201297	4.04775272	3.99256079
C	-7.66657110	-2.74786764	7.20656265
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C	-6.33350459	-2.13975684	9.14407750
C	-6.14636010	-3.49336855	9.44733531
C	-6.73298324	-4.47243828	8.64104697
C	-7.49238403	-4.09974552	7.52625631
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H	-5.54387876	-3.78068755	10.30801258
H	-6.59172806	-5.52824558	8.87182761
C	-9.25973048	-1.16893070	5.99285304
C	-9.18453502	-0.07003594	5.12938654
C	-10.07439137	1.00282168	5.26822490
C	-11.05015272	0.98528682	6.26864954
C	-11.13211374	-0.11407369	7.13364321

C	-10.24102696	-1.18012437	6.99705687
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H	-9.99921285	1.85495302	4.59272965
H	-11.74058003	1.82126920	6.37760765
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5_68

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S	-5.34285573	-2.78963531	3.58901650
N	-3.32266864	-1.17278187	2.80032237
H	-2.84647983	-0.65055059	2.06494344
C	-2.71928989	-1.08090911	4.13681501
H	-3.40000137	-1.63299776	4.79814013
H	-9.70862635	1.04967193	4.00559480
C	-2.74451962	0.38976771	4.61751024
N	-1.77336709	1.25542725	3.95412763
H	-2.52870776	0.38140485	5.69855333
P	-2.12531671	2.35004180	2.87975159
C	-0.53493642	3.01658143	2.28130551
C	0.65859164	2.58055134	2.87422305
C	-0.49654927	3.95539864	1.23858944
C	1.88413981	3.07831249	2.42191170
H	0.60449206	1.85309695	3.68074265
C	0.73036625	4.44761803	0.78700025
H	-1.41711480	4.29265933	0.76664540
C	1.92193233	4.00959527	1.37794211
H	2.81055825	2.73633723	2.88276383
H	0.75703756	5.17102629	-0.02731657
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C	-3.07809766	3.81547875	3.46944254
C	-3.08551803	4.04115843	4.85461447
C	-3.70585425	4.73491654	2.61392917
C	-3.70774350	5.17739596	5.37892893
H	-2.59739891	3.32203657	5.51123686
C	-4.32659401	5.86997689	3.13991790
H	-3.72577527	4.56275369	1.53993164
C	-4.32544144	6.09470866	4.52135302
H	-3.71414575	5.34536813	6.45569143
H	-4.81743120	6.57703444	2.47178076
H	-4.81318791	6.97960437	4.92952151
C	-3.00986515	1.81973707	1.35564524
C	-4.41244136	1.86390517	1.27725732
C	-2.27719298	1.22909545	0.30853958
C	-5.06809198	1.36422266	0.15161783
H	-4.99199114	2.29110560	2.08820859
C	-2.93932840	0.72598226	-0.81553812
H	-1.19067408	1.17576940	0.36596468
C	-4.33489019	0.80700493	-0.90035634
H	-2.36583184	0.27990597	-1.62773264
H	-4.85566768	0.41921168	-1.77189277
H	-3.78910224	0.72405901	4.51483164
H	-6.15219555	1.39367646	0.09552679
H	-0.33017490	-0.44606065	5.54850033
H	-8.48225679	2.65941845	1.33502563
H	-8.61276194	0.36395083	0.81244995
H	-3.89227764	-2.14161403	-1.54760423
H	-7.44604388	4.51443523	2.62826155
H	-2.16090690	-3.59027384	3.16642886
C	-1.33421770	-1.81934426	4.16713050
C	-0.41691599	-1.41186462	2.98926937
C	-0.61938015	-1.50410662	5.49875502
C	-1.60425570	-3.33960098	4.07994028
H	-0.85544925	-1.70038969	2.02233794
H	-0.24106664	-0.33213816	2.98965316
H	0.54682917	-1.93602592	3.07907170
C	-4.38755751	-1.92481575	2.44782685
C	-5.51746705	-3.39518677	-0.76340425
C	-4.85465454	-2.55788325	-1.87741566
C	-4.55695926	-4.52981872	-0.33639605
C	-6.83544877	-4.01391545	-1.28171314
H	-5.50970216	-1.73710685	-2.18667881
H	-4.65094488	-3.19962515	-2.74751741
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H	-4.31297182	-5.15993620	-1.20373930
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H	-6.62388087	-4.69307573	-2.12012638
H	-7.33007467	-4.59682858	-0.48975473
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C	-6.92858691	-1.45648667	0.36959478
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N	-7.46946158	-1.15372545	1.58101796
H	-7.11914874	-1.67386835	2.39707016
H	-0.65270726	-3.89198590	4.06517072
H	-2.19567191	-3.68562547	4.93981297
H	-1.26521021	-1.73413495	6.35985200
H	0.29088797	-2.11606859	5.58546265
C	-9.64906173	-0.48527498	2.48764339
C	-10.30885271	-1.61016486	1.96599590
C	-11.49974662	-2.06443779	2.53561834
C	-12.04915169	-1.39994831	3.64004488
C	-11.39914281	-0.27896321	4.16267995
C	-10.20573488	0.17743091	3.58826037
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H	-11.99937938	-2.93930560	2.11993781
H	-12.97587796	-1.75649717	4.08878806
H	-11.81640416	0.24426012	5.02283151
C	-7.65732551	1.10479967	2.58218203
C	-6.85836401	0.82789446	3.70020609
C	-6.29857353	1.87082841	4.44234847
C	-6.51468757	3.20005917	4.06680831
C	-7.29300630	3.48189260	2.94093533
C	-7.86651383	2.43737127	2.20750292
H	-6.66083786	-0.20218264	3.99456622
H	-5.68243018	1.64647078	5.31172278
H	-6.06168022	4.00790969	4.63447846
H	-6.20875456	-3.27087597	1.26372503

5_69

E = -19777.77

G = -19305.66

Nimag = 0

C	-6.03959210	-1.90243600	0.42888789
N	-4.78482784	-1.44554867	1.03089225
H	-4.43173436	-0.55004927	0.69435320
C	-8.56498740	-0.79711248	3.07715791
S	-4.91093931	-3.24257192	3.04212962
N	-2.96395418	-1.44304127	2.41434525
H	-2.62063736	-0.81166706	1.68758289
C	-2.37630640	-1.12186415	3.74608633
H	-1.34005712	-0.84144670	3.50436690
H	-10.70009174	-0.53020791	4.75877556
C	-2.24478021	-2.35718030	4.67121133
N	-0.97563226	-2.26683725	5.40853138
H	-2.26973016	-3.25761156	4.03964461
P	-0.84091511	-2.86833761	6.86274577
C	-0.87384338	-4.70276985	7.03071908
C	-0.52609219	-5.45723467	5.89897333
C	-1.22665751	-5.35780342	8.22192656
C	-0.52256708	-6.85356550	5.96039284
H	-0.26588767	-4.94053749	4.97574154
C	-1.21647546	-6.75405197	8.28269641
H	-1.51805853	-4.77983286	9.09741654
C	-0.86495537	-7.50232478	7.15270989
H	-0.25683078	-7.43588219	5.07851390
H	-1.48883677	-7.25895040	9.20918363
H	-0.86334590	-8.59101490	7.20016181
C	-2.10716328	-2.32092696	8.07517965
C	-3.40769927	-2.85347010	8.00107434
C	-1.85139678	-1.24693289	8.94452632
C	-4.43217327	-2.31488458	8.78208909
H	-3.61780126	-3.69445201	7.34210690
C	-2.87875471	-0.71466617	9.72692804
H	-0.85056121	-0.82295806	9.00480659
C	-4.17139647	-1.24485481	9.64348563

H	-5.43370501	-2.73484218	8.72263550
H	-2.67079056	0.11498891	10.40220811
H	-4.97171559	-0.82753402	10.25376913
C	0.76223841	-2.31988107	7.53096239
C	1.36915870	-1.18070225	6.97877626
C	1.35802172	-2.97183154	8.62126456
C	2.56286390	-0.69588386	7.51968979
H	0.89343139	-0.69556215	6.12940283
C	2.54941487	-2.47973399	9.16225543
H	0.90121298	-3.86316189	9.04593907
C	3.15121034	-1.34109987	8.61408987
H	3.00959388	-2.98775250	10.00923638
H	4.08025229	-0.95947587	9.03701249
H	-3.13222340	-2.41987657	5.31826405
H	3.03342658	0.18771274	7.08885850
H	-2.60955907	-0.25722671	6.48502068
H	-8.17886921	1.45469874	4.58112319
H	-8.66735101	0.21565936	2.65930358
H	-4.55430095	-0.30265122	-1.44506759
H	-7.40380694	1.60803757	6.93917807
H	-3.37388211	1.19472466	2.45530861
C	-3.05412511	0.14995278	4.37353755
C	-4.56424314	-0.04100474	4.61374130
C	-2.37764644	0.48992646	5.72104759
C	-2.85028407	1.34480657	3.41062967
H	-5.12221690	-0.16941378	3.67898047
H	-4.77519241	-0.90527227	5.25269593
H	-4.96670676	0.84965568	5.11414071
C	-4.19272196	-1.97797920	2.14294927
C	-5.95677645	-1.96762536	-1.12315499
C	-5.56643963	-0.61032287	-1.74956684
C	-4.89108378	-3.02723304	-1.48736314
C	-7.33160336	-2.42573610	-1.66035810
H	-6.27887942	0.17102526	-1.46250878
H	-5.55654590	-0.70065993	-2.84578754
H	-5.17111094	-4.01637459	-1.09587867
H	-4.79612502	-3.10290265	-2.58003741
H	-3.90892324	-2.76061048	-1.07310550
H	-7.27050609	-2.59364027	-2.74533022
H	-7.63748645	-3.37213540	-1.18859955
H	-8.10395294	-1.67148761	-1.46767106
C	-7.19753456	-1.04535125	1.01882492
O	-7.72107247	-0.07888984	0.44234853
N	-7.55595643	-1.47458181	2.25623662
H	-6.96488360	-2.20167902	2.69106737
H	-3.25396422	2.26342819	3.86087633
H	-1.78172546	1.50812546	3.20041047
H	-1.28559416	0.54439810	5.62267225
H	-2.75043380	1.46313156	6.07580598
C	-9.93683825	-1.48002854	2.97472666
C	-10.24010788	-2.35279486	1.92273486
C	-11.50851877	-2.93669025	1.82511375
C	-12.49093191	-2.64997934	2.77797754
C	-12.19520130	-1.77544351	3.83066443
C	-10.92696583	-1.19634067	3.92793113
H	-9.48173471	-2.58498683	1.17946218
H	-11.72673318	-3.61746852	1.00240118
H	-13.47780414	-3.10608155	2.70405993
H	-12.95188439	-1.54783962	4.58148198
C	-8.08168994	-0.69734273	4.51565438
C	-7.78158609	-1.86076031	5.23780595
C	-7.32691060	-1.77713168	6.55366970
C	-7.18971577	-0.52912453	7.17197815
C	-7.51015814	0.63235180	6.46516528
C	-7.94757020	0.54664012	5.13845225
H	-7.90098797	-2.83679716	4.76868152
H	-7.07834549	-2.68854832	7.09452822
H	-6.82386939	-0.46208036	8.19477369
H	-6.17847998	-2.92851970	0.79479749

5_70

E = -19778.96

G = -19305.80

Nimag = 0

C	-6.33313340	-1.85074315	0.76842999
N	-5.63335117	-1.04930860	1.80474752
H	-4.80026576	-0.60977352	1.41107095
C	-4.74104099	-5.05219501	2.11338160
S	-6.91139109	-1.67327864	4.12670128
N	-4.36784163	-0.90201673	3.70921481
H	-3.59062809	-0.68570477	3.07698033
C	-4.12708928	-0.38387264	5.06293053
H	-5.11728079	-0.24039727	5.51475965
H	-3.39100500	-2.98821365	0.91418727
C	-3.46899491	1.01297427	4.86393290
N	-2.30741663	0.91754137	3.98187613
H	-3.16180686	1.40236626	5.84720452
P	-2.04757306	1.73159471	2.66190625
C	-0.45498872	1.14067056	1.99948336
C	0.16510765	0.03437652	2.59907212
C	0.13565295	1.75983915	0.88696191
C	1.36300469	-0.45835110	2.07534036
H	-0.30811612	-0.42396817	3.46206723
C	1.33263185	1.26174608	0.36651446
H	-0.33555358	2.62310335	0.42086768
C	1.94530181	0.15003113	0.95790348
H	1.84365391	-1.31950905	2.53797043
H	1.78723102	1.74062388	-0.50010425
H	2.87746037	-0.23879626	0.54891410
C	-1.90310103	3.55739172	2.82530970
C	-1.56116093	4.05606582	4.09316734
C	-2.08590278	4.44738948	1.75395150
C	-1.40137408	5.43093885	4.28632338
H	-1.42393727	3.36088941	4.92004685
C	-1.92186457	5.82127637	1.94986000
H	-2.36767546	4.07377232	0.77160977
C	-1.57956733	6.31365619	3.21479148
H	-1.13975072	5.81390016	5.27223069
H	-2.06541514	6.50814406	1.11636149
H	-1.45594850	7.38552464	3.36599004
C	-3.23826586	1.53534752	1.26811406
C	-4.45225123	2.24624800	1.28252681
C	-2.99937894	0.60719462	0.23725218
C	-5.39073142	2.05914152	0.26592252
H	-4.65632950	2.96250877	2.07701880
C	-3.94075890	0.42618468	-0.78178423
H	-2.06974515	0.04192499	0.21694582
C	-5.13214744	1.15994840	-0.77314582
H	-3.74084214	-0.28571487	-1.58214588
H	-5.86197926	1.02192718	-1.56930029
H	-4.26112878	1.68628143	4.49097197
H	-6.32501158	2.61821653	0.28517588
H	-2.97492550	0.10911759	7.56372974
H	-4.70892545	-7.76241616	2.01319236
H	-4.70532528	-5.56432049	1.14144725
H	-7.75260100	0.48265991	0.53933501
H	-5.45276783	-9.38149051	3.74499325
H	-3.91274592	-3.18427374	4.88505958
C	-3.34682313	-1.38510339	5.98596060
C	-1.86011750	-1.53115305	5.60124204
C	-3.45678090	-0.87075144	7.43942102
C	-4.00702067	-2.77793181	5.89764749
H	-1.75874049	-1.85995211	4.56246134
H	-1.31498586	-0.58702711	5.71510945
H	-1.39285246	-2.29597830	6.24074505
C	-5.57969250	-1.18424720	3.17048932
C	-7.89550174	-1.69989610	0.58888962
C	-8.33102768	-0.29582159	1.05331716
C	-8.16540226	-1.83861645	-0.93140203
C	-8.70369355	-2.79313918	1.31886088
H	-8.18622036	-0.17887925	2.13387301
H	-9.39573198	-0.14873906	0.81846853
H	-7.78714836	-2.79671785	-1.31328818
H	-9.24667496	-1.78755542	-1.12432068
H	-7.67705262	-1.02732685	-1.49196952
H	-9.77672731	-2.63124823	1.13781696
H	-8.44349697	-3.79251779	0.94123183
H	-8.51966654	-2.76653557	2.39738300
C	-5.82566301	-3.31239205	0.72695315
O	-5.53340339	-3.84012010	-0.36062930

N	-5.65782950	-3.91836107	1.92882100
H	-5.94439575	-3.40155563	2.76494771
H	-3.50439090	-3.47323803	6.58640389
H	-5.07327167	-2.73134486	6.15006277
H	-4.51012846	-0.77954749	7.74541607
H	-2.96265110	-1.57596692	8.12413046
C	-3.31881253	-4.53915654	2.42334906
C	-2.51255734	-5.13997766	3.39786892
C	-1.21113303	-4.67972823	3.63052230
C	-0.69752158	-3.61291216	2.89074569
C	-1.49538346	-3.00415107	1.91610611
C	-2.79273009	-3.46384252	1.68591910
H	-2.90227963	-5.96431774	3.99043640
H	-0.60478867	-5.15055112	4.40391488
H	0.31114690	-3.24999915	3.08039802
H	-1.10485459	-2.16938288	1.33725721
C	-5.26821163	-6.02100736	3.15708629
C	-5.82065523	-5.56379237	4.36200480
C	-6.23993472	-6.47185389	5.33762662
C	-6.10646025	-7.84885168	5.12301893
C	-5.55704485	-8.31134255	3.92277677
C	-5.14212584	-7.39989000	2.94572338
H	-5.92459219	-4.49836879	4.55366757
H	-6.66847963	-6.10271100	6.26924624
H	-6.43140627	-8.55630563	5.88558219
H	-5.90988241	-1.43131425	-0.14961786

5_71

E = -19773.73

G = -19302.24

Nimag = 0

C	-5.48707336	-3.30391240	1.18216799
N	-4.66991179	-2.22191225	1.78548507
H	-3.88916210	-1.97592202	1.17756268
C	-4.76986235	-6.19171742	3.62734133
S	-5.65367285	-2.04739664	4.31514261
N	-3.64934633	-0.67871902	3.11931451
H	-3.23049339	-0.40026934	2.23113414
C	-2.80712484	-0.30150817	4.29994422
H	-1.81578501	-0.14273965	3.85098896
H	-3.44054286	-8.26844489	4.72584010
C	-2.63036594	-1.48139738	5.30598117
N	-1.28006300	-1.63629959	5.85224951
H	-2.94639995	-2.39028777	4.78387384
P	-0.12640098	-2.30647326	4.99913770
C	0.84830347	-1.17967270	3.90628749
C	1.07326426	0.12493947	4.37715192
C	1.35789003	-1.55984737	2.65512594
C	1.78739803	1.04108619	3.60345067
H	0.67363501	0.41396993	5.34708266
C	2.07261506	-0.63978389	1.87987630
H	1.19512693	-2.56927497	2.28291677
C	2.28497041	0.66046891	2.35033809
H	1.95519606	2.05218381	3.97396372
H	2.46237354	-0.93884363	0.90697144
H	2.83880179	1.37610556	1.74321035
C	-0.60608107	-3.67639419	3.87659927
C	-1.39925276	-3.38716991	2.75212568
C	-0.30342840	-5.01409335	4.17739017
C	-1.87503201	-4.41723825	1.94111154
H	-1.63486972	-2.35453776	2.50683071
C	-0.77921723	-6.04137789	3.36056157
H	0.29178920	-5.25413489	5.05466027
C	-1.56632352	-5.74560130	2.24389984
H	-2.49070121	-4.19285724	1.07334601
H	-0.54912483	-7.07604029	3.60841101
H	-1.95512392	-6.54615117	1.61610281
C	1.10428094	-3.00820145	6.14589119
C	0.69851103	-3.36834993	7.43947742
C	2.41479166	-3.27687649	5.72194987
C	1.59592127	-4.00608017	8.29947792
H	-0.31686800	-3.13790877	7.75193568
C	3.30808436	-3.91940560	6.58367135
H	2.73778612	-2.98589529	4.72399859
C	2.89821587	-4.28844195	7.87058812
H	4.32433468	-4.13032565	6.25189392
H	3.59565517	-4.79108525	8.54025633
H	-3.32375622	-1.35729733	6.14645058
H	1.27907306	-4.28527285	9.30410866
H	-2.12260852	0.71516350	6.78067376
H	-6.38552464	-7.77850879	2.13126017
H	-4.34362754	-6.83044854	2.84394190
H	-6.77783626	-1.10564854	0.17153031
H	-8.70604893	-8.53458300	2.63056405
H	-3.92832397	1.92764378	3.00747241
C	-3.21455606	1.08077685	4.90441006
C	-4.62727904	1.05513345	5.51927461
C	-2.18262568	1.46959973	5.98637736
C	-3.17365331	2.13970255	3.77786964
H	-5.37538595	0.75898643	4.77367375
H	-4.69120177	0.34453551	6.35343372
H	-4.87826017	2.05673428	5.90053694
C	-4.61253812	-1.64594118	3.02398902
C	-7.05370173	-3.09415576	1.04946044
C	-7.35848440	-1.58508251	0.97358654
C	-7.46526654	-3.76295908	-0.28708490
C	-7.87647815	-3.75702986	2.17856047
H	-7.12379346	-1.08407161	1.92057431
H	-8.42697181	-1.43827375	0.75804103
H	-7.18759220	-4.82546908	-0.29465148
H	-8.55369818	-3.68495126	-0.42142556
H	-6.97534110	-3.27095711	-1.14106233
H	-8.94589583	-3.58537408	1.98465208
H	-7.71290253	-4.84244221	2.21218339
H	-7.62393975	-3.33994710	3.15727059
C	-5.11545097	-4.72705881	1.67314175
O	-4.97077905	-5.64326852	0.84268317
N	-4.96464948	-4.87403047	3.00565557
H	-5.29020297	-4.09281256	3.59998859
H	-3.37848746	3.13909076	4.18920047
H	-2.18193185	2.16560336	3.29918857
H	-1.18044423	1.57334737	5.55006751
H	-2.46324917	2.43479736	6.43391646
C	-3.79800689	-6.13963114	4.79624305
C	-3.49129886	-4.95143317	5.46267672
C	-2.58733419	-4.94062284	6.52907557
C	-1.98621732	-6.12784490	6.95002036
C	-2.30529606	-7.32885604	6.30244276
C	-3.20520731	-7.33277739	5.23457665
H	-3.94347935	-4.01775887	5.14954874
H	-2.33553341	-3.99223924	6.99887340
H	-1.26328500	-6.11916477	7.76537623
H	-1.83869002	-8.26144413	6.62022358
C	-6.14375130	-6.74517276	4.00695701
C	-6.75374440	-6.39127679	5.21722864
C	-8.06222026	-6.79762134	5.49347061
C	-8.77023899	-7.56846030	4.56354319
C	-8.16084057	-7.93299535	3.35787889
C	-6.85363246	-7.52106979	3.08052117
H	-6.20436217	-5.79559979	5.94472033
H	-8.53002515	-6.51337337	6.43605114
H	-9.79041250	-7.88550605	4.77920880
H	-5.11922268	-3.30067936	0.14911940

5_72

E = -6218.59

G = -6105.62

Nimag = 0

C	-0.24706330	0.46103318	0.50853140
C	-0.04171670	1.91516773	0.16056872
C	0.98988053	0.80356164	0.33924935
H	-2.11814394	3.05889310	-3.14216978
C	-0.16568185	2.91254987	1.29165283
C	-0.35914935	2.33366059	-1.25574580
H	-2.20278839	4.72874692	-2.46651525
C	2.44875803	0.61876661	0.30652699
C	-1.25651960	-0.55555982	0.77729617
O	-0.65608645	2.65015600	2.38157421
O	0.40971556	4.09684400	0.96993591
C	0.34844723	5.12383973	2.01602409

H	0.86012732	5.98949074	1.59083588
H	0.85731212	4.76736461	2.91718964
H	-0.69706076	5.35627742	2.24268095
O	0.03334074	1.72811200	-2.24419924
O	-1.18018681	3.41128583	-1.28928232
C	-1.56795821	3.85622211	-2.63254575
H	-0.67443650	4.12175870	-3.20623348
O	-0.99549301	-1.70438593	1.11649532
O	-2.50186412	-0.05305807	0.59270412
C	-3.59274459	-1.00627249	0.83276346
H	-3.49747893	-1.85490709	0.14836335
H	-4.50556357	-0.44082302	0.63706718
H	-3.55590935	-1.35223298	1.87048795
C	3.13270305	1.50162728	-0.75475683
H	2.66766615	-0.44853785	0.15181849
H	2.83303107	0.87588081	1.31012745
H	4.21906814	1.34909058	-0.72410457
H	2.92156190	2.56231592	-0.56219684
H	2.76189214	1.25448640	-1.75693075

5_73

E = -5946.47

G = -5835.87

Nimag = 0

C	-0.27477435	0.45133390	0.43307219
C	-0.05709304	1.91648718	0.10481878
C	0.96681100	0.80259608	0.29859957
H	-2.03369004	3.16143402	-3.21896153
C	-0.23272650	2.89904916	1.24116856
C	-0.33782351	2.35100832	-1.31125200
H	-2.06395793	4.82894804	-2.53315853
C	2.42644664	0.62417215	0.29770088
C	-1.34121973	-0.52463340	0.67412443
O	-0.83766419	2.64197780	2.27417191
O	0.41834832	4.06186744	0.99802960
C	0.29599105	5.07744240	2.05054474
H	0.87185237	5.93065800	1.68673911
H	0.70953316	4.69222626	2.98792129
H	-0.75764075	5.34184476	2.18572029
O	0.03426795	1.73006277	-2.29826090
O	-1.10955971	3.46603880	-1.34989006
C	-1.46086363	3.93352942	-2.69572096
H	-0.54966861	4.16786976	-3.25495536
O	-1.06602352	-1.69089367	0.97227053
C	-2.74368994	0.00663259	0.53509177
H	2.78672646	0.88135016	1.31041751
H	4.21561205	1.36917330	-0.68907561
H	2.90520940	2.57208614	-0.55742459
H	2.78547675	1.26352292	-1.75720297
C	3.12917943	1.51328829	-0.74590806
H	2.65252757	-0.44199164	0.14594326
H	-2.88299666	0.84503012	1.23352593
H	-3.47436652	-0.78433738	0.73319735
H	-2.88698654	0.40743580	-0.48013671

TS5_53

E = -25999.87

G = -25398.01

Nimag = 1, 1574 i cm–1

C	-6.28125149	-2.27744247	2.49276532
N	-5.09046372	-1.42342164	2.44103782
H	-4.61189622	-1.39451090	1.53055142
C	-4.61178241	-5.59770467	3.38469091
S	-4.79196138	-1.44529507	5.13594075
N	-3.07857209	-0.65763519	3.18940412
H	-2.99194174	-0.36938957	2.21392212
C	-2.08455463	-0.05883115	4.08249243
H	-2.60134419	0.18445354	5.01943414
H	-2.08380520	-5.59605332	2.34871877
C	-1.53544618	1.25423040	3.42333085
N	-2.48444013	1.93205210	2.52747636
H	-0.67010784	1.01761794	2.79523850
P	-3.66421607	2.90551795	3.04498538
C	-3.07703963	4.55276438	3.57115955
C	-1.81185067	4.97573237	3.13486405
C	-3.86063188	5.39536647	4.37780332
C	-1.33846428	6.24041002	3.49239072
H	-1.20303378	4.31361787	2.52489746
C	-3.38635380	6.66224265	4.72423792
H	-4.83049915	5.05956597	4.74064187
C	-2.12666173	7.08497096	4.28196779
H	-0.35373632	6.56463414	3.15796354
H	-3.99578980	7.31726304	5.34589123
H	-1.75648562	8.07121245	4.55987676
C	-4.64917439	2.31950898	4.45369305
C	-4.07550417	2.32743766	5.73819684
C	-5.97506723	1.89942487	4.27953312
C	-4.82842871	1.91190977	6.83466148
H	-3.05355507	2.67478247	5.88226501
C	-6.72260659	1.48689702	5.38367208
H	-6.42352269	1.90206516	3.29154033
C	-6.15335663	1.49642950	6.65882663
H	-4.38222596	1.91276382	7.82846715
H	-7.75020935	1.15545273	5.24474393
H	-6.73845890	1.17087641	7.51833446
C	-4.77892110	3.11123659	1.62872948
C	-4.98076055	2.02161390	0.76343803
C	-5.46856012	4.31577941	1.42064574
C	-5.87852979	2.14063224	-0.29781947
H	-4.42863006	1.09721763	0.90051410
C	-6.36532477	4.42461178	0.35479726
H	-5.30069741	5.16773644	2.07563896
C	-6.57332128	3.33730611	-0.50165824
H	-6.89757818	5.36082247	0.19068513
H	-7.27371293	3.42600421	-1.33156619
H	-1.16612021	1.91219191	4.22399309
H	-6.03293176	1.29519458	-0.96577329
H	0.75659480	0.37747704	4.37988404
H	-4.07251339	-8.22162186	3.78673800
H	-4.41960439	-5.84276849	2.32972394
H	-6.96353585	0.34041011	1.92120684
H	-6.65476268	-2.20097908	3.52299532
H	-2.23896445	-2.72901075	4.97820157
C	-0.92039311	-1.06581381	4.41399797
C	-0.43726311	-1.77405669	3.13189363
C	0.25312731	-0.30460836	5.07689166
C	-1.41946274	-2.13947553	5.40116702
H	-1.21039286	-2.44827760	2.74734760
H	-0.18124214	-1.06592672	2.33859797
H	0.45479480	-2.37816599	3.34959774
C	-4.29810203	-1.15728006	3.52769544
C	-7.40710152	-1.76725368	1.54900927
C	-7.80599522	-0.35089846	2.02196232
C	-6.95907334	-1.69665343	0.07148533
C	-8.62247848	-2.71017689	1.69545208
H	-8.12135032	-0.36025654	3.07549125
H	-8.63752346	0.02977729	1.41118668
H	-6.67919966	-2.68899406	-0.29785752
H	-7.78285086	-1.30189411	-0.54201032
H	-6.09986497	-1.02622663	-0.05385647
H	-9.46692623	-2.32644567	1.10451025
H	-8.38346710	-3.72156860	1.34474370
H	-8.94406579	-2.76973833	2.74693385
C	-5.82169464	-3.74569897	2.27383055
O	-5.95204539	-4.38110516	1.21696036
N	-5.21202880	-4.26089944	3.37954009
H	-5.06117781	-3.63934835	4.18760783
H	-0.59727723	-2.82604695	5.64246006
H	-1.78296630	-1.68216451	6.33211946
H	-0.09437248	0.27616734	5.94556618
H	1.00039344	-1.02813866	5.43497353
C	-3.28750379	-5.57402988	4.13638738
C	-3.26639897	-5.55930011	5.53798552
C	-2.05197947	-5.55647875	6.22668791
C	-0.84404084	-5.57482086	5.52045637
C	-0.85739765	-5.57890712	4.12362477
C	-2.07552875	-5.57905312	3.43675287
H	-4.20555026	-5.56811639	6.09055655
H	-2.04712864	-5.54210107	7.31645220
H	0.10341118	-5.57559119	6.05884952

H	0.07869654	-5.58118824	3.56593876
C	-5.56358360	-6.66571075	3.93347718
C	-6.87837885	-6.36898991	4.30427075
C	-7.72001793	-7.37275142	4.80110375
C	-7.25407047	-8.68425391	4.92591855
C	-5.93855633	-8.98838532	4.55019874
C	-5.10067891	-7.98479860	4.06024032
H	-7.24633226	-5.35006213	4.20942976
H	-8.74145197	-7.12559891	5.09061458
H	-7.90803526	-9.46529129	5.31295853
H	-5.56522091	-10.00801227	4.64419692
C	-1.34016183	-0.15469696	-0.31381546
C	0.06782299	0.31995091	-0.53602431
C	-1.18857814	1.16347856	-0.28868101
H	2.42499820	-1.00608900	2.51066078
C	0.60589599	0.32971613	-1.95000225
C	1.08410101	0.25616925	0.58217849
H	3.39532446	-1.92435429	1.30089899
C	-1.60268747	2.47059142	-0.02186123
C	-2.26503821	-1.19974655	-0.08086592
O	-0.05492729	0.07398969	-2.94599960
O	1.90253047	0.74108872	-1.97345101
C	2.50599205	0.82895014	-3.30569996
H	3.52909618	1.16817178	-3.13069167
H	1.95253597	1.54781297	-3.91839744
H	2.49481566	-0.15594989	-3.78360609
O	1.17697643	1.07573128	1.48831508
O	1.85317821	-0.85943685	0.48887746
C	2.88753886	-0.98275091	1.52014500
H	3.57931996	-0.13621405	1.45137339
O	-3.47464390	-0.98001750	0.14686525
O	-1.72854932	-2.45399239	-0.07958831
C	-2.66760470	-3.51138087	0.30342044
H	-2.94308488	-3.39640407	1.35667865
H	-2.11858116	-4.44301969	0.14968606
H	-3.56817045	-3.47635705	-0.31605328
C	-0.61093079	3.61301673	-0.20112690
H	-1.99017695	2.24415613	1.33993281
H	-2.63129151	2.67939589	-0.34379668
H	-1.02171953	4.54846232	0.20246480
H	-0.36957091	3.79196525	-1.26198471
H	0.32593626	3.38895924	0.32720708

TS5_54

E = -25997.80

G = -25397.61

Nimag = 1, 1627 i cm–1

C	-4.92449829	-2.37021474	4.51885528
N	-4.26859868	-1.38319343	3.66534320
H	-4.34669524	-1.51648542	2.65288536
C	-2.17635152	-4.77262230	5.64357638
S	-3.01138384	-0.24783932	5.76640916
N	-2.73970605	0.17372850	3.06779138
H	-3.09883963	-0.11881309	2.15408479
C	-1.90012830	1.38155105	2.98690140
H	-1.49086444	1.32826387	1.97337137
H	0.47312972	-4.36800782	5.05745185
C	-0.69258407	1.37055773	3.93357674
N	0.27182646	0.30207633	3.56803337
H	-1.03436621	1.26376564	4.97017502
P	1.66750858	0.20606594	4.37461798
C	1.47029445	-0.11443993	6.15377086
C	0.28686593	-0.73806081	6.57504147
C	2.44232291	0.26943717	7.09343952
C	0.06195958	-0.95081670	7.93392105
H	-0.47058394	-1.01888147	5.84944021
C	2.22244670	0.02439697	8.45074523
H	3.35605064	0.76429703	6.76811899
C	1.02919436	-0.57768502	8.87024480
H	-0.86434917	-1.41960305	8.25576181
H	2.97564591	0.31508810	9.18254709
H	0.85745809	-0.75794324	9.93109447
C	2.66551069	1.73373877	4.28799169
C	2.17112800	2.89088628	4.92131790
C	3.85205531	1.80612829	3.54082793
C	2.83765765	4.10796501	4.77399919
H	1.27887396	2.83781975	5.54190196
C	4.52026751	3.02576819	3.40618675
H	4.25901381	0.91510771	3.06971955
C	4.00924596	4.17831792	4.01077451
H	2.44644277	5.00071727	5.26048575
H	5.44242851	3.07409583	2.82792771
H	4.52821317	5.12946892	3.89733811
C	2.63637836	-1.14309358	3.64983379
C	2.91027766	-1.15400766	2.27045408
C	3.10291732	-2.18226853	4.46777266
C	3.64647186	-2.20352488	1.72058761
H	2.51585564	-0.37348481	1.62560542
C	3.83040500	-3.23536411	3.90745284
H	2.88707784	-2.17124707	5.53181521
C	4.10443381	-3.24569664	2.53618201
H	4.18197147	-4.04846810	4.54115491
H	4.67157006	-4.06800245	2.10114074
H	-0.20349572	2.34596907	3.82584631
H	3.85049758	-2.21482776	0.65039783
H	-1.09926868	4.13880427	3.39683579
H	-1.20214352	-7.26974414	5.32052874
H	-1.75921376	-4.93758882	4.64033235
H	-6.71909974	-0.42609325	3.82151087
H	-4.90950909	-1.94523958	5.53015276
H	-4.54735913	1.77631922	2.16087234
C	-2.73901477	2.71296017	2.99826953
C	-3.38843824	2.99455152	4.36662533
C	-1.81774874	3.89331361	2.60297893
C	-3.84127871	2.58125829	1.91915544
H	-4.07059543	2.18757714	4.65857139
H	-2.63264265	3.09516635	5.15758557
H	-3.95991780	3.93435152	4.31680819
C	-3.34408738	-0.46914905	4.09536846
C	-6.41693093	-2.57710227	4.12572338
C	-7.15672227	-1.24822740	4.40419193
C	-6.59116635	-2.96021629	2.63857057
C	-6.99906482	-3.68690339	5.03012305
H	-7.09826883	-0.98188383	5.47006372
H	-8.21701861	-1.34279299	4.12850334
H	-6.03391340	-3.87421038	2.40527351
H	-7.65823684	-3.12608959	2.42746785
H	-6.24724402	-2.15722144	1.97060428
H	-8.08027998	-3.78423656	4.85489821
H	-6.52659871	-4.65574036	4.82473087
H	-6.84845395	-3.44299491	6.09303029
C	-4.06331190	-3.65690245	4.53866565
O	-4.16441844	-4.57942837	3.71940922
N	-3.14847389	-3.67384152	5.55422880
H	-2.95304545	-2.78472220	6.03094974
H	-4.40768367	3.52109255	1.84681344
H	-3.39748678	2.36934447	0.93531425
H	-1.26114355	3.66673125	1.68341458
H	-2.42874494	4.79064348	2.42469735
C	-1.03901441	-4.42816932	6.59796173
C	-1.27739935	-4.33406525	7.97778435
C	-0.22174987	-4.12833599	8.86759526
C	1.08975952	-4.02632567	8.39025421
C	1.33312099	-4.11282431	7.01877823
C	0.27376958	-4.30228787	6.12557116
H	-2.29148714	-4.44981945	8.35800740
H	-0.42153321	-4.05257931	9.93633591
H	1.91464585	-3.86762433	9.08348259
H	2.35129662	-4.03986595	6.64353479
C	-2.83776062	-6.08309527	6.07868804
C	-4.06261553	-6.11134967	6.75221131
C	-4.60599155	-7.32657410	7.18251702
C	-3.92848562	-8.52616776	6.94084173
C	-2.70159429	-8.50219868	6.26502093
C	-2.16093761	-7.28628435	5.83944911
H	-4.59787703	-5.18186010	6.93208494
H	-5.56348805	-7.33565491	7.70331331
H	-4.35350848	-9.47334189	7.27193628
H	-2.16759530	-9.43180189	6.06859208
C	-1.75761457	-0.83016894	0.02164327

C	-0.35452806	-0.47630019	-0.37969872
C	-0.81480496	-1.31603724	0.81962078
H	1.68639252	-3.08759466	-2.75552928
C	0.10145139	0.94236178	-0.08300275
C	0.32580044	-1.12439449	-1.55237399
H	0.23720690	-4.15912406	-2.72882042
C	-0.28075335	-1.87632297	1.98090554
C	-3.13857791	-0.58353426	-0.19232099
O	-0.64790792	1.90723344	-0.03806242
O	1.42538355	1.00152415	0.21793712
C	1.90651354	2.32356688	0.63368509
H	2.98761105	2.21420846	0.73348472
H	1.45723721	2.58593895	1.59632472
H	1.65179320	3.07196533	-0.12302797
O	1.05721500	-0.53006356	-2.33693996
O	0.01238114	-2.44266955	-1.65090285
C	0.59333406	-3.12971867	-2.80566890
H	0.24552654	-2.66198785	-3.73246872
O	-4.03478536	-0.87334838	0.62814338
O	-3.39827455	0.04688599	-1.37531187
C	-4.80077985	0.41066156	-1.57864021
H	-5.42641893	-0.48792818	-1.59238155
H	-4.82191107	0.91758472	-2.54597913
H	-5.13208896	1.07990281	-0.77789387
H	0.75572325	-2.20129106	1.86182850
C	-1.13853934	-2.81000846	2.82970466
H	-0.05285643	-0.71029764	2.77188723
H	-1.37106208	-3.73701150	2.28605947
H	-2.08808595	-2.34763777	3.11219284
H	-0.61441845	-3.08304178	3.75246791

TS5_55
E = -25984.68
G = -25383.55
Nimag = 1, 1416 i cm–1

C	-4.74995684	-1.02220424	0.61455250
N	-4.38370914	-0.84182124	2.04060834
H	-3.57129112	-0.21851698	2.10829538
C	-8.08133989	0.89443533	0.63462011
S	-6.52595607	-1.90792822	3.35790986
N	-4.33250311	-0.69177728	4.32558454
H	-3.44142854	-0.22255867	4.14570601
C	-5.01404349	-0.23363955	5.54759776
H	-6.07409958	-0.47869882	5.39644104
H	-8.61327645	0.29002890	-1.96543348
C	-4.96226633	1.31221418	5.59125080
N	-3.64113943	1.93087583	5.28033956
H	-5.34865975	1.64825078	6.56221685
P	-3.72717645	3.47856236	4.77037822
C	-4.20080009	4.65688094	6.08151378
C	-4.30717635	4.17734323	7.39575393
C	-4.36962784	6.02928439	5.82293011
C	-4.61040601	5.05569589	8.43992608
H	-4.12831436	3.12503690	7.60078834
C	-4.67028540	6.90212991	6.86888690
H	-4.24523329	6.41823003	4.81388872
C	-4.79803688	6.41565892	8.17604389
H	-4.69281953	4.67818389	9.45830630
H	-4.79729173	7.96483001	6.66618243
H	-5.03340755	7.10038382	8.99000279
C	-4.91084805	3.67659361	3.39347396
C	-5.99292650	4.57063558	3.45184461
C	-4.70548343	2.91343998	2.22668385
C	-6.81793090	4.74441672	2.33876140
H	-6.20912226	5.11773745	4.36433750
C	-5.52208947	3.10690291	1.11468289
H	-3.91801066	2.16767804	2.18317815
C	-6.57091326	4.03136755	1.16553013
H	-7.66778411	5.42115819	2.40109067
H	-5.35385024	2.51977877	0.21441792
H	-7.21532313	4.16989069	0.29892431
C	-2.07425682	4.02236649	4.22936106
C	-1.49787397	3.48898018	3.06373212
C	-1.33136829	4.90465467	5.03464329
C	-0.18572506	3.81553789	2.72463306
H	-2.03086029	2.77655796	2.44587318
C	-0.02108785	5.23395274	4.68010591
H	-1.75854654	5.31424936	5.94572303
C	0.55549979	4.68588591	3.53015056
H	0.55307466	5.90904991	5.31348309
H	1.58373889	4.93106924	3.26638168
H	-5.68233548	1.65423816	4.83390075
H	0.26247382	3.37257166	1.83653844
H	-4.98283775	0.55852645	8.32962339
H	-10.14064968	2.63204378	0.65323976
H	-7.78852475	1.57592985	-0.17521135
H	-4.62745987	-3.59155460	1.91427806
H	-3.85257091	-0.63906860	0.11821099
H	-4.59396313	-2.91017952	5.73298243
C	-4.58996388	-1.01536604	6.83299500
C	-3.07865007	-0.93569948	7.08690016
C	-5.34432619	-0.44158732	8.05421883
C	-5.01724281	-2.48911041	6.64959201
H	-2.51052719	-1.29657015	6.22313553
H	-2.76900234	0.09303032	7.29327868
H	-2.80327910	-1.55446929	7.95345711
C	-5.01736756	-1.10654231	3.21137635
C	-4.95445862	-2.49224466	0.05612266
C	-4.16193933	-3.48515007	0.92800246
C	-6.43803839	-2.92123036	-0.03247011
C	-4.37622685	-2.49760613	-1.38097411
H	-3.12270607	-3.15591449	1.06815113
H	-4.15073117	-4.47240437	0.44298309
H	-7.00964141	-2.25762715	-0.69558859
H	-6.48757451	-3.93700929	-0.45259479
H	-6.91805012	-2.92170731	0.95095131
H	-4.55284473	-3.47672074	-1.84918544
H	-4.85137878	-1.72289387	-1.99741636
H	-3.29194884	-2.31629888	-1.37257336
C	-5.85129759	-0.05142169	0.12652821
O	-5.73789275	0.51779796	-0.97468882
N	-6.88326265	0.12594725	0.97671572
H	-6.97190072	-0.56003437	1.74820997
H	-4.67329157	-3.08875484	7.50510024
H	-6.11053355	-2.57289411	6.57773906
H	-6.42679074	-0.38089865	7.86331783
H	-5.19041560	-1.09822811	8.92288215
C	-9.12879154	-0.07688969	0.09512199
C	-9.90492782	-0.84451098	0.97350714
C	-10.76785782	-1.82485351	0.47844405
C	-10.86707331	-2.04136304	-0.90184000
C	-10.09973389	-1.27141982	-1.78244202
C	-9.23168995	-0.29399724	-1.28435683
H	-9.82850616	-0.67615953	2.04700856
H	-11.36432221	-2.42125027	1.16880686
H	-11.54060031	-2.80613684	-1.28815452
H	-10.17337355	-1.43494071	-2.85758894
C	-8.57536122	1.71358535	1.82128520
C	-7.97958689	1.64106582	3.08390053
C	-8.46105836	2.41747491	4.14145686
C	-9.54186209	3.28065740	3.94762908
C	-10.14307800	3.35868160	2.68512230
C	-9.66521976	2.57558374	1.63295781
H	-7.12449025	0.99373714	3.24142078
H	-7.97990690	2.35832036	5.11705252
H	-9.91069115	3.89336863	4.76987359
H	-10.98444688	4.03194943	2.52107506
C	-0.72097427	0.04786124	3.20748974
C	0.03503965	-0.85484201	4.14326810
C	-0.71478726	0.45307960	4.46855796
H	-2.44753517	-3.76507312	5.33765098
C	1.54150697	-0.74369825	4.14926203
C	-0.56314506	-2.16952659	4.56608041
H	-3.37861355	-3.59862080	3.80582027
C	-0.96930348	1.27710073	5.57171573
C	-1.11114485	0.13387029	1.84955844
O	2.14387430	0.30873434	4.31174604
O	2.14144438	-1.93396498	3.88267585
C	3.60506745	-1.89328123	3.84000906
H	3.90954123	-2.91930904	3.62265609

H	3.99630070	-1.56539000	4.80868861
H	3.93727311	-1.20884467	3.05264480
O	-0.10207069	-2.89811535	5.43563067
O	-1.71142534	-2.43150990	3.88186355
C	-2.38684757	-3.67379327	4.25015951
H	-1.83479923	-4.52459528	3.83368705
O	-2.05769345	0.82018619	1.41150564
O	-0.35766768	-0.68151315	1.04674552
C	-0.73855813	-0.68421708	-0.36301003
H	-1.74475718	-1.09479390	-0.47892883
H	-0.00447442	-1.32729804	-0.85385121
H	-0.70784692	0.33179738	-0.76993972
C	-0.27678276	0.92344351	6.88428256
H	-2.43746463	1.47508425	5.55329483
H	-0.84972644	2.33080929	5.30882664
H	-0.74513302	1.44925602	7.72910348
H	0.78827569	1.20569563	6.85627620
H	-0.32880974	-0.15382709	7.08695887

TS5_56
E = -25989.54
G = -25386.60
Nimag = 1, 1624 i cm–1

C	-4.93037947	-3.07290425	4.90874835
N	-4.05755583	-2.15236406	4.13966050
H	-4.25419733	-2.20393060	3.13591142
C	-7.07054543	-0.36303313	6.61267265
S	-2.88335844	-0.69264936	6.11164978
N	-2.82606761	-0.40539184	3.40237107
H	-3.19347992	-0.76587697	2.51595219
C	-2.14954882	0.89725655	3.25312625
H	-1.80985723	0.87922326	2.21255705
H	-6.30134294	-1.11408857	9.08992910
C	-0.88407971	1.03633570	4.11065972
N	0.16870601	0.08573334	3.66705438
H	-1.14212557	0.88787568	5.16534907
P	1.52779397	0.00595283	4.53407429
C	1.33646091	-0.72622932	6.18950925
C	0.33473476	-1.69500954	6.35330771
C	2.17584606	-0.38845338	7.26457561
C	0.17309369	-2.32739444	7.58689417
H	-0.32875970	-1.92681378	5.52737133
C	2.01304962	-1.02883524	8.49508513
H	2.94911050	0.36781341	7.14045823
C	1.01347653	-1.99795077	8.65536245
H	-0.61778868	-3.06430698	7.71456432
H	2.66204315	-0.76974817	9.33085091
H	0.88658622	-2.49086095	9.61889312
C	2.26586341	1.65192054	4.79882549
C	1.62058176	2.54719012	5.67287902
C	3.37239120	2.08537006	4.05025817
C	2.07111135	3.86348008	5.78209960
H	0.77451764	2.21492807	6.27172669
C	3.82031749	3.40358141	4.16750460
H	3.88758732	1.39629115	3.38535813
C	3.16788070	4.29444305	5.02625616
H	1.56660616	4.55288593	6.45800569
H	4.68238834	3.73400575	3.58897943
H	3.51749973	5.32260370	5.11246561
C	2.71788445	-1.01439256	3.62255665
C	2.89700120	-0.80263822	2.24406690
C	3.48226868	-1.98445047	4.28946301
C	3.83501317	-1.55926889	1.54200808
H	2.28003562	-0.08152977	1.71850021
C	4.41959257	-2.73893244	3.57755916
H	3.34063112	-2.16019450	5.35321943
C	4.59787565	-2.52661070	2.20680339
H	5.00618934	-3.49682384	4.09517542
H	5.32660569	-3.11926272	1.65478643
H	-0.51440215	2.06125751	3.98407646
H	3.96267463	-1.40039788	0.47179186
H	-1.70520515	3.73328874	3.75204430
H	-9.43911737	0.93415893	6.81605212
H	-7.81233715	-1.02568951	7.08633629
H	-5.39617748	-3.49646803	7.72951199
H	-5.32610658	-3.71025094	4.10935484
H	-4.78703662	0.95785124	2.41840225
C	-3.14505088	2.11781623	3.31349707
C	-3.82071107	2.28906091	4.68690769
C	-2.38278140	3.41508112	2.94815267
C	-4.22968773	1.88316218	2.23346829
H	-4.42618669	1.41878119	4.95221260
H	-3.08678799	2.43382302	5.49007613
H	-4.48414340	3.16685542	4.65982189
C	-3.27598713	-1.07852433	4.49284845
C	-4.26719160	-4.08265022	5.94067847
C	-4.35088192	-3.61537026	7.41149278
C	-5.06482543	-5.40592047	5.81709014
C	-2.79918588	-4.33696189	5.54984655
H	-3.82945114	-2.66501768	7.55829491
H	-3.88936512	-4.37975985	8.05473634
H	-4.95976077	-5.83390661	4.80876712
H	-4.68863907	-6.13930488	6.54519418
H	-6.13308815	-5.23743037	6.01090093
H	-2.38128814	-5.12559556	6.19330846
H	-2.71600788	-4.66531958	4.50508883
H	-2.20124955	-3.42881651	5.67642234
C	-6.20326955	-2.39085941	5.47084566
O	-7.31836391	-2.92899376	5.35041704
N	-5.99880528	-1.20256517	6.07568446
H	-5.02546746	-0.89424141	6.23474489
H	-4.94721214	2.71560399	2.23742496
H	-3.77477514	1.81835103	1.23456514
H	-1.80296803	3.28586822	2.02426680
H	-3.10661231	4.22789845	2.78718564
C	-6.42653038	0.51838633	7.68352427
C	-6.08973337	1.85346092	7.43733230
C	-5.38839160	2.59372679	8.39495564
C	-5.02236385	2.00500503	9.60866796
C	-5.36268271	0.66995459	9.86289654
C	-6.05813501	-0.06808393	8.90347620
H	-6.36416148	2.31458784	6.49233373
H	-5.12332481	3.63026695	8.18771823
H	-4.47515372	2.58111683	10.35462509
H	-5.08125788	0.20430928	10.80728150
C	-7.78051970	0.43856001	5.52588183
C	-7.21816743	0.61588169	4.25850830
C	-7.85666320	1.41394987	3.30391898
C	-9.06961217	2.03902705	3.60874998
C	-9.64204100	1.85859870	4.87496867
C	-8.99941410	1.06271256	5.82620859
H	-6.27555452	0.13226303	4.02038973
H	-7.40385004	1.55003961	2.32310686
H	-9.56866376	2.66064190	2.86575435
H	-10.58905472	2.33923160	5.12002334
C	-1.98682247	-1.06156291	0.20756751
C	-0.69298684	-0.50676255	-0.30836595
C	-0.90839581	-1.46644761	0.86852622
H	0.47369804	-0.98605842	-4.18060270
C	-0.36979962	0.93391464	0.04599030
C	-0.08477168	-1.08299903	-1.55964092
H	1.74313666	0.26352299	-3.90244680
C	-0.18145761	-2.01857607	1.92461948
C	-3.40426418	-1.00364326	0.14546086
O	-1.19052606	1.83955714	0.08239754
O	0.93260151	1.07994395	0.41378962
C	1.29388963	2.40328079	0.93009130
H	2.37975754	2.37912678	1.04532866
H	0.81092426	2.55428215	1.90016220
H	0.98842303	3.18299107	0.22577839
O	-0.20152051	-2.24821333	-1.91178570
O	0.60335320	-0.13743247	-2.25683766
C	1.23669611	-0.61180831	-3.49066739
H	1.95216691	-1.40733094	-3.25861359
O	-4.15969963	-1.46814808	1.02548331
O	-3.86969556	-0.35074957	-0.95898821
C	-5.32298653	-0.19401291	-1.01427113
H	-5.80824470	-1.17514898	-1.04829658
H	-5.51029601	0.36714224	-1.93262890
H	-5.67149919	0.36228647	-0.13840525

H	0.87515163	-2.17468728	1.68567293
C	-0.80900680	-3.13480699	2.75335002
H	-0.06488564	-0.89246543	2.79709748
H	-0.24011688	-3.28678170	3.68075507
H	-0.81836334	-4.09177070	2.20684894
H	-1.83879171	-2.89548937	3.03147898

TS5_57

E = -25998.51

G = -25397.20

Nimag = 1, 1680 i cm–1

C	-6.11807436	-2.31349277	2.14153568
N	-4.93066190	-1.52811439	2.51820815
H	-4.07103809	-1.77518058	2.01249323
C	-5.20355367	-5.35297275	4.25978477
S	-5.95947357	-0.99664378	4.97101685
N	-3.42761073	-0.73167057	4.05197433
H	-2.74716275	-0.93550089	3.31236691
C	-2.97406876	-0.01085620	5.23717520
H	-3.89053089	0.21456263	5.79532258
H	-3.27164502	-4.16288189	2.71773482
C	-2.28070504	1.34020901	4.84240424
N	-2.66287194	1.84779269	3.52049539
H	-1.19506404	1.18858019	4.79694756
P	-3.84777316	2.90514339	3.26953226
C	-3.41631844	4.63623860	3.66854998
C	-2.07542626	5.02475210	3.51285370
C	-4.37765606	5.57943047	4.06696049
C	-1.69950449	6.34832320	3.75024429
H	-1.33389898	4.28950350	3.21125845
C	-3.99630953	6.90358729	4.30124375
H	-5.41616166	5.28166795	4.19662805
C	-2.66007295	7.28828389	4.14343413
H	-0.65856692	6.64657943	3.63074304
H	-4.74251168	7.63455717	4.61073917
H	-2.36606761	8.32081528	4.32928235
C	-5.39453684	2.59277154	4.17443813
C	-5.41665605	2.75238611	5.57183047
C	-6.55321856	2.18186273	3.49967562
C	-6.59068519	2.50330956	6.28020852
H	-4.52618083	3.08463086	6.10283303
C	-7.72726650	1.94312846	4.21529783
H	-6.54210780	2.04998700	2.42240266
C	-7.74876405	2.10494076	5.60216842
H	-6.60435239	2.62340381	7.36298427
H	-8.62295497	1.61968133	3.68714538
H	-8.66504158	1.91172849	6.15924518
C	-4.24618026	2.84190204	1.50289655
C	-4.05329483	1.64347868	0.79845875
C	-4.87770980	3.93347619	0.88430337
C	-4.50477542	1.53657684	-0.51634426
H	-3.57148832	0.80434938	1.28925327
C	-5.34227732	3.81008153	-0.42634865
H	-5.01456601	4.86841624	1.42421933
C	-5.16170844	2.60968123	-1.12272640
H	-5.84056591	4.65250666	-0.90509988
H	-5.52332370	2.51512166	-2.14630739
H	-2.45069897	2.06777681	5.64843409
H	-4.34047298	0.61701764	-1.06958137
H	-1.05737305	0.75601176	7.18368217
H	-6.50609778	-7.69854591	4.79396600
H	-5.35989011	-6.11299587	3.48041251
H	-6.32645513	0.19362783	1.17227112
H	-6.88873445	-2.03691864	2.87264267
H	-3.13893739	-2.76534585	5.68295328
C	-2.06824581	-0.90992979	6.14567642
C	-0.79016459	-1.35716906	5.39969239
C	-1.68913654	-0.11309733	7.41418899
C	-2.86591988	-2.16733598	6.55824927
H	-1.03635414	-1.87095632	4.46247743
H	-0.12240040	-0.51482780	5.17330210
H	-0.22811123	-2.06829465	6.02186966
C	-4.71104647	-1.08341674	3.80183415
C	-6.65748786	-1.92323573	0.73807236
C	-7.13737816	-0.45623609	0.83187060
C	-5.58085261	-2.05277701	-0.36043312
C	-7.86378553	-2.82798176	0.40225400
H	-7.97133423	-0.36533780	1.54316789
H	-7.47394843	-0.09911078	-0.15205891
H	-5.28031433	-3.09854058	-0.48235616
H	-5.97659184	-1.68403262	-1.31825940
H	-4.69013087	-1.45790378	-0.12337808
H	-8.33134492	-2.49257552	-0.53510198
H	-7.55356298	-3.87312459	0.28514531
H	-8.62275013	-2.77387023	1.19803341
C	-5.76959834	-3.80763007	2.37410986
O	-5.48047042	-4.61794840	1.47870529
N	-5.73389396	-4.09800404	3.70332379
H	-5.89507045	-3.31752840	4.35471246
H	-2.25564500	-2.79964442	7.21860046
H	-3.78963228	-1.88921693	7.08284657
H	-2.59149426	0.24299414	7.93481731
H	-1.12947809	-0.75808769	8.10766428
C	-3.69286832	-5.25976256	4.53507144
C	-3.11894798	-5.82297131	5.68321986
C	-1.74010444	-5.73233486	5.90715806
C	-0.91796046	-5.08016925	4.98532339
C	-1.48364842	-4.52317601	3.83387371
C	-2.85741162	-4.61579245	3.60994194
H	-3.74744677	-6.32303515	6.41662276
H	-1.31349477	-6.16342595	6.81307898
H	0.15300397	-4.99474497	5.16790276
H	-0.86483113	-3.99278597	3.11264803
C	-6.00523531	-5.72278591	5.49621765
C	-6.12343669	-4.81044307	6.55702796
C	-6.83591747	-5.15192798	7.70809442
C	-7.43130163	-6.41548718	7.81690409
C	-7.31083142	-7.33068666	6.76693259
C	-6.60094253	-6.98286619	5.61065946
H	-5.64835433	-3.83228252	6.48987307
H	-6.92342151	-4.43456991	8.52390678
H	-7.98464568	-6.68370030	8.71659520
H	-7.77003296	-8.31596569	6.84491958
C	-1.17231902	-0.46913347	0.44569658
C	-0.46972076	0.51259015	-0.44138788
C	-0.68007684	0.59172469	1.06915907
H	2.75512990	-0.45607585	-2.71806022
C	-1.27761667	1.40177214	-1.36660229
C	0.94113560	0.20804472	-0.88689279
H	2.64580758	1.16625886	-3.49722736
C	-0.35965607	1.37242773	2.18784730
C	-1.76033114	-1.74463408	0.62988046
O	-2.02371077	1.00627515	-2.24956540
O	-1.06590683	2.71105579	-1.06635913
C	-1.76908576	3.67482917	-1.91590741
H	-1.46789057	3.53835519	-2.96007713
H	-1.46244681	4.65523338	-1.54439399
H	-2.84702340	3.53852350	-1.81267154
O	1.71456711	-0.51231330	-0.27296346
O	1.24187052	0.84714607	-2.04948120
C	2.59793910	0.61479531	-2.55607079
H	3.33148458	0.99686253	-1.83869476
O	-2.22854530	-2.12162659	1.72517940
O	-1.78692080	-2.52416019	-0.48592110
C	-2.30617979	-3.88070365	-0.27094728
H	-1.68718591	-4.40061028	0.46749239
H	-2.23681475	-4.36368528	-1.24825707
H	-3.34147025	-3.84689089	0.07686336
H	-0.10219953	0.74239869	3.05141444
H	-1.61337789	1.74015050	2.71270245
C	0.55925116	2.57554446	1.99228846
H	1.58454143	2.27543292	1.71940607
H	0.62439465	3.16543900	2.91751900
H	0.17485987	3.22450577	1.19436436

TS5_58

E = -25995.55

G = -25393.12

Nimag = 1, 1408 i cm–1

C	-4.82508125	-2.25784509	4.40341937

N	-4.31275252	-1.11111080	3.65554387
H	-4.37617912	-1.16300752	2.63434118
C	-1.80428577	-4.43832519	5.25662758
S	-3.11053748	-0.10475912	5.85370680
N	-2.92139406	0.61701535	3.21146159
H	-3.33301303	0.45720276	2.28411508
C	-1.89257965	1.67458241	3.19864784
H	-1.47029150	1.60020533	2.18701399
H	0.88554576	-3.97981021	5.10257526
C	-0.72854505	1.46014403	4.17427285
N	0.14541703	0.32124568	3.78250248
H	-1.11140975	1.33420687	5.19239231
P	1.55519622	0.17512033	4.56491120
C	1.42918396	-0.23442462	6.33247626
C	0.19976418	-0.71148541	6.80851375
C	2.50040627	-0.02858603	7.21883389
C	0.03004676	-0.94850391	8.17209313
H	-0.62975275	-0.86043264	6.12263271
C	2.33288197	-0.30243699	8.57755543
H	3.45154532	0.35608857	6.85263054
C	1.09429011	-0.74948985	9.05454268
H	-0.92997021	-1.30376698	8.53981795
H	3.16335709	-0.15251792	9.26673542
H	0.96426923	-0.94996217	10.11762715
C	2.48884039	1.74513239	4.52088436
C	2.12039607	2.77451940	5.40765678
C	3.43854905	2.00044812	3.51766474
C	2.68292655	4.04550408	5.27676563
H	1.40024952	2.58087425	6.20063863
C	4.00128348	3.27293104	3.39528018
H	3.74859319	1.20807962	2.84180587
C	3.61881902	4.29805520	4.26752617
H	2.38930484	4.83922031	5.96275804
H	4.74148567	3.46333090	2.61884956
H	4.05514449	5.29112799	4.16577075
C	2.52907889	-1.09800351	3.72925487
C	2.62455796	-1.05895878	2.33034535
C	3.19430613	-2.09955236	4.45201945
C	3.37731573	-2.01597643	1.65272457
H	2.07562228	-0.31361136	1.77112872
C	3.93727369	-3.06441580	3.76788332
H	3.11471446	-2.13464398	5.53437225
C	4.03185726	-3.02215017	2.37132522
H	4.43931598	-3.85464577	4.32486454
H	4.60877905	-3.78100225	1.84355606
H	-0.13632672	2.38157605	4.13993479
H	3.41975269	-1.98937866	0.56443318
H	-0.66081135	4.25137776	3.62479632
H	-0.55691260	-6.62051017	4.26129057
H	-1.27629859	-4.30678746	4.30464645
H	-6.88367319	-0.51470246	3.99393013
H	-4.84499383	-1.94797226	5.45510884
H	-4.51152740	2.50684661	2.56170982
C	-2.52757688	3.11079044	3.29676859
C	-3.05249166	3.40752195	4.71592280
C	-1.46819910	4.16149726	2.88582693
C	-3.69949694	3.19358453	2.29013481
H	-3.78717195	2.65396906	5.02714854
H	-2.23973124	3.40756213	5.45531048
H	-3.53217415	4.39807751	4.73811259
C	-3.44060342	-0.18185609	4.16660798
C	-6.28435333	-2.62295021	4.00283450
C	-7.19378933	-1.45986767	4.46062578
C	-6.44682588	-2.83523154	2.48090008
C	-6.67577781	-3.91144903	4.76174191
H	-7.15009627	-1.33425549	5.55287837
H	-8.23707162	-1.66195001	4.17757593
H	-5.76668255	-3.61592615	2.12257925
H	-7.48347409	-3.13267407	2.26284199
H	-6.24756093	-1.90945401	1.92159154
H	-7.73879800	-4.13749175	4.59412581
H	-6.08193859	-4.76951078	4.42145322
H	-6.52182873	-3.78855521	5.84488386
C	-3.80224588	-3.41117113	4.26272805
O	-3.75577543	-4.18427899	3.29805671
N	-2.92043441	-3.48160334	5.30779991
H	-2.83501962	-2.64695382	5.90105247
H	-4.10629647	4.21520046	2.27507731
H	-3.36273576	2.94157615	1.27346591
H	-1.01935329	3.90424234	1.91506502
H	-1.94354320	5.14928783	2.79532889
C	-0.82268538	-4.20805151	6.39874631
C	-1.24969099	-4.28020369	7.73316107
C	-0.32697737	-4.19431309	8.77700182
C	1.03649879	-4.04053219	8.50053365
C	1.46687001	-3.95784315	7.17576832
C	0.54146228	-4.03885198	6.13144137
H	-2.30586430	-4.42556384	7.95552355
H	-0.67159949	-4.24874206	9.80946551
H	1.75593942	-3.96872542	9.31496013
H	2.52479303	-3.82776455	6.95542272
C	-2.29799918	-5.88625505	5.30340270
C	-3.49549415	-6.23983091	5.93328296
C	-3.88421815	-7.58054149	6.01120892
C	-3.07697287	-8.58173313	5.45938617
C	-1.87777126	-8.23124966	4.82709087
C	-1.49217495	-6.88977914	4.75238833
H	-4.13376072	-5.46327357	6.34840416
H	-4.82289055	-7.84356898	6.49884799
H	-3.38191986	-9.62631493	5.51613704
H	-1.24507617	-9.00259749	4.38836319
C	-2.05736643	-0.72459918	0.29964112
C	-0.62015029	-0.88280517	-0.10114572
C	-1.32627489	-1.29421647	1.23339493
H	0.22953952	-4.63243250	-1.28645063
C	0.17281334	0.40817206	-0.05956472
C	-0.16588044	-2.02029636	-0.97657619
H	-1.52904624	-4.92347528	-1.55923991
C	-0.95496575	-1.83938022	2.46475136
C	-3.30393678	-0.17021154	-0.08216224
O	-0.34060205	1.48728102	0.20914417
O	1.50183721	0.25562800	-0.29749391
C	2.28648531	1.49092562	-0.21173344
H	3.32499130	1.16846259	-0.31812382
H	2.11994214	1.97737369	0.75479747
H	2.00251379	2.17069422	-1.02214034
O	0.89043264	-2.08552616	-1.59291921
O	-1.09160423	-3.02548895	-0.96398679
C	-0.70057798	-4.22426218	-1.70023598
H	-0.56085932	-3.99025716	-2.76224510
O	-4.27413016	-0.04571340	0.69321634
O	-3.32738433	0.24063286	-1.38386383
C	-4.56942037	0.88359961	-1.80958348
H	-5.40665027	0.18323254	-1.72354370
H	-4.39835316	1.16077480	-2.85241404
H	-4.76111162	1.77047585	-1.19647857
C	0.05588181	-2.98636251	2.42608029
H	-1.81808440	-2.04063465	3.10655440
H	-0.36771031	-0.69814753	3.13966420
H	0.62538967	-3.05336539	3.35849633
H	0.77810328	-2.85286397	1.61433491
H	-0.45812383	-3.94610949	2.25993974

TS5_60

E = -25987.45

G = -25384.28

Nimag = 1, 1738 i cm–1

C	-5.84728316	0.93137987	2.20026931
N	-4.54819893	1.08507876	2.89396477
H	-4.36991270	2.06705018	3.13940488
C	-7.75180003	-1.22375918	4.74765124
S	-3.77287696	-1.49229890	3.29881727
N	-2.80679807	0.86092408	4.30847484
H	-2.99130056	1.86572928	4.38476039
C	-1.69263572	0.43144992	5.17733244
H	-1.02889232	1.30848965	5.18066940
H	-10.06669772	-1.88669739	3.46497343
C	-0.87165855	-0.73513757	4.61304217
N	-0.06877257	-0.32442031	3.43464552
H	-1.53852199	-1.56186247	4.35825202

P	1.40043768	-0.95115798	3.25517279
C	1.44277906	-2.68616340	2.69147800
C	0.21526913	-3.34600570	2.52315416
C	2.64619257	-3.35577551	2.40661712
C	0.19402698	-4.67494879	2.08822576
H	-0.71526741	-2.81323482	2.70974110
C	2.61775270	-4.68164410	1.97178340
H	3.59997380	-2.84002139	2.50855764
C	1.39248364	-5.34271052	1.81703599
H	-0.75935423	-5.18491737	1.95492792
H	3.55020104	-5.19826087	1.74717573
H	1.37380940	-6.37763144	1.47678011
C	2.30750986	-0.88207610	4.84846709
C	2.98027473	-1.98269375	5.40209277
C	2.23048173	0.32246991	5.57455349
C	3.59784952	-1.86805569	6.65187352
H	3.00710188	-2.93456983	4.87942872
C	2.85418805	0.43037921	6.81680500
H	1.65437507	1.15962680	5.19113814
C	3.54408657	-0.66133775	7.35616630
H	4.11509589	-2.72760973	7.07692360
H	2.78499638	1.36433802	7.37345936
H	4.02553551	-0.57654359	8.32991755
C	2.30051646	0.00644361	1.99842117
C	2.67246584	1.32850967	2.29217200
C	2.54983972	-0.51905793	0.72123261
C	3.26713264	2.12528142	1.31630604
H	2.47171621	1.73684088	3.27355138
C	3.16490493	0.27706923	-0.24848100
H	2.25035571	-1.53456783	0.47460235
C	3.51774550	1.59752996	0.04495988
H	3.35085723	-0.13186909	-1.24099415
H	3.97580463	2.22222248	-0.72120846
H	-0.20571865	-1.07523253	5.41508202
H	3.49784481	3.16434860	1.53704374
H	-0.22258381	-0.59199255	7.38410416
H	-8.20266500	-3.38139466	6.41776565
H	-8.64439097	-0.58189009	4.73418703
H	-7.35666580	-1.35190297	1.27129673
H	-6.10082732	1.97623793	1.98255855
H	-4.02254220	1.36673499	6.52590455
C	-2.15403771	0.21713584	6.66694714
C	-2.91583768	-1.11139509	6.85272853
C	-0.90366434	0.24627530	7.57834988
C	-3.07305609	1.39308694	7.07381749
H	-3.77951829	-1.17107285	6.18163793
H	-2.26841690	-1.97633673	6.65147543
H	-3.28262904	-1.19204683	7.88625088
C	-3.70440517	0.20883291	3.53032451
C	-5.87111017	0.19944190	0.78636213
C	-6.33875617	-1.27211028	0.86608223
C	-6.87860444	0.97844029	-0.09563386
C	-4.47291019	0.27831199	0.14338242
H	-5.67052306	-1.86683657	1.49543930
H	-6.34722963	-1.69992567	-0.14803009
H	-6.53868740	2.01300657	-0.25691727
H	-6.97196549	0.48884280	-1.07602962
H	-7.86906762	1.00894197	0.37742843
H	-4.53135422	-0.06910786	-0.89914298
H	-4.09388834	1.31005116	0.14114295
H	-3.75874035	-0.35411924	0.68354043
C	-7.01953032	0.46237735	3.09293140
O	-8.15682456	0.94075529	2.93061486
N	-6.71742739	-0.48495368	4.00992906
H	-5.80222506	-0.95536040	3.91459073
H	-3.29802909	1.33606205	8.14821522
H	-2.58949121	2.36224028	6.87621578
H	-0.33806381	1.17922521	7.43868107
H	-1.21239319	0.18700508	8.63255789
C	-8.06789119	-2.50250094	3.98354966
C	-7.08577744	-3.49065395	3.82041512
C	-7.33856913	-4.61566322	3.03568342
C	-8.58020960	-4.76748649	2.40398605
C	-9.56469299	-3.78875763	2.56676182
C	-9.30619929	-2.65933391	3.35306791
H	-6.11452186	-3.37032869	4.29863917
H	-6.56608135	-5.37429512	2.90989553
H	-8.77637197	-5.64445195	1.78715414
H	-10.53181962	-3.89869815	2.07622590
C	-7.31484405	-1.42516296	6.19738543
C	-6.59639580	-0.41170071	6.84992613
C	-6.21249925	-0.55581368	8.18396492
C	-6.53670843	-1.72122843	8.88685044
C	-7.25641343	-2.73456272	8.24552289
C	-7.64689339	-2.58544898	6.90955585
H	-6.32431329	0.48538120	6.29783239
H	-5.64544841	0.23622035	8.67037281
H	-6.22750270	-1.84084162	9.92493652
H	-7.51436683	-3.64691056	8.78335691
C	-1.60714129	3.69375012	2.96428460
C	-0.19110167	3.87550673	2.49853799
C	-1.15875426	2.68570602	2.23921485
H	-0.48793085	5.41064504	-1.20389281
C	0.83773095	3.70375826	3.58542684
C	0.14799580	4.69675349	1.27922538
H	-1.69629800	6.60873593	-0.60895499
C	-1.15171195	1.42867581	1.62763562
C	-2.60480993	4.25834512	3.79394864
O	0.65097888	3.01199803	4.58103203
O	1.96306955	4.43879239	3.39034680
C	2.94426236	4.36804307	4.47588770
H	3.74766391	5.04250787	4.17152814
H	3.31922244	3.34536635	4.58271360
H	2.48807736	4.69329333	5.41647426
O	1.22493005	4.68683929	0.69964954
O	-0.93639910	5.40569284	0.85308975
C	-0.74019213	6.12021921	-0.40855694
H	0.06236553	6.85756228	-0.30238195
O	-3.67339806	3.68860057	4.10656605
O	-2.26807827	5.49895308	4.25545795
C	-3.24594516	6.11022020	5.15462569
H	-4.19708605	6.25891304	4.63241452
H	-2.80452171	7.06769912	5.44033209
H	-3.40014810	5.47337777	6.03204924
C	-0.33274934	1.23495374	0.35179469
H	-2.15535962	0.99628881	1.57451108
H	-0.57917928	0.57854672	2.58648272
H	-0.03999914	0.18420464	0.23446448
H	0.57877335	1.84320562	0.36510640
H	-0.91877982	1.51869895	-0.53739420

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E = -26011.26

G = -25408.80

Nimag = 1, 1436 i cm–1

C	-6.04006263	-2.26943344	2.21916818
N	-4.71659815	-1.66673329	2.39309618
H	-4.10291439	-1.66125670	1.56669533
C	-5.29859469	-5.72350487	3.63870129
S	-4.97353342	-1.51893784	5.08967625
N	-2.85672387	-0.93342020	3.48851332
H	-2.63668470	-0.63421171	2.53907474
C	-2.14458078	-0.10414042	4.47296987
H	-2.87208409	0.14750130	5.25615740
H	-3.85687338	-7.21621085	1.86105702
C	-1.64615638	1.21510895	3.76529072
N	-2.16781071	1.39110152	2.39415328
H	-0.55867238	1.19383305	3.66914176
P	-3.06884198	2.66074282	1.97700475
C	-2.29537184	4.23863270	2.44444246
C	-0.90072751	4.33762838	2.28366281
C	-3.03043175	5.32325495	2.94603572
C	-0.25381550	5.53114231	2.60784475
H	-0.33141261	3.47968899	1.92938135
C	-2.37280204	6.51441376	3.26774464
H	-4.10547160	5.23868942	3.08934774
C	-0.98833624	6.61973997	3.09559545
H	0.82580629	5.61147844	2.48646931
H	-2.94119798	7.35743688	3.65887224
H	-0.47893154	7.54890617	3.34933549

C	-4.76799870	2.66754226	2.64450033
C	-5.06637320	1.96821357	3.82259060
C	-5.78990132	3.34386117	1.95429935
C	-6.37304097	1.95124399	4.31275064
H	-4.30086951	1.41048984	4.34804480
C	-7.09211488	3.33252135	2.45587328
H	-5.57351686	3.85841396	1.01973645
C	-7.38367397	2.63931981	3.63615413
H	-6.59676350	1.37600445	5.20951580
H	-7.88331560	3.85110474	1.91526578
H	-8.40498155	2.61862544	4.01560215
C	-3.29327860	2.66120022	0.17896341
C	-3.85585616	1.52535470	-0.42308771
C	-3.02286283	3.80726020	-0.58314752
C	-4.13701378	1.53370733	-1.78811349
H	-4.04586393	0.63338678	0.16139735
C	-3.31949345	3.81231102	-1.94905017
H	-2.58838533	4.68853830	-0.11625944
C	-3.87689512	2.67897514	-2.55054220
H	-3.11032140	4.70092931	-2.54355851
H	-4.10342340	2.68536320	-3.61654880
H	-1.89656964	2.07204291	4.40437387
H	-4.55747285	0.64473860	-2.25593750
H	0.23066926	0.92038516	5.65227832
H	-4.32483146	-7.74839252	5.20645045
H	-5.74652333	-6.29827159	2.81419075
H	-6.08217996	0.38136077	1.49677737
H	-6.59007958	-2.03427281	3.13975887
H	-2.08674767	-2.73752603	5.27484877
C	-0.96817232	-0.87121884	5.16413012
C	0.04302788	-1.39367147	4.12098506
C	-0.26916323	0.08399687	6.15909623
C	-1.54708369	-2.06560779	5.94796293
H	-0.44777242	-2.03970134	3.38516991
H	0.53566615	-0.57956861	3.57493567
H	0.82373819	-1.98222479	4.62554986
C	-4.15195095	-1.36150212	3.59548252
C	-6.83391342	-1.63398656	1.04086120
C	-7.03846892	-0.13826901	1.37079399
C	-6.11429790	-1.76749642	-0.31980032
C	-8.21143412	-2.33195460	0.97409418
H	-7.60808377	-0.01373312	2.30172427
H	-7.59049946	0.35559689	0.55843239
H	-5.97101791	-2.82160697	-0.58182019
H	-6.72031201	-1.27997393	-1.09808085
H	-5.13266425	-1.28187009	-0.31151874
H	-8.84285111	-1.83883803	0.22079535
H	-8.10607344	-3.38920655	0.69946517
H	-8.72889619	-2.27059790	1.94384854
C	-5.84762536	-3.80901693	2.17361907
O	-5.78682433	-4.48728512	1.13879511
N	-5.71620546	-4.33308455	3.42623628
H	-5.60116500	-3.66550662	4.20299093
H	-0.73366977	-2.62844586	6.42993297
H	-2.25189031	-1.72988967	6.72053607
H	-0.99232827	0.49737816	6.87943451
H	0.49587567	-0.46701040	6.72566433
C	-3.78460152	-5.87672281	3.54704380
C	-2.95190149	-5.21101415	4.45690369
C	-1.56887768	-5.39134546	4.41165692
C	-1.00288741	-6.24655948	3.45807044
C	-1.82662452	-6.90024519	2.53758321
C	-3.21305706	-6.70976159	2.58009481
H	-3.39139890	-4.55443379	5.20676659
H	-0.92980542	-4.86468192	5.11766469
H	0.07716084	-6.39006571	3.42606703
H	-1.39167875	-7.55335176	1.78091678
C	-5.86655825	-6.25553741	4.95634654
C	-7.04226087	-5.72121473	5.50365508
C	-7.57750462	-6.24014996	6.68756600
C	-6.94970660	-7.30861569	7.33589536
C	-5.78107927	-7.85267349	6.79094345
C	-5.24261822	-7.32777453	5.61249771
H	-7.54197852	-4.89434013	5.00299987
H	-8.48780727	-5.80716842	7.10208397
H	-7.36499925	-7.71198568	8.25904687
H	-5.28145968	-8.68413365	7.28795114
C	-0.82357283	-0.09510586	0.56378890
C	0.70812881	-0.00903988	0.34641347
C	-0.32449705	0.64689683	-0.53906943
H	3.66955632	1.66418457	2.56659437
C	1.40691749	-1.25743626	-0.11038422
C	1.50045377	0.93236028	1.21143456
H	4.60560724	1.90578861	1.04551307
C	-0.39909601	1.47683859	-1.57086809
C	-1.60268623	-1.32457415	0.52307203
O	2.29874634	-1.81593099	0.51448612
O	0.87388249	-1.73409103	-1.26907196
C	1.31008262	-3.08030262	-1.63236378
H	0.76990460	-3.31482504	-2.55241448
H	1.04391322	-3.77985115	-0.83277598
H	2.39236675	-3.09810646	-1.79792082
O	1.05730308	1.59827965	2.13732140
O	2.78214205	1.03543064	0.76422448
C	3.62193560	1.96855585	1.51580119
H	3.21400171	2.98200923	1.44146575
O	-2.80020164	-1.36067139	0.18906828
O	-0.96139834	-2.41274270	1.03295595
C	-1.78530499	-3.61564167	1.18161498
H	-2.45953171	-3.50047272	2.03619034
H	-1.07684879	-4.42055652	1.37575637
H	-2.36250897	-3.80071196	0.27126505
C	0.80482184	2.05035773	-2.26722790
H	-1.46912724	0.76375348	1.52953102
H	-1.38289770	1.76265852	-1.94041458
H	0.82100232	3.14954601	-2.17937829
H	0.79391486	1.81659264	-3.34380055
H	1.73507425	1.65756034	-1.83688561

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E = -25994.70

G = -25393.19

Nimag = 1, 1560 i cm–1

C	-4.81136140	-1.76481305	4.79007141
N	-4.27332592	-0.69922939	3.95211852
H	-4.45472664	-0.74542932	2.94463729
C	-2.16779133	-4.47530885	4.31110883
S	-2.53911730	0.10610833	5.85663434
N	-3.24862965	1.26256214	3.47111792
H	-3.84452619	1.13853530	2.65202142
C	-2.15191678	2.22981465	3.23268244
H	-2.23612708	2.44011095	2.15792305
H	0.10680874	-4.57467115	2.82158695
C	-0.76103217	1.60123036	3.43293115
N	-0.11149653	1.23730317	2.14397379
H	-0.85414203	0.73078868	4.08764983
P	1.50244695	1.34665203	2.15897476
C	2.03249821	3.04864884	2.57505978
C	2.14300888	3.43839829	3.92309896
C	2.14418342	4.01830326	1.56354663
C	2.33221156	4.78251273	4.25153567
H	2.08525645	2.69472229	4.71505289
C	2.34087534	5.35918305	1.89873582
H	2.07793161	3.72996084	0.51710700
C	2.42543423	5.74465223	3.24152128
H	2.40504612	5.07672488	5.29786053
H	2.42820951	6.10481670	1.10915137
H	2.57019765	6.79328321	3.49911970
C	2.15513265	0.96138809	0.51853133
C	1.47019509	1.42342114	-0.61673993
C	3.37726754	0.28432398	0.37613653
C	2.02109084	1.22493184	-1.88329851
H	0.50848684	1.91891679	-0.50479376
C	3.90972032	0.07323635	-0.89604323
H	3.90886202	-0.08309039	1.24957432
C	3.23612931	0.55075575	-2.02606140
H	1.49206988	1.58547510	-2.76359032
H	4.85124596	-0.46371860	-1.00469270
H	3.65588691	0.39001567	-3.01850839
C	2.28559216	0.30581205	3.43491059

C	1.48536057	-0.66856785	4.05424040
C	3.61202305	0.49535139	3.85845056
C	2.00068966	-1.43536399	5.09705769
H	0.47177369	-0.83816301	3.70597497
C	4.13437266	-0.30191471	4.87977205
H	4.23014935	1.26728976	3.40220190
C	3.32659853	-1.26159808	5.50367518
H	5.16670343	-0.16389700	5.19936538
H	3.73161802	-1.87089849	6.31098099
H	-0.13516903	2.31504818	3.97638240
H	1.36891142	-2.17241092	5.58180123
H	-0.48196625	4.35592960	2.99823601
H	-1.79517003	-6.91306759	3.22133453
H	-2.17436022	-4.47030442	3.21119454
H	-6.39939632	0.46616665	4.92961904
H	-4.43858002	-1.55987979	5.80240729
H	-4.44193895	3.32099321	4.48932472
C	-2.34584357	3.62665343	3.92605908
C	-1.86145949	3.65612749	5.39324627
C	-1.53395761	4.65202153	3.09671130
C	-3.84084182	4.00692064	3.87792426
H	-2.23111429	2.78402458	5.94572849
H	-0.76435026	3.66300259	5.45819128
H	-2.22582934	4.57218129	5.88182508
C	-3.37655097	0.24442426	4.36562764
C	-6.37025633	-1.72758488	4.85430018
C	-6.76930835	-0.38728133	5.51429881
C	-7.01387123	-1.82070443	3.45310634
C	-6.84995776	-2.89449096	5.74694805
H	-6.35564673	-0.31067415	6.53074993
H	-7.86451265	-0.31257010	5.57964565
H	-6.76064742	-2.77117016	2.97187066
H	-8.10749166	-1.74048753	3.54347516
H	-6.67716905	-0.99811897	2.80528327
H	-7.94079106	-2.84071107	5.87798929
H	-6.59857151	-3.86405959	5.30169037
H	-6.38678058	-2.83524322	6.74423425
C	-4.19889361	-3.10386673	4.32835091
O	-4.79279178	-3.93231708	3.62928503
N	-2.92370443	-3.30360523	4.77243949
H	-2.44827051	-2.54401700	5.27155316
H	-3.98041392	5.02903060	4.25845888
H	-4.22640460	3.97355832	2.84715406
H	-1.95321395	4.75940531	2.08489529
H	-1.55802137	5.63669483	3.58594930
C	-0.72694706	-4.44968121	4.80309077
C	-0.44255138	-4.45203288	6.17749852
C	0.87111291	-4.60454172	6.62761091
C	1.91374251	-4.77236246	5.70775370
C	1.63744125	-4.74922154	4.33856039
C	0.32375898	-4.58061722	3.88794677
H	-1.25468201	-4.36686044	6.89847652
H	1.07969456	-4.60923785	7.69739934
H	2.93707639	-4.90281048	6.05806569
H	2.44818211	-4.85865303	3.61980581
C	-2.80033268	-5.79524573	4.76946974
C	-3.64636705	-5.87462575	5.87931623
C	-4.14761946	-7.11084814	6.29924807
C	-3.80686233	-8.28096550	5.61147988
C	-2.95934117	-8.20518387	4.49915937
C	-2.45968846	-6.96794375	4.08379118
H	-3.92404569	-4.96727639	6.41120309
H	-4.81064526	-7.15927065	7.16307299
H	-4.20070271	-9.24369253	5.93637412
H	-2.68965308	-9.10971970	3.95409504
C	-1.61190572	-0.33627833	0.45041545
C	-1.43515607	-1.86353057	0.20918609
C	-1.05784283	-0.79536238	-0.78244491
H	2.44994739	-2.55343170	0.42659910
C	-2.68400993	-2.65353858	-0.11597701
C	-0.27908189	-2.66954728	0.71125932
H	2.56181110	-1.99469882	2.13283293
C	-0.59862829	-0.67729392	-2.01841940
C	-2.96022019	0.23773470	0.46053752
O	-3.36098997	-2.49388947	-1.12245895
O	-2.99730516	-3.50559988	0.88981191
C	-4.19757674	-4.31540110	0.66041786
H	-4.35123214	-4.85071579	1.59617495
H	-4.02253924	-4.99361463	-0.18255480
H	-5.04821479	-3.66105042	0.44649587
O	-0.14803742	-3.86357213	0.46451574
O	0.67660104	-1.92487634	1.33780041
C	1.98495548	-2.57914284	1.41850746
H	1.88109520	-3.60884825	1.76010132
O	-3.96169356	-0.17910623	1.05503533
O	-2.96291512	1.42918472	-0.22799860
C	-4.23045995	2.15449068	-0.24021235
H	-5.06816450	1.46244599	-0.35716721
H	-4.16353761	2.84147549	-1.08718287
H	-4.34554098	2.71997566	0.69199148
C	-0.12220017	-1.83266669	-2.85264336
H	-0.54102496	0.32043834	-2.45687903
H	-0.77052086	0.42512034	1.35369995
H	-0.25088441	-2.78377710	-2.32054983
H	0.94589182	-1.71631301	-3.10134932
H	-0.67197690	-1.89300329	-3.80530885

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E = -26007.43

G = -25405.99

Nimag = 1, 1446 i cm–1

C	-3.98185535	-3.29927460	0.93000074
N	-4.46548873	-3.03009481	2.29820126
H	-3.88251431	-3.50530190	3.00192221
C	-3.51898478	0.28239189	-0.45421972
S	-6.57980931	-1.34024490	1.92291977
N	-5.77382475	-2.65834784	4.12287336
H	-5.07456074	-3.25422703	4.57569536
C	-6.55110407	-1.78937022	5.01536986
H	-6.90861018	-0.96872578	4.38309246
H	-1.03434678	1.23871401	-1.01600787
C	-5.58606069	-1.21085239	6.07774869
N	-4.39937522	-0.60887544	5.46030752
H	-5.21953322	-2.02581132	6.71474599
P	-4.24711531	0.94310209	5.06142703
C	-4.00667674	2.09874206	6.45056040
C	-3.35712757	1.62628627	7.60172523
C	-4.39150707	3.44737229	6.35794528
C	-3.09332825	2.50339227	8.65585809
H	-3.06129234	0.58529194	7.68065411
C	-4.11859496	4.31952557	7.41491030
H	-4.89835046	3.81310060	5.46678220
C	-3.46921073	3.84856610	8.56256813
H	-2.59470709	2.13267489	9.55058757
H	-4.41512076	5.36549977	7.34406189
H	-3.26068526	4.53090770	9.38619003
C	-5.66726558	1.60196975	4.13728098
C	-6.89595883	1.75408918	4.80678914
C	-5.58572641	1.85125062	2.76021551
C	-8.03363551	2.13217481	4.09601069
H	-6.96286796	1.57849326	5.87916690
C	-6.72386645	2.25390572	2.05900599
H	-4.64250172	1.73013720	2.23515285
C	-7.94664383	2.38320529	2.72034965
H	-8.98608254	2.23823053	4.61404260
H	-6.65779375	2.45019433	0.99471383
H	-8.83566997	2.68178526	2.16525712
C	-2.76496972	1.03286537	4.02130272
C	-2.52084220	0.01002788	3.09011005
C	-1.86717501	2.10583761	4.14395577
C	-1.37696067	0.05928931	2.29235911
H	-3.21910590	-0.81592696	2.99626354
C	-0.72968536	2.15132145	3.33552017
H	-2.04249877	2.88831828	4.87877509
C	-0.48454034	1.12818843	2.41277411
H	-0.02915073	2.97964764	3.43559958
H	0.40921994	1.16089693	1.79002365
H	-6.12283309	-0.51380897	6.73353658
H	-1.19197142	-0.72979258	1.56834968
H	-8.08364162	-1.18995618	7.35054760

H	-3.45550623	2.98291034	-0.41983594
H	-2.86418693	0.76801225	0.28460840
H	-6.43315809	-4.65738476	1.45525040
H	-3.13585827	-3.96504175	1.13071892
H	-8.13578283	-3.71185602	3.79995653
C	-7.80600632	-2.51145453	5.60248554
C	-7.40566481	-3.72025621	6.47502991
C	-8.61895307	-1.49936102	6.44267748
C	-8.68523223	-3.00065854	4.43033963
H	-6.80280846	-4.44051914	5.90301468
H	-6.83221272	-3.41306955	7.35696435
H	-8.30642155	-4.24339869	6.82891421
C	-5.56134714	-2.39808585	2.79732353
C	-4.90598646	-4.14685758	-0.03326005
C	-5.69268890	-5.16239835	0.82179720
C	-5.88702079	-3.32742172	-0.89883426
C	-3.94638534	-4.90289354	-0.98592895
H	-5.01924240	-5.74061960	1.47172258
H	-6.22315868	-5.86549479	0.16339298
H	-5.34700188	-2.64629310	-1.56714407
H	-6.47223026	-4.01838468	-1.52447751
H	-6.57257266	-2.74017467	-0.28062491
H	-4.52652287	-5.49342796	-1.70941284
H	-3.31000074	-4.20111290	-1.54289370
H	-3.29209265	-5.58774486	-0.42613165
C	-3.28153329	-2.08277547	0.27013982
O	-2.09177770	-2.17902035	-0.08090224
N	-4.03404866	-0.97277730	0.10388459
H	-4.95907810	-0.95585460	0.58047163
H	-9.58492635	-3.49983139	4.81993273
H	-8.99283966	-2.15877464	3.79577712
H	-8.84828311	-0.59987233	5.85234774
H	-9.57119786	-1.95199790	6.75616623
C	-2.69951610	0.06934504	-1.72569656
C	-3.21856150	-0.66606841	-2.79724104
C	-2.48240177	-0.81512519	-3.97384341
C	-1.22290239	-0.21358149	-4.09625191
C	-0.70722350	0.53393701	-3.03197193
C	-1.44456136	0.67172554	-1.85110978
H	-4.19761274	-1.13065913	-2.70940901
H	-2.89130696	-1.39860800	-4.79866652
H	-0.64834105	-0.32793856	-5.01511989
H	0.27269375	1.00330612	-3.11761216
C	-4.66998209	1.23314200	-0.76991739
C	-5.92488598	0.76970706	-1.18673827
C	-6.91706652	1.67206029	-1.58211811
C	-6.66551313	3.04781955	-1.56749320
C	-5.41706513	3.51684390	-1.14147995
C	-4.42814034	2.61314830	-0.74460718
H	-6.13565434	-0.29612393	-1.20215364
H	-7.89037186	1.29724419	-1.89825656
H	-7.43936939	3.75069029	-1.87483293
H	-5.21575318	4.58743686	-1.11225836
C	-2.19795744	-2.14120894	5.71704460
C	-1.91742166	-2.51874803	7.19598392
C	-1.25535177	-1.38739673	6.46077848
H	-5.45814961	-2.22019791	9.21647038
C	-1.03104212	-3.70982809	7.45322024
C	-2.96898463	-2.24740184	8.24175412
H	-5.51290723	-4.02256108	9.24779008
C	-0.47106276	-0.33318092	6.65053256
C	-1.95855768	-3.07184481	4.61958562
O	-0.33341857	-4.26137563	6.61465670
O	-1.08202583	-4.07650723	8.76557735
C	-0.24872987	-5.22894973	9.11834732
H	-0.42816334	-5.39138085	10.18316277
H	0.80467420	-4.99995263	8.92745758
H	-0.55413146	-6.10066956	8.53055408
O	-3.03058740	-1.25152359	8.94813033
O	-3.87640780	-3.26481463	8.29162474
C	-4.87918475	-3.13963751	9.35118710
H	-4.38395554	-3.12354733	10.32841898
O	-2.71326683	-4.02078093	4.33550436
O	-0.88046128	-2.72710748	3.86765084
C	-0.57436430	-3.57602398	2.71619545
H	-0.80814212	-4.62016236	2.94278614
H	0.49752199	-3.44316215	2.54323460
H	-1.13610203	-3.23411190	1.84142405
C	0.10424755	0.06472534	7.98065163
H	-3.37499854	-1.34930030	5.53973833
H	-0.26242796	0.30537752	5.78849897
H	-0.24905788	1.06930759	8.26632474
H	1.20469677	0.10808497	7.95241953
H	-0.20247397	-0.63816969	8.76537585

TS5_64

E = -26000.18

G = -25395.81

Nimag = 1, 1673 i cm–1

C	-5.16806683	0.70966516	2.92904677
N	-4.22548881	1.05500789	4.01719325
H	-4.28745711	2.04150186	4.27674679
C	-6.79930530	-2.42181257	4.41067051
S	-2.85691438	-1.27158242	4.40271209
N	-2.60749014	1.14592385	5.59710377
H	-2.86684001	2.13826873	5.57627697
C	-1.37065141	0.93154640	6.36652327
H	-1.05534922	1.95904549	6.58647250
H	-8.29955215	-3.01768447	2.20739726
C	-0.23784383	0.28981121	5.54829042
N	-0.03915866	0.97153948	4.24402376
H	-0.48420234	-0.76255303	5.37865554
P	0.85119035	0.16128462	3.16475565
C	0.87553691	1.06334896	1.59490537
C	-0.10256755	2.02199680	1.30266623
C	1.80353349	0.68048521	0.60917256
C	-0.16047281	2.58750172	0.02796597
H	-0.81619267	2.32770145	2.05558881
C	1.72952936	1.23942479	-0.66630125
H	2.57562200	-0.05266403	0.83300727
C	0.74221535	2.18902888	-0.95985408
H	-0.91541575	3.34258440	-0.18575227
H	2.44612496	0.93904617	-1.43005866
H	0.68910698	2.62649764	-1.95664728
C	0.19099872	-1.49900937	2.78850511
C	-0.63968212	-1.69355891	1.67314682
C	0.37503949	-2.54477782	3.71072307
C	-1.29678691	-2.91118846	1.49577355
H	-0.78547628	-0.89131862	0.95544498
C	-0.29243139	-3.75690772	3.53252374
H	1.03120745	-2.41185634	4.56854425
C	-1.13486195	-3.93750341	2.43054434
H	-1.95381103	-3.05119573	0.63961313
H	-0.16168698	-4.55792156	4.25925351
H	-1.66155065	-4.88090181	2.29908410
C	2.56763850	-0.14379826	3.70971127
C	3.11077666	0.72070312	4.67368516
C	3.33557730	-1.20812106	3.20667831
C	4.41676960	0.52193478	5.12663255
H	2.52181573	1.55650772	5.04141045
C	4.64444315	-1.39490169	3.65679726
H	2.91044089	-1.89596406	2.47821419
C	5.18410237	-0.53250460	4.61896732
H	5.24006168	-2.21817714	3.26403265
H	6.20283791	-0.68479294	4.97443293
H	0.67526431	0.33591002	6.16110595
H	4.83746034	1.19292514	5.87490106
H	0.55079879	0.34161420	8.30061445
H	-7.72591404	-4.74968634	5.43312160
H	-7.84548465	-2.09792390	4.31785447
H	-5.50038465	-1.65102626	1.27529959
H	-5.68171157	1.66463702	2.76670217
H	-3.77766576	0.47553177	7.81631490
C	-1.59391824	0.26680048	7.77885632
C	-1.68582362	-1.27419416	7.72895065
C	-0.41717684	0.67913558	8.69647558
C	-2.90361720	0.82484802	8.38106772
H	-2.47353497	-1.60046532	7.04115176
H	-0.73976117	-1.72728227	7.39917523
H	-1.90785224	-1.65713210	8.73690737

C	-3.23442993	0.37001861	4.67667077
C	-4.55096277	0.31951446	1.51085385
C	-4.49853622	-1.20374987	1.25869783
C	-5.46723404	0.95714695	0.43822027
C	-3.13965062	0.91721829	1.38985256
H	-3.87823442	-1.70976300	2.00195410
H	-4.06929701	-1.38373113	0.26164071
H	-5.46965252	2.05462049	0.52425616
H	-5.10489737	0.69236178	-0.56616903
H	-6.49981526	0.59928683	0.54491829
H	-2.74566332	0.73183214	0.38058516
H	-3.14553200	2.00136112	1.55301479
H	-2.45625950	0.46548905	2.11476406
C	-6.31488798	-0.24987290	3.32436711
O	-7.45504360	-0.09274176	2.85111122
N	-5.96269878	-1.24223971	4.17054754
H	-4.94086468	-1.39598228	4.28528311
H	-3.00595936	0.49008514	9.42356607
H	-2.90994461	1.92594732	8.37209323
H	-0.37562204	1.77166509	8.82043396
H	-0.54628786	0.23022755	9.69245675
C	-6.49611079	-3.43675993	3.30927225
C	-5.27730807	-4.13097856	3.31089276
C	-4.92701505	-4.94130885	2.23102002
C	-5.79498110	-5.07383237	1.13931514
C	-7.01605838	-4.39276205	1.13838011
C	-7.36317701	-3.57456620	2.22009945
H	-4.59360129	-4.01659945	4.15084331
H	-3.97446185	-5.46865103	2.23545136
H	-5.51849019	-5.70402069	0.29400581
H	-7.69506305	-4.48912989	0.29108290
C	-6.56135390	-2.97183845	5.81401947
C	-5.78445089	-2.28937703	6.75908158
C	-5.57919995	-2.82961115	8.03378272
C	-6.15810135	-4.05343688	8.38189643
C	-6.94174548	-4.73812207	7.44322928
C	-7.13574450	-4.20252452	6.16817620
H	-5.32724550	-1.33940690	6.49850132
H	-4.96087187	-2.29167667	8.75159134
H	-5.99893274	-4.47480028	9.37420738
H	-7.39584945	-5.69418052	7.70360773
C	-0.66079135	3.62992177	4.34024888
C	0.45126302	4.66959320	4.03619220
C	0.13690637	4.13925668	5.40491087
H	2.94302922	3.08447552	1.30761722
C	0.03114532	6.10982416	3.87937210
C	1.67146087	4.20334379	3.29145944
H	2.44706702	4.35793887	0.13783887
C	0.59086182	4.22094791	6.64923158
C	-2.06374836	3.93032861	4.06002154
O	-1.08350530	6.54583005	4.13211334
O	1.07933439	6.88644111	3.48950316
C	0.77554146	8.31308083	3.35821821
H	1.70742523	8.76945158	3.01783112
H	0.46927927	8.72054253	4.32724714
H	-0.02366121	8.45732817	2.62397375
O	2.59389685	3.56471337	3.77797695
O	1.59522544	4.55168138	1.98035296
C	2.74161507	4.14853752	1.16748578
H	3.62002592	4.73923269	1.45310748
O	-3.00571227	3.83896225	4.86449392
O	-2.26448267	4.21980044	2.74012019
C	-3.62595213	4.60855723	2.39061422
H	-4.32694903	3.79307223	2.59201470
H	-3.59416926	4.82787972	1.32079746
H	-3.91695330	5.49573769	2.96379590
C	1.80816860	5.01800328	7.03486418
H	0.06741635	3.68397250	7.44331828
H	-0.30596233	2.25085182	4.18811896
H	1.54416266	5.86471119	7.68899399
H	2.31400112	5.40987137	6.14352955
H	2.52487365	4.39320173	7.59090924

TS5_65
E = -26007.71
G = -25404.59
Nimag = 1, 1024 i cm–1

C	-5.61044683	-2.47058952	2.60689786
N	-4.43227815	-1.62744976	2.47758851
H	-3.99685204	-1.56691296	1.55182870
C	-5.52118285	-5.85916308	4.40870421
S	-4.21315833	-1.32883485	5.15810812
N	-2.51539088	-0.61989646	3.16215208
H	-2.40973922	-0.45056414	2.16307823
C	-1.52603665	0.00515364	4.02477129
H	-2.01500015	0.12885484	5.00027593
H	-3.60481551	-4.00564724	5.23031461
C	-1.17449964	1.43324459	3.46439431
N	-1.56374741	1.68549955	2.05814226
H	-0.09329122	1.59722222	3.54328808
P	-2.72169364	2.76445578	1.71472164
C	-2.39127144	4.33657715	2.58195417
C	-1.05313327	4.70034760	2.80270589
C	-3.42697795	5.19028316	2.99377454
C	-0.75142936	5.91630531	3.41697054
H	-0.26187764	4.02470777	2.49388067
C	-3.11937720	6.40840371	3.60607524
H	-4.46566061	4.90629322	2.84015136
C	-1.78459811	6.77318408	3.81513905
H	0.28770852	6.19549722	3.58758462
H	-3.92335488	7.07171724	3.92282772
H	-1.54924249	7.72266446	4.29484139
C	-4.45147360	2.37362417	2.16503965
C	-4.73501805	1.82688566	3.42680051
C	-5.50777166	2.74641914	1.31476686
C	-6.05782949	1.65565482	3.83343565
H	-3.93807651	1.52635343	4.09875485
C	-6.83018460	2.59177960	1.73735077
H	-5.29934990	3.16520551	0.33299213
C	-7.10557667	2.05266167	2.99718507
H	-6.26052083	1.19746878	4.79979857
H	-7.64484646	2.88407205	1.07548472
H	-8.13828517	1.92396968	3.31981278
C	-2.75267002	3.11284221	-0.06336776
C	-3.02939921	2.07509909	-0.97056155
C	-2.60635698	4.43252797	-0.52084317
C	-3.13567729	2.36310943	-2.33064335
H	-3.13404219	1.05074886	-0.62011011
C	-2.72855997	4.70894528	-1.88413401
H	-2.40664007	5.23998246	0.17952787
C	-2.99310767	3.67657519	-2.78775828
H	-2.60919685	5.73183229	-2.23904619
H	-3.07953112	3.89545306	-3.85174441
H	-1.64527313	2.17773895	4.11930990
H	-3.31935216	1.55158815	-3.03307571
H	0.95920654	0.74278847	5.11878965
H	-7.81769319	-6.96499260	3.46935357
H	-5.47978632	-6.44088520	3.47519549
H	-6.17028994	-0.19388799	1.17619888
H	-6.17375970	-2.09469362	3.47081133
H	-1.32702380	-2.79976573	4.00220385
C	-0.26566254	-0.89819059	4.28523867
C	0.60395554	-1.07250742	3.02671091
C	0.56344578	-0.23934780	5.41285338
C	-0.73072705	-2.28847875	4.76843374
H	0.05903754	-1.59879663	2.23611764
H	0.95157013	-0.11563155	2.61749312
H	1.49200852	-1.67320711	3.27518308
C	-3.68802537	-1.19540472	3.53418077
C	-6.53872089	-2.35020842	1.35263710
C	-7.01629042	-0.88566254	1.26397092
C	-5.81909606	-2.73980835	0.04170003
C	-7.75554741	-3.27743266	1.56820132
H	-7.58529976	-0.60555287	2.16071636
H	-7.66597772	-0.75262245	0.38638321
H	-5.42458717	-3.76084661	0.09601540
H	-6.53427833	-2.67594649	-0.79212551
H	-4.98613524	-2.06189346	-0.18583944
H	-8.47128904	-3.14841985	0.74382151
H	-7.45623043	-4.33436729	1.59687900

H	-8.27127506	-3.04216733	2.51111390
C	-5.18375383	-3.92983247	2.88866860
O	-4.41426532	-4.56122263	2.15005918
N	-5.74526949	-4.46709043	4.00270118
H	-6.26618730	-3.86106773	4.63394270
H	0.14443361	-2.91519722	4.99464636
H	-1.34957389	-2.20530850	5.67032551
H	-0.04603753	-0.10681133	6.31993280
H	1.42092629	-0.87918041	5.66776383
C	-4.19908490	-6.08192475	5.14168684
C	-3.84380639	-7.39656161	5.48178562
C	-2.65184599	-7.65771251	6.16018902
C	-1.79880226	-6.60143986	6.50810538
C	-2.14928673	-5.29211110	6.16783856
C	-3.34464599	-5.03078549	5.48582590
H	-4.51260080	-8.21819080	5.22295734
H	-2.38732640	-8.68316730	6.41831118
H	-0.86752067	-6.80119836	7.03812082
H	-1.49078022	-4.46650931	6.42970934
C	-6.73371074	-6.30863358	5.21565751
C	-6.78008281	-6.13958650	6.60569734
C	-7.93003678	-6.48902781	7.32164846
C	-9.03991694	-7.01836504	6.65397257
C	-8.99641788	-7.19390949	5.26544554
C	-7.84923113	-6.83634389	4.55136864
H	-5.91163335	-5.74322287	7.12979943
H	-7.95657071	-6.35263627	8.40259363
H	-9.93324021	-7.29654224	7.21260446
H	-9.85526080	-7.61067083	4.73982838
C	-0.53995245	0.05036815	0.10491670
C	-0.05967329	0.80738820	-1.17771253
C	0.79265581	-0.11464058	-0.33710706
H	-0.88758199	0.39339573	-5.14687435
C	0.22586868	2.28365766	-1.14919968
C	-0.42725439	0.21698858	-2.51870587
H	0.87533958	0.55158728	-5.48421863
C	2.01308505	-0.63903789	-0.33231473
C	-1.54109174	-1.02338376	0.06332027
O	0.07132876	3.04919889	-2.08821806
O	0.72883859	2.67484603	0.05997582
C	1.10631011	4.08287071	0.11564510
H	1.52914923	4.22548777	1.11254788
H	0.22671112	4.71744804	-0.03120798
H	1.85313490	4.30438475	-0.65526974
O	-1.32187271	-0.59979773	-2.69226434
O	0.40179057	0.65189654	-3.50337304
C	0.12119253	0.10655560	-4.83127487
H	0.20919644	-0.98487830	-4.81522005
O	-2.77150170	-0.84969648	0.13515820
O	-0.98629146	-2.26531703	0.15083363
C	-1.93268298	-3.36783006	0.33496673
H	-2.45886107	-3.27928564	1.28857119
H	-1.31734171	-4.27116552	0.32302112
H	-2.65980993	-3.37862230	-0.48273240
C	3.08989518	-0.27765863	-1.31990717
H	-1.02118353	0.98649335	1.15848381
H	2.25780831	-1.36659951	0.44638459
H	3.45239147	-1.16862351	-1.85813883
H	3.96319923	0.16399951	-0.81198144
H	2.71830400	0.44029538	-2.06201825

TS5_66

E = -25997.64

G = -25399.52

Nimag = 1, 1190 i cm–1

C	-4.48111545	-2.25344797	4.60458358
N	-4.09059311	-1.00032857	3.96437686
H	-4.70298730	-0.65424256	3.22660839
C	-2.04026020	-4.93256523	3.40434408
S	-1.90230110	-0.76839515	5.51591845
N	-2.95614841	0.93853519	3.64801264
H	-3.63707552	1.05562563	2.88591382
C	-2.19101596	2.18087977	3.86638004
H	-2.42243158	2.76173708	2.96512937
H	0.02997815	-4.44550852	1.67195050
C	-0.67510024	1.96123590	3.87143401
N	-0.16732079	1.73139402	2.49535237
H	-0.44201008	1.12488043	4.54208678
P	1.43951079	1.66700019	2.33147403
C	1.87610354	1.79798755	0.58210354
C	0.98392682	2.39999353	-0.31764783
C	3.14482840	1.37938168	0.15392141
C	1.36508375	2.56710420	-1.65087692
H	-0.00468760	2.71087068	0.01015437
C	3.52420421	1.57423832	-1.17440819
H	3.82646648	0.89041535	0.84675528
C	2.63468322	2.16790385	-2.07728192
H	0.65796262	2.99733987	-2.35635302
H	4.50810870	1.24689324	-1.50915975
H	2.92758664	2.30417639	-3.11811292
C	2.17270744	0.21069888	3.14600924
C	1.30060915	-0.83840326	3.48337510
C	3.51560920	0.17183180	3.55675796
C	1.76515744	-1.90491007	4.25255303
H	0.26388837	-0.80769656	3.16107852
C	3.98189090	-0.91771119	4.29812841
H	4.18620630	0.99956333	3.32920761
C	3.10308943	-1.94920334	4.65521068
H	1.07926225	-2.69754089	4.53863110
H	5.02357504	-0.95079913	4.61639153
H	3.46214876	-2.78705968	5.25201710
C	2.25652460	3.08526717	3.15049646
C	2.38900323	3.10023277	4.55160053
C	2.63516862	4.21508727	2.40568606
C	2.89321717	4.23173735	5.19518038
H	2.11215022	2.22546055	5.13673644
C	3.14814432	5.34128331	3.05502467
H	2.54014776	4.21153133	1.32191764
C	3.27401312	5.35293680	4.44860329
H	3.45229900	6.20917150	2.47063745
H	3.67183124	6.23321234	4.95260389
H	-0.20729148	2.86423737	4.28290847
H	2.99079266	4.23762689	6.28032310
H	-1.25542640	4.65855637	4.59666961
H	-1.80945305	-7.26032496	2.05906217
H	-2.18900642	-4.78952472	2.32587217
H	-6.03414446	-0.17210453	5.53243042
H	-3.94295826	-2.26485571	5.56093940
H	-4.56070286	1.95120223	5.45449382
C	-2.71333266	3.06736541	5.05921762
C	-2.10400110	2.67736088	6.42327128
C	-2.33896574	4.53384796	4.73295052
C	-4.25177900	2.95448010	5.13534026
H	-2.35416148	1.64356523	6.68581988
H	-1.00897912	2.76897791	6.41974417
H	-2.49394900	3.34974624	7.20260846
C	-3.02442599	-0.22269300	4.33402928
C	-6.00430515	-2.28567244	4.93299647
C	-6.28587550	-1.15580186	5.95077403
C	-6.88441531	-2.07908738	3.67989968
C	-6.32417674	-3.64983611	5.58533064
H	-5.69714113	-1.29701199	6.86915934
H	-7.35216731	-1.15073913	6.21959604
H	-6.66784966	-2.83988799	2.92227078
H	-7.94569974	-2.14134822	3.96265821
H	-6.73267880	-1.08314106	3.23564142
H	-7.37024066	-3.66540414	5.92393437
H	-6.17569289	-4.47405043	4.87725881
H	-5.68175995	-3.82127849	6.46257020
C	-3.96163192	-3.45328188	3.77519382
O	-4.61501169	-4.03611112	2.89979243
N	-2.68793010	-3.81448474	4.10217926
H	-2.13219228	-3.16833553	4.67675166
H	-4.64371678	3.68087626	5.86223033
H	-4.71368646	3.16178010	4.15826259
H	-2.83993689	4.87119011	3.81320792
H	-2.65134394	5.19444350	5.55456234
C	-0.54489803	-4.97364221	3.69120419
C	-0.07822442	-5.32696623	4.97009440
C	1.29175833	-5.46798791	5.20628693

C	2.20886023	-5.26958614	4.16196074
C	1.75181920	-4.89485292	2.89241949
C	0.38066757	-4.74441083	2.66087863
H	-0.79094917	-5.51971827	5.77550126
H	1.64265812	-5.74555901	6.20317443
H	3.27640132	-5.39054514	4.34321606
H	2.46166597	-4.70536476	2.08357217
C	-2.67270079	-6.27812309	3.77692682
C	-3.44151998	-6.44870955	4.93200181
C	-3.94927873	-7.70910043	5.26545762
C	-3.69154659	-8.81186773	4.44463595
C	-2.92283048	-8.64506028	3.28522154
C	-2.41652116	-7.38507064	2.95647963
H	-3.65074144	-5.59394994	5.57056261
H	-4.55097761	-7.82724791	6.16684847
H	-4.08906153	-9.79320926	4.70234255
H	-2.71900437	-9.49753745	2.63736182
C	-1.93809946	0.66537804	0.70415192
C	-1.40499267	-0.10601506	-0.55388909
C	-2.25538253	-0.70821635	0.53439031
H	-3.00015482	2.07670526	-3.54001796
C	0.00986179	-0.60201366	-0.55079964
C	-2.08978917	0.23738816	-1.85167167
H	-1.34753508	2.36908899	-4.19724232
C	-2.64547953	-1.92294603	0.89775028
C	-2.93725476	1.72119494	0.56319659
O	0.64759204	-0.85184727	0.46010080
O	0.45867224	-0.82954370	-1.82115738
C	1.81013064	-1.37336921	-1.94014563
H	2.25674724	-0.87614471	-2.80805168
H	1.73827708	-2.45692678	-2.10948341
H	2.37820646	-1.16372563	-1.03033770
O	-3.17767349	-0.20522229	-2.20464761
O	-1.38458045	1.15822082	-2.55769524
C	-2.03087232	1.62518276	-3.77965465
H	-2.17298315	0.79201539	-4.47707594
O	-4.02625785	1.75850399	1.16089723
O	-2.49700839	2.76504634	-0.20682020
C	-3.41041699	3.90051088	-0.29203883
H	-4.35970346	3.59007504	-0.74231205
H	-2.89890407	4.62888163	-0.92579414
H	-3.59578365	4.31452565	0.70521398
C	-2.37930157	-3.15049702	0.06443348
H	-3.17842411	-2.05220999	1.83517874
H	-0.94713367	1.14906569	1.67870015
H	-1.43350587	-3.62915370	0.36773601
H	-2.29196135	-2.89602118	-1.00079564
H	-3.17920103	-3.89307099	0.18723528

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E = -26001.76

G = -25399.64

Nimag = 1, 1521 i cm–1

C	-3.05230310	-2.74191325	1.23302962
N	-3.84293305	-2.67105234	2.47816540
H	-3.31474374	-3.11288591	3.24125733
C	-3.30176348	0.61054046	-0.64565473
S	-6.13389178	-1.26846833	1.89075670
N	-5.45695801	-2.65565673	4.07884022
H	-4.74877099	-3.18439083	4.58350421
C	-6.35782962	-1.90974305	4.97018605
H	-6.74183243	-1.06602268	4.38564570
H	-0.72957437	0.68868316	-1.51521555
C	-5.50186240	-1.36128806	6.14343566
N	-4.27917109	-0.69954152	5.66206611
H	-5.17684175	-2.19696349	6.78258287
P	-4.24188569	0.88999909	5.37952823
C	-4.31645873	1.89858043	6.90197072
C	-3.98031008	1.28857309	8.12049315
C	-4.71135403	3.24613899	6.87517356
C	-4.03017353	2.02793856	9.30343692
H	-3.66563321	0.24824556	8.13232331
C	-4.74883873	3.98427994	8.06101460
H	-5.00319675	3.71349944	5.93629608
C	-4.40847030	3.37559345	9.27472071
H	-3.76958562	1.55405828	10.24927824
H	-5.05149268	5.03070524	8.03903756
H	-4.44281776	3.95115602	10.19944693
C	-5.62709291	1.51665951	4.37782231
C	-6.90843203	1.62175860	4.94924190
C	-5.43679940	1.84049054	3.02618416
C	-7.98682289	2.03710180	4.16916540
H	-7.06112348	1.38733684	6.00126024
C	-6.51278268	2.29293863	2.26154537
H	-4.45401845	1.74545332	2.57165896
C	-7.78665406	2.38211420	2.82562007
H	-8.98023068	2.10730167	4.61123187
H	-6.35617066	2.56103108	1.22339143
H	-8.62664857	2.72170027	2.21988698
C	-2.73104388	1.24560764	4.44833292
C	-2.14112244	0.23090889	3.68123428
C	-2.16175091	2.52596541	4.49225251
C	-0.96681159	0.49632808	2.97586592
H	-2.58523092	-0.75889207	3.65330514
C	-0.99517475	2.78716692	3.77254570
H	-2.60390818	3.30568466	5.10809197
C	-0.39551310	1.77159230	3.01861689
H	-0.54675439	3.77969229	3.81170574
H	0.52014049	1.97564449	2.46331345
H	-6.11480913	-0.70624920	6.77745034
H	-0.51768586	-0.29086434	2.37664325
H	-7.97073209	-1.78200698	7.34454678
H	-3.36327694	3.30835402	-0.73718952
H	-2.50625265	1.18548339	-0.14801690
H	-4.48668137	-5.11692271	1.67638760
H	-2.08931104	-3.11355810	1.60590471
H	-7.78975776	-3.67000060	3.42605162
C	-7.57860048	-2.77641163	5.41300361
C	-7.12761715	-4.08508423	6.09779118
C	-8.46287638	-1.95237861	6.37733187
C	-8.40383336	-3.12471283	4.15478170
H	-6.54903927	-4.70861683	5.40323833
H	-6.51275011	-3.89786078	6.98872217
H	-8.00848462	-4.66369905	6.41330981
C	-5.08354777	-2.23671901	2.82377899
C	-3.51894832	-3.82666194	0.18931354
C	-3.66107667	-5.16347715	0.95290888
C	-4.85102667	-3.49896309	-0.51518952
C	-2.41102220	-3.95682793	-0.88258146
H	-2.73810361	-5.40800471	1.49980947
H	-3.87011254	-5.97878637	0.24557387
H	-4.76235104	-2.59225801	-1.12593622
H	-5.11589366	-4.33359000	-1.18253158
H	-5.66356347	-3.35172910	0.20351186
H	-2.67140652	-4.76737570	-1.57870020
H	-2.30133572	-3.03009878	-1.46164345
H	-1.43842296	-4.19056546	-0.42547938
C	-2.62584443	-1.40321955	0.58706614
O	-1.41640735	-1.19685252	0.38136150
N	-3.60332443	-0.56968916	0.17754557
H	-4.56069006	-0.72759732	0.54968933
H	-9.26610853	-3.75039007	4.43011243
H	-8.77118630	-2.21224108	3.66509352
H	-8.71274442	-0.97459022	5.93826351
H	-9.40419980	-2.48745029	6.57104636
C	-2.75621013	0.16399978	-2.01139283
C	-3.59254212	-0.41032814	-2.97747150
C	-3.06505781	-0.88645606	-4.18083995
C	-1.69258975	-0.78311986	-4.43673050
C	-0.85442948	-0.19859280	-3.48154419
C	-1.38529550	0.26687333	-2.27444257
H	-4.66165796	-0.49015698	-2.79743716
H	-3.72720539	-1.33590808	-4.92087963
H	-1.28036182	-1.15462529	-5.37480801
H	0.21606759	-0.11604534	-3.67023556
C	-4.52863140	1.49382668	-0.80204996
C	-5.81565043	0.96226567	-0.97342706
C	-6.90385454	1.80094613	-1.22807095
C	-6.72295863	3.18543150	-1.30818139
C	-5.44555812	3.72581754	-1.12194124

C	-4.35810077	2.88342108	-0.87182000
H	-5.98203749	-0.10940976	-0.90040095
H	-7.89721033	1.37049341	-1.35228754
H	-7.57278972	3.84015181	-1.49896899
H	-5.29544681	4.80426606	-1.16763426
C	-2.28055373	-2.30102308	6.46862570
C	-0.83524823	-1.78131498	6.69837086
C	-1.73903992	-2.32259540	7.78115831
H	1.27613260	-3.87739946	4.01513589
C	-0.59717855	-0.30321728	6.77196069
C	0.23554454	-2.69076399	6.15676886
H	2.17197659	-2.38083588	3.55928803
C	-1.77539330	-2.45823175	9.10024427
C	-2.49674898	-3.47042404	5.62829575
O	-1.46921743	0.54780047	6.80880555
O	0.72909413	-0.01912434	6.92849693
C	1.02023598	1.41190484	7.02901726
H	2.10114961	1.47258168	7.17499826
H	0.48004131	1.84702209	7.87627295
H	0.71572370	1.91153310	6.10350653
O	0.45566088	-3.82831894	6.55409844
O	0.84672740	-2.12363782	5.08562794
C	1.79487361	-2.98705909	4.38608471
H	2.60785858	-3.28099069	5.05885422
O	-2.09410486	-3.61342762	4.46568051
O	-3.34266812	-4.38255672	6.22271960
C	-3.62854049	-5.57515757	5.42275138
H	-4.07343332	-5.30693365	4.45886567
H	-4.33518819	-6.15317401	6.02207894
H	-2.70425850	-6.13757398	5.25050311
C	-0.63950266	-2.07372371	10.00904019
H	-3.23938934	-1.34111017	6.04642202
H	-2.67473015	-2.88248227	9.55693657
H	-0.30953072	-2.92823128	10.62100081
H	-0.94562032	-1.27820865	10.70823549
H	0.22034208	-1.71192179	9.43022161

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E = -25995.03

G = -25391.56

Nimag = 1, 1707 i cm–1

C	-4.83493245	0.73626015	2.25521566
N	-3.75731634	0.76411813	3.27058107
H	-3.66547655	1.69338615	3.69517524
C	-7.29012290	-1.43884292	4.28313494
S	-3.08437119	-1.86144444	3.49786179
N	-2.64673801	0.21588024	5.17689668
H	-2.77664851	1.21940332	5.35272163
C	-1.66237652	-0.40781279	6.08137447
H	-1.37517441	0.44153988	6.71488692
H	-8.89949364	-2.95595316	2.66784578
C	-0.40016561	-0.86478631	5.33178923
N	0.13854605	0.23506655	4.50417578
H	-0.66319427	-1.72659432	4.71615143
P	1.12183483	-0.01667958	3.25014623
C	0.55605710	0.69093345	1.66272968
C	0.24335124	2.05983838	1.63331435
C	0.53197403	-0.05324466	0.47372215
C	-0.11076087	2.67132693	0.43195328
H	0.27830793	2.65428274	2.53871864
C	0.18037147	0.56714563	-0.72867774
H	0.79478867	-1.10794606	0.47706608
C	-0.14205712	1.92628528	-0.75226824
H	-0.35462398	3.73256103	0.41997223
H	0.15668494	-0.01751768	-1.64776021
H	-0.41970967	2.40496528	-1.69092655
C	1.42476854	-1.78477135	2.95566611
C	0.34518763	-2.60787119	2.58547103
C	2.69978157	-2.34162683	3.14350341
C	0.54526416	-3.97620774	2.40498691
H	-0.64964095	-2.18549045	2.45405013
C	2.89174814	-3.71401449	2.95684505
H	3.53731200	-1.70927418	3.42904542
C	1.81773538	-4.53089198	2.58811806
H	-0.29438174	-4.61020799	2.12182328
H	3.88270339	-4.14368278	3.09911788
H	1.97154236	-5.59989958	2.44446234
C	2.74487017	0.76657916	3.50371731
C	3.21170097	0.91979164	4.81690021
C	3.54975295	1.14124810	2.41605954
C	4.49784333	1.41633701	5.03833195
H	2.55585768	0.69753416	5.65378583
C	4.82986080	1.65065140	2.64647019
H	3.17811780	1.04294488	1.39770733
C	5.30743337	1.77781275	3.95658999
H	5.45391008	1.94931940	1.80460159
H	6.30741780	2.17405316	4.13263940
H	0.33989022	-1.19586884	6.07758971
H	4.85980969	1.53833448	6.05852940
H	-0.45087745	-1.26042306	8.34260421
H	-8.49489445	-2.82700255	6.32643528
H	-8.17608534	-1.01572221	3.78697496
H	-6.09605226	-1.36636234	0.75864952
H	-5.01281460	1.80645334	2.09382060
H	-4.29204787	-1.50878458	6.32588757
C	-2.23683258	-1.50004839	7.08261945
C	-1.96569974	-2.96062144	6.65208202
C	-1.54560761	-1.26322090	8.44533532
C	-3.75392288	-1.29440830	7.25482655
H	-2.40211197	-3.16786894	5.66999193
H	-0.88958777	-3.18195731	6.61302555
H	-2.41707108	-3.63728589	7.39365748
C	-3.14848910	-0.22522251	3.99786150
C	-4.51326303	0.15559004	0.81436235
C	-5.00789934	-1.29499614	0.61779621
C	-5.26673183	1.05843839	-0.19507618
C	-3.00058917	0.25084687	0.54527946
H	-4.52073533	-1.97797128	1.32019258
H	-4.77905173	-1.61606817	-0.40954431
H	-4.89180135	2.09258498	-0.15216852
H	-5.11807390	0.68132190	-1.21731150
H	-6.34408187	1.07338026	0.01970983
H	-2.79679550	-0.02060190	-0.50012461
H	-2.62563251	1.26994131	0.70524258
H	-2.43811524	-0.42424758	1.19851195
C	-6.19523353	0.24240511	2.80726645
O	-7.25038784	0.82594471	2.49834758
N	-6.12796895	-0.81657117	3.64189556
H	-5.23279536	-1.31984731	3.71375748
H	-4.13937076	-1.96265459	8.03873306
H	-3.98851909	-0.26189845	7.54490667
H	-1.85506896	-0.30041767	8.87216445
H	-1.81620872	-2.05794341	9.15616275
C	-7.22400023	-2.93644296	4.02434493
C	-6.21958984	-3.70665574	4.63028781
C	-6.10827412	-5.06934524	4.35110019
C	-7.00914858	-5.68095242	3.46931325
C	-8.01646663	-4.91964788	2.86800828
C	-8.11902212	-3.55048976	3.14258078
H	-5.52041458	-3.23752448	5.31987915
H	-5.32041017	-5.65684392	4.82199309
H	-6.92603118	-6.74612019	3.25442107
H	-8.72216392	-5.39004748	2.18342297
C	-7.35927000	-1.07525809	5.77105152
C	-6.77570727	0.10827344	6.24104862
C	-6.86624135	0.45986182	7.59028023
C	-7.53996211	-0.37106119	8.49015357
C	-8.13064422	-1.55240230	8.02743180
C	-8.04344569	-1.89971810	6.67578079
H	-6.22765513	0.74666253	5.55246618
H	-6.39891972	1.38002589	7.94060565
H	-7.60163159	-0.10341349	9.54483454
H	-8.65636476	-2.20892127	8.72082671
C	-0.47993753	2.84075642	5.04300524
C	-0.01439622	3.35168346	6.43546477
C	0.76019202	3.52711000	5.15946333
H	-1.55645810	6.25882491	8.82239234
C	0.44779965	2.35825773	7.46861019
C	-0.58849694	4.65884459	6.93017132
H	0.06495152	6.42284642	9.59259154

C	1.92304233	4.00264646	4.73404548
C	-1.71675823	3.33166931	4.43940007
O	1.47069195	1.69297289	7.40885216
O	-0.44508246	2.28802746	8.49846228
C	0.02945640	1.57829979	9.68817110
H	-0.84767217	1.47508400	10.33036406
H	0.79970175	2.18627048	10.17760452
H	0.43514620	0.60174614	9.41817818
O	-1.40469103	5.34099061	6.32655036
O	-0.00630565	5.02916831	8.10384963
C	-0.47588793	6.30378887	8.65134058
H	-0.24171327	7.11744295	7.95713485
O	-2.86041436	3.05590692	4.84052098
O	-1.49998948	4.01966340	3.28145230
C	-2.68633222	4.29005895	2.47247317
H	-3.07774290	3.34935823	2.07131498
H	-2.33682086	4.92931968	1.65850099
H	-3.45070641	4.79711949	3.06913108
C	2.96231954	4.59256873	5.64495867
H	2.15875031	3.94371134	3.66814468
H	-0.23572455	1.46195629	4.78318901
H	3.89059998	4.00311299	5.60086506
H	2.61094908	4.60695201	6.68451511
H	3.21802928	5.62189307	5.34689734

Int5_1

E = -26015.04

G = -25412.08

Nimag = 0

C	-5.80922779	-2.27692253	2.54933336
N	-4.56698762	-1.49178669	2.65988299
H	-3.88441549	-1.67151780	1.91905679
C	-4.36403441	-5.34175501	4.29416582
S	-4.91158772	-1.08713698	5.31615506
N	-2.68614627	-0.83338606	3.79611015
H	-2.29543058	-0.79285040	2.85139903
C	-1.94889628	-0.05603865	4.80066556
H	-2.70351878	0.29196014	5.51651841
H	-2.94324287	-3.83575478	2.46496528
C	-1.29773408	1.18044332	4.09226891
N	-2.07282628	1.67237341	2.95746216
H	-0.31654591	0.88245745	3.69622250
P	-3.21237824	2.75895481	3.06516977
C	-2.63097969	4.47762501	3.38508394
C	-1.33395463	4.80394607	2.95679027
C	-3.43336534	5.46201064	3.98303631
C	-0.84748562	6.10399096	3.11574909
H	-0.71556730	4.02951746	2.50568326
C	-2.94548111	6.76302885	4.13918292
H	-4.43686811	5.21344411	4.32401941
C	-1.65433774	7.08527189	3.70481492
H	0.15990362	6.35316232	2.78297841
H	-3.57210829	7.52538513	4.60149678
H	-1.27547150	8.09944992	3.82876211
C	-4.55723329	2.54032863	4.29103578
C	-4.24533419	2.63526542	5.65897956
C	-5.86152017	2.20669921	3.90063782
C	-5.22821764	2.39937726	6.61922038
H	-3.23646975	2.90155991	5.97289480
C	-6.84326729	1.97056234	4.86559567
H	-6.11172478	2.13346608	2.84618347
C	-6.52938884	2.06773144	6.22327641
H	-4.98029619	2.47003160	7.67803404
H	-7.85303012	1.70445410	4.55513979
H	-7.29509750	1.87769579	6.97508138
C	-4.00922476	2.81580183	1.42617370
C	-4.19013260	1.61035698	0.73030017
C	-4.42328520	4.02454167	0.84756693
C	-4.77797084	1.61439254	-0.53430214
H	-3.84640245	0.68600544	1.18341515
C	-5.01232097	4.02436592	-0.42078968
H	-4.27202739	4.96486883	1.37361029
C	-5.18994060	2.81996916	-1.10996751
H	-5.32568983	4.96543143	-0.87208084
H	-5.65289775	2.82189838	-2.09532041
H	-1.09776276	1.94020898	4.86680476
H	-4.90318578	0.68359964	-1.08080570
H	0.23181413	0.78372755	6.36729299
H	-5.64761169	-7.61181394	5.12796741
H	-4.70998977	-6.11370107	3.59108702
H	-6.25417195	0.25716719	1.66100883
H	-6.39060652	-2.02809577	3.44651367
H	-2.01732130	-2.81198148	5.38975559
C	-0.91225112	-0.93235597	5.58686270
C	0.22967611	-1.42411036	4.66770289
C	-0.33099832	-0.08326769	6.73996909
C	-1.62436337	-2.16744546	6.18297081
H	-0.17384349	-1.88799572	3.76002561
H	0.90832187	-0.61151676	4.37594745
H	0.82338161	-2.18908733	5.18863673
C	-4.00558569	-1.13375653	3.86786662
C	-6.65859795	-1.86464624	1.31583590
C	-7.11519929	-0.40496458	1.53792398
C	-5.86625643	-1.96430318	-0.00631988
C	-7.90400154	-2.77692391	1.25141371
H	-7.73790823	-0.32506772	2.44090440
H	-7.70036155	-0.05395434	0.67551529
H	-5.56234848	-2.99832402	-0.19900164
H	-6.48999328	-1.61705818	-0.84291644
H	-4.97127786	-1.33117665	0.01387077
H	-8.57626946	-2.43286060	0.45193645
H	-7.62268357	-3.81737788	1.04887235
H	-8.45997916	-2.74159624	2.20091502
C	-5.40330224	-3.77225128	2.64886183
O	-5.29877840	-4.54698100	1.68288988
N	-5.07446855	-4.10697204	3.92586705
H	-5.09854546	-3.35199413	4.62707476
H	-0.91158534	-2.75837419	6.77713381
H	-2.46260453	-1.86508258	6.82317274
H	-1.13501169	0.28269632	7.39702288
H	0.35405989	-0.69304944	7.34814469
C	-2.84082326	-5.20658703	4.13227360
C	-1.96663899	-5.91596397	4.96842404
C	-0.58109115	-5.80998367	4.80634156
C	-0.04975101	-5.00145010	3.79780364
C	-0.91597228	-4.30188376	2.95313495
C	-2.29705791	-4.40193404	3.12132073
H	-2.36634518	-6.54036803	5.76487350
H	0.08228483	-6.35570297	5.47749739
H	1.02910923	-4.90747733	3.67886995
H	-0.52157515	-3.65453652	2.17183809
C	-4.77435853	-5.72696219	5.70572271
C	-4.49184022	-4.86472446	6.77726793
C	-4.86705330	-5.20794732	8.07719563
C	-5.52080611	-6.42308192	8.32287041
C	-5.80008390	-7.28733680	7.26023214
C	-5.42933194	-6.93698716	5.95561772
H	-3.97260573	-3.92559745	6.59385996
H	-4.64695768	-4.52987728	8.90152762
H	-5.81022030	-6.69260769	9.33838668
H	-6.30656050	-8.23468762	7.44390326
C	-1.74236942	-0.41074020	-0.91276160
C	-1.47103409	0.25125506	-2.23384873
C	-1.40221142	0.83920488	-0.82537864
H	1.25944630	-1.36571385	-4.76895064
C	-2.65944566	0.63397834	-3.09159912
C	-0.16457726	-0.07501990	-2.91423027
H	0.66959439	-0.25138316	-6.05834171
C	-1.08247387	2.10232364	-0.15417393
C	-2.08835080	-1.65918441	-0.26438816
O	-3.67260230	-0.03959946	-3.21062578
O	-2.47025494	1.85289343	-3.65685920
C	-3.55082671	2.30395514	-4.53902114
H	-3.25571227	3.30482333	-4.86018279
H	-4.49407621	2.32944393	-3.98780269
H	-3.63561616	1.62418513	-5.39346825
O	0.85431151	-0.38040192	-2.31087303
O	-0.27676068	-0.01567210	-4.26454076
C	0.94632988	-0.34435457	-5.00650522
H	1.73893564	0.36289533	-4.74317273

O	-2.21274466	-1.78046557	0.95741200
O	-2.25297771	-2.65826564	-1.15050425
C	-2.58714610	-3.97025444	-0.56661025
H	-1.76753000	-4.30066953	0.07696605
H	-2.70454916	-4.63084148	-1.42757990
H	-3.51358637	-3.90159557	0.00802589
C	0.30850599	2.63717855	-0.55785154
H	-1.17611762	1.95433167	0.93321243
H	-1.85332670	2.83396221	-0.44992907
H	0.49398550	3.59038105	-0.04572672
H	0.36536080	2.80845707	-1.64134207
H	1.09509238	1.92458147	-0.27945528

Int5_2

E = -26013.70

G = -25409.14

Nimag = 0

C	-5.91049159	-2.34336371	2.19486118
N	-4.57588332	-1.82324059	2.50091825
H	-3.87805686	-1.80636770	1.74174533
C	-5.25282893	-5.69273029	3.82566004
S	-5.12659299	-1.39444717	5.11755161
N	-2.76926148	-1.23646313	3.77515069
H	-2.30598314	-1.39962593	2.87131478
C	-2.16305982	-0.16234732	4.57367335
H	-2.96540455	0.25133683	5.19762151
H	-3.76699820	-7.38548679	2.28332861
C	-1.61171681	0.94966501	3.62549728
N	-2.39886404	1.15548642	2.39442275
H	-0.59613990	0.69017482	3.30199582
P	-3.27127878	2.47762245	1.99073825
C	-2.41608165	3.93929358	2.61744620
C	-1.05100624	4.09361158	2.30937368
C	-3.08793176	4.90607541	3.38005227
C	-0.36741742	5.22029066	2.76238885
H	-0.53298857	3.33530973	1.72493349
C	-2.39157826	6.03056943	3.83317846
H	-4.14123946	4.78048176	3.62013048
C	-1.03733835	6.18749208	3.52406974
H	0.68821930	5.34453434	2.52529244
H	-2.90830031	6.78147911	4.42892837
H	-0.49817499	7.06496009	3.87920630
C	-4.97337011	2.51987539	2.60813305
C	-5.29143928	1.90058863	3.82431351
C	-5.97123332	3.16890721	1.85913316
C	-6.60432970	1.93233880	4.29506340
H	-4.53877126	1.36081498	4.38843045
C	-7.27893127	3.20531539	2.34250936
H	-5.73203356	3.62029164	0.89836967
C	-7.59486849	2.58969236	3.55998301
H	-6.84968321	1.42079902	5.22390502
H	-8.05614157	3.69914420	1.76056431
H	-8.62105501	2.60782236	3.92610579
C	-3.35502510	2.54472419	0.18853307
C	-3.61969137	1.36899049	-0.53233367
C	-3.15110305	3.76159289	-0.48198648
C	-3.64751486	1.40797386	-1.92315633
H	-3.75221009	0.42269729	-0.02155034
C	-3.19450234	3.78920168	-1.87744655
H	-2.93976077	4.67139445	0.07636258
C	-3.43222376	2.61365136	-2.59570681
H	-3.02348466	4.72794542	-2.40271792
H	-3.43743855	2.63781179	-3.68432459
H	-1.54548650	1.89533618	4.17369890
H	-3.80778853	0.48741562	-2.47767392
H	0.10960087	1.17146970	5.69571227
H	-3.87593192	-7.07905845	5.78145193
H	-5.69080970	-6.36769803	3.07506731
H	-5.66945487	0.24772285	1.35048761
H	-6.55460781	-2.02694683	3.02638375
H	-2.19881531	-2.50751896	5.98590621
C	-1.05387927	-0.69922170	5.53821309
C	0.06095900	-1.42455813	4.75097136
C	-0.45408016	0.48011103	6.33712345
C	-1.71107459	-1.68837537	6.52398309
H	-0.35826934	-2.20093318	4.09897892
H	0.64954777	-0.73641612	4.12907868
H	0.75556707	-1.90990531	5.45185767
C	-4.12198189	-1.47211522	3.72943227
C	-6.49517949	-1.72615561	0.89172485
C	-6.63742074	-0.20665849	1.12345113
C	-5.60374713	-1.97302198	-0.34762498
C	-7.89418538	-2.33958616	0.66139735
H	-7.30716889	0.00810521	1.96728367
H	-7.04022558	0.28122090	0.22484467
H	-5.51131575	-3.04424908	-0.55562407
H	-6.04951971	-1.47444501	-1.22111534
H	-4.59648571	-1.55962205	-0.21443888
H	-8.37425638	-1.85787250	-0.20280473
H	-7.82671440	-3.41699429	0.46480019
H	-8.53852281	-2.18144945	1.53981566
C	-5.79889659	-3.88743791	2.24324307
O	-5.66901534	-4.62073944	1.25431116
N	-5.78039337	-4.35087800	3.52726621
H	-5.72788666	-3.64711252	4.27665035
H	-0.95125772	-2.10959234	7.19852631
H	-2.48058658	-1.18694373	7.12689876
H	-1.24496564	1.04759452	6.85142782
H	0.23894176	0.09849686	7.10104041
C	-3.73879098	-5.72844481	3.65942738
C	-2.93033665	-4.81491880	4.34910042
C	-1.54133518	-4.87920037	4.23647057
C	-0.94397333	-5.84627148	3.41890407
C	-1.74656923	-6.74643676	2.71290301
C	-3.13941988	-6.68525465	2.83486516
H	-3.39013612	-4.05578313	4.97957383
H	-0.92143807	-4.17732977	4.78785937
H	0.14108067	-5.88855518	3.32551652
H	-1.29071148	-7.49179034	2.06132602
C	-5.73098182	-6.13350814	5.20854684
C	-7.04651711	-5.85107299	5.61116381
C	-7.51357209	-6.26654371	6.86070676
C	-6.67280590	-6.97696528	7.72597649
C	-5.36531592	-7.27076146	7.32755993
C	-4.89746790	-6.85140052	6.07676441
H	-7.70299544	-5.29486637	4.94361905
H	-8.53546622	-6.03391884	7.15992694
H	-7.03486928	-7.29748213	8.70246388
H	-4.70181700	-7.82361451	7.99232559
C	-0.81152618	-0.72698130	-0.71698259
C	0.11220749	-0.69093989	-1.89466206
C	-0.38774111	0.51886232	-1.08964418
H	3.87508470	-2.14325873	-2.46905444
C	-0.47354378	-1.01049487	-3.24168875
C	1.56415784	-1.04342037	-1.68871978
H	4.12680019	-0.85584502	-3.70387710
C	-0.22351817	1.84711911	-1.08283841
C	-1.56500123	-1.57491074	0.04831724
O	-0.20492778	-2.01380116	-3.89370560
O	-1.39049692	-0.08025141	-3.63612265
C	-2.10955091	-0.40935237	-4.86209300
H	-2.81073735	0.41518833	-5.01113524
H	-2.64372811	-1.35907254	-4.74514227
H	-1.41252546	-0.48068640	-5.70460536
O	2.05858964	-1.41898792	-0.63516908
O	2.28641792	-0.80804624	-2.82432265
C	3.71727829	-1.08836753	-2.71808485
H	4.16843197	-0.45427735	-1.94728947
O	-2.33111327	-1.20237637	1.01649326
O	-1.47913366	-2.91407904	-0.27815474
C	-2.23346328	-3.83060972	0.56927955
H	-1.96889269	-3.70748364	1.62411538
H	-1.94260714	-4.82939295	0.23386670
H	-3.31166211	-3.69973372	0.43896659
C	0.55437315	2.59434195	-2.13024709
H	-2.35695009	0.35843615	1.71169473
H	-0.75301755	2.43315555	-0.33494881
H	1.29752989	3.27821641	-1.68715439
H	-0.11688774	3.21118125	-2.75349969
H	1.08367115	1.89794140	-2.79439889

5_74

E = -6228.12

G = -6113.83

Nimag = 0

C	-0.11626913	0.15285461	0.21707659
C	0.12782850	1.69540334	-0.03915171
C	1.21346424	0.71133334	-0.01026350
H	-0.02021137	2.72478259	-3.96180184
C	-0.01819034	2.66764468	1.12211894
C	-0.33545215	2.28119979	-1.34939010
H	-0.56080897	1.04869798	-4.35031558
C	2.52366349	0.54562119	-0.06823232
C	-0.53027629	-0.24128643	1.60351749
O	0.89989053	3.32071043	1.58760958
O	-1.30449866	2.71402448	1.53464826
C	-1.56067943	3.61795407	2.66221602
H	-2.63306519	3.53721087	2.84939963
H	-1.28266231	4.64003797	2.38681375
H	-0.98081529	3.28797972	3.52990029
O	-0.69615449	3.44428813	-1.46761684
O	-0.27026567	1.38336730	-2.35839897
C	-0.67514431	1.89696356	-3.67304067
H	-1.71527659	2.23454278	-3.63333075
O	0.00977425	0.13380744	2.63314982
O	-1.60827696	-1.06986992	1.55249806
C	-2.10958082	-1.50582664	2.86203025
H	-1.32755207	-2.05838150	3.39229202
H	-2.96258663	-2.14862222	2.63668790
H	-2.41574625	-0.63368548	3.44809755
C	3.49682179	1.66249357	-0.30597489
H	4.19986285	1.74056881	0.53756844
H	2.97933573	2.62268082	-0.41570187
H	4.09714164	1.46673665	-1.20795392
H	2.92582239	-0.46240874	0.06778049
H	-0.62492638	-0.36680733	-0.59560943

TS5_69

E = -25735.34

G = -25136.25

Nimag = 1, 1625 i cm–1

C	-6.05602873	-2.05534187	2.32228086
N	-4.70720356	-1.47628079	2.31696397
H	-4.10616428	-1.71793179	1.52245737
C	-8.51533130	0.80296573	2.97742371
S	-4.86109009	-0.68637204	4.90872046
N	-2.70795380	-0.99368478	3.30615131
H	-2.33530529	-1.40050589	2.43860312
C	-1.82324835	-0.13846186	4.09741923
H	-2.44570246	0.27845484	4.89841419
H	-10.87104878	2.05525123	2.57302700
C	-1.36273036	1.02816398	3.18707611
N	-2.51557689	1.72869691	2.61125405
H	-0.78287149	0.61993253	2.35116537
P	-3.15992086	3.05801709	3.24696271
C	-2.12361136	4.54719192	3.04937058
C	-1.10192141	4.50796162	2.08801279
C	-2.32877206	5.70653323	3.81580703
C	-0.29137115	5.62887957	1.89049636
H	-0.92955292	3.60621945	1.50641224
C	-1.52273130	6.82746519	3.60521637
H	-3.10640797	5.72928679	4.57829641
C	-0.50459071	6.78871824	2.64363098
H	0.50745502	5.59135972	1.15058907
H	-1.68230693	7.72889218	4.19602011
H	0.12717537	7.66275272	2.48757854
C	-3.45938606	2.93942305	5.03221544
C	-2.35465592	3.06465268	5.89858882
C	-4.71314858	2.56985778	5.54009076
C	-2.50554574	2.81005803	7.26010299
H	-1.38267430	3.36139942	5.50836602
C	-4.85788757	2.33485506	6.90970576
H	-5.56518597	2.46258638	4.87709137
C	-3.76036125	2.44424401	7.76588782
H	-1.64916798	2.90021112	7.92739883
H	-5.82971142	2.04802025	7.30146666
H	-3.87962047	2.24564094	8.83073085
C	-4.67638657	3.30369406	2.27870932
C	-5.35145876	2.16699085	1.80154643
C	-5.06088110	4.58322271	1.84759361
C	-6.34853783	2.30856566	0.83693566
H	-5.06028433	1.18092302	2.14768113
C	-6.09105629	4.71882576	0.91419009
H	-4.53119047	5.46594235	2.19910481
C	-6.71482917	3.58155634	0.38889574
H	-6.38322275	5.71153380	0.57335127
H	-7.49103953	3.68869347	-0.36872579
H	-0.69091878	1.69826684	3.74003146
H	-6.83514476	1.42010476	0.43841283
H	0.85537746	0.63597761	4.85406362
H	-7.87069299	3.46007904	2.74105192
H	-8.44831381	1.30983223	2.00752505
H	-4.61820618	-2.86022023	-0.06289127
H	0.45036613	-3.42526142	0.99030161
H	-2.01664661	-2.61107186	5.25417162
C	-0.67123240	-0.95597440	4.75905556
C	0.13328744	-1.74867283	3.70418260
C	0.26439128	0.00333162	5.52965648
C	-1.30742641	-1.94428136	5.76222958
H	-0.49645392	-2.50598557	3.21883669
H	0.54558005	-1.09974208	2.92150590
H	0.97225970	-2.27123242	4.18756985
C	-4.05141143	-1.06893638	3.44665889
C	-6.12196268	-3.35799129	1.47077371
C	-5.68270070	-3.12839182	0.00544623
C	-5.18150027	-4.39542032	2.13154919
C	-7.57172695	-3.89307804	1.51618894
H	-6.28375512	-2.33970242	-0.46017082
H	-5.81327069	-4.06121475	-0.56334927
H	-5.47604261	-4.58186044	3.17523780
H	-5.23664486	-5.34681907	1.58263818
H	-4.13714101	-4.05722240	2.11946672
H	-7.62065213	-4.87349011	1.02072587
H	-7.90537288	-4.02398575	2.55715310
H	-8.26494664	-3.21059829	1.01088041
C	-7.11528034	-0.97061157	1.95970124
O	-7.61417949	-0.82058162	0.83316362
N	-7.45663196	-0.20808251	3.03156367
H	-6.86773301	-0.29200484	3.87804530
H	-0.52706543	-2.55650324	6.23809767
H	-1.85646114	-1.40278621	6.54562596
H	-0.31188784	0.65760599	6.20055546
H	0.96989385	-0.57681401	6.14250738
C	-9.91476906	0.18389000	3.07052233
C	-10.12060928	-1.15392628	3.41779185
C	-11.41952719	-1.66542015	3.52809760
C	-12.52320193	-0.84201804	3.28789293
C	-12.32148941	0.49953518	2.93624970
C	-11.02488677	1.00717372	2.83132030
H	-9.26610751	-1.80006007	3.60201220
H	-11.56641762	-2.71068520	3.79988294
H	-13.53402654	-1.24033772	3.37129700
H	-13.17563873	1.14909105	2.74580200
C	-8.31377053	1.83219987	4.08366599
C	-8.48002042	1.46250199	5.42669436
C	-8.33449844	2.40809311	6.44315146
C	-8.01941485	3.73577673	6.12934501
C	-7.85388264	4.10968392	4.79354247
C	-8.00296540	3.16149429	3.77617012
H	-8.74290795	0.43470371	5.67515831
H	-8.46830011	2.10981361	7.48279883
H	-7.89643900	4.47083900	6.92411293
H	-7.60002777	5.13828417	4.53840313
C	-1.17248453	-0.81977015	-0.13942824
C	-0.38469113	0.33032089	-0.71477250
C	-1.84283271	0.32359781	-0.25639437
H	1.65052029	1.67014076	2.50716570
C	-0.14649242	0.38256611	-2.20190374
C	0.57222327	1.12610757	0.15100425
H	2.73305547	0.23031532	2.42090687

C	-2.89799190	1.21096085	-0.04078530
C	-1.14311171	-2.15550459	0.32051430
O	-0.92680143	-0.04688446	-3.03944622
O	1.05930085	0.94338459	-2.49044168
C	1.37871526	1.03411541	-3.91901603
H	2.36494845	1.50092770	-3.95795522
H	0.63082283	1.65167962	-4.42632374
H	1.39877903	0.03240329	-4.35983889
O	0.61390367	2.34800471	0.19353565
O	1.34205098	0.31389383	0.92605564
C	2.23588487	1.01812223	1.85169734
H	2.95927734	1.61525258	1.28649848
O	-2.11988355	-2.63791987	0.96403728
C	0.09068955	-2.98620799	0.04976736
H	-3.86917594	0.71399977	0.06949438
H	-3.66017982	3.21671060	-0.35396448
H	-3.16652826	2.39963721	-1.85332299
H	-1.93122674	3.02237719	-0.73231957
C	-2.91584165	2.53963514	-0.79017557
H	-2.68237820	1.49928544	1.27514806
H	0.89025503	-2.39291994	-0.40790704
H	-0.17621601	-3.81508950	-0.62328005
H	-6.25538045	-2.34361779	3.36438210

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E = -25724.33

G = -25123.17

Nimag = 1, 1731 i cm–1

C	-5.33801960	-2.37595403	4.47284124
N	-4.49841717	-1.44272407	3.71563565
H	-4.76529358	-1.26359557	2.74543080
C	-6.92911361	0.19422009	6.83398817
S	-2.86704230	-0.92820675	5.80936165
N	-2.74809625	-0.08410516	3.21300381
H	-3.14049593	-0.24806113	2.27505550
C	-1.96349388	1.16562428	3.28420798
H	-1.57644046	1.27166443	2.26600277
H	-8.61528211	0.05898594	8.96538170
C	-0.73823274	1.10597286	4.20869342
N	0.29294423	0.17486857	3.69045502
H	-1.04651579	0.83487928	5.22531398
P	1.72611631	0.09649340	4.42673513
C	1.66248367	-0.44260462	6.16348473
C	0.59696073	-1.26809507	6.55440414
C	2.65509948	-0.07924801	7.08902908
C	0.52710551	-1.73126342	7.87022291
H	-0.18907223	-1.51616501	5.84465895
C	2.58295824	-0.55302322	8.40076393
H	3.47541666	0.56979261	6.78699112
C	1.52071785	-1.37913032	8.79060122
H	-0.30665579	-2.36217363	8.17648730
H	3.35231148	-0.27543029	9.12048661
H	1.46556671	-1.74267911	9.81636775
C	2.60149514	1.69838452	4.45826992
C	2.06053794	2.74098518	5.23628787
C	3.72291646	1.94678490	3.65053234
C	2.61507576	4.01999640	5.17389430
H	1.21921253	2.55062397	5.89968061
C	4.27894226	3.22737990	3.60029839
H	4.16554050	1.14454690	3.06583973
C	3.71990045	4.26668211	4.35005646
H	2.18796049	4.82391387	5.77214065
H	5.15042830	3.41262188	2.97317631
H	4.15029131	5.26638920	4.30215269
C	2.74508783	-1.09420363	3.51263836
C	2.91724899	-0.93334416	2.12618781
C	3.33497363	-2.18365633	4.17107390
C	3.67493684	-1.85742518	1.40776939
H	2.43112969	-0.11633934	1.60289218
C	4.09015784	-3.10809862	3.44220155
H	3.19862186	-2.31856205	5.24144683
C	4.26121802	-2.94637731	2.06375523
H	4.53964879	-3.95838298	3.95353965
H	4.84697405	-3.67151852	1.49958851
H	-0.32232542	2.12027279	4.22841501
H	3.79528822	-1.73280938	0.33227299
H	-1.29664316	3.88974370	4.04161006
H	-7.31029416	0.78220100	4.21678897
H	-7.95026785	-0.19873643	6.72396169
H	-5.99389005	-2.55495224	1.68830954
H	-3.31580961	-0.29654779	-2.27819015
H	-4.69154627	1.54900370	2.63800814
C	-2.87235617	2.43268386	3.50888826
C	-3.47844146	2.49094445	4.92506355
C	-2.03091091	3.70649902	3.24548725
C	-4.01405201	2.39350492	2.46510920
H	-4.13196214	1.63537491	5.11899325
H	-2.69872906	2.50452751	5.69910727
H	-4.08773908	3.39870194	5.03074929
C	-3.39389798	-0.78251558	4.17820478
C	-5.76340050	-3.60319994	3.61376300
C	-6.57967393	-3.19540382	2.36490201
C	-4.48442067	-4.34099975	3.15599040
C	-6.59112515	-4.55442689	4.50865615
H	-7.49450824	-2.66631406	2.65176845
H	-6.85007478	-4.09783647	1.79641283
H	-3.82594637	-4.56515012	4.00799154
H	-4.75915278	-5.28929601	2.67129323
H	-3.91605145	-3.74443133	2.43385249
H	-6.87024406	-5.45076959	3.93605230
H	-5.99992618	-4.87806353	5.37922655
H	-7.50649871	-4.06862781	4.86509240
C	-6.51032089	-1.57244775	5.12800960
O	-7.69849302	-1.64524481	4.77638239
N	-6.06541944	-0.75743957	6.11755719
H	-5.04397670	-0.71620722	6.27004886
H	-4.61022703	3.31344818	2.53304615
H	-3.60997204	2.31156486	1.44558288
H	-1.49625639	3.63357216	2.28763015
H	-2.69575720	4.58200961	3.20502688
C	-6.56705122	0.21594928	8.30937061
C	-5.23197287	0.34738984	8.72210740
C	-4.91298626	0.40878583	10.08090193
C	-5.92667143	0.34485667	11.04503707
C	-7.25929230	0.21801964	10.64044987
C	-7.57541980	0.15411410	9.27821448
H	-4.43493163	0.41255577	7.98224137
H	-3.87234853	0.51021989	10.38832451
H	-5.67806422	0.39396513	12.10497742
H	-8.05417639	0.16551226	11.38428390
C	-6.89564373	1.58344373	6.17851027
C	-6.66727262	2.75386984	6.91218613
C	-6.66494161	4.00231624	6.27727291
C	-6.89353360	4.09389117	4.90265205
C	-7.12546826	2.92777118	4.16405507
C	-7.12611970	1.68442977	4.79611256
H	-6.48852595	2.69899320	7.98342053
H	-6.47776371	4.90265753	6.86280982
H	-6.88626320	5.06497350	4.40795275
H	-7.29944702	2.98649186	3.09025593
C	-1.70569799	-0.71795549	0.11702147
C	-0.28998805	-0.32152036	-0.23910619
C	-0.76118931	-1.24743646	0.88932870
H	1.98686939	-2.68621060	-2.66358046
C	0.10610581	1.09550172	0.13661986
C	0.41546915	-0.88975854	-1.43755038
H	0.69276781	-3.93619484	-2.55985600
C	-0.23986671	-1.90697229	2.00263783
C	-3.05801303	-0.38040213	-0.14727562
O	-0.69646649	1.99103103	0.35749086
O	1.45063319	1.24396211	0.26102275
C	1.88782297	2.56785327	0.71778976
H	2.97838231	2.51975605	0.71645015
H	1.50929266	2.74841990	1.72856897
H	1.52507617	3.33919656	0.03131059
O	1.01164143	-0.21870846	-2.27257144
O	0.29154846	-2.24317481	-1.49595363
C	0.90739316	-2.87068344	-2.66628588
H	0.46503741	-2.47065905	-3.58448504
O	-3.98623919	-0.69683181	0.65033168

C	-3.34056308	0.39110801	-1.41790395
H	-0.03293619	-0.82386818	2.84478788
H	-1.04015432	-3.91144842	2.31467373
H	-2.16053055	-2.60145075	2.72922975
H	-0.81230253	-2.96846770	3.80918689
H	0.80198050	-2.21648257	1.87824344
C	-1.11299388	-2.90411315	2.75416259
H	-2.57149186	1.15711567	-1.58163313
H	-4.33264043	0.85362897	-1.36217109
H	-4.70859525	-2.74348491	5.29618832

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E = -25727.20

G = -25128.29

Nimag = 1, 1628 i cm–1

C	-1.96285243	-1.92128265	0.78932574
N	-2.44226644	-1.45400061	2.11788938
H	-1.89639450	-1.90595098	2.87184827
C	-4.84893400	-4.41975414	0.41376783
S	-4.87320974	-0.29319318	1.59037993
N	-3.87195497	-1.27991979	3.87784354
H	-3.14056154	-1.82252653	4.34303430
C	-4.96682794	-0.77282549	4.70691951
H	-5.69849850	-0.35695282	4.00404021
H	-2.99014859	-4.23955513	2.48560896
C	-4.44044290	0.37865635	5.59371511
N	-3.94640473	1.50691916	4.79620980
H	-3.60107222	0.02428096	6.20286598
P	-4.85923805	2.76251279	4.37503325
C	-5.28865161	3.82658886	5.78938289
C	-4.46369794	3.77451417	6.92458551
C	-6.38492095	4.70403926	5.74748359
C	-4.73579442	4.60768042	8.01340744
H	-3.62343142	3.08377547	6.95363646
C	-6.64611791	5.53690586	6.83780022
H	-7.02860884	4.73418953	4.86978697
C	-5.82176253	5.48944567	7.96930426
H	-4.09865524	4.56767672	8.89639950
H	-7.49312822	6.22134004	6.80688912
H	-6.02987364	6.13892661	8.81915944
C	-6.46030659	2.35527091	3.59673598
C	-6.68260948	2.50258806	2.21889365
C	-7.43133881	1.71946311	4.39199834
C	-7.84062855	1.97991078	1.63850269
H	-5.94996021	3.00641609	1.59528825
C	-8.58577729	1.19982629	3.80760775
H	-7.28563350	1.63224128	5.46672170
C	-8.78374731	1.31555514	2.42636646
H	-7.99405197	2.07538500	0.56430250
H	-9.33064188	0.70278988	4.42780008
H	-9.67811866	0.89489841	1.96812558
C	-3.86360877	3.72907328	3.21235934
C	-3.49754783	5.05176515	3.50247118
C	-3.41135129	3.10868452	2.03440857
C	-2.67509294	5.75092988	2.61434661
H	-3.83885986	5.52809008	4.41890305
C	-2.59365620	3.81609884	1.15357305
H	-3.69053860	2.07705290	1.82243442
C	-2.22414364	5.13519797	1.44235203
H	-2.23868068	3.33507936	0.24420461
H	-1.57814362	5.68147774	0.75551758
H	-5.21866478	0.69722323	6.29959881
H	-2.38148425	6.77476868	2.84310846
H	-6.35569453	-0.83058174	7.26759601
H	-6.13685499	-5.21568954	-1.87268486
H	-4.39396272	-5.11780089	-0.30430562
H	-3.78697670	-0.26633834	-0.75711843
H	0.30095161	-2.79931451	7.14987221
H	-5.57298949	-3.24967100	3.73367059
C	-5.65091801	-1.94319169	5.49041582
C	-4.62289777	-2.72662871	6.34071869
C	-6.76077683	-1.39137616	6.41422952
C	-6.30585142	-2.88555179	4.45784415
H	-3.87779265	-3.23089799	5.71428216
H	-4.09660675	-2.07017760	7.04878505
H	-5.13689878	-3.50549477	6.92293248
C	-3.67309068	-1.04096268	2.55612772
C	-1.71867091	-0.86333381	-0.35777743
C	-2.92325452	-0.66012488	-1.30127940
C	-1.31540452	0.47798998	0.27998053
C	-0.53691788	-1.40640709	-1.20092217
H	-3.21517901	-1.60533406	-1.78007946
H	-2.64155880	0.04908979	-2.09424739
H	-0.45576205	0.35758658	0.95503796
H	-1.03861070	1.19520320	-0.50666008
H	-2.14872726	0.89267923	0.85392934
H	-0.32667939	-0.71822955	-2.03228928
H	0.37318200	-1.49853765	-0.58916289
H	-0.77131726	-2.39546310	-1.61709871
C	-2.67751170	-3.21145371	0.30855361
O	-2.01821847	-4.18526351	-0.09729776
N	-4.02627780	-3.20419691	0.41295103
H	-4.48318221	-2.33149660	0.71404670
H	-6.74745790	-3.75951608	4.95635582
H	-7.09996567	-2.35634806	3.91144090
H	-7.44486223	-0.73639677	5.85836228
H	-7.34985433	-2.22838513	6.81705067
C	-4.85384643	-5.10155319	1.79487104
C	-5.90694115	-5.95920504	2.14642267
C	-5.92180359	-6.59898289	3.38952699
C	-4.87979430	-6.39342979	4.30043563
C	-3.82389310	-5.54678529	3.95467863
C	-3.81302041	-4.90644294	2.71262811
H	-6.73189747	-6.11258202	1.45238114
H	-6.75563679	-7.25130410	3.64951676
H	-4.89813119	-6.88173386	5.27459833
H	-3.00788479	-5.35748722	4.65029789
C	-6.24517153	-4.04680823	-0.06321217
C	-7.03608818	-3.17684870	0.70266202
C	-8.30206738	-2.79418611	0.25766985
C	-8.80155587	-3.29259500	-0.95287963
C	-8.02189059	-4.16801073	-1.71586319
C	-6.74558825	-4.53852147	-1.27324604
H	-6.65594772	-2.78391048	1.64079367
H	-8.89892379	-2.10600045	0.85588515
H	-9.79258354	-2.99959847	-1.29910373
H	-8.40401770	-4.56067604	-2.65804186
C	-0.90723036	-1.02067523	5.56363318
C	-0.46566593	0.08920978	6.47630806
C	-0.98223622	0.20949083	5.04119997
H	-3.48780574	0.17575215	9.17374483
C	0.97777121	0.36504400	6.77535126
C	-1.39529832	0.56633162	7.57839960
H	-2.54106869	-0.93349008	10.23617083
C	-1.32759897	1.20154220	4.13043520
C	-1.00058344	-2.42322346	5.45663406
O	1.35852957	1.00190505	7.75319506
O	1.80141181	-0.16632548	5.83666978
C	3.22679053	0.10304196	6.04258148
H	3.72765413	-0.37259486	5.19685127
H	3.55545822	-0.33465093	6.99078152
H	3.40549999	1.18322141	6.04931809
O	-1.96242860	1.64868779	7.59856397
O	-1.57223935	-0.40326016	8.51626655
C	-2.50278645	-0.05098962	9.59446906
H	-2.12525494	0.81952246	10.14090959
O	-1.47772319	-2.98600304	4.42346072
C	-0.56833599	-3.24537350	6.64995620
H	-1.45059058	0.84536788	3.10297450
H	-1.02767140	3.25776236	3.50308382
H	0.39729130	2.53872868	4.28477822
H	-1.00672305	3.02482481	5.26539691
C	-0.70276094	2.58631996	4.30469667
H	-2.71392950	1.37525407	4.45128786
H	-0.34529294	-4.27121166	6.33451007
H	-1.38943660	-3.26990911	7.38345435
H	-0.95895019	-2.28387022	1.04362605

TS5_73

E = -25730.71
G = -25132.71
Nimag = 1, 1692 i cm–1

C	-5.96588536	-2.50061860	2.46997521
N	-4.69027824	-1.85399281	2.77941306
H	-3.88194512	-2.07617187	2.18702384
C	-8.49089474	0.22907763	1.63043003
S	-5.67453406	-0.85288825	5.09134245
N	-3.15910949	-0.74182828	4.06139640
H	-2.50792732	-1.04156419	3.32087831
C	-2.60609414	-0.11840311	5.25858421
H	-3.44558632	-0.05236464	5.95943977
H	-9.55790330	-1.46074452	-0.20422496
C	-2.08275865	1.34150067	4.99172214
N	-2.55187438	1.90406818	3.72607172
H	-0.98470833	1.33160779	4.95781911
P	-3.47895045	3.20238966	3.51994405
C	-2.49533064	4.69226741	3.12824384
C	-2.44923228	5.24214928	1.84105995
C	-1.64531948	5.19464630	4.13166524
C	-1.56718087	6.28849657	1.55742731
H	-3.08647478	4.84341118	1.06031926
C	-0.77351739	6.24449583	3.84730450
H	-1.66123165	4.76069680	5.13100774
C	-0.73123847	6.79124644	2.55776959
H	-1.52799521	6.70592421	0.55185460
H	-0.11871972	6.63152505	4.62737472
H	-0.04233765	7.60532661	2.33478383
C	-4.48775753	3.63793569	4.97101408
C	-4.73697703	4.97635555	5.31877693
C	-5.06499774	2.59926443	5.71920225
C	-5.55193834	5.26688550	6.41628156
H	-4.30249466	5.78736570	4.73866132
C	-5.86750356	2.89794893	6.82021489
H	-4.93090224	1.55896676	5.43144939
C	-6.11007744	4.23027563	7.17290132
H	-5.74973297	6.30521000	6.68050582
H	-6.31417707	2.08535453	7.39253113
H	-6.74179067	4.46206791	8.02992354
C	-4.58023583	2.89506352	2.11355365
C	-4.57175432	1.63150811	1.50487436
C	-5.46856710	3.89074642	1.67111382
C	-5.43289065	1.37462979	0.43801966
H	-3.89497347	0.86655167	1.87375672
C	-6.32762686	3.62364789	0.60774525
H	-5.50124563	4.86091097	2.16425655
C	-6.30624367	2.36806984	-0.00865896
H	-7.02906546	4.38589649	0.27423294
H	-6.98420019	2.16135201	-0.83633729
H	-2.35848896	1.96450256	5.85343044
H	-5.43186677	0.39522132	-0.03324359
H	-0.52942683	0.56039585	7.05359786
H	-10.03143261	2.22940466	0.78247473
H	-8.19502644	0.29971637	0.57561867
H	-3.86796648	-3.75581140	0.94007461
H	-0.17102864	3.48877848	1.04066908
H	-2.52749544	-2.91859423	5.34609672
C	-1.53382375	-1.04690731	5.92238965
C	-0.32813531	-1.29660330	4.98749375
C	-1.05447492	-0.38727232	7.23568715
C	-2.20173733	-2.40062452	6.25742594
H	-0.63632527	-1.74422920	4.03246105
H	0.22314241	-0.37204564	4.77048120
H	0.37469433	-1.99209417	5.46991988
C	-4.43938931	-1.16294462	3.92478054
C	-5.78880744	-3.96371967	1.97075547
C	-4.89707375	-4.06067357	0.71467782
C	-5.14021797	-4.77156011	3.11992768
C	-7.19461560	-4.53573668	1.67715816
H	-5.28638965	-3.42928367	-0.09139705
H	-4.86057784	-5.10499345	0.36919027
H	-5.76934096	-4.74828076	4.02203589
H	-5.01213225	-5.81986062	2.81352969
H	-4.15248781	-4.36839323	3.38082158
H	-7.11655174	-5.60267676	1.42298448
H	-7.84758608	-4.44155501	2.55831421
H	-7.66841138	-4.01151950	0.83807703
C	-6.79996031	-1.57443531	1.54708353
O	-6.82740498	-1.65271646	0.30917564
N	-7.48879895	-0.63875536	2.25515661
H	-7.39089889	-0.65454436	3.27642310
H	-1.48988772	-3.05084317	6.78671048
H	-3.08403761	-2.25386582	6.89653000
H	-1.90515968	-0.18771801	7.90495184
H	-0.35876455	-1.05884488	7.75975910
C	-9.85108228	-0.47145099	1.68717359
C	-10.69831807	-0.32268031	2.79331250
C	-11.90259412	-1.02937661	2.86121382
C	-12.27295954	-1.88897780	1.81945818
C	-11.43025223	-2.03957277	0.71233980
C	-10.22459089	-1.33382165	0.64749701
H	-10.41984332	0.35651651	3.59811735
H	-12.55553109	-0.90589212	3.72526218
H	-13.21453083	-2.43540553	1.86961598
H	-11.71333406	-2.70557648	-0.10277614
C	-8.53159211	1.63242141	2.21574454
C	-7.74888881	2.04681784	3.29673459
C	-7.85858915	3.35652691	3.78190545
C	-8.73708970	4.26313017	3.18874001
C	-9.51753552	3.85542718	2.09929688
C	-9.41694115	2.54914810	1.62446268
H	-7.02968361	1.37051627	3.75308234
H	-7.24526765	3.67118004	4.61955492
H	-8.81029624	5.28283776	3.56690091
H	-10.20230545	4.55598653	1.62099034
C	-1.23370422	-0.25739383	0.60888072
C	-0.92950030	0.85923253	-0.35286369
C	-0.73403015	0.84646462	1.16026158
H	1.58908789	0.37071142	-3.50530821
C	-2.09881675	1.59033047	-0.98044074
C	0.32432224	0.78256413	-1.18520144
H	1.04181297	1.96663641	-4.14004127
C	-0.31827130	1.67241190	2.20600282
C	-1.72124881	-1.57906406	0.66130896
O	-2.99552326	1.04611106	-1.60676296
O	-2.02402878	2.93010984	-0.75624517
C	-3.07493171	3.72025931	-1.40445777
H	-3.08154634	3.51644645	-2.48083012
H	-2.80906168	4.76142757	-1.20973596
H	-4.04567386	3.47144877	-0.97083705
O	1.34337275	0.19781252	-0.84509712
O	0.17535420	1.44029999	-2.36801335
C	1.34401365	1.40719409	-3.25236812
H	2.19716077	1.88330536	-2.75846730
O	-1.98551553	-2.15065274	1.76221719
C	-1.94575024	-2.26906866	-0.66726179
C	0.34961911	3.00121685	1.87380698
H	1.40550737	2.86564932	1.58943328
H	0.31303340	3.68093675	2.73463692
H	-6.50741111	-2.56000479	3.42239361
H	0.13871461	1.11187468	3.03323514
H	-1.52759803	1.85136498	2.85205243
H	-1.02736024	-2.22361768	-1.27152683
H	-2.72704175	-1.73774744	-1.22985184
H	-2.23833932	-3.31196658	-0.51559808

TS5_75
E = -25719.11
G = -25117.99
Nimag = 1, 1698 i cm–1

C	-5.09038000	-2.99860200	2.53448100
N	-3.86589100	-2.18342600	2.69996800
H	-3.31435300	-2.14491000	1.83142600
C	-4.95613100	-5.29364700	5.59987900
S	-4.09530400	-1.21470000	5.24642300
N	-2.33109500	-0.60630900	3.30334300
H	-2.00911400	-0.73030400	2.33563900
C	-1.42365800	0.05647800	4.23530500
H	-1.99878800	0.16854600	5.16218600
H	-5.02947100	-6.67632400	7.93187400

C	-1.01813800	1.48570300	3.73443300
N	-1.86830700	2.03557200	2.67010100
H	-0.00733500	1.44832000	3.31366900
P	-3.17338700	2.93186600	2.97553800
C	-2.84073000	4.73037400	3.02954100
C	-1.86234300	5.23080400	2.15384200
C	-3.56581500	5.61127600	3.84690500
C	-1.61650800	6.60274500	2.09157200
H	-1.30228400	4.54740300	1.52291500
C	-3.31356900	6.98528300	3.78223500
H	-4.32035800	5.22880600	4.53156800
C	-2.34278900	7.48127400	2.90524700
H	-0.85835900	6.98752100	1.41017000
H	-3.87467500	7.66816300	4.41917200
H	-2.14925000	8.55241900	2.85782700
C	-4.03594200	2.53937500	4.52792000
C	-3.40271400	2.79253800	5.75910600
C	-5.31284600	1.95955100	4.50781500
C	-4.04286000	2.45573700	6.95074300
H	-2.42306600	3.26524600	5.78966000
C	-5.95170900	1.63537400	5.70535600
H	-5.80619000	1.75614400	3.56319500
C	-5.31870200	1.87900400	6.92517700
H	-3.54818400	2.64860100	7.90206300
H	-6.93667500	1.17211000	5.67963000
H	-5.81361000	1.61511400	7.85920100
C	-4.37440600	2.71730300	1.63301600
C	-4.25986700	1.62229200	0.76956700
C	-5.45477700	3.60752100	1.51007100
C	-5.20935700	1.43211200	-0.23461800
H	-3.43180400	0.93482900	0.89633800
C	-6.42533700	3.38376700	0.53324000
H	-5.53964400	4.46778200	2.17168800
C	-6.29781700	2.30029800	-0.34491000
H	-7.27070300	4.06508900	0.44369100
H	-7.04452600	2.13928600	-1.12188500
H	-0.94605900	2.14513100	4.60894500
H	-5.10560800	0.60271300	-0.92939600
H	1.11619100	0.84492700	5.22394700
H	-5.46684400	-3.34546700	7.44161200
H	-5.07489900	-6.22883800	5.03453400
H	-6.57900100	-1.73934400	4.68185800
H	-2.68915300	-2.27997100	-2.17032000
H	-1.20438400	-2.74919300	4.41036100
C	-0.16307500	-0.82805300	4.55576700
C	0.67232700	-1.10982000	3.28583100
C	0.70083400	-0.09643900	5.60891300
C	-0.62114700	-2.17908300	5.14436100
H	0.06289500	-1.57544900	2.49845500
H	1.12741400	-0.19993500	2.87352400
H	1.49218100	-1.80175800	3.52886100
C	-3.41317800	-1.35004100	3.68152200
C	-6.49386000	-2.24480800	2.54825200
C	-7.19082500	-2.24088800	3.92720600
C	-6.27557400	-0.80646500	2.05458400
C	-7.41317900	-2.98285400	1.54399300
H	-7.40324300	-3.25965600	4.27464700
H	-8.15226100	-1.71238600	3.83700100
H	-5.78483800	-0.80244200	1.07451500
H	-7.24138100	-0.29123200	1.94936200
H	-5.65124700	-0.23597400	2.74823300
H	-8.40215500	-2.50125500	1.52655400
H	-6.99462000	-2.94608500	0.52637800
H	-7.53776200	-4.03536000	1.82746500
C	-5.14972800	-4.30521000	3.35725600
O	-5.67167400	-5.32008900	2.85985400
N	-4.64341900	-4.25074100	4.61169700
H	-4.45082300	-3.29991200	4.98845500
H	0.25697600	-2.78097600	5.42077500
H	-1.24660500	-2.03620700	6.03360600
H	0.10745300	0.12960200	6.50802500
H	1.54494800	-0.73434800	5.91011800
C	-3.82639800	-5.46463000	6.60860200
C	-2.56779300	-4.88533200	6.41311100
C	-1.54748900	-5.06350000	7.35466300
C	-1.77368400	-5.83145900	8.50048300
C	-3.02946300	-6.42083500	8.69868400
C	-4.04829400	-6.23404700	7.76183700
H	-2.38651900	-4.28663600	5.52720200
H	-0.57730800	-4.59610700	7.19116300
H	-0.98108700	-5.96922400	9.23567200
H	-3.21694500	-7.02065700	9.58929800
C	-6.29174400	-4.94514700	6.25045100
C	-7.45994000	-5.61345900	5.86984600
C	-8.70178700	-5.21199600	6.37691600
C	-8.78025000	-4.13452000	7.26428100
C	-7.61090000	-3.46558600	7.65046700
C	-6.37436600	-3.87223800	7.14921700
H	-7.39822000	-6.43452700	5.15640700
H	-9.60768200	-5.73565800	6.07134700
H	-9.74686400	-3.81562200	7.65422700
H	-7.66682600	-2.62337300	8.34013800
C	-1.52463600	0.26316400	-0.80997800
C	-1.32770300	1.43912400	-1.73378000
C	-0.74065900	1.23236800	-0.34148000
H	0.26362000	1.38753600	-5.48395000
C	-2.44952300	2.43418700	-1.93777600
C	-0.36845000	1.28038200	-2.89098500
H	0.25542900	3.18999400	-5.45951700
C	-0.04153900	1.90305200	0.66431800
C	-2.24273300	-0.92947000	-0.57366900
O	-3.34069500	2.30688000	-2.76511300
O	-2.35058900	3.47405200	-1.06650200
C	-3.39526400	4.49500800	-1.18427000
H	-3.27389800	5.12908400	-0.30433400
H	-4.37862600	4.02393600	-1.19534400
H	-3.23868700	5.06677200	-2.10624400
O	0.40805900	0.34476600	-3.01824400
O	-0.44790500	2.33588700	-3.74364700
C	0.46658300	2.28344100	-4.88884000
H	1.50270000	2.27204900	-4.53574100
O	-2.11645500	-1.55636300	0.51958200
C	-3.17149100	-1.43506900	-1.65351000
C	0.70701600	3.18777200	0.33206600
H	0.94717600	3.74385800	1.24921700
H	0.09666300	3.83133500	-0.31452100
H	1.65586900	2.98277500	-0.18915200
H	0.50206000	1.21366400	1.32245300
H	-1.09679900	2.10851200	1.55369100
H	-3.39766800	-0.65861500	-2.39386700
H	-4.09825700	-1.81175600	-1.20088700
H	-4.97620100	-3.36089400	1.50505900

TS5_76

E = -25721.78

G = -25122.77

Nimag = 1, 1723 i cm–1

C	-5.48436351	0.70805215	2.04321719
N	-4.30430266	0.95300673	2.89038136
H	-4.20245264	1.95019734	3.12738269
C	-3.83001805	-1.36954029	-0.75211137
S	-3.46863262	-1.56914253	3.49435242
N	-2.81664130	0.85654554	4.57384983
H	-3.08450452	1.84758674	4.59393345
C	-1.63224419	0.58040244	5.41276754
H	-1.03242246	1.49753579	5.32446764
H	-2.41485135	0.01303413	-2.62365092
C	-0.74488921	-0.56364236	4.91534326
N	-0.01702269	-0.20147964	3.67443942
H	-1.34555342	-1.46512733	4.77191289
P	1.38151377	-0.93264410	3.36859163
C	1.24783113	-2.64984648	2.76784634
C	-0.04064329	-3.20604139	2.71775757
C	2.35775657	-3.41057124	2.35956877
C	-0.21404939	-4.51990337	2.27659269
H	-0.90363077	-2.60151384	2.98954411
C	2.17473149	-4.71850529	1.90675533
H	3.35876734	-2.98201315	2.38069871
C	0.88987869	-5.27541587	1.86988310
H	-1.21495999	-4.94827514	2.23539841

H	3.03362838	-5.30285175	1.57843052
H	0.75086646	-6.29584968	1.51431106
C	2.39301360	-0.96489552	4.89872384
C	3.05948312	-2.10970234	5.36018524
C	2.41916273	0.21533500	5.66897030
C	3.77159217	-2.06628893	6.56373313
H	3.01109872	-3.04034401	4.80177811
C	3.13033482	0.24994674	6.86753871
H	1.84873567	1.08632693	5.35521442
C	3.81362909	-0.88777348	7.31441825
H	4.28552949	-2.95948669	6.91729863
H	3.13766632	1.16192644	7.46340535
H	4.36495479	-0.85927169	8.25373889
C	2.27931904	0.02708641	2.11171667
C	2.60922228	1.35971383	2.41440772
C	2.58947605	-0.49494817	0.84868480
C	3.22331036	2.16620973	1.45948349
H	2.34961945	1.76854522	3.38190669
C	3.21718393	0.31309461	-0.10243890
H	2.31658798	-1.51219923	0.59246352
C	3.53185920	1.64093542	0.19901559
H	3.44231055	-0.09163514	-1.08805851
H	4.00245223	2.27373041	-0.55283233
H	-0.02254295	-0.76510741	5.71380110
H	3.42232889	3.21126080	1.68515901
H	-0.10311306	-0.34619216	7.66466190
H	-4.43753682	-2.82878198	-2.94566035
H	-4.30430550	-0.76641410	-1.53645332
H	-8.04603930	0.64261419	1.06290881
H	-2.07058857	6.25314951	3.71314335
H	-3.90355333	1.59581109	6.76614801
C	-2.03413062	0.44519558	6.92526282
C	-2.78800544	-0.87471871	7.18497205
C	-0.75886520	0.52362719	7.79800457
C	-2.94633452	1.63709263	7.30153181
H	-3.66288480	-0.95649569	6.52640778
H	-2.14655500	-1.74825774	7.00402669
H	-3.13113576	-0.91492779	8.22985467
C	-3.53316506	0.13929448	3.67879662
C	-6.76280778	0.06120209	2.74101324
C	-8.00926882	0.76627612	2.15246963
C	-6.88962630	-1.45515438	2.47993377
C	-6.70747265	0.33171041	4.25920514
H	-7.99200379	1.84326603	2.37990214
H	-8.92211893	0.33602426	2.59043624
H	-6.04152229	-1.99725605	2.90867241
H	-7.81856833	-1.82619061	2.93919033
H	-6.93623154	-1.67225069	1.40435590
H	-7.65543043	0.01279834	4.71706865
H	-5.89246165	-0.22381046	4.73815420
H	-6.56850554	1.40230166	4.46898293
C	-5.20292992	0.10626112	0.64600208
O	-5.97980260	0.36729019	-0.29059013
N	-4.09294184	-0.66029577	0.50541055
H	-3.63985847	-1.00239895	1.36931149
H	-3.15870300	1.61873170	8.38027059
H	-2.46089275	2.59618245	7.06396593
H	-0.17762464	1.42662686	7.55934253
H	-1.03925611	0.56746982	8.86076224
C	-2.33348797	-1.44917764	-1.04125218
C	-1.50589982	-2.32650555	-0.32650399
C	-0.15037655	-2.43621044	-0.64130844
C	0.39386991	-1.67046158	-1.67863957
C	-0.42153656	-0.78530399	-2.38810497
C	-1.77869269	-0.67615187	-2.06795462
H	-1.92792607	-2.94079185	0.46488804
H	0.47788965	-3.12706476	-0.08453987
H	1.44902456	-1.76308864	-1.93130131
H	-0.00258324	-0.17781792	-3.18994681
C	-4.45724139	-2.76359998	-0.78752427
C	-4.75831551	-3.47160340	0.38093975
C	-5.27476060	-4.76996466	0.30822980
C	-5.49593772	-5.37253469	-0.93406025
C	-5.19685858	-4.66732655	-2.10719532
C	-4.67820414	-3.37226560	-2.03145018
H	-4.59948546	-3.00945825	1.35104932
H	-5.50828421	-5.30899057	1.22656528
H	-5.90203546	-6.38224314	-0.99068261
H	-5.37104865	-5.12623080	-3.08036200
C	-1.70862297	3.63872628	3.15836976
C	-0.29200146	3.88213847	2.69068187
C	-1.21212873	2.66601918	2.40767844
H	-0.70473774	5.55254242	-0.94620449
C	0.75798619	3.72479176	3.75873579
C	0.00393931	4.74737533	1.49002252
H	-1.93180319	6.68944674	-0.27492536
C	-1.15840988	1.43484302	1.75613821
C	-2.73650178	4.21150806	3.93604372
O	0.62310046	3.00296539	4.74068933
O	1.84968168	4.50999312	3.55947370
C	2.85624315	4.44270473	4.62182073
H	3.61489680	5.17475593	4.33629210
H	3.28793124	3.43778161	4.66943766
H	2.40366147	4.69522114	5.58618744
O	1.06644873	4.78205898	0.88657787
O	-1.10606852	5.44810988	1.11764355
C	-0.95821961	6.22059943	-0.11632683
H	-0.17392548	6.97506604	0.00520566
O	-3.80899752	3.58332221	4.19131699
C	-2.49353814	5.59867426	4.48733892
H	-0.58813389	0.63193031	2.75012472
H	-0.03695855	0.24152961	0.33491281
H	0.63723260	1.86651226	0.59760897
H	-0.83182328	1.64735092	-0.37742476
C	-0.28947603	1.29053210	0.51105600
H	-2.14383209	0.96888008	1.65613042
H	-1.75991192	5.54112427	5.30722080
H	-3.42873648	6.01837334	4.87469337
H	-5.79032188	1.73217541	1.79181214

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E = -25725.32

G = -25124.82

Nimag = 1, 1550 i cm–1

C	-4.90803771	-1.77498326	5.28436396
N	-4.51175838	-0.68455606	4.39337604
H	-5.05165783	-0.58352300	3.53420307
C	-6.49372519	0.46823166	7.89607073
S	-2.57234064	0.17910492	6.05827931
N	-3.35499448	1.10633116	3.60744789
H	-3.83317648	0.83087574	2.73890439
C	-2.19388213	1.97195603	3.30021512
H	-2.27355705	2.09524401	2.21588004
H	-8.22110378	1.37302355	9.75539736
C	-0.83526702	1.25459969	3.51360504
N	-0.09681422	1.19106313	2.22880397
H	-1.02374926	0.24424358	3.88864528
P	1.51294788	1.28842444	2.18769604
C	2.13315025	2.78962952	3.02449941
C	2.26618216	2.76598261	4.42601598
C	2.34155639	3.99147652	2.32832658
C	2.57088870	3.93840352	5.11967000
H	2.13633141	1.83444628	4.97356529
C	2.65870403	5.15756896	3.02763294
H	2.26498525	4.02055252	1.24472629
C	2.76323519	5.13593845	4.42260241
H	2.66069239	3.91515374	6.20512415
H	2.82525838	6.08517782	2.48092403
H	3.00211693	6.04983991	4.96543036
C	1.95884008	1.37510470	0.43489955
C	1.27111840	2.30311044	-0.36831143
C	2.97733624	0.58967411	-0.11986458
C	1.62871526	2.46324862	-1.70590100
H	0.45716379	2.88547388	0.05585057
C	3.31206693	0.73737417	-1.46795195
H	3.50520163	-0.13797270	0.48840558
C	2.64916608	1.68086214	-2.25710498
H	1.09813008	3.18665346	-2.32389424
H	4.09362500	0.11381765	-1.90003151
H	2.91694980	1.79708057	-3.30673859

C	2.41841945	-0.03848681	3.04853267
C	1.68453524	-1.05817347	3.67260255
C	3.81708101	0.00197676	3.17781284
C	2.34688692	-2.03773270	4.41512715
H	0.60575757	-1.09489946	3.55907112
C	4.47629387	-0.99565945	3.89804812
H	4.38719289	0.81359217	2.72742897
C	3.74076723	-2.01286481	4.51985095
H	5.56200640	-0.97380405	3.98559306
H	4.25716781	-2.78391578	5.09079092
H	-0.24632181	1.76221405	4.28615118
H	1.77510567	-2.82668336	4.90231205
H	-0.18309411	3.95409702	3.78836640
H	-7.19110667	1.43664538	5.47910678
H	-7.51599768	0.17007164	7.62305541
H	-5.89473221	-2.24558725	2.61840739
H	-3.05285451	1.62518432	-1.43288638
H	-4.49517356	3.42986950	3.56826625
C	-2.32403837	3.43357721	3.84301637
C	-2.36971474	3.51328454	5.37937439
C	-1.12423417	4.25379771	3.31538361
C	-3.62821160	4.02610271	3.26145103
H	-3.23641517	2.97912735	5.78097819
H	-1.46690429	3.08032609	5.82962366
H	-2.44192214	4.56757839	5.68722616
C	-3.50786959	0.21290150	4.62003447
C	-5.14826843	-3.09857271	4.50653247
C	-6.21700281	-2.94884180	3.40028974
C	-3.80115303	-3.51266096	3.86842454
C	-5.58582706	-4.17693474	5.52275332
H	-7.16819625	-2.60410397	3.82139816
H	-6.37477865	-3.91932783	2.90793308
H	-3.02177206	-3.61877810	4.63794794
H	-3.91086498	-4.48063081	3.35983130
H	-3.45958357	-2.77942620	3.12707146
H	-5.65747358	-5.15297082	5.02173283
H	-4.84880780	-4.26719535	6.33552274
H	-6.56258155	-3.93645090	5.96065389
C	-6.07620159	-1.24879979	6.16086493
O	-7.27684827	-1.46855780	5.94356104
N	-5.61220950	-0.45789870	7.17265068
H	-4.61585817	-0.18918149	7.10776833
H	-3.77372936	5.05379051	3.62372042
H	-3.58987630	4.05102803	2.16137974
H	-1.00813799	4.14075647	2.22774953
H	-1.28119489	5.32011930	3.53475657
C	-6.35092126	0.35309989	9.40543749
C	-5.23387891	-0.23573199	10.00826565
C	-5.11664576	-0.27155756	11.40355044
C	-6.11735835	0.28047954	12.20836889
C	-7.23992302	0.86807878	11.61048862
C	-7.35230351	0.90439898	10.21899108
H	-4.45290570	-0.67556558	9.39154942
H	-4.24114883	-0.73371968	11.85964359
H	-6.02646765	0.25235118	13.29396673
H	-8.02768707	1.29645854	12.22984234
C	-6.24777010	1.88541985	7.36841315
C	-5.56777801	2.85693181	8.11146053
C	-5.32876838	4.12446278	7.56749228
C	-5.76971470	4.43152927	6.27875200
C	-6.44391692	3.46141334	5.52820256
C	-6.67623152	2.19578510	6.06764021
H	-5.22456765	2.62760305	9.11834779
H	-4.79053792	4.86946130	8.15324936
H	-5.57777832	5.41579524	5.85363857
H	-6.78584946	3.69133439	4.51970591
C	-1.48631229	-0.14360181	0.27573322
C	-1.37212691	-1.66023100	-0.06892514
C	-0.89403606	-0.53023417	-0.95551432
H	2.21780107	-3.23288394	0.06502782
C	-2.68250996	-2.30333791	-0.45969271
C	-0.30394890	-2.58171968	0.42933588
H	2.77597585	-2.12149890	1.36659002
C	-0.29237379	-0.35511742	-2.12318125
C	-2.79197922	0.50640278	0.36253479
O	-3.31067510	-2.02570910	-1.47362188
O	-3.11494501	-3.16780068	0.48986331
C	-4.41251912	-3.78055839	0.21587242
H	-4.58371545	-4.46379286	1.04862489
H	-4.38108168	-4.32138978	-0.73639993
H	-5.18696001	-3.00730016	0.18201701
O	-0.34531586	-3.80076719	0.30739282
O	0.79956528	-1.92054015	0.88862265
C	1.97544162	-2.77977031	1.03267634
H	1.79099035	-3.56110757	1.77604990
O	-3.75470963	0.06065596	1.02322431
C	-2.88708845	1.83675134	-0.36363031
H	-0.68655877	0.48452304	1.30564836
H	-0.08503595	-2.45508361	-2.57662665
H	1.25607892	-1.43444444	-3.16220842
H	-0.30125409	-1.41890461	-4.00784792
C	0.16501542	-1.47847371	-3.01114681
H	-0.09542257	0.66263701	-2.46004091
H	-1.94946524	2.40260548	-0.29061373
H	-3.72619085	2.42918070	0.01933011
H	-4.05025780	-1.93831073	5.95026029

TS5_79

E = -25730.78

G = -25130.97

Nimag = 1, 1630 i cm–1

C	-3.96729462	-3.34810220	0.66117807
N	-4.29402677	-2.88291994	2.03231293
H	-3.89355664	-3.51498002	2.73842850
C	-7.49233988	-4.67287548	-0.15408875
S	-6.14953492	-0.93500428	1.59184430
N	-5.62848213	-2.37285823	3.81403139
H	-5.02937798	-3.04441417	4.30753532
C	-6.54604530	-1.58560351	4.63705664
H	-6.85509610	-0.74529906	4.01111432
H	-6.15662414	-5.67850104	2.01132459
C	-5.78285698	-1.04706000	5.86468308
N	-4.50943550	-0.39546473	5.52912812
H	-5.52092154	-1.88248195	6.52323456
P	-4.30838702	1.15753897	5.15614317
C	-5.88566900	2.05497958	5.09732714
C	-6.79473721	1.81379080	4.05051763
C	-6.24464550	2.90676468	6.15635869
C	-8.05025107	2.42101265	4.06948969
H	-6.53096371	1.14543469	3.23222414
C	-7.50716868	3.50629879	6.16819982
H	-5.54340471	3.10027209	6.96519532
C	-8.40979879	3.26422689	5.12735269
H	-8.75099321	2.23116850	3.25705105
H	-7.78347511	4.16401976	6.99145484
H	-9.39302559	3.73355420	5.13997096
C	-3.38810420	1.42494988	3.60608085
C	-2.10885857	0.84609886	3.52732600
C	-3.84207970	2.25449880	2.57250048
C	-1.29417809	1.09522500	2.42591618
H	-1.74867867	0.22277425	4.33960091
C	-3.02081864	2.49653685	1.46647982
H	-4.81931867	2.72573610	2.62967616
C	-1.74935660	1.92380527	1.39386202
H	-0.30453198	0.64347780	2.36963190
H	-3.37827140	3.13902568	0.66258186
H	-1.11300607	2.11723523	0.53125436
C	-3.24999776	1.97479679	6.39572113
C	-3.17995676	1.42189535	7.68010183
C	-2.50098485	3.12004711	6.07978607
C	-2.37047102	2.01072295	8.65246800
H	-3.73858836	0.52186795	7.91040534
C	-1.69841678	3.71104990	7.05771184
H	-2.53318101	3.53829541	5.07526435
C	-1.63311651	3.15691541	8.34292186
H	-1.11474360	4.59850571	6.81502956
H	-0.99445530	3.61447835	9.09820999
H	-6.43810942	-0.37395074	6.43151349
H	-2.30315632	1.55660186	9.63948542
H	-8.37247442	-1.33002866	6.86425307

H	-8.46829686	-5.04132154	-2.67938848
H	-7.12512143	-5.46782793	-0.81921201
H	-1.92947612	-1.50708283	0.98127199
H	-0.33785097	-2.73712456	4.06212435
H	-7.94060071	-3.36164115	3.03919917
C	-7.84254648	-2.38743245	4.99854677
C	-7.50679843	-3.68336130	5.76852568
C	-8.76764801	-1.48761731	5.85147706
C	-8.57491894	-2.75141092	3.68858922
H	-6.83834205	-4.32856683	5.18340812
H	-7.02989399	-3.47429274	6.73567591
H	-8.42688760	-4.25418686	5.96020632
C	-5.31635787	-2.11618889	2.51682548
C	-3.41630262	-2.31265715	-0.40405499
C	-2.72895609	-1.14386893	0.32346982
C	-2.36365630	-3.08419519	-1.24108307
C	-4.49126202	-1.78033278	-1.37800088
H	-3.44208163	-0.57107481	0.92562123
H	-2.27673088	-0.46713839	-0.41572308
H	-2.80976235	-3.97034038	-1.71382235
H	-1.96372671	-2.43208667	-2.03102515
H	-1.52538040	-3.41554403	-0.60971392
H	-4.01280816	-1.09583165	-2.09449516
H	-4.95332443	-2.59826996	-1.94847256
H	-5.27776266	-1.23897903	-0.84425027
C	-5.04490746	-4.29956752	0.08575588
O	-4.72181734	-5.39346938	-0.41390341
N	-6.31833861	-3.86393339	0.19505638
H	-6.48159870	-2.91494464	0.55755031
H	-9.48208586	-3.33115769	3.90853328
H	-8.85709221	-1.84442607	3.13678617
H	-8.90276069	-0.50300215	5.37852401
H	-9.75732055	-1.95777134	5.94910299
C	-8.08576024	-5.33425505	1.09966217
C	-9.46802461	-5.50127466	1.25286718
C	-9.98910988	-6.10118173	2.40490988
C	-9.13297400	-6.54828373	3.41441719
C	-7.75048019	-6.40279740	3.25903752
C	-7.23203177	-5.80085676	2.11123364
H	-10.14563470	-5.14505307	0.47977561
H	-11.06820803	-6.20804452	2.51485865
H	-9.53884573	-7.00369886	4.31739442
H	-7.07339134	-6.74818774	4.03958830
C	-8.48545988	-3.80727765	-0.91131421
C	-9.02059600	-2.65629232	-0.31226481
C	-9.92874854	-1.85549508	-1.00653245
C	-10.32112367	-2.20153217	-2.30640903
C	-9.79489554	-3.34952993	-2.90643903
C	-8.87855955	-4.14719673	-2.20978134
H	-8.72606490	-2.38369608	0.69907147
H	-10.33514986	-0.96161781	-0.53337273
H	-11.03292510	-1.57834127	-2.84728361
H	-10.09521725	-3.62526299	-3.91717799
C	-2.42454973	-2.09708692	5.78906613
C	-2.16606125	-2.49828487	7.25922111
C	-1.36092781	-1.47876566	6.50400794
H	-5.47043521	-1.25392491	9.29840716
C	-1.46849721	-3.81642198	7.47674315
C	-3.09267511	-2.06808047	8.37256743
H	-6.16115284	-2.90443413	9.08712082
C	-0.39975645	-0.57816684	6.67400910
C	-2.37352618	-3.02714316	4.67107706
O	-0.72653875	-4.35467213	6.66794573
O	-1.76162822	-4.32516041	8.70530497
C	-1.11151516	-5.59983088	9.02359159
H	-1.45915188	-5.84950137	10.02809037
H	-0.02398355	-5.47679377	9.00314947
H	-1.41670385	-6.36203942	8.29981910
O	-2.80185674	-1.28588393	9.26589552
O	-4.30721840	-2.67327967	8.26379721
C	-5.26254371	-2.32889849	9.31858708
H	-4.85674647	-2.61004398	10.29622306
O	-3.21458298	-3.94952818	4.53416448
C	-1.33761236	-2.75644023	3.60409100
H	-0.10138808	0.03476426	5.81857770
H	0.25797782	0.75004248	8.22921128
H	1.36954009	-0.59629248	7.91960992
H	-0.16891030	-0.88376202	8.79012279
C	0.30363036	-0.32021883	7.97666004
H	-3.49995926	-1.20736782	5.61680722
H	-1.51704371	-1.77221828	3.15498104
H	-1.38015373	-3.52159930	2.82096946
H	-3.12506186	-4.02178198	0.85776300

TS5_80

E = -25716.01

G = -25109.89

Nimag = 1, 1502 i cm–1

C	-4.76837087	0.45268992	3.19048228
N	-3.95345581	0.87364732	4.34923974
H	-3.90103335	1.89906538	4.40099890
C	-2.11056387	-0.95374210	0.78374004
S	-2.73465973	-1.44004643	5.08391213
N	-2.47431431	1.10466397	6.03857293
H	-2.75367176	2.08100562	5.87967415
C	-1.19031683	1.06642324	6.76903182
H	-0.90392366	2.12432409	6.80131423
H	0.54811515	-1.26715718	0.34301764
C	-0.06187532	0.33923271	6.03579457
N	0.11450977	0.83401567	4.63639510
H	-0.27467970	-0.73314507	6.02179645
P	1.47899482	0.31328216	3.91836622
C	1.51526362	1.03495321	2.25718054
C	0.31139582	1.45466206	1.67324541
C	2.69353320	0.99975142	1.49559211
C	0.28750378	1.83956046	0.33300825
H	-0.59718860	1.45846427	2.26470426
C	2.65331483	1.34956558	0.14545271
H	3.63686332	0.70519042	1.95202260
C	1.45135057	1.76823556	-0.43663841
H	-0.64729209	2.17657124	-0.11238067
H	3.56564462	1.31456333	-0.44887455
H	1.42636996	2.04792775	-1.48950020
C	1.59089067	-1.49317999	3.66223239
C	0.50830139	-2.30422706	4.02913936
C	2.74935225	-2.08423995	3.12446727
C	0.61746680	-3.69289845	3.94612078
H	-0.42382253	-1.85674869	4.36211160
C	2.85683215	-3.47304528	3.05933242
H	3.56782382	-1.47436652	2.75244763
C	1.80010369	-4.27976932	3.49326269
H	-0.23360098	-4.31286122	4.22334360
H	3.76059732	-3.92467561	2.65151489
H	1.88436770	-5.36408900	3.43463628
C	2.95369434	0.78451133	4.91229025
C	2.86195608	2.03192054	5.55427515
C	4.06582035	-0.03612257	5.17017153
C	3.87728235	2.47032615	6.40263593
H	1.98872986	2.65628418	5.41906739
C	5.08200908	0.40739565	6.02129566
H	4.13906662	-1.02906318	4.74191100
C	4.99392530	1.66182552	6.63451043
H	5.93877485	-0.23755468	6.21368607
H	5.78537042	1.99941704	7.30303291
H	0.85237336	0.49580611	6.62526111
H	3.78661519	3.44174657	6.88456724
H	0.80183205	0.36498585	8.72375247
H	-1.17059030	-0.01018193	-1.56950668
H	-1.42163526	-0.10300328	0.76808498
H	-6.61633471	-0.22403249	1.34421913
H	-2.75877659	2.84143106	2.08036075
H	-3.45677851	1.21436024	8.41048881
C	-1.34292580	0.64615772	8.27432044
C	-1.65043276	-0.85452032	8.44405318
C	-0.03935775	1.00046616	9.03040234
C	-2.49957000	1.47336189	8.88135945
H	-2.54860562	-1.13596188	7.88166194
H	-0.82144862	-1.48110824	8.08700062
H	-1.81102497	-1.07923306	9.50964836
C	-3.04249198	0.24231869	5.14752975

C	-5.93487419	-0.59088438	3.40316200
C	-7.02225816	-0.20473231	2.36639870
C	-5.58181192	-2.07627650	3.16997934
C	-6.48948789	-0.40760800	4.83066318
H	-7.41288868	0.80533989	2.55970695
H	-7.85934777	-0.91552472	2.41581391
H	-4.78815271	-2.41164116	3.84281983
H	-6.48271592	-2.68331224	3.34669768
H	-5.26020982	-2.25036365	2.13644961
H	-7.40471511	-1.00550469	4.95130927
H	-5.75595963	-0.73536685	5.57874331
H	-6.73614265	0.64616428	5.02675684
C	-3.89382357	0.27445953	1.92753628
O	-3.97175041	1.10051188	1.00030193
N	-3.05130389	-0.78753755	1.89738984
H	-2.87756418	-1.28434630	2.78732413
H	-2.57592111	1.27612397	9.96030962
H	-2.33040545	2.55252951	8.74245158
H	0.24617652	2.04997650	8.86469886
H	-0.18788664	0.85698763	10.11062453
C	-1.29648806	-2.22964210	0.92101897
C	-1.91112328	-3.44880274	1.23423154
C	-1.19054954	-4.64273157	1.14977459
C	0.14621553	-4.62665617	0.74039887
C	0.77151435	-3.40897299	0.45789403
C	0.05641970	-2.21463241	0.55692745
H	-2.95943727	-3.46909590	1.52594637
H	-1.67596612	-5.58678174	1.39684261
H	0.70715427	-5.55800962	0.67004777
H	1.82268598	-3.38743075	0.17564181
C	-2.81094111	-0.99330888	-0.57673618
C	-4.05298590	-1.61367330	-0.74730824
C	-4.63291649	-1.70023688	-2.01511402
C	-3.96977994	-1.17401458	-3.13076181
C	-2.72158973	-0.56261516	-2.96602892
C	-2.14669816	-0.47620007	-1.69430753
H	-4.57697463	-2.01620880	0.11524070
H	-5.60616804	-2.17677613	-2.13306979
H	-4.42330776	-1.23824844	-4.11943656
H	-2.19643965	-0.15071988	-3.82776957
C	-0.62091684	3.53197106	4.36340839
C	0.35511828	4.69912288	4.02878516
C	0.00407233	4.25899141	5.42126897
H	3.59731925	3.69216533	1.72406005
C	-0.27662339	6.03347817	3.68385444
C	1.72696548	4.51882117	3.42676873
H	2.66293174	4.31207414	0.31904334
C	0.28833345	4.55488626	6.68438615
C	-2.01499487	3.64032048	3.93252070
O	-1.43903375	6.33905427	3.90655412
O	0.63701268	6.87712108	3.13060021
C	0.12806000	8.20993151	2.79491259
H	0.97958159	8.73331097	2.35547145
H	-0.21871511	8.71464765	3.70227341
H	-0.69419195	8.12271929	2.07774090
O	2.78281470	4.56986798	4.04009936
O	1.63473735	4.36982876	2.07877171
C	2.91005448	4.46486133	1.37027667
H	3.34254767	5.45837169	1.53676008
O	-2.98125873	3.52751015	4.72646441
C	-2.27459844	3.75906748	2.44706582
H	-0.20267022	2.11774267	4.40597277
H	0.81454240	6.41598433	7.64965459
H	1.80747955	6.00791721	6.21763115
H	2.05539481	5.16025914	7.76410579
C	1.29560220	5.59414722	7.09477601
H	-0.22923803	4.01803131	7.48243900
H	-1.35525897	3.93214763	1.87859916
H	-2.97695961	4.58622136	2.27696574
H	-5.29622566	1.38631320	2.96194609

TS5_81
E = -25728.57
G = -25126.42
Nimag = 1, 1335 i cm–1

C	-5.66508587	-2.36436096	2.06711613
N	-4.32258847	-1.78079013	2.10455497
H	-3.93561403	-1.40437850	1.22799094
C	-7.62468845	0.05328474	4.29988542
S	-3.99152435	-2.33738760	4.74093783
N	-2.45732774	-0.87124802	3.04879139
H	-2.46251493	-0.32519081	2.18555994
C	-1.68703736	-0.21748658	4.10882527
H	-2.28881990	-0.31166231	5.02425373
H	-7.73275854	-1.16846244	6.75412535
C	-1.62374318	1.29424219	3.75348477
N	-1.51542440	1.59973303	2.29183844
H	-0.79154317	1.74808801	4.30470884
P	-2.15469661	3.04073101	1.87906727
C	-1.23491275	4.44248688	2.60030012
C	0.00515913	4.16834298	3.19741841
C	-1.72143497	5.76244972	2.58303872
C	0.74935701	5.19848033	3.77542013
H	0.39305614	3.15384154	3.17804650
C	-0.96715105	6.79123111	3.14921902
H	-2.68391341	5.98934382	2.12953171
C	0.26562898	6.50988286	3.75020811
H	1.71137774	4.97819155	4.23667366
H	-1.34412118	7.81292829	3.12531489
H	0.84881249	7.31452775	4.19660573
C	-3.88593847	3.19258239	2.45738162
C	-4.28841225	4.07865687	3.46783333
C	-4.84540520	2.36411051	1.84183689
C	-5.63984965	4.18202538	3.80995702
H	-3.55651150	4.68374604	3.99555870
C	-6.18898684	2.46888813	2.19041227
H	-4.54930884	1.64003831	1.08784857
C	-6.59012876	3.39385099	3.16145093
H	-5.94272751	4.86542624	4.60061315
H	-6.90976347	1.80614689	1.71635262
H	-7.64079224	3.47705420	3.43356439
C	-2.22622318	3.26930900	0.07869131
C	-2.71557325	2.23318837	-0.73452725
C	-1.95122014	4.52685081	-0.48465775
C	-2.93147786	2.46271371	-2.09232032
H	-2.88544028	1.23745567	-0.33477301
C	-2.15881843	4.73952193	-1.84864132
H	-1.56734754	5.33802476	0.12501092
C	-2.65790745	3.71234510	-2.65293189
H	-1.92576854	5.71179733	-2.28081908
H	-2.82020048	3.88281319	-3.71650868
H	-2.54566909	1.75216294	4.13818325
H	-3.30178703	1.65078048	-2.71469443
H	0.38286304	0.82006845	5.71017587
H	-4.87616170	0.31756373	4.57095681
H	-7.99139705	0.63917803	3.44626279
H	-4.71083047	-1.97662926	-0.63007727
H	-1.10311228	-2.61674237	1.58134105
H	-0.81800892	-2.86032726	3.70656476
C	-0.29441291	-0.86126685	4.44270568
C	0.75783718	-0.59519246	3.35112901
C	0.18813985	-0.25898752	5.78429934
C	-0.45265375	-2.38578027	4.62591958
H	0.48661919	-1.08986705	2.41659304
H	0.88289957	0.47400274	3.13540482
H	1.73236913	-0.99255914	3.67107550
C	-3.57715794	-1.63207726	3.23301468
C	-5.92003298	-3.17618734	0.76708897
C	-5.74431477	-2.33030756	-0.51560868
C	-4.91243669	-4.34983140	0.74693740
C	-7.35675759	-3.74078347	0.83762266
H	-6.41469266	-1.46407587	-0.50204630
H	-5.97924860	-2.95248521	-1.39243942
H	-5.02274866	-4.98036264	1.64195109
H	-5.08443293	-4.97554479	-0.14080423
H	-3.87871987	-3.98265310	0.71330036
H	-7.55135678	-4.37381200	-0.03996493
H	-7.49165065	-4.35702881	1.73968483
H	-8.09887184	-2.93243065	0.85244893
C	-6.68617782	-1.22589310	2.37532786

O	-7.28681847	-0.56573090	1.51437585
N	-6.80271592	-1.00952103	3.71376434
H	-6.20329873	-1.56745849	4.33704456
H	0.52203832	-2.82965367	4.87781937
H	-1.16774362	-2.61676692	5.42461681
H	-0.55672934	-0.42066511	6.57804842
H	1.12569892	-0.74365886	6.09240262
C	-8.83113473	-0.57305193	4.99254417
C	-10.07664042	-0.58245557	4.35472868
C	-11.17899865	-1.19660725	4.96060859
C	-11.03856587	-1.81152895	6.20884838
C	-9.79262718	-1.80668343	6.85010429
C	-8.69619096	-1.18795011	6.24515867
H	-10.18289624	-0.10992765	3.37827991
H	-12.14598459	-1.19433548	4.45788340
H	-11.89503827	-2.29092030	6.68243878
H	-9.67853800	-2.28151748	7.82443500
C	-6.82238602	0.97847154	5.21526313
C	-7.50929311	1.86724243	6.05655456
C	-6.81168421	2.75396438	6.87915976
C	-5.41252073	2.75496556	6.88332207
C	-4.72453412	1.87229646	6.04769173
C	-5.42362704	0.99613861	5.21379532
H	-8.59872422	1.86286990	6.06933465
H	-7.36152850	3.44110692	7.52231582
H	-4.86476280	3.44243714	7.52744359
H	-3.63583194	1.86856971	6.04351275
C	-0.41318236	0.01286938	0.30601214
C	0.12218777	0.74422701	-0.99418690
C	0.93299653	-0.15692395	-0.07578074
H	-2.00802729	-0.28392694	-4.26230793
C	0.53836693	2.18741628	-0.99663153
C	-0.30751136	0.07709299	-2.28040999
H	-1.36941098	1.14948575	-5.15351924
C	2.18516818	-0.58125765	0.03247798
C	-1.43155741	-1.04312529	0.17048148
O	0.71516988	2.87663102	-1.98906076
O	0.83703989	2.62571057	0.26811517
C	1.50638841	3.92202914	0.29547677
H	1.87918615	4.03234824	1.31378522
H	0.79433046	4.72013959	0.06102618
H	2.32753146	3.93699592	-0.42870617
O	-0.41993531	-1.14039723	-2.38864559
O	-0.60501611	0.94005845	-3.27831031
C	-1.12070730	0.31399481	-4.49533654
H	-0.35335543	-0.32444733	-4.94632496
O	-2.63236877	-0.76894844	-0.06192070
C	-1.03402087	-2.46548697	0.49564274
H	2.44195683	-1.23939212	0.86702079
H	3.72808439	-1.09770730	-1.39330297
H	4.10069222	0.32157257	-0.40289197
H	2.90803889	0.44864593	-1.72114601
C	3.28431187	-0.20534758	-0.92338120
H	-0.88336330	0.88403957	1.41098664
H	-0.00608054	-2.67491814	0.17859289
H	-1.73489960	-3.15507181	0.01137372
H	-5.70882391	-3.07228781	2.90579178

TS5_82

E = -25728.76

G = -25128.05

Nimag = 1, 1772 i cm–1

C	-5.02307631	-1.96274553	4.31097114
N	-4.27703786	-0.79320394	3.81672563
H	-4.78559985	-0.14223366	3.21028376
C	-5.66548532	-0.26735836	7.67402943
S	-2.05963190	-1.28206608	5.28092955
N	-2.97446963	1.03975925	4.17009260
H	-3.71499724	1.42985888	3.57104254
C	-1.77866198	1.91493392	4.20178279
H	-2.12555836	2.78004758	3.61951310
H	-6.19524150	-1.44124923	10.09917607
C	-0.59852522	1.33457006	3.38331590
N	-0.61220739	1.89662209	2.00693575
H	-0.66785782	0.24114371	3.35656988
P	0.77824365	2.36599147	1.33977221
C	0.36776804	3.34757734	-0.13089379
C	-0.93358971	3.84656459	-0.29174213
C	1.37988653	3.72661402	-1.02827131
C	-1.22049531	4.71193027	-1.34928900
H	-1.70878086	3.56760790	0.41396592
C	1.09048009	4.60845645	-2.07034540
H	2.38946265	3.33830018	-0.91993767
C	-0.20956315	5.10152975	-2.23185050
H	-2.23538893	5.08564563	-1.47838041
H	1.87843177	4.90286762	-2.76257163
H	-0.43410176	5.78500380	-3.05012164
C	1.94856166	1.02442425	0.94533603
C	1.47604376	-0.29447883	1.01459038
C	3.29558896	1.27427743	0.62854968
C	2.34519480	-1.35695831	0.75904923
H	0.43261875	-0.48075483	1.24555827
C	4.15524479	0.20829822	0.35928053
H	3.68129183	2.29184038	0.61749474
C	3.68042077	-1.10808408	0.42583960
H	1.97829199	-2.38048469	0.81347683
H	5.19781969	0.40258369	0.11000896
H	4.35519863	-1.93931795	0.22346548
C	1.73299057	3.47867084	2.42944269
C	2.64576334	2.95378334	3.36078769
C	1.44529024	4.85402748	2.43329767
C	3.25880287	3.79845403	4.28936483
H	2.87825843	1.89062375	3.36182521
C	2.06601398	5.69314889	3.35934380
H	0.73965279	5.26642462	1.71441340
C	2.96912210	5.16651594	4.29014135
H	1.84339048	6.75965600	3.35679199
H	3.44762242	5.82352877	5.01565844
H	0.34525531	1.57610250	3.88539398
H	3.95986241	3.38602322	5.01418904
H	0.42981965	3.52648877	4.86037906
H	-5.83983680	1.90238244	9.31779711
H	-6.65707873	-0.67405229	7.92242084
H	-6.28674815	-0.89200921	1.97620135
H	-3.73890217	2.61597265	-0.89283789
H	-3.36855328	2.15714836	6.49311172
C	-1.40414812	2.53957550	5.59544275
C	-0.61725215	1.59741881	6.52877722
C	-0.53351362	3.78873910	5.30933879
C	-2.70049152	2.99773340	6.29049418
H	-1.19636426	0.70375737	6.77493717
H	0.32255138	1.26110656	6.06732473
H	-0.36408994	2.13542198	7.45528462
C	-3.13398514	-0.28793085	4.38517685
C	-5.80968798	-2.67518420	3.17218320
C	-6.80819734	-1.72213791	2.47340976
C	-4.80216462	-3.19217107	2.12255636
C	-6.55567857	-3.88676546	3.77841401
H	-7.53161330	-1.31480623	3.18816131
H	-7.35214556	-2.27573672	1.69412595
H	-4.03908825	-3.83240247	2.58946874
H	-5.33336566	-3.78722448	1.36489260
H	-4.29509885	-2.36511681	1.61837663
H	-7.04622869	-4.45501095	2.97471733
H	-5.84788618	-4.56085616	4.28547021
H	-7.31671673	-3.56918603	4.49946291
C	-5.89540661	-1.49104803	5.52166014
O	-7.13177238	-1.40649129	5.51669865
N	-5.13388751	-1.08943624	6.57668927
H	-4.11221526	-1.16740432	6.49473083
H	-2.46546141	3.49158099	7.24413108
H	-3.25528804	3.70989796	5.66315145
H	-1.04656607	4.48624734	4.63102846
H	-0.32643261	4.31668718	6.25153407
C	-4.74226040	-0.42357625	8.87253394
C	-3.42938691	0.06593117	8.80592845
C	-2.55891908	-0.08672909	9.88539380
C	-2.99865445	-0.72148952	11.05466142
C	-4.30869120	-1.20513168	11.13062831
C	-5.17580118	-1.05989898	10.04001496

H	-3.08789396	0.57032306	7.90767747
H	-1.53956305	0.29207982	9.81660289
H	-2.32292545	-0.83714670	11.90174415
H	-4.65728521	-1.69817115	12.03784336
C	-5.85492268	1.20727494	7.27232472
C	-5.97086201	1.60390758	5.93400770
C	-6.15919658	2.94672172	5.59715182
C	-6.23768453	3.91791555	6.59819462
C	-6.12800903	3.53265891	7.93876170
C	-5.94160384	2.18810020	8.27192431
H	-5.89895157	0.87353412	5.13870132
H	-6.22762482	3.22874905	4.54657792
H	-6.37316622	4.96751760	6.33801777
H	-6.17945499	4.28144017	8.72937558
C	-2.83488677	0.88413918	0.80997507
C	-2.58747238	0.10764741	-0.50947733
C	-2.42107722	-0.47965533	0.86554260
H	-5.73453442	-2.29378868	-1.32189171
C	-1.41403772	0.48211947	-1.37585840
C	-3.73405917	-0.48741133	-1.28170100
H	-6.82709209	-1.12891470	-0.49304363
C	-1.93829481	-1.57483818	1.43605589
C	-4.06349062	1.63215960	1.03466266
O	-0.27454745	0.05826558	-1.26871750
O	-1.80270601	1.40556123	-2.29820723
C	-0.77390141	1.77463065	-3.27058248
H	-0.58038609	0.92278564	-3.93298386
H	0.14221245	2.06459650	-2.75424057
H	-1.19404577	2.61455148	-3.82652968
O	-3.62511711	-0.93597312	-2.41727978
O	-4.87970687	-0.53509933	-0.55223253
C	-5.99367749	-1.23801258	-1.18788448
H	-6.22257821	-0.78167069	-2.15646653
O	-4.73958264	1.62254097	2.09256952
C	-4.47132911	2.58117531	-0.07997178
H	-1.70347910	1.53360806	1.30423523
H	-0.39667309	-3.01531415	1.00324046
H	-1.35672653	-2.52149675	-0.41483355
H	-2.03946057	-3.63475090	0.80743680
C	-1.40670311	-2.74487716	0.65777002
H	-1.94811028	-1.65966970	2.52322303
H	-4.62153110	3.58603601	0.33950521
H	-5.43683093	2.24366267	-0.48471613
H	-4.26963704	-2.66280185	4.69847062

TS5_83

E = -25732.77

G = -25132.55

Nimag = 1, 1714 i cm–1

C	-1.09136374	-2.02136065	3.93576938
N	-2.56834780	-1.87508712	3.86016777
H	-3.03376094	-2.64814280	4.35642487
C	-0.85665127	-3.09941991	0.26862068
S	-2.99862055	0.19936620	2.12503664
N	-4.57244954	-1.88353646	2.78050789
H	-4.64103038	-2.80011495	3.22695873
C	-5.84178110	-1.27672143	2.37230207
H	-5.63657434	-0.21115783	2.21299415
H	-2.41121271	-4.23126270	2.25672991
C	-6.82805510	-1.43342752	3.55410236
N	-6.35033330	-0.75469710	4.76933551
H	-6.92007858	-2.50245911	3.79933402
P	-6.92368275	0.69117166	5.20705065
C	-8.16348509	0.66177765	6.54798116
C	-8.20861704	-0.44911617	7.40186024
C	-9.05021638	1.73485000	6.74312970
C	-9.13050645	-0.48429296	8.45025502
H	-7.51372386	-1.26871161	7.26312116
C	-9.97064415	1.69379075	7.79328949
H	-9.02783952	2.59505252	6.07615252
C	-10.01080325	0.58552659	8.64825825
H	-9.15803211	-1.34781640	9.11379133
H	-10.65795887	2.52575009	7.94289078
H	-10.72982409	0.55636049	9.46662409
C	-7.77522907	1.47586051	3.79227745
C	-9.10932877	1.13045859	3.50981929
C	-7.07303363	2.31191534	2.90892320
C	-9.72862676	1.61544231	2.35695927
H	-9.66310132	0.48584106	4.19031328
C	-7.69971358	2.79487056	1.75771928
H	-6.04285888	2.58921502	3.11769905
C	-9.02465679	2.44603954	1.47873072
H	-10.76107236	1.34134367	2.14284307
H	-7.14887474	3.44339096	1.07731565
H	-9.50866557	2.82051559	0.57733013
C	-5.60848146	1.84159087	5.71106584
C	-4.41145521	1.83457337	4.98300797
C	-5.79478305	2.76626161	6.74954678
C	-3.41860253	2.77328895	5.26779208
H	-4.24591429	1.10204526	4.19761178
C	-4.79020774	3.69152947	7.04058248
H	-6.70348763	2.75162804	7.34526621
C	-3.60562653	3.70383883	6.29447733
H	-4.93042907	4.40053576	7.85603198
H	-2.82549200	4.42983266	6.52303374
H	-7.82809071	-1.10963838	3.24797982
H	-2.49475580	2.76355833	4.69195950
H	-8.41744546	-1.01427834	1.20929952
H	1.23421593	-3.05515437	-1.49138324
H	0.02805373	-3.74207447	0.38319861
H	-0.49368207	0.56534720	2.75354561
H	-7.44728305	-4.41003161	5.43672631
H	-4.42829340	-2.48924389	0.26641467
C	-6.38530955	-1.86445376	1.02705274
C	-6.87420542	-3.31919281	1.20871797
C	-7.54882831	-0.97023406	0.53961575
C	-5.25757003	-1.83796511	-0.02737617
H	-6.08831866	-3.94733064	1.64592447
H	-7.76676829	-3.37561933	1.84739340
H	-7.12945754	-3.75370329	0.23108005
C	-3.38691211	-1.24575286	2.96619765
C	-0.22169675	-0.80340750	4.43946802
C	0.32328261	0.09395588	3.30921033
C	-1.06974363	0.01921099	5.42428711
C	0.98340873	-1.42153941	5.19263899
H	0.93821505	-0.48214903	2.60289526
H	0.95697347	0.87937780	3.74868843
H	-1.45545484	-0.61863093	6.22729077
H	-0.45740740	0.81970201	5.86634797
H	-1.91890393	0.47512857	4.90814938
H	1.64901873	-0.62168810	5.54893959
H	0.64072785	-2.00262693	6.06112416
H	1.56077195	-2.08784575	4.53643941
C	-0.51393734	-2.74784139	2.69954512
O	0.25017907	-3.72034245	2.83877031
N	-0.93874145	-2.29517762	1.49428378
H	-1.55029687	-1.46942048	1.47337082
H	-5.64085316	-2.19099985	-0.99578827
H	-4.86422448	-0.81995099	-0.14830173
H	-7.23251827	0.08026372	0.47115407
H	-7.87868359	-1.29506430	-0.45850923
C	-2.08930596	-4.01203418	0.12682797
C	-2.56009425	-4.39024579	-1.13834272
C	-3.66985494	-5.23300868	-1.26385602
C	-4.32013640	-5.71688774	-0.12510228
C	-3.84888900	-5.35435631	1.14030132
C	-2.74529955	-4.50852472	1.26322155
H	-2.07129611	-4.00917848	-2.03300086
H	-4.03116601	-5.50255082	-2.25633493
H	-5.19316662	-6.36159728	-0.22324354
H	-4.34354846	-5.71172405	2.04282952
C	-0.65526223	-2.18303992	-0.92635427
C	-1.61942119	-1.21365432	-1.24244636
C	-1.43998113	-0.37059081	-2.34053278
C	-0.29845849	-0.49433059	-3.14389215
C	0.66298004	-1.46195145	-2.83668124
C	0.48378464	-2.30114257	-1.72974222
H	-2.51119373	-1.11506936	-0.62768220
H	-2.19294157	0.38225617	-2.57392457
H	-0.16083342	0.16071346	-4.00392817

H	1.55330029	-1.56504986	-3.45687664
C	-5.46545658	-2.85533154	6.23286430
C	-4.36210800	-2.52908646	7.30314057
C	-5.74297837	-3.05645525	7.61182406
H	-1.57498930	-5.45058860	8.08958437
C	-4.18831088	-1.07879051	7.65082610
C	-3.17700717	-3.45285560	7.28280890
H	-2.91526844	-6.64012991	7.89163284
C	-6.49615079	-3.39754687	8.64819139
C	-5.32064268	-3.97309088	5.30233240
O	-5.09613583	-0.26292092	7.57758311
O	-2.95745760	-0.78508373	8.13924854
C	-2.77698352	0.62775925	8.49147621
H	-1.72954737	0.70966018	8.78962420
H	-3.44701320	0.89424911	9.31600740
H	-2.99171104	1.25458575	7.62338896
O	-2.07383426	-3.16242357	6.84382569
O	-3.51067654	-4.69410439	7.73481981
C	-2.47631218	-5.70973515	7.52472807
H	-2.24066983	-5.77823767	6.45763843
O	-4.31970738	-4.14930309	4.57058724
C	-6.49876295	-4.92101401	5.22918357
H	-7.51437051	-3.75194426	8.46149876
H	-6.01533774	-4.31959157	10.54362499
H	-6.70754035	-2.69464777	10.67914566
H	-5.02028394	-2.90055254	10.13676727
C	-6.03215521	-3.32192221	10.07584837
H	-5.87391753	-1.70096488	5.57725520
H	-6.36099242	-5.68273935	6.01458082
H	-6.53274221	-5.42033562	4.25399580
H	-0.99834645	-2.76747104	4.73053739

TS5_84

E = -25726.40

G = -25126.54

Nimag = 1, 1756 i cm–1

C	-4.53458207	0.57561643	2.54758952
N	-3.45465311	0.60528687	3.56192318
H	-3.41268804	1.53248069	4.00320477
C	-3.09287913	-1.67795613	-0.23125385
S	-2.54761973	-1.97272188	3.82404213
N	-2.46060561	0.10771126	5.53801768
H	-2.65743945	1.10445717	5.69515107
C	-1.47794484	-0.42430879	6.50022054
H	-1.29432100	0.45131088	7.13688799
H	-0.36806761	-1.71439052	-0.21508779
C	-0.13311551	-0.78446060	5.84614881
N	0.36474231	0.31174581	4.98783728
H	-0.25195129	-1.70260459	5.26812214
P	1.40876699	0.05846713	3.78178184
C	0.75286468	0.27626520	2.09490502
C	-0.52218472	0.82188867	1.91310510
C	1.56439530	-0.00641961	0.98053751
C	-0.96756295	1.14066530	0.62799248
H	-1.16456827	0.98538171	2.77028874
C	1.12194516	0.32750619	-0.29963544
H	2.53688493	-0.47841162	1.11501250
C	-0.13863410	0.91492700	-0.47378890
H	-1.96305354	1.55430126	0.48324539
H	1.75309697	0.11905541	-1.16299348
H	-0.48374007	1.17289451	-1.47477152
C	2.07486054	-1.63078822	3.82612036
C	1.24179890	-2.67585746	3.38658991
C	3.32884332	-1.91568386	4.38974355
C	1.65906279	-3.99834258	3.53357876
H	0.27137907	-2.45701927	2.94536629
C	3.74325728	-3.24417276	4.51944021
H	3.98029902	-1.10815454	4.71617148
C	2.90623670	-4.28471783	4.10017028
H	1.00825407	-4.80451324	3.20283515
H	4.71977460	-3.46564495	4.94873906
H	3.22885909	-5.31958586	4.21040495
C	2.78417848	1.23986168	3.95328446
C	3.26932452	1.45392746	5.25436052
C	3.36306055	1.92328493	2.87314406
C	4.35076611	2.30653405	5.46681167
H	2.78006515	0.97886220	6.09986866
C	4.44170097	2.78307386	3.09396822
H	2.96785508	1.80808109	1.86824633
C	4.94558011	2.96261997	4.38600448
H	4.88207595	3.32037339	2.25458385
H	5.78572640	3.63632012	4.55241036
H	0.58122341	-0.99072087	6.66006695
H	4.70429615	2.48050980	6.48143043
H	-0.35717003	-1.24302930	8.87081092
H	-2.81945756	-2.18149001	-2.86546620
H	-2.50524737	-0.88797914	-0.72215067
H	-6.78838732	-0.12067486	1.03312983
H	-2.39554056	3.64016032	2.65875128
H	-4.01280203	-1.75958038	6.57659310
C	-2.02471005	-1.55477818	7.47383938
C	-1.60101046	-2.98828145	7.07611647
C	-1.45574639	-1.26071431	8.88086180
C	-3.56524522	-1.48330505	7.53929350
H	-1.94118938	-3.23452511	6.06518935
H	-0.51042836	-3.11765113	7.12026989
H	-2.04797944	-3.70119969	7.78578198
C	-2.85434965	-0.36719605	4.33144915
C	-5.92630361	0.03565267	3.05436918
C	-6.98298469	0.39355758	1.98309772
C	-5.96487636	-1.48386502	3.31583550
C	-6.26245867	0.77908010	4.36779770
H	-6.99488227	1.47477267	1.78269782
H	-7.98002948	0.09511995	2.33764257
H	-5.29313610	-1.77134563	4.13066530
H	-6.99070615	-1.77217237	3.59182466
H	-5.67597867	-2.05744966	2.42750508
H	-7.27088617	0.49984386	4.70559752
H	-5.55324232	0.51988918	5.16489472
H	-6.23839080	1.86979125	4.22338887
C	-4.12963003	0.09628468	1.13044874
O	-4.32478550	0.84346623	0.15241987
N	-3.61363966	-1.14375229	1.03073718
H	-3.29918201	-1.60175623	1.91289496
H	-3.93266479	-2.18033057	8.30714230
H	-3.90687349	-0.47134458	7.80087491
H	-1.81494606	-0.29087040	9.25151117
H	-1.77309680	-2.03938478	9.59021932
C	-2.16934367	-2.84501632	0.10505915
C	-2.69933295	-4.08108567	0.49933370
C	-1.84869122	-5.13384311	0.84602901
C	-0.46008148	-4.96398060	0.78854695
C	0.07175105	-3.73173884	0.39854580
C	-0.78203322	-2.67671218	0.06534537
H	-3.77869643	-4.22227527	0.52850149
H	-2.26909571	-6.09103947	1.15424560
H	0.20146671	-5.79024836	1.04653142
H	1.15060759	-3.58423552	0.36963351
C	-4.19258921	-2.10217389	-1.20138451
C	-5.51117727	-2.31609828	-0.79068604
C	-6.47723596	-2.75607530	-1.70262552
C	-6.13038856	-2.98600478	-3.03765257
C	-4.80966445	-2.77408441	-3.45480491
C	-3.84884885	-2.33622798	-2.54034928
H	-5.78412949	-2.13711326	0.24462071
H	-7.50220738	-2.91689952	-1.36838339
H	-6.88186995	-3.32623180	-3.74964556
H	-4.53001170	-2.94979348	-4.49349173
C	-0.29252661	2.95624700	5.27026267
C	0.12606854	3.60584121	6.61668705
C	0.81799527	3.84430773	5.30322896
H	-2.29384935	6.00051566	8.84417714
C	0.83548125	2.78441138	7.66562141
C	-0.68946859	4.77236011	7.10413692
H	-0.95967764	6.15380500	10.04689607
C	1.80141041	4.56906499	4.78848387
C	-1.56304146	3.22953945	4.61382467
O	2.04773393	2.72829615	7.80795078
O	-0.04816269	2.11522360	8.46005483
C	0.56668633	1.46082800	9.61747847

H	-0.26632176	1.07243331	10.20382969
H	1.14426063	2.19509755	10.18941015
H	1.22234237	0.64882057	9.28782121
O	-1.40543672	5.46503167	6.39481109
O	-0.49026333	4.99454068	8.43446619
C	-1.21749033	6.14038789	8.98574159
H	-0.89254176	7.06146219	8.49107799
O	-2.67292515	2.91687495	5.11229625
C	-1.48750780	3.84870204	3.23659151
H	0.01727179	1.57208068	5.17447271
H	3.74314396	5.22279973	5.46097249
H	2.44887127	5.38783774	6.67039982
H	2.55690388	6.52835840	5.29875555
C	2.68170739	5.47559969	5.60167957
H	1.99736575	4.49903606	3.71576798
H	-0.59974396	3.51453842	2.68808846
H	-1.39324848	4.93801051	3.37634001
H	-4.70639918	1.64530313	2.37069360

Int5_3

E = -25743.35

G = -25142.64

Nimag = 0

C	-5.17766279	-2.03193760	2.52694621
N	-3.84558358	-1.48141802	2.78614505
H	-3.12841097	-1.62701184	2.07450825
C	-7.47228430	1.01131241	2.29056662
S	-4.51868663	-0.71091148	5.28437244
N	-2.08013845	-0.86273068	4.10823294
H	-1.56138046	-0.99516578	3.23387359
C	-1.40193357	-0.03479520	5.11722562
H	-2.19594779	0.46087154	5.68977631
H	-8.56296303	-1.45999862	2.95599395
C	-0.57543330	1.04688782	4.36868359
N	-1.37014150	1.73819588	3.35744461
H	0.26262209	0.55539856	3.84837053
P	-2.24786413	3.01492952	3.66590068
C	-1.36471110	4.63413431	3.62421866
C	-1.89995556	5.79949252	4.19690321
C	-0.13594791	4.69285431	2.95098356
C	-1.21792469	7.01361793	4.08173303
H	-2.84567544	5.75440470	4.73579354
C	0.54712434	5.90731409	2.83822241
H	0.27761176	3.77897086	2.52803198
C	0.00429843	7.06897116	3.39966974
H	-1.63683039	7.91616584	4.52652826
H	1.50320087	5.94849766	2.31670725
H	0.53618094	8.01602014	3.31188180
C	-3.08505187	3.06342744	5.28849779
C	-2.29291881	3.34287424	6.42127103
C	-4.40785891	2.63438361	5.45553384
C	-2.82136353	3.18871737	7.70146457
H	-1.26451922	3.67977972	6.29812572
C	-4.93599954	2.49556164	6.74181975
H	-5.01961875	2.40046215	4.59126313
C	-4.14834153	2.76535598	7.86175107
H	-2.20347263	3.39878778	8.57431346
H	-5.96160238	2.15788977	6.86379753
H	-4.56279765	2.64258010	8.86239154
C	-3.43277236	3.11480964	2.27558223
C	-3.89257755	1.90715160	1.72386817
C	-3.73120097	4.32777524	1.63677319
C	-4.61144049	1.90939854	0.52796409
H	-3.63455826	0.97028110	2.20542191
C	-4.45708032	4.32746137	0.44181928
H	-3.36173263	5.26799471	2.03968487
C	-4.88593765	3.11930708	-0.11819886
H	-4.67289937	5.27052976	-0.06028591
H	-5.43875648	3.12706588	-1.05548568
H	-0.12275973	1.71037945	5.12217214
H	-4.95143552	0.96513133	0.10775370
H	0.83391440	0.67409971	6.77260353
H	-6.42663834	3.50322197	1.93081684
H	-7.12390633	1.37365234	1.31425820
H	-3.26378294	-3.24796644	0.66732199
H	-0.68129194	-3.65297473	-0.30921737
H	-1.98340779	-2.57339632	6.09302108
C	-0.56555033	-0.90185399	6.11820494
C	0.54714331	-1.68819814	5.39053959
C	0.05285805	0.02479393	7.19039007
C	-1.50604503	-1.90505985	6.82170688
H	0.12346243	-2.32708139	4.60193505
H	1.29119294	-1.02139155	4.93383491
H	1.07385309	-2.33896420	6.10470129
C	-3.42137134	-1.03453815	4.00826684
C	-5.12108485	-3.41109920	1.80876592
C	-4.33915277	-3.34829170	0.47687315
C	-4.42139961	-4.40549342	2.76516698
C	-6.57108041	-3.88853313	1.56142315
H	-4.67134035	-2.51363415	-0.14878849
H	-4.47570402	-4.28939226	-0.07696009
H	-4.98992071	-4.51918071	3.70023533
H	-4.34239762	-5.39250656	2.28646482
H	-3.40804222	-4.06595381	3.02020114
H	-6.56111060	-4.91965305	1.17897966
H	-7.14879804	-3.88142900	2.49861526
H	-7.08061999	-3.24789049	0.83280456
C	-6.06041268	-0.95703475	1.83506097
O	-6.31764124	-0.92727471	0.62302381
N	-6.54380362	-0.03885622	2.71644973
H	-6.19042051	-0.06598730	3.68567270
H	-0.93325049	-2.51657808	7.53558834
H	-2.30343543	-1.37912388	7.36299383
H	-0.72005570	0.66395285	7.64317769
H	0.50972339	-0.57847458	7.98930597
C	-8.89947823	0.48656355	2.09775899
C	-9.84982496	1.33895711	1.51636914
C	-11.17108101	0.92064058	1.34591687
C	-11.56041785	-0.36075231	1.75944167
C	-10.61703684	-1.21277307	2.34081846
C	-9.29219048	-0.79055394	2.50673959
H	-9.55366303	2.34207636	1.20808929
H	-11.89877367	1.59295320	0.89161316
H	-12.59097211	-0.68935442	1.62823203
H	-10.90906866	-2.21168644	2.66480571
C	-7.45408044	2.17309244	3.27437579
C	-8.04327233	2.04428641	4.54082749
C	-8.04900762	3.12252014	5.42788422
C	-7.46356728	4.34009767	5.06061918
C	-6.87915986	4.47379574	3.79887659
C	-6.88070094	3.39523228	2.90971060
H	-8.51317269	1.10314209	4.82503246
H	-8.50721425	3.01312427	6.41065729
H	-7.45684639	5.17531669	5.76017538
H	-6.41145208	5.41333861	3.50589229
C	-1.38287697	-0.29970212	-0.41815784
C	-1.71823242	0.31769001	-1.75740139
C	-1.36591355	1.00122206	-0.44189259
H	0.32209687	-0.75043892	-5.09729876
C	-3.17315169	0.22160471	-2.17113551
C	-0.66437694	0.26889318	-2.83221422
H	-0.86323672	0.18417225	-6.08364681
C	-1.05519157	2.32762728	0.09886793
C	-1.14165968	-1.60899680	0.16288556
O	-3.86615777	-0.76256872	-1.95907857
O	-3.61081429	1.36044256	-2.76018428
C	-5.00449766	1.31319499	-3.21976883
H	-5.21854819	2.32162204	-3.57885235
H	-5.66178129	1.03510164	-2.39078254
H	-5.09822092	0.57950511	-4.02786269
O	0.53493064	0.19704777	-2.59983946
O	-1.21208505	0.26834919	-4.07388249
C	-0.25122106	0.17826486	-5.17975756
H	0.42314451	1.03970328	-5.15417400
O	-1.15552892	-1.79412885	1.39039018
C	-0.90497629	-2.71539929	-0.82802294
H	-1.93687260	2.97012156	-0.04095003
H	0.34024392	3.96347571	-0.17206438
H	-0.03941356	3.10566622	-1.68714411

H	1.05301140	2.35673874	-0.49989744
C	0.15438766	2.97591586	-0.61416231
H	-0.88608128	2.21104668	1.17890412
H	-0.07722519	-2.43880347	-1.49833258
H	-1.80285251	-2.82845747	-1.45379018
H	-5.61878121	-2.20085534	3.51901398

Int5_4

E = -25744.53

G = -25143.82

Nimag = 0

C	-1.06205047	-2.36986707	3.97743234
N	-2.53695757	-2.20826958	3.89301400
H	-3.01741693	-3.06762623	4.22909894
C	-0.80449326	-3.17033399	0.24183853
S	-2.90964628	0.02614592	2.34111368
N	-4.51983509	-2.08971318	2.78779112
H	-4.61173774	-3.04891948	3.17011772
C	-5.74639684	-1.41318965	2.37456661
H	-5.47475537	-0.36337151	2.20462849
H	-2.43056174	-4.40333813	2.12155009
C	-6.72286033	-1.46554131	3.56649385
N	-6.15707929	-0.70528317	4.69297207
H	-6.89455064	-2.49807662	3.89548776
P	-6.82470731	0.62418396	5.37312417
C	-7.90301465	0.26739178	6.78523398
C	-7.69545050	-0.93636920	7.48051602
C	-8.86714302	1.18982487	7.22720010
C	-8.45538671	-1.21011859	8.61928872
H	-6.94550978	-1.64885755	7.14596455
C	-9.62322260	0.90346893	8.36551545
H	-9.02735468	2.12221882	6.68789747
C	-9.41670158	-0.29445171	9.06088031
H	-8.29191947	-2.14136711	9.15746430
H	-10.37335285	1.61437599	8.70950425
H	-10.00853674	-0.51409171	9.94896661
C	-7.79966352	1.42460863	4.07464177
C	-9.15142330	1.08466602	3.89290140
C	-7.15077308	2.26595437	3.15494311
C	-9.84527676	1.58241565	2.78842591
H	-9.65342108	0.42642171	4.59899238
C	-7.85398557	2.75763480	2.05466263
H	-6.10568320	2.53222113	3.29340988
C	-9.19712948	2.41360379	1.86923265
H	-10.89079331	1.31445667	2.64325422
H	-7.35044701	3.40689344	1.33995409
H	-9.74045699	2.79489629	1.00550830
C	-5.48370544	1.69398731	5.94618502
C	-4.31352381	1.77724561	5.17488246
C	-5.59539919	2.40569067	7.15102715
C	-3.26400094	2.58783087	5.60499806
H	-4.19548004	1.18687295	4.26777458
C	-4.53719020	3.21380989	7.57176749
H	-6.48438550	2.31324886	7.76985680
C	-3.37387914	3.30741077	6.79952540
H	-4.61655943	3.75892157	8.51154384
H	-2.54663655	3.93065274	7.13820075
H	-7.68971030	-1.04157790	3.28575017
H	-2.35159441	2.63490531	5.01255474
H	-8.33671022	-1.05252172	1.28076035
H	1.25085589	-3.04569940	-1.55887467
H	0.07610286	-3.82520655	0.30956161
H	-0.41369970	0.26323239	2.94724233
H	-7.15604268	-5.16277305	5.64338705
H	-4.40162440	-2.61851138	0.24668836
C	-6.33661273	-1.96899074	1.04076116
C	-6.86268447	-3.41005975	1.21735934
C	-7.48428976	-1.03526691	0.58809281
C	-5.22365901	-1.95180409	-0.02945369
H	-6.08198938	-4.06735613	1.61772354
H	-7.73129546	-3.44588392	1.89037189
H	-7.17190989	-3.82049990	0.24488608
C	-3.32952190	-1.48667900	3.04767250
C	-0.18153801	-1.19641263	4.56363830
C	0.38872564	-0.23746880	3.49774127
C	-1.02067639	-0.42445765	5.59735022
C	1.01040080	-1.87700719	5.28516064
H	1.02440195	-0.77443567	2.77919165
H	1.00840748	0.52346877	3.99649310
H	-1.37744986	-1.10960872	6.37418715
H	-0.40122657	0.35164668	6.07203581
H	-1.88396397	0.05426049	5.12477784
H	1.68089679	-1.10924245	5.69891561
H	0.65310803	-2.51219127	6.10749226
H	1.58689053	-2.50185477	4.58861554
C	-0.48096784	-3.01411493	2.69626353
O	0.26903222	-4.00447442	2.76666447
N	-0.88891271	-2.46423216	1.52555888
H	-1.49163141	-1.63350020	1.56499034
H	-5.62439509	-2.28638564	-0.99696298
H	-4.81588628	-0.93813566	-0.14512468
H	-7.13524511	0.00495275	0.50886709
H	-7.85408201	-1.34847872	-0.39942609
C	-2.04274616	-4.05971475	0.01676358
C	-2.48791898	-4.34942550	-1.28128016
C	-3.60620080	-5.16454771	-1.48630745
C	-4.29345918	-5.70582313	-0.39543063
C	-3.84964102	-5.42988507	0.90095059
C	-2.73453269	-4.61429323	1.10300368
H	-1.97337795	-3.91863066	-2.13824290
H	-3.94692607	-5.36479716	-2.50237412
H	-5.17541529	-6.32590894	-0.55515560
H	-4.37486639	-5.81835944	1.77240920
C	-0.59599749	-2.16526548	-0.87849513
C	-1.53787374	-1.14761991	-1.09483287
C	-1.35978227	-0.22849542	-2.13008217
C	-0.24287510	-0.32303254	-2.97123214
C	0.69530042	-1.33895621	-2.76454371
C	0.51866173	-2.25404364	-1.71886173
H	-2.41166092	-1.07094600	-0.45153647
H	-2.09476304	0.56137009	-2.28524526
H	-0.10642017	0.39166858	-3.78255351
H	1.56625074	-1.42001781	-3.41474930
C	-5.05421703	-3.81464821	6.30188946
C	-3.94622997	-3.29915612	7.19785754
C	-5.33096295	-3.81502348	7.64749216
H	-1.08560532	-6.03507102	8.29710614
C	-3.79004839	-1.82136041	7.37177880
C	-2.71028579	-4.13654367	7.32066446
H	-2.25729976	-7.32025971	7.82414280
C	-6.02348797	-3.91674494	8.78850527
C	-5.14808501	-4.48815889	5.09896064
O	-4.41469662	-0.97260821	6.74275598
O	-2.96306242	-1.48984975	8.39227746
C	-2.88947927	-0.04819685	8.66083149
H	-2.14163850	0.05366438	9.45039789
H	-3.86930129	0.31346285	8.98995728
H	-2.59118988	0.48608507	7.75613468
O	-1.57869178	-3.72852438	7.08319338
O	-2.99547761	-5.42784799	7.64345814
C	-1.85215709	-6.33675408	7.57549142
H	-1.43139845	-6.32983809	6.56436813
O	-4.24667716	-4.46410766	4.17631767
C	-6.41591289	-5.28921340	4.84293527
H	-7.04455163	-4.30692284	8.74146951
H	-5.44883946	-4.38728322	10.82893762
H	-6.09638817	-2.75349788	10.61571016
H	-4.45586463	-3.13514048	10.04223637
C	-5.47605824	-3.52966072	10.13597301
H	-5.41682694	-1.15112290	5.26582884
H	-6.15354234	-6.35591175	4.76371254
H	-6.86188247	-4.99294517	3.88301704
H	-0.97992998	-3.16867774	4.72235134

5_75

E = -5954.64

G = -5841.65

Nimag = 0

C	-0.50496586	0.76249325	0.82496233
C	0.08984039	2.12436095	0.28180629

C	0.89960669	0.91401412	0.46931410
H	-1.83934553	2.44378239	-3.27348411
C	0.21182374	3.21924571	1.31612647
C	-0.25745939	2.55816835	-1.13160337
H	-3.10586991	3.42612948	-2.44650388
C	2.10142746	0.39109913	0.29842115
C	-1.46672489	0.03745206	-0.08896192
O	0.28594844	3.02813357	2.52020855
O	0.25345306	4.43359468	0.71794654
C	0.39575333	5.57634261	1.63107981
H	0.40738315	6.45244054	0.98049193
H	1.33205844	5.48566281	2.19002205
H	-0.45480899	5.60408947	2.31866017
O	0.54752610	2.65368281	-2.04231335
O	-1.58062877	2.83332917	-1.22415526
C	-2.03461936	3.24767005	-2.55690350
H	-1.51034857	4.15953730	-2.85953649
O	-1.14671593	-0.29720761	-1.22764934
C	-2.83949291	-0.20222330	0.48706975
H	-2.76191735	-0.80195782	1.40656405
H	4.10449072	1.14742546	0.49958371
H	3.00819478	2.19419073	-0.45659254
H	3.65795228	0.68636722	-1.15014340
C	3.27919907	1.15631121	-0.22930357
H	-3.47762617	-0.71192529	-0.24254230
H	-3.28499172	0.76361093	0.77150361
H	-0.78182624	0.81567246	1.88095880
H	2.24891974	-0.66267125	0.55162182

DBU

E = -4900.72

G = -4773.84

Nimag = 0

C	1.64703963	-0.52856348	-0.75758136
C	-0.44418033	-0.81792912	0.34552667
C	0.56919166	1.42992424	0.34109566
N	-0.49302821	0.49942632	0.76177994
N	0.51260101	-1.37541204	-0.34032794
C	1.88385485	0.66981888	0.16876272
H	1.46319141	-0.17101946	-1.78722122
H	2.54680136	-1.16145167	-0.80225092
C	-1.63323975	-1.69393739	0.69726229
H	0.66698683	2.20566915	1.11387276
H	0.28896174	1.93066650	-0.60382668
C	-1.71739055	1.10962336	1.30757056
H	2.65752484	1.34040268	-0.23380817
H	2.22292355	0.30930856	1.15344523
C	-2.91010361	1.14340894	0.33035853
C	-3.69654267	-0.17731241	0.27356181
C	-2.87840143	-1.40030474	-0.17509433
H	-1.89358370	-1.60042474	1.76378871
H	-1.30199819	-2.72528991	0.52525269
H	-1.44523539	2.13490580	1.58870435
H	-2.01114154	0.59582859	2.23733067
H	-2.53712139	1.41427272	-0.67177529
H	-3.59411257	1.94731176	0.64868481
H	-4.56051982	-0.05579535	-0.39989328
H	-4.10696858	-0.37869597	1.27934718
H	-2.54877828	-1.27314106	-1.21998164
H	-3.53457250	-2.28473989	-0.15354127

TS5_85

E = -11108.64

G = -10854.80

Nimag = 1, 1552 i cm–1

C	-0.41387912	-7.06588444	-5.80726998
C	-2.70481518	-7.83358273	-5.81090568
C	-1.15335393	-8.75648150	-4.13541293
N	-2.50916514	-8.60016309	-4.71558893
N	-1.78361365	-7.05958368	-6.34851672
C	-0.08544820	-8.41797216	-5.17282941
H	-0.31622455	-6.25319498	-5.06815152
H	0.27682684	-6.85252600	-6.63446116
C	-4.06773649	-7.81759231	-6.46194906
H	-1.05619511	-9.80175897	-3.81413777
H	-1.06589902	-8.11413215	-3.24331793
C	-3.60265299	-9.35963484	-4.07570872
H	0.90662479	-8.40076948	-4.70191617
H	-0.09450621	-9.18791113	-5.95433205
C	-4.71423713	-8.48168297	-3.47544031
C	-5.73891364	-7.96602353	-4.49882749
C	-5.14811343	-7.09700826	-5.61981081
H	-4.39047867	-8.84574181	-6.67483983
H	-3.95455987	-7.30690388	-7.42265114
H	-3.13247973	-9.94295786	-3.27624029
H	-4.02054382	-10.08352274	-4.79396738
H	-4.24335431	-7.63852069	-2.94328439
H	-5.24436556	-9.08435045	-2.72067562
H	-6.51702493	-7.39269588	-3.97025319
H	-6.24414755	-8.83487100	-4.95675636
H	-4.71567137	-6.17309806	-5.20208482
H	-5.96122020	-6.79283459	-6.29629002
O	-3.15122823	-10.63398123	-9.03220844
C	-1.97897168	-10.27188522	-8.43108207
H	-3.34700747	-7.69046356	-9.84599050
C	-0.77392575	-8.09221425	-9.16606986
C	-1.07318094	-10.04030045	-10.84603595
O	-1.13104298	-11.39837145	-10.92860555
H	-2.60760230	-6.45767760	-10.88649717
C	-1.12271090	-11.93753923	-12.29004359
H	-1.98714661	-11.55921338	-12.84583514
H	-0.19764643	-11.64993687	-12.80022988
O	2.18763530	-8.31685261	-7.78619065
H	-3.59717929	-12.34349774	-7.89286655
C	0.19999299	-8.94478760	-8.89227198
C	-1.49171680	-6.89278370	-9.05083498
O	1.73392463	-10.53943969	-8.18618483
C	2.97526311	-10.85836690	-7.48948118
O	-0.97827223	-9.29945868	-11.81590846
C	1.44883349	-9.19298483	-8.25201193
H	-4.33953352	-10.82863752	-7.30220332
H	3.82907938	-10.39708940	-7.99855539
H	3.04774560	-11.94840876	-7.52106827
H	2.93048630	-10.50255544	-6.45395660
C	-1.06167604	-9.57937789	-9.40838615
H	-0.84947621	-6.00046406	-9.03687650
H	-1.77308940	-6.97521266	-7.67690690
C	-2.79075892	-6.74243110	-9.83804957
O	-1.74482970	-10.44746258	-7.24399962
C	-4.06870043	-11.40129502	-8.19331776
H	-4.94516564	-11.58380311	-8.81915081
H	-3.43464435	-5.97210019	-9.38843683
H	-1.18117368	-13.02107190	-12.16624206

TS5_86

E = -11107.91

G = -10854.24

Nimag = 1, 1568 i cm–1

C	-0.38942116	-7.13811302	-5.75930602
C	-2.69329036	-7.86265884	-5.83664126
C	-1.21164531	-8.83334994	-4.12483643
N	-2.54454034	-8.64984684	-4.74705120
N	-1.74254906	-7.10405439	-6.33755273
C	-0.10167317	-8.49697950	-5.11882171
H	-0.29765022	-6.32668002	-5.01765634
H	0.32931129	-6.93946066	-6.56447829
C	-4.03636986	-7.80567718	-6.52662811
H	-1.13980568	-9.88392362	-3.81362799
H	-1.14533150	-8.20321753	-3.22207653
C	-3.67594019	-9.37198712	-4.13206817
H	0.87015578	-8.49010653	-4.60669648
H	-0.08340173	-9.26206765	-5.90480051
C	-4.77273488	-8.45797512	-3.55798487
C	-5.75666185	-7.91028571	-4.60484001
C	-5.11527867	-7.05567906	-5.70914924
H	-4.38633629	-8.82184981	-6.75402815
H	-3.87959416	-7.29469439	-7.48315551
H	-3.24327232	-9.96980910	-3.32203863
H	-4.10359013	-10.08312336	-4.85710776
H	-4.28761956	-7.63008572	-3.01463417

H	-5.33965825	-9.04288933	-2.81609370
H	-6.53054892	-7.31619352	-4.09323593
H	-6.27562324	-8.76327403	-5.07711030
H	-4.66582351	-6.14602720	-5.27830138
H	-5.90324806	-6.72610014	-6.40331191
O	-3.13516677	-10.58020278	-8.90894317
C	-1.90834555	-10.27677129	-8.38846477
H	-0.47371425	-5.20016289	-10.08830732
C	-0.77483112	-8.07073798	-9.18316116
C	-1.12679954	-10.04094805	-10.83551122
O	-1.19611696	-11.40006479	-10.88865178
H	0.38222560	-5.74594601	-8.62994252
C	-1.24726130	-11.96752719	-12.23772742
H	-2.13295548	-11.59642872	-12.76409253
H	-0.34318377	-11.69507167	-12.79202276
O	2.19829243	-8.23660055	-7.84862367
H	-3.53813487	-12.39604322	-7.93311395
C	0.22420103	-8.90814848	-8.95185612
C	-1.44978181	-6.85078476	-9.02457613
O	1.80328127	-10.46766827	-8.26082332
C	3.04657414	-10.75876936	-7.55514367
O	-1.06610815	-9.31974664	-11.82240363
C	1.48274087	-9.12949230	-8.31924867
H	-4.10108668	-10.93763093	-7.06830216
H	3.89328076	-10.27671269	-8.05690416
H	3.14475263	-11.84672721	-7.58795337
H	2.98524663	-10.40583011	-6.51952075
C	-1.05469171	-9.55794084	-9.40586614
C	-0.61296815	-5.56782140	-9.05937164
H	-1.73953807	-6.96537411	-7.66728098
H	-2.40951004	-6.79236660	-9.55189967
O	-1.58014660	-10.53001347	-7.23899283
C	-3.98608916	-11.40264513	-8.05079638
H	-4.94476177	-11.46527284	-8.57030970
H	-1.09763534	-4.77079663	-8.47543385
H	-1.30478816	-13.04791578	-12.08872014

Int5_5

E = -11120.66

G = -10864.92

Nimag = 0

C	-0.21671162	-7.32325136	-5.69885345
C	-2.58319737	-7.98847859	-5.74312544
C	-1.10118816	-8.95133499	-4.03222322
N	-2.44381282	-8.69403999	-4.62207745
N	-1.57814140	-7.29046359	-6.25914979
C	0.00354240	-8.69047155	-5.05320254
H	-0.11685765	-6.51311782	-4.95958636
H	0.49364403	-7.15560604	-6.51561767
C	-3.90955794	-7.90708102	-6.44640126
H	-1.09294688	-10.00196316	-3.71541834
H	-0.98589762	-8.31883725	-3.13843285
C	-3.60264681	-9.33190866	-3.95239701
H	0.98155993	-8.72860574	-4.55746439
H	-0.03264432	-9.45725993	-5.83774755
C	-4.65675048	-8.33357750	-3.44742654
C	-5.62363481	-7.81796463	-4.52600196
C	-4.95459233	-7.05928295	-5.68248892
H	-4.28993735	-8.92423492	-6.60112293
H	-3.72687299	-7.47624375	-7.43623620
H	-3.18403973	-9.88052291	-3.10222641
H	-4.04731016	-10.07652334	-4.63124730
H	-4.13594956	-7.49199870	-2.96142095
H	-5.24229014	-8.84314263	-2.66630398
H	-6.37103983	-7.16327431	-4.05145056
H	-6.17648332	-8.67816770	-4.94231556
H	-4.47250352	-6.13951339	-5.31397846
H	-5.72767989	-6.75052436	-6.40144631
O	-3.23419182	-10.59693791	-9.17713039
C	-2.11577171	-10.17660363	-8.50551270
H	-3.48283166	-7.81135980	-10.04739383
C	-0.96295820	-7.96911280	-9.24431692
C	-1.08278758	-10.00190201	-10.85415575
O	-1.00542327	-11.36663918	-10.86063503
H	-3.03789581	-6.38571626	-11.00489771
C	-0.88878346	-11.97272276	-12.18600155
H	-1.76030608	-11.71150951	-12.79617332
H	0.02514857	-11.62493218	-12.67919207
O	2.04739971	-8.13482663	-7.81664978
H	-3.68159640	-12.21748384	-7.91152985
C	0.05380631	-8.79651596	-8.89985382
C	-1.69114314	-6.83142541	-9.35022631
O	1.58728288	-10.37787043	-8.15870026
C	2.83507420	-10.65347979	-7.47258085
O	-1.02308935	-9.31679953	-11.86720013
C	1.28279297	-9.01571646	-8.26885271
H	-4.64744755	-10.73985078	-7.62128470
H	3.68355092	-10.19890091	-7.99943357
H	2.92904944	-11.74376876	-7.47015936
H	2.80760263	-10.27176099	-6.44411493
C	-1.16515824	-9.47905617	-9.44145227
H	-1.19258830	-5.87731223	-9.15112029
H	-1.68514657	-7.01026576	-7.25456679
C	-3.06351763	-6.79772680	-9.98020979
O	-1.96404807	-10.32704797	-7.30013166
C	-4.18669514	-11.37051770	-8.38796700
H	-4.94000950	-11.71329451	-9.10143589
H	-3.76941994	-6.17355866	-9.40739175
H	-0.84836356	-13.04941083	-12.00503108

Int5_6

E = -11119.83

G = -10864.41

Nimag = 0

C	-0.24562891	-7.33384802	-5.76925014
C	-2.60804302	-8.01092895	-5.76448438
C	-1.10478744	-8.90222814	-4.03332532
N	-2.45413902	-8.67443939	-4.61978990
N	-1.61218255	-7.32699323	-6.31629724
C	-0.01074512	-8.67417641	-5.07385751
H	-0.14200577	-6.49495911	-5.06322367
H	0.45690263	-7.19562886	-6.59748259
C	-3.94044655	-7.95927674	-6.45808349
H	-1.08818371	-9.93995527	-3.67627183
H	-0.98457894	-8.23547804	-3.16547293
C	-3.60695016	-9.26942280	-3.90180828
H	0.97189843	-8.68787883	-4.58609214
H	-0.04863975	-9.46988983	-5.82892236
C	-4.64429046	-8.23724497	-3.43089626
C	-5.62527483	-7.76880682	-4.51873028
C	-4.97255523	-7.07142440	-5.72246386
H	-4.32723802	-8.98082736	-6.55949426
H	-3.76456365	-7.57510069	-7.47098758
H	-3.17906033	-9.78027980	-3.03289693
H	-4.07009934	-10.04169643	-4.53586091
H	-4.10867734	-7.37674473	-2.99709472
H	-5.22099565	-8.70107053	-2.61545693
H	-6.36101251	-7.08663102	-4.06498825
H	-6.18977644	-8.64503974	-4.88272932
H	-4.48267378	-6.13592001	-5.40792572
H	-5.75617695	-6.79665290	-6.44384722
O	-3.20161053	-10.64499407	-9.20598945
C	-2.08747307	-10.18971776	-8.54968711
H	-0.88427579	-4.84778848	-9.95481852
C	-0.92429679	-7.99303252	-9.29602700
C	-1.11198070	-10.01632573	-10.91979200
O	-0.96010514	-11.37438205	-10.92107778
H	0.14102997	-5.65787563	-8.74713312
C	-0.87214004	-11.98559479	-12.24648968
H	-1.78410908	-11.77765863	-12.81670731
H	-0.00239694	-11.59332929	-12.78420836
O	2.04834899	-8.20699609	-7.82565385
H	-3.60248545	-12.25560918	-7.91234718
C	0.09350258	-8.83819299	-8.99298746
C	-1.58783389	-6.81213804	-9.33775723
O	1.56874638	-10.44300553	-8.18081339
C	2.78268802	-10.73536984	-7.44179078
O	-1.13657174	-9.33800389	-11.93896381
C	1.28939310	-9.07772936	-8.30552976
H	-4.59497551	-10.79341514	-7.63279074

H	3.65853321	-10.29229075	-7.93216225
H	2.86122776	-11.82683647	-7.43553619
H	2.71591097	-10.35260163	-6.41569042
C	-1.15579581	-9.49163698	-9.50471121
C	-0.89963921	-5.49133266	-9.05893243
H	-1.72159423	-7.11157593	-7.32807874
H	-2.59808524	-6.79457080	-9.75086994
O	-1.92024528	-10.32241879	-7.34471618
C	-4.13041473	-11.42639877	-8.39499991
H	-4.88388199	-11.79483014	-9.09528163
H	-1.40089856	-4.91328874	-8.26257624
H	-0.76454443	-13.05670198	-12.06016599

TS5_87

E = -11118.35

G = -10864.75

Nimag = 1, 1490 i cm–1

C	9.99553720	4.07286449	4.87691395
C	7.99349308	3.87382593	3.52363802
C	7.99738011	5.47028397	5.40126294
N	7.33561617	4.81056330	4.25345141
N	9.22202898	3.48335566	3.77502909
C	9.06927339	4.55600731	5.99199442
H	10.59483857	4.91107428	4.48393124
H	10.70053269	3.31388536	5.23170501
C	7.28971991	3.26984768	2.33100639
H	7.22341571	5.69270380	6.14727738
H	8.43659533	6.42649525	5.07078907
C	6.00928867	5.33359014	3.85801252
H	9.63577107	5.09630426	6.76290973
H	8.58536697	3.68847036	6.46703585
C	6.01163381	6.12278005	2.53631103
C	5.98004548	5.23861615	1.27857293
C	7.15970637	4.26269773	1.15010483
H	6.29336583	2.91040937	2.63244951
H	7.85562905	2.39425097	2.00420341
H	5.69299127	5.98965732	4.67696267
H	5.28404391	4.50644014	3.81212221
H	6.89592302	6.78161800	2.52289517
H	5.12353838	6.77517336	2.53288101
H	5.94473510	5.88385252	0.38634204
H	5.04137843	4.65677554	1.28486373
H	8.10684034	4.81555496	1.05035429
H	7.03777218	3.67445209	0.22815330
C	12.78939316	-0.73299382	-0.54858268
H	9.83253203	2.67582870	2.95376644
H	9.70826512	3.86366135	-0.45645333
C	10.44966722	1.91401102	1.91350615
H	11.73935580	5.42561755	-0.82635273
H	11.89842496	4.02537851	-1.89744665
H	12.15095031	-1.04772528	-1.37709603
H	12.83908132	-1.50828086	0.22366946
H	13.79826150	-0.49306135	-0.90051052
C	11.96438582	2.11661524	1.68519233
O	12.66082804	2.76808201	3.92854073
C	9.77926949	0.63237600	1.71793608
C	10.89059931	2.78201953	0.87417718
H	15.13255720	3.76172562	3.58806975
O	13.85592949	0.63999910	1.49452652
O	13.63819315	3.72938990	2.10707501
C	14.52006653	4.46565725	3.01459881
H	13.92496321	5.08203624	3.69631708
H	12.82049146	4.08443880	-0.37022337
O	8.71485521	0.47103777	1.11410368
O	10.42181067	-0.39304089	2.37687975
C	9.78800963	-1.69884518	2.23731033
H	8.76889072	-1.67613184	2.63995502
H	10.41635899	-2.38477389	2.81118548
H	9.75718098	-1.99319635	1.18193590
C	11.85937889	4.32991771	-0.83844749
O	12.14444203	0.46140374	-0.00842661
C	12.76431019	2.88229373	2.71696107
C	12.76967644	1.01590968	1.06265767
H	15.14149297	5.08695830	2.36583629
C	10.72532263	3.64799804	-0.11994209

TS5_88

E = -11119.33

G = -10866.06

Nimag = 1, 1513 i cm–1

C	9.85023891	3.82256837	4.86607162
C	7.97895171	3.94226960	3.32922628
C	7.64437908	4.67589850	5.65369805
N	7.14717076	4.44120307	4.28016064
N	9.24149436	3.65774609	3.54029826
C	8.79467033	3.72002578	5.96713975
H	10.36239479	4.79644623	4.90528965
H	10.62486891	3.05292431	4.96946233
C	7.43722394	3.73206529	1.93356749
H	6.80493032	4.51333888	6.34209148
H	7.96984577	5.72513612	5.75390817
C	5.79769683	4.95324271	3.95845548
H	9.22626188	3.96571052	6.94733228
H	8.40740124	2.68996809	6.01090965
C	5.79488951	6.16749782	3.01189240
C	5.93890626	5.80175070	1.52507825
C	7.23363705	5.05724055	1.16168597
H	6.48954923	3.17378574	1.98316413
H	8.14787557	3.09582148	1.40120780
H	5.34986014	5.23418046	4.91851542
H	5.18142477	4.14034139	3.54343252
H	6.59930520	6.85573402	3.32083633
H	4.84149417	6.70177305	3.15268863
H	5.86975263	6.72001204	0.92030914
H	5.07947402	5.17002454	1.23848952
H	8.11117174	5.70257777	1.33078630
H	7.21450138	4.82559105	0.08735080
C	12.85154199	-1.06190528	0.07506322
H	9.92004231	2.98593590	2.65245132
H	11.84477813	3.71615731	-1.14560410
C	10.54618793	2.14198084	1.70295534
H	9.62791383	3.23668497	-2.36331664
H	9.40247290	4.70913250	-1.40522281
H	12.30167607	-1.49612352	-0.76300441
H	12.66902935	-1.62454389	0.99696850
H	13.92584859	-1.03107599	-0.13519859
C	12.07904553	2.26963990	1.50399738
O	12.41112583	3.92258945	3.26330995
C	9.84554191	0.85988740	1.74547254
C	11.04907899	2.74598244	0.51853236
H	15.06764185	4.29298621	3.35830165
O	13.79407047	0.63068066	1.92638334
O	14.01595288	3.59484001	1.67420729
C	14.82924656	4.61344946	2.33846689
H	14.28958237	5.56599941	2.36464546
H	8.79544757	3.14656896	-0.79464632
O	8.80208664	0.60561456	1.14061927
O	10.42025938	-0.01351988	2.64326134
C	9.73182338	-1.29144193	2.77826824
H	8.70882046	-1.13864737	3.14105958
H	10.31992515	-1.85836204	3.50453466
H	9.70286155	-1.81099589	1.81367217
C	9.61789181	3.63057242	-1.33388966
O	12.32193874	0.29284196	0.21294926
C	12.82277669	3.32714265	2.27906302
C	12.84862057	1.00916689	1.24373617
H	15.73503752	4.69323137	1.73322412
C	10.93405240	3.37520716	-0.64607676

5_76

E = -6227.83

G = -6113.67

Nimag = 0

C	-0.20725364	0.15804770	0.25812153
C	0.14573422	1.68274141	0.03005344
C	1.16230862	0.63446333	0.05774806
H	0.05930357	2.79847496	-3.87465187
C	0.04826360	2.64586276	1.20603424
C	-0.28154008	2.31256852	-1.27429476
H	-0.51825101	1.14379013	-4.29968003

C	2.45090314	0.33998191	0.07991316
C	-0.64802991	-0.24471443	1.63257268
O	1.00016048	3.23594832	1.68739897
O	-1.23572459	2.76212092	1.60980168
C	-1.44838818	3.66446181	2.74751627
H	-2.52520676	3.64411956	2.92523297
H	-1.10874636	4.67204271	2.48851531
H	-0.89649188	3.28961195	3.61518102
O	-0.60799842	3.48704064	-1.37200969
O	-0.23387578	1.43246773	-2.29973666
C	-0.61705454	1.98110928	-3.60652008
H	-1.64928057	2.34246927	-3.56725245
O	-0.10256813	0.09030428	2.67333733
O	-1.74753656	-1.04380622	1.55803817
C	-2.26487338	-1.49847781	2.85603114
H	-1.50059802	-2.08793363	3.37197359
H	-3.13602006	-2.10943021	2.61218652
H	-2.54582287	-0.63301955	3.46380883
C	2.98936444	-1.04333254	0.29566660
H	3.61425567	-1.35492342	-0.55562770
H	2.18008368	-1.77275881	0.42547407
H	3.63125372	-1.06777496	1.18996498
H	3.16879516	1.15251961	-0.05867507
H	-0.73833808	-0.31314622	-0.56953176

5_77
E = -2829.46
G = -2775.88
Nimag = 0

O	0.21609322	-1.86168956	0.20390394
C	0.14748770	-3.08342709	0.07205864
C	-1.08738528	-3.88912061	0.01334516
C	-2.30272780	-3.32636932	0.10316388
H	2.64831556	-2.67683109	0.96355140
H	2.60022677	-2.47026877	-0.81829686
O	1.24773448	-3.88732931	-0.04237923
C	2.53715294	-3.19086540	0.00341881
H	3.28681193	-3.97670638	-0.10793977
H	-0.96785766	-4.96626522	-0.10676363
C	-3.59624318	-4.06912893	0.05340226
H	-2.35800435	-2.24069186	0.22412593
H	-3.44808799	-5.14865558	-0.07631721
H	-4.21932196	-3.69112870	-0.77258207
H	-4.16904546	-3.89529941	0.97831341

5_78
E = -3061.82
G = -3006.82
Nimag = 0

C	-0.27654703	0.53390336	0.45740785
C	-0.00859791	1.99476383	0.17572247
C	0.98142178	0.86385139	0.36175280
H	2.91770286	1.13465203	1.16316847
H	-0.17967579	2.38716528	-0.83390277
O	-0.95989974	-1.70057733	0.89545969
O	-2.51921131	-0.04013367	0.62738381
C	2.41305488	0.53533038	0.38953388
C	-1.24478806	-0.52032156	0.68220576
C	-3.57062944	-1.04140379	0.84663410
H	-3.50559388	-1.81990364	0.07994084
H	-4.50767282	-0.48740111	0.76498567
H	-3.45983818	-1.48184001	1.84255867
H	-0.13092689	2.72886357	0.98116409
H	2.58306284	-0.52992353	0.58702427
H	2.87689959	0.80661310	-0.57161800

5_79
E = -2788.40
G = -2736.25
Nimag = 0

C	-0.25515130	0.53151306	0.43468372
C	0.01808977	1.97637502	0.06638472
C	1.00620165	0.86241851	0.33248578
H	2.93057046	1.19593847	1.13445898
H	-0.13692681	2.30808784	-0.96752488
O	-0.92918078	-1.64530732	1.02247665
C	-2.69685682	-0.04039935	0.63246954
C	2.43890864	0.54491811	0.39459498
C	-1.25794958	-0.48218094	0.72155187
H	2.91020448	0.76292586	-0.57666386
H	-0.10952283	2.75880059	0.82453302
H	2.61367263	-0.50509590	0.65762526
H	-2.87216170	0.79518000	1.32736224
H	-3.37060169	-0.87195374	0.86596007
H	-2.90453652	0.34137403	-0.37909860

5_80
E = -2825.27
G = -2771.07
Nimag = 0

O	0.15821312	-2.27183101	1.01822787
C	0.13201036	-3.26374166	0.29918907
C	-1.10914217	-4.07075239	-0.04420320
C	-2.37756926	-3.45187456	0.47459205
H	2.69384078	-3.12389805	1.06360193
H	2.44713113	-2.07803960	-0.37559097
O	1.23000835	-3.79779709	-0.29629565
C	2.49785021	-3.10931585	-0.01300151
H	3.25385479	-3.67885942	-0.55678290
H	-2.56979308	-2.42220990	0.16080259
C	-3.25373304	-4.08452020	1.25940820
H	-0.97169743	-5.08787913	0.35393795
H	-1.14587830	-4.16772532	-1.14216845
H	-4.17157551	-3.60013183	1.59267732
H	-3.08376523	-5.11003265	1.59290068

5_81
E = -3073.77
G = -3017.61
Nimag = 0

C	-0.21354472	0.31837619	0.20832311
C	0.18159401	1.80525154	-0.04254390
C	1.18899178	0.76108129	0.00943476
H	2.71542902	-0.68249383	0.11431496
H	-0.70075666	-0.21115898	-0.61181864
O	-0.31303545	0.50488379	2.61587618
O	-1.49088122	-1.13215595	1.53945400
C	2.45065261	0.36489381	-0.03319213
C	-0.65297234	-0.05962348	1.58002493
C	-1.97659533	-1.59699095	2.84659046
H	-1.12972972	-1.90097461	3.46954019
H	-2.62123248	-2.44806256	2.61946029
H	-2.54019947	-0.79733532	3.33714296
H	-0.11677003	2.22432051	-1.00570983
H	0.08503783	2.47204227	0.81739902
H	3.25914638	1.07376533	-0.21706536

5_82
E = -2799.75
G = -2746.57
Nimag = 0

C	-0.26705226	0.38985021	0.17102465
C	0.19903601	1.86327765	-0.01340245
C	1.15954519	0.77767572	-0.00371846
H	2.62573143	-0.73495856	0.04240560
H	-0.75596507	-0.09033703	-0.67925839
O	-0.41704209	0.57436316	2.55421593
C	-1.55362762	-1.30553289	1.56547948
C	2.40279850	0.32791926	-0.05443716
C	-0.71953454	-0.04823220	1.52911020
H	3.24112670	1.01123855	-0.19834061
H	-0.06481168	2.34142544	-0.95846070
H	0.12161157	2.48624870	0.88102258
H	-0.99938442	-2.12987125	1.09154835
H	-2.46953449	-1.15591358	0.97397332
H	-1.81135271	-1.56912956	2.59704968