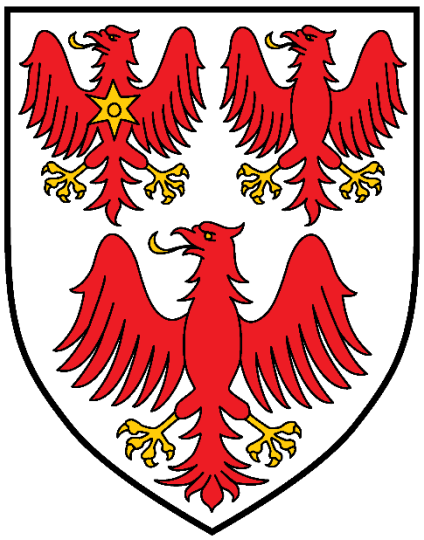
An Examination of Bonding, Structure and Reactivity of Exotic Main Group Systems





Appendix of Spectra and Calculated Coordinates

Agamemnon Elvis Crumpton
The Queen's College
Thesis submitted for the Degree of Doctor of Philosophy
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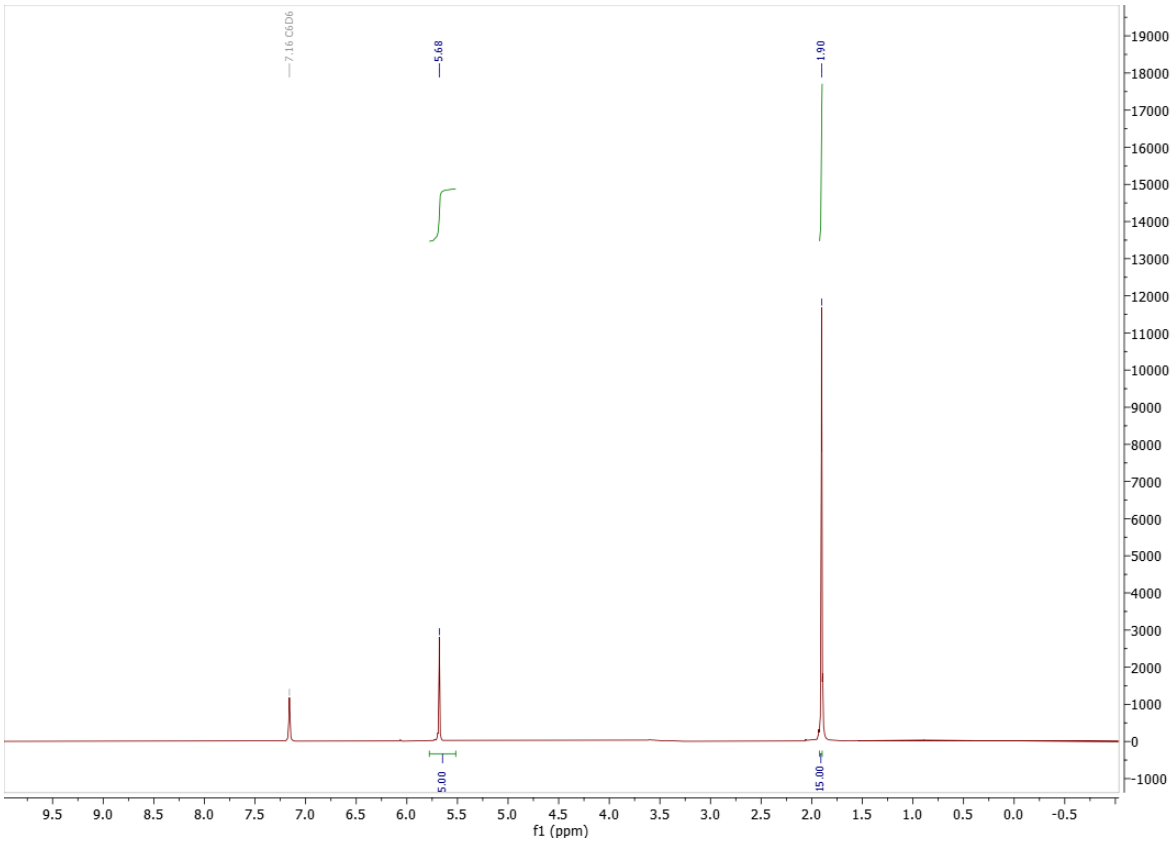
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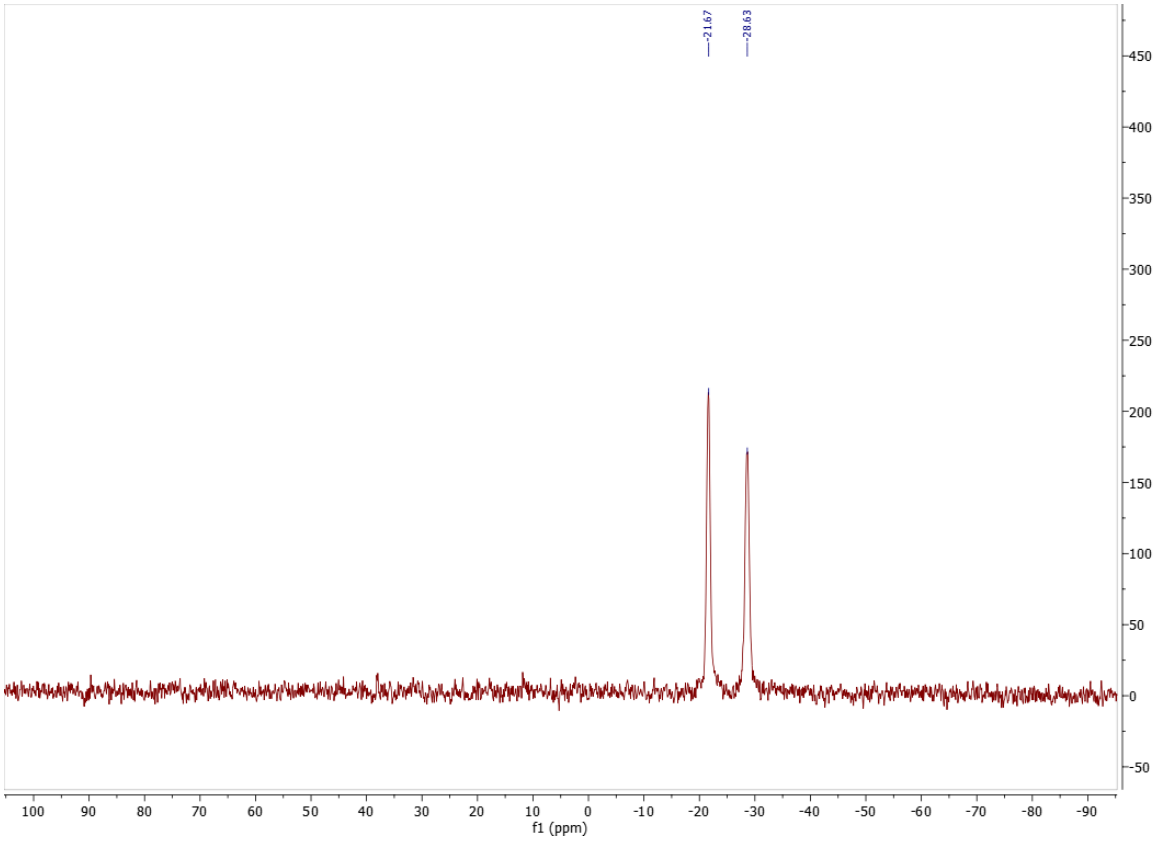
Chapter 2 Metathesis at [Be–Be]2+: A Route to a Nucleophilic Beryllyl Complex

Spectra

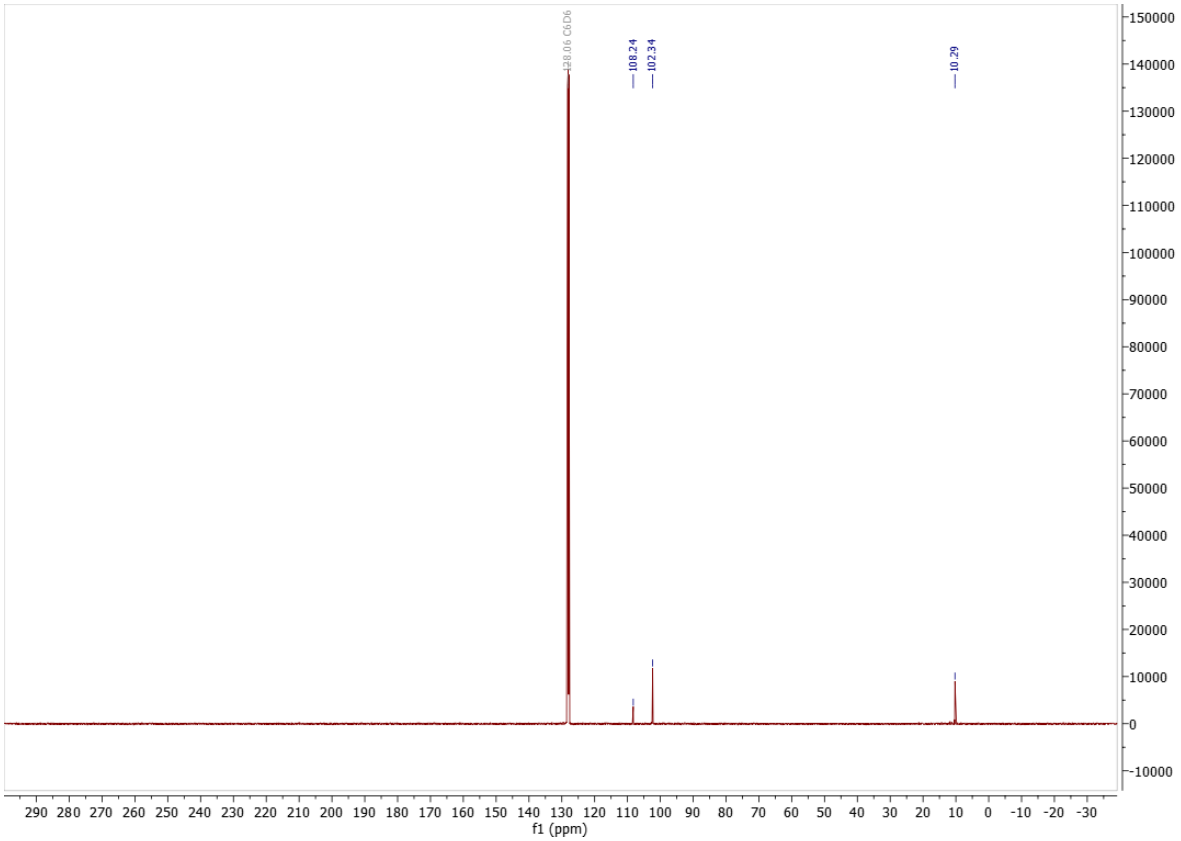
NMR



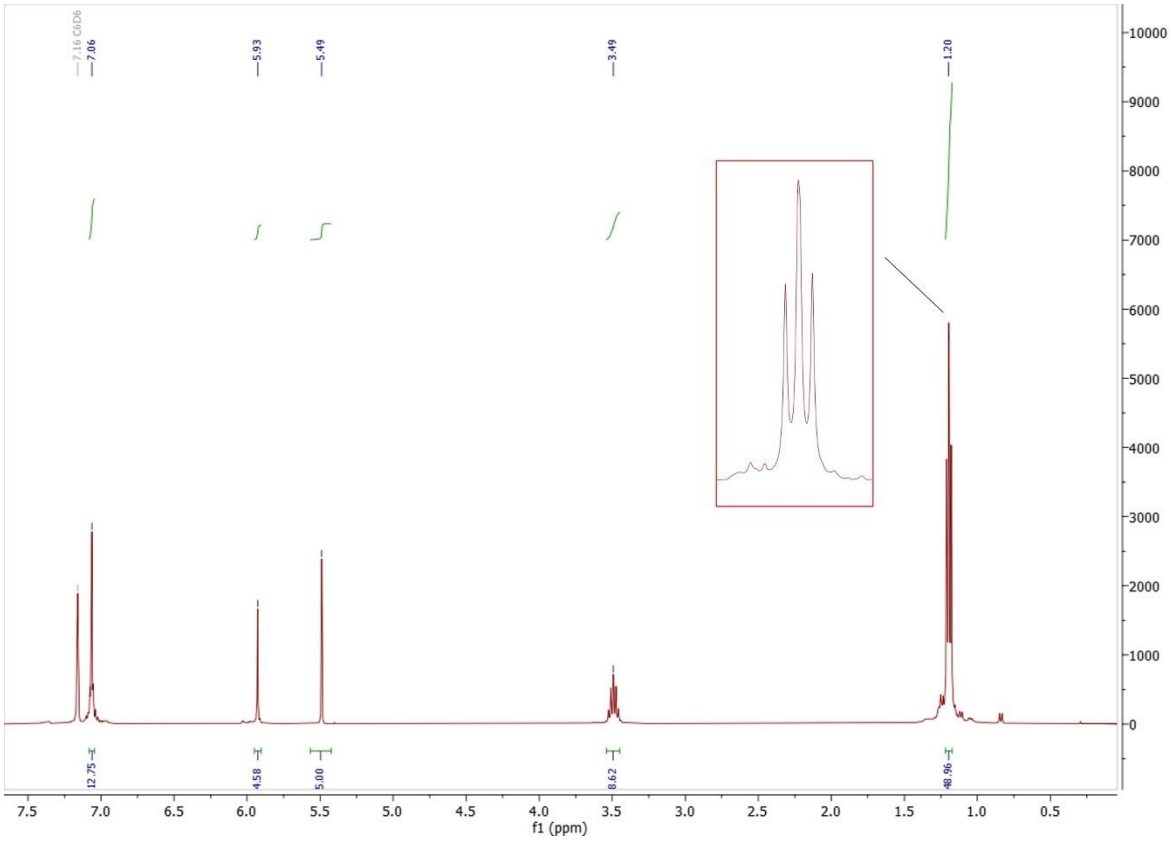
A 2.1: ^{1}H NMR spectrum of compound **2** in C_6D_6.



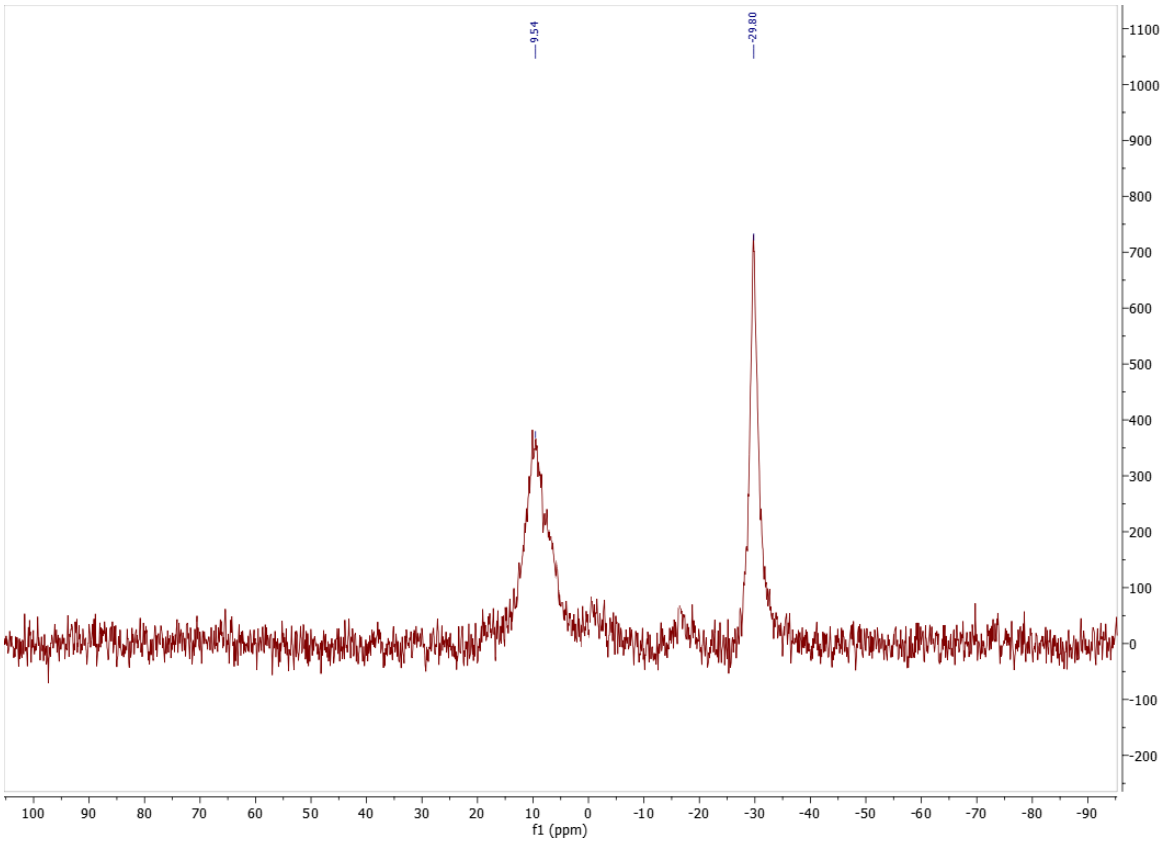
A 2.2: ^{9}Be NMR spectrum of compound **2** in C_6D_6.



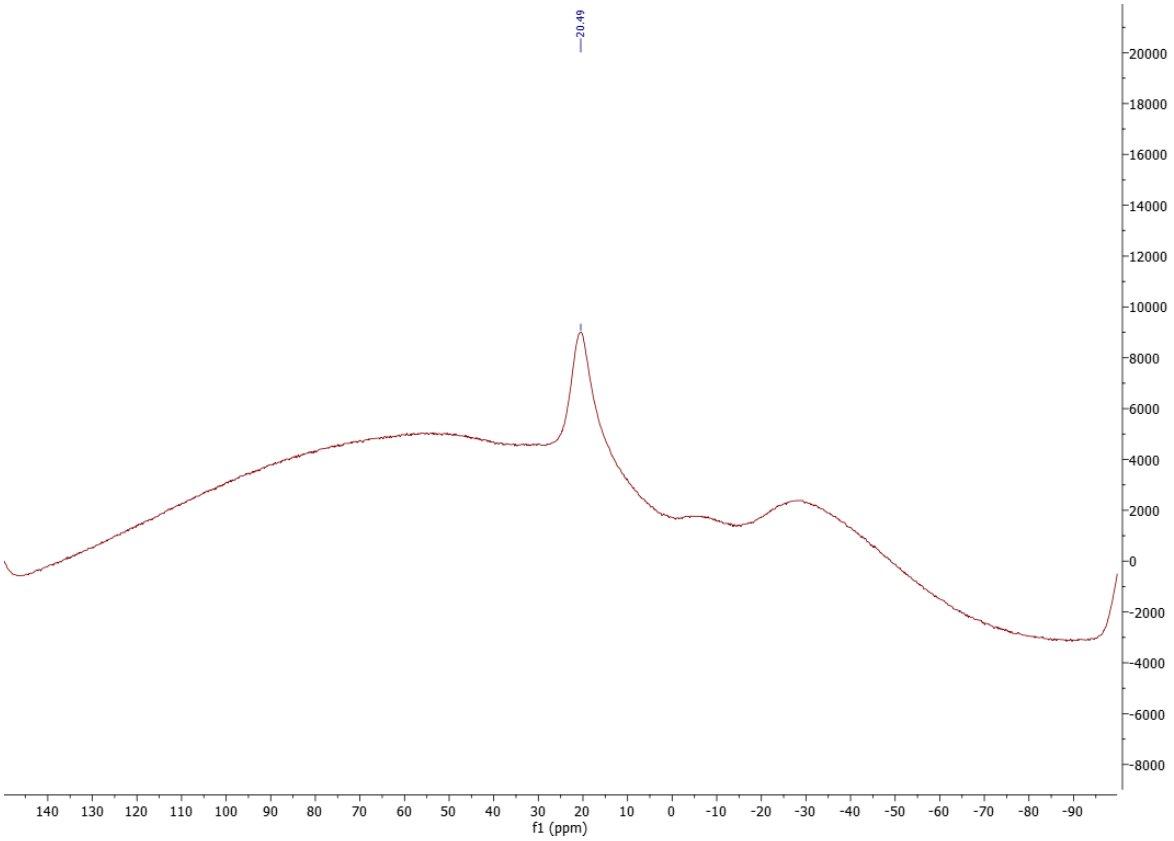
A 2.3: ^{13}C {^{1}H} NMR spectrum of compound **2** in C_6D_6.



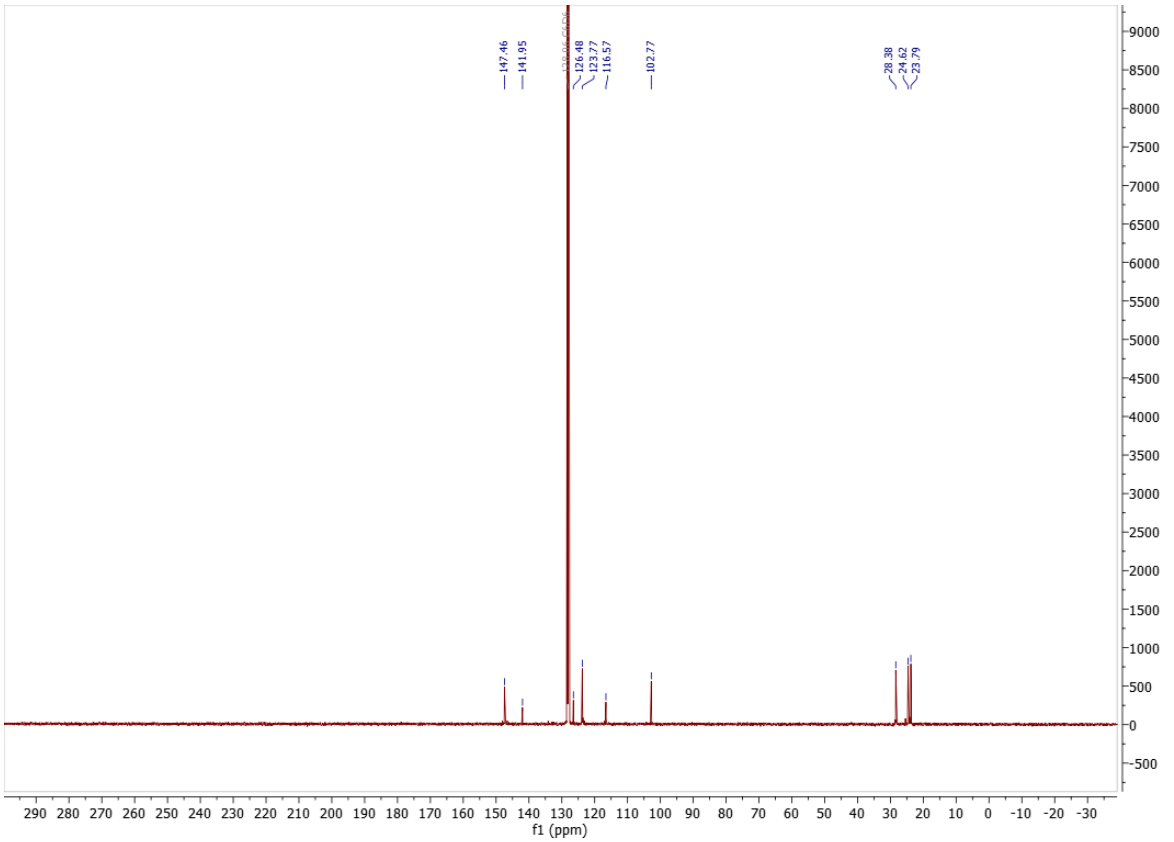
A 2.4: ^{1}H NMR spectrum of compound **3** in C_6D_6. The region from 1.15 – 1.25 ppm is also shown in an expanded view.



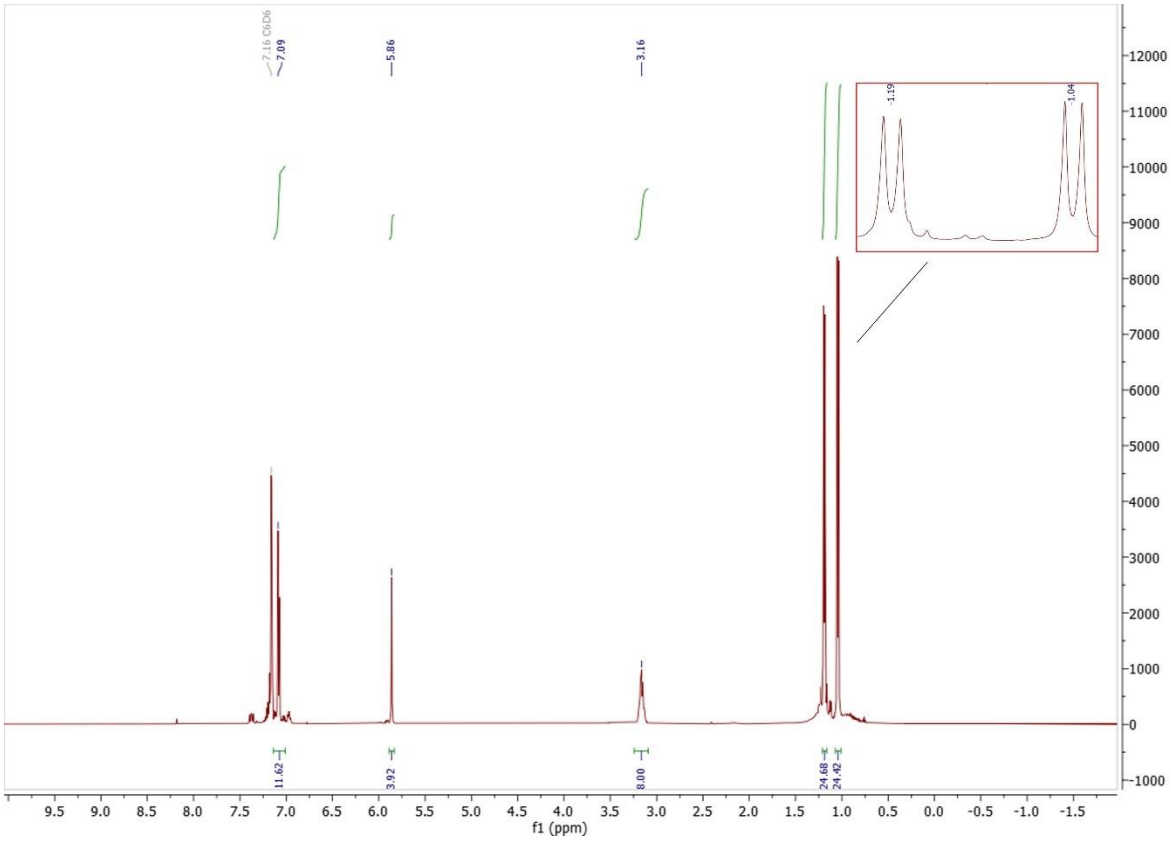
A 2.5: ^{9}Be NMR spectrum of compound **3** in C_6D_6.



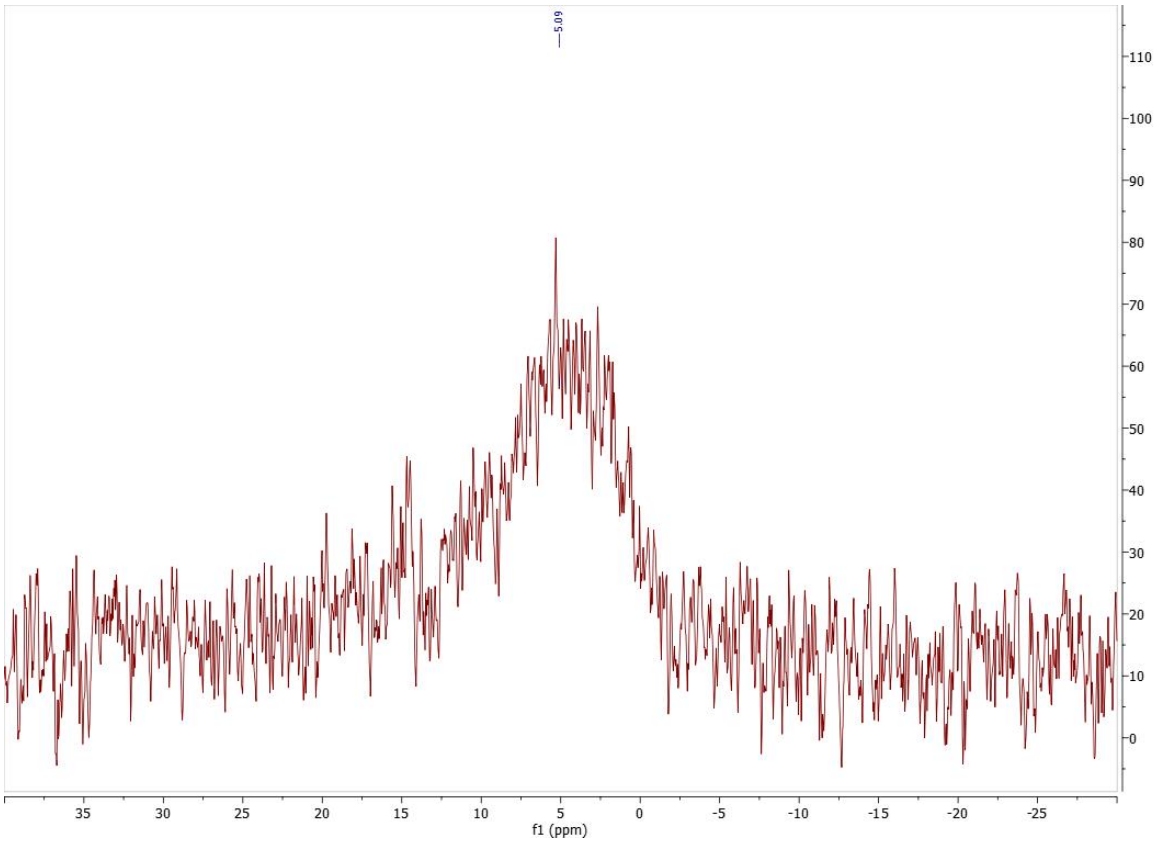
A 2.6: ^{11}B NMR spectrum of compound **3** in C_6D_6.



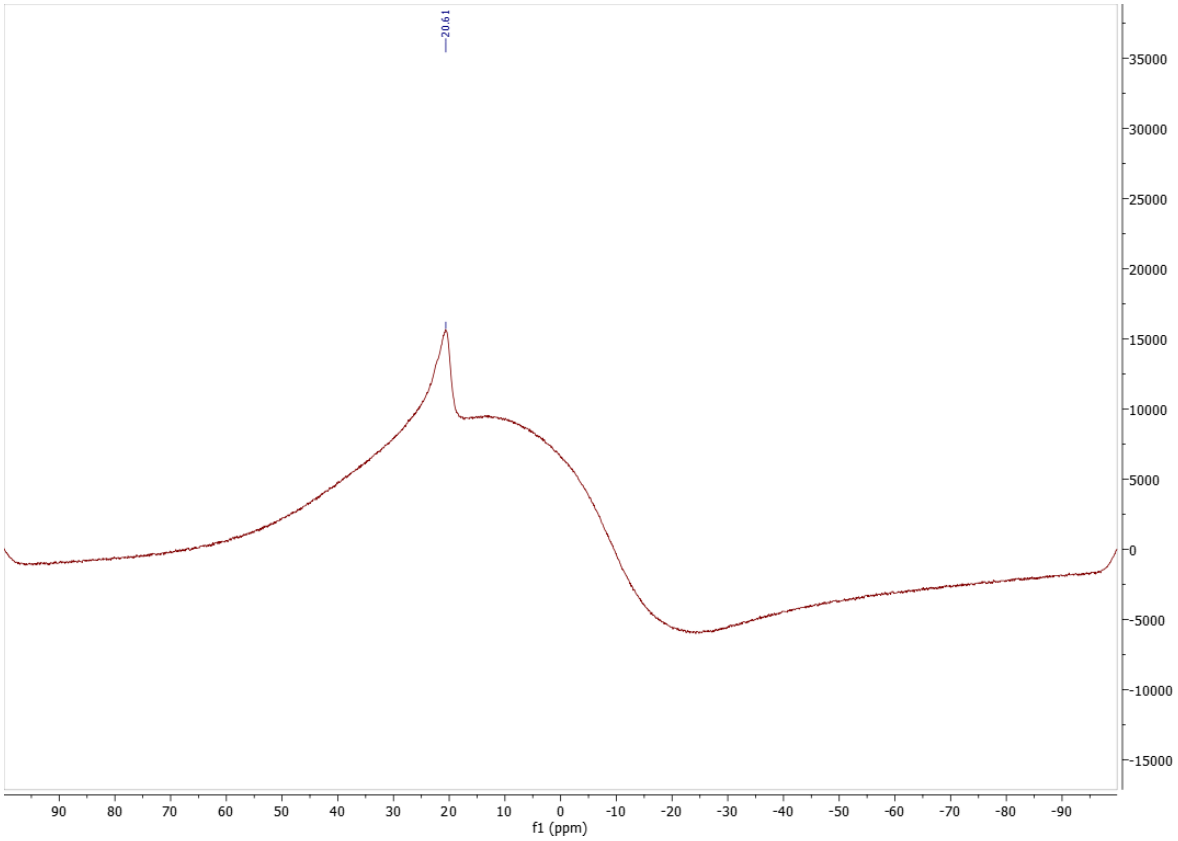
A 2.7: ^{13}C $\{^1H\}$ NMR spectrum of compound **3** in C_6D_6.



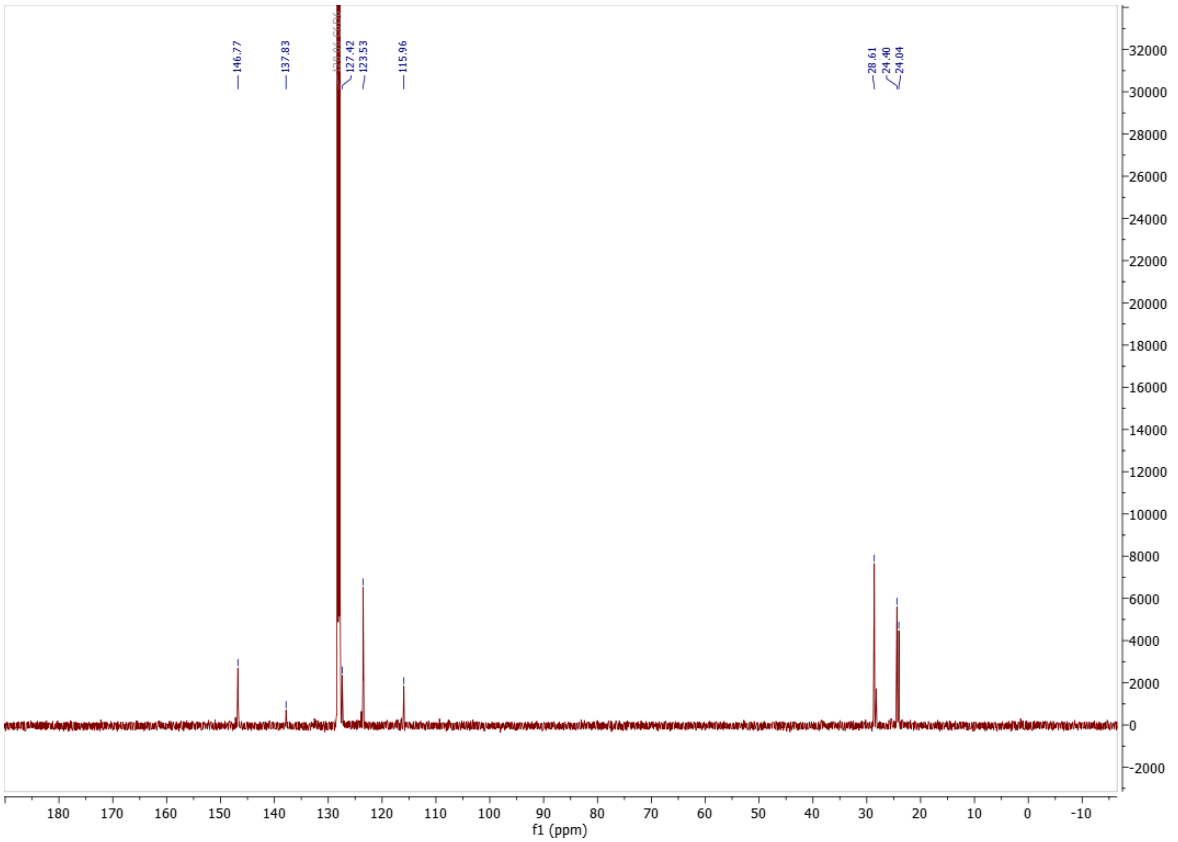
A 2.8: ^{1}H NMR spectrum of compound **4** in C_6D_6. The region from 1.00 – 1.25 ppm is also shown in an expanded view.



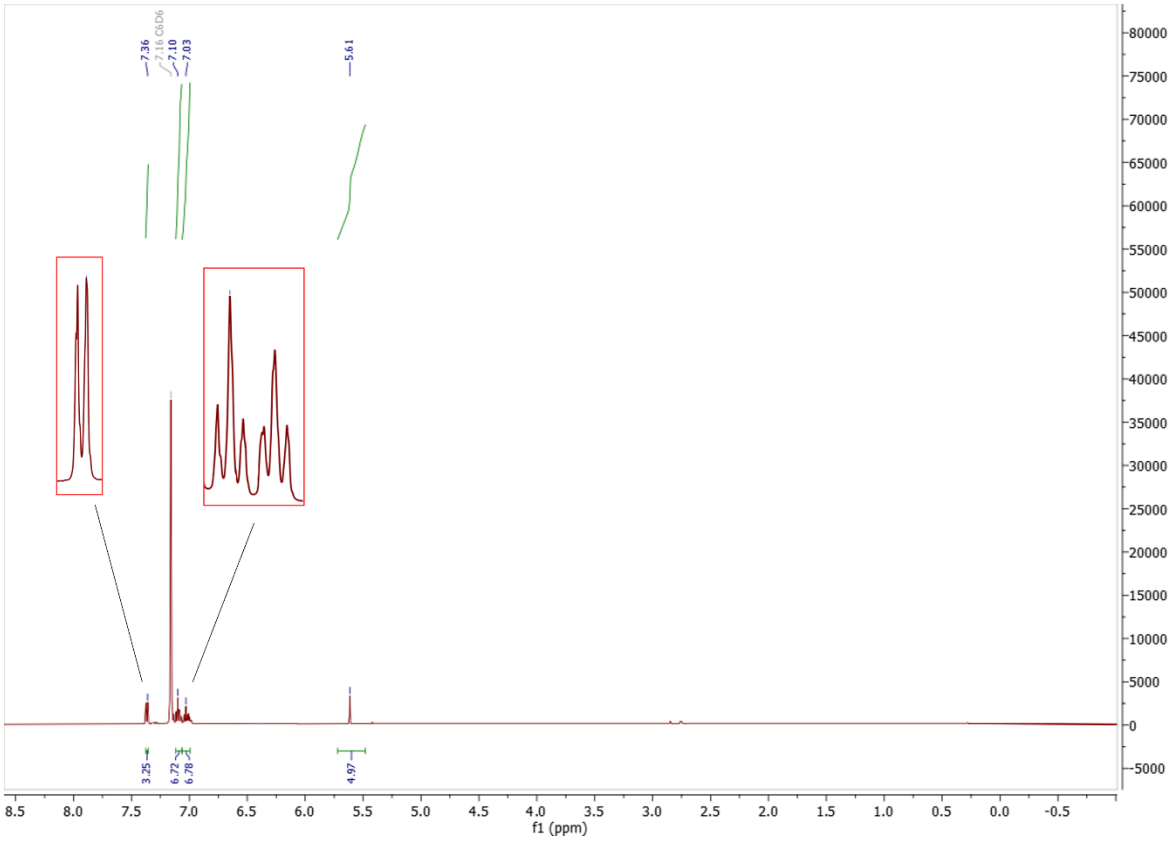
A 2.9: ^{9}Be NMR spectrum of compound **4** in C_6D_6.



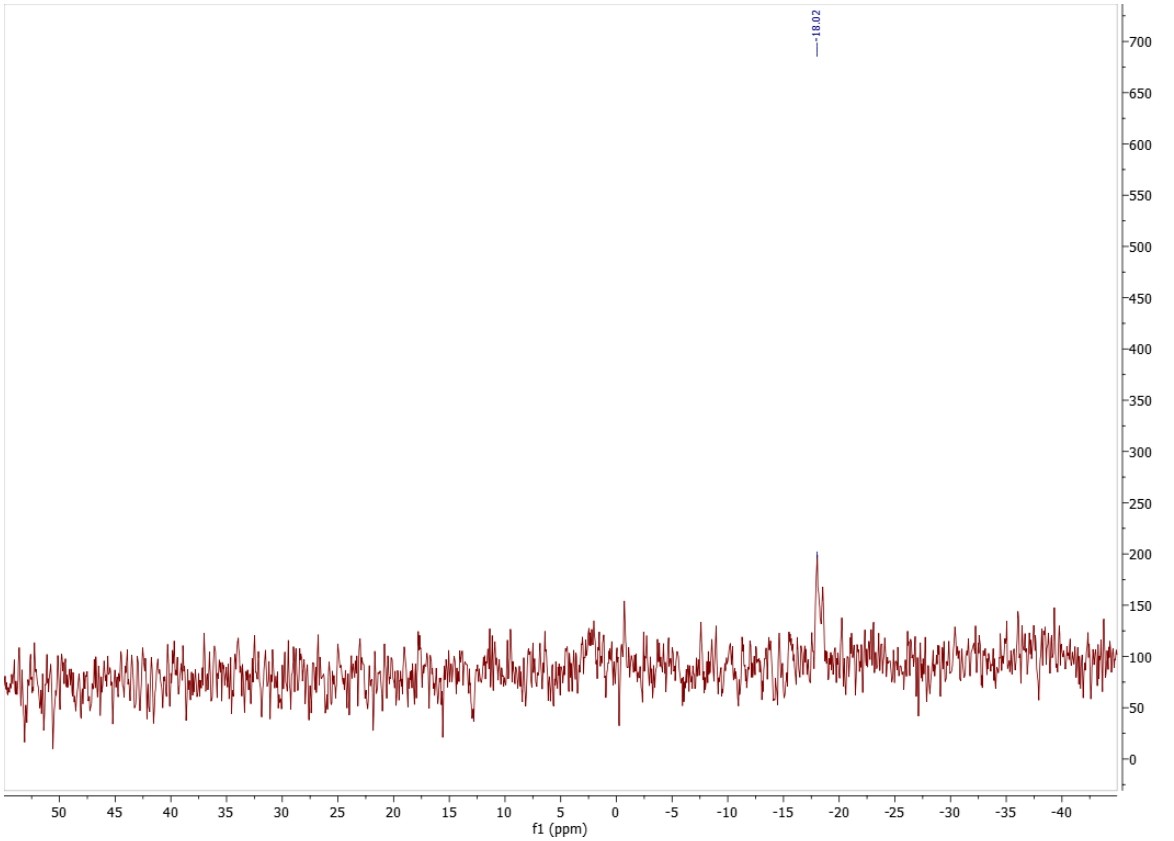
A 2.10: ^{11}B NMR spectrum of compound **4** in C_6D_6.



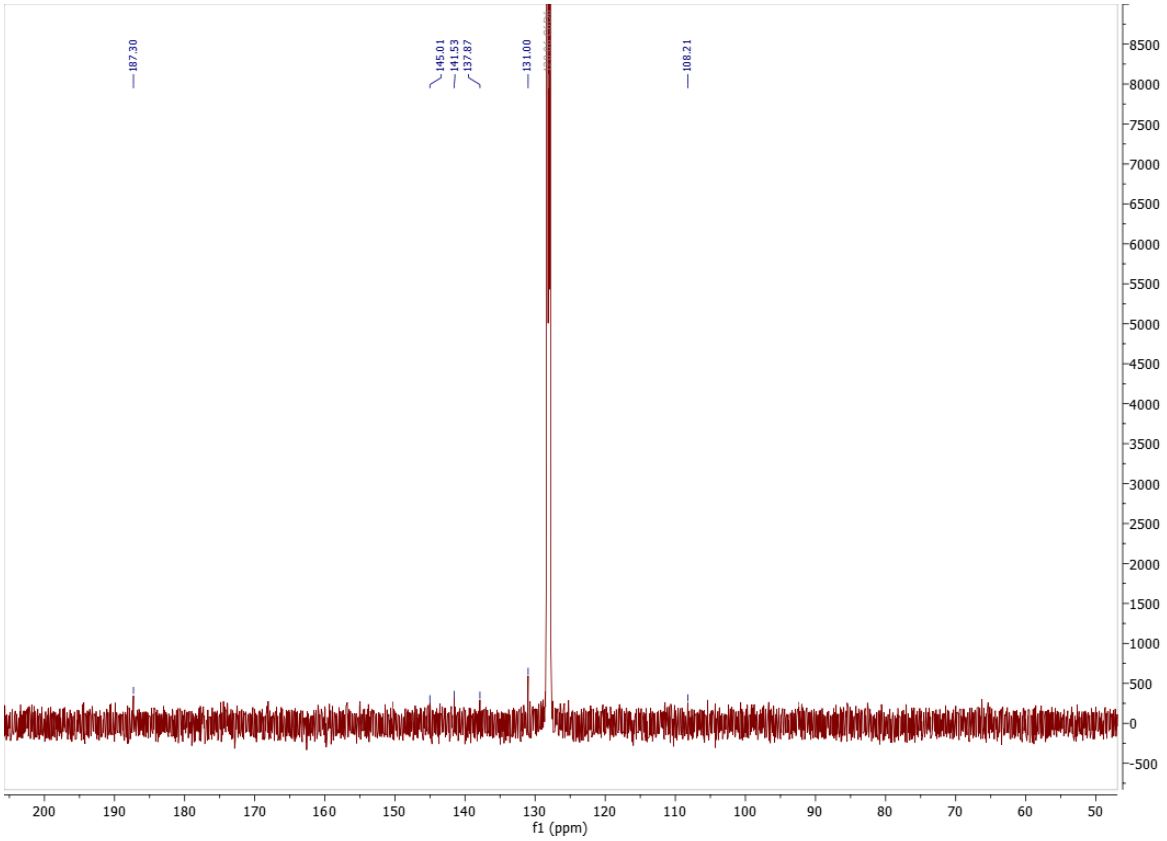
A 2.11: ^{13}C $\{^1H\}$ NMR spectrum of compound **4** in C_6D_6.



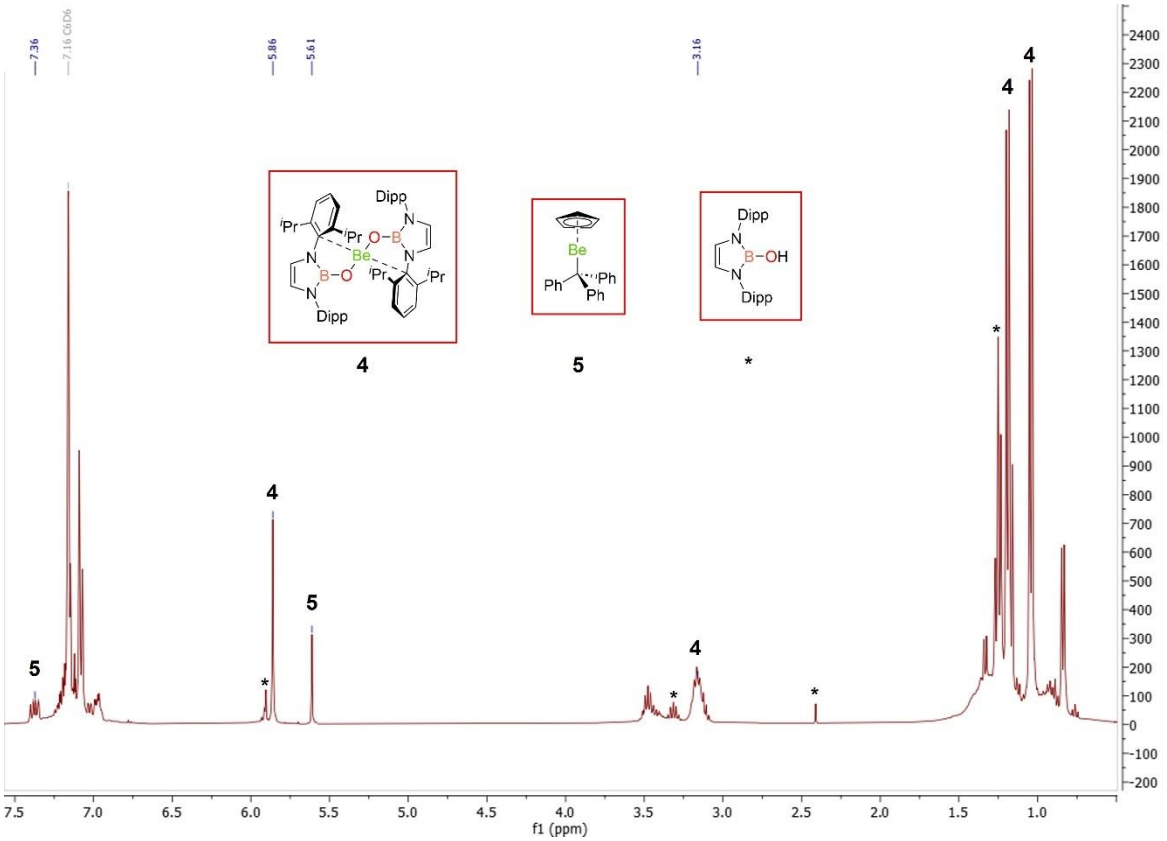
A 2.12: ^{1}H NMR spectrum of compound **5** in C_6D_6. The regions from 6.97 – 7.15 ppm and 7.35 – 7.40 ppm are also shown in an expanded view.



A 2.13: ^{9}Be NMR spectrum of compound **5** in C_6D_6.



A 2.14: ^{13}C {^{1}H} NMR spectrum of compound **5** in C_6D_6.



A 2.15: Crude ^{1}H NMR spectrum of the reaction between **3** and $[CPh_3][B(C_6F_5)_4]$.[5]

Coordinates

Complex **1**

Energy: –416.998808063663 E_h

Be	6.07532008500246	2.45977689338742	2.20273800246051
Be	7.89986786620247	2.43637172742399	3.14773957654565
C	8.72295665719373	2.56017023653347	4.91840088375154
H	8.17518465030222	2.68818759572111	5.84184311557989
C	9.17479314148642	3.60115345671017	4.06783513904426
H	9.03116091431724	4.66047210168856	4.23026417207326
C	9.75810156866362	3.00696285293050	2.91987102870861
H	10.13602726649374	3.53468133259237	2.05507457908347
C	9.66665788288205	1.59884268165880	3.06086303429876
H	9.96292404864714	0.86677721605390	2.32228731660589
C	9.02692488535839	1.32266962980387	4.29601231468681
H	8.75109395427939	0.34353265143868	4.66261751722224
C	5.19476592632372	3.05502847317773	0.56012623433937
H	5.69136119676751	3.57210600519213	-0.24932869842748
C	5.09867912557411	1.64850734865559	0.71421224420914
H	5.50934320453386	0.90721287658225	0.04263478702361
C	4.45865800111855	1.38600526258153	1.95222628063609
H	4.29704997390369	0.40986711124368	2.38837090205620
C	4.15914189326093	2.63020578709736	2.56321338769261
H	3.72974215734919	2.76719726167572	3.54609009191386
C	4.61410290351051	3.66170857649148	1.70292451722862
H	4.59144269682870	4.72156292135959	1.91598357326698

Complex **2**

Energy: –613.782804708877 E_h

C	-1.07207299702478	0.01111178526273	13.57119268584060
C	0.26812498187518	0.22310904367703	14.01338317090891
C	1.14661613169513	-0.14746096899675	12.95162254528438
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C	-1.02175068578165	-0.49040720345552	12.23599797928913
C	-2.31334813780022	0.29380539335423	14.35867213512124
H	-2.62390343683021	-0.58817057301908	14.93306906290073
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H	0.82624376195053	-0.04079268875301	16.07282374544684
H	-0.07804894421437	1.44335688316413	15.75303813157900
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H	0.15058179033766	-0.82491054721027	9.72228299911513
H	1.03591484081003	-2.12944407901664	10.52044197185627
C	-2.20094790872790	-0.82718447568986	11.37758815862786
H	-2.48504661353232	-1.88057057656518	11.49560996943751
H	-1.98606518879136	-0.66087621255621	10.31827515714082
H	-3.07220822227850	-0.22006839620362	11.63865221707895
C	-1.38787619092789	4.64374499501478	11.39319123211566
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C	-0.32462718856259	4.99686322942546	12.26248628090941
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H	1.88748304709615	4.88692506333030	11.99075895617923
C	0.58648646097041	4.28380242407730	10.28111403140325
H	1.30175708465454	3.95715251202897	9.53886468659845
C	-0.82474236680224	4.20299080006489	10.16863694619989
H	-1.37228209381238	3.80434351468152	9.32571035487615
Be	-0.17201313569643	3.13343633223863	11.67565371402980
Be	-0.11352643869031	1.20880007692028	12.39410120536737

Complex **3**

Energy: – 3269.994430592048 E_h

O	9.49685653283993	3.65150721716992	3.74549012713785
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C	9.46549548227494	1.31327973143519	1.29371061948204
C	8.14506264371357	-0.04733330216270	2.86449072188647
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H	9.53833821591504	3.44122637829722	1.27892233409745
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N	13.42527305662550	2.35554922503180	6.25553676615931
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H	13.42015118962436	5.66544292170540	1.21087987863747
H	14.13354016410710	4.13727370716825	0.66786223276972
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C	15.90904115055364	3.78391626765397	2.75817935610440
H	16.77903915286017	4.36976786978443	2.43776265506926
H	15.81521154242499	2.91994157631218	2.08984023038712
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C	12.59260924307710	6.69181396164517	7.39271427524393
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H	12.22617026352298	6.48081829684831	8.40446602070328
H	12.14130889863829	5.97313376469227	6.70119361052651
C	14.73885991960259	7.63876498741938	8.31357578706285
H	15.83337702063896	7.63537485633786	8.26717521469448
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H	14.38999446370403	8.65661576404618	8.10516685777325
Be	10.78103903878120	4.51486312458405	4.05690164864068
Be	10.93556856845234	6.59047884838957	3.53488714772793
C	13.76460195121430	0.61803486105406	3.23008799331768
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Complex **D**

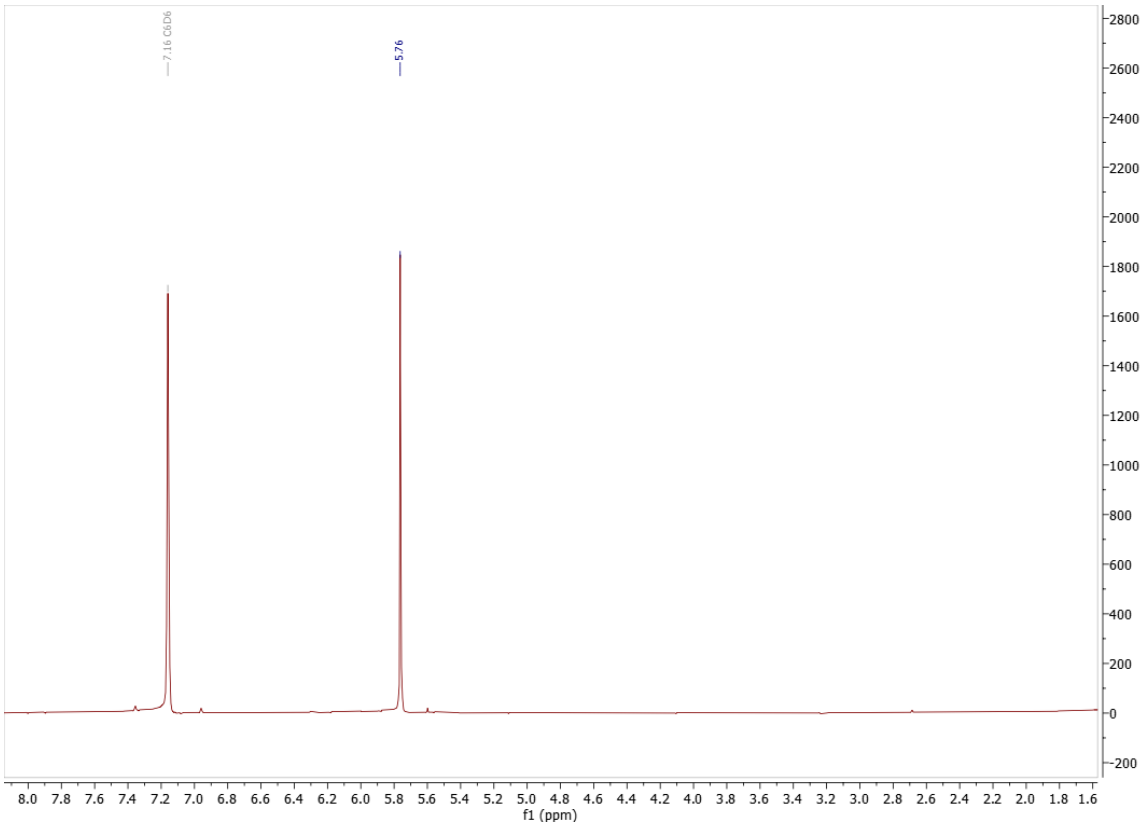
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C	-4.02066506635818	2.67337488048521	0.92172408863823
H	-4.57861003612839	3.58896362990833	0.69668796678856
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H	-0.60948180638095	4.46909304430810	0.77604161425458
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H	0.23925237894519	4.05789825689101	-1.59796336817831
H	1.08648085287719	2.56400071435438	-1.15613680586242
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C	3.75114646133910	2.23319614858329	-1.31588539791580
C	3.48779255797302	2.51984671855528	1.05375892163432
C	3.84526135455466	3.03202065865758	-0.18630934484985
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H	5.31621322003549	-0.28578149095765	-2.64150010029955
H	4.40272401634827	-0.67531085675096	-4.11452356761124
H	4.75391860792881	1.00903406896282	-3.70523569176728
C	1.51069062616988	1.41762165919630	3.20254353127243
H	1.70370634562869	2.49111011998517	3.31640383754600
H	0.62331835143973	1.28528437691356	2.57609112346755
H	1.29805328693158	1.00683979775333	4.19669692396327
C	3.92581026291170	0.82558299546579	3.53320817167518
H	3.71960652452393	0.31770109164322	4.48231815196704
H	4.83372979080060	0.39621226938065	3.10022108512814
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Be	0.00001104425326	0.00010474686207	0.00025332583825

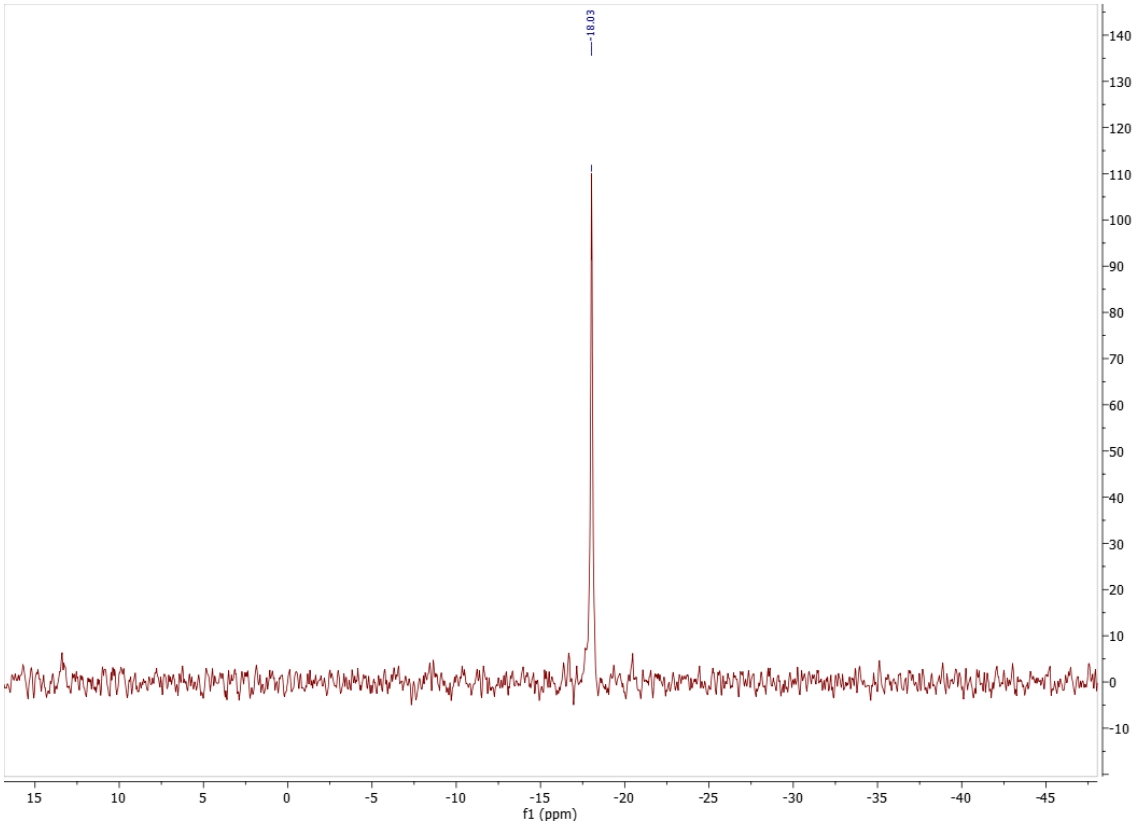
Chapter 3 - A Stable Hexavalent Nickel Complex

Spectra

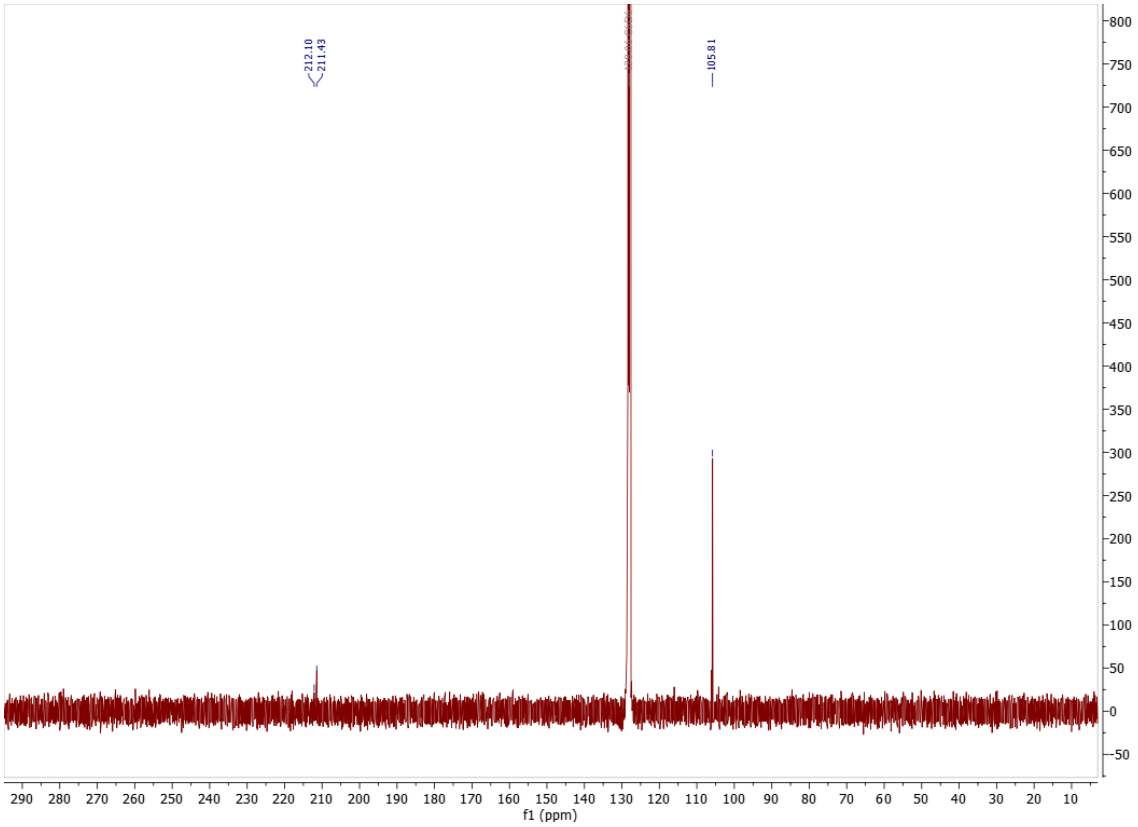
NMR



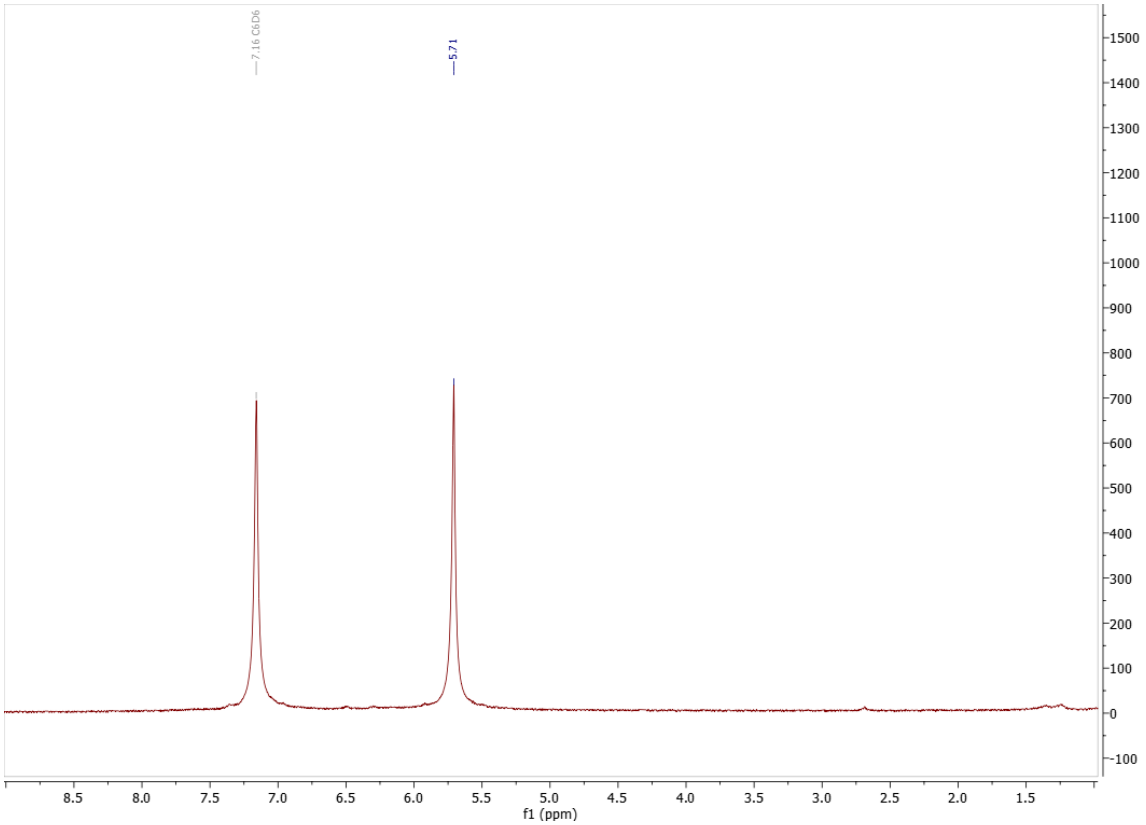
A 3.1: ^{1}H NMR spectrum of **2Be** in d_6-benzene.



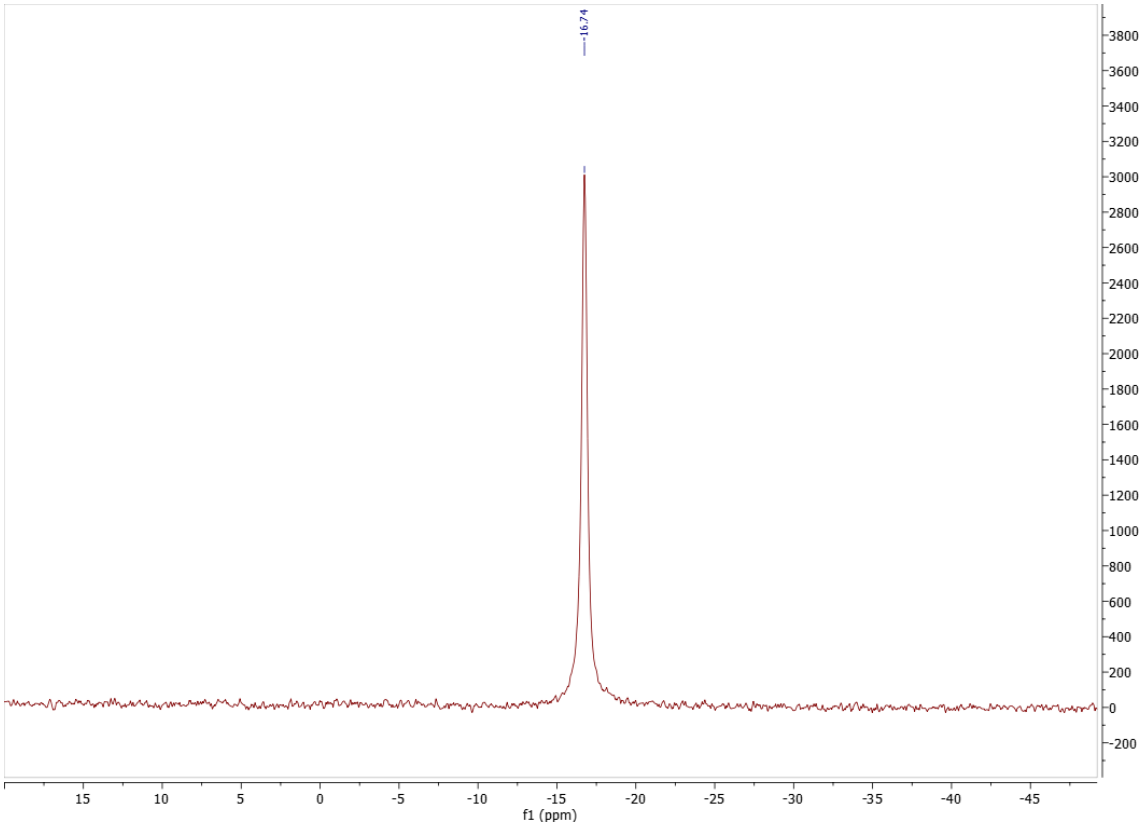
A 3.2: ^{9}Be NMR spectrum of **2Be** in d_6-benzene.



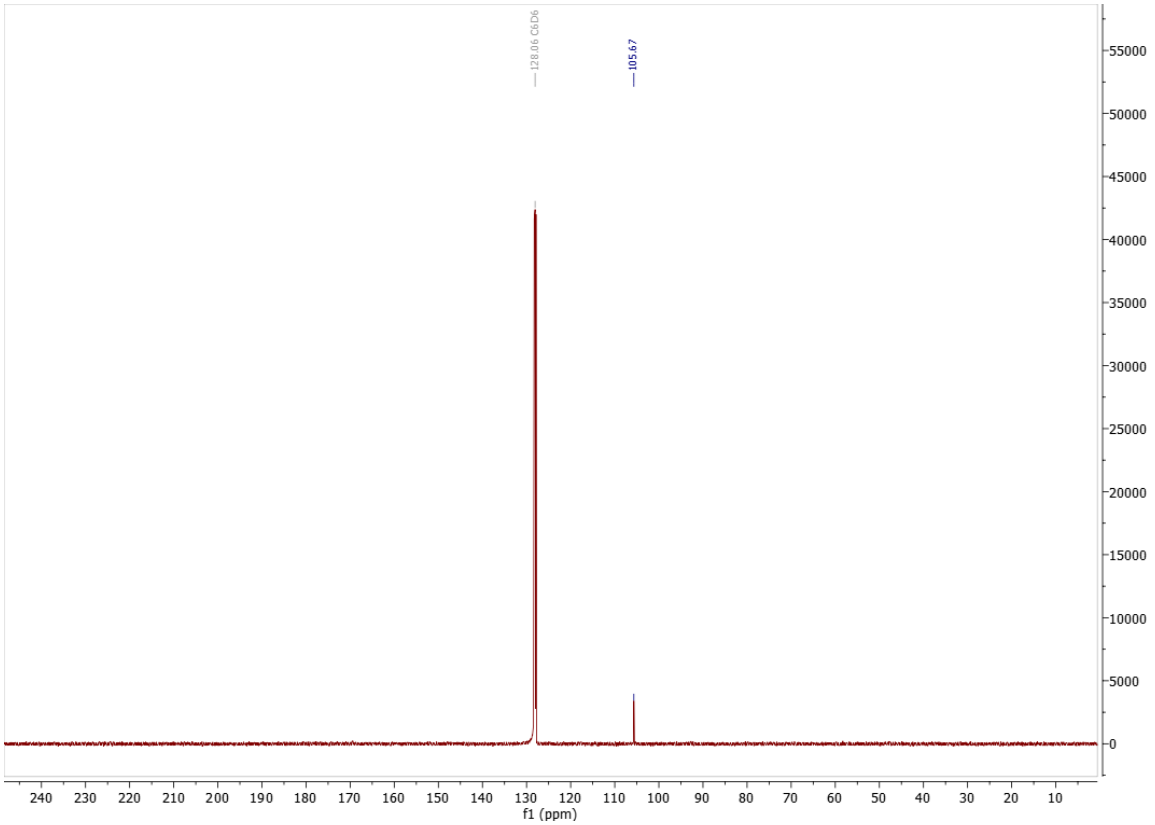
A 3.3: ^{13}C NMR spectrum of **2Be** in d_6-benzene.



A 3.4: ^{1}H NMR spectrum of **1** in d_6-benzene.

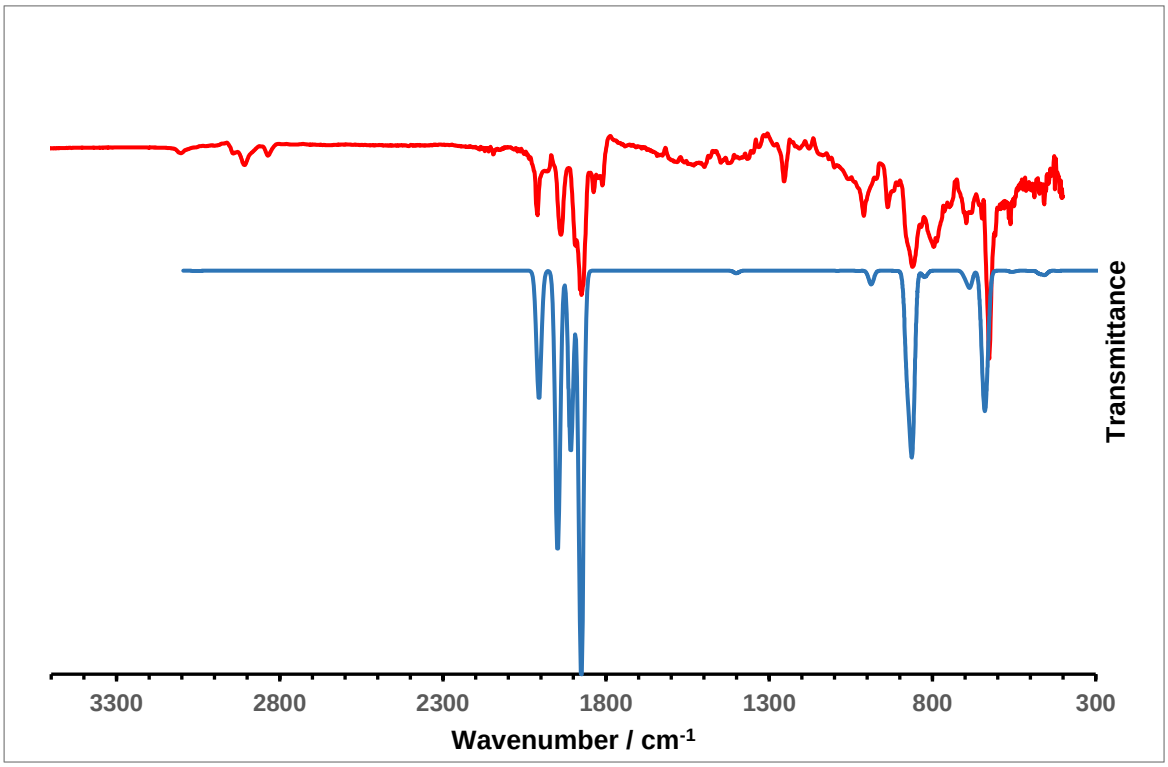


A 3.5: ^{9}Be NMR spectrum of **1** in d_6-benzene.

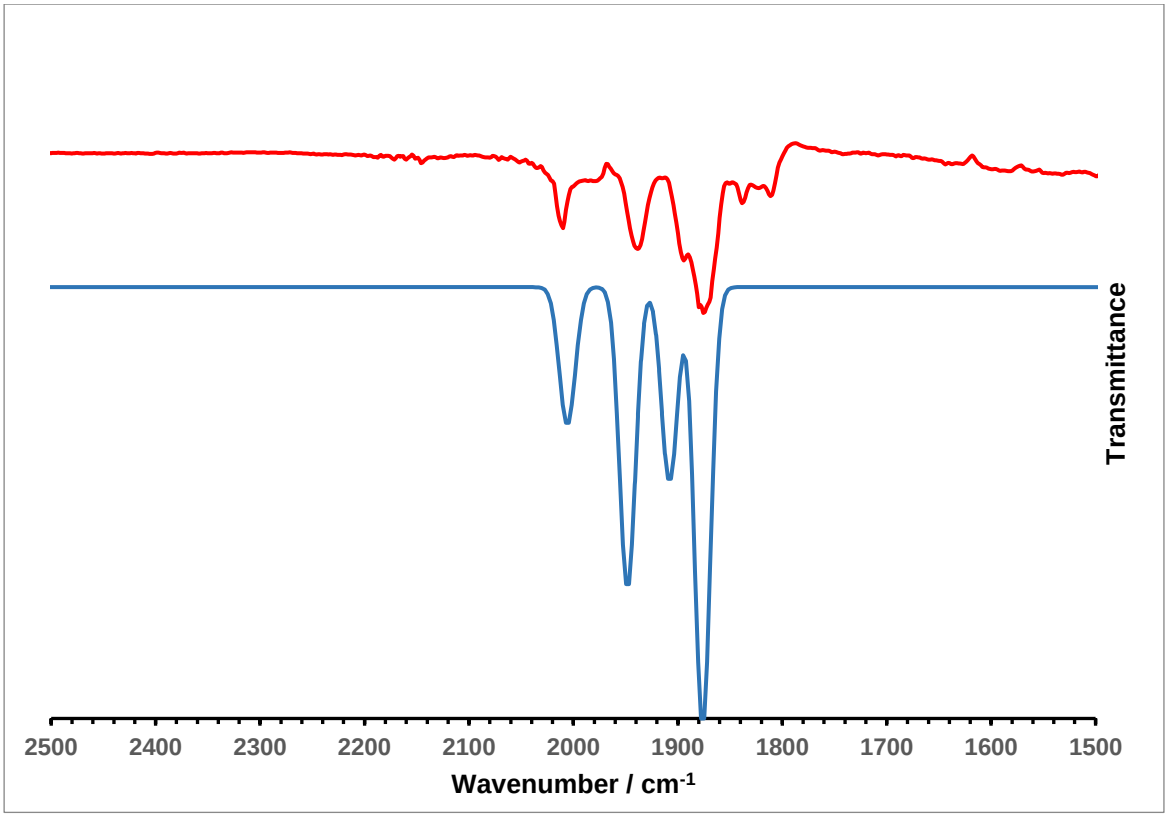


A 3.6: ^{13}C NMR spectrum of **1** in d_6-benzene.

IR



A 3.7: ATR IR spectrum of compound **2Be** (red) overlaid with the computationally simulated ATR IR spectrum for the complex (blue).



A 3.8: ATR IR spectrum (zoomed in on the carbonyl stretching region) of compound **2Be** (red) overlaid with the computationally simulated ATR IR spectrum for the complex (blue).

Coordinates

Complex **2**

Energy: -2134.478845633375 Eh

O	6.05783660634309	2.12095221119659	1.68696835234240
C	6.57559469835959	2.98317255036149	2.23177837380152
Be	8.32291922592767	5.96501022544080	4.14308554401101
C	7.78291155233141	7.34307845998614	5.33541863101351
H	6.77301285601338	7.48803842109537	5.69312275800542
C	8.75309286445708	6.48388075590280	5.91557786426881
H	8.60580356661411	5.87016210735295	6.79342859264898
C	9.89912612076490	6.48833961788235	5.07902175601073
H	10.78297498624469	5.87820642017896	5.20363546416262
C	9.63746892284311	7.34997288071545	3.98117821451001
H	10.28506277793037	7.50130661584912	3.12876758842780
C	8.33096939237243	7.87981682797231	4.14170527672735
H	7.80972170442223	8.50646471754284	3.43120398973689
Fe	7.37241686264238	4.32521669428620	3.08678434705100
O	6.09112705909992	4.32465690835981	5.69450176068391
O	6.05606271964811	6.52868267399514	1.68737979976102
O	10.07988137365915	4.32524074327215	2.03455459727133
C	6.59830102179116	4.32501874523803	4.65695247395187
C	6.57447097608358	5.66679416859955	2.23209081611653
C	9.00330634050638	4.32552871272553	2.45168155562328
Be	8.32326771770401	2.68576955992090	4.14324305504905
C	7.78402516773257	1.30834825893807	5.33657238999697
H	6.77441542440658	1.16382238449714	5.69526415329444
C	8.75498618959755	2.16751282428102	5.91548275958480
H	8.60871234671710	2.78160038625779	6.79324585744397
C	9.90024647706066	2.16238321872871	5.07786994714675
H	10.78437754458059	2.77232729776024	5.20139908587884
C	9.63732429230235	1.30039203344952	3.98061465480621
H	10.28409340520862	1.14851798997056	3.12767341974208
C	8.33082327153806	0.77097820468745	4.14256917442503
H	7.80874303337354	0.14419672795939	3.43279731083996

Complex **1**

Energy: -2134.478845633375 Eh

Ni	32.44518318442613	9.14533191512955	0.56918806355365
C	33.94133979665505	11.51588120923832	-2.20767742412570
H	34.57687951855608	10.95832543893769	-2.87621076974826
C	35.46365188716679	9.19528267926215	2.94119789324532
H	35.78192453307073	8.16525523386452	2.95852583147099
C	30.93595943118125	5.77025594934388	1.87097283124860
H	30.19079069737890	5.40018862403789	1.18692054952316
C	34.47417758544660	9.77517730951301	3.77250935875998
H	33.90893040180804	9.26375600446731	4.53486746257932
C	34.36512710344203	12.23917712478808	-1.06791883961046
H	35.38143429777514	12.32818522278884	-0.71895473301768
C	35.91506114758003	10.18954428438297	2.04101214890552
H	36.62862170312593	10.05072379925802	1.24578483954720
C	35.80948609406891	8.47135007360291	-1.44009019914415
H	36.32332883960425	9.39546473558685	-1.65258466802002
C	29.64256972217727	9.28705663878021	-1.76133056113405
H	29.79726579341239	10.27184936036369	-2.16985339263666
C	30.69094755055260	6.56558141859657	3.01198289333240
H	29.72431430009637	6.90863978608924	3.34270137734376
C	28.74240942298317	8.95775265975463	-0.72270745377107
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H	31.17884486184161	8.05898523580819	-2.80563444676300
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H	28.39767596645351	7.04623988410663	0.36676613508695
C	34.31712011445698	11.12664514697398	3.38149673892698
H	33.62307761966454	11.83764811356423	3.79596595910942
C	29.91149716538952	7.06740335592462	-1.27123753501186
H	30.31089211659211	6.06629992130127	-1.24996782691854
C	32.53095418574637	11.59627754073722	-2.27896905996674
H	31.91005245742538	11.09930138825334	-3.00668531821559
C	35.20440936217973	11.37888306972895	2.31100508011510
H	35.29065804352730	12.30747064597527	1.77151639176655
C	33.21390154102339	12.77245222111503	-0.43661690113379
H	33.19918160122157	13.33203775380172	0.48493389369451
C	31.93924815759446	6.88155611040207	3.60137792613586
H	32.09276311674454	7.51884058816997	4.45722255211285
C	35.10256352247667	6.56910433100340	-0.37570384296976
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C	36.02655425036819	7.63852033854112	-0.31558425305781
H	36.74347979709308	7.80634634586155	0.47106111608343
C	34.31214097474175	6.73894770392053	-1.53814130527788
H	33.47899561909405	6.12227140595293	-1.83558080971403
C	32.33322649809841	5.59746775382976	1.74769794276055
H	32.83358525331295	5.08349405786600	0.94356274682890
C	30.93708656556930	10.91762725035588	3.67978465824158
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H	34.01547459065605	6.38801652996364	2.97343053673782
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H	29.88909270684213	9.06259186319116	4.30570276992290
C	32.07974905835307	12.37488880573667	-1.18522547154252
H	31.05174000964556	12.56878369469703	-0.92479605761580
C	29.63748863463669	11.27608469763014	1.83170595718491
H	29.27067695084449	11.67901669361818	0.90126389793754
C	34.75132261124325	7.91218677154796	-2.19693706276305
H	34.31071796081525	8.33997734627054	-3.08317975386406
Be	33.09497809032789	10.80779565787605	-0.53336577229863
C	29.16690068770178	10.10885446930988	2.47930198217413
H	28.37158568481350	9.46644601018804	2.13881733694806
Be	31.08852564708986	9.93662358928952	1.93748443037619
Be	34.15886872997031	8.32424545904472	-0.34831421101076
Be	33.91671414411907	9.86130006276223	1.87222424118406
Be	30.59178025481635	8.55334083681253	-0.19509829760746
Be	31.87623777370656	7.53322302115172	1.74540839088747

Complex **1'**

Energy: -2759.344354704943 Eh

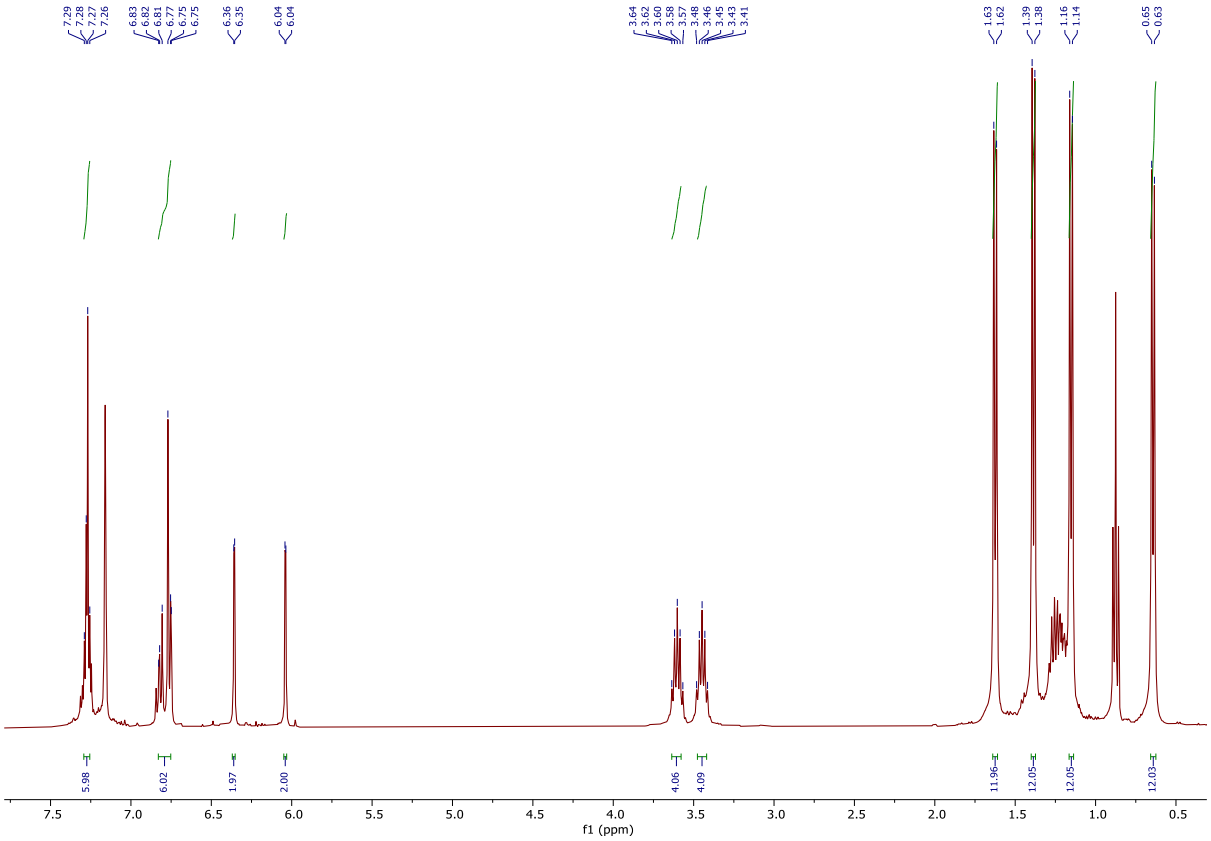
Ni	3.75865433261661	1.66997462579474	-0.00026223114634
C	3.92694197118924	5.34981177459967	1.22658442953969
C	2.66782913779898	5.35043025977009	0.58199363991505
C	4.92807384388135	5.36484450866492	0.23440388321309
H	4.09714752574283	5.27682430664224	2.28793015453703
C	2.88866249256623	5.36586556166995	-0.81154391440085
H	1.70832125843786	5.26878788312247	1.06662824530240
C	4.28783683823167	5.37486305596078	-1.03391688386482
H	5.99160949357181	5.33926905435252	0.40081240695621
H	2.13006203175063	5.30553892633815	-1.57543029729229
H	4.78453020984621	5.36300345750372	-1.99063016369426
Be	3.74863529690545	3.76128941560949	0.02131444238096
C	7.46068523368015	0.50558299117965	0.22289532402060
C	7.45613127082298	1.53425954618212	1.19174747165915
C	7.45731591244393	1.10443681254962	-1.05416520178190
H	7.40686621903498	-0.54955615970845	0.43024374479506
C	7.44993398314267	2.77206213639829	0.51983195228290
H	7.39357272832342	1.39835981102952	2.25882607863092
C	7.45062696324394	2.51386385737764	-0.87652026538363
H	7.40439330225445	0.58711673915271	-1.99884751522666
H	7.40289117560328	3.74135499944956	0.98678981096596
H	7.41950353791794	3.25562220860738	-1.65897722513617
Be	5.85494843739556	1.68002594382597	-0.00108020131758
C	2.55744191694672	1.59929995646201	3.68614916016010
C	3.35341443278096	2.76429195638418	3.69781678210308
C	3.42907651466185	0.47521356250657	3.67417130411323
H	1.48084147214969	1.56811749783516	3.65804743158720
C	4.71044836576510	2.37018496845635	3.69315455665174
H	2.98280588764059	3.77466242854332	3.64613339108851
C	4.75784534062583	0.95914263839872	3.67857895021080
H	3.12891959775193	-0.55989902656513	3.63523760646382
H	5.56010356173616	3.03054188590601	3.62501180657673
H	5.64709836088283	0.35386641977492	3.60879354126198
Be	3.75957153985175	1.64845404383914	2.08604288682041
C	0.07088770417757	0.46504015218052	-0.19462222901638
C	0.06570192093262	1.46568779824123	-1.18754388728837
C	0.06830870146689	1.10598527094818	1.07329842952791
H	0.10497939981255	-0.59838314745165	-0.36046911282556
C	0.05991446879355	2.72515343712981	-0.54357281678690
H	0.12919447397931	1.29522790576989	-2.24944938556692
C	0.06151428992265	2.50481666768558	0.85030402344840
H	0.09459128566735	0.60983249253815	2.02987763292595
H	0.12710775489919	3.68513220526492	-1.02952499518525
H	0.12276383175368	3.26415172522003	1.61334500568647
Be	1.66525235785960	1.65993715156019	0.00055452773019
C	3.92084224270715	-2.01175277273245	-1.23288087882450
C	2.68809772431525	-2.02468610092103	-0.55177150176556
C	4.95673107046374	-2.01670564739441	-0.27187585996988
H	4.04835892404908	-1.93546458739038	-2.30020028112152
C	2.95675454754050	-2.03778422844627	0.84250241886332
H	1.71496667647816	-1.98110305881263	-1.01107866349520
C	4.36766496473510	-2.03274844929042	1.00954940428912
H	6.00968324122259	-1.95001504782409	-0.48644677362739
H	2.22067078701621	-2.02244350055793	1.63077554244479
H	4.89195604716367	-1.98551698301532	1.95065972719628
Be	3.76869029025735	-0.42487285105272	-0.02187537188788
C	3.76087834860895	2.91118732799500	-3.67241465899128
C	2.61525444474625	2.08770729505753	-3.68040574545857

C	4.90561203250105	2.06663377487201	-3.68162992469066
H	3.76610313671967	3.98797467450093	-3.63327805766630
C	3.04154766874984	0.74058468770363	-3.69448854320546
H	1.59699895105728	2.43369843580273	-3.61490663344332
C	4.45338431035339	0.72672711556774	-3.69525251370135
H	5.93370936866594	2.39081812702660	-3.65029181609773
H	2.40248898632757	-0.12541716389457	-3.62926540667270
H	5.08001060269313	-0.14877926624419	-3.64033997991863
Be	3.75773782891923	1.69147813502834	-2.08490994822737

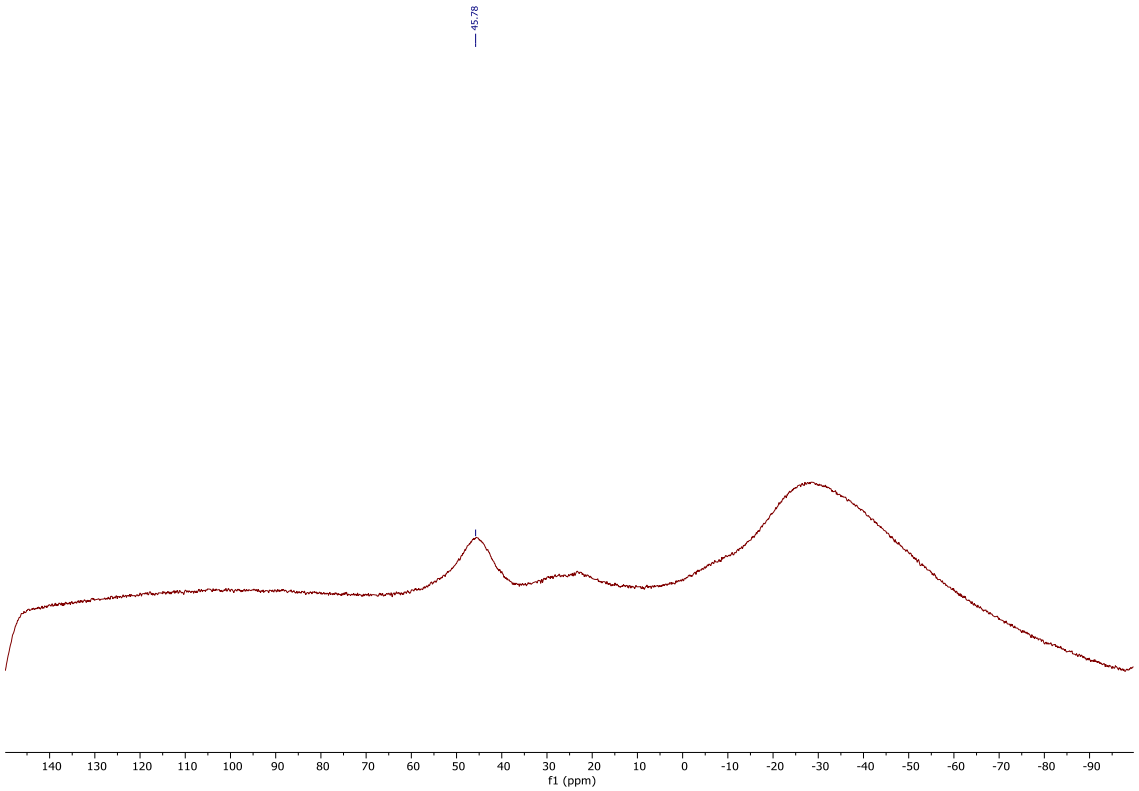
Chapter 4 - Synthesis of Homo-metallic Heavier Analogues of Cyclobutene and the Cyclobutadiene Dianion

Spectra

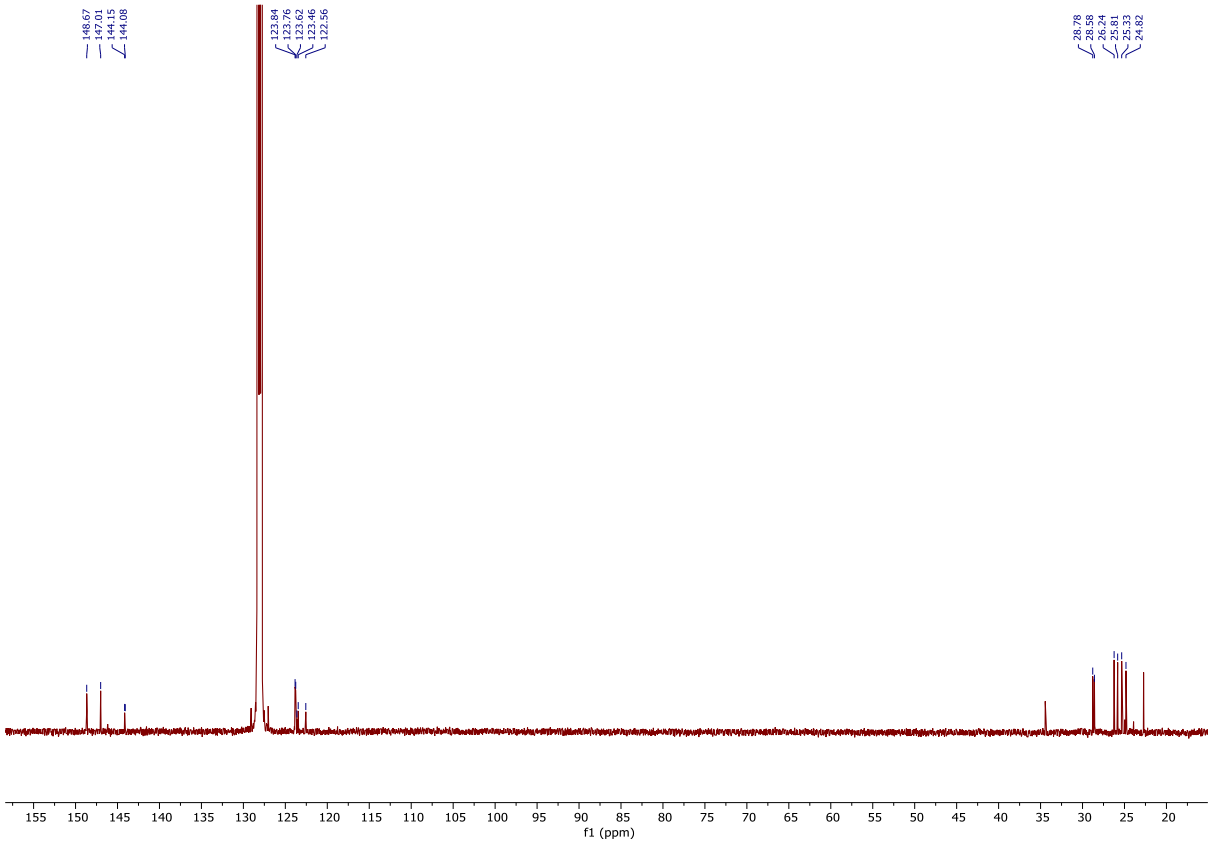
NMR



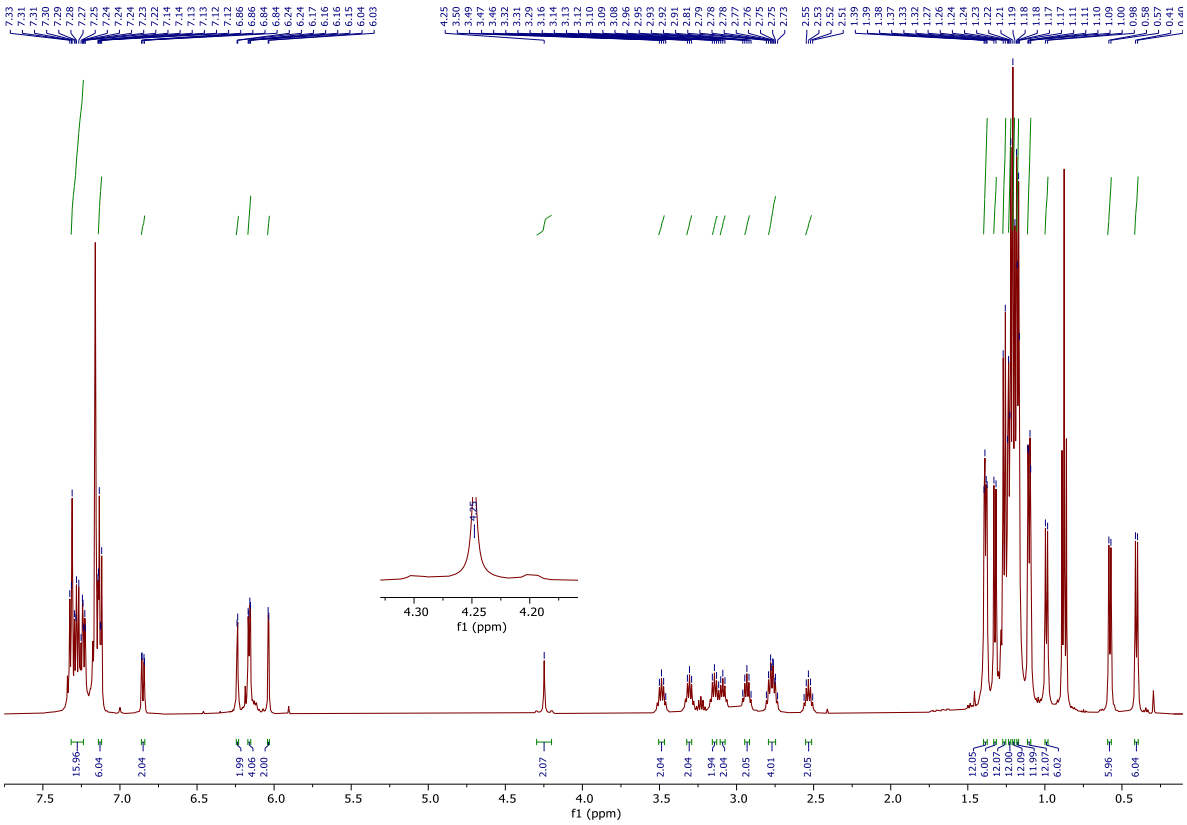
A 4.1: ^{1}H NMR spectra of **2** in C_6D_6 at 298 K.



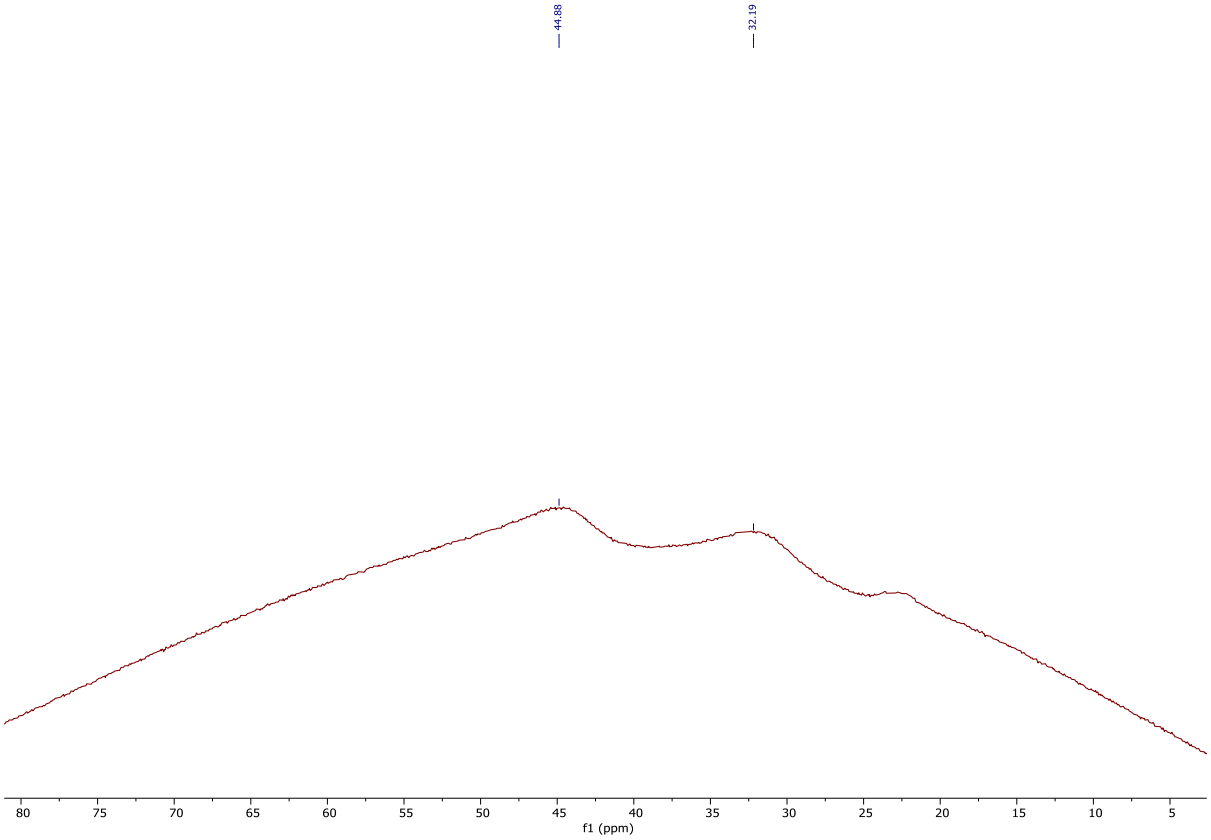
A 4.2: $^{11}B\{^1H\}$ NMR spectra of **2** in C_6D_6 at 298 K.



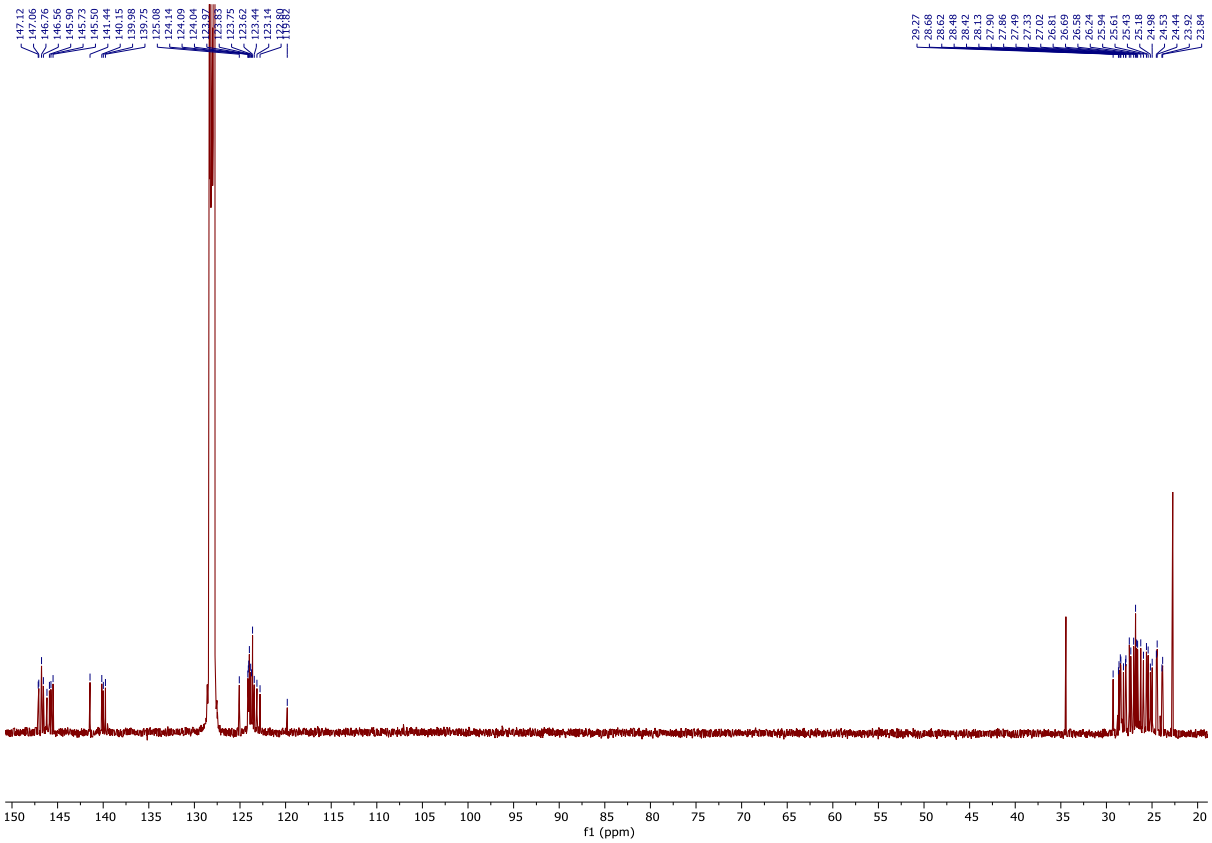
A 4.3: $^{13}C\{^1H\}$ NMR spectra of **2** in C_6D_6 at 298 K.



A 4.4: ^{1}H NMR spectra of **4** in C_6D_6 at 298 K.

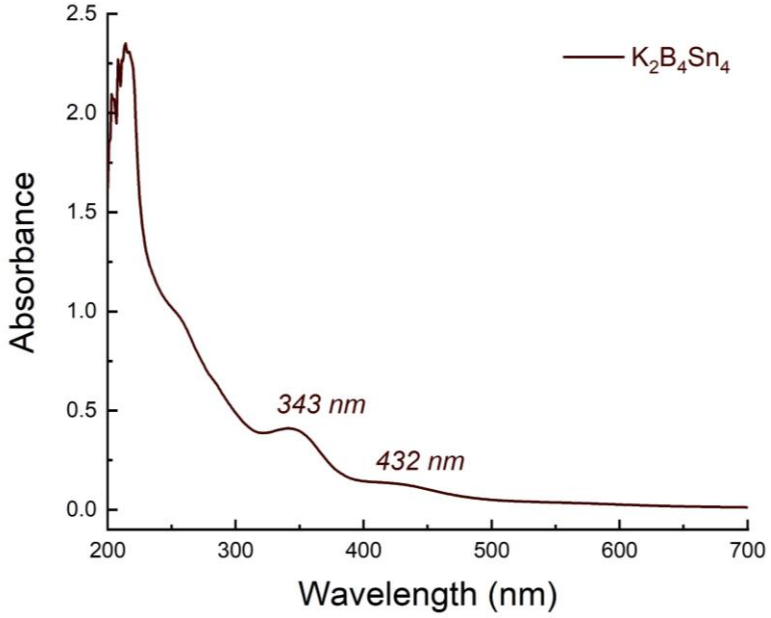


A 4.5: $^{11}B\{^{1}H\}$ NMR spectra of **4** in C_6D_6 at 298 K.

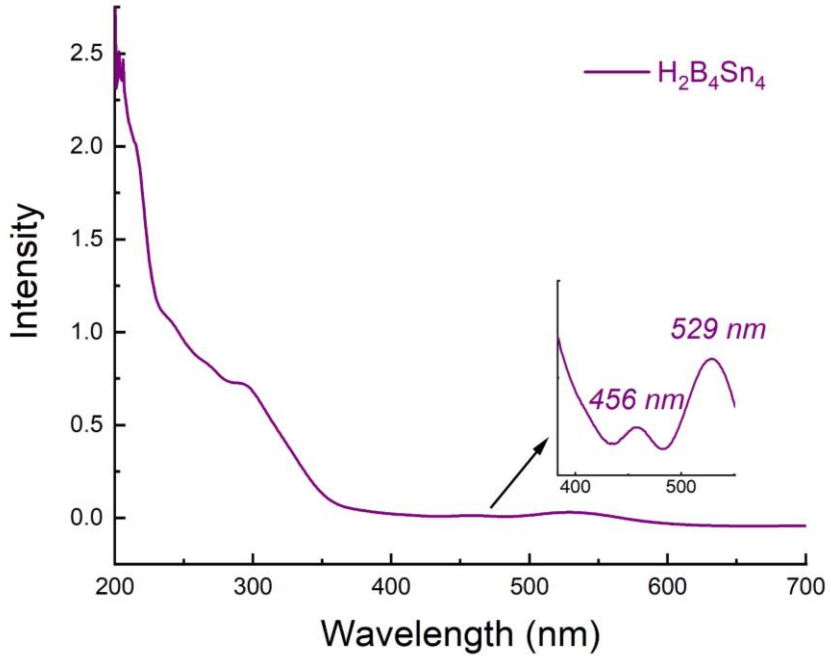


A 4.6: $^{13}C\{^{1}H\}$ NMR spectra of **4** in C_6D_6 at 298 K.

UV-Vis



A 4.7: UV-Vis spectrum of **2** in methyl-cyclohexane at 298 K.



A 4.8: UV-Vis spectrum of **4** in methyl-cyclohexane at 298 K.

Coordinates

K2Sn4

Energy: -5382.770116929179 Eh

Sn	7.93290493774198	9.73271962052571	18.18778129875407
K	6.55538705752630	11.10118616115493	21.89885676172339
N	9.65119567899513	8.15392890370708	20.70980679020758
N	10.08363214126653	7.29055081597023	18.66449688921043
C	9.24570197438354	8.87361163358544	21.86735545419220
C	7.94439297329200	8.99798212117212	23.89211053946865
H	7.19515312906388	8.57465203412297	24.55731096325445
C	10.20561128595172	7.04604744906534	17.26718274888351
C	8.25845311554722	8.32695439237942	22.70535632901593
C	9.88932063563281	10.08090893232666	22.18515168958052
C	8.58109105051099	10.19109500438132	24.22673290315983
H	8.33585525476881	10.69555203329889	25.15793542137581
C	10.57074041471174	7.10123862113196	20.83904186475149
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C	10.83166235125445	6.59007876158855	19.61335767222666
H	11.48907280647833	5.77552810382910	19.34105111819133
C	9.22847511619242	6.28075749134842	16.61723778020956
C	9.53354221508580	10.73485301015907	23.36967127655556
H	10.02520560875197	11.67102276322254	23.62279985375789
C	9.35379247130366	6.07779507625708	15.24200594213429
H	8.60758452393049	5.47902981580519	14.72568033711258
C	11.29284089745260	7.59609481335682	16.57391820886884
C	10.41997406900082	6.62236438770293	14.53586184715080
H	10.50645867735147	6.45175134611652	13.46616736656875
B	9.29989470732538	8.31995109715455	19.31253941806798
C	11.38280130628466	7.37514591969999	15.19872137667639
H	12.22013611522758	7.79582129789522	14.64658811068746
Sn	5.20635617640549	12.46571575581121	18.15108044717714
N	3.46598805249723	14.04753346047258	20.66023093726620
N	3.04829727306423	14.90244071905149	18.60850438684803
C	3.86447354354554	13.33499897755861	21.82460376741167
C	5.15329249801378	13.22421459998382	23.85802846605053
H	5.89911070675959	13.65154171414895	24.52452902385714
C	2.93899549050556	15.14303385161530	17.20948344909741
C	4.84790850269641	13.88630439525404	22.66397876701810
C	3.21672828198215	12.13139913028434	22.14783086935367
C	4.51195820008496	12.03520055726502	24.19833279882641
H	4.75012028222280	11.53795891516800	25.13525295811788
C	2.54341805625791	15.09894591741211	20.77817794982059
H	2.14048820861069	15.39830819817715	21.73622569246833
C	2.29148258180358	15.60519253325662	19.54858983175581
H	1.63505337921313	16.41775339121033	19.26807806530547
C	3.92143528123534	15.90761794052242	16.56671521703585
C	3.56395088651060	11.48621027989885	23.33965984712306
H	3.06894751255943	10.55301185541214	23.59721764754273
C	3.80908480384354	16.10646797593094	15.18977981952791
H	4.55952212138572	16.70452726128849	14.67877782082000
C	1.85893094228590	14.58996318912715	16.50756248339050
C	2.75022137031450	15.55871656391284	14.47511863332512
H	2.67373650233790	15.72616664989195	13.40416519798052
B	3.82901325140676	13.87688401319081	19.26652789537854
C	1.78177426146328	14.80697815837765	15.13097281513883
H	0.95036583306150	14.38348111474403	14.57207470731799
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N	3.48031890790762	8.14864747012671	16.47648324437391
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C	5.18670121592801	8.97441183665107	13.28925019833198
H	5.93459394766671	8.54641681611175	12.62550550097431
C	2.92498771937999	7.05760228494737	19.92431279322856
C	4.87208971078499	8.30962848829626	14.47936909659201
C	3.24471757633126	10.06903647752886	14.99209434511856
C	4.55223323527876	10.16727840104439	12.94947997374642
H	4.79796565199773	10.66692563041226	12.01581618737613
C	2.55992281721147	7.09607489710478	16.35229671523271
H	2.16448557347769	6.79560613691278	15.39148002637680
C	2.29854033465170	6.59103226129642	17.58041412830273
H	1.64031592629220	5.77845278048193	17.85663044730894
C	3.90055378577199	6.29327527555685	20.57769322162869
C	3.60128193317231	10.71686677640347	13.80446272623154
H	3.11127305207034	11.65278732577750	13.54726093991565
C	3.77479312080435	6.09671585238248	21.95381570140036
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C	1.83911258074575	7.61330397787142	20.61516123707572
C	2.70985654680153	6.64681391092581	22.65753257096094
H	2.62304194583899	6.48121787989943	23.72798662150985
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C	9.92341407101254	12.10147605200330	15.01444165036533
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C	10.39435496210857	15.57358635714035	22.66739332032506
H	10.46984908100193	15.74751305768402	23.73738632548709
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H	12.19052333634370	14.39194242260807	22.58043638100229
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H	11.40194728197891	11.52947355971968	21.72363107916589
H	11.69394099960468	9.91121482943836	21.02553130271946
H	10.46078173796344	10.96823860850564	20.32733872041858
C	7.52959832536821	7.07713565677202	22.30754118372709
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H	8.22055266609638	6.26604946380485	22.05675506789103
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C	7.56863806782428	15.10859670117458	14.88299729297210
H	6.90618349573928	15.44248363859669	14.08053516527248
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H	8.25957944656294	15.91836875578593	15.13815094973585
C	2.20605430574368	10.64853241473814	15.90337351947618
H	1.73421221685851	11.52200354973830	15.44707434680389
H	1.43882889665320	9.90663775441952	16.15042805372010
H	2.67304108063415	10.96400683909491	16.84623816872770
C	5.59846600067440	7.06005441113941	14.88253944444428
H	6.20254585243050	7.25332507310252	15.77850112465120
H	4.90580801173864	6.25155053051502	15.13696093211754
H	6.26427665847894	6.72309784380081	14.08414326696644
C	0.81499338286678	8.43546095573093	19.88557812056697
H	1.29675225837729	9.23113313253562	19.30560983640700
H	0.24833167956684	7.82823429717249	19.17063798659666
H	0.10755883688501	8.88881895886497	20.58491753084138
C	5.05600682124776	5.71808932100337	19.81036713134497
H	5.65386118589942	5.05553897905034	20.44228693923738
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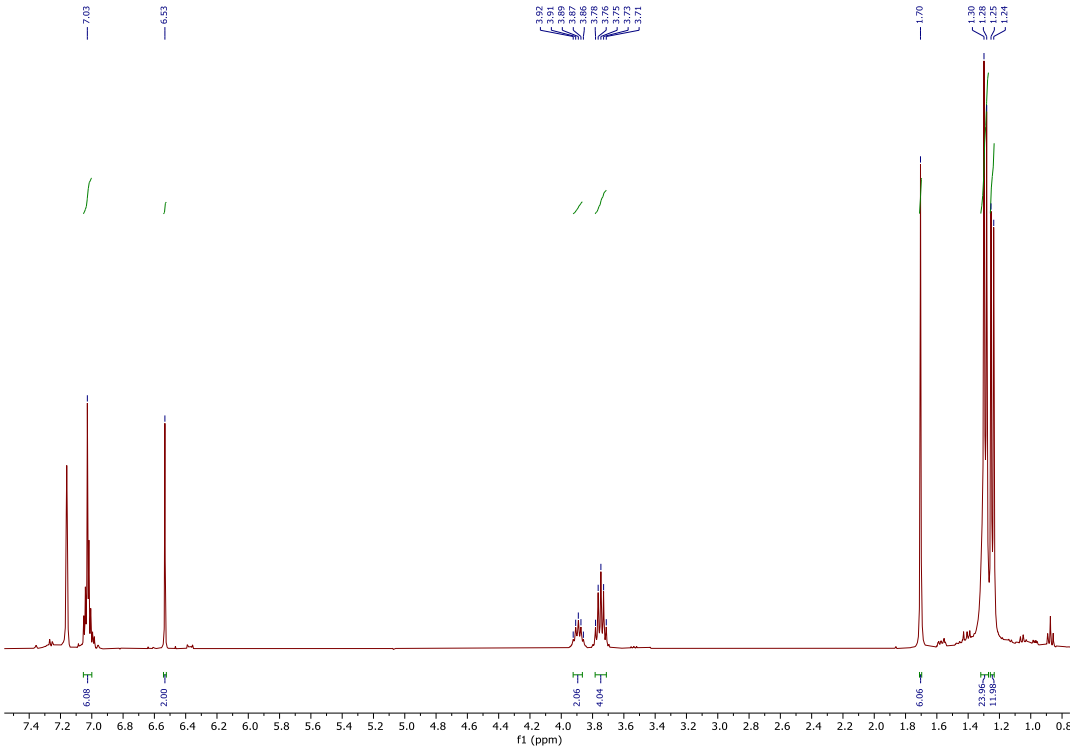
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H	3.98948930102803	10.01927314332363	15.63802836884184
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H	1.91650744912124	7.07229955700231	20.27902544971935
H	3.26371147409595	5.92017221150335	20.08520447941703
H	3.59700435310968	7.62148499704225	20.48247732206458
C	10.18962284438340	6.95023460250098	17.28296133535744
H	11.21634016337159	7.07043294717300	16.91114606930334
H	9.87552655337521	5.91187281552057	17.11083664141792
H	9.53275580333580	7.60978375285647	16.70707928962628
C	9.22348220709568	8.98094459801056	21.85935822556824
H	8.25459700264123	8.64438217470254	22.26950458551686
H	9.96656127348923	8.92180554086358	22.66305032969004
H	9.15082062693273	10.03160948243466	21.54647686827190

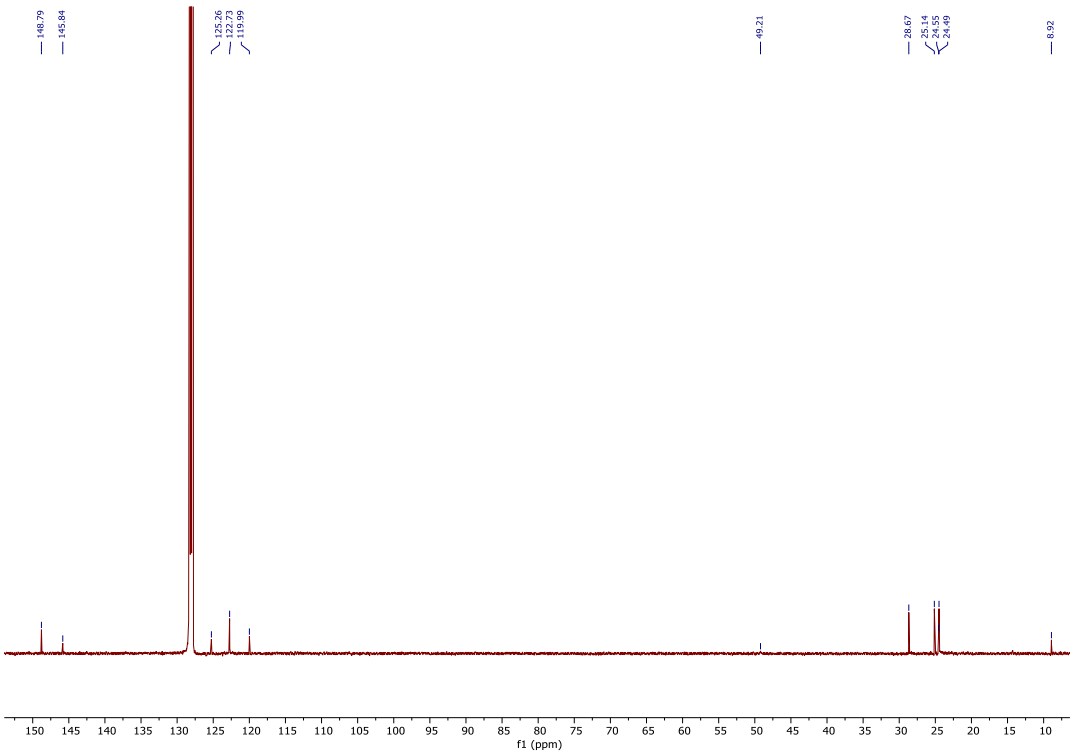
Chapter 5 - A Planar Per-borylated Digermene

Spectra

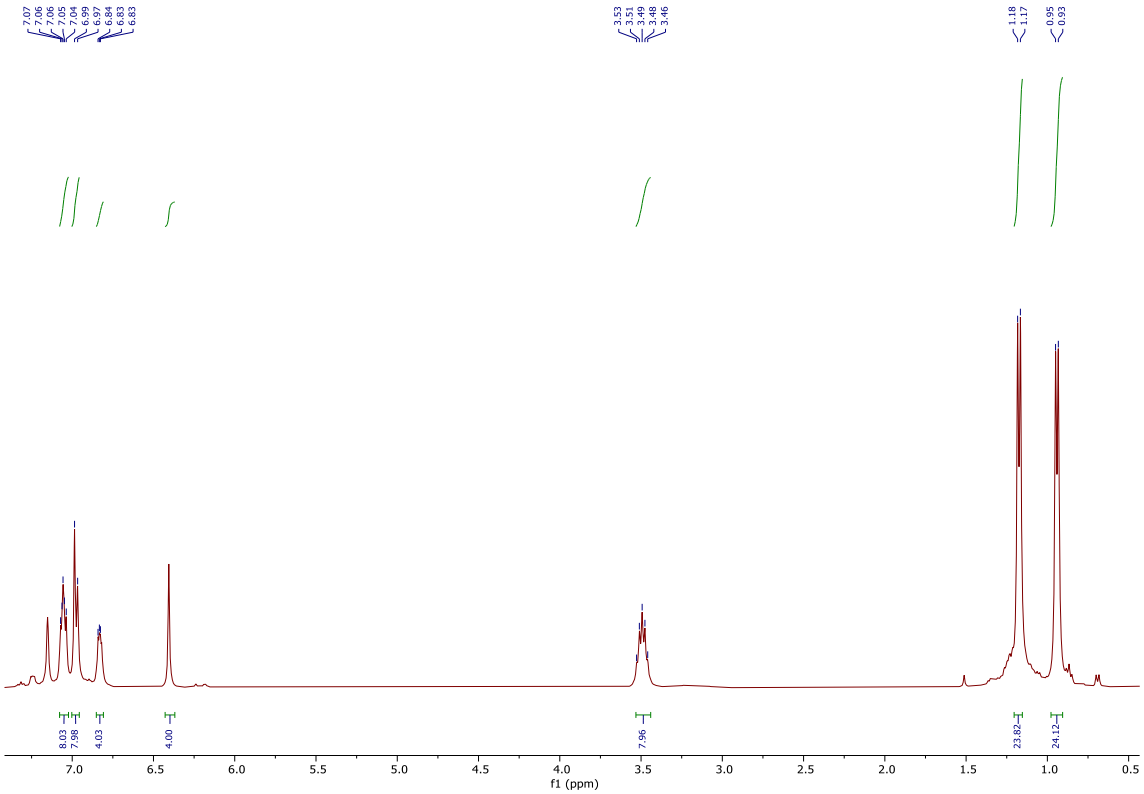
NMR



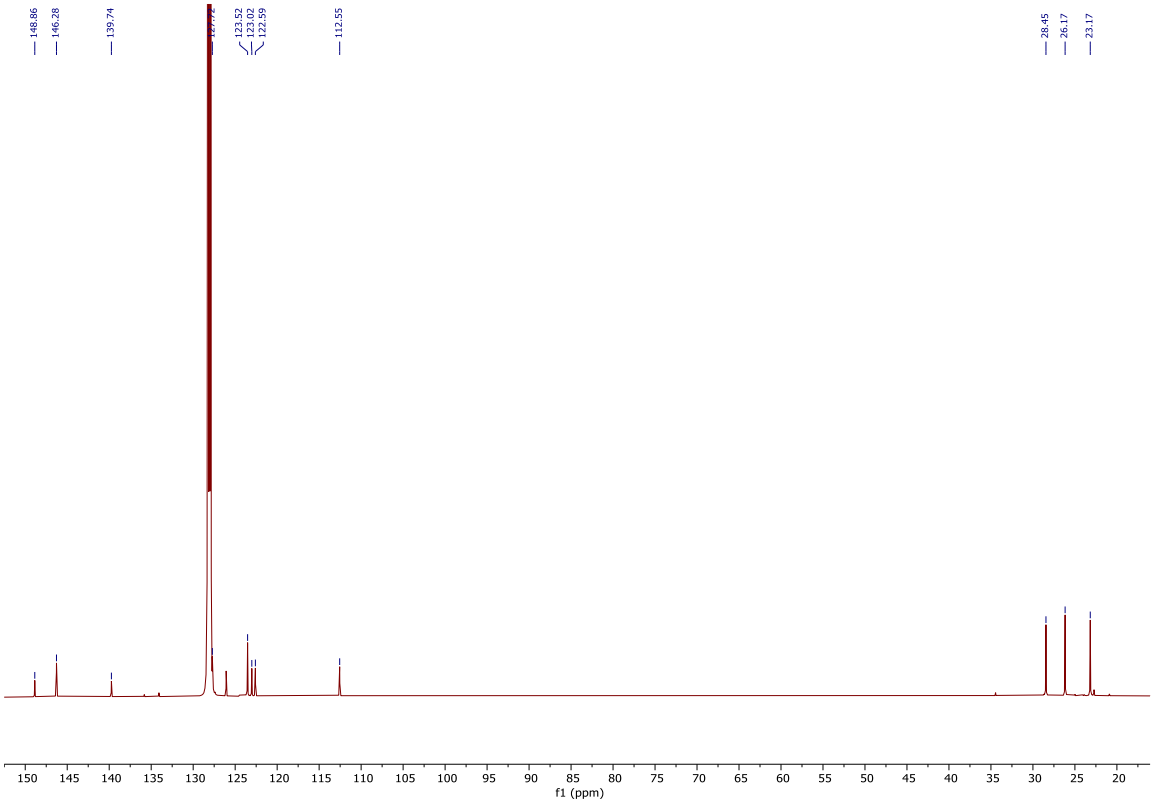
A 5.1: ^{1}H NMR spectrum of **2** in C_6D_6 at 298 K.



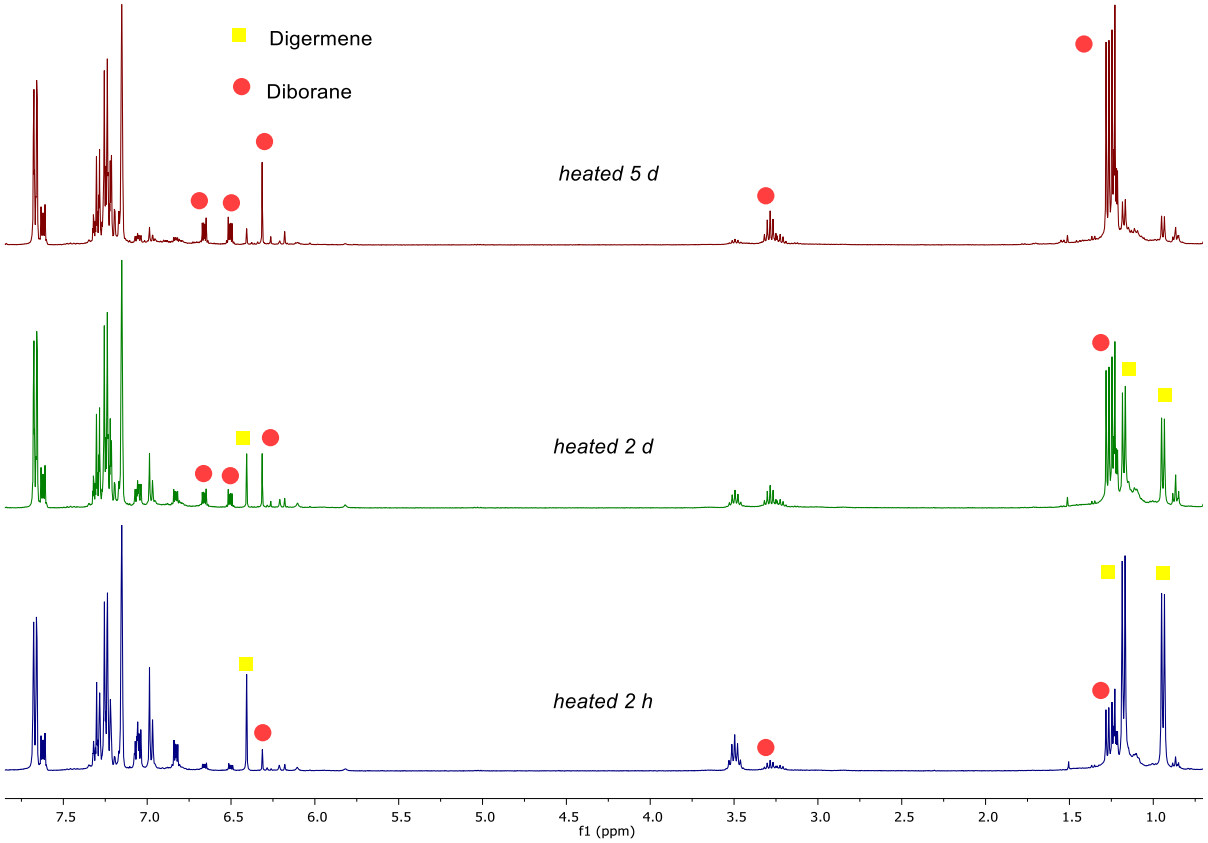
A 5.2: $^{13}C\{^{1}H\}$ NMR spectrum of **2** in C_6D_6 at 298 K.



A 5.3: ^{1}H NMR spectrum of **3** in C_6D_6 at 298 K.



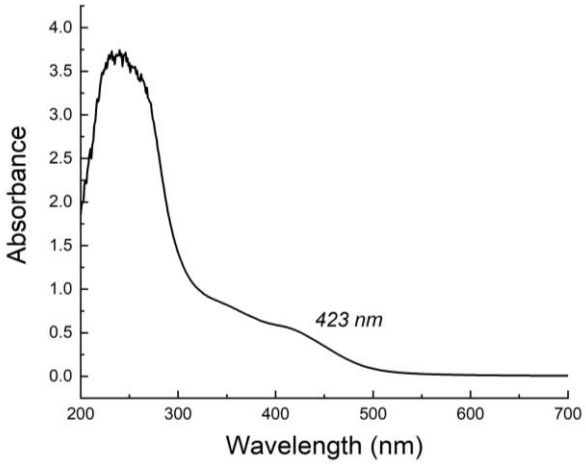
A 5.4: $^{13}C\{^{1}H\}$ NMR spectrum of **3** in C_6D_6 at 298 K.



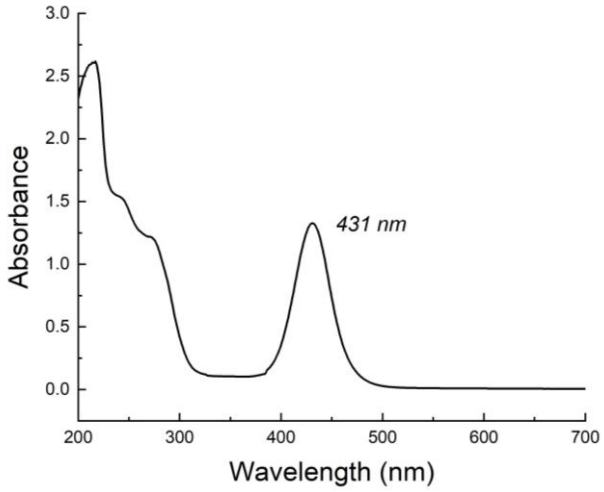
A 5.5: In situ 1H NMR monitoring of the thermolysis of digermene 3 in C6D6 at 353 K to yield diborane 4.

Figure s7:

Uv-Vis



A 5.6: UV-Vis spectrum of **2** (λ_{max} = 423 nm, ε = 1440 L $mol^{-1}cm^{-1}$) in methylcyclohexane.



A 5.7: UV-Vis spectrum of **3** (λ_{max} = 431 nm, ε = 4470 L mol^{-1} cm^{-1}) in pentane.

Coordinates

AgT1

Energy: -7259.972043256641 Eh

Ge	3.16486724076669	1.07820264868193	12.79535088520452
O	1.53689231212607	-0.02238922885554	15.12057355980833
O	0.30351205828426	1.35922174290930	13.77873954179761
N	6.05614847609506	0.38251875868758	13.73324387074482
N	5.26018045919828	-1.13491787338625	12.22446197764827
C	7.05359458396879	-0.55480259826917	13.45700889651509
H	8.03246110120769	-0.50446344286779	13.93247763479896
C	6.57905935057769	-1.46116699845253	12.55220680985482
H	7.08041352147039	-2.32298153437159	12.11362354780637
C	4.39359319393500	-1.98274277116940	11.46801151840095
C	4.38368273631352	-1.90124287160796	10.05892760549861
C	3.53713119705567	-2.76922756143109	9.35206556071581
H	3.51932943215427	-2.72791309249687	8.25907028991211
C	2.71114548184603	-3.66984931602065	10.02078738095158
H	2.05601908164200	-4.33767677467306	9.45318007871888
C	2.69935945197098	-3.70406124396722	11.41585245822532
H	2.02416102566385	-4.39311008992903	11.92975090383028
C	3.52923814500932	-2.86182395242351	12.16849755257094
C	5.25655510762554	-0.90608487031080	9.31644622324604
H	5.61655520849224	-0.17512322549328	10.05694572833460
C	4.47267392869080	-0.13397507777211	8.24937408517362
H	5.10543893836255	0.65382159364056	7.80785839145693
H	3.57141689482037	0.33790907327431	8.67372763282541
H	4.14882547217015	-0.78531330339675	7.42096876501178
C	6.48425904965571	-1.59377344024716	8.70468263414625
H	6.18423222637069	-2.35313853436946	7.96261919146404
H	7.08866881677601	-2.09870619461410	9.47460301666126
H	7.12632686925783	-0.85619894178643	8.19502477688173
C	3.50734118489290	-2.90764055016375	13.68915144530525
H	3.76801845420551	-1.89652354282985	14.04866043661999
C	2.13162032511176	-3.24498196544165	14.26651151022691
H	1.85634574364216	-4.29835474742456	14.09239977295969
H	1.34413038314331	-2.60820829689949	13.83464121889618
H	2.13517171149932	-3.08273365050954	15.35588053829469
C	4.57262526999412	-3.87406972104976	14.22750398142895
H	4.57621276952959	-3.87030381279794	15.33028200721684
H	5.58103041541701	-3.59782272489889	13.88486202940083
H	4.36647126147685	-4.90416786147303	13.89068724647027
C	6.09997740356936	1.30552129793418	14.82368453393885
C	6.24762066760580	2.68875117074956	14.56609200506453
C	6.21890856111741	3.56782664814857	15.65722343683327
H	6.31790570302643	4.64231052220325	15.48257269066200
C	6.06244410070221	3.09381551086408	16.96082372626068
H	6.04605555242768	3.79664734136147	17.79932818956179
C	5.91615246723224	1.72772691360310	17.19399557903945
H	5.77928043466074	1.36496978182363	18.21759121239830
C	5.91598359973695	0.80884708940644	16.13363564899704
C	6.47119485266000	3.18999110465490	13.15259230140352
H	5.94535572100664	2.49696151745569	12.48078358828389
C	5.90667599356235	4.58610292112826	12.89681443431858
H	6.46682627382332	5.37129184435251	13.43217691830722
H	4.84710828132948	4.66010674231141	13.18989625329793
H	5.97498837446185	4.82481363446995	11.82198827949157
C	7.96024004192325	3.11686324735030	12.78681767000547
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H	8.55958620497755	3.77153391905417	13.44216012151990
C	5.69825398224475	-0.67004726953372	16.41423007718665
H	5.64709993625036	-1.19362834558078	15.44620036090906
C	6.87556443964624	-1.26674105849797	17.19463336603186
H	6.97889668527620	-0.79393702223176	18.18572093561554
H	7.82644553716410	-1.12536921492640	16.65704542269459
H	6.72915315123579	-2.34805871459986	17.35166908432797
C	4.36741790489703	-0.91941286691946	17.13379648394804
H	4.20646089717083	-2.00195562257713	17.27123668669837
H	3.52063638526510	-0.51795494844744	16.55664802982144
H	4.35198228807509	-0.45433874236992	18.13361234943320
C	0.26880461637081	0.07674518246701	15.62987639984632
C	-0.26721194968883	-0.51509464837488	16.76408664009654
H	0.33065557409632	-1.17321173472050	17.39853770337169
C	-1.61010832311023	-0.21688706801236	17.04766323995469
H	-2.07804264549945	-0.65890108002985	17.93144244081082
C	-2.36334807688094	0.63511055105050	16.22621908709845
H	-3.40547560454928	0.84276136850228	16.48369937176470
C	-1.81054265714895	1.22887676966373	15.07977455540934
H	-2.38247726070485	1.89568828313357	14.43040798508402
C	-0.48434811503177	0.92446931473934	14.80864232241485
B	4.89660821239788	0.04805154874541	12.95344397991244
B	1.55917499822323	0.77967127427132	13.97603504849020
Ge	2.92312865452807	2.54270720523934	11.10746775068555
O	5.78327618166900	2.26111413535419	10.11890373879122
O	4.54695785902797	3.64226965221967	8.77937277450385
N	0.82437438345383	4.75590252539816	11.66658780282765
N	0.03477881684508	3.23445967007922	10.15853209720778
C	6.56854255406739	2.69463954984541	9.08649355976408
C	5.81361484647953	3.54219374387659	8.26672809475619
C	6.34677841440161	4.13285226203149	7.13054880019838
H	5.74749935635517	4.79081170905745	6.49726177615056
C	7.68868627628892	3.83359957554819	6.84343362084558
H	8.15441322943933	4.27461904323740	5.95799296505426
C	8.44369809549859	2.98173944252333	7.66340097274077
H	9.48495359727236	2.77320852587371	7.40311823230005
C	7.89376571876057	2.38917726611849	8.81184372865963
H	8.46707042552735	1.72241990624476	9.46005142247903
C	-0.96388184781339	4.17239676851488	10.42819272919483
H	-1.94094256066774	4.12060881151175	9.94919760165890
C	-0.49322275450040	5.08110230338523	11.33270255288068
H	-0.99662485927389	5.94380009736909	11.76717939725660
C	1.68817561395159	5.60460165024469	12.42518952407727
C	2.55626602592057	6.48175685322970	11.72689390567503
C	3.38433645407673	7.32385195454247	12.48168659800873
H	4.06242155872145	8.01138738364664	11.96957934038546
C	3.36717699190317	7.29132793082317	13.87673848172004
H	4.02103543320908	7.95895139993257	14.44603974394873
C	2.53747323403749	6.39261023211064	14.54341746179379
H	2.55108133924462	6.35267070530337	15.63651480295019
C	1.69257425963267	5.52479110601246	13.83438157251587
C	2.58405655207053	6.52539001108619	10.20624541169208
H	2.32624639725692	5.51333760540979	9.84730027407288
C	3.96145578224601	6.86374112018351	9.63356694945667
H	4.23465135670566	7.91775610222922	9.80708915228794
H	3.96219489770391	6.69975759063280	8.54445727493118
H	4.74824464118779	6.22875312455878	10.06936179816240
C	1.51963871614192	7.48954722727632	9.66213048026736
H	0.51017947903541	7.21233043653362	10.00082571536934
H	1.52073742553692	7.48428040539884	8.55935080705755
H	1.72292921647195	8.52038715031802	9.99840835523164
C	0.81561622412740	4.53146718588321	14.57456345589541
H	0.45913515335742	3.79897233426509	13.83384549855175
C	-0.41488140917903	5.22097334965491	15.17863892708560
H	-0.11820012506702	5.98195748390273	15.92038549528116
H	-1.05971454985154	4.48482642274419	15.68686548518450
H	-1.01529566916772	5.72430191990276	14.40456289317336
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H	2.49703336800777	3.28843613572754	15.22822392817888
H	0.95858261100557	2.97437344097579	16.08676624409542
H	1.91330229042869	4.41412141486783	16.47602708777259
C	-0.00331065408335	2.30841363963315	9.07043458889436
C	0.18657937419746	2.80143591911010	7.75992911491892
C	0.19308915124183	1.87935415907919	6.70236348988978
H	0.33432532795401	2.23922898745617	5.67835999082561
C	0.04776832796136	0.51373932467636	6.93892219514150
H	0.06956379353441	-0.19157715669239	6.10262656554220
C	-0.11482652411835	0.04339651204065	8.24310504838736
H	-0.21309978722987	-1.03070316877097	8.42046667272577
C	-0.15049742399798	0.92572943059069	9.33139838435294
C	0.40166027171307	4.28007800271638	7.47608118468325
H	0.45559725043871	4.80513761743990	8.44319489325396
C	1.72916777153190	4.53105557144082	6.75106868401006
H	1.74094564015963	4.06724084904387	5.75063857655753
H	2.57847755638814	4.12990592142455	7.32462736938992
H	1.88851074012065	5.61388291013145	6.61403101170044
C	-0.77963312941866	4.87342198916165	6.69902313129469
H	-0.63546577814909	5.95458946251899	6.53886070225359
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H	-0.88591026260928	4.39783843163714	5.70956028723691
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H	0.14220285377050	1.12300718958251	11.41758196793582
C	-1.87183233138734	0.50414172328951	11.10384958832807
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H	0.10654738537159	-1.20309494714315	12.08272682680512
H	1.24154859165464	-1.04321010122085	10.72001312819562
H	-0.37757305097391	-1.75338627670410	10.47154610021994
B	4.52728191393106	2.84086501472969	9.92443527376707
B	1.19105148449086	3.57117111408997	10.94227070788629

AgT2

Energy: -6894.225375096725 Eh

Ge	10.38021755853584	8.19476496370919	4.83616457650537
C	10.11168325152853	6.39755272266373	5.66192518852775
C	10.10447937546076	6.13079203167316	7.05140858744615
C	9.94949503340770	4.81678831017454	7.49286241319771
H	9.94301471480409	4.62728200284767	8.56349465380961
C	9.80280859388135	3.74568370679245	6.61803537819014
C	9.79600233011196	4.02245437939636	5.25782577506012
H	9.67119577108012	3.19911215022926	4.55741123530984

C	9.93212168965218	5.32176605001612	4.76624413754695
C	10.25851565096243	7.19419133959803	8.12414994079714
H	10.39375227952620	8.16021758623947	7.62407649340554
C	11.49528073335816	6.93880850615900	8.99759142462020
H	12.41279471318891	6.93898477718113	8.40185324391943
H	11.42766696720258	5.97097320891779	9.50582089660598
H	11.58727435443235	7.71107822781589	9.76801715098605
C	9.00251297782306	7.29949675670451	8.99968662700750
H	8.10476725647355	7.45227499500768	8.39507590045378
H	9.08793112797691	8.14997054411173	9.68516532562373
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H	9.57309695997299	1.67407927221674	6.24870437867228
C	8.33660006286474	2.17358387820492	7.92682567781023
H	7.47095004352956	2.48170299542598	7.33205747277716
H	8.35663463627812	2.78991655567182	8.83279237467174
H	8.19392171841894	1.13140163565708	8.23363126704523
C	10.84844435231405	1.88599036244082	7.95951258038375
H	10.74683176830833	0.83739831088344	8.26044306470121
H	10.93954277710610	2.48755724314648	8.87066496044726
H	11.77744341276902	1.99542844318896	7.39107262304292
C	9.86728919391763	5.50187438523687	3.25965796687272
H	9.90562868648373	6.57926246501551	3.04576026472654
C	8.53749899386990	4.99307823157754	2.68829100929134
H	8.46675553722693	5.21912747655419	1.61834406673594
H	7.68987167223021	5.46294661064844	3.19789195929825
H	8.44115836650700	3.90854590531054	2.80416800051172
C	11.06933810648015	4.84558157351452	2.56990978300369
H	11.02263078489778	4.97902008164562	1.48372476744092
H	11.09033779584934	3.76900421507389	2.77263325243407
H	12.00926416803462	5.28022734711037	2.92497863080237
C	11.97218003451337	8.13769500960207	3.64051247199736
C	11.88767681392836	8.40988045068786	2.26008924611780
C	13.03662576164291	8.30050731405277	1.47351172941994
H	12.97151499328383	8.51253838511372	0.40827945116421
C	14.26791317844190	7.93888040299885	2.00502043223810
C	14.33857655511020	7.68318421658613	3.37200237718604
H	15.29259134604119	7.40351488175450	3.81349982737855
C	13.21711121371526	7.77219319732012	4.19592201005660
C	10.60552939493212	8.84161052529045	1.56642699226213
H	9.81019936537927	8.84967131346881	2.32676062850614
C	10.73513310663110	10.26022135709214	0.99893931040015
H	11.49563628628924	10.29053432288370	0.21052536557038
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H	9.78451104955227	10.59126424956085	0.56696332911559
C	10.17622307535932	7.87877887412826	0.45107926640009
H	9.21068267078555	8.19260017728589	0.03837507555847
H	10.07885340490809	6.85218169586668	0.81034257005811
H	10.90175218154640	7.87816236154241	-0.36987515940617
C	15.49823238584270	7.86400985902993	1.12508971823969
H	15.16060371016301	7.98715638920009	0.08649788813575
C	16.46284167211405	9.01491365881632	1.44381500484392
H	17.33176049479812	8.99244153764201	0.77648741481082
H	16.82677053451135	8.94040854000325	2.47530735743044
H	15.96345906412453	9.98294407949661	1.33165231246638
C	16.20510918689236	6.50776632874520	1.23143655404995
H	15.51321363632611	5.68593201912173	1.02142349889776
H	16.61687557631297	6.35258960476771	2.23475310686695
H	17.03667336185673	6.45070344516565	0.52051479655233
C	13.39508937632569	7.46090954642994	5.67262070625340
H	12.43609532061241	7.64700826865828	6.17320204342762
C	13.74736793604539	5.98364109487611	5.88721360581653
H	12.96577342103772	5.33449585035771	5.47833756420916
H	13.85255121510957	5.75878431087219	6.95445484190885
H	14.69402351554790	5.73114460285322	5.39585491966008
C	14.41868384175208	8.39061321573374	6.33466077097898
H	15.42238316931281	8.24606873488289	5.92017455764090
H	14.47219835250541	8.19362831587269	7.41150499853408
H	14.14170540720061	9.44119120095819	6.19423339213695
Ge	10.00342881069319	10.22625096524065	5.86609779112001
Si	10.00182149760852	12.24599742943697	4.58335898761929
C	8.61069944057976	10.37474926701494	7.27002960671453
C	8.10475423800367	10.99902731919685	9.55293844651715
C	9.00232500867888	10.97651084433359	8.48527176663111
H	8.40425188448223	11.45021465315150	10.49600197543285
C	6.82648659058570	10.45778444003393	9.44932571106672
C	6.43430115070162	9.92978278866255	8.22294624810109
H	5.42533828856577	9.53789524196565	8.11194050500353
C	7.29775946380777	9.88531947816051	7.12761229455182
C	10.38228105374636	11.59704929349801	8.66217034055762
H	10.74350955564987	11.87982078606725	7.66051862641656
C	11.38523906910417	10.59322069691079	9.24219472776295
H	11.52617245196854	9.74389113767155	8.56785727741023
H	11.03309063589898	10.21419915793077	10.20894032041548
H	12.36090229809927	11.06914684646896	9.39430017043291
C	10.36734607330299	12.87981519941500	9.49805323902004
H	11.33384605602115	13.38745417288137	9.41214307106994
H	10.20478288110505	12.66739071060851	10.56091470098827
H	9.59019525347275	13.56881035078325	9.15713062909502
C	5.88927772527973	10.45113892436340	10.63916230428244
H	6.41887912426575	10.93563404039304	11.47150689784702
C	4.61206474626490	11.25475445062617	10.36355238022174
H	4.85034900453930	12.27968395735032	10.06199667474202
H	3.97910334514841	11.29428216221802	11.25715173734067
H	4.02594584480862	10.79591492359134	9.55960769850731
C	5.55443770131362	9.01580973633964	11.06696721492101
H	4.99476475652753	8.49552490242223	10.28149445131248
H	4.94081330779398	9.01331904990927	11.97490277387286
H	6.46630634008519	8.44207880200894	11.26175327539790
C	6.76233326242046	9.35007190718899	5.81155293970133
H	7.55540103913689	9.47399162955207	5.06536538630364
C	5.55512986991651	10.16432305638370	5.32923661461856
H	5.80369470023290	11.22875432038070	5.26250663315552
H	4.69821978564248	10.05520554814157	6.00359719173003
H	5.24338173378307	9.82925095869573	4.33363326038970
C	6.43524767368122	7.85380468487905	5.87780656236318
H	6.05576665532678	7.50459929690642	4.91026238750862
H	5.66740737710758	7.64616991762436	6.63247299834462
H	7.32283738319880	7.26130337672503	6.12467596376097
C	9.74033969671083	13.68156185350233	5.77750182902844
C	8.47304561798082	13.90343462884011	6.33799664269041
H	7.65679781581588	13.21996268190804	6.11289604867525
C	8.24008667433056	14.99128902579886	7.17195275829931
H	7.25075493780617	15.14793251167782	7.59315251722160
C	9.27447388160220	15.87669778348154	7.46804693792434
H	9.09278407751077	16.72927301752146	8.11683803421375
C	10.54236309841032	15.66107227487739	6.93749652672305
H	11.35334779705819	16.34599382749516	7.17011767347811
C	10.77242417854683	14.57205672710123	6.09998638161722
H	11.76387956321697	14.41921130399804	5.67885883113836
C	11.66606907550096	12.44846579567604	3.72312333658587
C	11.85015240159081	13.45176960010489	2.75969745496695
H	11.03196880063080	14.12709546578844	2.51616704930177
C	13.06063637853486	13.58491702039345	2.08834798702591
H	13.18319785404665	14.36567263332475	1.34258885250345
C	14.11137723893142	12.71095642707482	2.36246288788978
H	15.05362286881514	12.81002125618311	1.82993251257481
C	13.94901902241364	11.71256589860059	3.31705801646604
H	14.75630792185089	11.01728598032271	3.53151057677300
C	12.73804191206606	11.58894121473514	3.99200124607309
H	12.61834459443161	10.79235632207709	4.72275896892980
C	8.57621120643210	12.35241043115105	3.34312436947255
C	8.09626523283836	13.61227086038535	2.95154771758563
H	8.51344826382007	14.51211169645982	3.39888163086375
C	7.07685703140059	13.73262927119968	2.01216431848721
H	6.72098176451425	14.71796806305433	1.72363823262356
C	6.50749990010547	12.59303846680413	1.45035718690981
H	5.70636278133875	12.68594328297625	0.72222842322760
C	6.96247723117589	11.33537904854766	1.83410777931074
H	6.51701684140254	10.44027047784225	1.40768591913864
C	7.98468037833642	11.22136186897070	2.77081676307787
H	8.32586977204667	10.23300713276715	3.07047221933857

AgT3

Energy: -6734.000432627332 Eh

Ge	0.50066828608298	2.60491247784651	0.39362470651086
Si	1.76163500975425	0.60052053161450	1.03223597635032
Si	-1.94457566768007	2.45748438765024	0.00922176265010
C	3.56847179389426	1.14046944839875	1.11789356040183
H	3.68110020164330	2.02639141219290	1.74261579884035
H	4.20258967182136	0.34724589829994	1.53163606207193
H	3.94216446428383	1.39588085527142	0.12175573279265
C	1.35874244743886	-0.25496723904076	2.73274636164450
C	2.08690818771517	-1.60486311822734	2.85292963401878
H	3.16488490676082	-1.51548860757753	2.67869960564597
H	1.95276249398374	-1.99855956559048	3.87097676763048
H	1.68815911215540	-2.35289479399495	2.16114186970298
C	1.86241357749734	0.65597731838926	3.86255390739558
H	2.94413200955880	0.81884722828218	3.81207553719999
H	1.36700796514756	1.63162304947017	3.84327574801646
H	1.64400238737560	0.19057737163273	4.83454536851773
C	-0.13698653345105	-0.48738730835000	2.96714475036864
H	-0.67908098414006	0.46378166110887	2.99152513206029
H	-0.58647165433398	-1.12874377247907	2.20291148361306
H	-0.28954901704484	-0.97690771722754	3.94008529237027
C	1.67291084821578	-0.59627336068541	-0.50381376286790
C	2.88779212131771	-1.54314878741881	-0.51173154100657
H	2.93597084769608	-2.18509964749759	0.37141065550882
H	2.82476995062467	-2.20085047636920	-1.39101407961785
H	3.83222276193161	-0.99426721502345	-0.58407743374681
C	1.73017939081416	0.22969111716520	-1.80003167644751
H	1.78864379970599	-0.44614959016366	-2.66604709471403
H	0.84033549871756	0.85495298238651	-1.92041167942962

H	2.60256723461736	0.89335022564017	-1.83231498760309
C	0.38759973196371	-1.43176290697046	-0.51568739499263
H	0.33346070970292	-2.02985527510066	-1.43706803080300
H	0.34032315465867	-2.12756195792449	0.32842127655684
H	-0.50206187416286	-0.79648064527698	-0.47951351130658
C	-2.53142259440893	0.73391666982160	0.53330745130129
H	-2.45773515805846	0.01740469951982	-0.28964808271515
H	-1.98351718519117	0.32873769862780	1.38169271095185
H	-3.58913297618178	0.78936498749368	0.81663803259267
C	-2.66590204929077	3.69255840730989	1.32614708636540
C	-2.66443101991704	2.66357444562581	-1.77647326779188
C	-4.20411865991578	3.68842469865099	1.31923395741000
H	-4.62487645244834	2.68628269207693	1.45571975550272
H	-4.57244902568292	4.31100356672177	2.14758863271373
H	-4.61178176798919	4.10968228983916	0.39477036315629
C	-4.09250881273049	2.08803321751091	-1.85187340096971
H	-4.78478808525100	2.57875241700764	-1.16189276185241
H	-4.48297058938353	2.23456445292195	-2.86943503229998
H	-4.11468890345447	1.01372145181665	-1.64643899801118
C	-1.79269143296504	1.85062311702091	-2.74691829528262
H	-0.76479681003634	2.21583231724806	-2.77985588490227
H	-1.76031268171832	0.79026875621208	-2.46819542052837
H	-2.20579145861082	1.91031181122489	-3.76446443271764
C	-2.71773770924977	4.13108353965509	-2.21690378216419
H	-3.49568770203547	4.68224341032011	-1.67822872943595
H	-1.77101277654782	4.64871683429552	-2.04290695936367
H	-2.94744228649514	4.20289405659752	-3.29011308952802
C	-2.18513318033388	5.13206908722632	1.11190873618503
H	-2.62122372571821	5.58048111387757	0.21478683441233
H	-2.47552565774365	5.75857021843377	1.96785507317361
H	-1.09546074637924	5.18014591242971	1.01911095228763
C	-2.19250101709938	3.22012336422502	2.71344374159707
H	-2.54792784890718	2.20966092305252	2.94523217098817
H	-1.09763905672847	3.22420053850499	2.79121830332383
H	-2.58368646824846	3.89597312347619	3.48742339593350
Ge	1.89132718091988	4.45471908179985	0.02233952174852
Si	3.25525910230168	5.19227574456263	1.96131858850115
Si	1.73565203729422	5.56805041774428	-2.16998008388020
C	2.52242010828259	6.92673211998466	2.44081497998101
C	2.73496897680482	4.06072732886078	0.38596933123238
H	3.25811368381850	3.10406925339101	0.39170837518140
H	2.94033610595249	4.54361424553698	4.34808022607602
H	1.66357984226850	3.85221786792429	0.32730102758079
C	5.21747469766265	5.18776253673416	1.89860669878856
C	3.15802084640170	7.46981860833163	0.73205023207770
H	2.68333622256917	8.42727230043709	3.99155597034510
H	3.00608986312492	6.79492776286360	4.58139921604780
H	4.23064783928691	7.65694431365627	3.63581250004602
C	1.01411983775002	6.77000274689039	2.69756244474390
H	0.80167617821105	6.07405911861888	3.51595742099533
H	0.58177873987736	7.74464706284034	2.96668476839853
H	0.49098639244945	6.40511601906564	1.80863059462787
C	2.70768009060740	7.94091618770579	1.30812888397084
H	3.75812638751653	8.18140511795214	1.12222425819394
H	2.28370793589867	7.54824763742205	0.37904567098156
H	2.18511382666754	8.87993363086179	1.54279313609955
C	5.86430229090391	6.52932131750014	1.50921369190722
H	5.58240282750607	6.87153495914281	0.51157521503199
H	5.63450638279822	7.32879154358137	2.21793816407150
H	6.95675766841886	6.40462981096565	1.50967256085177
C	5.72391867463041	4.84023512680202	3.31459078322418
H	6.82271042309244	4.87592094342021	3.32197105647295
H	5.36725552949405	5.54816695617945	4.07082014109947
H	5.42652690840461	3.83495964209202	3.62699024032175
C	5.74654945609710	4.11630153213271	0.93290963754688
H	5.39141273195609	3.11575208557526	1.19066488042222
H	5.45613083761204	4.31751764280528	-0.10254011225656
H	6.84544580227167	4.09695719361739	0.97322213584445
C	0.75014059197219	7.24209660981692	-2.36527149081311
C	1.60194772506115	8.51810088805570	-2.26518772704391
H	2.34260408778510	8.58843815815965	-3.06637647312258
H	0.94342418029424	9.39403135876580	-2.35665635032071
H	2.12655150492466	8.60831618895006	-1.31153374168079
C	-0.35166036726374	7.31779749188548	-1.29832965122346
H	-0.98610795895135	8.19834617470079	-1.47621222275773
H	-0.99896078213457	6.43631122141443	-1.31501888852952
H	0.06270082395447	7.40059218392377	-0.28839672395315
C	0.07759114788866	7.24471079293694	-3.75318033034508
H	-0.46402253798749	8.19142724541662	-3.89174426284171
H	0.80645115364572	7.15998868950218	-4.56705807250384
H	-0.64732182727981	6.43237125763568	-3.86351452039548
C	3.55961271305566	5.64470821451204	-2.81921540782353
C	3.62910766154187	6.20558298905606	-4.24923746262865
H	3.30028444409372	7.24694970395463	-4.31044871323656
H	4.66965034320546	6.17197852069145	-4.60398422027889
H	3.02876781226033	5.61802188879799	-4.95237699423836
C	4.43432875144528	6.49231521654637	-1.89282473033864
H	5.49182681143427	6.42748783383322	-2.18891916493324
H	4.15024314883605	7.54892704696371	-1.89717983910357
H	4.35555087195882	6.12969404420925	-0.86417132909695
C	4.12260636201905	4.21116682930778	-2.85082541753708
H	3.60239528773868	3.58730089511655	-3.58508959677435
H	5.18597326690869	4.23685734200981	-3.12951279449593
H	4.04105463559569	3.71395025120861	-1.87617162386139
C	0.91070928091522	4.28403562562288	-3.28695969931290
H	1.30605354166777	3.28757014486821	-3.06989763076239
H	-0.17100802774452	4.24732795894976	-3.16335150136652
H	1.10917092876072	4.51218567301045	-4.34073043262068

AgT5

Energy: -7582.557187425953 Eh

Ge	-0.01977615713869	-0.02082401457343	0.01171913740199
C	-2.03509129659921	-0.01220351383422	-0.00716071239783
C	0.71714856437146	1.85293181792629	-0.01026434817432
H	-3.20293194725218	3.39433991234530	-1.92567835556404
H	-2.70499641976994	3.27263744842591	-0.23517925201529
H	-1.51066252668523	3.10729822357549	-1.52768536449744
H	-2.59765026648068	1.16758608308379	-3.80140329002211
H	-1.55736387298935	-0.09858513116163	-3.13068903951463
H	-3.29170749679780	-0.38846316316077	-3.34083012242789
H	-5.25060698293529	1.34186750840657	-2.06522706949715
H	-5.15535530765411	-0.12151704220346	-1.07578498739165
H	-5.18805614442236	1.47608135671844	-0.30543215098729
H	-4.75800992263203	-0.82880029375866	2.86228804507302
H	-5.28952169544296	0.04196310671572	1.41865137260995
H	-4.56620688322788	-1.56506054017138	1.26995261416307
H	-3.05925471669098	1.95682981149672	3.39094182398182
H	-1.89985120402206	2.44415092851544	2.14778042268533
H	-3.63291930363674	2.46283835079767	1.79892255405187
H	-2.22435077591039	-0.76017141196922	3.98993456289525
H	-1.91969194735541	-1.98411528681660	2.75104051161640
H	-0.74015166063593	-0.69973362881230	3.02884072551823
H	2.36414944479500	4.21010543209206	2.82212797269098
H	2.62383232221049	4.52421766113984	1.10525243253314
H	0.98203521911796	4.53841642688860	1.76599985935911
H	1.61186839104686	1.80418843123246	3.94545864264789
H	0.01400656046346	1.63142688549315	3.20726789158477
H	1.20573483109600	0.32596079047796	3.06982803813215
H	3.95601636498107	1.29709754693999	2.36760862210693
H	3.56582144630290	0.51587703862387	0.83774955845120
H	4.24286812232601	2.14968959340240	0.84584531646103
H	3.52176308767030	2.60821248818299	-2.87319329656340
H	3.82692807794390	2.97912565555806	-1.17478473590158
H	3.56014330068523	1.30652280255233	-1.67975601004359
H	1.38391733011916	4.87535603993381	-2.60712685192735
H	0.05535138530407	4.73434180445537	-1.45196335624971
H	1.70411820750184	4.98566914383273	-0.87277576106182
H	1.11958713187150	2.31388765901068	-4.06189072202887
H	0.55831771719268	0.85457042113495	-3.22843387167000
H	-0.46906783350115	2.29141786081034	-3.29336109397875
H	-2.24963040860979	-1.05659024271790	-0.29388386139904
H	-0.19365895425356	2.43987990710226	0.19719676023297
Si	-2.92316203234650	1.02236746938669	-1.32937182223043
Si	-2.77118186235866	0.11496848987233	1.74294482449181
Si	1.81297492078857	2.17813916962229	1.51164898008578
Si	1.38815427943111	2.60067520996297	-1.63082211299624
C	-2.53332257982750	2.86485759286400	-1.23654486672724
C	-2.54705008120649	0.36307946136613	-3.05900741344285
C	-4.80280874258016	0.91177072188095	-1.16044503323724
C	-4.51283430443448	-0.61514625479319	1.81481779394590
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H	-4.52904051566866	-0.31461171861599	10.28963208244742
H	-2.81492934413020	-0.76806677292591	10.34414888630414
H	-3.72528287583784	-0.98099309063817	8.84958222776143
B	0.33450536923245	4.86377040491293	8.81460085486307
Li	-3.21594472350662	4.10036253657265	10.71836205208922

A

Energy: -925.88458947 Eh

C	-0.73141786028157	-0.71088848941938	3.29598699426037
O	-1.19231295230013	-1.22043537210293	2.26868201697425
B	0.61985928169994	-1.29297258041109	3.89710209025885
O	1.33749936152234	-2.31715069176105	3.30485551746022
C	2.42212493765578	-2.51965899713677	4.13299600797316
O	1.22036425425723	-0.85122132251498	5.06513994483015
C	2.35240211739349	-1.63098595056829	5.20266374366299
C	3.30624307405761	-1.60001746842740	6.19959337600177
H	3.24179399890565	-0.90309732779531	7.02832477336250
C	4.35435421167274	-2.51622778615160	6.07545518718745
H	5.13191437231051	-2.53380576094617	6.83265841765151
C	4.42489606520655	-3.40876275418991	5.00125219276340
H	5.25598353663618	-4.10465823332442	4.94301849690879
C	3.45146438942573	-3.42921235646694	3.99855719357002
H	3.49699652418938	-4.11782542479460	3.16167251830127
B	-1.51263448609596	0.50204282673457	3.96298391943439
O	-2.70368149109957	1.00285242715050	3.46735097028191
C	-3.03833675220216	2.03713560024612	4.31656264664762
O	-1.09530215091483	1.18847898185701	5.09184153616389
C	-2.06274075330634	2.15185747807846	5.30351051002567
C	-2.12861867690105	3.10567957005154	6.29885755806414
H	-1.36253451452840	3.18595342646233	7.06261190047909
C	-3.23688830162241	3.95627127186223	6.26196165788909
H	-3.33725830227127	4.72471554900345	7.02206057290781
C	-4.21709566481393	3.84124530124819	5.27143509292383
H	-5.06198319173466	4.52275784225924	5.27933577798726
C	-4.13759552380452	2.87050962382085	4.26917265345167
H	-4.89259550305632	2.77371061723635	3.49635673257686

AltCO

Energy: -5931.10079758 Eh

Ge	0.42899493465522	-1.06360989123466	0.06298513354682
Ge	2.34352632212455	0.07630747920904	-0.70844492607182
B	-1.23043809800455	0.10676348755790	-0.10014577232413
N	-1.16791859336825	1.52346325737180	-0.37271117512097
N	-2.64796943703421	-0.16578156787016	-0.03460854877070
C	-2.46011761946402	2.03072836176810	-0.46231287905608
C	-3.34422380764037	1.02252045574636	-0.26208724759699
H	-2.64878149730725	3.07630732267721	-0.66517306245515
H	-4.42505339682473	1.05065981799835	-0.27517085133777
B	0.61238771797574	-2.88278196068304	0.98973687695426
N	1.09216630138914	-2.98058198233631	2.34328144113987
N	0.58447852072088	-4.24232021075616	0.51411828421887
C	1.33174407920434	-4.32766962809219	2.63809232565720
C	1.03532432641307	-5.07559173024027	1.54901389982017
H	1.70546444532767	-4.64293515952036	3.60302188019623
H	1.11712059799031	-6.14563534695782	1.41457854701149
C	-0.03507178523613	2.37735894914107	-0.53599037288939
C	0.60075200737520	2.89466839956342	0.60160322296864
C	0.39800874328378	2.68064237899703	-1.83430105156468
C	1.69725024563985	3.73780613147574	0.41252942066113
C	1.49491078029926	3.53184799901003	-1.98062218869671
C	2.13951334521638	4.05638341211086	-0.86668785507885
H	2.20640539748336	4.14628703446203	1.28166127333924
H	1.84985588261185	3.77227914633040	-2.97943393969624
H	2.99492566012595	4.71359317421109	-0.99557794620992
C	-3.38836925800233	-1.36324582297714	0.20065907736529
C	-3.46209125530328	-2.34424680967887	-0.80020001876251
C	-4.10551179984238	-1.47846867107686	1.40306375569718
C	-4.30094864635667	-3.43945089547971	-0.58414395994144
C	-4.91344149693179	-2.60175032329941	1.58726332625314
C	-5.02345857611325	-3.56842216247471	0.59505567630122
H	-4.37833466984693	-4.19881246550912	-1.35739523345400
H	-5.46653932207292	-2.70806358743924	2.51727549775306
H	-5.66794718700578	-4.43029972770669	0.74537436480119
C	1.03797551272088	-1.96908081640994	3.35525791035116
C	-0.21475741182103	-1.69948552416153	3.93600847446119
C	2.19244022574288	-1.28524949373560	3.75659699861533
C	-0.30230488690575	-0.69493815056118	4.89897598880119
C	2.06338535754567	-0.28767445423977	4.72938347671580
C	0.82976466460079	0.01389166412017	5.28884049840818
H	-1.26616125726310	-0.47747989699660	5.35264782105698
H	2.95132634907907	0.25383230994295	5.04686095454941
H	0.75057475610533	0.79328027767290	6.04179610474391
C	-0.03637576474963	-4.80281078720021	-0.64837070728402
C	0.61799252471357	-4.78389606626752	-1.88861949970828
C	-1.29746376675392	-5.40548501969778	-0.49549566062926
C	-0.03370757331575	-5.34661145932481	-2.99011326999137
C	-1.90682026221278	-5.96863338157032	-1.61750242703399
C	-1.28526791407988	-5.93368047758420	-2.86007417496309
H	0.46386282378509	-5.33495198159583	-3.95661089366531
H	-2.88200090399221	-6.43654995414378	-1.50861670532046
H	-1.77280643928962	-6.37334039262916	-3.72589168923947
C	-1.42871896051627	-2.48736790528671	3.53493909178741
H	-1.72153648189248	-2.27413334567916	2.50011219166090
H	-1.23807548989926	-3.56479188491478	3.59212687500913
H	-2.27772519959967	-2.24704620053973	4.17957264237319
C	3.54026460343755	-1.57320608311803	3.16189506725968
H	4.32813593022933	-1.39313925608876	3.89894734873721
H	3.62162914250930	-2.59931948882552	2.79795783585271
H	3.72773997658994	-0.90883324972943	2.30891899319547
C	-0.27980271253005	2.07201279993681	-3.02928611652992
H	-0.23380593313902	0.97686205038390	-2.98241204330897
H	-1.34037735667306	2.34308834417480	-3.07485935991917
H	0.20187754944179	2.39928102954961	-3.95375024348678
C	0.13208446526777	2.53245191941168	1.98178525613129
H	0.66838836670499	3.11369000872851	2.73595549946255
H	-0.94280341564013	2.70717480222407	2.10040907320381

H	0.30762422137682	1.46810181035781	2.18583296278397
C	-2.68022896834169	-2.23036792554570	-2.07831667306380
H	-1.63764425239687	-2.54185415222669	-1.92912958543947
H	-3.10707290042355	-2.88107836769801	-2.84592794088350
H	-2.66011487226985	-1.20170486305339	-2.45138418769795
C	-1.98652585545748	-5.43869934128881	0.83874588713929
H	-2.04487131693276	-4.43456595131455	1.27237962223858
H	-3.00285399447067	-5.82372520065158	0.73437334780815
H	-1.44887737482640	-6.06712741411033	1.55694077643838
C	-4.02206883179946	-0.41942347601743	2.46826596357930
H	-3.00090489188617	-0.04078972264220	2.58063591090279
H	-4.65741376944228	0.44110616147663	2.22766701731970
H	-4.35533876621834	-0.82063159914172	3.42893984261703
C	1.99002538002096	-4.19927416639042	-2.04468777939852
H	1.95699442412872	-3.10328562679250	-2.02138657977523
H	2.65247743894476	-4.51579919818249	-1.23435980168615
H	2.42777473119079	-4.50290593231993	-2.99909874329296
C	3.21892970588333	-1.58423858568065	-0.23642101207439
O	3.88977858323819	-2.49889401892051	-0.00750152346941

AltCo_TS

Energy: -5931.07382438 Eh

Ge	0.38459031616465	-1.05944058757209	0.07941110862115
Ge	2.16384945607370	0.26349184656631	-0.62017337881520
B	-1.29578991567542	0.06636398234166	-0.06376072500313
N	-1.18361559881336	1.47358552038339	-0.36905379164513
N	-2.71997276413465	-0.15578839485244	-0.00588204533274
C	-2.46025720344680	2.02605096029705	-0.48552347595559
C	-3.37673487200313	1.05356844334876	-0.26289333432282
H	-2.61425204423049	3.07108230680490	-0.71799291682798
H	-4.45618164166078	1.11827563339692	-0.27821611986634
B	0.65457211793534	-2.86530726999828	0.98865034754011
N	1.10275969933637	-2.98992413222015	2.35297232054026
N	0.65530279891580	-4.21717700821761	0.48545807925593
C	1.34425177753839	-4.34168621844383	2.62554106158346
C	1.08159859618618	-5.06989542252137	1.51355834312280
H	1.69853334304856	-4.67495651140281	3.59186084995810
H	1.17592147959799	-6.13654821618239	1.36039314328873
C	-0.01394556161033	2.25902700612185	-0.56441152938698
C	0.60743480846437	2.85680727802864	0.55163037075534
C	0.44271241344844	2.49168179714952	-1.87654064685606
C	1.68195432743916	3.71613175419963	0.32440578921337
C	1.52294497916662	3.36424819018755	-2.05592171765256
C	2.12945648792272	3.97563745015895	-0.96844022071409
H	2.16795364604508	4.18965489293956	1.17323322778168
H	1.88295950986055	3.55747144100090	-3.06292944821266
H	2.96505640076343	4.65185739832961	-1.12489644824632
C	-3.48185758848375	-1.33065058542620	0.26078372025888
C	-3.59384565520871	-2.32115323308919	-0.72722123971996
C	-4.15656033089804	-1.43119002588127	1.48768314607054
C	-4.42588120222667	-3.41269715613328	-0.47158366850757
C	-4.96525625487012	-2.54751180456258	1.70982829977291
C	-5.10904457795953	-3.52596979287241	0.73316887100516
H	-4.53269110162552	-4.18106304131049	-1.23284354016429
H	-5.48795068258631	-2.64283691552210	2.65849427748745
H	-5.75015407252411	-4.38433602238864	0.91496363599007
C	1.01012596007567	-2.00306958652587	3.38594637127150
C	-0.25102162242203	-1.77606307846412	3.96338161852173
C	2.14172878132767	-1.29050227006424	3.80083071473900
C	-0.36963821914927	-0.78845922867234	4.94132424252576
C	1.98404836376327	-0.31194242938085	4.78730856839671
C	0.73992002082645	-0.05441991827593	5.34718820236170
H	-1.34203211725094	-0.60191910022960	5.39062898292767
H	2.85488886803720	0.25102733119021	5.11439684308837
H	0.63576800412270	0.71102388585607	6.11131947144493
C	0.04146703198770	-4.73772287573344	-0.69795493432090
C	0.71182477418232	-4.68119756404321	-1.92789625951875
C	-1.23446912898544	-5.31717083884725	-0.58588113042163
C	0.06594984326569	-5.18471016864155	-3.06049182636822
C	-1.83883511206772	-5.82220269619078	-1.73808969593739
C	-1.19905040572324	-5.75088954766875	-2.96987940444826
H	0.57593352586967	-5.14242410866224	-4.01963737457691
H	-2.82661935872331	-6.26973474383237	-1.66219147196601
H	-1.68424517102218	-6.14386315729139	-3.85916546966195
C	-1.44484132419222	-2.57843556640470	3.53346100086633
H	-1.73934347356012	-2.33034936796143	2.50652771222661
H	-1.22954961500765	-3.65236817097795	3.55030748547514
H	-2.29989758060263	-2.38107084677454	4.18492332745530
C	3.49024885474086	-1.52630181338879	3.18793293437925
H	4.28536725115988	-1.21984768028633	3.87315802422256
H	3.64106281344910	-2.57342868802202	2.91396740207724
H	3.59131399671642	-0.92936998180461	2.27165337178454
C	-0.25655470639173	1.87187188907939	-3.05279136998441
H	-0.47827797453685	0.81574570670741	-2.87145211770493
H	-1.21364338429432	2.37323763023570	-3.24342310017884
H	0.35789407744280	1.95550472754775	-3.95233576442388
C	0.11301549871962	2.57666245656929	1.93951883794868
H	0.64207694372193	3.19339668417699	2.67000510471388
H	-0.96222660268548	2.76755885742989	2.02534343926153
H	0.27172391655412	1.52083839461348	2.19755496150154
C	-2.85535408981835	-2.21201784360196	-2.03084564800035
H	-1.78612156770177	-2.42153189617207	-1.89594935365640
H	-3.24540733557380	-2.93334619729728	-2.75329282013452
H	-2.93237671071524	-1.20445042632972	-2.45286248930868
C	-1.94643981388608	-5.37787562064961	0.73531513314457
H	-2.02869300375413	-4.37957426695525	1.17854511302900
H	-2.95538917328067	-5.77568006462933	0.60876852673967
H	-1.41201240626985	-6.00511529012411	1.45677884849922
C	-4.00958926420891	-0.36804067377693	2.54105393015992
H	-2.96475622822581	-0.05545070118005	2.64678196254740
H	-4.58495497393703	0.53045872363187	2.28880743760632
H	-4.36616095446958	-0.73545428571542	3.50689998708855
C	2.09712844085307	-4.11605733725635	-2.03501145430364
H	2.08782668759962	-3.02698616638915	-1.90276743405592
H	2.75114823551960	-4.53088559026214	-1.26176629286071
H	2.52776928947155	-4.33639205229151	-3.01519533089626
C	3.75761237430062	-1.97162323781137	-0.10458892224831
O	4.51702874479949	-2.79552904110879	0.06734755395537

B

Energy: -925.81932214 Eh

C	-3.62206606384772	-0.18370403526730	-0.00792371667216
O	-4.93238856933718	-0.06347162668720	0.00827080316173
B	-2.88889011533983	-1.56903089519774	-0.02839631391845
O	-2.38175213709096	-2.13944871869483	-1.19283132432952
O	-2.36481075310879	-2.16315289550853	1.11633128910396
C	-1.51271254021666	-3.12260398925601	-0.75006071159623
C	-1.50230951358537	-3.13674304021056	0.64088192571015
C	-0.75161118965343	-3.99463678680190	-1.49948134383304
C	-0.73035917972457	-4.02372510177808	1.36105133735447
C	0.03945555066225	-4.89967448356626	-0.78192292743125
H	-0.76762228502795	-3.97549875404861	-2.58401330787952
C	0.04981413054706	-4.91388635914374	0.61355152409104
H	-0.73033061668811	-4.02677167219105	2.44585937690965
H	0.65861473529347	-5.60543268258662	-1.32689591228752
H	0.67681781055407	-5.63062319888828	1.13471702736723
B	-5.58963340161162	-1.31050258321446	0.00271926788205
O	-5.95427969640704	-1.95707363830682	-1.15417620050196
O	-5.92293411353169	-1.98404378546085	1.15371812386837
C	-6.53009264647292	-3.14084403227938	-0.70149664550380
C	-6.51114185707272	-3.15724745131638	0.68925303290379
C	-7.05382370394656	-4.17618657832237	-1.44317346659556
C	-7.01452382672125	-4.21001835411806	1.42041720479990
C	-7.57052925288219	-5.25376520839821	-0.71451816489639
H	-7.06188873247612	-4.15342188752240	-2.52752438371720
C	-7.55130876895231	-5.27031219203447	0.68096188910690
H	-6.99275691637733	-4.21294357423972	2.50481160894372
H	-7.99561763239433	-6.09590791570711	-1.25130836915299
H	-7.96169422459013	-6.12509896825296	1.20914336711264

C

Energy: -1851.87321201 Eh

C	-3.34832486424208	0.13434231582379	-1.58783467636208
C	-3.10506177776765	1.46098461351688	-1.59767495600276
O	-1.77516813283595	1.86197978118410	-1.68315057538674
O	-4.67612823972459	-0.26791563512964	-1.69708602655740
B	-4.15917544619005	2.59104324148007	-1.56052473361725
O	-3.79206919348047	3.92559228743330	-1.68203407512460
O	-5.52380433897631	2.44706503154484	-1.36147861363144
C	-4.97076555007418	4.63239494172148	-1.54635746683932
C	-6.01883626383037	3.73741941840938	-1.35341720113780
C	-5.16624023911507	5.99738069009878	-1.58427502707296
C	-7.32270660887514	4.15591703344954	-1.18799996327578
C	-6.48370964676672	6.43631066209924	-1.41715917481365
H	-4.34208658813327	6.68645105814369	-1.73510149909215
C	-7.53596648859040	5.53778201645082	-1.22394013375146
H	-8.13231355852965	3.44937158968286	-1.03909972346418
H	-6.69094628749109	7.50163887864798	-1.43873157979674
H	-8.54464295411522	5.91887640442831	-1.09862330873668
B	-1.19459569948604	2.54302435318710	-0.66557878097394
O	0.08576923550063	3.06957377055441	-0.76822965407851
O	-1.77409128244225	2.77894856922504	0.57765685480249
C	0.30826832727556	3.66486554093373	0.46089589128890
C	-0.81170755509937	3.49320087109544	1.27133339082203
C	1.42856524268242	4.34005989494361	0.89449498213438
C	-0.87164572674695	3.98778166982139	2.55569286764219
C	1.38240809178450	4.84843432835846	2.19881938821401
H	2.29607264676759	4.46887706207412	0.25591717594962
C	0.26029915522422	4.67635596665725	3.00948027477897
H	-1.74970476866833	3.84817992030755	3.17735987140244
H	2.24156891219453	5.38846569509017	2.58439009190738
H	0.26082009249474	5.08504552794502	4.01527884991690

B	-2.29573082008638	-0.99443378210409	-1.50355018631125
O	-2.65968850715187	-2.33130401692294	-1.60725874426350
O	-0.93628541742406	-0.84570166887991	-1.27462015209306
C	-1.48451817440485	-3.03458535582989	-1.42908850163030
C	-0.44147475992717	-2.13533783146442	-1.22882865244733
C	-1.28833091606258	-4.39996349964351	-1.43464840139437
C	0.85796516694510	-2.54994862433534	-1.02323325535567
C	0.02462137254140	-4.83487856951131	-1.22661795333363
H	-2.10866968826625	-5.09223805235527	-1.59147013834958
C	1.07188354977111	-3.93216071344980	-1.02602601151210
H	1.66379247894428	-1.84025798023075	-0.86887080102552
H	0.23227391291619	-5.90033203669978	-1.22147986028659
H	2.07716306837520	-4.31023479712702	-0.86839272321691
B	-5.28179658891040	-0.92731929354158	-0.67983950316635
O	-6.55996059609263	-1.45497556985363	-0.80214810445062
O	-4.73270954450038	-1.13710423368352	0.58177107367425
C	-6.81274321165973	-2.02386224486698	0.43358778364942
C	-5.71245461306080	-1.83577543170769	1.26703084803879
C	-7.94416152894047	-2.68863416926104	0.85425258344622
C	-5.68446781252306	-2.30240018352910	2.56290695720495
C	-7.93034948955831	-3.16882215435941	2.16995807357646
H	-8.79613656040491	-2.83033491384106	0.19774192675133
C	-6.82804491835346	-2.98048177474844	3.00374775309818
H	-4.82164059569548	-2.15005240799041	3.20264988782947
H	-8.79931441792892	-3.69973446600933	2.54611203400898
H	-6.85348531128433	-3.36696633723261	4.01781781841511

CO

Energy: -113.30818479 Eh

C	-2.10091442505908	-2.73860000000000	0.03590000000000
O	-0.97068557494092	-2.73860000000000	0.03590000000000

CO2

Energy: -188.57583811 Eh

C	-2.75423810626167	-1.29955982184698	-0.00000400782435
O	-2.75360502520709	-2.46274592275283	0.00006307708683
O	-2.75479429853123	-0.13637261540018	-0.00005906926248

I1

Energy: -6630.36265007 Eh

Ge	-0.23350789273348	1.62654366728895	0.05914414473345
Ge	0.86246380067753	-0.38056942815373	1.06580997566996
C	-0.41142124178148	-0.25560924808853	2.77826569773185
O	-0.76461761131285	-1.14969036644953	1.75575914002494
B	0.65454205744416	-0.69167967002680	3.78837216561191
O	1.23000727826434	-1.97577481492450	3.83913027409761
C	2.14108301640575	-1.92412686675862	4.86532733132358
O	1.17020570449973	0.11619305598263	4.81758096769576
C	2.10090795232267	-0.66323263715382	5.45991849925970
C	2.91513134740416	-0.32866480441723	6.52257955059289
H	2.87460199323928	0.65526211712786	6.97890160500223
C	3.79195040241591	-1.32242226813872	6.97749501973023
H	4.45209269241378	-1.10353372211836	7.81124208201841
C	3.83266578824218	-2.58361084776074	6.38258913482781
H	4.52452780331729	-3.33008641815606	6.76065887186865
C	2.99836634264819	-2.91161573603084	5.30584038373584
H	3.02223715924512	-3.89013739226848	4.83733517809272
B	-1.32227918391738	0.95388319240391	3.03198627757344
O	-2.58758706252891	1.14229331895675	2.45029134434384
C	-3.07158377020579	2.31152648771870	2.99793884094933
O	-1.05626141794639	1.97183681517894	3.96235246545387
C	-2.14702350302955	2.80873354335742	3.91264440576041
C	-2.36316693249455	3.97784012639494	4.61383539570928
H	-1.63448906984629	4.35445011390560	5.32437872283913
C	-3.56708188089885	4.64548651626582	4.35774961894120
H	-3.78127403668838	5.56994649571898	4.88567929267427
C	-4.49181269053911	4.14843429056169	3.43841501280053
H	-5.41363365620893	4.69377431779768	3.25850558613376
C	-4.25889407847410	2.96184632118754	2.73332305600172
H	-4.96621883167133	2.58017813942123	2.00593041120364
B	0.91815813730197	3.30429198989759	-0.10563988590985
N	2.28387688447235	3.36368155402767	0.37048283472289
C	2.76012301807425	4.65320559673278	0.21900401656735
H	3.76126910950192	4.93278668658662	0.51906887493399
C	1.78001792905953	5.42811358576219	-0.32960553926560
H	1.80444945255753	6.48078750976296	-0.57854420260884
N	0.65190001847127	4.65475513351220	-0.54159905825519
C	-0.52055675403995	5.20281281045357	-1.15151521809701
C	-0.58669148859962	5.24437007166212	-2.55010309327927
C	0.57190567630776	4.78488294341273	-3.39096736325020
H	0.28436307917555	4.72220014952106	-4.44343879999418
H	1.41320365100768	5.48366524548051	-3.30965625969886
H	0.94326733393126	3.80579538610344	-3.06894875211926
C	-1.43390279422015	5.66555262025127	1.16007839791409
H	-0.48193001400438	6.08628144929931	1.50139319070485
H	-1.49135349346074	4.63511551659598	1.52786909583991
H	-2.25049855327437	6.22819998101983	1.61910845666829
C	-1.54699738432400	5.69593864132499	-0.33655808338080
C	-2.68574376829561	6.20592213875921	-0.96301178568361
H	-3.50062201213076	6.58253330151195	-0.35002596382532
H	-3.68805221977352	6.61905746281927	-2.81840816246409
C	-2.79005726755612	6.22661141773429	-2.34901507842536
C	-1.74650406343141	5.75451557678556	-3.13752845011290
H	-1.82315916440080	5.78593420918465	-4.22154695598162
C	3.09075165842806	2.32801485987601	0.94376267156105
C	3.88461990744057	1.54230444891879	0.09743755111386
C	3.91722513599742	1.79838494718570	-1.38253055489913
H	4.32969446297294	2.79007999973244	-1.60321858128749
H	4.53248498178400	1.05085580494565	-1.88925317994883
H	2.91095383126284	1.76905029008479	-1.81348701722669
C	4.65440881839030	0.52962559772844	0.67260905379927
H	5.26948448365874	-0.09645394431955	0.03141774370144
C	4.64179332773348	0.32141619439813	2.04714834478109
H	5.24165950316925	-0.47331115550704	2.48182000399021
C	3.86365843903494	1.12688437628798	2.86948808448367
H	3.85945303917105	0.96382764648959	3.94391179209826
C	3.07306884892067	2.14637336857574	2.33365965972879
C	2.22292858561508	3.01344103863622	3.21545264778008
H	2.41179798505237	4.07728329612734	3.03498120513390
H	2.41229680976945	2.79280582220116	4.26798110969765
H	1.15769377663989	2.83724013612986	3.02827243329072
B	-3.03052344250198	0.82883757475658	-1.17001928086252
N	-2.46740799214128	-0.21121358458936	-1.98391868878823
C	-3.50261752480150	-0.99758057023984	-2.47760478095601
H	-3.32635899167664	-1.82473041539170	-3.15052824237478
C	-4.68334799503698	-0.51549570569746	-2.00531578199313
H	-5.68532550822765	-0.87985413990366	-2.18671552876219
N	-4.44713538885578	0.60193503767189	-1.21006740376212
C	-5.50975040081099	1.25878519054184	-0.51691644064793
C	-6.10052818374089	0.60947484984697	0.57769143034201
C	-5.57441103576145	-0.70760791126023	1.07575966464562
H	-6.03531630121145	-0.96325284189625	2.03277499842294
H	-5.77785806282055	-1.52216830991914	0.37159314099717
H	-4.48779936874613	-0.66618684975912	1.21329187488237
C	-5.27358778875920	3.20345658980616	-2.11720709584094
H	-5.14629979678756	2.52233107896684	-2.96534151319522
H	-4.27819778729947	3.56675746504778	-1.83420922299171
H	-5.86555093530785	4.06241024614513	-2.44390865987288
C	-5.93546197189273	2.51966192977617	-0.95551239720940
C	-6.99062806490332	3.12841738876705	-0.27258269301947
H	-7.33516645506953	4.10679351827812	-0.59759695888472
H	-8.42648604438914	2.98237527606461	1.32083962442127
C	-7.60412352904359	2.49644662633215	0.80316314963391
C	-7.16105161941502	1.24765186414012	1.22414754956972
H	-7.62550066986416	0.76485310086812	2.08009817654098
C	-1.09630231079989	-0.41170581861934	-2.29944876291714
C	-0.44727841900925	-1.57944618176336	-1.86432904867363
C	-1.17188699455094	-2.63553302339362	-1.07962664850441
H	-1.78325360110359	-3.26862102169149	-1.73302729870261
H	-0.45665422186399	-3.27849772438987	-0.56095985711269
H	-1.83291829014050	-2.18741776455585	-0.33271005391330
C	0.91199640671309	-1.71648254583157	-2.15250018451833
H	1.43472859258616	-2.60523264055256	-1.80932775579172
C	1.60370633738464	-0.72732167740897	-2.84289138829565
H	2.66394224155729	-0.84899694103006	-3.04468808346807
C	0.94022259578217	0.41147191807077	-3.27975580092070
H	1.47209558201543	1.16746097765344	-3.85213236044188
C	-0.42674680258003	0.58624412082512	-3.03273163952868
C	-1.16723207249745	1.75355554367674	-3.63288473566712
H	-2.14562491603097	1.44157973693040	-4.01176423850045
H	-0.58959196142711	2.17326836626730	-4.45993397341304
H	-1.34498457135549	2.56152738887991	-2.91428795596508
C	-2.21978715284827	1.92754077684828	-0.41403412504126
O	-2.70017437841945	2.95495030721556	0.04944531588171

I1a

Energy: -5931.08108759 Eh

B	1.70582234957849	1.09801561098356	-0.47008175080224
N	1.56547326482236	1.35530025625018	-1.89518055448826
N	1.70852813458328	2.44098278982792	0.09759194384539
C	1.50823050632734	2.71796415774144	-2.11457847887237
C	1.57057840655760	3.36994255270562	-0.91806269315943
H	1.42875185191476	3.13606267757153	-3.10954194603927
H	1.51818510624592	4.43235122286107	-0.72141897913201
C	1.72639147919385	0.43129880400540	-2.97707410814813
C	2.99951528522685	0.29845447991262	-3.55315611996319
C	0.62525159190020	-0.30541895708463	-3.43198418507400
C	3.15537278745082	-0.60518131869881	-4.60568808548094
C	0.82385219076750	-1.19767053480447	-4.48835719081857
C	2.07642308390040	-1.34843040126373	-5.07056941837352
H	4.13608980349713	-0.72568831400686	-5.05874938075504
H	-0.02012736117124	-1.77694437521855	-4.85419992138037

H	2.21318319805511	-2.04809160691822	-5.89046899050671
C	1.78970898059225	2.84331353381671	1.46933546522174
C	0.62857286056299	3.27265629113140	2.12958594349303
C	3.03792661572522	2.81771525855709	2.10848516185318
C	0.73141571233592	3.63118549165615	3.47531332835023
C	3.09583841956809	3.18198995136402	3.45541526176856
C	1.95179563981183	3.57797725395966	4.13747033983241
H	-0.16305690040361	3.94959405722769	4.00505524929851
H	4.05503674951652	3.16107967496029	3.96652416743572
H	2.01366057886703	3.85661333080647	5.18600147384255
C	-0.72261920983674	-0.15608375436816	-2.79323498957571
H	-0.71746458470365	-0.58064085978816	-1.78315187059263
H	-1.00908767979992	0.89447664380909	-2.68347802237076
H	-1.48897747383243	-0.67228799191210	-3.37746640212684
C	4.16661423992806	1.10005475973457	-3.04839347079473
H	5.09499286421237	0.76190841288025	-3.51494538594157
H	4.04388150335692	2.16756144678244	-3.26497748625882
H	4.26810091570422	1.00773468558974	-1.96064882894894
C	-0.69110833323816	3.35852452725521	1.41735509551403
H	-0.84449398605977	2.51831923514576	0.73528992456557
H	-1.51450145680381	3.37600361002029	2.13670760474771
H	-0.75448490945818	4.27575678715835	0.81868611425460
C	4.28352629020144	2.41719724872271	1.37351695977738
H	4.30992566222736	1.33129970914939	1.20711775871754
H	4.33541166549688	2.88821422787739	0.38646242989280
H	5.17264851984496	2.69439716158284	1.94564940418710
Ge	0.68045141921035	-0.37813609093348	0.95939247263299
Ge	2.73333171789627	-0.79414753041761	0.15545430364096
C	-1.36966936427947	-0.29886202456225	0.94976750300762
O	-1.98357922810256	0.46213038512632	0.21343949844086
B	-2.03430744849139	-1.36108655674565	1.87998098695524
N	-1.48193417843563	-1.97118294511972	3.05534996247308
N	-3.33513744360520	-1.94509835229278	1.73020989495212
C	-0.21978383868676	-1.73066561103663	3.68132289485980
C	-2.42244925394424	-2.86147396705432	3.56599665392669
C	-3.52612567680262	-2.85065659881565	2.76948565554299
C	-4.29491490702261	-1.75506097331213	0.68874259696585
C	-0.02002098880739	-0.52099743529669	4.36618358324961
C	0.78617861508007	-2.70379523119521	3.57873256648128
H	-2.24060312848697	-3.42691487159737	4.46952176898690
H	-4.43523467942596	-3.42963101990892	2.85963866479577
C	-5.41072408065141	-0.94509037899713	0.93401036198127
C	-4.07912608285850	-2.37230760297229	-0.54997922730362
C	-1.10858853722567	0.50946671574410	4.46860116494864
C	1.23354973256671	-0.28788071989728	4.93270862027315
C	2.02251676553685	-2.43174847766840	4.16399149596318
C	0.55749029026942	-3.97743151813033	2.81433770585732
C	-5.58835375991524	-0.26210648664594	2.26076302497704
C	-6.33494730250096	-0.76974513600499	-0.09708117441167
C	-5.02508708520981	-2.16971399103192	-1.55703306935160
C	-2.85716852597256	-3.21197969293119	-0.79684501027693
H	-0.87470905349403	1.23122516009128	5.25517240130498
H	-2.08023314429341	0.05198573604806	4.68117854063648
H	-1.20798357398588	1.06758131447475	3.52860083022860
H	1.41223230272173	0.65036054736920	5.45128922753767
C	2.24788235362114	-1.23167642195087	4.82894490810633
H	2.82083630984632	-3.16422446343786	4.07799313101871
H	-0.15025891728350	-4.63798147016570	3.32806287452538
H	0.13878068788998	-3.76947353854906	1.82305838470282
H	1.49736508489343	-4.51936205051588	2.68571283655813
H	-4.69073113729586	0.30664514366600	2.52909049512448
H	-6.43884662245762	0.42310943439903	2.22987135744849
H	-5.76009132683721	-0.98347716786358	3.06788265226076
H	-7.20538702411010	-0.14108575753453	0.07257478368993
C	-6.14514720550830	-1.37762110819379	-1.33304884773242
H	-4.87687856995480	-2.64213043284496	-2.52476888420806
H	-2.67838537192658	-3.91625252353582	0.02247302590356
H	-1.95922236016060	-2.58669222216419	-0.88164144354292
H	-2.96042423893250	-3.77566409955531	-1.72745188645664
H	3.22074918628810	-1.03101921454501	5.26879857301011
H	-6.87214477182122	-1.23034813047749	-2.12682122667902
C	29.69201904400484	13.30243269070393	12.26869652777854
C	28.30726629983194	13.27786253251212	12.05770838022305
C	27.84513543424447	13.01410779068006	10.76716966520890
H	26.77420810107187	12.99276965968641	10.58215826691823
C	28.73650584579438	12.78356359294805	9.72560530215321
H	28.36123218151225	12.58206365974802	8.72617009159814
C	30.10692524233254	12.81461508199283	9.95771168958031
H	30.80186519950766	12.64567573285815	9.13927659468358
C	30.60867997254612	13.07710076560153	11.23338627227327
C	27.34870740731081	13.55549113105532	13.18083473400205
C	32.08807768011236	13.15480853119372	11.48568661650570
C	31.20645515199709	15.40032846492350	16.62296230489061
C	30.42209133107447	15.28299704852160	17.78333135032138
C	30.72027203655772	16.10435177732182	18.87126411903879
H	30.11275736164256	16.03139914473513	19.77003417677906
C	31.76578342128128	17.01864126569679	18.81005979848617
H	31.98283348709809	17.65530080645060	19.66321754276094
C	32.53637867831534	17.11203758443898	17.65817574240225
H	33.36552043146247	17.81407718260075	17.61513784872035
C	32.28069659944207	16.30037383080451	16.54934992278138
C	29.26630980801369	14.32297734171126	17.86059049472003
C	33.15541764866400	16.39677988295849	15.33199136892864
C	28.48413875559012	21.38899514267957	11.70649189695690
H	28.24282018902434	22.37528069280233	11.33325708071486
C	28.10940821335276	20.80005804365652	12.86946858798443
H	27.49217606200713	21.19413166449158	13.66531879776044
C	29.84334126030945	20.83958762495747	9.71508718859410
C	29.13043891598171	20.53361259899104	8.54830680660916
C	29.69980376162562	20.87155544299656	7.31870119287424
H	29.16034592978910	20.64223101351143	6.40313843138305
C	30.94363174260224	21.49019700515951	7.25769149441609
H	31.37464143908836	21.74619993034374	6.29370037555418
C	31.63941203291661	21.77789965859115	8.42680884293354
H	32.61499681959933	22.25499753914643	8.37638866304974
C	31.10126386946465	21.45627415064976	9.67444924076450
C	27.79719992828460	19.84454285109893	8.62572908950846
C	31.85062785686507	21.74655164917687	10.94418353928154
C	28.44366189900238	18.66400766971796	14.04054828069292
C	27.31526207711233	17.81727284166662	14.05650957741079
C	27.05565966482876	17.08590998386913	15.21568247697331
H	26.18270311791057	16.43882147552642	15.24927152768100
C	27.89106375499219	17.18838170685734	16.32356559543966
H	27.66728892525922	16.62326212953508	17.22313599265408
C	29.01412862057148	18.00479874685868	16.28661161873355
H	29.67183517555331	18.06685998767654	17.14901247035332
C	29.31140366020321	18.75859818229548	15.14912930464742
C	26.42232080681807	17.72691227200367	12.85543226741131
C	30.48979689803327	19.68793146125428	15.12112527007208
H	32.81375572614925	22.21457687367115	10.72627099228233
H	32.02930440094683	20.82448607296434	11.50997930187834
H	31.28061062672057	22.41311603776194	11.60132480748524
H	30.16268982990472	20.73352477722164	15.17707365404905
H	31.05163877360915	19.57591562163086	14.18804451175961
H	31.15413772370787	19.48523006046604	15.96525641470195
H	27.34824575857094	19.75898846649259	7.63305808897762
H	27.10435055576072	20.38550775411641	9.27932854854829
H	27.90377518375245	18.83684993235916	9.04563152402572
H	25.99831264217743	18.70475689098059	12.60066971370926
H	25.60378067314895	17.02496606944334	13.03335336372504
H	26.99480667998841	17.38934237069233	11.98252517480448
H	26.32183309459119	13.34559113156594	12.87065522075795
H	27.40555117412728	14.60773620338335	13.48864159651691
H	27.57880538755216	12.95262538231473	14.06593013743269
H	28.71578294276693	14.28374111529201	16.91501549083673
H	28.57942016751758	14.62108223758978	18.65737689883475
H	29.60195185173201	13.30259639578434	18.07853049146341
H	33.34386766023521	15.41177404008305	14.89371080471085
H	34.11216153737983	16.85978036243898	15.58803159284268
H	32.68417950246518	17.00480992379164	14.54856743352423
H	32.64571635059281	12.99338942522665	10.56033619775002
H	32.41317054189937	12.41064239572840	12.22114561663670
H	32.36276848274229	14.13805052500370	11.88644661671806

I1b

Energy: -5817.76412651 Eh

Ge	30.13864214473899	16.55288701142242	13.06767111178272
Ge	30.50992398122104	17.60538140015573	11.13363202484203
B	30.37127295480311	14.87320887084185	14.20358328711218
B	29.42660414742303	19.27306776308312	11.72151414743532
N	30.18455221779239	13.58953878423589	13.58025597111519
N	30.90731555040917	14.56167121335885	15.50744151601966
N	29.28083653625008	20.49983376287820	10.98030067318540
N	28.65549533188140	19.51190261963924	12.92297164252117
C	30.61558150885912	12.59531096582432	14.45322169367477
H	30.59769502395352	11.54831290265749	14.18218488485085
C	31.03277049835740	13.17456498012598	15.60750491926255
H	31.42814309565940	12.70574269511197	16.49773951319336

I2

Energy: -6743.69847122 Eh

Ge	-0.78266631850286	4.73807688446385	-6.66102838362734
Ge	0.54794758033872	3.54100336507283	-4.86233179752852
B	1.83542253824691	2.31894075558609	-5.93124691879254
O	2.22152322110908	2.57396311872117	-7.25632746947865
C	2.91980332080811	1.46023034266011	-7.66647461535852
O	2.31562497644691	1.07383352474108	-5.52953432550243
C	2.97621300535000	0.54934904094530	-6.61740387147333
C	3.60609653901412	-0.67182694247089	-6.73917426957817
H	3.64989513148397	-1.37181235840610	-5.91104792588190
C	4.18722775737629	-0.94951113077288	-7.98198635178453
H	4.69343848919422	-1.89883205119679	-8.12871631918874

C	4.12871657507810	-0.03472980893420	-9.03609896937673
H	4.58639895463904	-0.28808079083862	-9.98750085891673
C	3.48804745717681	1.20165624301712	-8.89676594419317
H	3.42822980789485	1.91572490519864	-9.71176225584030
B	-0.54129241839449	3.13560629400206	-7.99789151310482
O	-0.60155827620681	1.80015076566006	-7.58392445453949
C	-0.32096988333610	1.04585898312240	-8.70227202313463
O	-0.29211698333285	3.20210736207787	-9.37235581743978
C	-0.13250714229827	1.89488740948324	-9.78743982094772
C	0.19084412471420	1.41942140145060	-11.04152100928886
H	0.34045495994231	2.08877153921759	-11.88243085100060
C	0.32600702799950	0.03130035379402	-11.16408164978023
H	0.58560129925031	-0.39033507077451	-12.13033231732660
C	0.13964734546457	-0.82013783856005	-10.07318396136774
H	0.26070457445714	-1.89082357483847	-10.20574945045441
C	-0.19371093164365	-0.32399508622749	-8.80772035806826
H	-0.33068001165630	-0.97496439982791	-7.95013359220996
B	1.67544840281850	4.83991722401046	-3.69883067231213
N	1.33098834834402	6.07277031070597	-3.03046553709593
C	2.49240957866599	6.63913308115592	-2.49110930317141
H	2.46333455978161	7.57782807989486	-1.95462909960687
C	3.54824389815935	5.83895726890840	-2.76440685356066
H	4.58864057633669	5.96321125923838	-2.49673822507644
N	3.10551668547748	4.73633939382090	-3.49772756475334
C	4.03092028251196	3.74608860517726	-3.94987379500486
C	4.50923853987550	2.79088261872878	-3.04288816355551
C	4.14047745882859	2.85617012938306	-1.58947544201144
H	4.42821199737018	1.93560544092899	-1.07832750154435
H	4.65141966181459	3.69348589702279	-1.09865141809335
H	3.06781744324355	3.01414068175376	-1.45333415676211
C	4.08425436282506	4.91124348299992	-6.19291471148195
H	4.57021063532140	5.84460032903279	-5.88192972516812
H	3.00788679202332	5.09315412356007	-6.16975126093356
H	4.37337273811923	4.69595221218993	-7.22419182195193
C	4.47833957419668	3.78601427914974	-5.27974962506850
C	5.35093234046901	2.78596643356167	-5.71463657944516
H	5.69052255039298	2.79206556234232	-6.74728211543234
H	6.44905799190123	1.01122752212772	-5.20336104931962
C	5.78433203167591	1.79229321842254	-4.84488332773074
C	5.37824033334052	1.80521493802209	-3.51607516071799
H	5.73775855630240	1.04394613514999	-2.82811750000270
C	0.12693867543423	6.84366306836102	-2.99704038659355
C	-0.73251511573989	6.74236857173429	-1.89311328158227
C	-0.49552878974766	5.72890550565567	-0.81093179073096
H	0.56425737701978	5.63852091434668	-0.55597606353900
H	-1.05711147394720	5.98780766047694	0.09058525000766
H	-0.83361970787002	4.73901532942857	-1.14224715395560
C	-1.84577881238455	7.58292546010953	-1.84060459263092
H	-2.51711967866324	7.51800783378831	-0.98773181890344
C	-2.11159746520070	8.47941600161085	-2.86866330066622
H	-2.98887473541540	9.11868865602385	-2.81841274184146
C	-1.25781715766872	8.55698624524224	-3.96173700797183
H	-1.46288166048426	9.25975922189654	-4.76552023874448
C	-0.11364735853901	7.75836299835699	-4.03348187195916
C	0.85807063540409	7.92633849078968	-5.16679473710521
H	1.65877016426284	8.62222304115437	-4.88530398286138
H	0.35781006276608	8.32850640450607	-6.05181880981530
H	1.34072811650397	6.98188395108850	-5.42984604562163
B	-0.92341278782526	2.33592046976715	-3.99872025762752
N	-2.35784412265250	2.35178083361570	-4.20730868665967
C	-2.94445773185980	1.35087587209230	-3.42540943302951
H	-4.01517578168957	1.19966776184856	-3.41431165494165
C	-1.97898449707256	0.69324345599826	-2.74797051611713
H	-2.06680046643042	-0.12793384905331	-2.04939307491587
N	-0.73358595282718	1.24718902229308	-3.06769386697190
C	0.43879537037554	0.55446380684201	-2.63141409891673
C	0.85789387918189	-0.57060915860710	-3.35707221880528
C	0.13781987901664	-0.99847224892474	-4.60402920351947
H	0.71409236838757	-1.75819406457649	-5.13906593863193
H	-0.84780858489238	-1.41759015764407	-4.36655993881940
H	-0.02730517809594	-0.15062945343607	-5.27598889706901
C	0.58721055697107	2.14406183454667	-0.68312300274609
H	-0.47873670171375	2.06367237704162	-0.44247177412367
H	0.70692333303727	3.05490553661219	-1.28126496799789
H	1.14796680941869	2.26796945544263	0.24720482169552
C	1.07056320200449	0.94377153691457	-1.44468504659997
C	2.14889900962767	0.18342631475020	-0.98813034964582
H	2.63984267062929	0.46561632815339	-0.06054712918016
H	3.43587411061126	-1.50253225857248	-1.33757807293556
C	2.59248783068265	-0.92275494579617	-1.70290500240963
C	1.95224413188164	-1.29328504807897	-2.88010723840614
H	2.29632916222328	-2.16169188922736	-3.43657989783121
C	-3.16678535123802	3.02857015260325	-5.17197367222765
C	-3.60901405847604	2.31989494294361	-6.30350666182449
C	-3.29818893702554	0.86220133215357	-6.50045303393383
H	-4.06017739103810	0.24056995112134	-6.01359497099644
H	-3.29425364388264	0.61262085249709	-7.56523485207024
H	-2.33093185945064	0.59144578302905	-6.07409552647219
C	-4.39201466444085	2.99721911954640	-7.24113361534626
H	-4.72090180071272	2.46832836608875	-8.13253664643564
C	-4.75930671749675	4.32325143478572	-7.04374160772207
H	-5.36874904301972	4.83394352436726	-7.78411554253056
C	-4.35593665145732	4.99085894559507	-5.89467335483053
H	-4.65333401158373	6.02328304933400	-5.72931896266970
C	-3.55810540483712	4.35536053476132	-4.94061090165510
C	-3.11638018935450	5.08540340224342	-3.71020661405995
H	-3.18088534125857	4.45368221197188	-2.81848471060534
H	-3.71832288794094	5.98343561621506	-3.55615621016916
H	-2.07168246699483	5.40660316287091	-3.80047352170305
C	0.76408565115946	5.41000310575576	-7.62408034793121
O	1.52756720691806	5.97529116588643	-8.27269977110375

I2a

Energy: -6044.39029175 Eh

B	1.79202748483513	1.27826211942330	-0.27366130403688
N	1.06832406940798	1.43404815305652	-1.52376350436613
N	2.09512393181993	2.65339773947649	0.10053744703847
C	0.97979077758231	2.78334456734591	-1.83251424127887
C	1.59293283467892	3.51213482460811	-0.86043336751260
H	0.49555306171581	3.12695315443170	-2.73670482129808
H	1.72054409498746	4.58409158409106	-0.79240230691551
C	0.52430090465804	0.46098760818281	-2.41888182313042
C	1.39046604109906	-0.25056113339976	-3.25937083214216
C	-0.86493770542694	0.27604208559603	-2.45298826613943
C	0.83576735545441	-1.20862166428977	-4.11117427875755
C	-1.37919473554213	-0.68732673643799	-3.32028332108049
C	-0.53602353795089	-1.43280111499430	-4.13527595491922
H	1.49229910731870	-1.77557860200189	-4.76635225748411
H	-2.45106459067833	-0.86855745257701	-3.33291445399555
H	-0.95130347864216	-2.18754983753889	-4.79751167300893
C	2.82144863933012	3.13987907730064	1.23194410770743
C	2.12127728883407	3.74747160605496	2.28753946683740
C	4.22103244296737	3.02990516706877	1.23803450770846
C	2.84987233544266	4.17284889843825	3.39939278788345
C	4.90985685093770	3.47312274687850	2.36986590063998
C	4.23114887377086	4.02526635671964	3.44848508653246
H	2.32123246235000	4.62839289725483	4.23285148678967
H	5.99381686123126	3.39310354004891	2.39176508102697
H	4.78214445508177	4.36006043635037	4.32296122090645
C	-1.77925811710179	1.06332477330278	-1.56032793297299
H	-1.43818460193683	1.03281410959249	-0.51798971270746
H	-1.81857341241011	2.12018216150960	-1.84830210117883
H	-2.79236517482540	0.65656182419420	-1.60536667431054
C	2.86960050844778	0.02338493519569	-3.27604494160218
H	3.33442599067913	-0.45141798622588	-4.14374898690309
H	3.07287052700746	1.09906898585183	-3.31426476827090
H	3.36708128715999	-0.35600499015107	-2.37524401677394
C	0.63703826582837	3.97128003341171	2.22134658935873
H	0.11644641475962	3.08697432397707	1.83982537644327
H	0.24176783850789	4.20610102202864	3.21307058380174
H	0.39743814106577	4.80901206310779	1.55509710532718
C	4.98112704315588	2.49458980437931	0.05562883917443
H	5.00791313594765	1.39805220973426	0.05785045259993
H	4.52035551671656	2.79973975107719	-0.88880288263929
H	6.01266995543365	2.85611127091511	0.07728542309806
Ge	0.62926064422715	0.23761885815572	1.74100319566937
Ge	2.77599400491180	-0.35169470372465	0.69683660116558
C	-0.56208995664508	-1.21320122756513	0.82462758618307
O	-0.37767945441668	-1.62230570114434	-0.32803353086012
B	-1.80054109180503	-1.69370828906053	1.65653850624458
N	-1.86519276653512	-1.71391495685699	3.09126574332538
N	-3.06715916912793	-2.21603861544709	1.22396632635657
C	-0.84296335013071	-1.34976013958832	4.01541459282648
C	-3.10293597428630	-2.22511293883291	3.47274765571407
C	-3.82574895541893	-2.50942142013267	2.35622519145093
C	-3.59557546231333	-2.35623612289418	-0.09564656499767
C	-1.00868643867643	-0.18887985307612	4.79201390947998
C	0.30929702706394	-2.14855914072460	4.11260360130774
H	-3.36619253968778	-2.37665500931986	4.51050106360955
H	-4.82597805078926	-2.91401829065549	2.28009457058750
C	-4.50567063303571	-1.39940912098144	-0.56652916933619
C	-3.19561463465073	-3.44874501728603	-0.87717252386964
C	-2.22232114844599	0.68021274340881	4.62692369269412
C	0.00876957461782	0.16230875077328	5.67707085475145
C	1.30981946052443	-1.75011522908302	5.00366722745975
C	0.47495981305583	-3.40379398586149	3.29961090050103
C	-4.90408073544169	-0.22542553547051	0.28415739812360
C	-5.02326280860806	-1.55874280861023	-1.85385010994834
C	-3.73633053531832	-3.57260847718777	-2.15838632215948
C	-2.20718979575378	-4.45082150830417	-0.35508308251054
H	-2.09676322710018	1.61908349138332	5.17132407013562
H	-3.13059695229447	0.19013444260945	4.99460052409697

H	-2.38914655882401	0.90851050833109	3.56748378748671
H	-0.09765977887641	1.06428127061757	6.27403663677265
C	1.16179132703622	-0.60859453811191	5.77982938306461
H	2.21033008773613	-2.35278077366389	5.08820698343949
H	-0.46665658538575	-3.95416140158241	3.21086459968041
H	0.81665963063123	-3.17744615574000	2.28170051333267
H	1.22225670034245	-4.05502302715741	3.76004309927293
H	-4.03022070108015	0.23854969726144	0.75475962965529
H	-5.41859663680402	0.52747982598079	-0.31842581162359
H	-5.57745956469355	-0.52743593726650	1.09492009715487
H	-5.72473563522913	-0.82201465896760	-2.23767515951914
C	-4.64469631872394	-2.63861610533889	-2.64336177646960
H	-3.43835788271576	-4.41442095531277	-2.77824188857621
H	-2.47932776474295	-4.79691403944802	0.64779713016497
H	-1.21052601433177	-3.99909588710264	-0.28645886193801
H	-2.14751276443581	-5.31556916784019	-1.02068070603808
H	1.95060967501808	-0.31449027776754	6.46628634607863
H	-5.05542394209331	-2.74953647486794	-3.64322979088528
C	2.00369890286760	-1.80661878627833	-0.43879026508273
O	2.03749696287013	-2.86714288364229	-0.88294415707856

I2b

Energy: -5931.08288685 Eh

Ge	29.45636586542975	16.21877440352287	14.96805249372915
Ge	29.48568392112266	17.71404693407011	13.17733426306247
B	30.79279447038359	14.81371944932195	14.17191753097426
B	28.68043315323672	19.38640860703418	12.37893968105133
N	30.77581975639706	13.96748406084491	12.99096222500309
N	31.84438524189264	14.24370670674972	14.97410791610396
N	29.00229750355126	20.02024287416089	11.13439395167124
N	27.61319229300863	20.16617868365771	12.92610252371289
C	31.75301715947066	12.97461164388736	13.13534915357397
H	31.91103495742949	12.21684807148802	12.38072971608275
C	32.39338446861168	13.14173302802378	14.31788701024628
H	33.20426015294606	12.56557312581822	14.74295355142200
C	29.96719796588846	14.04432110898243	11.82008554159069
C	28.57235605933809	13.90210408631237	11.93689341532183
C	27.78966652697570	14.02388177123522	10.78717577701880
H	26.71074589425675	13.91899484647730	10.87182967236046
C	28.37013983518354	14.25499867112044	9.54677880612566
H	27.74689843978782	14.34875391385183	8.66177233939309
C	29.75077905041467	14.35541002786077	9.44164903171193
H	30.21158672372039	14.52733973877376	8.47161597343924
C	30.57247842591783	14.24665305854728	10.56603651686483
C	27.91166737295537	13.61012502494156	13.25244345743894
C	32.06465130092614	14.33581171697687	10.38819390873790
C	32.28374162304394	14.67390373344606	16.26056421628077
C	31.80954091558392	14.00365552151826	17.39805836153035
C	32.23843604369350	14.44347069682767	18.65123674122386
H	31.87691239039211	13.93809903958114	19.54323248318706
C	33.11014639318498	15.52100708997021	18.76588560740619
H	33.43558317820048	15.85245211035341	19.74805751268193
C	33.56361157031620	16.17678151046421	17.62726168908463
H	34.24404301854471	17.01960097656699	17.71958954642774
C	33.15780076726992	15.76609576017084	16.35524199048722
C	30.83977654435482	12.86353247815799	17.26507411934533
C	33.63940572221235	16.48050877308677	15.12328807046882
C	28.16009646740814	21.12477872538363	10.97060830088841
H	28.21417276167532	21.75744577729279	10.09516322024450
C	27.33070304635111	21.21215924301363	12.04208369437127
H	26.55241098403993	21.93458105517599	12.24695979630550
C	29.97818299352278	19.61452959724562	10.17763323404068
C	29.65552768209894	18.58959976392264	9.27541387860752
C	30.64254199572504	18.16437984791417	8.38383003536732
H	30.41179198008944	17.36795753457627	7.68099716063995
C	31.90454039866496	18.74743310303706	8.38901526027676
H	32.66254263016823	18.40447655914413	7.69026833300174
C	32.20039906812156	19.76955401884784	9.28467091945785
H	33.18971482099870	20.21992115774719	9.28870526948588
C	31.24360041544779	20.21837111510426	10.19590876314213
C	28.29256367445447	17.95817659147971	9.28098340047151
C	31.56345217433483	21.29385159804869	11.19530845883753
C	26.91669582841240	19.96177662574870	14.15509257241101
C	25.85527464053234	19.04702567718106	14.18922147549259
C	25.20254952857640	18.84285345964689	15.40676216206035
H	24.37681740740956	18.13748255053377	15.45362572802600
C	25.60009938205162	19.52633568858810	16.55004344227724
H	25.08320432918096	19.35526253832271	17.49017147530437
C	26.66083571422043	20.42387895293702	16.49583576703754
H	26.97604270300243	20.94935626819827	17.39365726817794
C	27.33939352277882	20.65405248628247	15.29790605899065
C	25.44597140415380	18.29287960576713	12.95477455053229
C	28.50836950186597	21.59589808277576	15.23288057238134
H	32.60736447570903	21.60410109743556	11.10781168179223
H	31.38783857890585	20.94021404453522	12.21818537006793
H	30.92782126977711	22.17529459354479	11.05465288778800
H	28.32958457344245	22.41285789259924	14.52485670925742
H	29.40920542619737	21.07312822804949	14.88993700632616
H	28.71119538541388	22.02803616302607	16.21568508249038
H	28.15295404487968	17.33841803894011	8.39196620372385
H	27.50182835497043	18.71479886337708	9.31483471038215
H	28.16147929248263	17.31508718604245	10.16073609459596
H	25.33279021142270	18.96091300294548	12.09469079151437
H	24.50181682578000	17.76794201823150	13.12003361598781
H	26.20523044961650	17.54856012465535	12.68140418125758
H	26.93437888883512	13.14577859525130	13.09275134055014
H	27.73872800055325	14.53332980290052	13.82863809129224
H	28.52224581811091	12.95343154611434	13.87915281164284
H	31.27373102596656	12.02608119421830	16.70776868364506
H	29.94547093118008	13.17806722533419	16.71360946592574
H	30.53235137296886	12.50140697727666	18.24906467630374
H	33.98141694811203	15.77600351663751	14.35824356153342
H	34.45902094385925	17.16050400601373	15.36919878917235
H	32.83106693645026	17.06997874710029	14.67207092214972
H	32.30613660079379	15.02902441758829	9.57692647210292
H	32.48171825643595	13.35637831668292	10.12190853902881
H	32.57144098039653	14.66977995426147	11.29431711276514
C	31.02757084938353	17.40381737272487	12.09507022839588
O	32.05375556741978	17.15291185678998	11.63438461771371

I3

Energy: -6743.68157724 Eh

Ge	-1.89322122826005	4.51669856718258	-6.00775751281780
Ge	0.09869420789328	3.40049950900821	-4.89563744303742
B	1.53609910901081	2.57561401775740	-6.13052383865486
O	1.67990884294744	2.83961349488976	-7.50228809129511
C	2.86980648796219	2.24272543604773	-7.88021710340776
O	2.61076987556071	1.81026918387246	-5.68347714739752
C	3.42587648093167	1.61335215876782	-6.77242879369482
C	4.62393567571712	0.93113349146174	-6.84090727920179
H	5.04129348230992	0.43906459163632	-5.96906281534166
C	5.25949937682946	0.91526678169240	-8.08673119353789
H	6.20530962470709	0.39220355925802	-8.19121420317591
C	4.70611421326622	1.55888072943728	-9.19643665433412
H	5.23024551312907	1.53055034217204	-10.14691361173820
C	3.48849606411554	2.24358268407734	-9.11399584205464
H	3.05754063702619	2.74822101082566	-9.97217022664275
B	1.12670552374409	5.02858761045505	-4.12735466771301
N	0.75511326072426	6.41392146330943	-4.30698478243086
C	1.75080100020885	7.23046725218620	-3.75554158431096
H	1.67889672160561	8.30923363212454	-3.77155629323016
C	2.73183715870121	6.44542450994140	-3.25354206379994
H	3.64947934912514	6.73239376042296	-2.75769349907049
N	2.39945230393928	5.10064674778938	-3.45560633768202
C	3.37481307349986	4.08327917281132	-3.21321994810415
C	3.31224879130613	3.32218176639755	-2.04057243914420
C	2.19904198992320	3.52208503975001	-1.05356298423874
H	2.39448090811892	2.96973840344330	-0.13070445036420
H	2.05978718538178	4.58090716988625	-0.81094455054633
H	1.24915243049687	3.16682404922621	-1.47012651552674
C	4.42759258466599	4.70419940725133	-5.42726882750619
H	4.64047549087646	5.76194967453403	-5.23328534071630
H	3.45656939722185	4.67402833948819	-5.93573182736350
H	5.18792052485648	4.31720369218225	-6.11032516024266
C	4.39750384216954	3.90284072589671	-4.15699142003955
C	5.37336548394126	2.93986550558509	-3.89971891886392
H	6.16629608763913	2.78309835534745	-4.62665558171065
H	6.09898242253849	1.43204144915914	-2.54912274317945
C	5.33096202921807	2.17709933485479	-2.73842001470849
C	4.30824394210567	2.36856096023897	-1.81764249760332
H	4.27788229605861	1.77701700890442	-0.90651384119237
C	-0.29164973393071	6.96580852242774	-5.09783499520633
C	-1.35851641912355	7.63856478399550	-4.48150136170378
C	-1.40206789402110	7.80928394595635	-2.99153691533996
H	-0.68257961096935	8.56888473232566	-2.66315456936985
H	-2.39765595384722	8.12246677214077	-2.66978151653360
H	-1.14178039819735	6.87923652155840	-2.47971720832447
C	-2.36916532312736	8.15831590220895	-5.29142431067424
H	-3.20950476304232	8.66601571907475	-4.82508898155484
C	-2.32343930051060	8.01952486093232	-6.67361787265602
H	-3.12923033935594	8.41334388011607	-7.28605537834044
C	-1.24239933748236	7.38683017569626	-7.27441839318945
H	-1.18575209204338	7.30715598437310	-8.35686588986903
C	-0.19162232646946	6.87187474102961	-6.50216595127883
C	1.05340564147812	6.34214541565971	-7.16146448688823
H	1.94656793615969	6.72115621756157	-6.65383946908860
H	1.08201175993468	6.65009875006658	-8.20902683649491
H	1.10975755481342	5.25000244939090	-7.14357400920630
B	-0.72896796530599	1.97910563206650	-3.64453892162538
N	-1.91918389327559	2.12264453893732	-2.83724530184361
C	-2.20213185709867	0.89796243134785	-2.22445783259280
H	-3.05542159635213	0.77582113621393	-1.57140374874651

C	-1.26788742959385	-0.00895961383086	-2.59069814589521
H	-1.17341534151370	-1.04715864523460	-2.30364554797583
N	-0.35623940310245	0.59531507868349	-3.46276161265952
C	0.68798428905895	-0.18130927654965	-4.05254436826420
C	0.56619748279683	-0.58725836313133	-5.39006890495957
C	-0.63551612448954	-0.22428660674286	-6.21479409698884
H	-0.69905747334147	-0.86029655974913	-7.10155895152115
H	-1.56379535670802	-0.31930022677664	-5.64261611315527
H	-0.59255875440224	0.81477813545803	-6.56080217448882
C	1.86559999775054	-0.19415602017582	-1.81226255077730
H	1.18887758858542	-0.81200232115558	-1.20980896525860
H	1.57681910457662	0.84721132001985	-1.64762685304030
H	2.88096767234088	-0.34165336266619	-1.43736933513591
C	1.78416504743784	-0.56328783881385	-3.26619212230296
C	2.79663042544895	-1.31812958734761	-3.86128373561895
H	3.65993980103146	-1.60646686323317	-3.26626527415532
H	3.50557760963374	-2.28739732750654	-5.64502824012945
C	2.70857865895713	-1.70258939811808	-5.19370978016121
C	1.59705943909164	-1.34686756471369	-5.94691462187351
H	1.51932382441209	-1.66176289797253	-6.98473609033436
C	-2.87236693800468	3.18421687950896	-2.77295210836716
C	-4.06093854533834	3.06390350348710	-3.51276462622787
C	-4.32125699379838	1.86495751718627	-4.38022076807421
H	-4.57115646990798	0.98386394032885	-3.77754671329230
H	-5.15444913561250	2.06060176041685	-5.05981396042828
H	-3.44254668409847	1.60802038721410	-4.98028362810810
C	-4.99911100546344	4.09435157867380	-3.42875293520765
H	-5.91543563161875	4.02169888711957	-4.00898211800723
C	-4.77124926115664	5.20331743044035	-2.62352185977462
H	-5.51383282938393	5.99440080159289	-2.56513427724106
C	-3.59669099932629	5.29624486869739	-1.88697736587499
H	-3.42529644202498	6.15419195435812	-1.24228351871314
C	-2.62823778561278	4.29216930860097	-1.95106883282481
C	-1.36220440644440	4.39855925278637	-1.15090935305776
H	-1.13591697754451	3.46031560680358	-0.63427743928594
H	-1.43795879247820	5.19954996835756	-0.41036293082116
H	-0.50556611605531	4.61822257988918	-1.80044933328038
C	-1.66937425084654	3.34132733026926	-7.60524032254577
O	-2.46930060623769	2.42772062574836	-7.31116912732714
B	-0.80312384800060	3.27442291942268	-8.91530591649774
O	-0.21161536228713	4.38072759442922	-9.50854130744953
C	0.48676803290595	3.87505323700892	-10.58413106489018
O	-0.53184122644185	2.10705232030786	-9.61536133971427
C	0.29194893854517	2.49679435473100	-10.64811641955805
C	0.87979316999910	1.71628155252406	-11.62253692487999
H	0.72529606256084	0.64316963614663	-11.65982583320458
C	1.69083680196429	2.38445205658239	-12.54526185355163
H	2.17894181125553	1.81391520825028	-13.32932706031607
C	1.89032652464116	3.76612675462193	-12.47868393922437
H	2.53090286559185	4.24727033017174	-13.21125444350724
C	1.28440650221346	4.54685417209014	-11.48843552982799
H	1.43465478558835	5.61964441143448	-11.42789685906935

I3a

Energy: -6044.38912637 Eh

B	1.64731660454333	1.29046227659194	-0.23497835997845
N	0.91945135135792	1.86839466395923	-1.35917718377913
N	2.48417448424561	2.40567887509991	0.20545096833757
C	1.32418380567236	3.17654038491017	-1.54156559044608
C	2.25679603895381	3.49942339338615	-0.59761539820114
H	0.92222740259577	3.79017182020244	-2.33706941476849
H	2.77776098385419	4.43665154397133	-0.45230516892614
C	-0.00649301020456	1.27660336671264	-2.28221984601246
C	0.50683445606896	0.66362413855589	-3.43361012106682
C	-1.38294780579895	1.36673125928258	-2.03757813849188
C	-0.39401623634935	0.08312032498684	-4.32630621368443
C	-2.25021689198036	0.76971795392649	-2.95536364026454
C	-1.76148733780145	0.12349788534830	-4.08371258194941
H	-0.01189905748286	-0.41533517714730	-5.21300573134974
H	-3.32145903783435	0.81852520678729	-2.77706513717561
H	-2.45061794384694	-0.34278039536550	-4.78222487882939
C	3.39344530697690	2.45474215820659	1.30915189018317
C	2.96459062148338	3.02299413342607	2.51882130505275
C	4.69248718742224	1.95099961886969	1.14372957720888
C	3.84768403233266	3.00653502472115	3.60033695886720
C	5.54563116264445	1.96363105088527	2.24932487660637
C	5.12327046399766	2.47110016555416	3.47188294109296
H	3.52574425179817	3.42693036047675	4.54977688710122
H	6.55517668645185	1.57544761155964	2.14058292338016
H	5.79765728170907	2.46482794806311	4.32366656867320
C	-1.93082840859092	2.06716353705839	-0.82620048269600
H	-1.84975149535809	1.43019597863186	0.06331067407481
H	-1.38588379840275	2.99003436573548	-0.60427205312085
H	-2.98684584799156	2.30991075964159	-0.97261774402729
C	1.98580916327453	0.61176736499531	-3.68941072020476
H	2.19020262659173	0.16360555486106	-4.66459253507101
H	2.43414416618298	1.61126058018210	-3.66395829489549
H	2.49598872449125	0.01074887117868	-2.92741586383233
C	1.61965297145060	3.68146203726339	2.65030522669206
H	0.84202953909472	3.13451697880799	2.11040579986398
H	1.32702615901473	3.74651772408558	3.70176998134427
H	1.64849361468910	4.70037486637829	2.24349268821454
C	5.17731956788313	1.43541769084450	-0.18231032653922
H	4.81900226522115	0.41459684991598	-0.36297399048407
H	4.81560746330533	2.05167972157975	-1.01120282765383
H	6.27004736351179	1.42005797619768	-0.20617033978415
Ge	0.47555759889048	0.36429436072087	1.59793305300614
Ge	2.23188656009275	-0.77521877000758	0.17557531290778
C	-0.63490342487475	-1.01862401309827	0.80597333431854
O	-0.58198440903700	-1.49446836976608	-0.48356774263172
B	-1.71852858235995	-1.72346676634097	1.62910692789715
N	-2.00375970418805	-1.55175845126146	3.03466484121435
N	-2.72226108469792	-2.65986362008916	1.17613602132076
C	-1.29757438099800	-0.75680109091053	3.98566351288490
C	-3.09902835007632	-2.33251394151524	3.36524850710997
C	-3.53574187544242	-2.98627872357103	2.24921037699722
C	-2.96609909050120	-3.15618542010297	-0.14317173352458
C	-1.77624511149982	0.52917558070206	4.27906435304864
C	-0.13225284034819	-1.27220116285575	4.57229423167655
H	-3.48320473107164	-2.38093114796256	4.37527088127927
H	-4.37062571222548	-3.66639974706615	2.14514056383666
C	-3.87046413296955	-2.47259170901359	-0.96399591481923
C	-2.26039657472514	-4.28079742092115	-0.58388679323997
C	-3.00598341765820	1.06046289978549	3.60011210809623
C	-1.05015548243408	1.30994932571159	5.17804748740014
C	0.56631527802541	-0.45701236451065	5.46499279861688
C	0.35955068861962	-2.65044943576933	4.23207097642231
C	-4.56137280541608	-1.23024137515640	-0.47666067020926
C	-4.07487564876271	-2.95305335266106	-2.25840072836246
C	-2.49207823884651	-4.73207854720311	-1.88408146684746
C	-1.24403153831466	-4.94408200465353	0.30110691954512
H	-3.21380131649953	2.08283563543106	3.92439891447209
H	-3.88539644754158	0.44265763057574	3.81238753732843
H	-2.87452814915747	1.06153635735366	2.51062026682687
H	-1.39909902219651	2.31265826106278	5.41141071014713
C	0.11412345116861	0.82299993532626	5.76252867277007
H	1.47519783368816	-0.83421140175284	5.92637543530904
H	-0.44602136616734	-3.38992685772393	4.28868885869055
H	0.75248191648958	-2.68114364045444	3.20785547581835
H	1.16161116121629	-2.95063095072177	4.91048523132884
H	-3.82803191509089	-0.45465149138748	-0.22285658120201
H	-5.22875534056105	-0.83280434975165	-1.24534157565871
H	-5.14926634413499	-1.41945919802633	0.42840015577064
H	-4.76822581144962	-2.43242479771873	-2.91427205906513
C	-3.39253607210083	-4.07509966585007	-2.71501892006001
H	-1.94839284037721	-5.59991039079769	-2.24821727033387
H	-1.64917726868909	-5.15760277092852	1.29577968416013
H	-0.37416169756012	-4.28963738789165	0.44283402895153
H	-0.89476550946585	-5.87886698713333	-0.14399977543715
H	0.67215519794336	1.44527598172045	6.45670782439172
H	-3.55757804834652	-4.43503315618203	-3.72668379879249
C	0.72546259646538	-1.54757802903043	-1.02075439310721
O	0.86041549525713	-2.13068035778043	-2.06294466364487

I3b

Energy: -5931.06687553 Eh

Ge	29.66306918549051	16.53773528631531	14.74730785394257
Ge	27.68857238650101	17.43324015619149	14.09452393799267
B	30.67284489565036	14.88756336069716	14.08609490594923
B	28.23386327042998	19.87289663879016	12.25424011364488
N	30.27317681587071	13.57132517037607	13.64874722302769
N	32.10745044315627	14.82204450213717	14.14668931882759
N	28.90269818882202	21.00359001954292	11.68052508097188
N	27.59274957170883	19.21617190832891	11.15579692793562
C	31.42650989279290	12.79749971120454	13.47797961006842
H	31.37293263888161	11.76093348339713	13.17551579995966
C	32.52046631561329	13.54472713838352	13.76912786833862
H	33.56512215535258	13.26528682381502	13.74353012529333
C	28.98092767296295	13.05071519032413	13.34940262341103
C	28.04049396597561	12.89111437913094	14.37999693717627
C	26.78345643126533	12.37657576744870	14.05386423155827
H	26.04697691776650	12.24850246196442	14.84309944252111
C	26.47335857050450	12.01490355165283	12.74914917884417
H	25.49256433640491	11.61004636063566	12.51555610685572
C	27.42024170950699	12.16948644994622	11.74424119608233
H	27.17706577148423	11.89517623851895	10.72021374704389
C	28.68334733847619	12.69377671812997	12.02335479221547
C	28.35825834408623	13.24328544651327	15.80618338681847
C	29.68037476557640	12.88905843546298	10.91344061430949
C	33.01691390312671	15.85388119941775	14.52970805596975
C	33.41484398136930	15.94153186530144	15.87128687256157
C	34.29470641876679	16.96391399519968	16.23130496552562

H	34.61136718069351	17.05032904915254	17.26749299939349
C	34.76186171973049	17.86703440495939	15.28298755170841
H	35.44733696233856	18.65637182168689	15.57863639529459
C	34.35399208563638	17.76357088994424	13.95798131901654
H	34.72223627931189	18.46952378918400	13.21792058532848
C	33.47199376296697	16.75718139069534	13.55898163053661
C	32.88908275532312	14.97211582696846	16.89146703778326
C	33.01745438886363	16.64645745714094	12.13043673688190
C	28.65468682710826	21.00086722601102	10.30995200803852
H	29.06798187733450	21.75619490995033	9.65554791784319
C	27.86727019486123	19.93665687711850	9.99568652187928
H	27.47494661748253	19.63915326188650	9.03282188864315
C	29.78308000940455	21.93895615502933	12.30374614306967
C	31.05408712104960	21.50279821379187	12.70359301714652
C	31.90197434499081	22.42819952254501	13.31529003079001
H	32.89129170709572	22.10876001838695	13.63289824631589
C	31.49509840602334	23.74133815747288	13.51979814696727
H	32.16684632411702	24.44891262704523	13.99761766848381
C	30.22727001468530	24.14966894416848	13.12066843874116
H	29.90472934531148	25.17310075018337	13.29456284973452
C	29.34786759990014	23.25470848623367	12.50943481437826
C	31.49268484349462	20.07966591597177	12.49927132067872
C	27.96130604117875	23.67981925218843	12.11387391495563
C	26.86599294803048	17.98740299480389	11.15862709380357
C	27.53187683139840	16.81533351115698	10.76172469072521
C	26.81628250870943	15.61846861559626	10.77618940650815
H	27.31769341928199	14.69827518852760	10.49277682913879
C	25.48418642861709	15.58993382074444	11.17155146728085
H	24.94731442483334	14.64556718438686	11.18793037166122
C	24.84031800498837	16.76171041973278	11.55232908985124
H	23.79814716142463	16.73601601212223	11.85941008042664
C	25.51709691028330	17.98297028172351	11.54947248124466
C	28.98028079293866	16.85257625601462	10.36885673349805
C	24.83278685688833	19.25049543117915	11.97376697044517
H	27.73955198824523	24.67490695842838	12.50673349683298
H	27.21330689338791	22.97682647564617	12.49700907488804
H	27.84036579481502	23.70986201971301	11.02496843310653
H	25.02090877101831	20.06415590772554	11.26573958425905
H	25.20034106654211	19.58532452084134	12.95200241033497
H	23.75430161393684	19.09571021866072	12.05509126614573
H	32.57138806159326	19.98691632025751	12.64728949736688
H	31.24234807321780	19.71827974674817	11.49601019528268
H	31.00357843122061	19.40500814072546	13.21607344658474
H	29.15063818394649	17.50985413335205	9.50936979349643
H	29.33530888018431	15.85096788446601	10.11732122728588
H	29.58884415664058	17.23854678895098	11.19662159371682
H	27.70077640538787	12.69689511646517	16.48787605544332
H	28.20607530556360	14.31465839241806	15.99632389628976
H	29.39876462187108	13.01780502354360	16.05789322322543
H	33.10693890949169	13.93591360858355	16.61060393662708
H	31.79878486981832	15.05403007007302	16.97948283425296
H	33.32965516297753	15.16719418381997	17.87207661169638
H	33.22040901713183	15.65011214231073	11.72231468531809
H	33.52195463138313	17.38867798989460	11.50681656340725
H	31.93561502631548	16.80681445038987	12.04718365186536
H	29.16813483069069	12.95671797879190	9.94926841570604
H	30.38722060580724	12.05330612444603	10.85247842387801
H	30.27202476816001	13.79689097848900	11.06595305525775
C	28.22536004684041	19.42239704864751	13.74570088965450
O	28.53072760996291	20.11353107407614	14.70155771303475

I4
Energy: -6743.67634027 Eh

Ge	2.34677198709125	3.67094059122008	-0.93856347229728
Ge	2.14896337391348	3.26990379017852	1.29319004394635
C	2.69979089655398	1.48968841704658	2.06355227610307
O	3.14851569735313	0.54875201158340	1.41927845161902
B	2.60972333285386	1.48296604178917	3.64597769394149
O	3.61776134175055	1.06988672912810	4.50125944942876
C	3.17823397415857	1.42357375176428	5.76271210743952
O	1.52796789822653	2.01448700431069	4.33820498960744
C	1.91080688560654	1.99090557250236	5.66503963318478
C	1.22616616281614	2.45972110882120	6.76683899961431
H	0.24310089440075	2.90954594336059	6.67609004541451
C	1.88045949057039	2.34005281081770	7.99698625818198
H	1.38798737659907	2.70275298683135	8.89385602755701
C	3.15281500106477	1.77150513009662	8.09629710099723
H	3.62740713118431	1.69658074185047	9.06984901282943
C	3.83363522220404	1.29657091224722	6.97016990313354
H	4.82308659006343	0.85642923739948	7.03626784660919
B	2.43774207752046	4.53723677174933	2.86918289258498
O	1.63058808579208	5.59121369582412	3.29174320171625
C	2.10963410545748	5.95047926916600	4.53462921586832
O	3.40443843970994	4.24112014294709	3.83947998306297
C	3.18123963743464	5.12893559162015	4.86888733585108
C	3.85919575473030	5.25166239873501	6.06394858267506
H	4.68750712556897	4.59750327383339	6.31590330384569
C	3.41061955986032	6.25459147614654	6.92979766329021
H	3.90848587880347	6.38898506405558	7.88518759209874
C	2.33653678661854	7.08268251426376	6.59436488998402
H	2.01682365419685	7.84932800788738	7.29347317876053
C	1.65813802422702	6.94550699275356	5.37788950294690
H	0.82050870599258	7.58131635465003	5.11024778133729
B	2.62378584901032	5.61334593553381	-1.50034393479525
N	3.49894827246731	6.55441875624013	-0.83611745189782
C	3.46251060634648	7.76469075021668	-1.52627198748855
H	4.05822630113583	8.61191232512354	-1.21591508301783
C	2.61486956707468	7.65483060516534	-2.57763933495261
H	2.34319926075772	8.39446317601758	-3.31853649826536
N	2.08038337851082	6.36723523869017	-2.60160740669813
C	1.13018835760971	6.01246248075290	-3.60649148318388
C	1.59805733270386	5.66577066427984	-4.88096125881275
C	3.07116955977488	5.65446828003578	-5.17488494040491
H	3.26063098363257	5.30636713075786	-6.19266303011692
H	3.50243757503192	6.65639299027052	-5.06947230839473
H	3.61250013840280	5.00280868028343	-4.48008175748408
C	-0.70804424463917	6.53348174293045	-1.95269106711822
H	-0.29334629568707	7.51279459087511	-1.68781734504982
H	-0.38735232227144	5.83462780729422	-1.17082048300386
H	-1.79861360646180	6.59861018087100	-1.92667429483275
C	-0.23708503691719	6.09742003881462	-3.31184105700007
C	-1.14642244893609	5.78235193486617	-4.32379824457968
H	-2.21169161151194	5.83742158220475	-4.11442314552436
H	-1.42490751333839	5.16232296239478	-6.36262972405756
C	-0.70420790290988	5.40618295701884	-5.58701282764689
C	0.65742183501837	5.35422710317145	-5.86468421927724
H	1.00121278195312	5.07385716997083	-6.85722348536177
C	4.29608796150163	6.43480985065023	0.34397418527446
C	5.47129583151267	5.67101734221639	0.30861994080191
C	5.90880435318342	4.96707296017824	-0.94363660436245
H	5.82737049811826	5.61787249449380	-1.82080852020920
H	6.94316020988133	4.62566040454912	-0.85188953236834
H	5.28532688265179	4.08814561594462	-1.14685589397397
C	6.23955925872284	5.59280897140668	1.47261439743224
H	7.14838202719151	4.99645523784980	1.46521612640341
C	5.86817537041797	6.27949735148128	2.62207274902456
H	6.47816520447651	6.20949816000555	3.51847348991379
C	4.71747252854393	7.05863429684957	2.62640886123649
H	4.42848938567696	7.59807918674907	3.52519095965574
C	3.90767110199924	7.14471017036548	1.49221333359812
C	2.65864627688619	7.98194991255802	1.50935725049189
H	2.80058147299825	8.92430173752140	0.96764347174050
H	2.37862300681882	8.22284072722104	2.53767400210564
H	1.82254027091753	7.45897834726727	1.03405959170181
B	1.98366484168658	1.97765468142231	-2.03468885765336
N	2.80489815999293	1.38449867187410	-3.05610004594782
C	2.21216112543585	0.18870360797623	-3.47265929209194
H	2.66444174677042	-0.43570740982944	-4.23048261270453
C	1.07096096340765	-0.00861049713946	-2.77103806007587
H	0.36452893041786	-0.82433502148329	-2.83548735161477
N	0.88918701215774	1.04849191905178	-1.87693982363770
C	-0.19770589478758	1.06481293405583	-0.94963872390861
C	-0.24346180105238	0.11237719037863	0.08032717053408
C	0.76159578216273	-1.00079245335151	0.18299070620169
H	0.85138250882154	-1.33997161554076	1.21834532047086
H	0.44599260084014	-1.85999053337216	-0.42245443905359
H	1.74895168335139	-0.69370653782690	-0.16463546408851
C	-1.20158261191356	2.96993806299689	-2.27208415924117
H	-1.11334698212469	2.42375981649826	-3.21827072252745
H	-0.35704046124855	3.66525451386027	-2.23968857717651
H	-2.11994121343278	3.56221467669760	-2.29372823019881
C	-1.20173713367677	2.03324633478450	-1.09989164713422
C	-2.21822637007911	2.09055985241434	-0.14576983779172
H	-2.99485556846698	2.84474998997215	-0.24538867586870
H	-3.04077839633725	1.25423131395355	1.65727070419594
C	-2.24988583317795	1.19238249927389	0.91494076312866
C	-1.27925063645234	0.20372278544964	1.01405568601705
H	-1.31373553219097	-0.51249706145935	1.83144697807195
C	4.05324012079942	1.81658537658284	-3.59425460106979
C	5.20982363713838	1.72260550060734	-2.80369254262550
C	5.17049495264706	1.12502569769046	-1.42489793150379
H	4.60892893361541	0.18501332302804	-1.41629086908751
H	6.18419729187370	0.93242268055399	-1.06426041468748
H	4.67411979802939	1.78127877450736	-0.69928525471246
C	6.41677989476005	2.16372068673568	-3.35241269637051
H	7.32162663274766	2.10234333829104	-2.75296383629678
C	6.47527815322767	2.65666816907104	-4.65068113800591
H	7.42319473803797	2.99346968377328	-5.06118061100284
C	5.32496905497738	2.70355656905032	-5.42989305727988
H	5.37207076290084	3.07882024378660	-6.44931649103608
C	4.09684416249914	2.28143223253272	-4.91756597420304
C	2.85423247245219	2.32776667818813	-5.76167325581123

H	2.52776089551809	1.32190635986322	-6.04881357516019
H	3.03341525351580	2.89595786910900	-6.67762243377097
H	2.02118722857350	2.78902596930049	-5.22028087911502

I5

Energy: -6743.69097369 Eh

Ge	0.13117387458927	-0.11480179967664	-0.57807159584673
Ge	-0.55999014616177	-0.69690685454326	1.65239091985037
O	0.38231727545608	-2.14187156392202	2.33074082082311
C	0.72734133947807	-1.00496458042032	3.18217147854131
B	-0.05078954872871	-0.87112705281518	4.49514567651364
O	0.31234688344610	-0.05308732577811	5.57080563120094
C	-0.68996262196745	-0.21092976917251	6.50138818844606
C	-0.82624237233904	0.39899056226771	7.73128520936028
C	-1.96033390418175	0.05352134714952	8.47693015073154
C	-2.89809283973684	-0.86032321947896	7.99492895415128
C	-2.74682967840412	-1.47297893871634	6.74462365086666
C	-1.62677026298711	-1.12293222222311	6.01953029671061
O	-1.23770265669068	-1.56179919240405	4.77466769183373
H	-0.09045088185901	1.10788111075652	8.09688871195014
H	-2.11003114863455	0.50802609043970	9.45145636787620
H	-3.76546981025566	-1.10386215432032	8.60078209744627
H	-3.47053929366799	-2.18479292965775	6.36119624291739
B	2.09738563044365	-0.36844756210597	2.92802289002435
O	2.58808826066404	0.77567986943270	3.57270243227232
C	3.80766808918114	1.02705263995699	2.98667534252782
C	4.68796167506620	2.05950336900614	3.23710702730727
C	5.86251671655104	2.07709395493330	2.47459788904274
C	6.12270415966214	1.09894226296051	1.51378497500725
C	5.22186148458717	0.05449411363628	1.27145520533818
C	4.06872158341751	0.04843251593033	2.02922203280979
O	3.02514388128482	-0.84497469070921	1.99522560566344
H	4.47715931196875	2.81533631390937	3.98675561691340
H	6.58495122408994	2.87118348028781	2.63663440213813
H	7.04354466810865	1.14618163560341	0.94057944941524
H	5.41458660596500	-0.71132292716412	0.52729067578546
B	-0.20701602973125	-1.77317320731062	-1.76471072590613
N	-1.28967628882972	-2.70970364463144	-1.60530919660549
C	-1.06181630975046	-3.80659014063323	-2.44304462051843
C	0.09244226479402	-3.61211810538529	-3.12255437894713
N	0.65469480195998	-2.38913724549735	-2.73358169299614
H	-1.74939973252781	-4.63979553537574	-2.48884882200858
H	0.57106146879545	-4.24946837209865	-3.85301624076530
C	-2.35880985574018	-2.67401076127900	-0.66244522440490
C	-2.27834958116021	-3.47301407494668	0.48930191382713
C	-3.29586149468673	-3.35930267251369	1.43957658607028
C	-4.36502393745621	-2.49327689825505	1.24064130105018
C	-4.43966425433609	-1.73278246628569	0.07951591263279
C	-3.43787544171355	-1.80828218720793	-0.88997332088149
C	-1.12494052923065	-4.41002921234922	0.70864514993063
H	-1.08831554494311	-4.73248889970278	1.75136875857609
H	-1.21543532209530	-5.30017433662127	0.07468528472768
H	-0.17098255591473	-3.93289003107119	0.46445448503291
H	-3.23414445488594	-3.94847254743308	2.35086655110881
H	-5.14478399600723	-2.41374710133395	1.99298897830923
H	-5.28260216257500	-1.06502713396337	-0.08062223308601
C	-3.50592913785214	-0.97151796251751	-2.13611095759509
H	-2.73112659962890	-0.19465366502677	-2.12848058575909
H	-3.33606694074462	-1.57517423319674	-3.03403940955719
H	-4.47955312486711	-0.48095971286962	-2.21862682476456
C	1.90026399752872	-1.93662384555250	-3.26019480083062
C	1.95263402264181	-1.49087908663063	-4.58918495225043
C	3.17885473033461	-1.05096777291071	-5.08965247554132
C	4.31617136194113	-1.05070152751107	-4.28987995395558
C	4.24677841037155	-1.51206982224488	-2.98066718385611
C	3.04232435207139	-1.97610726640425	-2.44530949365473
C	0.71838060218287	-1.47763219141077	-5.44492550723322
H	-0.09316859848104	-0.92829282120354	-4.95325989544142
H	0.34937320768322	-2.49077497519235	-5.63773168572477
H	0.92310189208051	-0.99802579096448	-6.40392783436438
H	3.23418419609325	-0.69996455089985	-6.11698692715688
H	5.26302415127433	-0.70132254472042	-4.69248607638794
H	5.14171555461253	-1.53438673048852	-2.36362394675217
C	2.98772671164056	-2.52362451469356	-1.04709504786736
H	2.37476407987733	-3.42939120002724	-0.99798261856748
H	3.99370365149819	-2.76058311946973	-0.69037595943959
H	2.55058768527348	-1.80800165416944	-0.34029020941362
B	-0.66602526746368	1.70594601449788	-1.04897371796528
N	-0.78031778519195	2.44134905082865	-2.28938399704877
C	-1.27917936811765	3.71254834056102	-2.00924154113845
C	-1.49396946445002	3.83058850866190	-0.67418385101984
N	-1.11782347477020	2.64846412603913	-0.04918131753214
H	-1.42152872843796	4.44847264475147	-2.78853271796722
H	-1.87866071425523	4.67380447460926	-0.11638365628470
C	-0.42668753783518	2.12920538567759	-3.63775909266194
C	0.92803198858318	2.00144407801518	-3.98840910477192
C	1.24673022483503	1.87177279238913	-5.34106716308841
C	0.25537265760023	1.83903385000080	-6.31322311221226
C	-1.08048020642809	1.91637116416175	-5.94312371915697
C	-1.44500641438093	2.07248966739321	-4.60402806674783
C	2.02664870945931	2.01691719319623	-2.96233682328065
H	2.16283630206317	1.01993775644062	-2.51880518261235
H	2.97859474343395	2.28621411125440	-3.42749258542977
H	1.82063307149201	2.71394301914749	-2.14450627395656
H	2.29205545546217	1.79626723873141	-5.62729083202862
H	0.52476261033390	1.73920945997494	-7.36113744978297
H	-1.86015128448259	1.86886678127304	-6.69956837664182
C	-2.89916122569642	2.20353616046331	-4.23738838277821
H	-3.09773096517714	1.85393234128244	-3.22171742210517
H	-3.51719098245729	1.63097210014330	-4.93495992121556
H	-3.22748993852319	3.24883867360432	-4.28929323431211
C	-1.25241887187338	2.49594922231536	1.36476688360186
C	-0.14810050255882	2.75946018341609	2.18804410390593
C	-0.31252922228869	2.62164722255430	3.56775182103644
C	-1.53511892658424	2.23554931046782	4.10445921882192
C	-2.61553628097069	1.97185801483927	3.27043776556833
C	-2.49362333073598	2.09990300079721	1.88526695199558
C	1.17388663529988	3.16445510021233	1.60101576826835
H	1.62811783538851	2.33122676890346	1.04820814630629
H	1.87004976155003	3.46247956255331	2.38794203276764
H	1.06167654302420	3.99235436085791	0.89285990764478
H	0.53372518018181	2.80795286729229	4.22238987472217
H	-1.64521954108906	2.13188124273807	5.18049420811962
H	-3.56753852408659	1.66147387485762	3.69348608417172
C	-3.64357956181675	1.79078847394359	0.97134614425846
H	-4.53624833233760	1.53587116833446	1.54759212682035
H	-3.87813231447480	2.63582486543462	0.31472580892464
H	-3.40245911315665	0.93849356900992	0.32395512842637

I6

Energy: -6857.00903032 Eh

Ge	-1.14755485753825	1.68678355651593	-0.17777493079116
Ge	0.23774494795914	-0.14899549029668	1.12505644930526
C	-0.50345210863615	-0.43421395802076	3.03981369349127
O	-1.08889765650838	-1.18199947400401	1.94136635060421
B	0.66275512381954	-1.10838318506161	3.76044227283069
O	1.32028038489764	-2.25436590031951	3.27382400717055
C	2.35028962598424	-2.48564753324488	4.15447345830846
O	1.26079390727740	-0.67512122865723	4.95472729774837
C	2.31326778398249	-1.53155639670163	5.16984285391295
C	3.23573933030770	-1.51887140838443	6.19594909946753
H	3.19776191632456	-0.77135958228433	6.98181024416725
C	4.21749778233608	-2.51795897985356	6.16775742390763
H	4.96458328744252	-2.54676451774829	6.95507530599414
C	4.25406147467474	-3.47354274151163	5.15177128532515
H	5.02912971004950	-4.23379087698108	5.16157529020655
C	3.31048694426862	-3.47562080787233	4.11609626682853
H	3.32980595223556	-4.21506821408155	3.32211422324916
B	-1.32382684009846	0.66183607659231	3.70574330138698
O	-2.65416470029634	1.00708148589450	3.40500427693779
C	-2.99691044770004	1.97908328558189	4.31965997971329
O	-0.85961383144206	1.42649700259590	4.79166736122555
C	-1.91000043349876	2.23252392584689	5.15292834754501
C	-1.96496046438601	3.16853328153122	6.16587678386430
H	-1.11178196674922	3.35532934785455	6.81011745225767
C	-3.17602422798783	3.85464588463605	6.32018002084731
H	-3.26588478396671	4.59886729330402	7.10565689358564
C	-4.26614154585276	3.59875525025747	5.48796259758269
H	-5.19084239247315	4.14852070378085	5.63484876945046
C	-4.19574745639163	2.64688129467794	4.46315443610417
H	-5.03329821879830	2.45198891726133	3.80256153554017
B	0.04166344042200	3.34751961924836	-0.53556672922135
N	1.22269566122795	3.59384241253115	0.24889042903859
C	1.77092260444092	4.81720628236100	-0.13224152716139
H	2.66724023552795	5.20549789586315	0.33208424523832
C	1.00481061236741	5.35909987271585	-1.10876167331229
H	1.12708264703705	6.29657666465833	-1.63387007792458
N	-0.06307327122605	4.50350844975590	-1.38988241227478
C	-0.90344554598616	4.80044122809230	-2.50841786813785
C	-0.37341051100176	4.58456473354768	-3.79372809087814
C	1.00398643683131	4.00967807787466	-3.97305129553502
H	1.18158880046331	3.75839589721550	-5.02138302231384
H	1.77656038754470	4.72050775893226	-3.65900011558908
H	1.14128028566048	3.10587288304373	-3.36793883451353
C	-2.73679120837879	5.64231822738066	-0.95560771034336
H	-1.96830953665417	5.63490614318117	-0.17959235131757
H	-3.49057658291942	4.89062837509198	-0.69075699337231
H	-3.23829846928841	6.61504658104031	-0.94227462747527
C	-2.16910099966320	5.36775304033511	-2.31975165419476
C	-2.91919803247513	5.69289612855060	-3.45564887257495
H	-3.90302596210064	6.13708290446394	-3.32495690569749
H	-3.02205851107102	5.72507334621204	-5.60025668982075

C	-2.42421810580655	5.46552852267458	-4.73106609318453
C	-1.15634533671738	4.91651532607125	-4.89763344379622
H	-0.76415911755200	4.74365113064722	-5.89670774721625
C	1.90130419527091	2.77595743057201	1.20814780194667
C	2.87263477526283	1.87331706058909	0.75099913392439
C	3.13586357083259	1.69880342609419	-0.71807003794771
H	3.31907429824338	2.65772128201635	-1.21472514224039
H	3.99954599971807	1.04921695015838	-0.87955926730037
H	2.27382333727401	1.23875045450984	-1.22062816222044
C	3.55875614661598	1.11247836448801	1.70001110701614
H	4.30867830236129	0.39977160926804	1.36675118883059
C	3.28121688642046	1.24758822928268	3.05525092396361
H	3.81615489737022	0.64065931928613	3.78094998524994
C	2.31254325306328	2.14684003970651	3.48561595733220
H	2.08384277128999	2.23499391077899	4.54353130040453
C	1.60861392424134	2.93005878594612	2.57034889566432
C	0.55373167682440	3.89620521618359	3.02754543361379
H	0.71647550282847	4.89748925326376	2.61463185734452
H	0.53605957899420	3.96022263109741	4.11753651949294
H	-0.44268945953407	3.57488346446302	2.69942211367675
B	-2.31299326349454	0.62781731804555	-1.49653975489876
N	-1.86478737763887	-0.31782850070653	-2.47400917808981
C	-2.97864590321435	-0.98394538750931	-2.99566890138721
H	-2.88043310666538	-1.73896259083638	-3.76353784973362
C	-4.09721952161108	-0.51371022889930	-2.39144802300922
H	-5.12968860210254	-0.79655180436157	-2.54431044581651
N	-3.73561747954767	0.47040778796361	-1.46408398714005
C	-4.68397223256333	1.12409924954196	-0.62490477912801
C	-5.02532415112597	0.53623081424006	0.60262224803073
C	-4.41672824421806	-0.76650626460464	1.03033838469840
H	-4.87203585711158	-1.11428928826229	1.96070974655629
H	-4.54848737388777	-1.53842961711753	0.26412811498958
H	-3.33793712372761	-0.66957926114849	1.20623897725788
C	-4.88320908100845	2.90561617380087	-2.39791631982937
H	-5.15634436160859	2.21705584403279	-3.20581019539427
H	-3.80404496649468	3.07571238423321	-2.48473544410858
H	-5.39379261302098	3.85698611392268	-2.56651786070318
C	-5.24508443695096	2.33523568950025	-1.05692164256811
C	-6.14420286401932	2.98306106213016	-0.20942440342979
H	-6.58344499492373	3.92749905691368	-0.52067415540645
H	-7.19207444202377	2.93820190838980	1.66683135595237
C	-6.48676056360982	2.42520843389719	1.01845172947021
C	-5.94142113922714	1.20902263991931	1.41389817132926
H	-6.22352704045056	0.76729318005257	2.36619030245346
C	-0.52623910573824	-0.58693661829518	-2.88726703547915
C	0.18850145117983	-1.62983048797673	-2.28334877662037
C	-0.46733885577039	-2.56683572514308	-1.30763895739445
H	-1.01032081410757	-3.35318395860801	-1.84783802232073
H	0.27733732306290	-3.05124956643190	-0.67076513463496
H	-1.19581354543623	-2.06152558054630	-0.66720005345608
C	1.52400844907044	-1.80756396684432	-2.65742379190974
H	2.10303710887091	-2.59849510982220	-2.18744095902531
C	2.11134379088360	-0.99051132223755	-3.61569799129532
H	3.15267013259878	-1.13915000679937	-3.88815638861320
C	1.36691847691964	0.00634937641786	-4.23965026069396
H	1.81941170067561	0.62555411933427	-5.01046129269137
C	0.03251689140805	0.21741029171515	-3.89090776610221
C	-0.81068148748459	1.24555161955785	-4.58894285229031
H	-1.69093572083586	0.78021512176487	-5.04710800350288
H	-0.24004012212136	1.74955900424300	-5.37181326669905
H	-1.18534252120304	2.00485062245516	-3.89398859183274
C	-2.51649274749090	2.68885405155384	0.79691887768115
O	-3.11367948123012	3.31325748202446	1.54700228184479

I7

Energy: -6857.00657637 Eh

Ge	-0.23350789273348	1.62654366728895	0.05914414473345
Ge	0.86246380067753	-0.38056942815373	1.06580997566996
C	-0.41142124178148	-0.25560924808853	2.77826569773185
O	-0.76461761131285	-1.14969036644953	1.75575914002494
B	0.65454205744416	-0.69167967002680	3.78837216561191
O	1.23000727826434	-1.97577481492450	3.83913027409761
C	2.14108301640575	-1.92412686675862	4.86532733132358
O	1.17020570449973	0.11619305598263	4.81758096769576
C	2.10090795232267	-0.66323263715382	5.45991849925970
C	2.91513134740416	-0.32866480441723	6.52257955059289
H	2.87460199323928	0.65526211712786	6.97890160500223
C	3.79195040241591	-1.32242226813872	6.97749501973023
H	4.45209269241378	-1.10353372211836	7.81124208201841
C	3.83266578824218	-2.58361084776074	6.38258913482781
H	4.52452780331729	-3.33008641815606	6.76065887186865
C	2.99836634264819	-2.91161573603084	5.30584038373584
H	3.02223715924512	-3.89013739226848	4.83733517809272
B	-1.32227918391738	0.95388319240391	3.03198627757344
O	-2.58758706252891	1.14229331895675	2.45029134434384
C	-3.07158377020579	2.31152648771870	2.99793884094933
O	-1.05626141794639	1.97183681517894	3.96235246545387
C	-2.14702350302955	2.80873354335742	3.91264440576041
C	-2.36316693249455	3.97784012639494	4.61383539570928
H	-1.63448906984629	4.35445011390560	5.32437872283913
C	-3.56708188089885	4.64548651626582	4.35774961894120
H	-3.78127403668838	5.56994649571898	4.88567929267427
C	-4.49181269053911	4.14843429056169	3.43841501280053
H	-5.41363365620893	4.69377431779768	3.25850558613376
C	-4.25889407847410	2.96184632118754	2.73332305600172
H	-4.96621883167133	2.58017813942123	2.00593041120364
B	0.91815813730197	3.30429198989759	-0.10563988590985
N	2.28387688447235	3.36368155402767	0.37048283472289
C	2.76012301807425	4.65320559673278	0.21900401656735
H	3.76126910950192	4.93278668658662	0.51906887493399
C	1.78001792905953	5.42811358576219	-0.32960553926560
H	1.80444945255753	6.48078750976296	-0.57854420260884
N	0.65190001847127	4.65475513351220	-0.54159905825519
C	-0.52055675403995	5.20281281045357	-1.15151521809701
C	-0.58669148859962	5.24437007166212	-2.55010309327927
C	0.57190567630776	4.78488294341273	-3.39096736325020
H	0.28436307917555	4.72220014952106	-4.44343879999418
H	1.41320365100768	5.48366524548051	-3.30965625969886
H	0.94326733393126	3.80579538610344	-3.06894875211926
C	-1.43390279422015	5.66555262025127	1.16007839791409
H	-0.48193001400438	6.08628144929931	1.50139319070485
H	-1.49135349346074	4.63511551659598	1.52786909583991
H	-2.25049855327437	6.22819998101983	1.61910845666829
C	-1.54699738432400	5.69593864132499	-0.33655808338080
C	-2.68574376829561	6.20592213875921	-0.96301178568361
H	-3.50062201213076	6.58253330151195	-0.35002596382532
H	-3.68805221977352	6.61905746281927	-2.81840816246409
C	-2.79005726755612	6.22661141773429	-2.34901507842536
C	-1.74650406343141	5.75451557678556	-3.13752845011290
H	-1.82315916440080	5.78593420918465	-4.22154695598162
C	3.09075165842806	2.32801485987601	0.94376267156105
C	3.88461990744057	1.54230444891879	0.09743755111386
C	3.91722513599742	1.79838494718570	-1.38253055489913
H	4.32969446297294	2.79007999973244	-1.60321858128749
H	4.53248498178400	1.05085580494565	-1.88925317994883
H	2.91095383126284	1.76905029008479	-1.81348701722669
C	4.65440881839030	0.52962559772844	0.67260905379927
H	5.26948448365874	-0.09645394431955	0.03141774370144
C	4.64179332773348	0.32141619439813	2.04714834478109
H	5.24165950316925	-0.47331115550704	2.48182000399021
C	3.86365843903494	1.12688437628798	2.86948808448367
H	3.85945303917105	0.96382764648959	3.94391179209826
C	3.07306884892067	2.14637336857574	2.33365965972879
C	2.22292858561508	3.01344103863622	3.21545264778008
H	2.41179798505237	4.07728329612734	3.03498120513390
H	2.41229680976945	2.79280582220116	4.26798110969765
H	1.15769377663989	2.83724013612986	3.02827243329072
B	-3.03052344250198	0.82883757475658	-1.17001928086252
N	-2.46740799214128	-0.21121358458936	-1.98391868878823
C	-3.50261752480150	-0.99758057023984	-2.47760478095601
H	-3.32635899167664	-1.82473041539170	-3.15052824237478
C	-4.68334799503698	-0.51549570569746	-2.00531578199313
H	-5.68532550822765	-0.87985413990366	-2.18671552876219
N	-4.44713538885578	0.60193503767189	-1.21006740376212
C	-5.50975040081099	1.25878519054184	-0.51691644064793
C	-6.10052818374089	0.60947484984697	0.57769143034201
C	-5.57441103576145	-0.70760791126023	1.07575966464562
H	-6.03531630121145	-0.96325284189625	2.03277499842294
H	-5.77785806282055	-1.52216830991914	0.37159314099717
H	-4.48779936874613	-0.66618684975912	1.21329187488237
C	-5.27358778875920	3.20345658980616	-2.11720709584094
H	-5.14629979678756	2.52233107896684	-2.96534151319522
H	-4.27819778729947	3.56675746504778	-1.83420922299171
H	-5.86555093530785	4.06241024614513	-2.44390865987288
C	-5.93546197189273	2.51966192977617	-0.95551239720940
C	-6.99062806490332	3.12841738876705	-0.27258269301947
H	-7.33516645506953	4.10679351827812	-0.59759695888472
H	-8.42648604438914	2.98237527606461	1.32083962442127
C	-7.60412352904359	2.49644662633215	0.80316314963391
C	-7.16105161941502	1.24765186414012	1.22414754956972
H	-7.62550066986416	0.76485310086812	2.08009817654098
C	-1.09630231079989	-0.41170581861934	-2.29944876291714
C	-0.44727841900925	-1.57944618176336	-1.86432904867363
C	-1.17188699455094	-2.63553302339362	-1.07962664850441
H	-1.78325360110359	-3.26862102169149	-1.73302729870261
H	-0.45665422186399	-3.27849772438987	-0.56095985711269
H	-1.83291829014050	-2.18741776455585	-0.33271005391330
C	0.91199640671309	-1.71648254583157	-2.15250018451833
H	1.43472859258616	-2.60523264055256	-1.80932775579172
C	1.60370633738464	-0.72732167740897	-2.84289138829565
H	2.66394224155729	-0.84899694103006	-3.04468808346807
C	0.94022259578217	0.41147191807077	-3.27975580092070

H	1.47209558201543	1.16746097765344	-3.85213236044188
C	-0.42674680258003	0.58624412082512	-3.03273163952868
C	-1.16723207249745	1.75355554367674	-3.63288473566712
H	-2.14562491603097	1.44157973693040	-4.01176423850045
H	-0.58959196142711	2.17326836626730	-4.45993397341304
H	-1.34498457135549	2.56152738887991	-2.91428795596508
C	-2.21978715284827	1.92754077684828	-0.41403412504126
O	-2.70017437841945	2.95495030721556	0.04944531588171

P

Energy: -5855.87914762 Eh

Ge	3.98898275646565	5.00087104615493	14.71897969641263
Ge	4.15188734439594	6.99647118052639	12.93571497692433
N	0.29736422892568	5.23697531276517	14.32291135187683
N	0.41373203397508	7.30478153706212	13.39148551892119
N	7.04728449066337	6.40788897435502	14.07835742422205
N	6.44958603723091	4.55144330900014	12.90422466389162
C	0.59425818135430	3.94893299158410	14.84982420029351
C	-0.99477077307691	5.72462971270318	14.13604069860942
H	-1.87048789961475	5.15178792458718	14.40985578711578
C	0.92522934963462	2.91249490086203	13.96448586980251
C	-0.92474529759111	6.96454249050572	13.58015953046694
H	-1.73024185753281	7.63443923227609	13.31082359036125
C	7.07908284087777	7.70809017503559	14.65824032231837
C	1.27270792445706	1.67070196744677	14.50068438769572
H	1.53519108889459	0.85811092141794	13.82773763199679
C	5.79427444975247	2.23755272194703	13.30407187120024
C	0.84269232875602	8.51690506074358	12.78171829314329
C	0.93009132990565	3.14411396791828	12.47998156501406
H	0.01548456315377	3.64850322036131	12.15063054594544
C	5.75797963232309	3.37931479316734	12.48107355864168
C	0.61214711722919	3.76675086583727	16.23956375776753
C	1.28677283426255	9.57141133841870	13.59140461416594
C	7.37124946632610	8.81226997194393	13.83867922727043
C	1.28928449988570	1.46964195123739	15.87644385672787
H	1.56254663161420	0.49813883298611	16.27913989112123
C	0.86376770420442	8.60163449164738	11.38212196563916
C	8.19525565163126	5.75433725949107	13.63335797360904
H	9.18542763985525	6.14081977367119	13.83415790254725
C	5.06604508524639	1.11456054078113	12.91120457549833
H	5.07425742105606	0.23130778783935	13.54499795994459
C	7.84008535923838	4.63451314703614	12.95376814657358
H	8.47470478352070	3.88435780494071	12.50150679089908
C	6.78372835774389	7.86245331456072	16.02136006045672
C	2.75849733094698	6.10894144333902	13.83005568123143
C	1.73984548178769	10.73706976837544	12.96988832932601
H	2.08698700704316	11.56451697064314	13.58373715058098
C	0.95947073959912	2.50990587946703	16.73854647026259
H	0.98219731590404	2.35362937592459	17.81422168268013
C	1.29574294963042	9.43623647836199	15.08797264510151
H	2.03584943546828	8.69075582227692	15.40406355159597
C	0.44151654958899	7.42881452291429	10.54272291075408
H	1.02682556032529	6.53804445461040	10.80247713034503
C	6.77770583346475	9.15297589663264	16.55621052844092
H	6.55475788085856	9.28656381418499	17.61190015650134
C	6.58757054959677	2.22568003793587	14.58045458233727
H	6.43809396965488	3.14896627899824	15.15022530188057
C	7.05972036854830	10.25599670593929	15.76002380097098
H	7.05002016661862	11.25337728188112	16.19069500620048
C	0.30166640866545	4.91237656743173	17.16100640118716
H	-0.72629111185656	5.26851713184804	17.03024242718690
C	7.35591090545211	10.08459567356895	14.41239812789282
H	7.56987084583775	10.94862976465686	13.78826077092042
B	1.24966761420009	6.22012658861955	13.85446075997998
C	1.75322082684153	10.84514538367801	11.58373100509247
H	2.10880262456974	11.75836948015931	11.11456477576878
C	4.32597100773266	1.11974990146770	11.73387582276512
H	3.76186006375246	0.23762566342023	11.44345372934663
C	1.31953006223285	9.78401678529871	10.79635353154696
H	1.34403927924600	9.86460322162895	9.71240428492585
C	7.67561640408830	8.63399096085959	12.37772141105736
H	8.67458927403304	8.20920149402894	12.22428675450087
C	5.02494309159242	3.39684189911088	11.28425742811641
C	4.31009991901468	2.25015848388125	10.92804024811464
H	3.73855824150894	2.25132093918862	10.00296619366652
B	5.87043829025946	5.67774266754455	13.62942765696512
C	6.48704524708128	6.67596479419480	16.89248467960996
H	7.14565246755770	5.83247109917902	16.66446597355220
C	4.99585903456849	4.60923853650378	10.39967416987898
H	4.19749443802225	5.30242018999110	10.70660863366792
H	6.59399374390810	6.93734263649756	17.94854709931640
H	5.45785219549997	6.31954947167433	16.74291610785358
H	7.63275649720581	9.59473128042090	11.85844721571400
H	6.96236247456233	7.94859905794303	11.90738783702212
H	4.79117547985661	4.32448405652792	9.36378969766747
H	5.93583595268187	5.16558154923911	10.44046341512793
H	6.29452632790038	1.37752791300088	15.20443038800350
H	7.66270838817945	2.14546030866696	14.38098313996247
H	0.58215770647343	7.64240211834301	9.48023543432754
H	-0.61037866002564	7.17067181182129	10.70858117317433
H	1.54582350776731	10.38962866101402	15.56027466058186
H	0.32458753006023	9.09910666581302	15.46580724414765
H	0.43355860644683	4.61642324024347	18.20471396302402
H	0.95804683568557	5.76579226946475	16.95234035703004
H	1.02885201002821	2.19793607375797	11.94174261479447
H	1.77242273556775	3.78643644701391	12.19246585122251

T1

Energy: -6630.35546304 Eh

Ge	3.20078539030829	2.22307735034489	12.70761552093919
Ge	3.92741799849768	4.36486848682756	12.03177548371118
O	2.14221113383799	2.17616309578411	15.63074839822169
O	1.01935563874220	0.73964701566490	14.24417003049998
O	4.92699146857375	2.24661015246411	9.81928364237142
O	5.99693404131043	4.27099679007459	9.79482187437047
N	5.78953588059252	0.54321789343915	12.79218492656850
N	4.06220129078963	-0.88265321034957	12.42402213937327
N	0.64929414572403	4.14347420322365	12.11785276358611
N	1.46909632211455	3.69137801552562	10.03817936599558
C	6.25182375152783	-0.77126334423822	12.88433287474909
H	7.28563701823651	-0.99462265483296	13.10774795573030
C	5.22291277905503	-1.62262298931086	12.66404812038822
H	5.21803857451739	-2.70408617192908	12.65506086839405
C	2.82616243887195	-1.54207806852837	12.16151883635910
C	2.40959564572664	-1.68521218580959	10.83116648659598
C	1.19583090042833	-2.33098433145455	10.58724777135564
H	0.85439101675140	-2.45054707354943	9.56198997134046
C	0.43477571863680	-2.83290817244772	11.63768482258142
H	-0.50893345173588	-3.33109324095896	11.43296999893964
C	0.88758084093430	-2.71614601880468	12.94717395815156
H	0.30137069462069	-3.12793253310816	13.76519754669425
C	2.09657192997001	-2.07790445456276	13.23113228708825
C	6.69185806307764	1.64329645024883	12.91797798407317
C	7.66632088931838	1.83921038497113	11.92217664456992
C	8.49131820126998	2.96068680863659	12.01163655627172
H	9.22608340619693	3.13680037061774	11.22959026169543
C	8.37735958433328	3.84838327415728	13.07469270874983
H	9.01856445015081	4.72398182451024	13.12455080681368
C	7.46015018504829	3.59901276450271	14.08690844755333
H	7.39888005740337	4.26780586086189	14.94222006041746
C	6.61480590256807	2.48703712283638	14.03755238070904
C	1.25061912269506	1.43282434664921	16.37471096938636
C	1.00152419210050	1.48516756575186	17.73034010122369
H	1.53833656602206	2.16766828994148	18.38098472233134
C	0.00846109981246	0.62526995068519	18.21245215721576
H	-0.22675283821942	0.63208780737728	19.27241256109809
C	-0.68710420929517	-0.23852885938983	17.36255863251237
H	-1.45134600976989	-0.89020745795880	17.77496632310608
C	-0.41911322405134	-0.28424399020796	15.99000376270102
H	-0.95114563658909	-0.95036174834488	15.31823215512894
C	0.56333552281214	0.56882420243830	15.52978150668012
C	5.82093901692251	2.26980178278116	8.77707241627662
C	6.48171533275786	3.49278091787781	8.77069447629570
C	7.45514310901148	3.79563774757887	7.83861583911363
H	7.96736437785767	4.75247988657273	7.84337335555280
C	7.74181749643410	2.80491577829345	6.89269652369136
H	8.49925078652392	2.99654668995182	6.13862909152234
C	7.07486061133589	1.57654944515436	6.89921867594893
H	7.32448587213548	0.83157366709803	6.14957254183746
C	6.09365170252739	1.28418797070493	7.85122620350258
H	5.56885322406052	0.33416256304003	7.86452242489086
C	0.24557281043622	4.31940568762399	9.92313318790156
H	-0.19030448644015	4.54169624222658	8.95813887642956
C	-0.24801548274464	4.57571751201523	11.16477584067152
H	-1.18658740219708	5.03894100231054	11.43888878642593
C	0.22646627902096	4.18282561760765	13.48824801388933
C	0.65810032986236	5.20802702806586	14.34168056241926
C	0.16865745732182	5.21940518943623	15.65162553427108
H	0.50032455467611	6.00463601495888	16.32649967667410
C	-0.74317740885957	4.26977289328882	16.08760898120726
H	-1.10965926264475	4.29473397960263	17.11002815462794
C	-1.19832554377505	3.29165496037867	15.21164504404952
H	-1.92093410437118	2.55237763932409	15.54766545304767
C	-0.73321533121176	3.23655083647795	13.89774924762188
C	2.10278685969183	3.24991298771099	8.83139175920832
C	2.87939348259084	4.14122139989179	8.08072211339272
C	3.43188092347851	3.67557008612847	6.88413448820896
H	4.05915894583084	4.34314529227209	6.29854416233731
C	3.18796443196582	2.38316432116984	6.43980210791813
H	3.63296477508789	2.03799155630951	5.51078508263339
C	2.37787529783629	1.53113373534489	7.18172666466455
H	2.16861826295043	0.52656833403702	6.82240573885977

C	1.81345863503348	1.95337032769509	8.38593928983195
B	4.36968935062452	0.52248494573712	12.49382361014484
B	1.98249928840924	1.75130942918514	14.30927593111596
B	5.01791315645962	3.50082718194560	10.44882031254287
B	1.82537297672313	3.56700710840589	11.45025013032791
C	3.27986075548000	-1.20320138166059	9.70399048769137
H	4.26468298217482	-1.68384435311107	9.74713583583769
H	2.82415082546226	-1.43711384704364	8.73843886836612
H	3.45635821330864	-0.12335233254300	9.75163255612374
C	2.61543910727245	-1.99813558366620	14.63870641114765
H	1.82086522770789	-2.21114387582120	15.35784334842920
H	3.42147317990698	-2.72469469227180	14.79794745859896
H	3.03357889315805	-1.01100371628399	14.85940772183726
C	7.86173448344197	0.85968439547321	10.79836912694013
H	8.53443178631792	0.04991660340650	11.10790654030773
H	6.92163539345378	0.39988946331738	10.48807302589702
H	8.31262913751451	1.35206165352180	9.93270629383307
C	5.67794891686576	2.21981749861892	15.18157641994496
H	4.74043204659471	2.77676094384177	15.06502209117610
H	5.42208338461372	1.15960804892194	15.26107156335108
H	6.13347168502610	2.54324497085118	16.12254036697879
C	1.57979213291679	6.30275047674129	13.88883456235326
H	2.62925105067478	6.02327088454149	14.03538617799199
H	1.46331066462948	6.51751557644924	12.82360784725912
H	1.38670631696896	7.21508761478055	14.46049637914379
C	-1.28254399335840	2.20928020121521	12.94677168271349
H	-2.06911988347440	2.64411345759416	12.31787486921204
H	-0.50994960196920	1.81548823934864	12.28112974747093
H	-1.71888587673904	1.37559275144740	13.50279211003496
C	0.88040127552380	1.06704686320595	9.16091489850530
H	-0.10299573496365	1.53858489206630	9.27404949784367
H	0.74803828141400	0.10941583391163	8.65304617447772
H	1.25199852628071	0.86968467467119	10.17225198599961
C	3.07036740466910	5.57446330993421	8.49363198980736
H	3.10798879070975	5.69183397281007	9.57994789277081
H	3.99460427381014	5.97511709726139	8.06872335714604
H	2.23828520332566	6.18956332153818	8.12709901853857

T1a

Energy: -5931.07504479 Eh

B	1.89494204167051	0.28568959713104	-1.49870321413126
N	1.51795400767475	0.63866453954742	-2.85253152307282
N	3.19307839843523	0.91671661634406	-1.34242356104209
C	2.50038369521140	1.44560278458956	-3.40646466663141
C	3.51414987899044	1.59641363739095	-2.51131466282489
H	2.40635325698513	1.85964655442178	-4.40169760522757
H	4.44218385269986	2.14058202921388	-2.62104577529882
C	0.27817420908286	0.39733081036186	-3.52347260072646
C	0.07768306451271	-0.82485397801284	-4.18011344167132
C	-0.70027026534998	1.40197101620138	-3.50996078060777
C	-1.15086292459502	-1.03921342731115	-4.80976386685195
C	-1.91453173251377	1.14764732695425	-4.14950015377731
C	-2.14034182316361	-0.06327617379448	-4.79188206019322
H	-1.32481728883369	-1.98206814180892	-5.32276299714474
H	-2.69375928618751	1.90530698769135	-4.12765182693770
H	-3.09352118363622	-0.24724784271429	-5.27967559022409
C	4.07587925961638	0.92081120983689	-0.21869207828608
C	3.73027005351829	1.67670790195466	0.91237385546992
C	5.27683704842850	0.19676006736000	-0.28473583749476
C	4.59739343666633	1.65921464175372	2.00665614342765
C	6.11630812304355	0.20907119227257	0.83074892912100
C	5.77839268705323	0.92778628819215	1.97100784588462
H	4.34176957896571	2.23712113674582	2.89129082121766
H	7.04260094947850	-0.35922899635053	0.80046532646698
H	6.44147890637290	0.92405911637647	2.83166434738938
C	-0.45392941277423	2.71337047699686	-2.82122130150250
H	-0.02893848535071	2.55634640963437	-1.82549613267322
H	0.25208490930364	3.33305317581305	-3.38731857588979
H	-1.38825314038708	3.26962384293827	-2.71376335980047
C	1.15131241353171	-1.87369668333563	-4.21909548347956
H	1.26889970605811	-2.34762823228856	-3.23460545926676
H	0.90431244156879	-2.65185346169347	-4.94611989177162
H	2.12412586451279	-1.44332658728674	-4.47840737379599
C	2.47068913148893	2.49375754385194	0.95452747437774
H	1.58954478065826	1.85426611868132	1.09799764413193
H	2.50800738459715	3.21072635434148	1.77886349877730
H	2.31532613945291	3.03869115781004	0.01772265152079
C	5.66439914956496	-0.57500000149366	-1.51549166016295
H	4.80305986523987	-1.08538006257592	-1.95858837007399
H	6.07905268575586	0.08665848048907	-2.28552505824971
H	6.42456389433508	-1.32192986636208	-1.27253591737389
Ge	0.71533411289846	-0.72338900025197	-0.08669773563738
Ge	2.30351356362769	-2.27379488507478	-0.50588548667412
C	-1.28966957468991	-0.33437600880924	-0.20336546533190
O	-1.66625178136833	0.74590240845898	-0.63606851942225
B	-2.28011899031808	-1.47322415033881	0.21591176268402
N	-2.03421858425716	-2.70041142910650	0.92535409362190
N	-3.68617017330150	-1.50455204745884	-0.08874458272353
C	-0.81130450517128	-3.23089509579365	1.43422652438039
C	-3.23386086848934	-3.39947818471070	1.02452840453777
C	-4.21785121718917	-2.68675923674111	0.41378197883601
C	-4.47250527938209	-0.60139573066126	-0.86978951000036
C	-0.33679334182560	-2.79007519383367	2.67479078355455
C	-0.10547982800373	-4.15501550907939	0.64961139146926
H	-3.29714769757275	-4.34646563026879	1.54292058176124
H	-5.26698883072819	-2.92779686555952	0.30801807728092
C	-4.94358452605470	0.57960606898975	-0.28441729320261
C	-4.74290327613612	-0.93222623897438	-2.20414161089565
C	-1.10576937663667	-1.78358442865631	3.48124317211744
C	0.89082875541553	-3.28392254371767	3.12478926594597
C	1.12926120274745	-4.60936141128918	1.12315610566632
C	-0.63775833060816	-4.59827390760165	-0.68258471140041
C	-4.61500574160835	0.91711781563612	1.14139212525634
C	-5.70653014789835	1.44293708868412	-1.07233797397657
C	-5.51147254580213	-0.04404930339888	-2.95868969942578
C	-4.19008838288379	-2.19054631732086	-2.81181428861149
H	-0.69851694052108	-1.70775272814268	4.49227879392281
H	-2.16701193202826	-2.04419485498545	3.54479999041369
H	-1.04652170299808	-0.79110551116897	3.01677227499643
H	1.27750453737539	-2.94931760957124	4.08363674383670
C	1.62409070122065	-4.17346170295946	2.35305450056846
H	1.69377790160902	-5.32666160493747	0.53226973194731
H	-1.58727473392156	-5.13507399115754	-0.57666615120760
H	-0.82592610191788	-3.73155933730501	-1.32766087471900
H	0.07772236020899	-5.25474991897271	-1.18401987406304
H	-3.55280735754240	1.17168088999117	1.23818560610852
H	-5.20367176808645	1.77312047256070	1.48080040435187
H	-4.80797763430666	0.07115021315265	1.80950189302478
H	-6.08001574773316	2.36596974665908	-0.63616152018662
C	-5.98961105249354	1.13498983572320	-2.39853613936174
H	-5.72711056335546	-0.28097684782588	-3.99756383417188
H	-4.57146525840146	-3.08619735879418	-2.30909234663092
H	-3.09715851522611	-2.21421462491471	-2.72676954591733
H	-4.45100505694557	-2.25322984078400	-3.87100294524084
H	2.58528242311783	-4.53590465151593	2.70603434625537
H	-6.58527563312057	1.81775848301422	-2.99813702347361

T1b

Energy: -5817.76340363 Eh

Ge	1.29852373792492	6.79991920920874	11.54151905928732
Ge	0.79236225824072	8.04544495774429	13.45689904435908
N	3.84526890666871	6.42100597136282	13.39678912239442
N	3.84560842527826	4.91803304720639	11.70131605177884
N	-1.20079975516627	5.36909358577222	13.29602274742577
N	-1.76978403267728	6.95279198953740	11.76735541811862
B	3.01630765970831	5.92837471175263	12.32100073406313
B	-0.60155640092766	6.35666918249274	12.41102918572136
C	5.06033082300463	5.73043472251637	13.40474836377979
C	3.33663615250376	2.14275945341647	12.21015434441734
C	5.05797985897047	4.83009050932831	12.39219339398506
C	3.55760459594857	7.43385658642408	14.35192646451492
C	3.85536820879092	8.77486893252263	14.04445697401490
C	3.58964754209921	9.74686899371498	15.01067386128238
C	3.06193746654976	9.39634746083296	16.24978164998287
C	-1.73094021750409	8.29664691520086	8.30904578998448
C	2.78101622661139	8.06791932806510	16.54053921673055
C	-2.28509254134201	9.72873575185501	12.32519702104124
C	3.02469970740644	7.06306832138763	15.59972564340763
C	4.43534947920911	9.13836828924580	12.70928463536336
C	-1.96213809155917	9.64482192379906	8.54228340861399
C	-1.30926272429152	5.94234302787786	16.11765529250076
C	-2.57795392205787	5.38329202704811	13.13991624221751
C	-2.14800366648100	10.10390531142229	9.84198764250774
C	2.75627721427591	5.62102020965861	15.91129444975493
C	-2.91850533570017	6.33275346538357	12.22646043975913
C	-0.60042150822628	4.44365944713874	14.20329057733594
C	-0.01307034779441	3.28006246841215	13.68687737763834
C	0.51375212369703	2.35381314488969	14.59007452575863
C	-2.08978015912473	9.22573469983836	10.92426826321684
C	0.44328297451356	2.57389687563632	15.96076376745286
C	3.56794995943693	4.07083508231704	10.58870461012975
C	3.59348091508431	4.60456286541584	9.29109950694934
C	3.28967844596703	3.75653894204427	8.22314826888647
C	2.98931803989290	2.41648781368880	8.43625175409316
C	-0.15439628884204	3.72860149048673	16.45060740690102
C	3.00516523407727	1.89753856037202	9.72585821714447
C	-1.47004982735651	5.92161048427686	9.06040013872406
C	3.30103037049067	2.71225359033012	10.81996860334159
C	3.95723758004499	6.04059733548721	9.03985098123067
C	-0.68507118018257	4.68486215515882	15.58282612153093
C	0.01658900798333	3.02030694880434	12.20766949848963
C	-1.83283248692249	7.86933501572470	10.66851634741411

C	-1.67037663435588	7.38136302037304	9.36421380452154
H	5.83481380660555	5.94165122923588	14.12959384234677
H	2.83416737733648	1.17219979430065	12.23980772056350
H	5.83324395731785	4.13714482802676	12.09492356927373
H	3.80769313942273	10.78790270192379	14.78701297650764
H	2.86378042441834	10.16647565258397	16.98981971621343
H	-1.59654397095263	7.93499587087234	7.29222274716562
H	2.36717575043944	7.79660875025562	17.50835456646028
H	-1.35401734717907	9.65785736797436	12.90711751110687
H	5.35508343690314	8.57737090572633	12.51036135923280
H	-2.00501678690910	10.34120753405052	7.70941088673202
H	-0.85054756749347	6.83041890691852	15.66468669628508
H	-3.22093385432622	4.71100460977422	13.69243957860033
H	-2.34117553901410	11.15771307476335	10.02545091423362
H	2.15675611880863	5.14898600485484	15.12534767556432
H	-3.90002966836904	6.60247609716176	11.86000906144388
H	0.96641051155511	1.44274905234638	14.20788692730390
H	0.85058129244788	1.83917206415085	16.64982301803033
H	3.30209514920427	4.15628847238492	7.21217699323373
H	2.75368752615615	1.77193075269243	7.59391135920730
H	-0.20673143016975	3.90164694139233	17.52263088911562
H	2.78291941369090	0.84636330767127	9.89325937686476
H	-2.37218320060588	5.50688508020468	8.59358004952977
H	4.79347953921155	6.35637993062886	9.67190875870745
H	-0.97417956999952	3.16109013409987	11.76178961200309
H	2.22260167924467	5.52201822592063	16.85893497700463
H	3.69261916227429	5.05410304842646	15.97946613605308
H	0.35227364796964	2.00114288927853	12.00194889715971
H	0.69520699792772	3.71318322737450	11.69445286204715
H	4.65761426494777	10.20707553972785	12.66214691407822
H	3.73205029186962	8.89217839232712	11.90405147998200
H	4.23139619977340	6.18654944289808	7.99154375875743
H	3.11526768882165	6.70677489541558	9.26752318338263
H	4.36818507835452	1.99668649063425	12.55224444968717
H	2.85541198411553	2.81201939822524	12.93044206352856
H	-1.18645843990520	5.99975466615731	17.20211287839307
H	-2.38037308030069	5.99273641656792	15.89156773764359
H	-2.59677885044146	10.77608313467246	12.31809695558294
H	-3.03227266955218	9.14260060985854	12.87019903369851
H	-0.64375661194077	5.78925957573150	8.35446057765290
H	-1.24617404644516	5.33684118008322	9.95320410901966

T2

Energy: -6743.66913495 Eh

Ge	-1.17663935512688	4.46908815126717	-6.56738320575351
Ge	0.45952651826447	3.49422098871649	-4.89461189229940
B	1.79352243918747	2.30624075193465	-5.93864783592064
O	2.20777450939719	2.55413936965199	-7.25856825648603
C	2.95864804361239	1.46182702143729	-7.63198589890697
O	2.29301880221761	1.07356915900078	-5.51393032823840
C	3.00766877896140	0.56271332212070	-6.57258932449092
C	3.69098151428244	-0.63257600541950	-6.65736277682940
H	3.73294814063134	-1.32150837270077	-5.81991800501457
C	4.33481470439151	-0.89652336039548	-7.87207620337140
H	4.88614732099944	-1.82481426137138	-7.98787877464681
C	4.28491011081028	0.00740652193967	-8.93544255106803
H	4.79288089853461	-0.23357115689245	-9.86436037578460
C	3.58872056318959	1.21719212652147	-8.83423592847346
H	3.53514316588872	1.92194771600598	-9.65759917880846
B	-0.74153959576596	2.78116162033201	-7.78556748891919
O	-0.60874719958378	1.42218052400443	-7.44185228279123
C	-0.16577132434463	0.77822169511618	-8.57618034585771
O	-0.42670133589282	2.94407144369677	-9.14499154803129
C	-0.04624906147653	1.70325667453728	-9.60711395244186
C	0.40401496889488	1.34888162374687	-10.86274402114907
H	0.49691488154601	2.07945766496498	-11.65989568257130
C	0.73753969328056	0.00237156279766	-11.04665755342954
H	1.10057757053191	-0.32482752094105	-12.01623874709850
C	0.61798334789555	-0.92643307998595	-10.01088457161986
H	0.89499628412399	-1.96111194657388	-10.18826141267890
C	0.15670252464058	-0.55352190525346	-8.74390322844235
H	0.07183187540678	-1.26625180955635	-7.93011394120028
B	1.54944636910566	4.87509842658539	-3.78795753210399
N	1.20093927176557	6.16308405837203	-3.22739470074559
C	2.35205689232659	6.76185567490354	-2.70056161950828
H	2.31774327518078	7.73963030067505	-2.23956814182301
C	3.40971166846607	5.94239719164464	-2.89553540566562
H	4.44698290786873	6.08625273667246	-2.62519628061916
N	2.97439804772251	4.78845659923735	-3.55098991327136
C	3.91207865212743	3.78911119627707	-3.94905442013729
C	4.34376807785882	2.84369461652057	-3.01057975342972
C	3.88671803990177	2.92124544721782	-1.58310473982473
H	4.21040003963450	2.03927119050347	-1.02717648840954
H	4.29956231399556	3.81014022839834	-1.09100361672572
H	2.79806777471724	2.99900077388898	-1.51586795603197
C	4.04335877821414	4.91673417028450	-6.20865482782273
H	4.47859553440202	5.86952570153729	-5.88224355433371
H	2.96005251963794	5.06267251922287	-6.25763080378632
H	4.40704384275479	4.69649863872814	-7.21545896426512
C	4.41691867396433	3.81393604259119	-5.25827305041490
C	5.31822895672439	2.81654430760874	-5.63672383395071
H	5.70576241973293	2.81018570008236	-6.65233711810947
H	6.40578364039008	1.05936554061656	-5.04892925238800
C	5.71691576762429	1.83796997934477	-4.73332372224086
C	5.24126531185044	1.85859705350501	-3.42767835862341
H	5.56840484498368	1.10544703981999	-2.71506622245304
C	-0.00523771362231	6.92682136562749	-3.26573630960116
C	-0.77800422662505	7.05063571034988	-2.10369886193989
C	-0.39075975950370	6.33641107262326	-0.83933335571973
H	0.49050173379317	6.79653462134576	-0.37676885905063
H	-1.20804739528091	6.36509354763736	-0.11391104897905
H	-0.12979524261235	5.29110555921741	-1.03580081723266
C	-1.91915895249500	7.85441449869719	-2.14975482867996
H	-2.53257864840560	7.95499368826855	-1.25735853712631
C	-2.27798825062192	8.51456205802794	-3.31891930287670
H	-3.17281551172950	9.13078305073793	-3.34183916465815
C	-1.48723169846601	8.39657129805640	-4.45648151096910
H	-1.75713482579076	8.92789604534893	-5.36551235405951
C	-0.32830104548679	7.61840636716150	-4.44311272524909
C	0.58444446018422	7.57167962990684	-5.63389209688674
H	1.57491922642055	7.96784693622800	-5.37783123499632
H	0.17503620364734	8.15841494351048	-6.45981505040517
H	0.73640960404766	6.54560713385314	-5.98521299393440
B	-0.88926470443874	2.11368181222420	-4.10272148951056
N	-2.30952768035566	2.14619188750640	-4.37952564737458
C	-2.91683242804545	1.00969312146971	-3.83157345914308
H	-3.98317086847730	0.84324541986492	-3.89818807737854
C	-1.96526714539275	0.25007330889077	-3.24439436649854
H	-2.06711632839000	-0.69146199214640	-2.72209833809557
N	-0.71982474397555	0.87497651876886	-3.38728981934863
C	0.43762456423681	0.26189242221336	-2.82326922482695
C	0.99466809832326	-0.85948606978598	-3.45290000525373
C	0.42074306692926	-1.38936865113196	-4.73574405044143
H	1.13911500174951	-2.04464410669795	-5.23597604926444
H	-0.49312971077641	-1.96825354939199	-4.55336573612395
H	0.15580990453051	-0.57316857319375	-5.41385108039418
C	0.29994704242021	1.94068931535960	-0.94302549630308
H	-0.77486229502152	1.78141736073137	-0.79983995396649
H	0.40342589000349	2.84575468019287	-1.55508605249011
H	0.75934975962583	2.13019802508150	0.03082254843545
C	0.94054199880956	0.75670710671640	-1.61287263519939
C	2.03319400732377	0.10687218251809	-1.03650918702494
H	2.42666524646504	0.46986548946792	-0.09076795852352
H	3.46640343456041	-1.48757087348394	-1.19692992107025
C	2.61295157434619	-0.99480452924844	-1.65477987524744
C	2.09650026433236	-1.47195253165732	-2.85410708252498
H	2.54971750479899	-2.33466173092977	-3.33664616486987
C	-3.10215239302124	3.19337841477787	-4.92726759135708
C	-3.79218634022214	3.01489093989958	-6.14574652038776
C	-3.75407219476182	1.72274786902360	-6.91178881285370
H	-4.67684829629562	1.15954295829622	-6.72277520395500
H	-3.70541362066769	1.91391872197089	-7.98881382264022
H	-2.91059199377155	1.09488851700611	-6.62715320787069
C	-4.61158885639859	4.05879514435054	-6.59626054662324
H	-5.13040205654226	3.94372526766679	-7.54449673668026
C	-4.77718431350875	5.21294477258724	-5.84839513653676
H	-5.41700941831841	6.00936587914009	-6.21778142872147
C	-4.14404950889486	5.34842342972492	-4.61481235274879
H	-4.29757190362140	6.24146539709521	-4.01537699566859
C	-3.31694901125986	4.34289502386395	-4.12880067049788
C	-2.69888161729767	4.43357623579642	-2.76756870352099
H	-2.88735150300869	3.51967255425699	-2.19286318418207
H	-3.09431431262162	5.29332804746720	-2.22385933344634
H	-1.61212684901350	4.55155629467428	-2.83479530276449
C	1.41566793116053	5.24084998614465	-8.57694486384192
O	2.12479852458034	5.15710669337406	-9.45421807188001

T2a

Energy: -6044.38259539 Eh

B	1.77840761726234	1.45853073877993	-0.36347086504850
N	1.66766976495461	1.37729594243538	-1.80035742322413
N	1.85219135210691	2.87717322176296	-0.10680128294813
C	1.66923001148764	2.67083861998185	-2.33269878116594
C	1.78412601981641	3.56521176696197	-1.32265199466676
H	1.60760910207696	2.84635502094602	-3.39811537107699
H	1.83995055898424	4.64413569527231	-1.36927803148692
C	1.52011911152150	0.23144714520873	-2.63244376742231
C	2.65570831597925	-0.52288117959033	-2.96721168811490
C	0.24130476459465	-0.10201597653119	-3.11006301594952
C	2.48520534442850	-1.64874648250068	-3.77444985519670
C	0.11546263253592	-1.23215789745798	-3.91960595718916
C	1.22519802393118	-2.00430363268601	-4.24343515030550

H	3.35344208086640	-2.24637206851572	-4.04040563456064
H	-0.86764332938859	-1.50868807975356	-4.29190390401547
H	1.10927285837474	-2.88401094709416	-4.87053373774349
C	1.87829514616421	3.57084813868231	1.13796757118518
C	0.70493208333476	4.19958653153186	1.58573184181685
C	3.06385501452697	3.60019299763418	1.88581992601943
C	0.74035189105641	4.86497727947011	2.81194750129564
C	3.05548732092911	4.27066869260548	3.11087628127163
C	1.90430881120052	4.89904159021802	3.57124790401732
H	-0.16279034047706	5.34657808303715	3.17814327955555
H	3.96651302223210	4.30246453506888	3.70343837957190
H	1.91450371517890	5.41745229361696	4.52605575254273
C	-0.95630609086900	0.72451349910302	-2.74097645148478
H	-1.03958561129751	0.83920468165675	-1.65438335140536
H	-0.88911237196281	1.73511646533351	-3.15998834233812
H	-1.87435349914775	0.26009439945690	-3.11091680813382
C	4.01828452974641	-0.12492244404338	-2.47375788584483
H	4.79355470924300	-0.71593302359061	-2.96789611652787
H	4.21108924268006	0.93708903076848	-2.65887070081431
H	4.10694214975988	-0.27792047365479	-1.39110228089505
C	-0.56679199112429	4.12098093018923	0.78882137041758
H	-0.77981268793152	3.08911473198419	0.48191929287214
H	-1.41070423368754	4.48713971042162	1.37889063988962
H	-0.50733345086254	4.71721961405328	-0.12875896858710
C	4.31318433596890	2.92381606363865	1.39261299165264
H	4.26327582732416	1.83592857439113	1.53615108370203
H	4.46565108139549	3.09332853563589	0.32232440296881
H	5.18722825150974	3.28775440980434	1.93909669940290
Ge	0.26563031895832	0.72415830091732	2.43524964610115
Ge	2.03955800434897	-0.12156048391453	0.99064303206792
C	-1.28615405391023	-0.14122727715484	1.41754871181226
O	-1.83097503276423	0.60469450246801	0.58973904050460
B	-1.83485469041267	-1.55775051431016	1.79878941842956
N	-1.26228617129556	-2.42391776224076	2.79272918523790
N	-3.02753346283347	-2.23447049528908	1.37312710394597
C	-0.06762304657049	-2.19813657888376	3.53437861023994
C	-2.07479578843896	-3.54502817681789	2.93279938016608
C	-3.13288361029121	-3.42739923934354	2.08563276528829
C	-4.03794501354692	-1.80947494236849	0.45570957500960
C	-0.07127104368126	-1.20260647048048	4.53573572218324
C	1.08096883207353	-2.95319965083245	3.25120362707960
H	-1.83838649437545	-4.34430279447400	3.62173708120668
H	-3.95592743739433	-4.11153144821436	1.92863317817277
C	-5.22394032548122	-1.26421535461436	0.96580954898892
C	-3.81340450454747	-1.94085253210460	-0.91987263438261
C	-1.35007965119791	-0.57856755018682	5.03373295354655
C	1.13604140867359	-0.93400320211428	5.19846176880372
C	2.25080315493657	-2.66501281837955	3.95506625957737
C	1.07175954684589	-4.05165930991445	2.22574360898932
C	-5.41607499206204	-1.08883876806108	2.44635781393993
C	-6.20652718229841	-0.86002011840053	0.06040754935479
C	-4.81988499525825	-1.52484798946759	-1.79370543272089
C	-2.51517757221717	-2.48247384136965	-1.44273699166335
H	-1.13830862529888	0.35175154136524	5.56600688656025
H	-1.83919740659897	-1.26853976512950	5.73387924078958
H	-2.06300503883020	-0.36463143524870	4.23523420326522
H	1.15234388577657	-0.15925189949349	5.96033438308959
C	2.28548582983223	-1.65350106892005	4.90810354132610
H	3.15152366782617	-3.23127839652011	3.73220416030790
H	0.86726892481816	-5.01916665481945	2.70105773982488
H	0.30487804622425	-3.89684655932388	1.46491229477855
H	2.04643030201990	-4.12509431722296	1.73512531917985
H	-4.57677621353377	-0.53654102504083	2.88492006564509
H	-6.33872520769759	-0.54118510451391	2.65255635973574
H	-5.46555279978590	-2.05252751993303	2.96560950216199
H	-7.13033343692970	-0.42976885625612	0.43868489713259
C	-6.00851454992859	-0.99137089653339	-1.30949384369782
H	-4.66367541667037	-1.62315191745343	-2.86513610383491
H	-2.19355649918542	-3.37353372518838	-0.89440557806924
H	-1.71991900401158	-1.73488616159696	-1.33905039519794
H	-2.59935346717240	-2.73273950261213	-2.50345008301490
H	3.21229631396142	-1.42779215407209	5.42728170144956
H	-6.78196100998179	-0.67199767387705	-2.00236167336842
C	0.98852217895217	-1.69187291889218	-0.41917454060425
O	0.91097299453146	-2.73399944739831	-0.87636298137473

T2b

Energy: -5931.07250912 Eh

Ge	29.48237151642648	16.24884231529987	15.03528851699450
Ge	29.50452884879160	17.78238738923367	13.34649615133095
B	30.76553024091699	14.82538222505682	14.19252054036892
B	28.71225621360965	19.39025755763466	12.40729080127207
N	30.70271243338502	13.98900602156212	13.00704481821195
N	31.84509837942302	14.24895258265082	14.95193405447340
N	29.06257966976670	20.00108152721947	11.15680159393660
N	27.60889066640311	20.16131150885328	12.89643215779035
C	31.68430592913576	12.99391599393751	13.10778703963847
H	31.81473470287257	12.24408591424246	12.34007023010553
C	32.36713614936957	13.15062630164764	14.26706496905002
H	33.19101242777779	12.56925832918777	14.65863299813548
C	29.85263963661738	14.06359056403583	11.86543647435540
C	28.46651005053123	13.88387659407015	12.02432570629363
C	27.64728720067101	13.98404537829310	10.89777665465656
H	26.57469800551017	13.84904180827657	11.01423982478745
C	28.18367224751277	14.22842466813552	9.64022272056933
H	27.53172850609684	14.30391960742497	8.77429311931107
C	29.55696067723856	14.36804215574169	9.49371543326144
H	29.98384577693062	14.55230974828948	8.51034530962141
C	30.41366376670106	14.28379942739756	10.59360011447693
C	27.85468673395657	13.56950104155129	13.35878281643532
C	31.89760855068477	14.40805365924671	10.37206349516792
C	32.33053852130730	14.65611498743874	16.22954931321988
C	31.88728231900069	13.97268749754121	17.37144107930254
C	32.36481204264010	14.38562706283229	18.61620900900719
H	32.02761024465150	13.86969727818482	19.51170527657574
C	33.25413847401112	15.44986438793969	18.71835976736780
H	33.61753475109538	15.76061276367557	19.69398632731020
C	33.67668194636467	16.11895217942801	17.57556945670603
H	34.37035220541090	16.95193938112666	17.65809618675687
C	33.22187127641829	15.73495874566461	16.31188643165109
C	30.90057009621417	12.84550769806501	17.25317595313707
C	33.66617610269078	16.46595288854780	15.07626533250126
C	28.19727202312398	21.07866893436717	10.93559664967714
H	28.26525090903846	21.68668570892707	10.04384154928345
C	27.33102019257160	21.17516213756040	11.97621653765546
H	26.53027736358296	21.88455699542330	12.13526431244299
C	30.06922368741825	19.61064368199268	10.22654102534126
C	29.79658727059171	18.56023521083643	9.33568198544174
C	30.80673041263018	18.16568513168509	8.45599104458650
H	30.61450764738873	17.35164690547652	7.76170103963453
C	32.04236995409534	18.80301195164564	8.46080847692325
H	32.81888417282699	18.48409105295250	7.77109026191566
C	32.28822010956930	19.84920768866977	9.34398725503276
H	33.25712939206216	20.34187884720634	9.34710568188073
C	31.30716878044907	20.26973107455978	10.24291853105330
C	28.46330759540992	17.87025714154431	9.34611603550165
C	31.57331852317945	21.37198080695409	11.22847201702934
C	26.87323550083014	19.96422888130092	14.10425963828626
C	25.82217496282196	19.03666099928930	14.11345850923509
C	25.13342487485187	18.83643175787960	15.31157452808469
H	24.31606122893106	18.12044927553730	15.33922856727463
C	25.48532970232052	19.53661678014890	16.45970633167870
H	24.94111755088322	19.36777082954808	17.38469710299463
C	26.53466211281368	20.44852506685333	16.42987967013270
H	26.81287975858322	20.98828980732653	17.33140380389342
C	27.24859277204934	20.67558534169672	15.25204142471589
C	25.46119023213949	18.26679405462739	12.87405160902563
C	28.40184677800037	21.63829813892303	15.21362320313445
H	32.60604215820505	21.71968204323567	11.14968784041890
H	31.39628893089842	21.02817601441448	12.25440595524632
H	30.90738194550081	22.22672769452344	11.06503717509623
H	28.23007672025430	22.44299738021665	14.48990357070316
H	29.32417265259108	21.13027829713934	14.90807797525520
H	28.56317499714370	22.08633222500901	16.19698812079924
H	28.34719301455895	17.24428829262839	8.45824056973378
H	27.64058769797048	18.59148828435675	9.38565176399406
H	28.36533951298732	17.21979864713697	10.22523290787809
H	25.34679942967590	18.92842547253186	12.00906486138643
H	24.52872895695523	17.71627709721737	13.02135218682713
H	26.24761239593455	17.54403732554244	12.62041581102158
H	26.88831500274800	13.07479806248843	13.22667076790944
H	27.67813333563815	14.48600204095385	13.94105151814043
H	28.50500990098032	12.92865904493391	13.96162148923727
H	31.31142558528810	12.00744882953131	16.67923552048763
H	29.99718584404743	13.17450008757606	16.72570620404403
H	30.61291171530101	12.47878860641103	18.24146615519343
H	33.98026241907888	15.77185394473273	14.28982369121502
H	34.49597171441624	17.13960331803263	15.30500356186509
H	32.84363719763869	17.06357240031073	14.66293986750181
H	32.10228434814352	15.12145406834093	9.56765918593862
H	32.32569024627603	13.44313917117215	10.07301453380913
H	32.42611032482725	14.73079768752469	11.26975415735537
C	31.23443573188274	17.47164700364076	11.95404458517561
O	32.31689017274729	17.27119721802552	11.65039879812476

T3

Energy: -6743.67336386 Eh

Ge	-1.82531033483492	4.08874371403804	-5.77781805658025
Ge	0.36401757743792	3.23157403406219	-4.85848011157408
B	1.54554626867528	2.14066711461492	-6.14822005726305
O	1.12750902722243	1.48500846558265	-7.30306688854841
C	2.25595621066940	0.91355454577939	-7.84334964787366

O	2.92512841026366	1.98914315934463	-5.97947444197665
C	3.34928677226627	1.21793134827680	-7.03916647681412
C	4.61931339975029	0.75998934119094	-7.32199785923699
H	5.46295480910563	0.99212157179869	-6.68015668879353
C	4.75203678185748	-0.03149909764224	-8.46853475835031
H	5.73132955906773	-0.41895822005958	-8.73269301553275
C	3.65447528746982	-0.33516998031761	-9.27779776524459
H	3.79777196075557	-0.95227900868494	-10.15953811347244
C	2.37139015413379	0.13683578112694	-8.97811190253340
H	1.51036601329750	-0.09593999117636	-9.59617916683180
B	1.41455384259907	4.89741206736766	-4.20297875817544
N	1.13758046843039	6.25633506348901	-4.61225352984354
C	2.07635351158307	7.11199801993109	-4.02492277769964
H	2.05558576013683	8.17963636582973	-4.19659924743555
C	2.93174820642240	6.38023250735568	-3.27655743024869
H	3.77759403790416	6.70639588616531	-2.68643152657835
N	2.57289925043262	5.02876428800099	-3.35151265675774
C	3.47360685567196	4.05626596109981	-2.81509705003223
C	3.26564411683774	3.55711301085594	-1.52335525527502
C	2.04860838310734	3.94782914664853	-0.73540803635538
H	2.11885136348883	3.58339600809616	0.29285371699874
H	1.90993609039694	5.03404021399958	-0.71741361685125
H	1.14477155984905	3.52189283073835	-1.18692446753938
C	4.86130122792058	4.31379905793321	-4.91723146570585
H	5.23924049185773	5.33851930758207	-4.81226397588976
H	3.94920724843868	4.36549553672949	-5.51643542333830
H	5.60595304250897	3.73206836676898	-5.46680049953423
C	4.60401286238190	3.70370399222613	-3.56911738042888
C	5.51281910582320	2.80134302122714	-3.01347822400397
H	6.38535090889038	2.50592769559925	-3.59103782420032
H	6.04922786300499	1.60886782586469	-1.30666378532328
C	5.32482428199617	2.29856414059896	-1.73143753343186
C	4.21519700901045	2.68414071588170	-0.98972735327384
H	4.07149107221706	2.29847705880694	0.01633802618306
C	0.26339208283459	6.76446993190687	-5.62120673462608
C	-0.89688964716796	7.45614210078446	-5.24893697909869
C	-1.25300930589152	7.62422812281654	-3.80090920344756
H	-0.50674513367306	8.22474338416694	-3.26837437871482
H	-2.22629741111683	8.11002582357662	-3.69658490688510
H	-1.29402488738707	6.65123884336528	-3.30049629768637
C	-1.72245678534681	7.95676889137263	-6.25680403446595
H	-2.63542224335687	8.47900919956493	-5.98220876863899
C	-1.39684298219141	7.78024367319584	-7.59617426749757
H	-2.05212856201260	8.16742153631063	-8.37157413022669
C	-0.22583699942519	7.11808416163879	-7.94732567642483
H	0.04438376298664	7.00877735182707	-8.99480485771377
C	0.62866225068836	6.60717901516256	-6.96720492987220
C	1.91595540114419	5.93145695568541	-7.34663901853851
H	2.75575403378459	6.32588526245021	-6.76437964269441
H	2.12294874722869	6.07437420264069	-8.41026442703940
H	1.87265475555025	4.85190292584633	-7.15889166330556
B	-0.51501349894439	1.87983882240503	-3.55506097370276
N	-1.80608162896838	2.02669129527165	-2.92602979503642
C	-2.12637458791437	0.83592970633868	-2.26159317734035
H	-3.05152292671556	0.72163725789360	-1.71357464900257
C	-1.11713784896219	-0.04936982026465	-2.43407767542300
H	-1.01996950415015	-1.05668764272080	-2.05254527390992
N	-0.12174618395981	0.53659930920915	-3.22187864043320
C	1.00392305141713	-0.20819005212950	-3.68869835341621
C	0.94179498796684	-0.80002805797319	-4.95974878278667
C	-0.32832723617196	-0.78191467382285	-5.76404171230090
H	-0.15609030646826	-1.18616437302312	-6.76444590345501
H	-1.09755602261113	-1.39100401577046	-5.27282999859611
H	-0.74121620304968	0.22399166430782	-5.87572079553971
C	2.09035070098150	0.15156372286316	-1.44468962688474
H	1.38531770358569	-0.43254139944784	-0.84071022140510
H	1.76356487420642	1.19371111474116	-1.39887856377804
H	3.07826191951828	0.07760463656384	-0.98650377246732
C	2.12054005435766	-0.35426954995875	-2.85715712945557
C	3.23597783596033	-1.02668590209093	-3.36096539725045
H	4.11935310684187	-1.12968567643764	-2.73554649974878
H	4.09913584079319	-2.07287581013468	-5.02942540943437
C	3.22058596217899	-1.56348982833089	-4.64312262498604
C	2.07649982116305	-1.46759669159126	-5.42727387981930
H	2.05622281161927	-1.91588907493379	-6.41740456770752
C	-2.79562662097792	3.02824255968457	-3.14120998667172
C	-3.85217551811017	2.75407180994418	-4.03660732015964
C	-3.94443632298281	1.44564216929002	-4.77190398755485
H	-4.39604844205955	0.67495392914568	-4.13578801582176
H	-4.56411364570151	1.55606233417265	-5.66467398143402
H	-2.96261955533776	1.07691640133411	-5.08040883940205
C	-4.84725407009363	3.72544592378052	-4.20084695083542
H	-5.66050766938509	3.53186682690829	-4.89516981163335
C	-4.79491041966116	4.92348881982010	-3.50462448229365
H	-5.57430368471386	5.66679596656560	-3.64582024764323
C	-3.74434054833668	5.17800512303481	-2.62841129332643
H	-3.70930369379934	6.11665875573961	-2.08183641587129
C	-2.73143624153861	4.24071179685086	-2.43043932929747
C	-1.60297180997650	4.51410634292225	-1.48023905093321
H	-1.43011053890530	3.66405958465618	-0.81243988370616
H	-1.81004478314297	5.40328547007224	-0.87939466495080
H	-0.66639216908024	4.68415188311688	-2.02564793220290
C	-1.80885498055025	2.81433898601896	-7.26208734032137
O	-2.21879945001984	1.74126897930190	-7.70092250784060
B	-1.19629699101828	3.74497374980108	-8.47419756917995
O	0.10660636757244	3.71839141118261	-8.95012460349989
C	0.07102570051885	4.41325247302253	-10.14231898263596
O	-2.03871958287210	4.43641963319018	-9.34013715915347
C	-1.22928362801573	4.84897824631227	-10.37831816231781
C	-1.56228617143419	5.59660476805005	-11.48901243402450
H	-2.57812834750492	5.93580550302888	-11.66258226660825
C	-0.51769816856365	5.89224551138123	-12.37177877677729
H	-0.72865667209403	6.47796875174987	-13.26114648716264
C	0.78692742359198	5.45221583661245	-12.13568537350754
H	1.56953482810998	5.70217656047577	-12.84530158191399
C	1.11051601363101	4.69546218444870	-11.00429916635841
H	2.12029163007826	4.34969898946402	-10.80852021981335

T3a

Energy: -6044.38661963 Eh

B	1.75902763663787	1.22551970327128	-0.31750591769789
N	1.00625473810515	1.52859378722165	-1.52334985153473
N	2.17258001732886	2.54756327914688	0.14276185272594
C	1.00808818547224	2.89739949356415	-1.73542191563769
C	1.70078354545775	3.50714428811400	-0.73363313298932
H	0.52893887399509	3.34055433823170	-2.59833677660887
H	1.90002959953087	4.56053796758220	-0.58966350607658
C	0.42081089600605	0.64798428752611	-2.48738214871134
C	1.24120753498412	0.08257622004783	-3.47387870076248
C	-0.95931832915664	0.40631117779585	-2.43926887279742
C	0.65366319120258	-0.78102001230749	-4.39946282446310
C	-1.50587328549947	-0.47216461569764	-3.37579618472646
C	-0.70565302173629	-1.06666827910829	-4.34381024676751
H	1.27549294465737	-1.23732735981672	-5.16532296812729
H	-2.56843403066567	-0.69738533677265	-3.33226784262399
H	-1.14565764796234	-1.75288353591559	-5.06220583360571
C	2.90981863923644	2.90563658317107	1.31411043067198
C	2.22868405097155	3.48306446461411	2.39976027669617
C	4.29691639700049	2.69457472916046	1.33932637795531
C	2.95966031800413	3.78140828967941	3.55037881295929
C	4.98924331147250	3.01284663935499	2.51069801869817
C	4.32694073107269	3.53810051797523	3.61231070879919
H	2.44391702127480	4.21106301226138	4.40546372702140
H	6.06416075196048	2.85400998818029	2.54653570714317
H	4.88021925348659	3.77440304316568	4.51698442259602
C	-1.82949407628893	1.06703258828967	-1.41174800571946
H	-1.43725096692146	0.91914002976009	-0.39810327481083
H	-1.88403371699809	2.15038775975660	-1.57182903754083
H	-2.84215619999948	0.66044244130508	-1.45663992081544
C	2.71240889278990	0.38263070307212	-3.53027057240881
H	3.14306015654187	0.01122554514669	-4.46342559659397
H	2.90591638175483	1.45828398194477	-3.45781053791076
H	3.24547518815725	-0.09088764121746	-2.69566641233354
C	0.76012782513810	3.79530791962434	2.33384962696675
H	0.19707250964823	2.96692669231366	1.89125830632333
H	0.36688771334198	3.98535530762217	3.33611694625995
H	0.57332443869889	4.68658005361686	1.72274550038774
C	5.04428404596974	2.17527236951694	0.14250386221633
H	5.02302655140110	1.07913276618534	0.10258505429989
H	4.60579349628411	2.53472211339339	-0.79297279878180
H	6.09062585125336	2.48956356576944	0.18684068650360
Ge	0.78966371838430	0.13156133407866	1.67579443393493
Ge	2.68403562056594	-0.62156884110155	0.29236813278338
C	-0.47119211859147	-1.24901652555539	0.84879680326806
O	-0.35841843721218	-1.68854346902780	-0.33879361348525
B	-1.70453894495488	-1.70368169628348	1.67368418977635
N	-1.82140027043453	-1.61875302412471	3.10607893648416
N	-2.94191352377116	-2.30884231093814	1.24591871503940
C	-0.86192392675419	-1.13098843291546	4.04252724256627
C	-3.04872859004461	-2.14367652137106	3.48438221455359
C	-3.72475184627674	-2.54044194524688	2.37000403754170
C	-3.43978050243560	-2.53222850792785	-0.07497218445590
C	-1.06815341254187	0.13228895178936	4.62160059704243
C	0.26537807234583	-1.91244206840481	4.34020013981265
H	-3.34252638613900	-2.22269693411963	4.52224982041426
H	-4.70876975230743	-2.98333759646003	2.29621250022701
C	-4.38953872254148	-1.64179895406613	-0.59625645968462
C	-2.97323712998853	-3.63375599488867	-0.80467398294665
C	-2.24996658887222	0.97082562935480	4.22901767561622
C	-0.11187321606467	0.60879033609895	5.51603464987312
C	1.20333954296349	-1.39142156048916	5.23542284651328
C	0.46710645202865	-3.26876737791816	3.72210154387791

C	-4.87702958751792	-0.46665152914892	0.20601254055295
C	-4.86601884188624	-1.86986664793837	-1.88886142836829
C	-3.47330164792252	-3.82498196150468	-2.09409038779222
C	-1.96717554786721	-4.58201230591625	-0.21931155298700
H	-2.19494488018956	1.95572269430063	4.69887040827637
H	-3.19875549719918	0.50433126440232	4.51573085090569
H	-2.27425381043077	1.10505901775949	3.14019749390424
H	-0.24737484527137	1.59038311077191	5.96273971449457
C	1.01781462960567	-0.14435275131068	5.81771533831158
H	2.08605704753128	-1.97823713311588	5.47540206993842
H	-0.46600825171549	-3.84009900995279	3.69330795528956
H	0.82727104241777	-3.18392668561755	2.68925224924276
H	1.21063369175988	-3.83654554305598	4.28691316353239
H	-4.05092671446319	0.03435511543737	0.72191604895313
H	-5.37766018825364	0.25853643413522	-0.44092504698383
H	-5.59205937551809	-0.77731478380255	0.97697042321840
H	-5.59576063009640	-1.18447587958177	-2.31303761896240
C	-4.41107913144728	-2.95198734069423	-2.63343224878530
H	-3.12040635577591	-4.67236608735710	-2.67614887065108
H	-2.24988330062007	-4.88986111219390	0.79297333343308
H	-0.98226144211797	-4.10619998241299	-0.15336476398318
H	-1.87297179133604	-5.47403297719926	-0.84348348508974
H	1.75967981166785	0.24533521288795	6.50897209157149
H	-4.78800388594326	-3.11501311823494	-3.63942521567935
C	1.39295262541166	-1.77102080162198	-0.87452487160154
O	1.47988817621192	-2.65326521806343	-1.62598069767213

T3b

Energy: -5931.06256764 Eh

Ge	30.12607415315350	17.59811368112429	14.35576786449753
Ge	29.09317649995878	16.67928880265482	12.25534184147241
B	31.04119598363250	15.69752425215917	14.31419818642130
B	28.13131111171773	18.74179767464598	11.90269355324191
N	30.52808574508083	14.34398875484735	14.35010497887629
N	32.46688882708156	15.52339789996063	14.40562048236540
N	28.83170421413663	20.01153501012207	11.92539205441654
N	27.16380316981196	18.90567420767113	10.83732646928987
C	31.60410623343603	13.45666873673598	14.47119273716545
H	31.45707626101661	12.38889141446424	14.55562850378180
C	32.76305003663943	14.16027620920350	14.49729857579069
H	33.77868462391051	13.79947689527465	14.59141021179197
C	29.18603473863533	13.90569075910356	14.16594139141306
C	28.20155319120752	14.28557016860024	15.09380786855220
C	26.88284449275167	13.88892211616739	14.86280706395717
H	26.11308458684798	14.18455343264974	15.57114645200239
C	26.54875056887735	13.12825696642161	13.75010403588412
H	25.51755782310209	12.82937089650592	13.58491415586595
C	27.53442399927684	12.75978477391316	12.84217721734658
H	27.27072246850182	12.18513863346665	11.95779218418330
C	28.86212174098409	13.14647119224344	13.02618930881612
C	28.53089806751278	15.11708491902525	16.30020179513134
C	29.89403004706126	12.80674800288707	11.98530319769690
C	33.46609773351628	16.53850832872759	14.33159386013447
C	33.85840706450736	17.20066593598546	15.50344829521662
C	34.83023659148757	18.19920022289483	15.40300520394647
H	35.14749472469718	18.72203852746214	16.30179312306708
C	35.39479994546256	18.52220780623435	14.17428415676300
H	36.15457531824857	19.29680646271202	14.11391332841482
C	34.98766872142048	17.85872477666991	13.02158710615329
H	35.42598602811358	18.11688655603610	12.06051092537612
C	34.01347119275788	16.86059577278033	13.08055653816602
C	33.23981256455423	16.84807628774842	16.82630963934859
C	33.54875487201092	16.15201776257325	11.83950169792647
C	28.30544837728792	20.83036368179850	10.93867968316755
H	28.67769298670763	21.83216284844474	10.77102896554540
C	27.30964614873656	20.16747942691497	10.28588279109485
H	26.69307245059639	20.50629389259271	9.46407401017173
C	29.89563543968838	20.44472428913200	12.77503123276845
C	31.21926195592635	20.15261560692713	12.41250200482594
C	32.23527983880312	20.50613215419021	13.30478780770500
H	33.26470804632368	20.26024164647516	13.05847449214760
C	31.94055932444864	21.16075486372698	14.49503433185994
H	32.74262359852773	21.42481056440831	15.17878354973521
C	30.62550029870511	21.48271150587855	14.80891890183545
H	30.39847347634137	21.99947841076630	15.73784557788928
C	29.57906407657924	21.12289503341735	13.95857790798655
C	31.54072263210893	19.49374268910218	11.10157549350283
C	28.15040002957046	21.41509628242340	14.31878871903414
C	26.20896320513931	17.96446920155546	10.33648209436806
C	26.58482800173862	17.11107929824044	9.28962204450184
C	25.65254740183661	16.17385411500556	8.84018429698114
H	25.92894853530923	15.49563592959562	8.03693506706335
C	24.38440688756265	16.10439316628136	9.40510631814166
H	23.67145487337925	15.36643919596360	9.04798497054170
C	24.02113554355553	16.98639502090695	10.41599589001504
H	23.02222924497471	16.94432585349428	10.84253679818107
C	24.92406359201465	17.93803972395581	10.89542342438611
C	27.93651895022372	17.22370026109510	8.64260390788871
C	24.51479623359984	18.92943226733226	11.94802919777304
H	28.09877639515024	22.00347995013087	15.23802757554874
H	27.58824895851208	20.48636898300681	14.47180007805500
H	27.64011341783523	21.96851681220214	13.52294485810694
H	24.53138707733310	19.95009633148423	11.54728548124822
H	25.19191082045306	18.90876666155698	12.80665654487138
H	23.50134349638979	18.71820463034313	12.29790107843086
H	32.60584726800193	19.25365554658908	11.04544089699193
H	31.28848797677245	20.15108994952951	10.26080707419913
H	30.96596408292775	18.57051558307718	10.96814541595847
H	28.02767701560347	18.16703132934937	8.09044831767299
H	28.09748031085640	16.40129269197537	7.94127906215164
H	28.74033766426304	17.21161777948149	9.38582951624807
H	27.76190103289371	14.99770189308182	17.06828725361027
H	28.56212705637708	16.19084220069176	16.05265253376369
H	29.50610378000312	14.85838180616641	16.72213522915321
H	33.29190074933356	15.77089294323255	17.01671358330609
H	32.17746861464251	17.12187776821926	16.84429102070835
H	33.74370796926554	17.37417711096257	17.64082416524228
H	33.73176091974742	15.07334687155284	11.90150446602679
H	34.06119982650694	16.54109573756393	10.95608521192482
H	32.46820915620531	16.27927769256703	11.69973308027500
H	29.40549713673266	12.55625683986914	11.03999838744186
H	30.51079836062761	11.95034176017845	12.28058755197634
H	30.57671034286319	13.64677589816367	11.81564991165287
C	27.80490706566433	17.68983487891441	13.27424535449526
O	26.94240132417653	17.96775980077554	14.07491615732757

T4

Energy: -6743.65854315 Eh

Ge	1.56109883752504	3.83349132670153	-0.48824225751888
Ge	0.24008011382842	3.55416646583349	1.44978121079889
C	0.59532778285584	1.61122185641386	2.06160753757115
O	0.01624077443581	0.64361312434804	1.56937816321075
B	1.43641776386378	1.44945122498187	3.39947135274513
O	2.40412984121359	0.48404392890260	3.63443638471574
C	2.88937210192627	0.76512497829136	4.89548189919000
O	1.26659106107440	2.28484743986432	4.49925107919293
C	2.19350869259542	1.84919853261505	5.42340867947051
C	2.46921959994273	2.36209215195085	6.67382707636224
H	1.92397901003593	3.21138408927246	7.07180311722619
C	3.50073172701126	1.74008516303155	7.38494388653470
H	3.76100030635735	2.11213838618980	8.37106281805862
C	4.20287871072720	0.65505533397675	6.85485540181007
H	4.99574188066952	0.19722030388994	7.43824244503317
C	3.90661619594489	0.13991681761590	5.58771098413113
H	4.44352743191795	-0.70514214563819	5.17022852319564
B	2.40992942976727	4.32739968749875	1.59994705664541
O	2.87937291555475	5.63107847530069	1.78109953814281
C	3.80350911200097	5.56294715434899	2.79728505535296
O	3.08685383722402	3.45460251766035	2.46577972266792
C	3.91137795824045	4.24540243619032	3.23195265013469
C	4.74149044332812	3.87881488438417	4.27352460917399
H	4.81551549650831	2.84950787932678	4.60643813024668
C	5.48791610039474	4.90282550132588	4.85740557567612
H	6.15785217319437	4.66468399220837	5.67786858958505
C	5.39499016850738	6.22523112262869	4.40904963490497
H	5.99303455050514	6.99299025048669	4.89029026382490
C	4.54424021207418	6.58491564218406	3.36209305870401
H	4.45756902425963	7.60881138645236	3.01719892399057
B	1.22950370241821	5.77129341662032	-1.16585144055472
N	2.08586144964613	6.86923245237035	-1.55800425004328
C	1.28593056916643	7.95161482129719	-1.93563152885757
H	1.72060206715188	8.87796235446419	-2.28456059595018
C	-0.01772003159312	7.61708485158393	-1.79750587558319
H	-0.90253983008319	8.19905125726078	-2.01648647199320
N	-0.10112397798469	6.31031874044222	-1.32029128678150
C	-1.37421833608362	5.70683245733339	-1.08589046963030
C	-1.95338595087089	4.94527791827708	-2.10728134186139
C	-1.27947614552311	4.82338432672739	-3.44284010670186
H	-1.94292583239745	4.34776587125684	-4.16693728773109
H	-0.98395416880735	5.80613385029291	-3.82617488416137
H	-0.36867982045678	4.21689553799084	-3.38128472255167
C	-1.42067413543657	6.83145635455975	1.17735704454896
H	-1.50520307469297	7.88091152654468	0.86859905584928
H	-0.35619341621232	6.62418721634167	1.32807440062127
H	-1.93449652026783	6.71382254480957	2.13451190429906
C	-2.01713866949715	5.92243760299592	0.14030852168964
C	-3.24162171311724	5.28642403589620	0.35722310247202
H	-3.74820239476660	5.42332948156881	1.30924344566225
H	-4.76061359257092	3.98967223991293	-0.43663847512472
C	-3.81134189057906	4.48347818585853	-0.62503377522519
C	-3.17871298832648	4.32546003362287	-1.85319785508492
H	-3.63801262942693	3.72106465172614	-2.63148895285738

C	3.50250943149681	7.04917552460495	-1.52518624089596
C	4.29837829941952	6.43344662859883	-2.50027744156133
C	3.69786335291159	5.51323512723357	-3.51984907485094
H	2.78962567220010	5.93277918503517	-3.96534316637822
H	4.41604359840404	5.29684146586406	-4.31488532904856
H	3.40922133586108	4.56085294572964	-3.05681451925090
C	5.67198303412894	6.68342539008189	-2.49232031529191
H	6.29830372265021	6.21250734417537	-3.24597447910353
C	6.23982996662153	7.51344570335342	-1.53462677603143
H	7.31154830890277	7.69224956135247	-1.53605248938019
C	5.43489653340819	8.11947172528772	-0.57701796401681
H	5.87710624306523	8.77541597793642	0.16885803000605
C	4.05364558809069	7.91388144862952	-0.56469249864527
C	3.19001139711457	8.62992066710816	0.43592669936523
H	2.64428186382316	9.45733959117397	-0.03175831745153
H	3.80482179371752	9.05332151456067	1.23434044646207
H	2.44657938992168	7.95962444183263	0.87564659746262
B	2.64299767941999	2.39443381624994	-1.51058754223784
N	3.86654671003938	1.73273980349792	-1.13437526839658
C	4.19607729612506	0.80420166055796	-2.12855181848779
H	5.08822028407799	0.19753650237593	-2.05638814258951
C	3.25693161768786	0.83193449508749	-3.09800407094745
H	3.19208727574545	0.24991191205241	-4.00687844660965
N	2.27969175716865	1.78010952148777	-2.76865691748474
C	1.10650839379071	1.86052220156887	-3.58312983106946
C	-0.09706242936975	1.31583409061831	-3.09529065841561
C	-0.18517656199275	0.69024003190626	-1.73403136776670
H	-0.22805215399147	1.43914321744386	-0.93658378467008
H	-1.08491896393871	0.07529725490894	-1.65358508723353
H	0.68766481781401	0.06311121001935	-1.52376760677453
C	2.49863163363971	2.85545990695888	-5.47558788624367
H	3.25296228672723	3.04133156748454	-4.71195853360597
H	2.33435400484001	3.77854769087176	-6.04080018155424
H	2.91143059441120	2.11652875614704	-6.17356275292286
C	1.20413423564792	2.35661520745865	-4.89294856782741
C	0.05991716673940	2.34362491264283	-5.69589995177432
H	0.12470816863175	2.73376814676674	-6.70912046599675
H	-2.01845583102194	1.82579922866217	-5.86212183542678
C	-1.13971617957721	1.83285121578267	-5.22284063303855
C	-1.21397994388338	1.32327906472853	-3.93206992387576
H	-2.14649269824569	0.90154593972294	-3.56567318232456
C	4.64066132513724	1.74126643140208	0.06817026617597
C	4.53097379910426	0.63917150539013	0.93029568765116
C	3.54123502008916	-0.46093469238832	0.66919047040748
H	3.85535906323003	-1.10094153433143	-0.16345083445570
H	3.42458618436182	-1.08482952233581	1.55740631148763
H	2.55982071450665	-0.05369696184392	0.40289553509604
C	5.36292028469931	0.59339548486757	2.05008970090857
H	5.28860091666257	-0.25461780300175	2.72549582700612
C	6.26842397072306	1.61391214968494	2.30886663784844
H	6.90966950845451	1.56236911137248	3.18479563781655
C	6.34339589674642	2.70872903690196	1.45669027474842
H	7.04076806062502	3.51615657907819	1.66673295304123
C	5.53363792875011	2.79061563586124	0.32282642211973
C	5.62457942535440	3.97664021613678	-0.59008716931950
H	5.59715624952065	3.68193313284483	-1.64391143907649
H	6.54241315389253	4.54028140968432	-0.40603821839988
H	4.78560587643664	4.66755259104761	-0.43639799657149

T4a

Energy: -6044.37141882 Eh

B	1.29738187805477	1.38674568566561	-0.27601393582215
N	1.05416092941971	1.99291892442196	-1.58202086926228
N	2.42958024831118	2.17176806147429	0.22516602403530
C	1.95981682087538	3.02045285862084	-1.78917740384824
C	2.77344326235483	3.13323110928198	-0.70246068508681
H	1.96073151309057	3.60158875878676	-2.70167113882644
H	3.57484156642800	3.83833576394362	-0.52543739605033
C	0.14585610218656	1.63728115695098	-2.62939034482010
C	0.65235818896459	0.94161542635774	-3.73815252984603
C	-1.19867409293185	2.02004769272855	-2.54679501189550
C	-0.22224771020315	0.63088508403943	-4.77775868926404
C	-2.04485565610249	1.67934506366269	-3.60528678368860
C	-1.56245303743166	0.99424867084139	-4.71256728067407
H	0.15114290876271	0.07751374936152	-5.63532804092453
H	-3.09273538523844	1.96420672267287	-3.55513221159949
H	-2.23443875126337	0.73803963153567	-5.52671065365620
C	3.02722236946881	2.14294623142784	1.52341725911991
C	2.60643681000261	3.07947660342093	2.48174266421293
C	4.03269798787523	1.20377326139211	1.79901203241521
C	3.17209567588730	3.01704212574286	3.75677671121933
C	4.57234558637728	1.17722769032656	3.08677019976336
C	4.13935264084043	2.06819886042987	4.06172301482281
H	2.84453549042957	3.72480397828986	4.51405035882205
H	5.35223195645599	0.45547238185708	3.31642315694291
H	4.56803621295407	2.03124766948745	5.05954260082477
C	-1.74373564563478	2.75511348721446	-1.35582474156809
H	-2.04119769336250	2.04524368251025	-0.57017764707549
H	-1.00995729628595	3.44051642512130	-0.92188599873182
H	-2.63774558009849	3.32209191165293	-1.62969516671486
C	2.08698887648872	0.49856270784910	-3.78051093163838
H	2.25407357439076	-0.17593203005565	-4.62347580463318
H	2.77353121233189	1.34736389586794	-3.87837830719538
H	2.35941035561852	-0.02602737699931	-2.85701571162290
C	1.60593463133346	4.15150473828327	2.15116702882095
H	0.81206086025609	3.78345433312850	1.49493513018659
H	1.14853428672433	4.54252039514248	3.06379139034346
H	2.09003034833673	4.98795108428874	1.63172604492382
C	4.55158098001978	0.27973710131333	0.73517239997760
H	3.82172250202853	-0.50662415449310	0.50613865193133
H	4.74526143931740	0.81712169781997	-0.19910181558603
H	5.47797231482327	-0.19826310550264	1.06346239621829
Ge	-0.23461485272314	1.06748401928733	1.37902683635074
Ge	1.06977016227146	-0.82202292859241	0.16789575948089
C	-1.03804218840690	-0.59087068697935	0.71836255187303
O	-1.52334218199372	-0.71917263012890	-0.68311761299881
B	-1.64525868152779	-1.65976720279025	1.64522827845219
N	-1.50561548157306	-1.70725879140231	3.08050788936836
N	-2.42359382812127	-2.83033870194530	1.32481799745262
C	-0.90086475049141	-0.73535348003362	3.92709810284250
C	-2.16437505026667	-2.84186684053791	3.55992956579219
C	-2.70672049201627	-3.51298525779616	2.51316179274328
C	-2.86687523922868	-3.32218558610445	0.06030449489362
C	-1.66760480104685	0.36106439896419	4.35456575686776
C	0.44624508303983	-0.88614644767007	4.29658333859037
H	-2.20346235259162	-3.07497483061410	4.61527395833502
H	-3.28126587194451	-4.42926275299640	2.51460517219889
C	-4.06929503227560	-2.83994737965240	-0.47178189092664
C	-2.07994425638947	-4.26109778742272	-0.61847513006827
C	-3.10562083533514	0.49182778392267	3.94079325018761
C	-1.05067360395928	1.33007981381493	5.14675986489285
C	1.03088307259966	0.11424982480423	5.07549277494445
C	1.23141836546391	-2.08438348762552	3.85356403943163
C	-4.86341706313072	-1.79564242111110	0.26042927089906
C	-4.48646699978065	-3.32922551345447	-1.71027202024582
C	-2.52800834687930	-4.72641964874528	-1.85653780066162
C	-0.77300336724496	-4.72504423046142	-0.04016334892746
H	-3.57535664041734	1.34389631542190	4.43812558006769
H	-3.67485318795306	-0.41328666850827	4.17838828477262
H	-3.18742227781558	0.63854721941702	2.85598426720528
H	-1.62839220924927	2.18680427470030	5.48450188437486
C	0.29078599821984	1.21340925071870	5.49431477656399
H	2.07830112966274	0.02624745053872	5.35134030922246
H	0.75309241621371	-3.01645274487520	4.17375113936017
H	1.30076005457179	-2.12152229536409	2.75787641512912
H	2.24636053171459	-2.05158398324769	4.25749650074805
H	-4.31565913896747	-0.84521427122596	0.28878054998866
H	-5.82322747792978	-1.62201305711867	-0.23270119885677
H	-5.04884892266575	-2.08617788005521	1.30007599203032
H	-5.41636077277831	-2.96469153835161	-2.13965690654532
C	-3.72259787591680	-4.26649172023150	-2.39782365622636
H	-1.92433376178796	-5.44744531078921	-2.40171201286141
H	-0.90984446390222	-5.20043969051763	0.93758007376264
H	-0.09091038221250	-3.87932193731988	0.11529918507420
H	-0.28579199992991	-5.43789662830300	-0.70971982308080
H	0.76234316808475	1.98256114788834	6.09980131207388
H	-4.05712308342726	-4.63511730584860	-3.36349936553512
C	-0.46232317502749	-1.19191027678023	-1.33111429799742
O	-0.14141564954323	-1.72067403958890	-2.35287226552064

T4b

Energy: -5931.06576282 Eh

B	1.12676634876333	1.59378573297241	-0.42195591059125
N	1.80746014763656	1.41811259679817	-1.68003436748493
N	0.57563024340157	2.92059519960411	-0.51834550319345
C	1.64514069691929	2.56709986996343	-2.46039983996641
C	0.90908086602804	3.46685796467115	-1.76059732632412
H	2.07762739615157	2.65878255204140	-3.44748656275521
H	0.60696997589466	4.46614362954010	-2.04407013593267
C	2.43362016007317	0.24041567491657	-2.17059092287867
C	3.76458415276050	-0.04116843777698	-1.80231207377585
C	1.71487763826401	-0.60212854030242	-3.04273083395578
C	4.36458015225946	-1.18777260731295	-2.32589366220150
C	2.36594688657690	-1.72498012389289	-3.56305910347341
C	3.67617228738449	-2.01484128845061	-3.20922828342654
H	5.38887106293850	-1.42177991665142	-2.04804500390472
H	1.82567841985085	-2.38102998925651	-4.24038914363802
H	4.16450813945761	-2.89637559801639	-3.61464236152513
C	-0.25509184711829	3.61179551050884	0.41339868353960
C	-1.63819458004880	3.66289611552403	0.18295642417095
C	0.33055520613454	4.21984040472704	1.53278939115830
C	-2.43499444778042	4.34997285155140	1.10073441026209

C	-0.50254005705733	4.88710297115252	2.43383708003600
C	-1.87430319152480	4.95589819210366	2.21906032176256
H	-3.50792620472747	4.39875947078718	0.93355436175927
H	-0.06391688255841	5.36440447293625	3.30665646939807
H	-2.50824302161678	5.48419953392506	2.92621500953742
C	0.29353865341419	-0.28750135599831	-3.40915664217705
H	-0.29708365010002	-0.04212593867437	-2.51936086973879
H	0.24164982298187	0.58182382575476	-4.07549118207658
H	-0.16802670153355	-1.13713392031309	-3.91801975765180
C	4.51175410260725	0.87602585549660	-0.87916638406272
H	5.55876030988610	0.57399371292820	-0.79991944332554
H	4.46526176492265	1.91217893037586	-1.23040107768395
H	4.06950976474768	0.86228304391809	0.12484902422393
C	-2.24812078466409	2.98356237656098	-1.01034427413325
H	-1.89176126959918	1.95185253546030	-1.09359390866843
H	-3.33821735556033	2.97129000374079	-0.92848377560150
H	-1.97950458659398	3.49348618064006	-1.94319820818937
C	1.81496338480094	4.15777375499967	1.76015015395544
H	2.12385538661140	3.14792373139734	2.05776663259160
H	2.36896366825611	4.40326605382170	0.84813181690583
H	2.11204498154622	4.85109581837057	2.55129345644268
Ge	1.04182673037864	0.30852954685353	1.21726442587021
Ge	1.57014404728432	-1.57761715159332	-0.06312805451488
C	-0.76391854434192	-0.81603096360809	0.63683434201992
O	-1.44534473903278	-0.32772372020752	-0.25711767319599
B	-1.37603454404932	-1.69655538066529	1.77279156829225
N	-0.76414453111256	-2.70904319503306	2.58547536415445
N	-2.72218770628328	-1.58844419893780	2.26253960225313
C	0.53625784908220	-3.29394264862676	2.50052047309658
C	-1.71336619789418	-3.16853409119991	3.49719236556304
C	-2.87627011102663	-2.48709290285419	3.31381230763857
C	-3.76685604569824	-0.69813423600180	1.86381492325939
C	1.52800478982788	-2.87799367344525	3.40427855469956
C	0.76438591690859	-4.31298933813756	1.56025184083457
H	-1.48817775534750	-3.95872717607005	4.20039471037016
H	-3.80478845266086	-2.56692463898839	3.86285691098678
C	-3.72673781359179	0.63527474319382	2.29163800059227
C	-4.79677337491917	-1.18936418771492	1.05086006065484
C	1.23611844936382	-1.82098351163170	4.42856313620007
C	2.78387141796379	-3.47931884422165	3.32006821145221
C	2.03155745617366	-4.90011493576648	1.52232519179609
C	-0.32873215516626	-4.77146929458678	0.63638142103534
C	-2.59351090432758	1.15201129021799	3.13071553354004
C	-4.76590133386436	1.48088246181132	1.89557684116808
C	-5.81412134654802	-0.31175284290939	0.67364306876438
C	-4.78413447413463	-2.61469645696736	0.57430002018511
H	2.14547381701376	-1.54664175742620	4.96863843654528
H	0.49373042651297	-2.16937173518242	5.15608552607519
H	0.82682431553775	-0.92128014266409	3.95382723441304
H	3.56987096398218	-3.15876628857750	3.99868677613813
C	3.03397098115880	-4.48141317414545	2.38768672421996
H	2.22820011745498	-5.68696638241029	0.79914741911566
H	-1.24709950004171	-5.00035070490021	1.18795586093095
H	-0.57800535406764	-3.99444054784872	-0.09681262610413
H	-0.01609371364917	-5.66277154456741	0.08739629339093
H	-1.68505363677094	1.28451950954583	2.52619789774562
H	-2.84601223493009	2.12447606597338	3.56057695405515
H	-2.33937241592612	0.45849268053949	3.93916435264736
H	-4.75508899646265	2.51602898219261	2.22612102444029
C	-5.80102830603943	1.01382318019666	1.09469047855856
H	-6.61816471825654	-0.67413226759741	0.03810292068500
H	-4.88362617060279	-3.32076650973855	1.40647620374523
H	-3.83737929489292	-2.84767023389573	0.07312493601205
H	-5.60317882734651	-2.79418560474637	-0.12634289380331
H	4.01701282507541	-4.94138983738131	2.33949475211375
H	-6.60139394451910	1.68538080918197	0.79625190495144

T5

Energy: -6743.63944804 Eh

Ge	0.01106899682611	0.44320700008663	-0.61431800300641
Ge	-0.49078695359309	1.15891299581540	1.55142502009186
O	0.80147497513778	-1.87795797427083	1.71769595233565
C	0.16042405759267	-1.10604607609944	2.40536610640877
B	-0.85148001440695	-1.60698397930156	3.52074597026600
O	-1.97166120936597	-0.89672371119852	3.91623851059666
C	-2.56738259931401	-1.68295994927503	4.88005151436257
C	-3.73769783701393	-1.45698983604651	5.57482582351715
C	-4.10786858302139	-2.44061823735432	6.49742440798345
C	-3.33309894475984	-3.58647855142098	6.69703209934050
C	-2.15000873952351	-3.80451538745097	5.98354867204363
C	-1.79716018098825	-2.82634755513901	5.07668836989900
O	-0.70666236625932	-2.78879277737018	4.22988471417805
H	-4.33267385373057	-0.56497730154534	5.40990848176783
H	-5.01981327321679	-2.30901078678083	7.07151533817033
H	-3.65597640727739	-4.32726661219136	7.42193326177830
H	-1.54311780525520	-4.69215839527850	6.12792441368460
B	1.02935893740837	0.48106203218465	2.77746795698030
O	0.93085842445477	0.57772381461561	4.20653682374060
C	2.21602486442990	0.66725155771340	4.66554815230726
C	2.65402728335595	0.80631199244287	5.96828458590142
C	4.03840142008087	0.88436656671508	6.15943908711858
C	4.92610139078166	0.81765625365395	5.08342145156227
C	4.47133581876638	0.66961845993866	3.76797053838190
C	3.10288676196661	0.59600434283172	3.58786533990963
O	2.40926507152892	0.45391697597003	2.42350006941026
H	1.95485948214982	0.85640994156969	6.79673027923121
H	4.42770093647031	0.99948093581966	7.16637453140576
H	5.99407412716375	0.88058422020940	5.26927494971261
H	5.15395941865788	0.61179806862707	2.92619474907437
B	0.00304381036640	-1.49494191000518	-1.29783816943280
N	-0.89922585749638	-2.57583682069643	-0.95668562265343
C	-0.47360524260171	-3.72857239093274	-1.62697100779439
C	0.63392125906986	-3.44901761725613	-2.34961927586958
N	0.96714326513053	-2.10062907311480	-2.17823766077342
H	-1.00832867346953	-4.66339169947923	-1.54196970240174
H	1.22627987819383	-4.10650427512740	-2.97028008552021
C	-2.00533263763840	-2.61229238426380	-0.05741448479803
C	-1.98817241989680	-3.49181149117319	1.04351198847488
C	-3.07435842848940	-3.46817391292132	1.92378146410368
C	-4.14991323082728	-2.61330967443201	1.72285559980590
C	-4.17243444118537	-1.78993926213517	0.60472083466857
C	-3.11720381189622	-1.79001457253334	-0.30928061966596
C	-0.87465871245489	-4.47392777579559	1.28917650162470
H	-0.79760274269326	-4.69236050368051	2.35729067220052
H	-1.07441263128714	-5.42057803699284	0.77183832622898
H	0.08848787913502	-4.09851956824591	0.94185015023647
H	-3.06518458150654	-4.13508322099113	2.78304062950097
H	-4.97510350077995	-2.60166784627598	2.42950356572843
H	-5.02839294817315	-1.14587422943933	0.41918182306234
C	-3.20311289411719	-0.95090036078575	-1.54919367960073
H	-2.57999138164619	-0.05135123626173	-1.47525431871765
H	-2.85406016996957	-1.49570199349691	-2.43248154750472
H	-4.23150571483956	-0.62102828210987	-1.71924538183001
C	2.10432694994407	-1.53666942822885	-2.82956545683257
C	2.08587440413796	-1.40088825583825	-4.22717763269317
C	3.20583558514650	-0.85262337429734	-4.85487946565167
C	4.31190790705995	-0.45045825822023	-4.11570555710087
C	4.32275248352141	-0.61824464209281	-2.73624384690769
C	3.23021031250728	-1.17899188572519	-2.06930100240887
C	0.88925081471069	-1.82291281490220	-5.03293762883198
H	-0.04175313927971	-1.46043033063355	-4.58414913451313
H	0.80948784597721	-2.91397998717854	-5.09384534007148
H	0.95898887173031	-1.43617780874077	-6.05245410752878
H	3.19892404512352	-0.73054478998179	-5.93528404429557
H	5.17301888422079	-0.01786694081553	-4.61752028085232
H	5.19947542822894	-0.33179102050351	-2.16065942626557
C	3.29546976823060	-1.43683736893385	-0.59052750169245
H	2.92815968764660	-2.43935058308949	-0.34865336960630
H	4.32500167129129	-1.34119691508224	-0.23487881270461
H	2.67661892029125	-0.74317829706265	-0.01058764950479
B	-0.14331928352165	2.17463605761035	-1.71461257037111
N	-0.75467755534107	2.57327637687422	-2.95911092012246
C	-0.55052140408511	3.93773897053190	-3.15325750499560
C	0.15240578003840	4.43812778238122	-2.10559673883091
N	0.41667631364585	3.41177419097160	-1.20488572828258
H	-0.92590931341633	4.44753239999469	-4.03043224107805
H	0.49433927228266	5.44971754910660	-1.93421207518400
C	-1.56506273620364	1.83359748817677	-3.87300656551363
C	-0.97130401517002	1.29780554518069	-5.02219704894434
C	-1.78051309401313	0.58592295820993	-5.91014485057986
C	-3.14002793532152	0.43057017759437	-5.66290355178632
C	-3.71637514983413	1.00639776095766	-4.53593573287323
C	-2.94109543220426	1.72991077151999	-3.62738800834782
C	0.48834497737993	1.52061457825037	-5.29551425630689
H	1.11173315123924	1.14967491502573	-4.47514618087852
H	0.79273202776361	1.01604777219715	-6.21524453769533
H	0.70792350700211	2.58923331915060	-5.40133886148049
H	-1.33607209561308	0.15489069464213	-6.80378057388069
H	-3.75669029691056	-0.13038130106361	-6.35971885552216
H	-4.78385630446252	0.90344025205246	-4.35761762277608
C	-3.57094476449089	2.42139075307395	-2.45026808832908
H	-3.04980695529517	2.19674971662069	-1.51375595714141
H	-4.61823100409573	2.12773220771544	-2.34487746350881
H	-3.53149789591944	3.51026695011201	-2.57736212274436
C	1.04201076117119	3.68464042990628	0.05180005239137
C	2.37247703196866	3.29113604482531	0.26315182410619
C	2.94753958886126	3.55954814119379	1.50494451585117
C	2.22776325485450	4.20757257843272	2.50217565192702
C	0.92001010551900	4.61263689152305	2.26554265312268
C	0.30372703670231	4.36125918732998	1.03781812135302
C	3.14935242513662	2.57307975071662	-0.80140805971826
H	2.80196742607347	1.53725420988165	-0.91009501713287

H	4.21190978304276	2.54074815964619	-0.54687534871768
H	3.03124842296247	3.04771124764815	-1.78098157130409
H	3.97026854686363	3.24332132264405	1.69321355504584
H	2.68933421689130	4.39588399254127	3.46768616962768
H	0.35513947684180	5.11414712166975	3.04721683051984
C	-1.11734158476422	4.79111183708820	0.79444072187320
H	-1.62306231491855	4.98713607975702	1.74323587775170
H	-1.15955402693434	5.70716615718060	0.19296049275355
H	-1.68045050703738	4.02592763833728	0.24978754635409

T6

Energy: -6856.99783633 Eh

Ge	-1.05545481849138	1.64118231325378	-0.15949751817823
Ge	0.28053316905340	-0.09787490825209	1.11166903779428
C	-0.45565523222211	-0.44012702710563	3.00672702344336
O	-1.03542028918859	-1.17884793470426	1.90497130239182
B	0.71548068260387	-1.11776685938501	3.72319456005057
O	1.35758761678980	-2.27367240211096	3.24370254160748
C	2.38539709721814	-2.51226576699566	4.12484847113647
O	1.31888494571190	-0.68362607724706	4.91372097663017
C	2.36154665526130	-1.55137968119810	5.13396901763112
C	3.28448878870986	-1.54371653491571	6.15963109747431
H	3.25651172652957	-0.79076090379865	6.94070091718190
C	4.25281904334538	-2.55598935718471	6.13779900876918
H	4.99984031835824	-2.58949389226482	6.92498905176140
C	4.27602296082271	-3.51881035028580	5.12823922762646
H	5.04093689914287	-4.28920448632827	5.14285295448068
C	3.33216863208526	-3.51531610604938	4.09286282914107
H	3.34133221384237	-4.26024396439510	3.30385698764387
B	-1.28435036839804	0.64366401484103	3.69006201825523
O	-2.61886795571647	0.98534940189066	3.40089331937199
C	-2.96998751799468	1.92400453178289	4.34671264301784
O	-0.82424036834217	1.38517125828267	4.79271507326229
C	-1.88184357733647	2.16857042312889	5.18088722080982
C	-1.94351878488271	3.07309372707453	6.22156694973812
H	-1.08892834838821	3.25267562665797	6.86597285173971
C	-3.16392500655386	3.73507237101477	6.40453092230418
H	-3.25978542016844	4.45388655170504	7.21262252138317
C	-4.25656574816967	3.48547234304920	5.57376792575689
H	-5.18934681406768	4.01416539124867	5.74481423425099
C	-4.17922301191154	2.56537091040348	4.52078774849370
H	-5.02082684317105	2.37456704491552	3.86399209709828
B	0.06625410163057	3.32878938637796	-0.54907337600055
N	1.22694947154752	3.62280167258855	0.25742484696116
C	1.74074508365178	4.85952101199576	-0.11493213160717
H	2.61630032370135	5.27862850109991	0.36233975835080
C	0.97139817091764	5.37652745678790	-1.10501048365261
H	1.07152675540955	6.31809880907789	-1.62791128938112
N	-0.05849742995594	4.48609854086414	-1.40496441652247
C	-0.88125918583579	4.75782352508613	-2.54365013678756
C	-0.33216160056578	4.50456828239962	-3.81370468579895
C	1.04064407325397	3.90877094371313	-3.95141552902966
H	1.25336034732294	3.66891600533381	-4.99582162763971
H	1.81285360263913	4.60012049386550	-3.59551733656774
H	1.13711178174425	2.99329234440104	-3.35588226228942
C	-2.72594666291818	5.66610778399910	-1.04326725067031
H	-1.97519648179561	5.63712351056906	-0.25071865134795
H	-3.51862915149281	4.95244907019289	-0.78685537089647
H	-3.18415262273774	6.66016606086294	-1.05420638023016
C	-2.14204235640713	5.34554453724338	-2.39052923666887
C	-2.87034426962079	5.64952139042784	-3.54641793633092
H	-3.85117404066706	6.10754600014563	-3.44353167966722
H	-2.93614859715316	5.63071802403577	-5.69252082264438
C	-2.35625778404145	5.38562269640103	-4.80713370536058
C	-1.09176205995663	4.81934272868658	-4.93856847501277
H	-0.68427549642422	4.61960110856897	-5.92640419658330
C	1.90940137826721	2.83116912023135	1.23578574093262
C	2.92056092207479	1.95910757436493	0.80616396489340
C	3.22706063857666	1.79031422551875	-0.65518590023646
H	3.39250308471887	2.75336769769777	-1.14997930512228
H	4.11447020359237	1.16779945564355	-0.79246570083278
H	2.39128207132517	1.30348001158395	-1.17661753544252
C	3.60686482827950	1.22389354928990	1.77496380764509
H	4.38822044597988	0.53570524107945	1.46305112732820
C	3.29092250747202	1.35386802711370	3.12213443964946
H	3.82647268138059	0.76652460745162	3.86319375002934
C	2.28188408903829	2.22097703870929	3.52482527474269
H	2.02244197938909	2.30295783285809	4.57609858234694
C	1.57541756294719	2.97742352353747	2.58920906254039
C	0.47002726539005	3.90105111175912	3.01311986153728
H	0.59009896537163	4.90146630824116	2.58425077240260
H	0.43043830630030	3.98299867053187	4.10137601225430
H	-0.50293864899908	3.52342719085487	2.67263185022286
B	-2.29491643342931	0.66122352811713	-1.48143877842578
N	-1.88216268434708	-0.29222244313885	-2.47170197701172
C	-3.01426344122457	-0.91736335005622	-3.00139255317959
H	-2.94025224460450	-1.66920621214235	-3.77514682864559
C	-4.11684237737378	-0.41798447918201	-2.39327652166050
H	-5.15782086855690	-0.66727988164893	-2.54705871603075
N	-3.72618933460104	0.54409711541343	-1.45259896663237
C	-4.68053387648181	1.18889788799445	-0.61353073379876
C	-5.01814696279593	0.59387341477025	0.61280364137473
C	-4.38123112678118	-0.69379385644633	1.04332379517693
H	-4.81666132282890	-1.04198670551894	1.98297693228966
H	-4.51339912872898	-1.47284462529217	0.28395588885256
H	-3.30141612666487	-0.58009460460703	1.20034828300413
C	-4.92400912018933	2.95340825043139	-2.39727182524464
H	-5.21987240706987	2.27456201955830	-3.20567009298250
H	-3.84337774319847	3.10342033674949	-2.49756382011421
H	-5.42175320121716	3.91366113167892	-2.55403249804542
C	-5.27816832566168	2.37963422580721	-1.05606747892477
C	-6.20641961244527	3.00120691679677	-0.22007148061013
H	-6.67229992604309	3.92998149660345	-0.53955809805585
H	-7.27041886815867	2.93007512133088	1.64634061742313
C	-6.54257662102833	2.43776682734118	1.00695995466536
C	-5.96266841472136	1.24071112163180	1.41249469904353
H	-6.24310633709470	0.79211291272269	2.36204636200035
C	-0.55390457963902	-0.59538049804140	-2.89570368543608
C	0.15042361719229	-1.63723709464856	-2.27801376588364
C	-0.50965839604238	-2.54497040222972	-1.27820750421227
H	-1.07357400599430	-3.32972504301748	-1.79911885042822
H	0.23418227787809	-3.03244675218863	-0.64270542343908
H	-1.21985970412471	-2.01709386475986	-0.63610907646068
C	1.47876679485381	-1.84503675785585	-2.66208888976535
H	2.04971132056391	-2.63504583584262	-2.18086328599120
C	2.06893295883214	-1.05958150607723	-3.64467478062082
H	3.10480743567920	-1.23098654701241	-3.92441472196082
C	1.33310183378559	-0.06598476996135	-4.28380107888183
H	1.78641746791033	0.52880408397150	-5.07313148695458
C	0.00633325092422	0.17444600318643	-3.92539355554414
C	-0.82811898701910	1.19865300561066	-4.63854373678355
H	-1.69849600479383	0.72936957137950	-5.11181220116485
H	-0.24653186351345	1.70399397041582	-5.41248510365628
H	-1.21772758273403	1.95522137115401	-3.94936703389708
C	-2.82072229441191	2.86579527457790	0.87737511956000
O	-3.33801193192216	3.50806891420465	1.65744281547113

T7

Energy: -6856.97367217 Eh

Ge	-1.00200714751106	1.68212557640523	0.44591201665926
Ge	-0.47137923203305	-0.45207858279108	2.01117700560748
C	-1.28404926587999	0.36499384281988	3.77840832025658
O	-1.96822564517927	-0.69398715336301	3.07637581344875
B	-0.27003992463303	-0.04572086381823	4.83820089510932
O	0.15236880213815	-1.37148416012427	5.04986737163700
C	1.12755439013685	-1.29304413199930	6.01543700562291
O	0.41765110732904	0.82915060407701	5.69486930205101
C	1.28551273237399	0.03562618734435	6.40754393355667
C	2.20896699561559	0.41278752672810	7.36089925853479
H	2.32524115332568	1.45022860507856	7.65729504130908
C	2.98401348850605	-0.61120042106055	7.92056816461133
H	3.72367171956077	-0.36147596307856	8.67507467403950
C	2.82566197172678	-1.94090551411021	7.52884264636740
H	3.44433054127147	-2.70853165940611	7.98354890127357
C	1.88479462786664	-2.31038893766930	6.55899992691516
H	1.75494627200714	-3.34148997789790	6.24661044071208
B	-1.94482342745870	1.73898814103700	3.70929228684261
O	-3.14335461049856	2.00486713383893	3.02943694859874
C	-3.38728302689336	3.34206947305561	3.22545170953566
O	-1.47759719029239	2.89979240994156	4.34922203537604
C	-2.38779857760623	3.88226163076490	4.03349102177155
C	-2.38195452530326	5.21149980023952	4.40168311501732
H	-1.60011382252342	5.62120326788776	5.03305178931857
C	-3.42834854384390	6.00106656711890	3.90805880096395
H	-3.46317692954885	7.05461556378815	4.16876926950360
C	-4.42015911069946	5.46454954840203	3.08605813309299
H	-5.21308721511558	6.10789882350121	2.71681591810710
C	-4.41924320496635	4.11061800875525	2.72753490361897
H	-5.18393421603139	3.67954705628929	2.08993760832033
B	0.68485764752261	2.69497553908091	-0.21684961758101
N	2.01617875090422	2.31370652775969	0.19055893457850
C	2.89431500302414	3.35094695930133	-0.11311959291436
H	3.94775327015264	3.28989754722126	0.12444769870421
C	2.20169622841621	4.36431187554366	-0.68928148266612
H	2.56169235735940	5.32188114764841	-1.03913187564009
N	0.85319593610051	4.02003630200491	-0.76463076763351
C	-0.09727227926315	4.96872969920883	-1.25637892070811
C	-0.08384015398351	5.29649260921783	-2.62149376427223
C	0.92190379046082	4.69493583847974	-3.56057830760269
H	0.57296074326608	4.77212555314076	-4.59301855124783
H	1.88259836423264	5.22081770503296	-3.49563138308764
H	1.11273259192402	3.64247388915947	-3.33547143173390

C	-0.95034743543607	5.31266624620642	1.11589198584745
H	0.04579724223953	5.03472645085731	1.47246425907118
H	-1.63286338568642	4.48967041427711	1.36230759938936
H	-1.29629747214729	6.18416115033100	1.67754984639372
C	-0.96725035333045	5.60122243834115	-0.35659762829809
C	-1.87967076300996	6.52866112064610	-0.86545679051456
H	-2.56834148714037	7.01559067461658	-0.17932547238387
H	-2.63643690162326	7.54916685001841	-2.59821592356954
C	-1.91525946030250	6.83015347031072	-2.21970393042800
C	-1.01525627256905	6.22420082663903	-3.08888174930182
H	-1.02788292999573	6.47195436530367	-4.14755728602344
C	2.45782677032868	1.20027252785247	0.97330994816721
C	2.96796002126467	0.06447229985593	0.33192414226092
C	3.13275463723247	0.03032902429956	-1.15990069196793
H	4.03629122701756	0.57897474746660	-1.45567248262901
H	3.23433407446782	-0.99782333005547	-1.51660760847820
H	2.29397218384552	0.50365989270680	-1.67523428089230
C	3.37260983934182	-1.01276543070948	1.12438108632819
H	3.75345523038135	-1.91001754425694	0.64288369628093
C	3.31053177186882	-0.93919008582550	2.51082168265097
H	3.63004213758494	-1.78300382429389	3.11614506779430
C	2.85140008689538	0.21834794595541	3.12899273256071
H	2.83149142773567	0.28330445011734	4.21395986520871
C	2.41371754497358	1.30779461414408	2.37272899845763
C	1.90718549013839	2.55384500439793	3.04088942132724
H	2.40729866591509	3.44814622500504	2.65370480259318
H	2.06009091863947	2.49890436183248	4.12074227165251
H	0.83165386868401	2.68830409891529	2.87094207512639
B	-2.46050325410933	1.02018269699432	-1.37743755744521
N	-2.08362818826774	0.63508156214381	-2.71791416974768
C	-3.02995586001481	-0.25644772549032	-3.20276297453590
H	-2.93767504415839	-0.69435824170255	-4.18770858399180
C	-3.99031752531948	-0.45731851621943	-2.25993944674148
H	-4.87735183971377	-1.07458461352196	-2.31082943574855
N	-3.68786585373897	0.28285519354429	-1.13458372696620
C	-4.53406896459892	0.21165196015499	0.02328396439940
C	-4.34233781115808	-0.86291779959633	0.90633339349416
C	-3.34622272677775	-1.94747714243367	0.61081588905757
H	-3.08671484760835	-2.48756227419474	1.52334293244421
H	-3.76470040194852	-2.66585927798367	-0.10624328773601
H	-2.42971020956065	-1.55258159760698	0.16083348675388
C	-5.89824875630249	2.20216461074561	-0.81750712486105
H	-6.95933899125501	2.13614630714305	-1.08193587853004
H	-5.30786534008478	2.10546515417889	-1.72965771003994
H	-5.72136474656778	3.20459389393639	-0.41458269464156
C	-5.56664948379417	1.14230002222421	0.19840912922687
C	-6.35476807845129	1.02980116085743	1.34786613328868
H	-7.15772237998517	1.74649633758794	1.50616324986601
H	-6.75563079501541	-0.05008608987564	3.16041238023871
C	-6.13950105258190	0.01356877286439	2.26786804836766
C	-5.15058481791161	-0.93542564863547	2.03915568900050
H	-4.99264542586843	-1.74314522227308	2.74818384136467
C	-0.91381060254215	0.85989115276208	-3.51245502746548
C	0.15021289394261	-0.04540224497248	-3.39587530967638
C	0.11156118707426	-1.15956781124585	-2.38744013911733
H	-0.81450078841048	-1.73880844938586	-2.47052681169971
H	0.95805959857669	-1.83567953174080	-2.52639929000502
H	0.14984214973512	-0.77167401754398	-1.36158979592311
C	1.22927276087004	0.10057442660806	-4.27013529664704
H	2.06551673086175	-0.59002849389897	-4.19840562410678
C	1.22795483384438	1.09522423592529	-5.24187075899590
H	2.06649412571692	1.18376133953144	-5.92695915168120
C	0.15340378348375	1.96967704201317	-5.34532573471860
H	0.15377364267725	2.74410335842803	-6.10763588784918
C	-0.93393387736049	1.87524793999328	-4.47468017981317
C	-2.09988374882720	2.81806132909837	-4.57533985006106
H	-3.02010079367534	2.28706456358164	-4.84619274598678
H	-1.91076093012612	3.58407052680846	-5.33161865604077
H	-2.28942532155448	3.32038447703569	-3.62032381191089
C	-2.38702811254960	2.57108807606559	-0.51536769350750
O	-3.15280166021320	3.44157518858270	-0.79411265481020

T8

Energy: -6856.99543939 Eh

Ge	-0.11739577737897	1.60674600631858	0.16449941270472
Ge	1.07899564336103	-0.32976072767909	0.94827039480130
C	-0.64325473888197	-0.17473859460968	2.50298726591510
O	-1.04512256594962	-1.08414570447312	1.63218706217841
B	0.50086370593496	-0.53967786325990	3.50207230540960
O	0.91691853253322	-1.86384707522526	3.74628653442807
C	1.78132727265591	-1.77937945683789	4.80867380474392
O	1.05465097092345	0.33140540637509	4.45662618389456
C	1.85837988256688	-0.45601861626077	5.24279393774577
C	2.64951533675806	-0.08042958133389	6.30959091438431
H	2.69662847224920	0.95097822021902	6.64413872340447
C	3.38269679602434	-1.09731717409848	6.93412443835053
H	4.01981242588590	-0.84807666964969	7.77716852659446
C	3.30933110143519	-2.42054797076862	6.49703499241421
H	3.89173853487918	-3.18319948902332	7.00491712277419
C	2.49734340153489	-2.79030415492598	5.41753127958378
H	2.43056813088314	-3.81711978081055	5.07307761024702
B	-1.49735563426512	1.09887479028166	2.79120214318832
O	-2.86058927978237	1.19552924637979	2.49308243912749
C	-3.26972362886204	2.39055123363725	3.04479019898497
O	-1.08193340320649	2.18965343130971	3.57029425727014
C	-2.19844684077028	2.98233031691174	3.70850082990783
C	-2.31607441147699	4.18989670009941	4.36523861544375
H	-1.47233996770393	4.64027133533589	4.87807556880448
C	-3.57352269539391	4.80314316985528	4.31976346406687
H	-3.71473689632215	5.75671414298252	4.81964675970503
C	-4.64327176434473	4.21771842856503	3.64066177806108
H	-5.60332423497344	4.72470762975455	3.61703208312838
C	-4.51049673913947	2.98866378174035	2.98370364418432
H	-5.33463603628817	2.53150642989766	2.44757335742060
B	0.99668010714262	3.31026178489482	0.02330844653150
N	2.37523942814158	3.33633528839519	0.45079919219025
C	2.88949219843498	4.61029142388093	0.24778882556542
H	3.90689892765889	4.86677142973191	0.51099008190660
C	1.91882089369312	5.39535768633029	-0.29530304268061
H	1.96857851738719	6.43707027887344	-0.58307033782596
N	0.75525283878677	4.65082862478179	-0.44754272192891
C	-0.40104223458165	5.19760226986076	-1.08815617282183
C	-0.43907547078504	5.22353159549842	-2.48887500898937
C	0.72238082431890	4.72188818792041	-3.30080478644917
H	0.46355470499668	4.68451750091780	-4.36189081270920
H	1.59664053758387	5.37303758190764	-3.18506176019598
H	1.03140712829646	3.72032534970626	-2.97990844160690
C	-1.36794771015495	5.67714262719852	1.19404625550588
H	-0.43989542521087	6.13554032855390	1.55331426032684
H	-1.39083796724918	4.64770933619770	1.56521240059981
H	-2.21621860878518	6.20720197403970	1.63418180225930
C	-1.44805707028758	5.69653085564023	-0.30372807650557
C	-2.57388185725219	6.19838601501969	-0.95939703749990
H	-3.40333114028931	6.57740711296443	-0.36777962912939
H	-3.53283793682997	6.59798285381742	-2.84088355135816
C	-2.64572961162321	6.21013041530643	-2.34755330980624
C	-1.58333495472012	5.73244083225692	-3.10696496153329
H	-1.63651380636625	5.75044534641254	-4.19273774740097
C	3.15951497242915	2.27312837733058	0.99588769496952
C	3.85603066747205	1.42595238166162	0.11877007033151
C	3.79585317438886	1.64249491502809	-1.36646875425068
H	4.16550177342734	2.63882681367004	-1.63517084413904
H	4.39881929600623	0.89561404704435	-1.88843475903382
H	2.76709132022664	1.57269676699319	-1.73719010450706
C	4.61551920253840	0.39044337828463	0.66948711382818
H	5.15659350970359	-0.27907605186747	0.00593167160664
C	4.68744730551240	0.21673165040785	2.04710328099515
H	5.28010710003513	-0.59397928618637	2.46136912889688
C	3.99964699967129	1.07378326558577	2.89769166425224
H	4.05672978911451	0.93292377715694	3.97351203733384
C	3.22114484837106	2.11656195156963	2.38888900295666
C	2.46520130428669	3.04117560542845	3.29707120095477
H	2.69533357367179	4.08960065314248	3.07917396584756
H	2.70706362455310	2.83474637850913	4.34178787728713
H	1.38407808748405	2.91220702886289	3.17150112286831
B	-2.91992239017502	0.74897117914648	-1.03887970772777
N	-2.36961205282689	-0.22906732367517	-1.93802291726634
C	-3.41137068045133	-1.00532090314924	-2.43436825824726
H	-3.24552889828278	-1.78477934093865	-3.16463382641125
C	-4.58012133664862	-0.58165490795502	-1.88608133334584
H	-5.58088243386681	-0.96033321286704	-2.04276524360338
N	-4.33399709487322	0.49561960873226	-1.03972186371074
C	-5.40796233917506	1.10892144315840	-0.32435219858245
C	-5.99162981136370	0.41101250314386	0.74327569368490
C	-5.43273446569738	-0.90423082973127	1.20865078484444
H	-5.86468403318751	-1.18010303594087	2.17370607455583
H	-5.64915147828360	-1.71018106201518	0.49781559663924
H	-4.34408539556553	-0.85142458703924	1.31471108268143
C	-5.24615863551577	3.08030504845236	-1.90199204262073
H	-5.11019773676554	2.41708411487801	-2.76331693844636
H	-4.25636806256468	3.45953497897710	-1.62132755047760
H	-5.86138746934435	3.92983012348485	-2.20982749266760
C	-5.88408799294852	2.35660620626316	-0.75065747914059
C	-6.98060528984125	2.90263372025406	-0.07974266270248
H	-7.36591839253023	3.86857421434842	-0.39599226846324
H	-8.44625293964579	2.65579200703811	1.47378410757588
C	-7.58881594955633	2.22037260883710	0.96797504848981
C	-7.09590497129527	0.98584989029176	1.37650546236447
H	-7.55928079656892	0.46232650494902	2.20898288617907
C	-1.03326603697192	-0.35853468071811	-2.41319845659270
C	-0.30536371523570	-1.52144236544027	-2.11612969253156
C	-0.90536671986366	-2.63988427084597	-1.31241396704505

H	-1.56176461976393	-3.26469256421441	-1.92975860800444
H	-0.11730223520568	-3.28058466761024	-0.90855066344607
H	-1.49841976703949	-2.25430458927175	-0.47905431184450
C	1.01284836736350	-1.60145608383428	-2.56881516481215
H	1.59767700106259	-2.48667715741259	-2.33230048637367
C	1.58311674519548	-0.56665002924160	-3.30160353589839
H	2.61151805049662	-0.64604704150106	-3.64239279233924
C	0.83670869425879	0.56416770314480	-3.60712832390893
H	1.27351149285397	1.36038103522634	-4.20509907043759
C	-0.48849600068627	0.68627845809726	-3.17886733420715
C	-1.31132353423967	1.88059615661833	-3.58308194688668
H	-2.33715075845089	1.59048856267058	-3.83114379591174
H	-0.86423628481198	2.36655920644770	-4.45417944572146
H	-1.37268552020041	2.63460787903886	-2.78960618455731
C	-2.13533707885626	1.86029367488773	-0.26564330494916
O	-2.62828129701388	2.90661527187802	0.12645320635655

V

Energy: -5817.77816606 Eh

Ge	-0.29103532809259	0.05603609309268	0.03627576021832
Ge	2.02106213133224	0.14500622020020	0.12545957514878
B	-1.09925511359080	1.82543756449256	-0.49771309692252
N	-0.22355196403780	2.84838175546315	-1.02045692907775
N	-2.37662048063650	2.48274006117934	-0.39309079601451
C	-0.95159220341978	4.02692143771644	-1.19969086119915
C	-2.23710242614264	3.80595305378040	-0.83233162405686
H	-0.49531988819465	4.93134481245299	-1.57879647317593
H	-3.07380414206627	4.49120061331128	-0.83698191645483
B	-1.00805962063557	-1.76810648006235	0.51904089793359
N	-0.11736015392579	-2.70781157719746	1.15973716194659
N	-2.20466829324526	-2.53405860694330	0.27873202897906
C	-0.75967051619118	-3.94265373005575	1.27594724867934
C	-2.00697478837159	-3.83617286428120	0.75763681298445
H	-0.27648460080408	-4.80086054486265	1.72294577680910
H	-2.77813862447942	-4.59019374442213	0.67838568190709
C	1.18307602726112	2.79233153597030	-1.22989870094284
C	2.04465169904345	3.22645359813742	-0.20391016207716
C	1.67883503699515	2.36816964520903	-2.47778974001322
C	3.42090375384144	3.25976748088801	-0.46581529147864
C	3.05486251087748	2.42102534564790	-2.69529060943762
C	3.91903746048459	2.87182562706721	-1.70073703004061
H	4.09715836133250	3.59706870311959	0.31525299663348
H	3.45073720551932	2.10567993391975	-3.65714762944425
H	4.98835296337839	2.90707234204224	-1.88844935716356
C	-3.62537307878077	2.02904914692961	0.12457712424982
C	-4.69443490416686	1.82500708207821	-0.76114635797220
C	-3.77331608410319	1.86184610683725	1.50993989535320
C	-5.93589836618649	1.47501781166974	-0.22996185948776
C	-5.02887932457437	1.49358184406035	1.99903565364517
C	-6.10535325484728	1.31365322502966	1.13947367639425
H	-6.77133046762790	1.30883528448469	-0.90504104660731
H	-5.16108926282723	1.36507182804895	3.07064537768690
H	-7.07779112790609	1.03659268007137	1.53762984384243
C	1.24785844024352	-2.53085544353168	1.52126978746585
C	1.56492199519972	-2.03457281890363	2.79979215145527
C	2.25049682366640	-2.91294005346111	0.60954435856927
C	2.90797538537695	-1.95806278479009	3.16486176413736
C	3.58772719049439	-2.81522815557506	1.01781039137645
C	3.91223559385374	-2.35264095894509	2.28431366948326
H	3.16705696214732	-1.58377849459524	4.15184835020930
H	4.37197000240625	-3.10948234638088	0.32527998868168
H	4.95357180540646	-2.28577667747176	2.58604841201361
C	-3.41766741274358	-2.19940619832461	-0.39235023932206
C	-3.41246503924498	-2.05364453359620	-1.78825328081991
C	-4.60034878489066	-2.09403822188662	0.35513336002903
C	-4.62877274799739	-1.80961283033039	-2.43018205366345
C	-5.79621330265790	-1.86827855702312	-0.32674331881439
C	-5.81367855220655	-1.73061409254194	-1.70900846870848
H	-4.64163248348475	-1.69842389398114	-3.51173381444505
H	-6.71844326014609	-1.77856353608995	0.24136596687467
H	-6.75275636684483	-1.54989216251316	-2.22510556178768
C	0.47585065703962	-1.59982631638816	3.73454147064215
H	-0.06397683977489	-0.74256809787412	3.31223118444861
H	-0.26159660201768	-2.39502968967530	3.88861192657891
H	0.88977358092398	-1.30867314592661	4.70290276102921
C	1.89367015236191	-3.48747832547128	-0.73280753840839
H	2.76082909193479	-3.47691036314196	-1.39773259899268
H	1.55380748680413	-4.52582880680471	-0.63038835801113
H	1.08038089810886	-2.92677141850575	-1.20293324979984
C	0.73784658522977	1.88060982449413	-3.53907678806300
H	0.22081723475130	0.97433993942223	-3.19899190913172
H	-0.03551291895767	2.62475627158661	-3.75826284016119
H	1.27831639810207	1.64987094960194	-4.46014482784434
C	1.49525834753719	3.71947460210449	1.10500452823023
H	2.28712954236981	3.77809125125462	1.85563622152392
H	1.05809282160357	4.71903805713823	0.98741411195837

H	0.70345583232615	3.06210242996476	1.47665788097841
C	-4.50332728183848	1.95944464735085	-2.24590934363003
H	-3.60190522570698	1.42863855158314	-2.57134970300332
H	-5.36290375917574	1.54630160054958	-2.77964477101064
H	-4.38342527516117	3.00611094170302	-2.54911330093741
C	-4.57941356670606	-2.20197055092144	1.85432944050058
H	-3.76514727114580	-1.60305215963039	2.27664797250631
H	-5.52527031105165	-1.85068980653386	2.27436132936874
H	-4.42058361595135	-3.23463801533281	2.18670941499508
C	-2.62706215100064	2.09693216872106	2.45319567008683
H	-1.87548076748210	1.30049239995365	2.37630461659704
H	-2.11112131277516	3.03649524819483	2.22703158235137
H	-2.98243206591187	2.13071022300074	3.48648998938425
C	-2.14287803904443	-2.18085055221793	-2.58272054845848
H	-1.47993581972698	-1.32250520099320	-2.41434916011969
H	-1.57791604646718	-3.07284588397583	-2.29043065821899
H	-2.36374914298635	-2.23847229836427	-3.65177199833876

Vlm

Energy: -5931.08223560 Eh

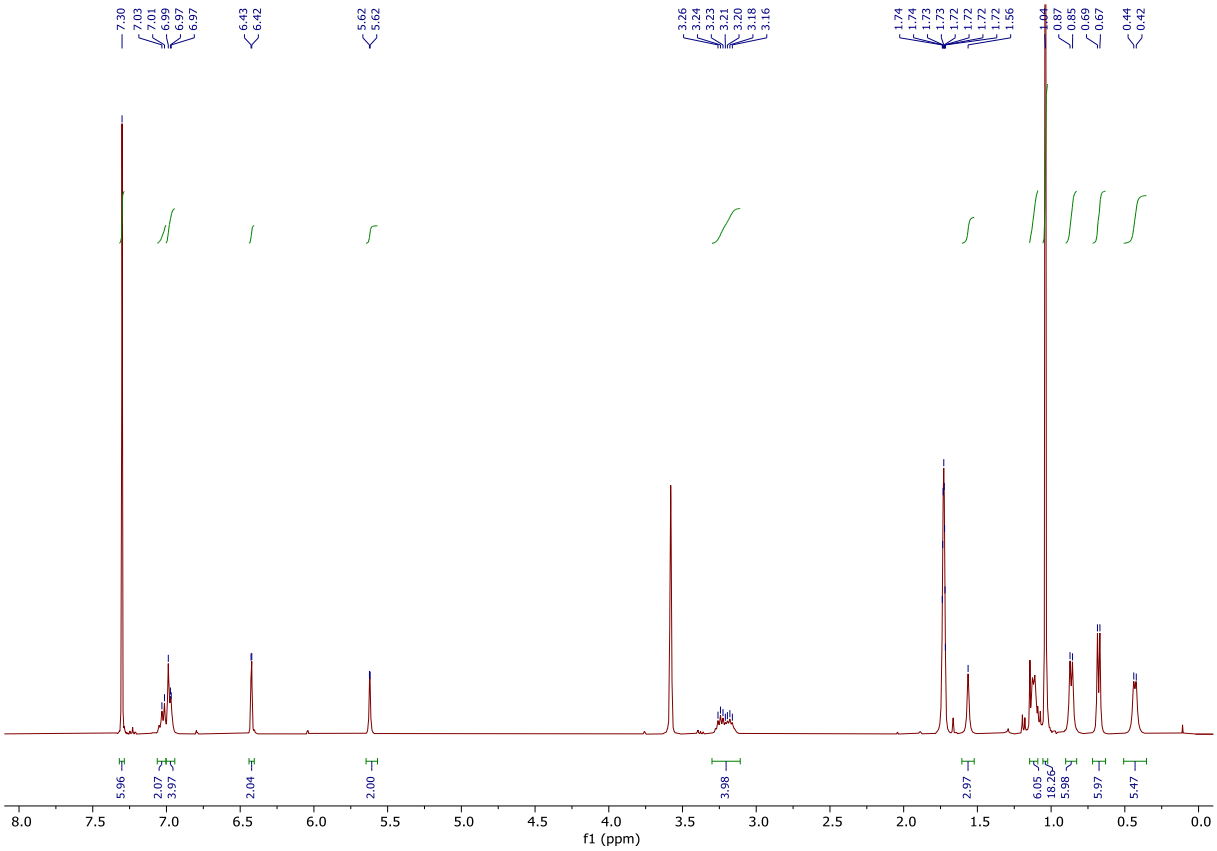
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H	0.89462753535702	4.29457848188969	-1.89049959317180
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C	4.18051263490957	0.07775135653721	-1.97283461689368
C	2.49424398609457	-0.62412777003728	-3.61425568119742
C	5.05596444434902	-0.87798101274500	-2.49612756283156
C	3.39860663737443	-1.56764392890322	-4.10514085885099
C	4.67058909247750	-1.68928664930562	-3.55597346006555
H	6.04690747509185	-0.98154811913786	-2.06171447005530
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H	5.36247913073174	-2.42727107073569	-3.95209589342679
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C	-2.70383511311934	3.58800350724064	0.55648824931865
C	-1.01592254089915	3.59894560740977	2.27462594576320
C	-2.32780551495171	3.82214960473151	1.87417741144521
H	-3.73498376637717	3.74485779765967	0.24961800395711
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C	4.59180668263194	0.97295139142378	-0.83899463556134
H	5.56719663376316	0.67525934398867	-0.44677537651230
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H	3.85797789510145	0.93434539472703	-0.02607799350463
C	-2.18602090780440	2.83210793707606	-1.79316326760639
H	-1.91904073580648	1.80331385843540	-2.05743039356942
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H	1.53388237774496	3.32375778485180	2.79456389741465
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Ge	2.23892875873731	-2.24525436933260	-0.59608050689271
C	-1.19206650480759	-0.59688500284931	0.79584548479429
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B	-1.65626843435836	-1.41357146385169	2.04423085409572
N	-0.95556485229729	-2.44677295169856	2.75467809959782
N	-2.90889163843628	-1.28197588874661	2.73651772758392
C	0.35348038947271	-2.95655277620629	2.52552228108622
C	-1.76314038480577	-2.89558350158424	3.79711801053788
C	-2.92672470764191	-2.19200803453034	3.78887346367192
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C	1.39293719847475	-2.56214565117514	3.37401903784842
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C	1.14807562568244	-1.57791640023905	4.48047638480568
C	2.67493574204078	-3.07252948154100	3.13714226817305
C	1.86595537951971	-4.28953640313956	1.21535478799573
C	-0.59075382124252	-4.33004740106997	0.61596410018243
C	-2.91767522887382	1.09341245508282	4.32086259622689
C	-5.05948841452375	1.70571868199515	3.13285149638274
C	-5.97998145762129	0.30564146806512	1.40122461726011
C	-4.85845313404973	-1.84813632240897	0.71220978564079

H	2.09237857816229	-1.25089680703607	4.92138628752020
H	0.52821042803549	-2.00721611429936	5.27565600897922
H	0.61158665586461	-0.69982129989825	4.10169719889506
H	3.49249983227046	-2.77314311896638	3.78710159318430
C	2.91400959792668	-3.91654825077874	2.06754775483261
H	2.04241768448441	-5.01640575954348	0.42673289018609
H	-1.32158815727085	-4.85001927187177	1.24668618619397
H	-1.11636734803618	-3.50891990453176	0.12016895368672
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H	-1.93933602047697	1.11594660378251	3.82641837202587
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H	-2.86789139234122	0.32401725423631	5.09966857723796
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C	-6.03950724945678	1.45658677384397	2.17946748320235
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H	-4.69785794214734	-2.74741588237514	1.31629010391642
H	-4.01440246698151	-1.77058406134083	0.01596151321416
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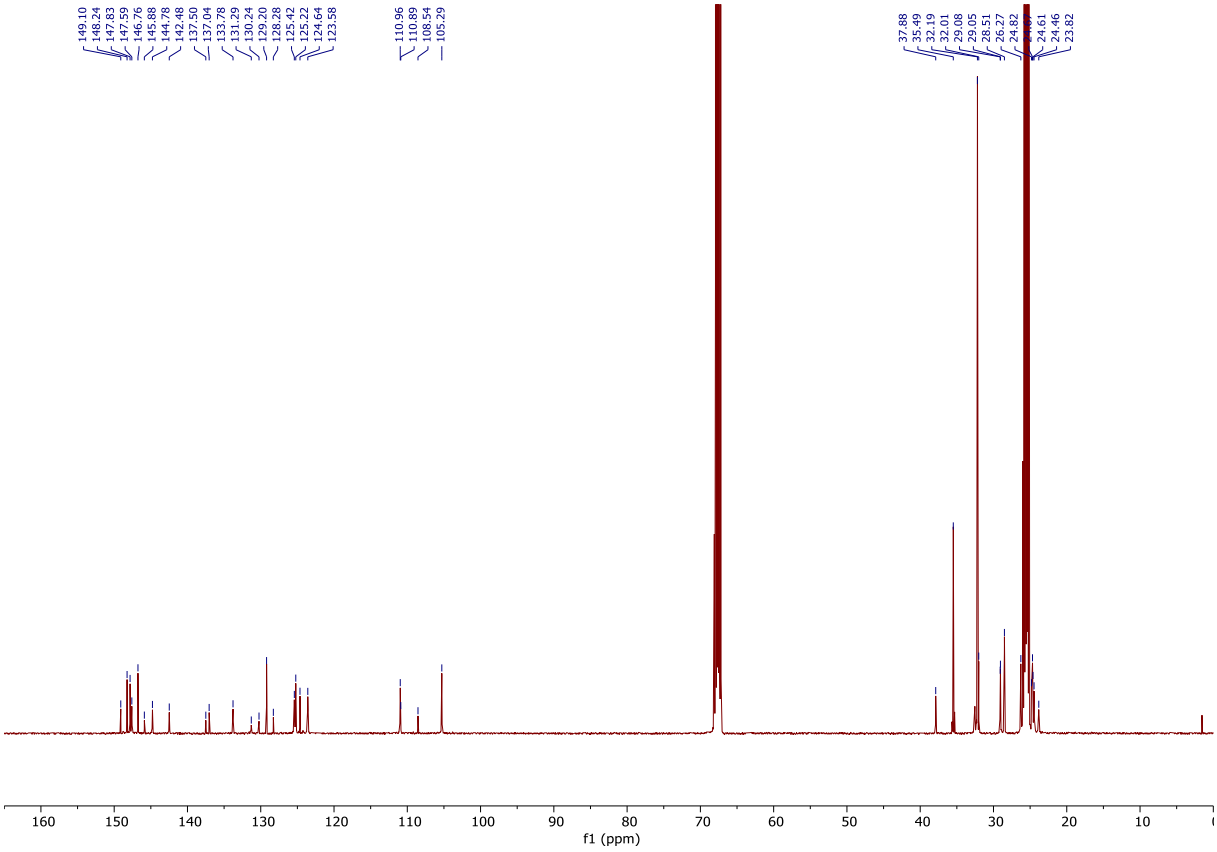
Chapter 6 - Coordination and Homologation of CO at Al(I): Mechanism and Chain growth, Branching, Isomerization and Reduction

Spectra

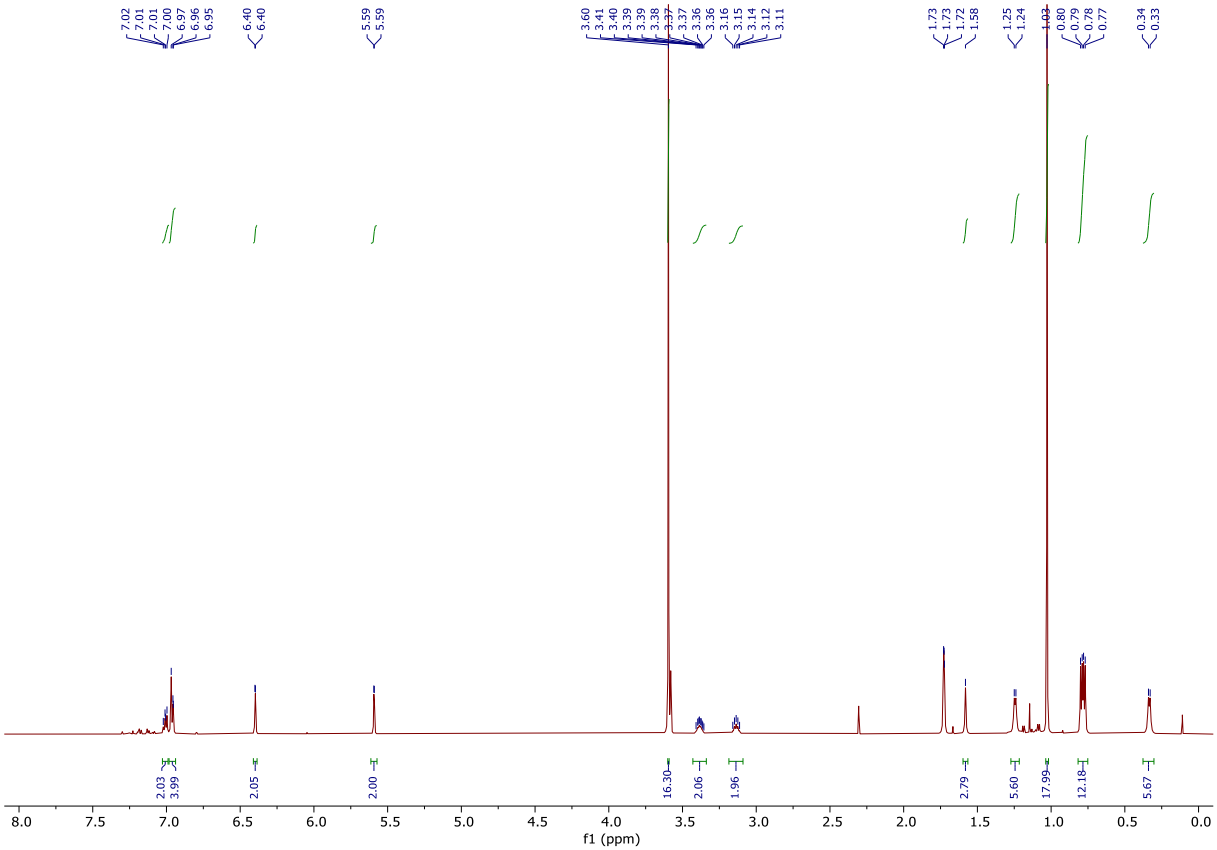
NMR



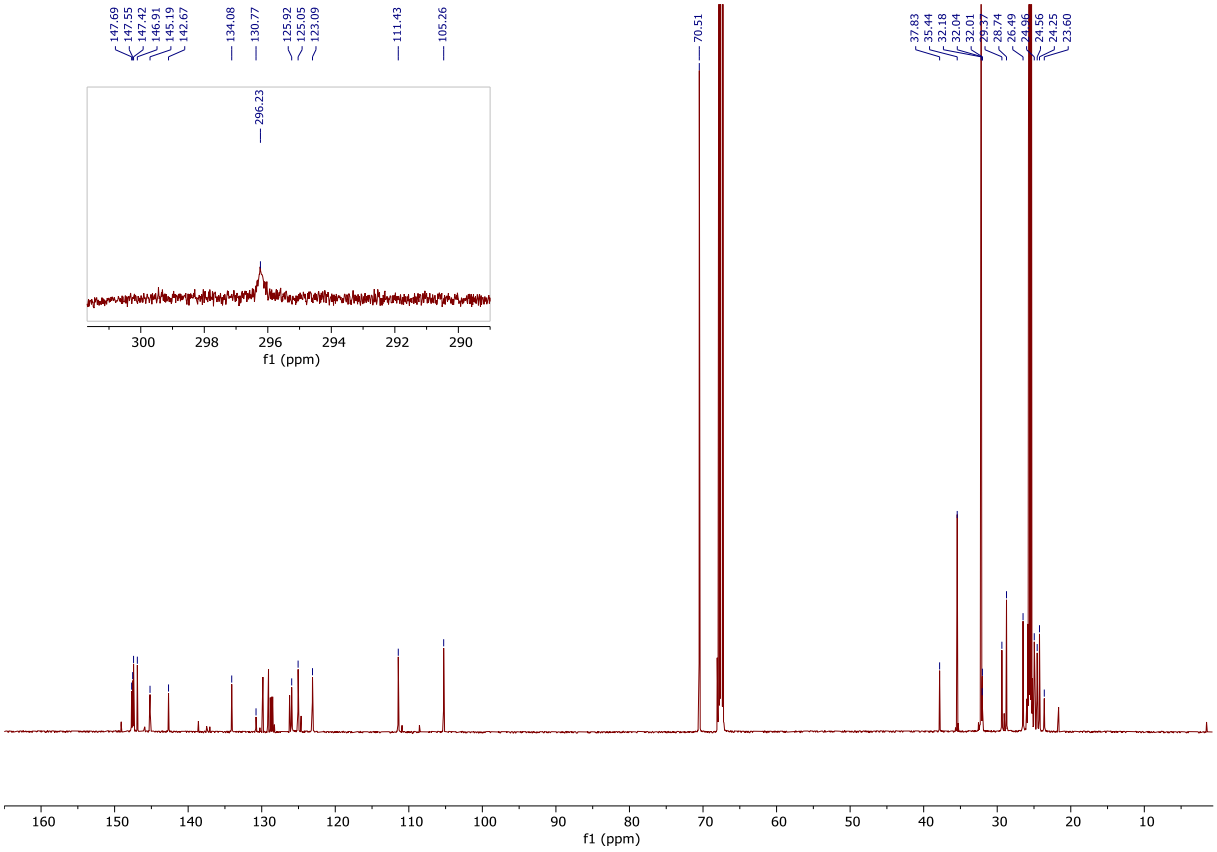
A 6.1: ^{1}H NMR spectrum of [**2**-K(C_7H_8)]$_2$ in THF-d_8.



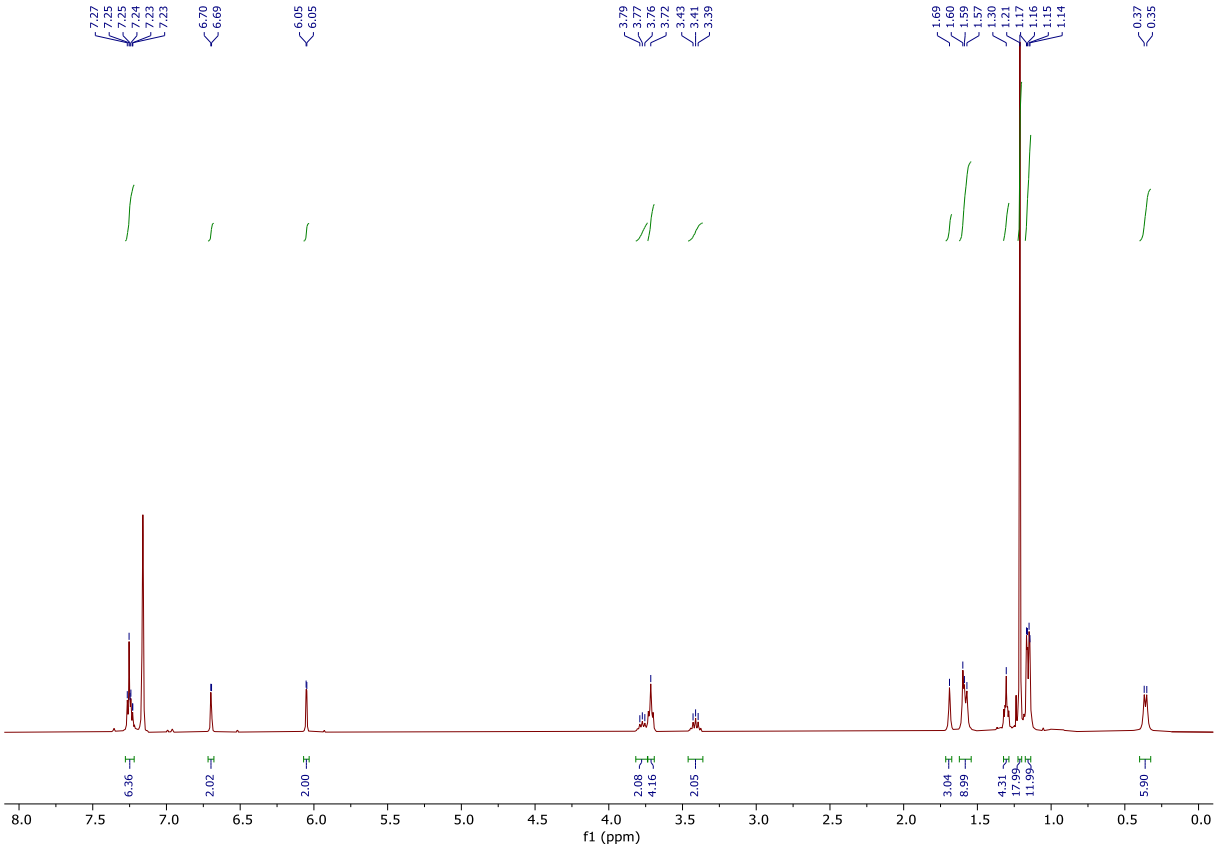
A 6.2: $^{13}C\{^{1}H\}$ NMR spectrum of [**2**-K(C_7H_8)]$_2$ in THF-d_8.



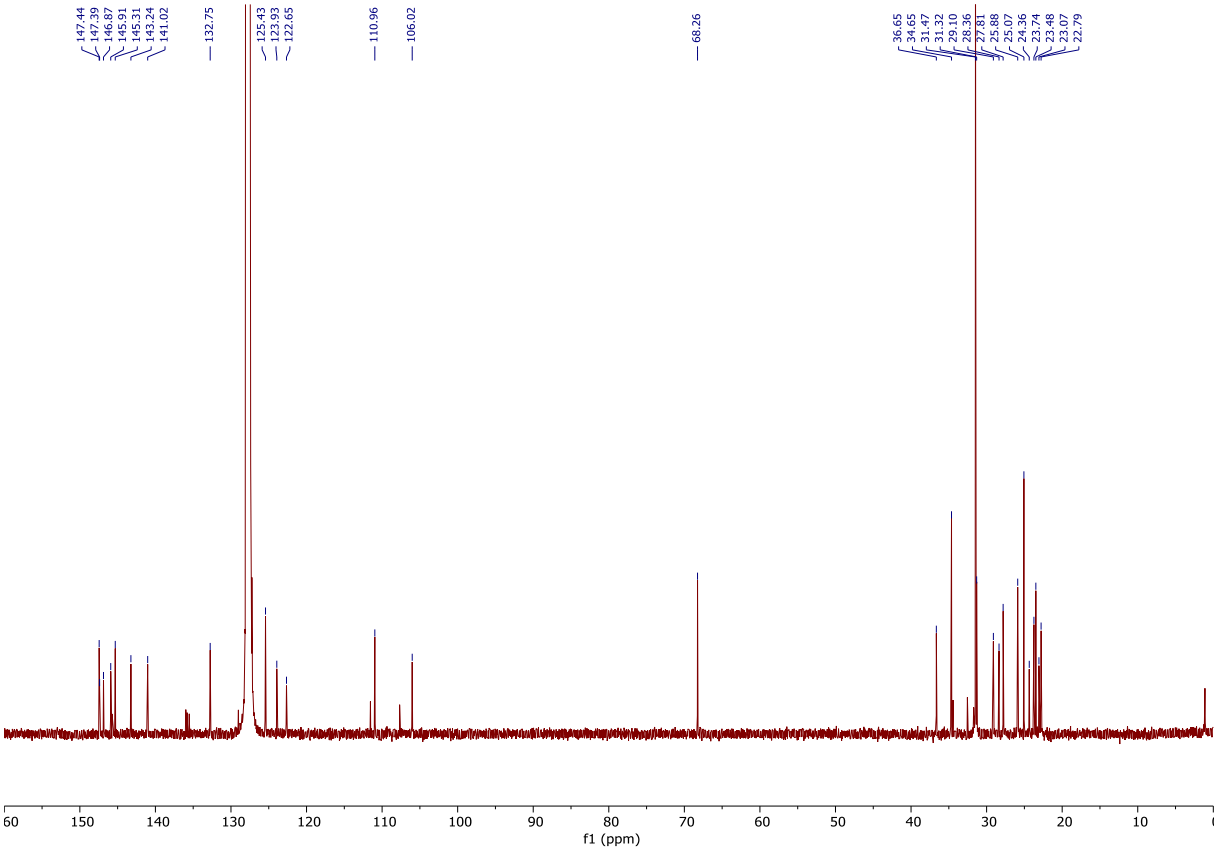
A 6.3: ^{1}H NMR spectrum of [**2**-K(12-c-4)]$_2$ in THF-d_8.



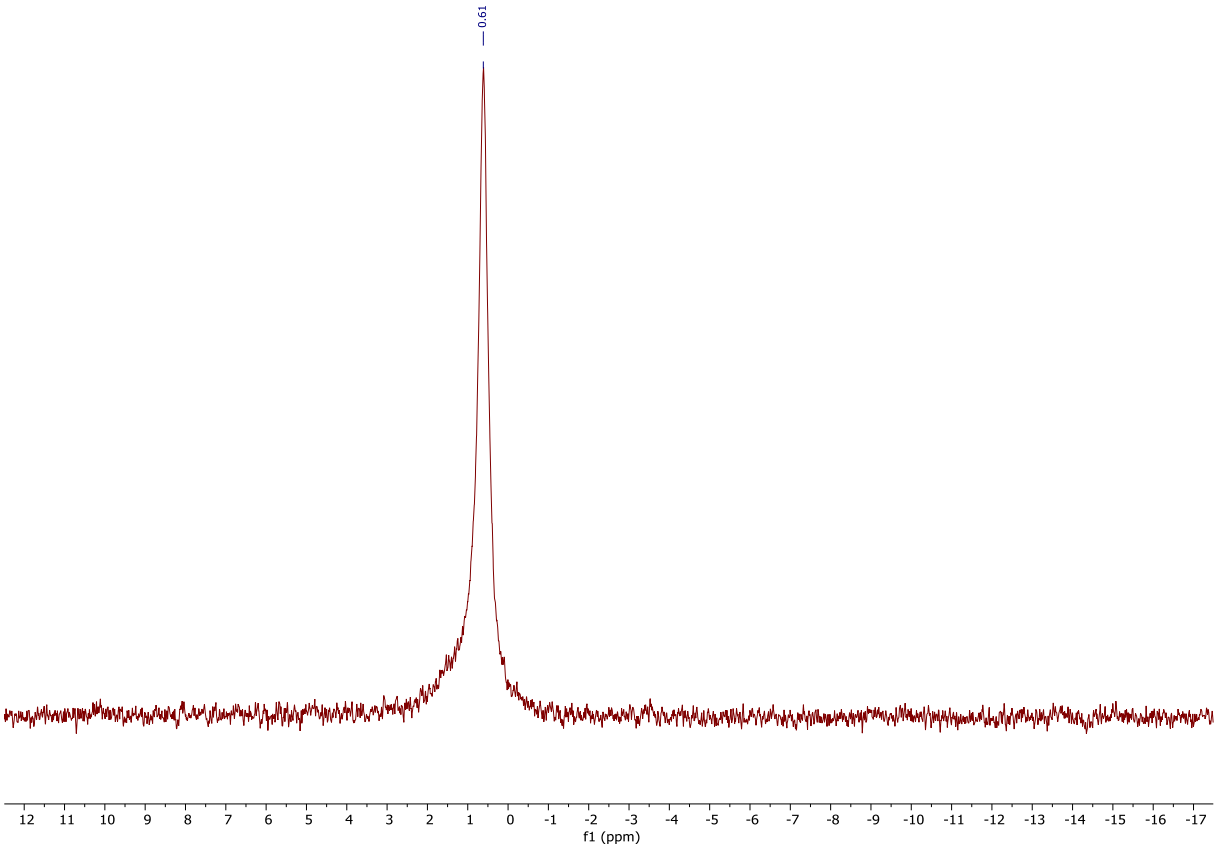
A 6.4: $^{13}C\{^{1}H\}$ NMR spectrum of [**2**-K(12-c-4)]$_2$ in THF-d_8.



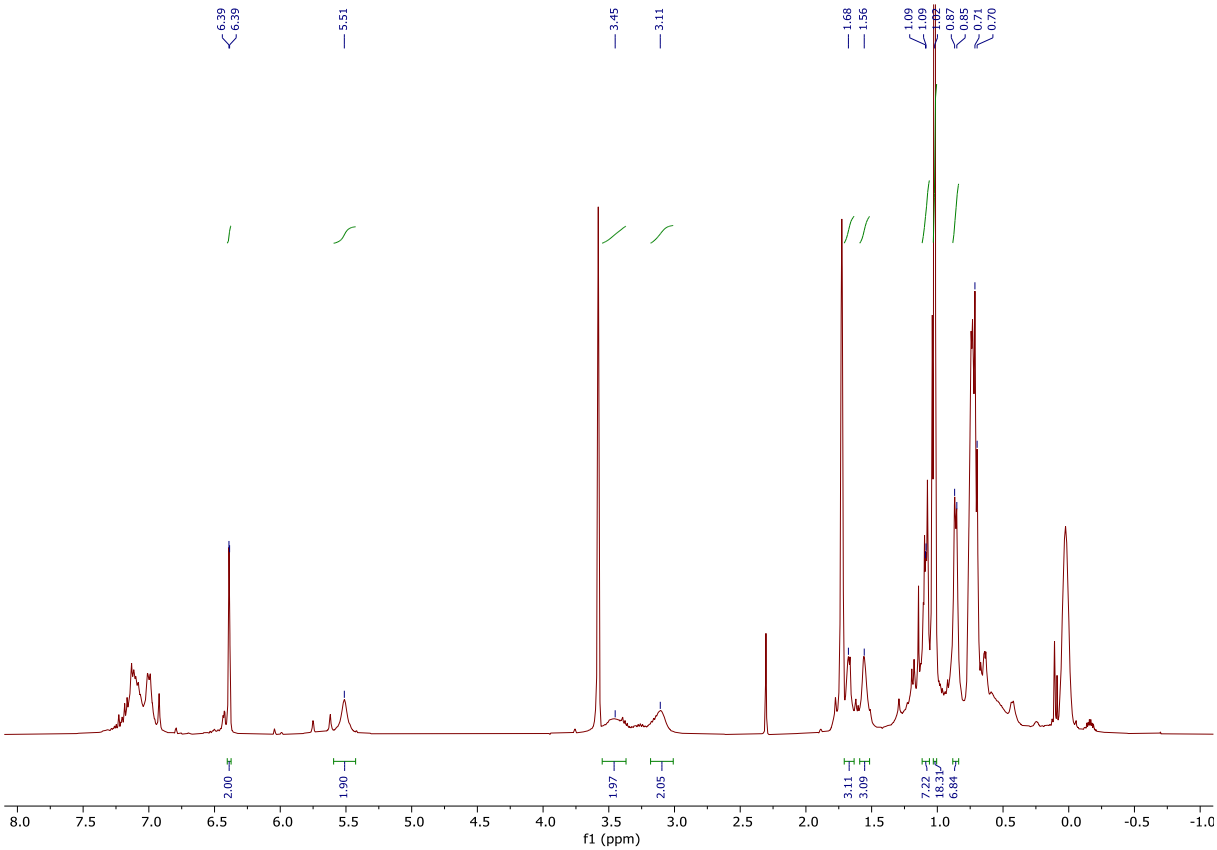
A 6.5: ^{1}H NMR spectrum of [**2**-Li(THF)]$_2$ in C_6D_6.



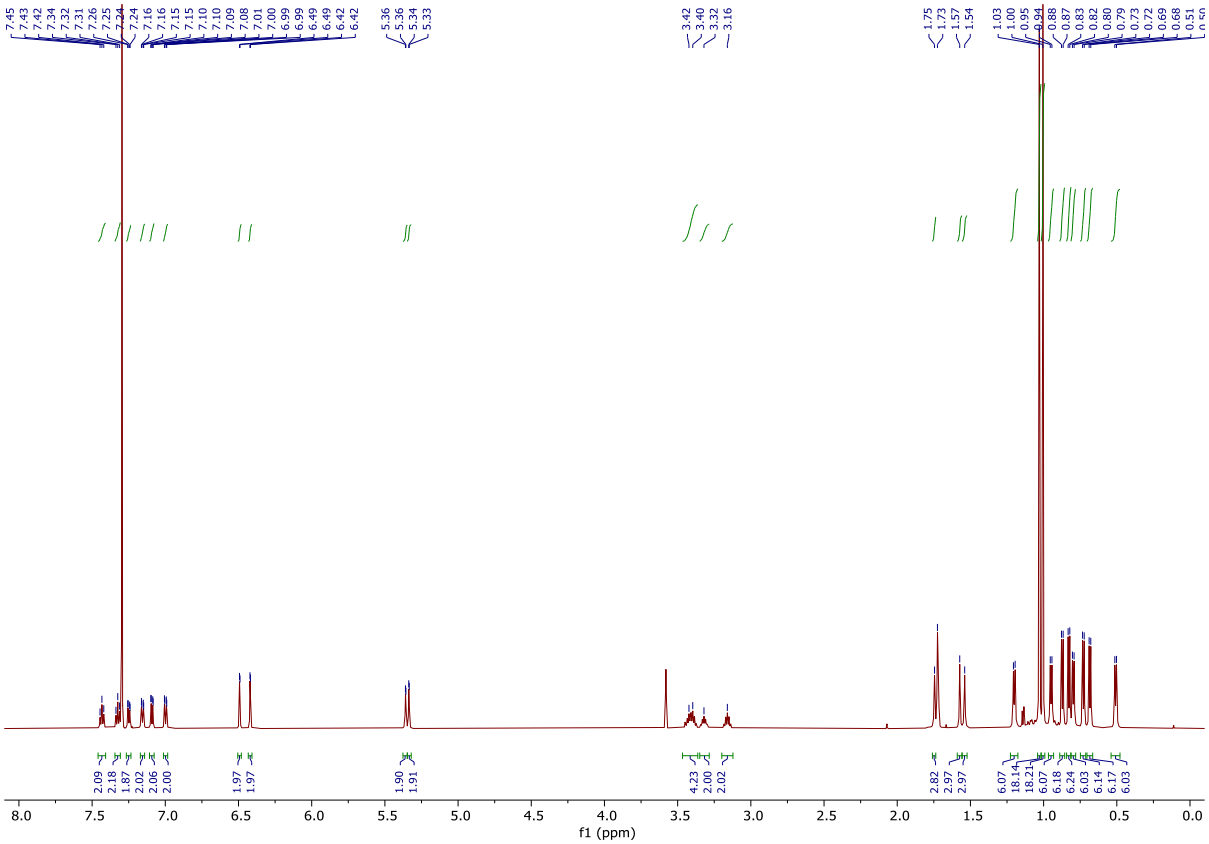
A 6.6: ^{13}C NMR spectrum of [**2**-Li(THF)]$_2$ in C_6D_6.



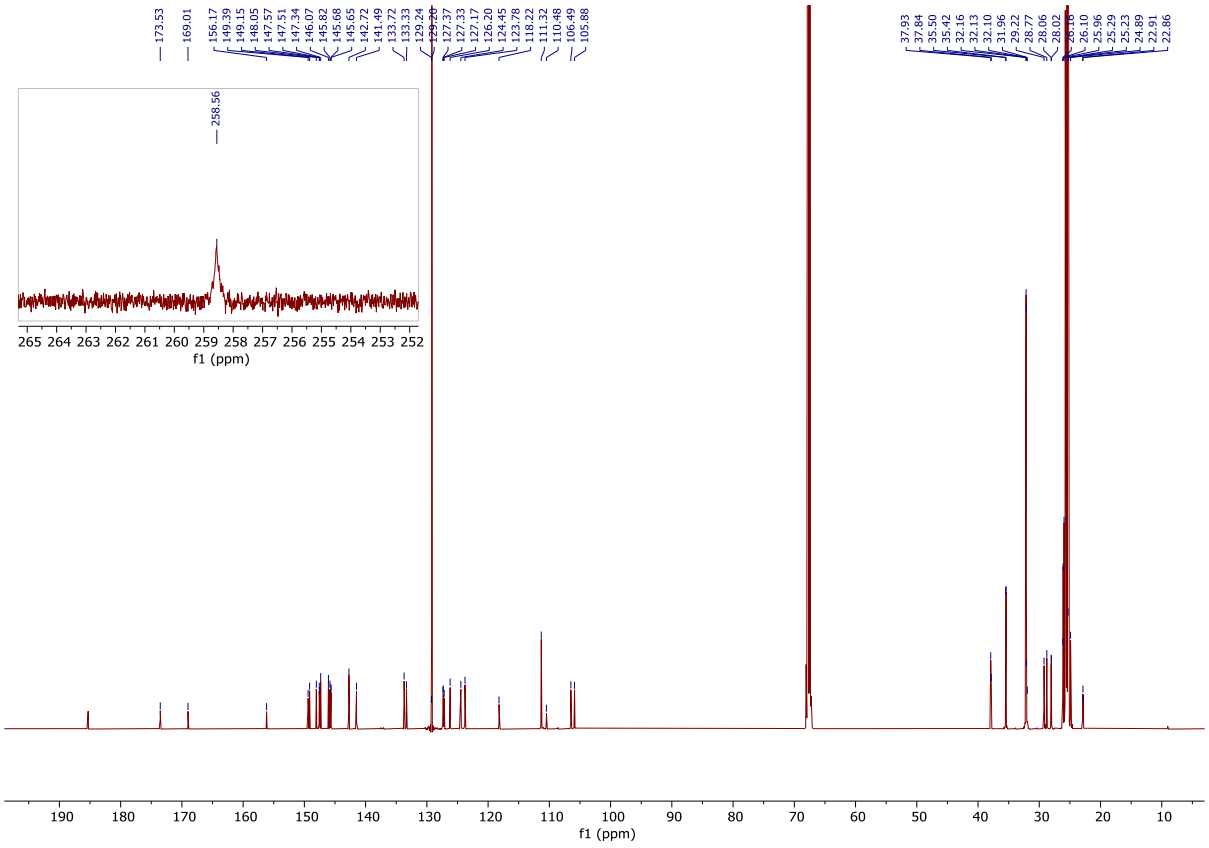
A 6.7: ^{7}Li NMR spectrum of [**2**-Li(THF)]$_2$ in C_6D_6.



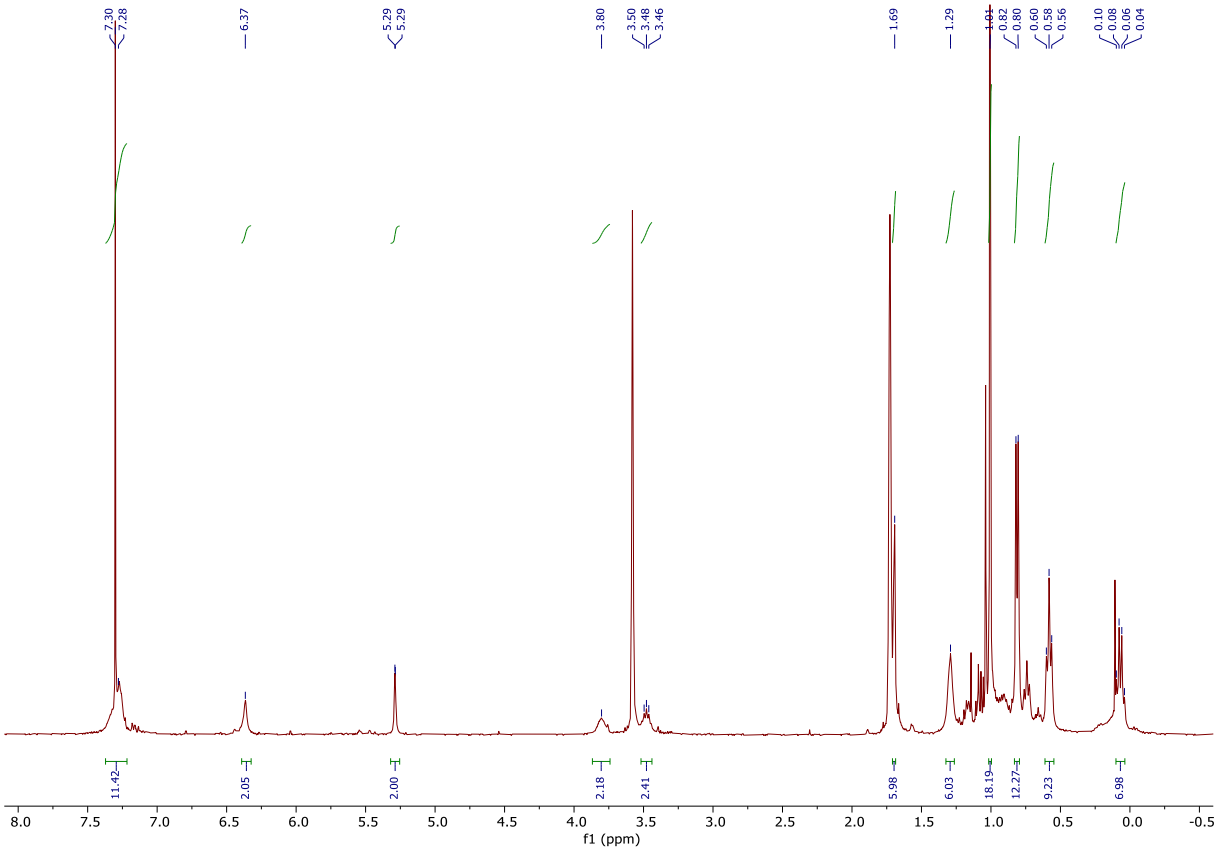
A 6.8: ^{1}H NMR spectrum of [**2**-K(THF)]$_2$ in THF-d_8.



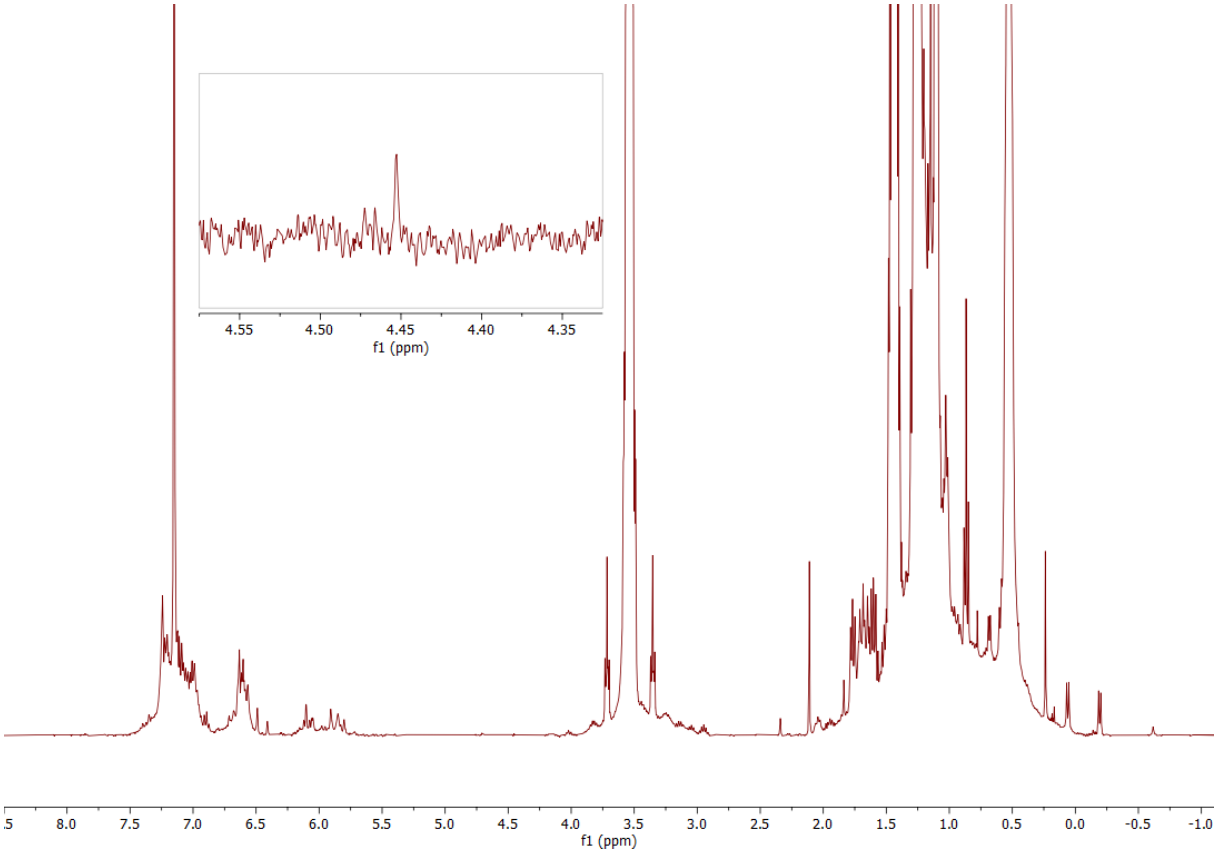
A 6.9: ^{1}H NMR spectrum of **3** in THF-d_8.



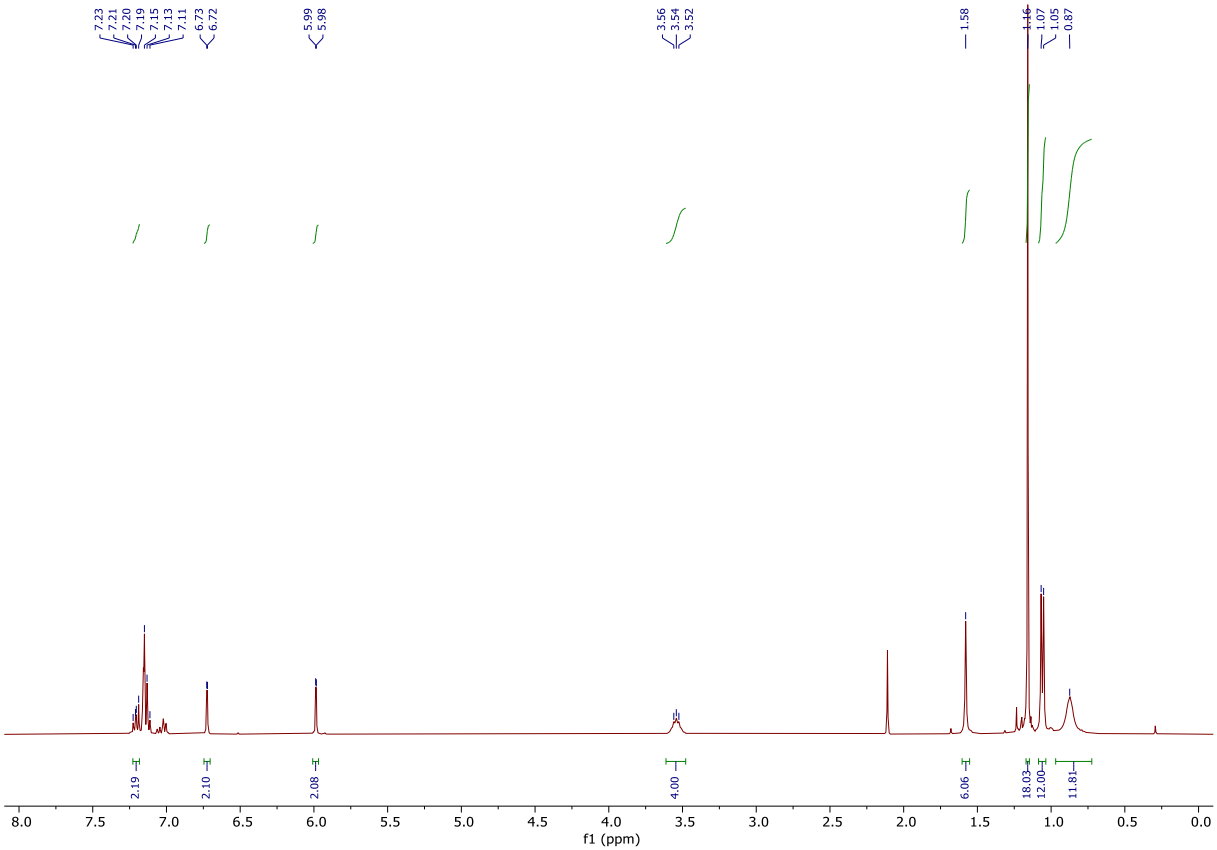
A 6.10: ^{13}C NMR spectrum of **3** in THF-d_8.



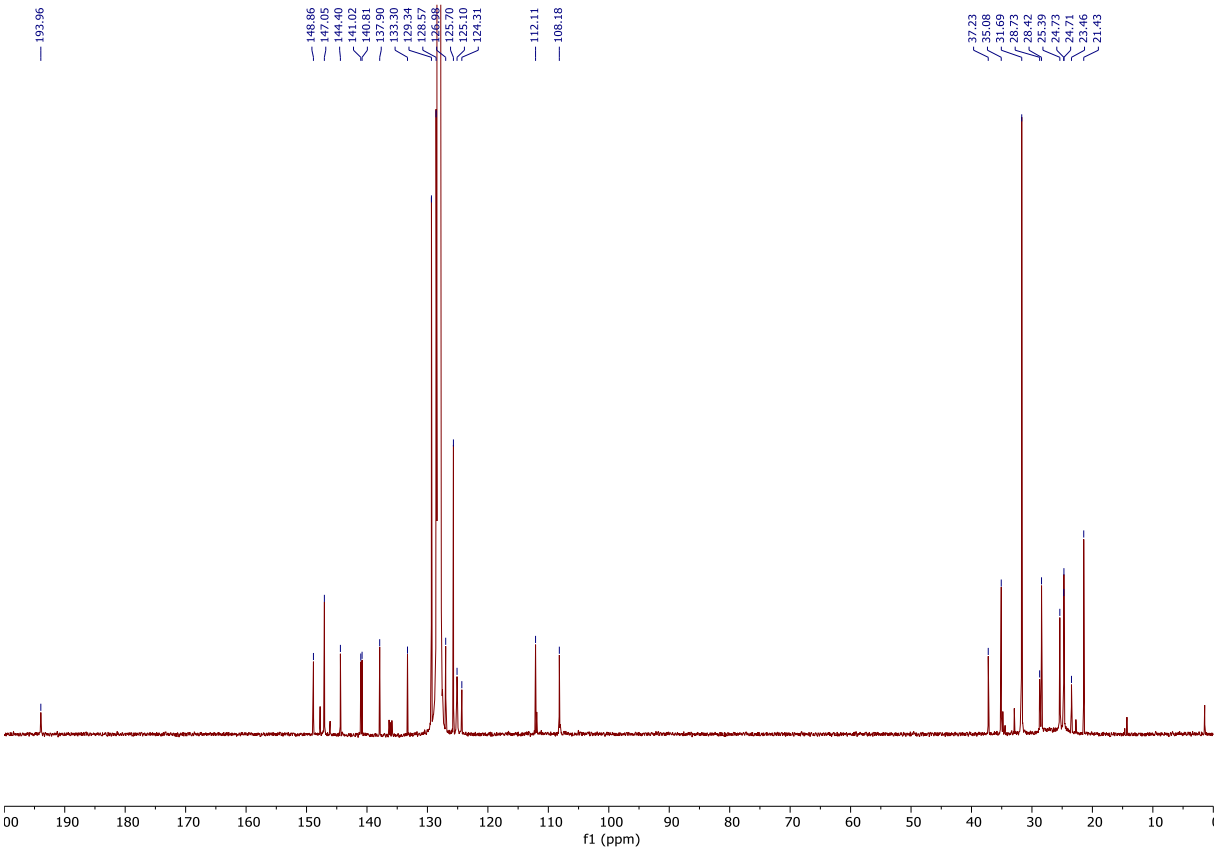
A 6.11: ^{1}H NMR spectrum of [**4**-$K_2(BEt_3)$]$_2$ in THF-d_8.



A 6.12: *In situ* ^{1}H NMR spectrum showing formation of [**4**-$K_2(BEt_3)$]$_2$ in THF-d_8.



A 6.13: ^{1}H NMR spectrum of **5** in C_6D_6.



A 6.14: ^{13}C NMR spectrum of **5** in C_6D_6

Coordinates

Gaussian outputs

A_SVP

SCF Done: E(RB3LYP) = -4489.00104413 A.U.

Al	3.23944	0.00005	0.23096
O	4.97777	0.00044	-0.82476
O	1.92181	-0.00018	-1.21798
O	1.69663	-0.00010	1.50880
N	3.77066	1.77475	0.51423
N	3.77148	-1.77437	0.51436
C	0.67148	-0.00003	0.78256
C	5.72446	-1.17118	-0.66999
C	5.72384	1.17249	-0.67024
C	5.03903	-2.14195	0.06433
C	0.78837	-0.00008	-0.66324
C	7.03447	-1.23770	-1.10615
C	7.69438	2.45586	-0.86031
H	8.72781	2.59179	-1.17977
C	5.03793	2.14300	0.06399
C	2.94655	2.87143	0.91570
C	7.61704	0.00104	-1.80868
C	2.78983	3.18375	2.28375
C	5.72147	3.35262	0.26770
H	5.23183	4.16473	0.80670
C	7.03967	3.50873	-0.19877
C	7.69569	-2.45353	-0.85979
H	8.72922	-2.58893	-1.17915
C	7.03379	1.23962	-1.10642
C	5.72322	-3.35117	0.26827
H	5.23397	-4.16346	0.80735
C	7.04152	-3.50665	-0.19812
C	2.39066	3.70075	-0.09008
C	2.94777	-2.87159	0.91522
C	1.73365	4.87453	0.29847
H	1.30818	5.52757	-0.46573
C	7.74412	4.82593	0.01939
C	3.36326	2.28595	3.36866
H	3.68239	1.35483	2.88093
C	1.62699	5.22411	1.64349
H	1.12947	6.15429	1.92960
C	2.79077	-3.18444	2.28311
C	2.52635	3.35901	-1.56832
H	3.03686	2.39134	-1.63819
C	9.14804	0.00147	-1.77351
H	9.52788	0.00170	-0.74137
H	9.54694	0.88521	-2.29175
H	9.54743	-0.88217	-2.29153
C	3.36317	-2.28656	3.36850
H	3.68198	-1.35514	2.88113
C	2.13389	4.37406	2.62519
H	2.02323	4.64273	3.67811
C	7.13710	0.00073	-3.28208
H	7.50881	-0.89468	-3.80392
H	7.50832	0.89623	-3.80414
H	6.03900	0.00043	-3.34048
C	7.74659	-4.82354	0.01989
C	2.39267	-3.70089	-0.09101
C	1.15879	3.20438	-2.24504
H	0.48813	2.54246	-1.67714
H	1.27105	2.78684	-3.25817
H	0.64179	4.16816	-2.33583
C	2.13548	-4.37527	2.62395
H	2.02466	-4.64436	3.67675
C	2.31158	1.91649	4.42199
H	1.96004	2.80018	4.97852
H	2.73312	1.21158	5.15560
H	1.43995	1.43734	3.95249
C	3.39199	4.38600	-2.31503
H	2.92776	5.38575	-2.29719
H	3.51333	4.09302	-3.37054
H	4.39233	4.46505	-1.86553
C	2.52861	-3.35857	-1.56909
H	3.03847	-2.39053	-1.63846
C	4.61225	2.91462	4.00551
H	5.38114	3.12130	3.24572
H	5.04914	2.23898	4.75897
H	4.36677	3.86558	4.50663
C	4.61220	-2.91462	4.00586
H	4.36704	-3.86584	4.50665
H	5.04829	-2.23889	4.75970
H	5.38161	-3.12067	3.24643
C	1.73623	-4.87519	0.29694
H	1.31138	-5.52822	-0.46762
C	1.62939	-5.22530	1.64182
H	1.13234	-6.15588	1.92746
C	2.31072	-1.91794	4.42137
H	1.43902	-1.43927	3.95152
H	2.73143	-1.21289	5.15533
H	1.95945	-2.80196	4.97756
C	1.16119	-3.20461	-2.24625
H	0.64499	-4.16876	-2.33782
H	1.27354	-2.78641	-3.25910
H	0.48978	-2.54354	-1.67823
C	3.39523	-4.38470	-2.31584
H	4.39548	-4.46318	-1.86603
H	3.51671	-4.09131	-3.37122
H	2.93171	-5.38478	-2.29845
O	-1.92180	0.00019	1.21799
O	-1.69662	0.00013	-1.50878
C	-0.67146	0.00007	-0.78254
C	-0.78836	0.00012	0.66325
Al	-3.23943	-0.00005	-0.23095
O	-4.97777	-0.00046	0.82477
N	-3.77065	-1.77474	-0.51428
N	-3.77147	1.77438	-0.51433
C	-5.72445	1.17117	0.67002
C	-5.72383	-1.17250	0.67019
C	-5.03902	2.14195	-0.06429
C	-7.03446	1.23768	1.10617
C	-7.69438	-2.45587	0.86022
H	-8.72782	-2.59179	1.17966
C	-5.03793	-2.14299	-0.06406
C	-2.94654	-2.87143	-0.91572
C	-7.61703	-0.00108	1.80867
C	-2.78984	-3.18379	-2.28376
C	-5.72148	-3.35260	-0.26781
H	-5.23183	-4.16470	-0.80682
C	-7.03968	-3.50872	0.19865
C	-7.69568	2.45351	0.85983
H	-8.72921	2.58891	1.17919
C	-7.03379	-1.23964	1.10637
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H	-1.12952	-6.15434	-1.92953
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C	-2.52635	-3.35893	1.56830
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H	-7.50879	0.89459	3.80394
H	-7.50830	-0.89633	3.80410
H	-6.03898	-0.00052	3.34046
C	-7.74658	4.82353	-0.01983
C	-2.39267	3.70090	0.09105
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H	-0.48810	-2.54244	1.67713
H	-1.27106	-2.78674	3.25816
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H	-2.02470	4.64442	-3.67670
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H	-2.73312	-1.21159	-5.15560
H	-1.44002	-1.43723	-3.95239
C	-3.39205	-4.38586	2.31503
H	-2.92786	-5.38562	2.29722
H	-3.51340	-4.09285	3.37052
H	-4.39239	-4.46489	1.86550
C	-2.52862	3.35854	1.56913
H	-3.03846	2.39049	1.63847
C	-4.61219	-2.91479	-4.00564

H	-5.38109	-3.12156	-3.24590
H	-5.04909	-2.23917	-4.75910
H	-4.36660	-3.86572	-4.50677
C	-4.61218	2.91464	-4.00586
H	-4.36701	3.86586	-4.50665
H	-5.04825	2.23890	-4.75970
H	-5.38160	3.12069	-3.24645
C	-1.73625	4.87521	-0.29688
H	-1.31141	5.52823	0.46768
C	-1.62943	5.22534	-1.64176
H	-1.13240	6.15593	-1.92739
C	-2.31069	1.91796	-4.42133
H	-1.43899	1.43929	-3.95145
H	-2.73139	1.21291	-5.15528
H	-1.95941	2.80198	-4.97751
C	-1.16120	3.20459	2.24629
H	-0.64502	4.16874	2.33790
H	-1.27355	2.78635	3.25913
H	-0.48977	2.54354	1.67826
C	-3.39526	4.38465	2.31589
H	-4.39551	4.46313	1.86607
H	-3.51675	4.09123	3.37126
H	-2.93175	5.38474	2.29853
H	-8.82031	-4.75053	0.19416
H	-7.62505	-5.17771	-1.05666
H	-7.32727	-5.60986	0.63567
H	-8.82321	4.74690	0.19116
H	-7.33206	5.60684	0.63768
H	-7.62522	5.17706	-1.05606
H	7.33211	-5.60683	-0.63767
H	8.82323	-4.74689	-0.19102
H	7.62517	-5.17709	1.05611
H	7.62506	5.17775	1.05649
H	8.82029	4.75055	-0.19434
H	7.32723	5.60986	-0.63584

B_SVP

SCF Done: E(RB3LYP) = -4490.40613834 A.U.

C	-1.99597	-0.78521	-1.51878
O	-1.66928	-1.18788	-2.52350
C	-0.48912	0.30616	0.37209
C	0.48442	0.29932	-0.37040
C	2.00065	-0.79066	1.52452
O	-1.58330	0.32821	1.05441
O	1.57774	0.30787	-1.05459
O	1.67492	-1.19441	2.52887
Al	3.13008	-0.03742	-0.21812
N	3.71584	-1.53186	-1.19200
N	3.63353	1.67577	0.36551
C	5.00521	-1.99882	-0.95351
C	2.84316	-2.38245	-1.93971
C	4.84648	1.81919	1.03256
C	2.96816	2.89653	0.02432
C	5.65513	-1.42865	0.14665
C	5.74211	-2.95072	-1.67389
C	2.44460	-3.61996	-1.37450
C	2.37892	-1.98994	-3.21715
C	5.54791	0.63203	1.27282
C	5.48930	3.00035	1.43949
C	2.04604	3.47305	0.92890
C	3.29891	3.54824	-1.18632
O	4.85819	-0.49149	0.80965
C	6.96119	-1.64930	0.54039
C	7.06767	-3.24813	-1.30682
H	5.28345	-3.44867	-2.52966
C	1.62203	-4.46900	-2.12552
C	2.85502	-4.04259	0.03206
C	1.53228	-2.86009	-3.91644
C	2.83224	-0.67869	-3.84292
C	6.84637	0.52290	1.73475
H	4.99459	3.96064	1.28999
C	6.78387	2.95196	1.98776
C	1.62460	2.75550	2.20255
C	1.53163	4.74273	0.63954
C	2.75820	4.81673	-1.43448
C	4.23039	2.91066	-2.20720
C	7.47807	-0.87981	1.76930
C	7.67320	-2.59340	-0.22095
C	7.83061	-4.28677	-2.09274
H	1.31863	-5.43015	-1.70514
C	1.16498	-4.09635	-3.38631
H	3.44264	-3.22581	0.47086
C	3.74994	-5.29096	0.02642
C	1.63020	-4.25602	0.93247
H	1.16088	-2.57371	-4.90080
H	2.94089	0.05017	-3.03020
C	1.81310	-0.09252	-4.82385
C	4.21185	-0.84502	-4.50037
C	7.46326	1.72863	2.11248
C	7.44127	4.23721	2.42845
H	1.82653	1.68806	2.03944
C	0.12669	2.90109	2.49617
C	2.46504	3.19823	3.41144
H	0.82404	5.20211	1.32943
C	1.89881	5.42137	-0.52039
H	3.01575	5.33987	-2.35769
H	4.31841	1.84393	-1.95015
C	3.66093	2.98855	-3.62891
C	5.64580	3.50607	-2.14183
C	9.00787	-0.80850	1.78640
C	6.98475	-1.61153	3.04309
H	8.70887	-2.82670	0.02703
H	7.77331	-4.09177	-3.17561
H	8.89211	-4.31327	-1.80681
H	7.41288	-5.29430	-1.92548
H	0.51367	-4.76492	-3.95447
H	3.21429	-6.16014	-0.38892
H	4.06064	-5.54891	1.05190
H	4.65667	-5.12887	-0.57290
H	0.93762	-3.40362	0.90030
H	1.93406	-4.40546	1.98089
H	1.05812	-5.14467	0.62688
H	1.71349	-0.70345	-5.73538
H	2.12773	0.91200	-5.14222
H	0.82006	-0.00828	-4.35659
H	4.96232	-1.18413	-3.77170
H	4.55938	0.10912	-4.92852
H	4.16890	-1.58735	-5.31436
H	8.48279	1.72532	2.49819
H	7.35105	5.01765	1.65606
H	6.96447	4.63233	3.34161
H	8.50972	4.09283	2.64531
H	-0.12939	3.92101	2.82234
H	-0.16828	2.21518	3.30534
H	-0.48697	2.66743	1.61730
H	3.53774	3.02231	3.25051
H	2.15836	2.65025	4.31756
H	2.32381	4.27460	3.60496
H	1.49412	6.41610	-0.72356
H	2.63393	2.59906	-3.66311
H	4.27922	2.39767	-4.32229
H	3.64404	4.02313	-4.00663
H	5.62553	4.58258	-2.37981
H	6.31018	3.01093	-2.86872
H	6.08432	3.38825	-1.14097
H	9.39731	-0.29504	0.89522
H	9.44212	-1.81775	1.82471
H	9.36112	-0.27292	2.67910
H	7.30903	-1.06923	3.94472
H	7.39100	-2.63427	3.07785
H	5.88712	-1.67838	3.06042
Al	-3.13294	-0.03546	0.22048
N	-3.70444	-1.53060	1.20126
N	-3.65471	1.67049	-0.36729
C	-4.98564	-2.01701	0.95815
C	-2.82298	-2.36287	1.95909
C	-4.86669	1.79796	-1.03911
C	-2.99810	2.89826	-0.03527
C	-5.63946	-1.45771	-0.14541
C	-5.71202	-2.97803	1.67712
C	-2.39891	-3.59536	1.40222
C	-2.37303	-1.95542	3.23714
C	-5.55409	0.60193	-1.27648
C	-5.52108	2.96990	-1.45397
C	-2.08296	3.47608	-0.94600
C	-3.32856	3.55387	1.17342
O	-4.85259	-0.51175	-0.80764
C	-6.94126	-1.69568	-0.54293
C	-7.03225	-3.29367	1.30587
H	-5.24984	-3.46835	2.53540
C	-1.56525	-4.42583	2.16193
C	-2.79231	-4.03064	-0.00518
C	-1.51502	-2.80683	3.94549
C	-2.85090	-0.64694	3.85070
C	-6.84951	0.47580	-1.74226
H	-5.03758	3.93635	-1.30738
C	-6.81338	2.90436	-2.00604
C	-1.66043	2.75459	-2.21695
C	-1.57621	4.75082	-0.66553
C	-2.79487	4.82694	1.41311
C	-4.25264	2.91475	2.20011

C	-7.46456	-0.93449	-1.77443
C	-7.64313	-2.64819	0.21747
C	-7.78377	-4.34163	2.09044
H	-1.24186	-5.38312	1.74784
C	-1.12242	-4.03886	3.42342
H	-3.39157	-3.22618	-0.45093
C	-3.66499	-5.29464	-0.00055
C	-1.55751	-4.22569	-0.89605
H	-1.15381	-2.50913	4.93020
H	-2.94551	0.07983	3.03400
C	-1.85994	-0.05103	4.85429
C	-4.24383	-0.82156	4.47724
C	-7.47868	1.67295	-2.12724
C	-7.48377	4.18014	-2.45463
H	-1.87156	1.68883	-2.05470
C	-0.15978	2.88904	-2.50227
C	-2.49195	3.20306	-3.42985
H	-0.87484	5.21139	-1.36113
C	-1.94313	5.43275	0.49249
H	-3.05187	5.35302	2.33473
H	-4.32286	1.84358	1.95619
C	-3.69023	3.01946	3.62279
C	-5.67720	3.48668	2.12289
C	-8.99507	-0.88096	-1.79446
C	-6.96035	-1.66305	-3.04577
H	-8.67487	-2.89547	-0.03333
H	-7.73213	-4.14508	3.17332
H	-8.84400	-4.38225	1.80150
H	-7.35242	-5.34373	1.92517
H	-0.46225	-4.69269	3.99848
H	-3.11718	-6.15237	0.42266
H	-3.96343	-5.56256	-1.02712
H	-4.57891	-5.14600	0.59137
H	-0.87903	-3.36194	-0.86046
H	-1.85047	-4.38213	-1.94646
H	-0.97325	-5.10394	-0.58439
H	-1.77629	-0.66059	5.76836
H	-2.19097	0.95079	5.16421
H	-0.85681	0.04211	4.41076
H	-4.97555	-1.16858	3.73363
H	-4.60773	0.13139	4.89429
H	-4.21337	-1.56074	5.29465
H	-8.49679	1.65653	-2.51634
H	-7.40716	4.96419	-1.68440
H	-7.00679	4.57797	-3.36652
H	-8.54922	4.02221	-2.67672
H	0.10612	3.90765	-2.82445
H	0.13441	2.20265	-3.31136
H	0.44703	2.64899	-1.62024
H	-3.56668	3.03579	-3.27256
H	-2.18635	2.65158	-4.33420
H	-2.34123	4.27802	-3.62403
H	-1.54428	6.43115	0.68921
H	-2.65671	2.64843	3.66605
H	-4.30119	2.42617	4.32055
H	-3.69334	4.05846	3.98854
H	-5.67434	4.56640	2.34685
H	-6.33583	2.99059	2.85436
H	-6.11100	3.34921	1.12253
H	-9.39202	-0.37014	-0.90508
H	-9.41756	-1.89523	-1.83139
H	-9.35287	-0.35142	-2.68894
H	-7.28908	-1.12634	-3.94914
H	-7.35468	-2.69048	-3.07922
H	-5.86198	-1.71725	-3.06079

C_SVP

SCF Done: E(RB3LYP) = -4488.74073197 A.U.

C	-1.56337	-0.50561	-1.22783
O	-1.16044	-0.84346	-2.28271
C	-0.68071	0.08780	0.03103
C	0.68057	0.08774	-0.03144
C	1.56324	-0.50520	1.22780
O	-1.50475	0.35326	0.96525
O	1.50469	0.35274	-0.96570
O	1.16019	-0.84258	2.28277
Al	3.17750	-0.06579	-0.12008
N	3.70283	-1.57568	-1.11001
N	3.71810	1.70161	0.23349
C	4.99627	-2.04083	-0.88430
C	2.82373	-2.44948	-1.82314
C	4.93340	1.86953	0.88889
C	2.99211	2.89632	-0.06376
C	5.68356	-1.42764	0.16973
C	5.70762	-3.02739	-1.58531
C	2.45538	-3.68305	-1.22830
C	2.34383	-2.09262	-3.10467
C	5.62747	0.69102	1.18966
C	5.59293	3.06491	1.22227
C	2.21255	3.51172	0.94284
C	3.11044	3.47769	-1.34857
O	4.91750	-0.45340	0.81380
C	6.99965	-1.63779	0.53458
C	7.04178	-3.31504	-1.24570
H	5.22206	-3.55748	-2.40599
C	1.66667	-4.57301	-1.96623
C	2.84813	-4.04973	0.19821
C	1.52977	-3.00429	-3.78963
C	2.74567	-0.77632	-3.75342
C	6.93588	0.59286	1.62325
H	5.10585	4.02056	1.02549
C	6.89806	3.03285	1.74606
C	2.01386	2.87845	2.31296
C	1.61647	4.74814	0.66406
C	2.49330	4.71305	-1.58164
C	3.91529	2.79374	-2.44492
C	7.55604	-0.81345	1.71071
C	7.68315	-2.61753	-0.20662
C	7.77695	-4.39101	-2.00744
H	1.38793	-5.53231	-1.52519
C	1.20827	-4.24311	-3.23895
H	3.42174	-3.21376	0.61840
C	3.74459	-5.29537	0.25708
C	1.60320	-4.22954	1.07838
H	1.14688	-2.74577	-4.77699
H	2.85617	-0.03765	-2.95019
C	1.68211	-0.22853	-4.70976
C	4.11500	-0.90705	-4.43916
C	7.57130	1.81142	1.92013
C	7.57503	4.33273	2.10689
H	2.47454	1.88130	2.28482
C	0.52462	2.69840	2.64443
C	2.72804	3.67476	3.41673
H	1.01788	5.23767	1.43342
C	1.76844	5.35541	-0.57883
H	2.58407	5.18496	-2.56104
H	3.86163	1.71089	-2.25512
C	3.34430	3.03528	-3.84583
C	5.40121	3.18453	-2.38845
C	9.08616	-0.75569	1.68220
C	7.09130	-1.47714	3.03159
H	8.72527	-2.84529	0.01852
H	7.66764	-4.25767	-3.09547
H	8.85066	-4.39490	-1.77007
H	7.37632	-5.38997	-1.76416
H	0.58290	-4.94461	-3.79614
H	3.21828	-6.18333	-0.12954
H	4.03879	-5.50968	1.29726
H	4.66111	-5.15684	-0.33375
H	0.92863	-3.36447	1.02320
H	1.88542	-4.36360	2.13461
H	1.02206	-5.11334	0.77536
H	1.58077	-0.84826	-5.61514
H	1.95625	0.78316	-5.04095
H	0.70130	-0.17723	-4.21436
H	4.88881	-1.22900	-3.72676
H	4.42993	0.05632	-4.87232
H	4.07355	-1.64900	-5.25349
H	8.60015	1.81983	2.28018
H	7.45279	5.08275	1.30942
H	7.13799	4.76384	3.02382
H	8.65150	4.19404	2.28425
H	0.01519	3.66770	2.75599
H	0.40467	2.14485	3.58913
H	-0.01356	2.14385	1.86384
H	3.80539	3.76180	3.21473
H	2.60244	3.17934	4.39309
H	2.31249	4.69241	3.50144
H	1.30433	6.32500	-0.77509
H	2.26925	2.80780	-3.88589
H	3.85945	2.39625	-4.57906
H	3.48560	4.07800	-4.17203
H	5.52040	4.26801	-2.55467
H	5.97085	2.65519	-3.16964
H	5.84921	2.94281	-1.41541
H	9.45527	-0.29006	0.75670
H	9.51306	-1.76595	1.75853
H	9.46801	-0.18042	2.53764
H	7.44590	-0.89444	3.89579
H	7.49021	-2.50067	3.10538
H	5.99421	-1.53208	3.08289

Al	-3.17758	-0.06583	0.12001
N	-3.70229	-1.57578	1.11020
N	-3.71885	1.70130	-0.23367
C	-4.99552	-2.04152	0.88458
C	-2.82282	-2.44900	1.82359
C	-4.93425	1.86871	-0.88901
C	-2.99310	2.89626	0.06317
C	-5.68312	-1.42870	-0.16946
C	-5.70645	-3.02829	1.58575
C	-2.45364	-3.68242	1.22898
C	-2.34331	-2.09165	3.10514
C	-5.62794	0.68992	-1.18953
C	-5.59418	3.06382	-1.22260
C	-2.21363	3.51141	-0.94365
C	-3.11152	3.47808	1.34777
O	-4.91752	-0.45419	-0.81362
C	-6.99918	-1.63935	-0.53415
C	-7.04053	-3.31647	1.24628
H	-5.22062	-3.55810	2.40645
C	-1.66456	-4.57183	1.96720
C	-2.84584	-4.04949	-0.19758
C	-1.52890	-3.00277	3.79039
C	-2.74582	-0.77533	3.75345
C	-6.93634	0.59125	-1.62302
H	-5.10738	4.01966	-1.02605
C	-6.89933	3.03123	-1.74629
C	-2.01483	2.87767	-2.31353
C	-1.61772	4.74803	-0.66532
C	-2.49456	4.71361	1.58039
C	-3.91625	2.79437	2.44436
C	-7.55601	-0.81530	-1.71027
C	-7.68225	-2.61928	0.20720
C	-7.77524	-4.39263	2.00820
H	-1.38519	-5.53103	1.52634
C	-1.20663	-4.24150	3.23996
H	-3.41951	-3.21371	-0.61811
C	-3.74197	-5.29537	-0.25648
C	-1.60060	-4.22922	-1.07733
H	-1.14631	-2.74388	4.77778
H	-2.85606	-0.03685	2.95000
C	-1.68289	-0.22708	4.71021
C	-4.11545	-0.90619	4.43856
C	-7.57218	1.80954	-1.92007
C	-7.57678	4.33082	-2.10725
H	-2.47535	1.88045	-2.28502
C	-0.52558	2.69773	-2.64496
C	-2.72919	3.67345	-3.41756
H	-1.01922	5.23736	-1.43487
C	-1.76978	5.35572	0.57736
H	-2.58541	5.18586	2.55962
H	-3.86244	1.71147	2.25488
C	-3.34520	3.03643	3.84517
C	-5.40221	3.18495	2.38788
C	-9.08615	-0.75806	-1.68157
C	-7.09122	-1.47892	-3.03117
H	-8.72430	-2.84746	-0.01783
H	-7.66603	-4.25902	3.09621
H	-8.84893	-4.39705	1.77079
H	-7.37415	-5.39145	1.76513
H	-0.58099	-4.94258	3.79738
H	-3.21555	-6.18307	0.13059
H	-4.03568	-5.51004	-1.29672
H	-4.65875	-5.15694	0.33394
H	-0.92614	-3.36407	-1.02203
H	-1.88247	-4.36340	-2.13363
H	-1.01945	-5.11293	-0.77408
H	-1.58179	-0.84664	5.61574
H	-1.95748	0.78458	5.04110
H	-0.70184	-0.17556	4.21528
H	-4.88885	-1.22855	3.72592
H	-4.43082	0.05724	4.87127
H	-4.07419	-1.64787	5.25315
H	-8.60107	1.81756	-2.28004
H	-7.45528	5.08080	-1.30962
H	-7.13952	4.76228	-3.02391
H	-8.65310	4.19163	-2.28512
H	-0.01629	3.66705	-2.75692
H	-0.40556	2.14380	-3.58943
H	0.01271	2.14359	-1.86414
H	-3.80655	3.76036	-3.21552
H	-2.60356	3.17770	-4.39375
H	-2.31384	4.69115	-3.50266
H	-1.30581	6.32544	0.77328
H	-2.27014	2.80902	3.88527
H	-3.86030	2.39765	4.57865
H	-3.48654	4.07926	4.17101
H	-5.52153	4.26849	2.55357
H	-5.97169	2.65593	3.16940
H	-5.85031	2.94269	1.41502
H	-9.45531	-0.29250	-0.75605
H	-9.51271	-1.76848	-1.75777
H	-9.46832	-0.18299	-2.53699
H	-7.44613	-0.89640	-3.89536
H	-7.48978	-2.50260	-3.10483
H	-5.99411	-1.53349	-3.08261

D_SVP

SCF Done: E(RB3LYP) = -5690.32630903 A.U.

Al	-3.14853	0.00697	0.23888
O	-5.06965	-0.03269	-0.76291
O	-2.00092	-0.01453	-1.22701
O	-1.75165	0.06299	1.51325
N	-3.80059	-1.78495	0.58660
N	-3.85525	1.78743	0.53751
C	-0.61424	-0.00269	0.83513
C	-5.82682	1.12201	-0.58055
C	-5.80347	-1.19165	-0.52165
C	-5.14933	2.10400	0.14538
C	-0.74972	-0.00023	-0.73126
C	-7.15417	1.17071	-0.97206
C	-7.79338	-2.47750	-0.57221
H	-8.83770	-2.62068	-0.85047
C	-5.09879	-2.13272	0.23165
C	-2.98825	-2.90941	0.89106
C	-7.73082	-0.08173	-1.64930
C	-2.54248	-3.15235	2.21483
C	-5.79222	-3.31825	0.53741
H	-5.29398	-4.10226	1.10947
C	-7.12644	-3.49285	0.13221
C	-7.84374	2.36196	-0.69154
H	-8.88934	2.47146	-0.98001
C	-7.13011	-1.28551	-0.90736
C	-5.86866	3.28715	0.39757
H	-5.39370	4.10174	0.94598
C	-7.20185	3.41908	-0.02664
C	-2.69991	-3.84763	-0.14495
C	-3.08003	2.91940	0.90119
C	-1.98852	-5.01305	0.17521
H	-1.76492	-5.73739	-0.61129
C	-7.83239	-4.78785	0.45451
C	-2.89192	-2.20621	3.35109
H	-3.23409	-1.27180	2.89463
C	-1.55101	-5.26076	1.47902
H	-0.99916	-6.17511	1.71018
C	-2.70518	3.13887	2.25109
C	-3.13071	-3.61632	-1.59322
H	-3.80379	-2.75390	-1.60883
C	-9.26106	-0.09579	-1.61476
H	-9.64227	-0.07187	-0.58341
H	-9.65089	-0.99744	-2.10890
H	-9.66824	0.77026	-2.15630
C	-3.14388	2.18561	3.34985
H	-3.43869	1.25024	2.86256
C	-1.82185	-4.32874	2.48168
H	-1.48226	-4.52491	3.50076
C	-7.25186	-0.11699	-3.12252
H	-7.63414	0.75965	-3.66841
H	-7.61524	-1.03002	-3.61949
H	-6.15404	-0.10685	-3.18216
C	-7.93504	4.71253	0.23519
C	-2.74749	3.87696	-0.10114
C	-1.94495	-3.24614	-2.50280
H	-1.54527	-2.25229	-2.24769
H	-2.27691	-3.18121	-3.55059
H	-1.13840	-3.99861	-2.46773
C	-1.98201	4.29950	2.57232
H	-1.68875	4.47555	3.60924
C	-1.67609	-1.86895	4.22077
H	-1.27774	-2.75395	4.74338
H	-1.95204	-1.13340	4.99089
H	-0.87415	-1.42958	3.60995
C	-3.91287	-4.81280	-2.15187
H	-3.27835	-5.70786	-2.25852
H	-4.31377	-4.57282	-3.14924
H	-4.75979	-5.06735	-1.49780
C	-3.12372	3.67452	-1.56854
H	-3.83188	2.84194	-1.62008
C	-4.05504	-2.77428	4.18029
H	-4.93771	-2.95719	3.54836
H	-4.34529	-2.06744	4.97461
H	-3.77785	-3.72763	4.66067

C	-4.38386	2.74407	4.06789
H	-4.15736	3.69848	4.57211
H	-4.74141	2.03401	4.83124
H	-5.20525	2.92227	3.35727
C	-2.03907	5.02868	0.27262
H	-1.77574	5.76642	-0.48837
C	-1.65187	5.24347	1.59790
H	-1.09718	6.14492	1.86953
C	-2.01600	1.85207	4.33041
H	-1.15883	1.41581	3.79775
H	-2.36430	1.11468	5.06963
H	-1.67432	2.73647	4.89259
C	-1.91519	3.26163	-2.42684
H	-1.08799	3.98770	-2.35859
H	-2.20427	3.20260	-3.48767
H	-1.55584	2.25786	-2.15217
C	-3.83088	4.90537	-2.15096
H	-4.69402	5.19229	-1.53201
H	-4.19814	4.68721	-3.16610
H	-3.15679	5.77433	-2.22530
O	2.00039	0.01281	1.22528
O	1.75232	-0.06161	-1.51527
C	0.61410	-0.01584	-0.83691
C	0.74955	-0.02064	0.72955
Al	3.14846	-0.00629	-0.24016
O	5.06926	0.03560	0.76282
N	3.79846	1.78652	-0.58638
N	3.85783	-1.78580	-0.53922
C	5.82831	-1.11770	0.57961
C	5.80137	1.19593	0.52306
C	5.15253	-2.10028	-0.14711
C	7.15559	-1.16465	0.97163
C	7.78919	2.48492	0.57568
H	8.83313	2.62957	0.85463
C	5.09568	2.13638	-0.23005
C	2.98457	2.90954	-0.89197
C	7.72995	0.08798	1.65045
C	2.54145	3.15223	-2.21666
C	5.78734	3.32327	-0.53449
H	5.28817	4.10685	-1.10636
C	7.12102	3.49974	-0.12832
C	7.84712	-2.35459	0.69040
H	8.89278	-2.46269	0.97919
C	7.12766	1.29157	0.90950
C	5.87385	-3.28205	-0.40001
H	5.40034	-4.09702	-0.94911
C	7.20715	-3.41218	0.02441
C	2.69152	3.84634	0.14396
C	3.08433	-2.91972	-0.90024
C	1.97718	5.00976	-0.17703
H	1.74953	5.73279	0.60948
C	7.82505	4.79608	-0.44941
C	2.89573	2.20749	-3.35259
H	3.24077	1.27426	-2.89580
C	1.54244	5.25735	-1.48174
H	0.98855	6.17030	-1.71356
C	2.70773	-3.14201	-2.24918
C	3.12154	3.61642	1.59271
H	3.79475	2.75409	1.60949
C	9.26018	0.10452	1.61660
H	9.64188	0.08232	0.58540
H	9.64835	1.00626	2.11189
H	9.66852	-0.76146	2.15739
C	3.14068	-2.18841	-3.34991
H	3.43515	-1.25219	-2.86409
C	1.81856	4.32697	-2.48447
H	1.48111	4.52303	-3.50429
C	7.25028	0.12088	3.12349
H	7.63365	-0.75578	3.66859
H	7.61205	1.03391	3.62163
H	6.15245	0.10902	3.18263
C	7.94253	-4.70417	-0.23854
C	2.75607	-3.87705	0.10384
C	1.93567	3.24767	2.50274
H	1.53752	2.25230	2.25117
H	2.26701	3.18682	3.55096
H	1.12790	3.99850	2.46431
C	1.98829	-4.30572	-2.56797
H	1.69394	-4.48393	-3.60422
C	1.68218	1.86606	-4.22384
H	1.28102	2.74986	-4.74631
H	1.96187	1.13207	-4.99415
H	0.88142	1.42310	-3.61412
C	3.90333	4.81391	2.14993
H	3.26842	5.70887	2.25504
H	4.30404	4.57545	3.14775
H	4.75033	5.06780	1.49574
C	3.13088	-3.66996	1.57088
H	3.83346	-2.83260	1.62123
C	4.05783	2.77974	-4.18034
H	4.93908	2.96575	-3.54733
H	4.35156	2.07402	-4.97436
H	3.77785	3.73213	-4.66100
C	4.37921	-2.74467	-4.07209
H	4.15297	-3.69974	-4.57519
H	4.73266	-2.03417	-4.83695
H	5.20344	-2.92091	-3.36426
C	2.05221	-5.03225	-0.26756
H	1.79299	-5.77020	0.49469
C	1.66376	-5.25007	-1.59204
H	1.11247	-6.15416	-1.86183
C	2.00842	-1.85781	-4.32646
H	1.15235	-1.42291	-3.79094
H	2.35232	-1.12014	-5.06745
H	1.66641	-2.74331	-4.88672
C	1.91921	-3.26344	2.42780
H	1.09788	-3.99652	2.36260
H	2.20804	-3.19780	3.48830
H	1.55121	-2.26395	2.14914
C	3.84576	-4.89524	2.15560
H	4.71141	-5.17706	1.53784
H	4.21058	-4.67330	3.17081
H	3.17743	-5.76860	2.23042
H	8.91226	4.71340	-0.30447
H	7.64171	5.10651	-1.49033
H	7.46471	5.61407	0.19849
H	9.02748	-4.58847	-0.09915
H	7.60272	-5.50022	0.44672
H	7.76632	-5.06613	-1.26393
H	-7.59641	5.50643	-0.45316
H	-9.02053	4.59768	0.09924
H	-7.75543	5.07693	1.25911
H	-7.64657	-5.09947	1.49463
H	-8.91984	-4.70265	0.31292
H	-7.47588	-5.60616	-0.19512
K	-0.03859	2.69383	0.08427
K	0.03918	-2.71645	-0.08864

Toluene_SVP

SCF Done: E(RB3LYP) = -271.394519887 A.U.

C	-1.90652	-0.00046	0.00892
C	-1.20116	-1.20696	0.00212
C	0.19567	-1.20363	-0.00954
C	0.91650	0.00062	-0.01227
C	0.19487	1.20411	-0.00952
C	-1.20220	1.20639	0.00212
H	-2.99913	-0.00093	0.01526
H	-1.74165	-2.15693	0.00219
H	0.73880	-2.15296	-0.01871
H	0.73726	2.15383	-0.01868
H	-1.74331	2.15600	0.00217
C	2.42465	0.00026	0.00949
H	2.80490	-0.02689	1.04590
H	2.83616	-0.87825	-0.51093
H	2.83610	0.90416	-0.46516

E_SVP

SCF Done: E(RB3LYP) = -6231.87250233 A.U.

K	-0.69591	3.25814	-1.33326
Al	3.15384	-0.24058	0.11736
O	4.96146	0.56097	-0.56890
O	1.46302	-0.91803	0.65993
O	1.40250	1.81061	-1.48216
N	3.87402	-1.73128	-0.87840
N	3.84879	0.51689	1.74099
C	5.67678	-0.29270	-1.40575
C	5.04720	-1.52871	-1.59366
C	5.72091	-2.42593	-2.44459
H	5.27705	-3.39806	-2.66337
C	6.98852	-2.10601	-2.96351
C	7.61652	-0.89729	-2.62096
H	8.62386	-0.69759	-2.98710
C	6.95805	0.03998	-1.80620
C	7.52873	1.36847	-1.27876
C	7.04046	1.51192	0.17525
C	7.77372	2.00602	1.26742
H	8.80001	2.34847	1.13216
C	7.19661	2.05597	2.54771
C	5.88865	1.58666	2.76359
H	5.46452	1.60746	3.76841

C	5.12498	1.07104	1.69896
C	5.74445	1.11009	0.44496
C	7.97437	2.62263	3.71145
C	6.93643	2.53023	-2.11460
H	5.83892	2.52212	-2.07398
H	7.24274	2.43680	-3.16822
H	7.28844	3.49903	-1.72698
C	9.05618	1.40450	-1.36964
H	9.44321	2.36289	-0.99414
H	9.38422	1.31046	-2.41501
H	9.51462	0.59213	-0.78699
C	7.67411	-3.08631	-3.88447
C	3.15363	-2.90583	-1.22602
C	2.39137	-2.91889	-2.42013
C	1.72317	-4.09602	-2.78118
H	1.12796	-4.11127	-3.69694
C	1.79778	-5.24005	-1.98891
H	1.26921	-6.14922	-2.28584
C	2.54805	-5.22255	-0.81104
H	2.60366	-6.12693	-0.20273
C	3.23565	-4.06483	-0.40907
C	4.08127	-4.05337	0.86247
H	3.96291	-3.05636	1.31532
C	3.66088	-5.10409	1.89826
H	2.58584	-5.08490	2.13724
H	4.20899	-4.94575	2.83883
H	3.89245	-6.12528	1.55717
C	5.57995	-4.21586	0.55746
H	5.76973	-5.18651	0.07036
H	6.16585	-4.18015	1.49009
H	5.94869	-3.42570	-0.10631
C	2.29648	-1.68794	-3.31107
H	2.89999	-0.89766	-2.84888
C	2.88157	-1.95326	-4.70670
H	3.92702	-2.28993	-4.64550
H	2.85520	-1.03247	-5.31138
H	2.30284	-2.72055	-5.24711
C	0.85766	-1.17057	-3.40560
H	0.20375	-1.88788	-3.91587
H	0.82270	-0.22745	-3.97195
H	0.42769	-0.97489	-2.41490
C	3.09988	0.88787	2.89414
C	2.79448	-0.06406	3.89161
C	2.24800	0.37565	5.10440
H	2.02730	-0.34696	5.89223
C	2.00229	1.72918	5.33295
H	1.59893	2.05852	6.29348
C	2.22671	2.65142	4.31151
H	1.97698	3.70358	4.47131
C	2.74445	2.24807	3.07527
C	2.87040	3.25401	1.93813
H	3.30846	2.73166	1.07918
C	3.78624	4.43647	2.27897
H	3.39201	5.02200	3.12584
H	3.87301	5.11939	1.41780
H	4.79652	4.09044	2.54047
C	1.47719	3.73567	1.50782
H	0.80668	2.88402	1.32153
H	1.54356	4.34399	0.59227
H	1.00736	4.35435	2.28522
C	3.11764	-1.52948	3.65577
H	3.04955	-1.68360	2.56994
C	4.56257	-1.85066	4.06446
H	5.27194	-1.20675	3.52544
H	4.81523	-2.90040	3.84264
H	4.70566	-1.68638	5.14496
C	2.11606	-2.48203	4.31833
H	2.19639	-2.47079	5.41664
H	2.30244	-3.52095	4.00331
H	1.07732	-2.21274	4.06645
C	0.69016	-0.01483	-0.01576
C	1.67261	0.85263	-0.74853
C	1.64720	6.01219	-1.64607
H	2.10223	6.33802	-0.70743
C	0.46578	6.62175	-2.09033
H	0.00779	7.41497	-1.49399
C	-0.12254	6.22128	-3.29494
H	-1.03842	6.70037	-3.64850
C	0.48165	5.20489	-4.04945
H	0.03156	4.88336	-4.99195
C	1.65418	4.59371	-3.59587
H	2.10609	3.78591	-4.17711
C	2.25954	4.98597	-2.38581
C	3.49592	4.28188	-1.89505
H	3.25372	3.22587	-1.69173
H	3.88714	4.73558	-0.97374
H	4.29367	4.30587	-2.65375
O	-1.46304	0.91805	-0.65992
O	-1.40248	-1.81059	1.48216
C	-0.69016	0.01486	0.01576
C	-1.67260	-0.85259	0.74855
K	0.69597	-3.25806	1.33363
Al	-3.15385	0.24058	-0.11739
O	-4.96145	-0.56097	0.56893
N	-3.87411	1.73136	0.87822
N	-3.84876	-0.51699	-1.74098
C	-5.67682	0.29276	1.40568
C	-5.04729	1.52882	1.59348
C	-5.72105	2.42610	2.44431
H	-5.27722	3.39827	2.66299
C	-6.98866	2.10619	2.96324
C	-7.61661	0.89741	2.62079
H	-8.62396	0.69772	2.98691
C	-6.95809	-0.03991	1.80614
C	-7.52872	-1.36846	1.27880
C	-7.04043	-1.51199	-0.17520
C	-7.77368	-2.00615	-1.26735
H	-8.79998	-2.34857	-1.13208
C	-7.19656	-2.05614	-2.54764
C	-5.88861	-1.58683	-2.76353
H	-5.46447	-1.60764	-3.76834
C	-5.12494	-1.07116	-1.69891
C	-5.74442	-1.11017	-0.44491
C	-6.93640	-2.53014	2.11472
H	-5.83888	-2.52201	2.07411
H	-7.24272	-2.43664	3.16833
H	-7.28838	-3.49898	1.72717
C	-9.05617	-1.40454	1.36966
H	-9.44317	-2.36296	0.99423
H	-9.38423	-1.31043	2.41502
H	-9.51464	-0.59222	0.78695
C	-3.15376	2.90595	1.22573
C	-2.39149	2.91914	2.41984
C	-1.72329	4.09631	2.78076
H	-1.12809	4.11166	3.69653
C	-1.79788	5.24025	1.98837
H	-1.26930	6.14945	2.28519
C	-2.54818	5.22263	0.81051
H	-2.60380	6.12695	0.20211
C	-3.23579	4.06488	0.40867
C	-4.08145	4.05328	-0.86284
H	-3.96314	3.05620	-1.31556
C	-3.66103	5.10382	-1.89880
H	-2.58599	5.08453	-2.13779
H	-4.20915	4.94537	-2.83934
H	-3.89254	6.12508	-1.55786
C	-5.58010	4.21588	-0.55781
H	-5.76984	5.18662	-0.07088
H	-6.16604	4.18003	-1.49042
H	-5.94886	3.42584	0.10610
C	-2.29665	1.68830	3.31094
H	-2.90018	0.89799	2.84884
C	-2.88174	1.95382	4.70653
H	-3.92717	2.29054	4.64528
H	-2.85544	1.03310	5.31132
H	-2.30297	2.72114	5.24685
C	-0.85785	1.17089	3.40554
H	-0.20390	1.88827	3.91564
H	-0.82291	0.22790	3.97211
H	-0.42792	0.97496	2.41487
C	-3.09986	-0.88807	-2.89409
C	-2.79440	0.06378	-3.89164
C	-2.24799	-0.37608	-5.10441
H	-2.02726	0.34646	-5.89231
C	-2.00237	-1.72964	-5.33286
H	-1.59906	-2.05908	-6.29338
C	-2.22677	-2.65177	-4.31132
H	-1.97707	-3.70395	-4.47102
C	-2.74446	-2.24829	-3.07511
C	-2.87036	-3.25408	-1.93783
H	-3.30840	-2.73162	-1.07894
C	-3.78618	-4.43661	-2.27847
H	-3.39196	-5.02224	-3.12527
H	-3.87290	-5.11941	-1.41720
H	-4.79647	-4.09064	-2.53999
C	-1.47712	-3.73563	-1.50750
H	-0.80662	-2.88392	-1.32140
H	-1.54343	-4.34378	-0.59184
H	-1.00731	-4.35443	-2.28481
C	-3.11737	1.52925	-3.65588
H	-3.04942	1.68339	-2.57005
C	-4.56219	1.85063	-4.06481

H	-5.27174	1.20686	-3.52588
H	-4.81472	2.90042	-3.84308
H	-4.70513	1.68634	-5.14533
C	-2.11553	2.48162	-4.31830
H	-2.19565	2.47034	-5.41662
H	-2.30180	3.52057	-4.00335
H	-1.07688	2.21218	-4.06619
C	-1.64718	-6.01210	1.64648
H	-2.10227	-6.33794	0.70788
C	-0.46574	-6.62166	2.09069
H	-0.00778	-7.41487	1.49432
C	0.12264	-6.22118	3.29526
H	1.03854	-6.70026	3.64879
C	-0.48152	-5.20478	4.04980
H	-0.03138	-4.88326	4.99228
C	-1.65407	-4.59361	3.59628
H	-2.10597	-3.78582	4.17754
C	-2.25949	-4.98587	2.38624
C	-3.49587	-4.28177	1.89552
H	-3.25362	-3.22579	1.69204
H	-3.88720	-4.73554	0.97430
H	-4.29355	-4.30561	2.65430
C	-7.97427	-2.62303	-3.71130
H	-7.58166	-3.61140	-4.00676
H	-9.03898	-2.74836	-3.46505
H	-7.90278	-1.97249	-4.59759
C	-7.67428	3.08652	3.88413
H	-8.73945	2.84419	4.01348
H	-7.20816	3.08247	4.88466
H	-7.60201	4.11688	3.50070
H	7.58067	3.61016	4.00826
H	7.90431	1.97103	4.59709
H	9.03875	2.74957	3.46463
H	8.73913	-2.84363	-4.01433
H	7.60239	-4.11661	-3.50075
H	7.20755	-3.08268	-4.88479

F_SVP

SCF Done: E(RB3LYP) = -7413.11017902 A.U.

K	0.15561	-1.87282	2.22147
K	0.54707	1.93003	2.80925
Al	-3.11649	0.03939	-0.22353
O	-1.47501	0.10839	-1.17102
O	-4.96386	-0.05928	0.78144
O	-1.28585	0.25994	2.41117
N	-3.94295	1.76097	-0.70628
N	-3.77335	-1.75236	-0.74601
C	-0.73831	0.17536	0.04960
C	-1.63522	0.17557	1.10555
C	-5.70596	-1.20957	0.52564
C	-5.05624	-2.10504	-0.32710
C	-5.73129	1.10253	0.70211
C	-7.00548	-1.32121	0.99299
C	-5.15264	2.08707	-0.10771
C	-7.54301	-0.16816	1.85625
C	-7.01729	1.12569	1.21335
C	-3.09762	-2.86092	-1.33571
C	-7.74338	2.31466	1.02955
H	-8.75503	2.40768	1.42445
C	-3.36081	2.82532	-1.44286
C	-7.18450	3.38547	0.31624
C	-2.60950	-3.90954	-0.49843
C	-2.75321	3.91767	-0.76580
C	-2.96551	-1.32168	3.60238
H	-3.62499	-1.39072	2.71911
H	-2.20641	-2.11704	3.44960
C	-5.80005	-3.24709	-0.68643
H	-5.35781	-3.99559	-1.34383
C	-9.07214	-0.17998	1.93158
H	-9.52969	-0.08452	0.93592
H	-9.43316	0.64606	2.56108
H	-9.42814	-1.11340	2.39094
C	-5.91080	3.26428	-0.26490
H	-5.52599	4.07657	-0.88190
C	-7.10661	-3.43835	-0.21013
C	-3.42154	1.34408	3.50864
H	-3.64680	1.49429	2.43970
H	-4.36965	0.97988	3.93828
C	-3.04350	-3.01277	-2.75022
C	-7.70799	-2.47764	0.61796
H	-8.73239	-2.63186	0.95714
C	-2.22458	4.97834	-1.51723
H	-1.75420	5.81671	-0.99830
C	-3.46835	2.85131	-2.86035
C	-1.32800	0.38549	4.95744
H	-0.93389	1.42166	5.02088
H	-1.98920	0.31813	5.83920
C	-2.58230	-3.78616	1.02183
H	-2.55700	-2.70980	1.24638
C	-7.94745	4.67781	0.15486
C	-2.29942	4.99358	-2.90905
H	-1.88591	5.83072	-3.47666
C	-2.92537	3.93437	-3.57029
H	-3.00919	3.96398	-4.65762
C	-2.54312	-4.21060	-3.29037
H	-2.51005	-4.34443	-4.37082
C	-2.68018	3.98561	0.75279
H	-3.12857	3.06967	1.15350
C	-2.13587	-5.08979	-1.08994
H	-1.77748	-5.90210	-0.45636
C	-7.85175	-4.69627	-0.58586
C	-6.96010	-0.31104	3.28198
H	-7.30475	-1.25017	3.74157
H	-7.27986	0.53265	3.91297
H	-5.86428	-0.32314	3.26059
C	-3.12857	2.70053	4.15605
H	-2.17064	3.13269	3.81751
H	-3.05570	2.61950	5.25299
H	-3.90481	3.45466	3.93941
C	-3.76348	-1.70041	4.85341
H	-3.10866	-1.80059	5.73564
H	-4.31203	-2.65299	4.74569
H	-4.50824	-0.92790	5.10410
C	-2.10821	-5.25072	-2.47199
H	-1.73969	-6.18007	-2.91253
C	-3.54436	-1.91657	-3.68743
H	-3.14167	-0.96431	-3.30258
C	-1.33746	-4.45595	1.62456
H	-1.40789	-5.55317	1.58994
H	-1.24050	-4.19907	2.69194
H	-0.40560	-4.19769	1.10070
C	-3.45919	5.18560	1.31325
H	-3.03695	6.14130	0.96109
H	-3.41600	5.18328	2.41265
H	-4.51648	5.14604	1.01887
C	-4.22272	1.75325	-3.59411
H	-4.09983	0.83342	-3.00599
C	-0.16034	-0.58347	5.16119
H	0.34226	-0.47776	6.13774
H	0.63951	-0.44498	4.40956
H	-0.49036	-1.63588	5.09311
C	-1.22503	4.02397	1.22441
H	-0.68559	3.14685	0.84117
H	-1.18686	4.03916	2.32356
H	-0.69815	4.92128	0.87296
B	-2.27941	0.17138	3.62569
C	-3.05379	-2.09568	-5.12993
H	-1.96932	-2.25884	-5.19424
H	-3.28778	-1.20363	-5.72453
H	-3.55117	-2.94916	-5.61713
C	-3.69972	1.49491	-5.01027
H	-3.84539	2.36371	-5.67036
H	-4.24644	0.65858	-5.46629
H	-2.62781	1.23577	-5.02781
C	-3.81835	-4.36918	1.73011
H	-4.74038	-3.84417	1.46650
H	-3.68737	-4.29459	2.82053
H	-3.94328	-5.43346	1.46969
C	-5.07833	-1.79815	-3.68730
H	-5.53758	-2.76507	-3.94682
H	-5.40196	-1.06144	-4.43810
H	-5.47107	-1.48777	-2.71385
C	-5.72976	2.06003	-3.63048
H	-6.14000	2.17887	-2.61955
H	-6.27750	1.24411	-4.12806
H	-5.92125	2.99165	-4.18828
C	0.73825	0.17537	-0.04952
O	1.47494	0.10804	1.17108
C	1.63517	0.17597	-1.10546
Al	3.11645	0.03936	0.22359
O	1.28581	0.26082	-2.41106
N	3.94293	1.76078	0.70686
N	3.77339	-1.75252	0.74560
K	-0.15551	-1.87214	-2.22199
K	-0.54753	1.93059	-2.80913
B	2.27943	0.17262	-3.62555
C	5.15259	2.08708	0.10833
C	3.36070	2.82495	1.44365
C	5.05631	-2.10503	0.32665
C	3.09771	-2.86131	1.33494
C	2.96553	-1.32045	-3.60267

C	3.42159	1.34527	-3.50805
C	1.32812	0.38713	-4.95730
C	5.73126	1.10281	-0.70178
C	5.91069	3.26431	0.26583
C	2.75335	3.91755	0.76677
C	3.46790	2.85050	2.86116
C	5.70603	-1.20933	-0.52584
C	5.80015	-3.24714	0.68574
C	2.60973	-3.90971	0.49730
C	3.04351	-3.01361	2.74940
H	3.62489	-1.38978	-2.71934
H	2.20645	-2.11589	-3.45029
C	3.76370	-1.69868	-4.85372
H	3.64619	1.49565	-2.43899
H	4.36995	0.98090	-3.93699
C	3.12920	2.70163	-4.15591
H	0.93404	1.42333	-5.02048
H	1.98937	0.32001	-5.83904
C	0.16047	-0.58178	-5.16141
O	4.96389	-0.05902	-0.78143
C	7.01730	1.12615	-1.21296
C	7.18436	3.38573	-0.31528
H	5.52583	4.07642	0.88304
C	2.22451	4.97797	1.51836
C	2.68073	3.98587	-0.75182
C	2.92474	3.93334	3.57129
C	4.22215	1.75223	3.59473
C	7.00559	-1.32080	-0.99314
H	5.35792	-3.99583	1.34293
C	7.10674	-3.43823	0.20947
C	2.58264	-3.78584	-1.02291
C	2.13613	-5.09017	1.08840
C	2.54319	-4.21164	3.28914
C	3.54426	-1.91768	3.68700
H	3.10901	-1.79862	-5.73608
H	4.31232	-2.65125	-4.74625
H	4.50842	-0.92602	-5.10405
H	2.17106	3.13394	-3.81817
H	3.05711	2.62039	-5.25289
H	3.90536	3.45573	-3.93885
H	-0.34210	-0.47575	-6.13794
H	-0.63941	-0.44360	-4.40976
H	0.49052	-1.63421	-5.09368
C	7.54314	-0.16754	-1.85609
C	7.74333	2.31509	-1.02882
C	7.94718	4.67816	-0.15405
H	1.75426	5.81650	0.99956
C	2.29895	4.99276	2.91022
H	3.13014	3.07051	-1.15268
C	3.45873	5.18674	-1.31176
C	1.22568	4.02278	-1.22383
H	3.00826	3.96261	4.65866
H	4.09931	0.83255	3.00637
C	3.69901	1.49352	5.01076
C	5.72919	2.05901	3.63131
C	7.70813	-2.47729	-0.61835
C	7.85191	-4.69623	0.58487
H	2.55735	-2.70942	-1.24711
C	1.33785	-4.45544	-1.62595
C	3.81876	-4.36861	-1.73128
H	1.77785	-5.90231	0.45454
C	2.10839	-5.25153	2.47041
H	2.51006	-4.34582	4.36954
H	3.14144	-0.96533	3.30250
C	3.05377	-2.09736	5.12945
C	5.07822	-1.79904	3.68688
C	9.07227	-0.17925	-1.93130
C	6.96037	-0.31015	-3.28191
H	8.75501	2.40823	-1.42362
H	1.88528	5.82971	3.47798
H	3.03527	6.14199	-0.95985
H	3.41618	5.18440	-2.41120
H	4.51590	5.14833	-1.01677
H	0.68726	3.14482	-0.84105
H	1.18784	4.03824	-2.32298
H	0.69768	4.91936	-0.87219
H	3.84462	2.36215	5.67111
H	4.24567	0.65707	5.46662
H	2.62710	1.23438	5.02812
H	6.13950	2.17812	2.62043
H	6.27690	1.24297	4.12871
H	5.92063	2.99049	4.18936
H	8.73256	-2.63137	-0.95750
H	1.40826	-5.55267	-1.59170
H	1.24095	-4.19818	-2.69325
H	0.40595	-4.19736	-1.10205
H	4.74077	-3.84371	-1.46736
H	3.68790	-4.29361	-2.82169
H	3.94366	-5.43299	-1.47125
H	1.73990	-6.18105	2.91064
H	1.96932	-2.26068	5.19374
H	3.28767	-1.20550	5.72435
H	3.55127	-2.95096	5.61632
H	5.53761	-2.76602	3.94593
H	5.40176	-1.06265	4.43802
H	5.47089	-1.48815	2.71356
H	9.52973	-0.08399	-0.93558
H	9.43329	0.64694	-2.56059
H	9.42836	-1.11255	-2.39084
H	7.30516	-1.24914	-3.74168
H	7.28007	0.53372	-3.91268
H	5.86454	-0.32240	-3.26062
H	7.54273	5.46195	-0.81813
H	7.87638	5.06203	0.87625
H	9.01208	4.55387	-0.40020
H	8.93138	-4.59914	0.39664
H	7.71131	-4.94473	1.64884
H	7.48972	-5.56059	0.00151
H	-7.88048	5.05913	-0.87666
H	-9.01144	4.55453	0.40537
H	-7.54010	5.46309	0.81538
H	-7.71196	-4.94393	-1.65012
H	-7.48883	-5.56096	-0.00345
H	-8.93109	-4.59961	-0.39666

A_TZVP

SCF Done: E(RB3LYP) = -4495.03167268 A.U.

Al	3.21969	0.00003	0.21619
O	4.93002	0.00009	-0.87327
O	1.91223	-0.00010	-1.22261
O	1.69491	0.00005	1.50125
N	3.76287	1.75832	0.51798
N	3.76319	-1.75807	0.51838
C	0.67195	0.00005	0.77712
C	5.68662	-1.16720	-0.70508
C	5.68633	1.16763	-0.70549
C	5.02257	-2.12348	0.05018
C	0.78321	0.00002	-0.66276
C	6.98272	-1.23278	-1.15656
C	7.65138	2.43471	-0.90374
H	8.67323	2.56694	-1.22918
C	5.02209	2.12394	0.04957
C	2.95861	2.86324	0.93891
C	7.55321	0.00025	-1.86804
C	2.82075	3.16273	2.30319
C	5.71417	3.31914	0.26302
H	5.24457	4.11935	0.81803
C	7.01646	3.47472	-0.22000
C	7.65196	-2.43389	-0.90297
H	8.67385	-2.56596	-1.22835
C	6.98241	1.23338	-1.15698
C	5.71492	-3.31847	0.26396
H	5.24546	-4.11866	0.81911
C	7.01726	-3.47387	-0.21896
C	2.40896	3.70661	-0.04723
C	2.95899	-2.86322	0.93888
C	1.77447	4.87795	0.35711
H	1.35354	5.53842	-0.38929
C	7.73201	4.78200	-0.00170
C	3.39502	2.25614	3.37431
H	3.68725	1.32567	2.89003
C	1.68476	5.21323	1.69865
H	1.20587	6.13768	1.99671
C	2.82075	-3.16294	2.30309
C	2.52435	3.38524	-1.52729
H	3.02364	2.42437	-1.62014
C	9.08127	0.00044	-1.85845
H	9.47480	0.00067	-0.84183
H	9.46547	0.87731	-2.37898
H	9.46569	-0.87651	-2.37866
C	3.39427	-2.25625	3.37451
H	3.68606	-1.32551	2.89049
C	2.18628	4.35105	2.66070
H	2.09024	4.60945	3.70721
C	7.05611	-0.00008	-3.33270
H	7.42086	-0.88761	-3.85226
H	7.42065	0.88736	-3.85258
H	5.96741	-0.00022	-3.37882
C	7.73311	-4.78092	-0.00030
C	2.40987	-3.70657	-0.04755
C	1.14923	3.25507	-2.18660

H	0.48702	2.59741	-1.62301
H	1.24660	2.85541	-3.19777
H	0.64878	4.21812	-2.25510
C	2.18656	-4.35151	2.66020
H	2.09028	-4.61011	3.70664
C	2.36046	1.91180	4.44883
H	2.04002	2.79778	5.00017
H	2.78391	1.21107	5.17015
H	1.47872	1.44973	4.00483
C	3.38014	4.41886	-2.27089
H	2.92309	5.40989	-2.22742
H	3.47834	4.14228	-3.32292
H	4.37924	4.48494	-1.84151
C	2.52568	-3.38499	-1.52754
H	3.02465	-2.42392	-1.62010
C	4.66174	2.86317	3.99089
H	5.41693	3.05015	3.22672
H	5.08929	2.18622	4.73392
H	4.43962	3.81114	4.48635
C	4.66120	-2.86267	3.99127
H	4.43950	-3.81090	4.48643
H	5.08814	-2.18565	4.73459
H	5.41670	-3.04900	3.22726
C	1.77556	-4.87815	0.35641
H	1.35504	-5.53860	-0.39022
C	1.68557	-5.21369	1.69786
H	1.20687	-6.13834	1.99562
C	2.35928	-1.91271	4.44887
H	1.47733	-1.45113	4.00475
H	2.78213	-1.21179	5.17036
H	2.03927	-2.79895	5.00004
C	1.15078	-3.25524	-2.18736
H	0.65069	-4.21846	-2.25616
H	1.24842	-2.85545	-3.19845
H	0.48811	-2.59786	-1.62398
C	3.38214	-4.41821	-2.27092
H	4.38109	-4.48399	-1.84115
H	3.48065	-4.14149	-3.32288
H	2.92542	-5.40941	-2.22772
O	-1.91222	-0.00005	1.22257
O	-1.69490	0.00017	-1.50128
C	-0.67195	0.00010	-0.77715
C	-0.78320	0.00004	0.66272
Al	-3.21968	-0.00004	-0.21618
O	-4.93004	-0.00031	0.87322
N	-3.76284	-1.75827	-0.51833
N	-3.76318	1.75815	-0.51800
C	-5.68662	1.16703	0.70531
C	-5.68635	-1.16780	0.70516
C	-5.02255	2.12347	-0.04974
C	-6.98273	1.23252	1.15677
C	-7.65139	-2.43494	0.90317
H	-8.67324	-2.56724	1.22856
C	-5.02208	-2.12398	-0.05004
C	-2.95849	-2.86316	-0.93919
C	-7.55326	-0.00067	1.86794
C	-2.82037	-3.16254	-2.30348
C	-5.71413	-3.31916	-0.26368
H	-5.24450	-4.11928	-0.81878
C	-7.01644	-3.47484	0.21927
C	-7.65196	2.43369	0.90343
H	-8.67385	2.56570	1.22882
C	-6.98244	-1.23365	1.15663
C	-5.71489	3.31850	-0.26328
H	-5.24544	4.11880	-0.81828
C	-7.01724	3.47381	0.21965
C	-2.40902	-3.70660	0.04698
C	-2.95907	2.86333	-0.93854
C	-1.77449	-4.87793	-0.35733
H	-1.35370	-5.53845	0.38909
C	-7.73197	-4.78209	0.00073
C	-3.39437	-2.25580	-3.37462
H	-3.68607	-1.32513	-2.89041
C	-1.68458	-5.21313	-1.69887
H	-1.20569	-6.13759	-1.99691
C	-2.82107	3.16319	-2.30273
C	-2.52468	-3.38534	1.52704
H	-3.02397	-2.42446	1.61988
C	-9.08131	-0.00084	1.85831
H	-9.47480	-0.00084	0.84168
H	-9.46553	-0.87782	2.37862
H	-9.46574	0.87599	2.37871
C	-3.39483	2.25666	-3.37417
H	-3.68711	1.32609	-2.89012
C	-2.18591	-4.35087	-2.66095
H	-2.08969	-4.60920	-3.70746
C	-7.05620	-0.00069	3.33262
H	-7.42095	0.88673	3.85238
H	-7.42077	-0.88824	3.85228
H	-5.96750	-0.00058	3.37878
C	-7.73308	4.78091	0.00126
C	-2.40981	3.70663	0.04788
C	-1.14969	-3.25526	2.18663
H	-0.48732	-2.59762	1.62319
H	-1.24726	-2.85562	3.19778
H	-0.64931	-4.21834	2.25521
C	-2.18691	4.35178	-2.65985
H	-2.09080	4.61046	-3.70629
C	-2.35984	-1.91205	-4.44935
H	-2.04000	-2.79819	-5.00078
H	-2.78304	-1.21106	-5.17056
H	-1.47774	-1.45047	-4.00554
C	-3.38065	-4.41899	2.27039
H	-2.92363	-5.41004	2.22690
H	-3.47902	-4.14251	3.32243
H	-4.37967	-4.48499	1.84083
C	-2.52540	3.38492	1.52786
H	-3.02434	2.42383	1.62041
C	-4.66147	-2.86230	-3.99094
H	-5.41666	-3.04877	-3.22666
H	-5.08876	-2.18528	-4.73405
H	-4.43985	-3.81048	-4.48624
C	-4.66140	2.86358	-3.99117
H	-4.43923	3.81163	-4.48645
H	-5.08857	2.18665	-4.73443
H	-5.41690	3.05037	-3.22727
C	-1.77559	4.87824	-0.35608
H	-1.35498	5.53866	0.39054
C	-1.68578	5.21388	-1.69753
H	-1.20712	6.13855	-1.99529
C	-2.35979	1.91263	-4.44833
H	-1.47819	1.45057	-4.00405
H	-2.78286	1.21198	-5.16996
H	-2.03922	2.79875	-4.99936
C	-1.15039	3.25517	2.18746
H	-0.65036	4.21841	2.25631
H	-1.24785	2.85523	3.19851
H	-0.48777	2.59791	1.62388
C	-3.38178	4.41805	2.27146
H	-4.38080	4.48382	1.84186
H	-3.48011	4.14123	3.32341
H	-2.92511	5.40928	2.22827
H	-8.81096	-4.66631	0.10492
H	-7.52618	-5.18601	-0.99176
H	-7.40747	-5.53058	0.72907
H	-8.81207	4.66480	0.10508
H	-7.40903	5.52929	0.72992
H	-7.52710	5.18518	-0.99105
H	7.40896	-5.52949	-0.72871
H	8.81209	-4.66484	-0.10429
H	7.52725	-5.18491	0.99215
H	7.52618	5.18614	0.99070
H	8.81100	4.66618	-0.10582
H	7.40756	5.53035	-0.73021

E_TZVP

SCF Done: E(RB3LYP) = -6238.45718919 A.U.

K	-0.70695	3.26524	-1.30844
Al	3.14183	-0.23244	0.10864
O	4.93145	0.59110	-0.58821
O	1.47027	-0.90780	0.65129
O	1.38527	1.80803	-1.49277
N	3.86333	-1.70745	-0.88962
N	3.83815	0.51371	1.72543
C	5.65083	-0.26467	-1.42329
C	5.02900	-1.49497	-1.60985
C	5.70078	-2.38383	-2.45990
H	5.26706	-3.35036	-2.67567
C	6.95556	-2.05882	-2.98204
C	7.57803	-0.85675	-2.63953
H	8.57630	-0.65702	-3.00188
C	6.92233	0.07065	-1.82391
C	7.49769	1.38752	-1.28642
C	7.01103	1.51979	0.16431
C	7.74706	1.99526	1.25330
H	8.76569	2.33089	1.12025
C	7.17915	2.02924	2.52943
C	5.88050	1.56113	2.74446
H	5.46693	1.56983	3.74352
C	5.11329	1.06603	1.68141
C	5.72354	1.11872	0.43346

C	7.96337	2.58544	3.68952
C	6.91887	2.55970	-2.11154
H	5.83103	2.55961	-2.07839
H	7.23062	2.47445	-3.15407
H	7.27498	3.51181	-1.71410
C	9.02223	1.41730	-1.37672
H	9.40755	2.36293	-0.99546
H	9.34436	1.33172	-2.41445
H	9.47293	0.60484	-0.80645
C	7.64003	-3.02656	-3.91144
C	3.16433	-2.89634	-1.23302
C	2.40634	-2.92830	-2.41955
C	1.75902	-4.11070	-2.77134
H	1.16777	-4.13950	-3.67746
C	1.85363	-5.24380	-1.98016
H	1.34324	-6.15400	-2.26870
C	2.60678	-5.21002	-0.81399
H	2.68153	-6.10353	-0.20939
C	3.27254	-4.04650	-0.42037
C	4.12560	-4.02725	0.84055
H	4.01260	-3.03968	1.29144
C	3.72037	-5.07789	1.87842
H	2.65544	-5.06804	2.11825
H	4.26725	-4.91086	2.80649
H	3.96068	-6.08730	1.53969
C	5.61849	-4.19216	0.52198
H	5.79713	-5.15257	0.03243
H	6.20488	-4.16487	1.44295
H	5.97976	-3.40580	-0.13415
C	2.29505	-1.71276	-3.32193
H	2.88860	-0.91647	-2.88026
C	2.86774	-1.99318	-4.71719
H	3.90672	-2.31785	-4.66094
H	2.82736	-1.08770	-5.32608
H	2.29374	-2.76573	-5.23395
C	0.85258	-1.21620	-3.41908
H	0.21330	-1.95035	-3.90257
H	0.80612	-0.29868	-4.00711
H	0.43200	-1.00158	-2.43894
C	3.10555	0.87763	2.89207
C	2.81504	-0.07503	3.88169
C	2.28459	0.35349	5.09668
H	2.07426	-0.36777	5.87485
C	2.04015	1.69682	5.33632
H	1.64835	2.01581	6.29370
C	2.25562	2.62087	4.32592
H	2.01156	3.66237	4.49594
C	2.75908	2.22968	3.08896
C	2.88500	3.25098	1.97162
H	3.33146	2.75405	1.11410
C	3.78307	4.43464	2.34224
H	3.37685	4.99366	3.18809
H	3.86887	5.12583	1.50067
H	4.78464	4.09614	2.60514
C	1.49407	3.73086	1.54317
H	0.84638	2.88390	1.31626
H	1.56716	4.36880	0.66025
H	1.01195	4.30693	2.33208
C	3.13771	-1.53565	3.64386
H	3.07091	-1.69158	2.56777
C	4.57890	-1.85473	4.05804
H	5.28455	-1.22386	3.51893
H	4.82491	-2.89827	3.85000
H	4.71571	-1.68110	5.12775
C	2.14203	-2.48679	4.31090
H	2.22892	-2.47274	5.39859
H	2.32896	-3.51577	3.99687
H	1.11156	-2.22059	4.06477
C	0.68517	-0.00871	-0.02120
C	1.66274	0.85813	-0.75730
C	1.59409	6.05941	-1.63376
H	2.01894	6.39232	-0.69477
C	0.41814	6.64350	-2.10196
H	-0.06087	7.42414	-1.52455
C	-0.13555	6.22935	-3.30889
H	-1.04491	6.68508	-3.67847
C	0.49741	5.22605	-4.04217
H	0.07549	4.89519	-4.98262
C	1.66502	4.64158	-3.56570
H	2.13863	3.84762	-4.12974
C	2.23438	5.04742	-2.35259
C	3.47420	4.37558	-1.83563
H	3.25766	3.32824	-1.61349
H	3.84290	4.85459	-0.92959
H	4.27154	4.40046	-2.58040
O	-1.47029	0.90778	-0.65131
O	-1.38529	-1.80807	1.49273
C	-0.68520	0.00869	0.02117
C	-1.66276	-0.85817	0.75726
K	0.70696	-3.26524	1.30849
Al	-3.14186	0.23240	-0.10866
O	-4.93154	-0.59110	0.58816
N	-3.86334	1.70742	0.88963
N	-3.83819	-0.51370	-1.72547
C	-5.65091	0.26470	1.42324
C	-5.02902	1.49495	1.60984
C	-5.70078	2.38383	2.45990
H	-5.26702	3.35033	2.67571
C	-6.95558	2.05886	2.98201
C	-7.57810	0.85683	2.63946
H	-8.57638	0.65714	3.00178
C	-6.92242	-0.07058	1.82382
C	-7.49783	-1.38741	1.28630
C	-7.01114	-1.51970	-0.16441
C	-7.74716	-1.99514	-1.25343
H	-8.76580	-2.33074	-1.12041
C	-7.17922	-2.02913	-2.52955
C	-5.88055	-1.56106	-2.74454
H	-5.46696	-1.56976	-3.74359
C	-5.11334	-1.06600	-1.68147
C	-5.72363	-1.11868	-0.43354
C	-6.91911	-2.55962	2.11143
H	-5.83127	-2.55958	2.07833
H	-7.23090	-2.47437	3.15394
H	-7.27524	-3.51172	1.71397
C	-9.02238	-1.41712	1.37655
H	-9.40774	-2.36272	0.99527
H	-9.34454	-1.33153	2.41427
H	-9.47303	-0.60463	0.80627
C	-3.16430	2.89627	1.23308
C	-2.40629	2.92816	2.41960
C	-1.75896	4.11053	2.77145
H	-1.16770	4.13928	3.67757
C	-1.85356	5.24367	1.98033
H	-1.34315	6.15386	2.26891
C	-2.60672	5.20996	0.81417
H	-2.68147	6.10351	0.20962
C	-3.27249	4.04648	0.42049
C	-4.12559	4.02730	-0.84040
H	-4.01259	3.03977	-1.29137
C	-3.72042	5.07804	-1.87821
H	-2.65549	5.06823	-2.11807
H	-4.26732	4.91107	-2.80627
H	-3.96074	6.08741	-1.53938
C	-5.61847	4.19216	-0.52176
H	-5.79712	5.15253	-0.03213
H	-6.20490	4.16492	-1.44271
H	-5.97969	3.40574	0.13432
C	-2.29501	1.71257	3.32192
H	-2.88856	0.91630	2.88022
C	-2.86769	1.99291	4.71720
H	-3.90667	2.31760	4.66096
H	-2.82732	1.08740	5.32604
H	-2.29369	2.76543	5.23400
C	-0.85254	1.21601	3.41905
H	-0.21326	1.95012	3.90258
H	-0.80608	0.29844	4.00702
H	-0.43195	1.00145	2.43889
C	-3.10558	-0.87758	-2.89211
C	-2.81505	0.07512	-3.88168
C	-2.28452	-0.35334	-5.09665
H	-2.07418	0.36795	-5.87479
C	-2.04002	-1.69665	-5.33633
H	-1.64816	-2.01561	-6.29369
C	-2.25551	-2.62075	-4.32597
H	-2.01141	-3.66223	-4.49600
C	-2.75905	-2.22961	-3.08901
C	-2.88497	-3.25095	-1.97170
H	-3.33156	-2.75409	-1.11421
C	-3.78289	-4.43470	-2.34244
H	-3.37653	-4.99364	-3.18827
H	-3.86868	-5.12591	-1.50090
H	-4.78447	-4.09629	-2.60542
C	-1.49403	-3.73070	-1.54314
H	-0.84645	-2.88369	-1.31610
H	-1.56715	-4.36870	-0.66027
H	-1.01176	-4.30667	-2.33203
C	-3.13780	1.53572	-3.64383
H	-3.07101	1.69163	-2.56773
C	-4.57901	1.85473	-4.05800
H	-5.28463	1.22380	-3.51891
H	-4.82508	2.89824	-3.84993

H	-4.71581	1.68111	-5.12772
C	-2.14219	2.48693	-4.31085
H	-2.22907	2.47289	-5.39853
H	-2.32917	3.51589	-3.99679
H	-1.11170	2.22079	-4.06472
C	-1.59400	-6.05950	1.63380
H	-2.01890	-6.39238	0.69482
C	-0.41800	-6.64358	2.10189
H	0.06099	-7.42418	1.52441
C	0.13576	-6.22947	3.30880
H	1.04516	-6.68519	3.67830
C	-0.49718	-5.22622	4.04217
H	-0.07521	-4.89540	4.98261
C	-1.66485	-4.64177	3.56581
H	-2.13844	-3.84786	4.12993
C	-2.23427	-5.04757	2.35272
C	-3.47416	-4.37575	1.83588
H	-3.25767	-3.32840	1.61377
H	-3.84291	-4.85474	0.92985
H	-4.27144	-4.40070	2.58071
C	-7.96343	-2.58529	-3.68966
H	-7.67101	-3.61799	-3.90090
H	-9.03408	-2.58207	-3.48317
H	-7.78974	-2.00811	-4.59934
C	-7.64003	3.02661	3.91143
H	-8.71414	2.84384	3.95393
H	-7.24902	2.93462	4.92877
H	-7.48187	4.05950	3.59630
H	7.67103	3.61818	3.90065
H	7.78960	2.00836	4.59924
H	9.03403	2.58213	3.48306
H	8.71413	-2.84373	-3.95399
H	7.48195	-4.05945	-3.59627
H	7.24899	-2.93463	-4.92878

F_TZVP

SCF Done: E(RB3LYP) = -7420.48092645 A.U.

K	0.15280	-1.87784	2.22393
K	0.55597	1.93138	2.81454
Al	-3.10522	0.03652	-0.22364
O	-1.48073	0.10192	-1.16496
O	-4.93858	-0.06659	0.80712
O	-1.27250	0.25833	2.41136
N	-3.93038	1.75070	-0.68668
N	-3.76997	-1.73948	-0.74945
C	-0.73552	0.16649	0.05616
C	-1.62677	0.16899	1.10529
C	-5.68900	-1.21004	0.53414
C	-5.04878	-2.09317	-0.32372
C	-5.71026	1.09428	0.72118
C	-6.97948	-1.32146	1.00236
C	-5.13529	2.07425	-0.08118
C	-7.51678	-0.17466	1.86576
C	-6.98646	1.11743	1.23417
C	-3.10696	-2.85069	-1.34996
C	-7.70793	2.30163	1.05810
H	-8.71105	2.39291	1.44875
C	-3.36273	2.82362	-1.42324
C	-7.15175	3.36802	0.35212
C	-2.62762	-3.90341	-0.52706
C	-2.75956	3.90991	-0.74968
C	-2.93965	-1.33220	3.60618
H	-3.60363	-1.41210	2.73920
H	-2.18635	-2.12070	3.45399
C	-5.79376	-3.22467	-0.68816
H	-5.36192	-3.96323	-1.34816
C	-9.04324	-0.18270	1.93471
H	-9.49245	-0.08016	0.94656
H	-9.39867	0.63373	2.56310
H	-9.39785	-1.11078	2.38267
C	-5.88914	3.24713	-0.23125
H	-5.51060	4.05437	-0.84173
C	-7.08989	-3.41644	-0.21003
C	-3.41175	1.32147	3.51858
H	-3.65146	1.47804	2.46388
H	-4.34345	0.95592	3.95939
C	-3.06187	-2.99268	-2.75776
C	-7.68284	-2.46685	0.62303
H	-8.69874	-2.61868	0.95813
C	-2.25011	4.97315	-1.49573
H	-1.78408	5.80395	-0.98165
C	-3.48961	2.85949	-2.83085
C	-1.31984	0.37939	4.95224
H	-0.93315	1.40790	5.01412
H	-1.97480	0.30833	5.82661
C	-2.59912	-3.80029	0.99017
H	-2.59699	-2.73813	1.23468
C	-7.91299	4.65894	0.20336
C	-2.34215	4.99795	-2.87794
H	-1.94658	5.83481	-3.43928
C	-2.96643	3.94587	-3.53476
H	-3.06535	3.98481	-4.61057
C	-2.57658	-4.18364	-3.30517
H	-2.55077	-4.30845	-4.37711
C	-2.67669	3.97640	0.76416
H	-3.11690	3.06827	1.16511
C	-2.16762	-5.07589	-1.12574
H	-1.81627	-5.88809	-0.50460
C	-7.83914	-4.66756	-0.58715
C	-6.94787	-0.32687	3.29279
H	-7.30549	-1.25552	3.74073
H	-7.26443	0.51080	3.91656
H	-5.86215	-0.35035	3.28059
C	-3.12154	2.67862	4.16496
H	-2.18163	3.11499	3.81459
H	-3.03615	2.59357	5.25055
H	-3.90457	3.41346	3.95830
C	-3.72379	-1.71163	4.86525
H	-3.06274	-1.81477	5.72964
H	-4.26622	-2.65557	4.75567
H	-4.45897	-0.94588	5.12121
C	-2.14753	-5.22685	-2.50087
H	-1.79156	-6.14731	-2.94552
C	-3.56371	-1.89503	-3.68550
H	-3.17485	-0.94998	-3.29725
C	-1.34225	-4.45259	1.57920
H	-1.39226	-5.54061	1.52963
H	-1.25242	-4.20643	2.63957
H	-0.42637	-4.16914	1.06017
C	-3.45043	5.17540	1.32728
H	-3.03254	6.11990	0.97112
H	-3.39727	5.17378	2.41639
H	-4.49991	5.13561	1.04239
C	-4.25079	1.77243	-3.56546
H	-4.13848	0.85522	-2.98951
C	-0.14964	-0.58275	5.16036
H	0.34163	-0.46628	6.13001
H	0.64140	-0.44338	4.41388
H	-0.47506	-1.62648	5.09835
C	-1.22247	4.02611	1.22668
H	-0.68490	3.15621	0.85113
H	-1.18084	4.05181	2.31596
H	-0.71038	4.91599	0.86519
B	-2.26455	0.16040	3.62346
C	-3.07039	-2.06017	-5.12594
H	-1.99510	-2.21960	-5.18848
H	-3.30409	-1.16964	-5.70485
H	-3.56388	-2.90157	-5.61625
C	-3.73627	1.51886	-4.98255
H	-3.87107	2.38753	-5.62819
H	-4.29331	0.70095	-5.43606
H	-2.67805	1.24700	-5.00373
C	-3.81587	-4.42969	1.68645
H	-4.74442	-3.93519	1.42610
H	-3.68924	-4.36418	2.76830
H	-3.90259	-5.48499	1.41516
C	-5.09596	-1.79502	-3.69412
H	-5.53431	-2.75563	-3.97186
H	-5.41867	-1.05677	-4.42954
H	-5.49544	-1.50965	-2.72674
C	-5.75196	2.09467	-3.60352
H	-6.16017	2.20449	-2.60151
H	-6.29842	1.29618	-4.10899
H	-5.92820	3.02593	-4.14745
C	0.73553	0.16651	-0.05605
O	1.48075	0.10179	1.16506
C	1.62677	0.16918	-1.10517
Al	3.10524	0.03655	0.22373
O	1.27248	0.25873	-2.41123
N	3.93037	1.75069	0.68694
N	3.77004	-1.73951	0.74934
K	-0.15268	-1.87759	-2.22396
K	-0.55636	1.93143	-2.81470
B	2.26457	0.16085	-3.62332
C	5.13526	2.07433	0.08144
C	3.36263	2.82357	1.42350
C	5.04882	-2.09315	0.32351
C	3.10707	-2.85078	1.34978
C	2.93957	-1.33181	-3.60614
C	3.41186	1.32182	-3.51828
C	1.31992	0.37997	-4.95212

C	5.71023	1.09445	-0.72102
C	5.88906	3.24724	0.23156
C	2.75956	3.90990	0.74991
C	3.48929	2.85936	2.83114
C	5.68900	-1.20990	-0.53426
C	5.79381	-3.22470	0.68777
C	2.62769	-3.90340	0.52679
C	3.06208	-2.99295	2.75756
H	3.60374	-1.41172	-2.73930
H	2.18626	-2.12027	-3.45378
C	3.72340	-1.71131	-4.86538
H	3.65116	1.47860	-2.46352
H	4.34371	0.95606	-3.95861
C	3.12209	2.67886	-4.16510
H	0.93326	1.40848	-5.01395
H	1.97491	0.30895	-5.82647
C	0.14972	-0.58216	-5.16035
O	4.93857	-0.06643	-0.80708
C	6.98642	1.11767	-1.23405
C	7.15165	3.36821	-0.35184
H	5.51051	4.05442	0.84210
C	2.24992	4.97306	1.49594
C	2.67694	3.97645	-0.76393
C	2.96595	3.94568	3.53503
C	4.25044	1.77235	3.56582
C	6.97947	-1.32125	-1.00252
H	5.36198	-3.96335	1.34768
C	7.08991	-3.41640	0.20956
C	2.59919	-3.80012	-0.99041
C	2.16770	-5.07596	1.12535
C	2.57681	-4.18397	3.30486
C	3.56428	-1.89552	3.68538
H	3.06214	-1.81448	-5.72961
H	4.26584	-2.65525	-4.75590
H	4.45853	-0.94558	-5.12156
H	2.18206	3.11541	-3.81530
H	3.03720	2.59355	-5.25072
H	3.90511	3.41366	-3.95826
H	-0.34155	-0.46557	-6.12999
H	-0.64132	-0.44292	-4.41385
H	0.47516	-1.62589	-5.09848
C	7.51675	-0.17434	-1.86579
C	7.70785	2.30189	-1.05791
C	7.91285	4.65915	-0.20303
H	1.78393	5.80386	0.98183
C	2.34172	4.99777	2.87817
H	3.11779	3.06864	-1.16487
C	3.45003	5.17594	-1.32687
C	1.22276	4.02519	-1.22669
H	3.06469	3.98455	4.61085
H	4.13817	0.85510	2.98992
C	3.73585	1.51890	4.98290
C	5.75160	2.09465	3.60391
C	7.68285	-2.46670	-0.62337
C	7.83918	-4.66758	0.58649
H	2.59702	-2.73793	-1.23479
C	1.34233	-4.45241	-1.57951
C	3.81600	-4.42936	-1.68672
H	1.81633	-5.88808	0.50413
C	2.14767	-5.22707	2.50046
H	2.55114	-4.30894	4.37678
H	3.17569	-0.95031	3.29724
C	3.07101	-2.06063	5.12585
C	5.09657	-1.79601	3.69393
C	9.04321	-0.18234	-1.93474
C	6.94785	-0.32639	-3.29284
H	8.71095	2.39323	-1.44859
H	1.94601	5.83457	3.43950
H	3.03140	6.12020	-0.97094
H	3.39726	5.17420	-2.41599
H	4.49945	5.13689	-1.04160
H	0.68584	3.15479	-0.85135
H	1.18132	4.05099	-2.31597
H	0.70997	4.91464	-0.86514
H	3.87056	2.38765	5.62846
H	4.29290	0.70107	5.43654
H	2.67764	1.24699	5.00403
H	6.15984	2.20442	2.60192
H	6.29807	1.29621	4.10945
H	5.92778	3.02595	4.14780
H	8.69874	-2.61848	-0.95852
H	1.39237	-5.54043	-1.53002
H	1.25249	-4.20615	-2.63985
H	0.42645	-4.16902	-1.06044
H	4.74452	-3.93488	-1.42620
H	3.68946	-4.36366	-2.76857
H	3.90274	-5.48471	-1.41561
H	1.79175	-6.14758	2.94502
H	1.99567	-2.21968	5.18845
H	3.30507	-1.17023	5.70482
H	3.56424	-2.90226	5.61604
H	5.53462	-2.75680	3.97151
H	5.41956	-1.05798	4.42945
H	5.49609	-1.51063	2.72658
H	9.49242	-0.07990	-0.94658
H	9.39863	0.63417	-2.56304
H	9.39784	-1.11037	-2.38280
H	7.30549	-1.25499	-3.74088
H	7.26438	0.51136	-3.91651
H	5.86213	-0.34991	-3.28063
H	7.57658	5.39833	-0.93603
H	7.76656	5.09502	0.78690
H	8.98215	4.50941	-0.35504
H	8.91573	-4.53384	0.47646
H	7.63538	-4.95634	1.61902
H	7.54431	-5.50715	-0.04968
H	-7.76677	5.09482	-0.78658
H	-8.98228	4.50917	0.35543
H	-7.57670	5.39813	0.93634
H	-7.63526	-4.95623	-1.61969
H	-7.54434	-5.50720	0.04896
H	-8.91569	-4.53382	-0.47720

Orca Outputs

Al

Energy: -1704.49889290 Eh

Al	-4.69220829178926	-2.89787105042429	-0.51731076816904
N	-4.06999865752601	-1.68313705243470	1.05830579488710
N	-3.64541102976739	-2.33474385567379	-2.21824590371118
C	-4.48906500649870	-0.38854238513946	1.16201952168973
C	-3.12065985402218	-2.13186324463910	1.99723459295563
C	-3.85246538484750	-1.11554684735690	-2.80756545993065
C	-3.04756605115819	-3.34307759697314	-2.99812263765923
C	-5.17394526913904	0.14681366502376	0.05398199625722
C	-4.27568103991502	0.51727121787840	2.23064727909316
C	-1.78152118065175	-1.67323617042553	1.92057928054095
C	-3.49748539901882	-3.05473262513551	3.00012057166998
C	-4.75093290383225	-0.24119686495367	-2.16845464396436
C	-3.24101375367168	-0.59457236309604	-3.97342820530492
C	-3.71302686963590	-3.85908928626866	-4.14042799809116
C	-1.80023445751636	-3.88621059068299	-2.61011729766392
O	-5.31570891580129	-0.74837532076533	-1.00364776925635
C	-5.44238566044344	1.48990277895000	-0.14483737360632
C	-4.63119194970684	1.86949779177334	2.11741762786574
H	-3.76986179944342	0.16229451583244	3.13171628880669
C	-0.83867233148506	-2.17070401238636	2.82920182973918
C	-2.52649889973660	-3.52939810352919	3.89039938564904
C	-4.97917228513398	1.08020014438911	-2.51604203476192
H	-2.53595266355868	-1.22205767151453	-4.52387493801000
C	-3.48540638062233	0.71844964814880	-4.40176764211357
C	-3.09973297069956	-4.86853869684785	-4.89164008523411
C	-1.22418166299488	-4.90433074570285	-3.38040861925423
C	-5.87022054154066	1.89808042391115	-1.56447698847013
C	-5.18653691388498	2.36451468659334	0.92650382763634
C	-4.40299996526000	2.80355482984914	3.28409483896730
H	0.19796145520879	-1.82428347330521	2.76217689550407
C	-1.20122643710069	-3.09755622181581	3.80730436954132
H	-2.82102585563391	-4.24158987692245	4.66783928177904
C	-4.33618049508631	1.56158233299768	-3.66881697711034
C	-2.82729598810610	1.22757537865427	-5.66415930839519
H	-3.61728684632707	-5.25958323722413	-5.77379981974378
C	-1.85948028613350	-5.39151837120579	-4.52301152888751
H	-0.25390431932745	-5.31225273180901	-3.07955557496711
C	-5.71088336559360	3.40467640362501	-1.79340026275438
C	-7.35078018814667	1.50800122736186	-1.79186658622559
H	-5.38993931320531	3.43258868396214	0.83329586455951
H	-3.48643659201059	2.54402143891561	3.83893557533544
H	-4.31404856643693	3.85099254881098	2.95229554340639
H	-5.23883354148297	2.76086625655363	4.00647531299372
H	-0.45269619585659	-3.47970582785259	4.50780766233297
H	-4.47862406653528	2.59341842408193	-3.99459174260492
H	-1.81215795520397	0.81579349378211	-5.78679029027052
H	-3.40124615638234	0.94005002224270	-6.56425088817603
H	-2.75012363480253	2.32706372231549	-5.66490935982207
H	-1.39549346449169	-6.18352635162445	-5.11819219159316
H	-4.66985899509166	3.72810157176666	-1.64364702901785
H	-6.35164323689787	3.97327717693585	-1.10176321056269
H	-6.01336440523192	3.67754854798129	-2.81625413005748
H	-7.65759100954645	1.75400629913358	-2.82209097649253
H	-8.00178648125766	2.05487487788387	-1.08960715766122

H	-7.50133869869753	0.43088977780004	-1.63450208186052
C	-1.09028255004375	-3.33994708367355	-1.40088571154663
H	-0.92801893735359	-2.25538523817226	-1.49793005450630
H	-1.67644011452093	-3.48139747421151	-0.47833430978453
H	-0.11417205991406	-3.82876578673052	-1.25666415514176
C	-5.07641890321514	-3.34623674233717	-4.52082753359286
H	-5.55639560995690	-4.01051472031119	-5.25632004565957
H	-5.72261287782789	-3.27498126389374	-3.63136879742160
H	-5.02902067552986	-2.33277266206078	-4.95429514863912
C	-1.39420882107602	-0.64840849686030	0.88750290582691
H	-1.70234167243619	0.36408459436755	1.20022954566375
H	-0.30551090560053	-0.63817772426436	0.72232226219397
H	-1.90130478693823	-0.84205873861034	-0.06761545068563
C	-4.94004604442793	-3.47030020542459	3.11741153103401
H	-5.59107886999524	-2.58605546858445	3.22258559845731
H	-5.27940762425424	-3.99086919888140	2.20637525558221
H	-5.09627446522976	-4.12838776379620	3.98692252741337

AlCO

Energy: -1817.81252538 Eh

Al	-2.78279773111628	-0.29668804541265	-0.42315073242778
N	-3.62072325647613	-1.70090311494346	0.76171716241120
N	-3.60479257133634	1.54899020256739	-0.37543777968839
C	-4.86158958111542	-2.20103237440151	0.48853681772124
C	-2.87115543245270	-2.24034709479574	1.82648246214963
C	-4.85696359210161	1.76729546267476	-0.87268531067864
C	-2.82166106247634	2.68188707990279	-0.05534415381363
C	-5.57601153343238	-1.56359836444932	-0.54642797943939
C	-5.54822388495731	-3.26606427665414	1.11419539418687
C	-1.67738662762172	-2.94368799549740	1.54260941911302
C	-3.25660353263782	-2.00697838256290	3.16995993234312
C	-5.57825822702853	0.62932909817313	-1.28884153028868
C	-5.55964924504705	2.98918248209212	-0.98446812217112
C	-2.10414615648398	3.35079221491948	-1.07437392898146
C	-2.74920988743839	3.13691213581611	1.28113355327741
O	-4.86520501455106	-0.55231578402847	-1.17043553106447
C	-6.90736396774300	-1.75791229371349	-0.85534004824813
C	-6.88196891602427	-3.55893213318145	0.78273728967658
H	-5.04320916214203	-3.84151073500641	1.89367307464327
C	-0.90228649784672	-3.42627280142579	2.60425290394310
C	-2.45985251542767	-2.51428247731421	4.20308725571459
C	-6.91297144044284	0.59208015611996	-1.63841638170317
H	-5.06121390170841	3.91685725250650	-0.69376643898700
C	-6.90056957757211	3.01568591325720	-1.40373626223537
C	-1.30899170746999	4.45318753383059	-0.73633510160839
C	-1.94287125552138	4.24153858064603	1.58192723647292
C	-7.52026962993257	-0.79975881664691	-1.89364099571674
C	-7.57149761874710	-2.79508490408591	-0.17170962142682
C	-7.57410032749074	-4.71296706447067	1.47166588569351
H	0.02440409202700	-3.96492378846398	2.38195664629735
C	-1.28929387441020	-3.22386298788340	3.92907172605898
H	-2.75530604542173	-2.32796773272548	5.24078394999470
C	-7.58483827062718	1.82841561096149	-1.70779388471060
C	-7.60681728542003	4.34698475744675	-1.52231777785680
H	-0.74753405720213	4.96543378458795	-1.52427278554220
C	-1.22221034123385	4.89828135123200	0.58342280618740
H	-1.88447865931550	4.58998970801909	2.61799560187832
C	-9.04897636696483	-0.77359086361264	-1.80132820083851
C	-7.10586497727621	-1.27096105264157	-3.31021475383763
H	-8.62135223452080	-3.01265896031269	-0.37515154832775
H	-7.39759835724558	-4.69960604543352	2.56057352059448
H	-8.66269643587321	-4.69074161297899	1.30454168619479
H	-7.20195513959874	-5.68528459562579	1.10098137882989
H	-0.67022082652041	-3.60131106824055	4.74835161530586
H	-8.63758788930564	1.87386370207971	-1.99151578179728
H	-7.39172893528202	4.99613495036209	-0.65700182014265
H	-7.27958549474640	4.89827395640999	-2.42265969465435
H	-8.69928256443071	4.22258457591275	-1.59043508254772
H	-0.59300297481020	5.75762601662120	0.83389946059914
H	-9.38791136957394	-0.44562276752972	-0.80695319032012
H	-9.46684082373914	-1.77287564926202	-1.99762310314200
H	-9.47271045224822	-0.09126401000375	-2.55402920883616
H	-7.49744445955033	-0.57993238347099	-4.07496332378944
H	-7.50067779062564	-2.28108752261556	-3.50915561415382
H	-6.01113908587501	-1.30450115141864	-3.40618472854354
C	-1.25466993667290	0.20187232683617	0.96440616169945
O	-0.10459191708208	0.24503731350454	1.13553269982539
C	-1.26159910317288	-3.16922012550761	0.11138020584802
H	-0.16731109954133	-3.24571054900224	0.01797235258892
H	-1.70436346063016	-4.09379057118354	-0.28650659696744
H	-1.61759920291606	-2.34683157923846	-0.54395428236280
C	-4.48299812200117	-1.18915928544694	3.47321883295181
H	-4.54289171501946	-0.31943440316941	2.80277451998444
H	-5.40915386090832	-1.76655409427490	3.31228466549482
H	-4.47637658278505	-0.83533700638351	4.51593189207015
C	-3.52173812503465	2.42229125413785	2.35417280549629
H	-4.56922819273714	2.26132765952770	2.05643789988608
H	-3.08321693475684	1.42461275853750	2.52925905842612
H	-3.50306431095183	2.98271061170968	3.30193585149774
C	-2.21729233772003	2.87925976800205	-2.50060171880054
H	-1.51825223928139	3.42289736544351	-3.15534774234032
H	-2.00838845457688	1.79970436271464	-2.57252819234257
H	-3.24008242056486	3.03003632947540	-2.88791012047942

AlCO2

Energy: -1931.14676808 Eh

Al	1.93754715434101	-0.47119791363263	-1.04788872150696
O	3.83164275840279	-0.48473584120976	-0.84247159152694
O	-0.13302699856110	-0.44045545962057	-1.23155021419414
O	2.73203171590060	-1.41976945859080	-3.92322950209588
N	1.42213684720480	-1.83671916073858	0.25388290808326
N	1.56361232244511	1.43241912057292	-0.80569074057077
C	4.25264770028650	-0.87078946050257	-2.00887944391677
C	2.85368768213490	-1.05783920742628	-2.77189624909392
C	-0.69528295644393	0.82633415302524	-1.09842516849090
C	0.25474510965613	1.84005167214020	-0.88171298040657
C	-0.78078905787694	-1.40929055486432	-0.46794896964051
C	-2.06817959557415	0.96203153105159	-1.05359603110404
C	0.09361845825132	-2.17286622305807	0.32634514895155
C	-2.89680821614896	-0.32733057734747	-1.19717964737705
C	-2.15948535934293	-1.41787175529810	-0.40053083771585
C	2.58491727027142	2.41375579103181	-0.83408946632402
C	-2.74031783643901	-2.39288967867717	0.43048985147224
H	-3.82505691156085	-2.46809427558367	0.52122426612085
C	2.32035111300379	-2.40675262536165	1.19048487079641
C	-1.92586533911583	-3.27241221437565	1.16244516680312
C	2.81507528871415	3.15578498345952	-2.01684445681822
C	3.27102671199115	-3.36639924018530	0.77651109787250
C	-0.28101374468881	3.13417673518968	-0.72117259626960
H	0.39806382158857	3.97433069580342	-0.55921631140358
C	-4.33137361220543	-0.13604904393811	-0.69717552581342
H	-4.35491749583262	0.15098934795081	0.36493533796211
H	-4.91096189760024	-1.06373938736126	-0.81840812027463
H	-4.84409276998169	0.64524686854798	-1.27856863100227
C	-0.52627213823669	-3.15788782866814	1.12238781695411
H	0.09407221759566	-3.80847039057189	1.74292978234891
C	-1.67052497120172	3.34297797980968	-0.72247801365867
C	3.40686949748746	2.60443660708478	0.29791385593753
C	-2.56070123855440	2.26654292215985	-0.86800413697486
H	-3.63507799025816	2.45285470155776	-0.82967400688775
C	4.17441410164842	-3.87168104871064	1.72241110353437
H	4.91312901101137	-4.61320242853996	1.40273496231485
C	2.27840081028964	-1.97761962644022	2.54034962675402
C	-2.55422227358594	-4.35956299235181	2.00319291756601
C	4.14719194909231	-3.44771999078379	3.04940014118788
H	4.86538132270808	-3.84924987330865	3.77035034499977
C	3.19983350657254	-2.50563111705825	3.45195747009852
H	3.17498377645552	-2.16324694665968	4.49141468029621
C	4.41753100303700	3.57243622497445	0.24702663938272
H	5.05165497410494	3.72159606596962	1.12636238356267
C	3.83075183523233	4.11980869160898	-2.02573397805968
H	4.01018264402907	4.69172476501427	-2.94148814393219
C	-2.20260540012970	4.74855384923596	-0.56282526753557
C	-2.92813475211950	-0.73415804935131	-2.69211918440712
H	-3.41480794893744	0.05160799642795	-3.29264964844394
H	-3.48754142870417	-1.67521509665400	-2.82019117085296
H	-1.91180824624970	-0.88465828230328	-3.08325067617332
C	4.62637310926913	4.33701675765147	-0.90056081748053
H	5.42079367040717	5.08865001384292	-0.92458316243793
H	-2.02837750467807	-4.48295339339283	2.96420944178275
H	-3.61291555950002	-4.14503543526660	2.21872706690991
H	-2.51441567722053	-5.33671722915708	1.48866388540787
H	-1.68877593701779	5.28432865204953	0.25276743272888
H	-2.04843349969574	5.34267680989339	-1.48135663228930
H	-3.28189258717035	4.75133267487792	-0.34378119093020
C	2.01002583945737	2.87788406353866	-3.25913781992573
H	2.44146577586028	3.39476968627083	-4.12970120156776
H	1.98296264277850	1.79782786961409	-3.47528019345435
H	0.96110098883951	3.20293224346808	-3.15367929989165
C	3.21205258621315	1.75782599896201	1.52534815760104
H	2.15386970989328	1.72129414503009	1.82394581065767
H	3.53547420189006	0.72146292766296	1.33200560458512
H	3.80234170060476	2.14312441792025	2.37105818013630
C	1.25263703649111	-0.97166276225045	2.99280337247891
H	1.10027019010251	-0.18847363212502	2.23750983782631
H	0.26800717483283	-1.44490252874819	3.14796804610547
H	1.55507622362600	-0.49610961978288	3.93844303350755

C	3.33629827204823	-3.84473123264232	-0.64987149540377
H	4.05988586807717	-3.24751177971155	-1.23195877043340
H	3.66496391068090	-4.89544294223819	-0.69486229489178
H	2.36482900937549	-3.75525113917500	-1.15491420335203

AlCO4

Energy: -3863.486423476073 Eh

Al	3.02088864681998	-0.23340273393893	-0.32974336856260
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O	1.49040855972494	-1.03853175695990	0.22803031122868
O	1.06922937560470	1.68206344905455	-1.89843647859580
N	3.82564770354608	-1.71823799670855	-1.33034738697159
N	3.64498865606541	0.55397595481710	1.38040365930200
C	5.74372554315591	-0.37412636979138	-1.54490395557988
C	5.09549670119319	-1.59105391238340	-1.82393955953716
C	5.86735694057454	-2.52632727184088	-2.54732558625711
H	5.42278736075890	-3.48639491519844	-2.81772480065326
C	7.20213963947595	-2.24972707524216	-2.88588668714124
C	7.80730982807490	-1.04223811163451	-2.50510638165950
H	8.85539190432815	-0.86568478459794	-2.75308154747788
C	7.06502155440740	-0.07218506817043	-1.80476501003022
C	7.57704800443646	1.28428537955589	-1.29716809113572
C	6.93492876348197	1.51261575633138	0.08022961030950
C	7.55002795605135	2.09769595422791	1.20330992047172
H	8.58343429304510	2.44492662849571	1.15188516247467
C	6.83349623885614	2.23934339035030	2.40292319577108
C	5.51669247169851	1.76798485091898	2.51516351888334
H	4.97952885213788	1.85404217564272	3.46253289614688
C	4.87197734463030	1.14612116942579	1.42310375362593
C	5.62245172329247	1.11173171744732	0.23101407213254
C	7.48188311023588	2.90002075122226	3.59853428389340
C	7.08661676677071	2.39270708859098	-2.26259874708134
H	5.98968302258254	2.39187984379147	-2.33577703699254
H	7.49865124316883	2.23240473651042	-3.27295931389620
H	7.40542517192730	3.38449680951241	-1.90120696485394
C	9.10635408456192	1.32219990218530	-1.22517322534915
H	9.45491644843721	2.30310537578875	-0.86698767887666
H	9.54602317622647	1.16495790677718	-2.22233573663774
H	9.49780032265032	0.54768952419331	-0.54828250808120
C	7.99201405767382	-3.28402002924040	-3.65547298481275
C	3.06740962760885	-2.81025082616135	-1.82998564112631
C	2.63764839145138	-2.79477015732403	-3.17717612556696
C	1.97576784870275	-3.91636494631115	-3.69001597936860
H	1.64971175480897	-3.90872750874075	-4.73453408907709
C	1.70226887327779	-5.02151760300876	-2.88368653839871
H	1.17399069218618	-5.88666050733029	-3.29596663260603
C	2.08483134620543	-5.00465542037395	-1.54263821874835
H	1.85384096499599	-5.85740282812946	-0.89643305726552
C	2.76908595147086	-3.90962080832876	-0.99946456014406
C	2.67755313145033	0.92970741910140	2.35380600021692
C	2.12484575892303	-0.02451483205358	3.23298698221810
C	1.16347675563050	0.38924581181218	4.16513584315500
H	0.72685737499297	-0.35769528780287	4.83487054172395
C	0.74174997349173	1.71290437795407	4.23029168636124
H	-0.01333341389829	2.01519821084527	4.95907027005790
C	1.25656008015802	2.64278492493166	3.32759410009322
H	0.88063239373591	3.66837710263450	3.32827167542472
C	2.20913378659618	2.26937773032355	2.37566474258211
C	0.64337880235824	-0.07170576950798	-0.21970938947783
C	1.46182363463181	0.82424528885732	-1.11897227475837
O	-1.49047796263979	1.03861156952274	-0.22802598322165
O	-1.06928112867313	-1.68203502801858	1.89837242912236
C	-0.64343083324478	0.07176281347673	0.21967136144017
C	-1.46188339651635	-0.82422392994855	1.11890101191925
Al	-3.02094438702515	0.23331624075474	0.32954129940324
O	-4.94951279824925	-0.50880141180025	0.82921590502925
N	-3.82573006878794	1.71821955459498	1.33029382359609
N	-3.64500722775536	-0.55396613712828	-1.38049995745851
C	-5.74411490550973	0.37445500849475	1.54420667377963
C	-5.09619028869214	1.59151614430736	1.82272178899827
C	-5.86844143395649	2.52719152483820	2.54517803747839
H	-5.42421592516584	3.48765527896804	2.81470348112546
C	-7.20373461981802	2.25138197372613	2.88213617381162
C	-7.80871747426753	1.04372263941346	2.50154771142987
H	-8.85662614767436	0.86682674597701	2.75001004249088
C	-7.06556338319332	0.07259619880775	1.80372250735798
C	-7.57729768708063	-1.28417225257871	1.29677302078985
C	-6.93511660513634	-1.51254696690938	-0.08051354587713
C	-7.55053755303990	-2.09663003916879	-1.20387658958857
H	-8.58397817665506	-2.44375761220262	-1.15246578066364
C	-6.83415423789100	-2.23785321853128	-2.40362227478044
C	-5.51724390179703	-1.76685858364206	-2.51564062541208
H	-4.98055406943053	-1.85182257917412	-3.46335631559671
C	-4.87223483360622	-1.14586407296694	-1.42324347959509
C	-5.62258374108935	-1.11165173589193	-0.23117509514354
C	-7.08656199515599	-2.39212763276936	2.26258018171953
H	-5.98963339386726	-2.39105518540710	2.33577127120445
H	-7.49864410364470	-2.23155920344900	3.27287572350888
H	-7.40516780171433	-3.38411524286338	1.90155162691287
C	-9.10658038008662	-1.32255113607770	1.22484484587387
H	-9.45485128717344	-2.30368432109607	0.86699468016928
H	-9.54622986430913	-1.16511481026870	2.22198560252530
H	-9.49831541801217	-0.54838794015959	0.54772337042917
C	-3.06624831393361	2.80720310794472	1.83461273470105
C	-2.64364413315102	2.78906115914472	3.18425023881935
C	-1.97902344742476	3.90700694376479	3.70145333309550
H	-1.65690795906674	3.89619509655130	4.74720857731758
C	-1.69449097222722	5.01068112483585	2.89690291997742
H	-1.16313988529306	5.87252143988255	3.31213340433970
C	-2.06800757241744	4.99533674384887	1.55330822454663
H	-1.82743584929890	5.84634646401627	0.90831263071359
C	-2.75506489266203	3.90424568054489	1.00563792874283
C	-2.67923254289717	-0.93019598439376	-2.35543656345103
C	-2.12794856771139	0.02309255572544	-3.23657913018245
C	-1.16965293631890	-0.39220043269754	-4.17125391392825
H	-0.73321993295079	0.35420849286269	-4.84172253794432
C	-0.74900202914732	-1.71620821873894	-4.23659425883384
H	0.00481631564779	-2.01916644886076	-4.96650675547836
C	-1.26106169545960	-2.64471509798697	-3.33093150602418
H	-0.88452587394866	-3.67008317058457	-3.33035203732559
C	-2.20988701951948	-2.26958251342634	-2.37597613973579
C	-7.48358792769254	-2.89565734847952	-3.60024100702238
H	-6.98124105148986	-3.84468121158629	-3.85940363035760
H	-8.54602568380911	-3.12019451088068	-3.41352572192410
H	-7.42565579657828	-2.25283369083616	-4.49568270408123
C	-7.99260997815694	3.28413466004756	3.65480101610437
H	-9.03890441348908	2.97081928893834	3.79948076449572
H	-7.55469003034237	3.46198819411392	4.65301597283985
H	-8.00057012739307	4.25822442475150	3.13510631926525
H	6.97751658003431	3.84823543616929	3.85677218633092
H	7.42572544603300	2.25813166217756	4.49475658138522
H	8.54373446045825	3.12674651022926	3.41114971231962
H	9.03751597080917	-2.96924561101281	-3.80272643273599
H	8.00264837685492	-4.25604780086437	-3.13191491590457
H	7.55312541495819	-3.46661999228077	-4.65237236139658
C	3.15973741785830	-3.88228400920839	0.44963465268039
H	2.51622753674165	-3.16634464727030	0.98223886981758
H	3.04314101069826	-4.87308800785496	0.91639682831120
H	4.19943606980596	-3.54459795042798	0.58278582271048
C	2.86477826944665	-1.57537525950471	-4.03141905302589
H	3.93745053187321	-1.37568656709816	-4.19041701591200
H	2.39209275382007	-1.69547178402156	-5.01776890457918
H	2.43553475741010	-0.68057965198774	-3.55227668777020
C	-2.66763003027051	-3.27139080411984	-1.34655670643207
H	-3.72615312365178	-3.55507493816976	-1.47389449507538
H	-2.05817043921938	-4.18565464260847	-1.40716896424415
H	-2.56018576481062	-2.86356472098040	-0.32951607362834
C	-2.46929669074843	1.48210813576934	-3.13996658846538
H	-3.45420412748226	1.64216606755659	-2.68087045920052
H	-1.70713023123735	1.96075598756595	-2.50283772970036
H	-2.45039815516176	1.96245323573605	-4.13262795965181
C	-3.13326838766969	3.87857025608963	-0.44678921841144
H	-2.48521373853111	3.16241775651226	-0.97371375768856
H	-4.17186058447703	3.54128431156625	-0.58897150226594
H	-3.01236741430664	4.86980984692406	-0.91149114977017
C	-2.87705077607806	1.56867056332340	4.03537379687513
H	-3.95066320717465	1.37719004530172	4.19835582141158
H	-2.45757028107182	0.67201701477800	3.55119387546039
H	-2.39920319594510	1.68142611344597	5.02008277347663
C	2.67018319478410	3.27278364295065	1.34928429061749
H	3.72880729088617	3.55486730531811	1.47926985442505
H	2.56422493249593	2.86733378704563	0.33113353257102
H	2.06168790870739	4.18764130743924	1.41064214120766
C	2.47130881960473	-1.48253264009538	3.13956186998680
H	3.45921279592183	-1.64011189549893	2.68593427043441
H	2.44896392722226	-1.96179972192905	4.13268832685520
H	1.71399751535602	-1.96471113941333	2.49930217453895

AlCO4’

Energy: -1931.19776524 Eh

Al	1.95548233423161	-0.41221372881062	-0.89159878482505
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O	2.64768138429326	-1.01564364526114	-3.88930609310879
N	1.44594797524785	-1.83948406821381	0.27701316067087
N	1.57537103973272	1.46033869096094	-0.73793430662678
C	4.05151747510347	-0.64712106780811	-1.88713977111293
C	2.82277349722296	-0.81738096401714	-2.68503275806692
C	-0.67520655178481	0.83653202368218	-1.06534749407703

C	0.26297044898291	1.85997944490618	-0.85058710221738
C	-0.75495373769651	-1.40747472199446	-0.44343535486463
C	-2.05015166686059	0.96128313168633	-1.04485458134493
C	0.11466896708921	-2.18710659195711	0.33642469990720
C	-2.87318552306536	-0.33202848941684	-1.18920518078720
C	-2.13453664593504	-1.42346712051897	-0.39457325297276
C	2.59453575252457	2.44483072765419	-0.80980542276231
C	-2.71563169381105	-2.41994159654144	0.41104861309420
H	-3.80064360334909	-2.50445598996354	0.48789273266279
C	2.33761708216037	-2.45104957193831	1.19831959646858
C	-1.90438413560670	-3.31034468460106	1.13477340450534
C	2.85301753282888	3.09791088075738	-2.03822213087874
C	3.21191063821732	-3.46850082830256	0.75983671545517
C	-0.27935184058493	3.15385197640233	-0.72767085137419
H	0.39158365905877	4.00244701862826	-0.57587083011621
C	-4.30973895647316	-0.14691318602241	-0.69120571123798
H	-4.33680374654702	0.13975821724511	0.37114150812013
H	-4.88450467704465	-1.07698699198572	-0.81412039422237
H	-4.82462731795936	0.63183902266460	-1.27341349609712
C	-0.50320595915246	-3.18911371599812	1.10940929449030
H	0.11290408817993	-3.84908727196597	1.72404385390013
C	-1.67111574763431	3.35400161227254	-0.75505359713787
C	3.37716197313694	2.72692885599919	0.32997169518067
C	-2.55145123553464	2.26701259401560	-0.89091894978788
H	-3.62733054509841	2.44695773538149	-0.87330238978696
C	4.11622461001805	-4.02264747810334	1.67607038956437
H	4.79840127407784	-4.80924355616414	1.33983247752372
C	2.35298656055833	-2.01824902232034	2.54346137605623
C	-2.53607232353334	-4.41494503780527	1.94974532166461
C	4.15486750439381	-3.58777325132022	3.00192827535713
H	4.87122757633943	-4.02602704846642	3.70270325728608
C	3.27319012119027	-2.59467099075991	3.43021892715702
H	3.29695045044810	-2.25269751740846	4.46947643002718
C	4.40102363525161	3.67869685338575	0.23262468927738
H	5.00786157740266	3.89784488768519	1.11637014333584
C	3.87971042005018	4.05015395176279	-2.09330973135842
H	4.08435579037411	4.55369914169705	-3.04301915080475
C	-2.21508636634913	4.75875211529766	-0.63484389789109
C	-2.89940042220783	-0.73727442784085	-2.68508187245252
H	-3.38937659480854	0.04688943048488	-3.28447361462223
H	-3.45572231496265	-1.67963664759751	-2.81488322038402
H	-1.88176619793737	-0.88298887157730	-3.07592193703330
C	4.65149586691858	4.34415651404728	-0.96804714681838
H	5.45422775706944	5.08445197608644	-1.02996396464696
H	-2.01700946903474	-4.55491989318899	2.91188326575752
H	-3.59716930761259	-4.20806233278422	2.15852870461082
H	-2.48715044305084	-5.38102636337520	1.41601674315811
H	-1.70620570039684	5.32049445167969	0.16578501482656
H	-2.06247760934154	5.32665410455214	-1.56981627446296
H	-3.29470625327724	4.75802634604483	-0.41953149086233
C	2.05896460185609	2.75762563020075	-3.27296649845408
H	2.48969126391088	3.24590821744783	-4.15995525475253
H	2.04352812891024	1.67124602391066	-3.44984955258065
H	1.00792502611163	3.08052452819112	-3.18474238342161
C	3.12210407155821	2.00064629637532	1.62256476494072
H	2.05347312205111	2.01551200454425	1.88716073543809
H	3.41930533228985	0.94248059423820	1.53988423549049
H	3.69428158393972	2.44959898345150	2.44866619598278
C	1.38454117426933	-0.96755466114123	3.01967139640340
H	1.28501950387583	-0.15190694140179	2.28999556634572
H	0.37386171672078	-1.39065979458885	3.15162944415813
H	1.70258322590790	-0.54204005402522	3.98330086464990
C	3.16471726923418	-3.95009898916130	-0.66542324066361
H	3.55593366269314	-3.18698845150814	-1.35814717664595
H	3.76350737448256	-4.86470835013453	-0.79185821495358
H	2.13100053912613	-4.15854568681462	-0.98322537620392

AlCOCO

Energy: -1931.14377413 Eh

Al	1.77532145627600	-0.07981646781830	-0.19964621954945
O	4.70143919677360	0.08511975910389	0.33904421612642
O	-0.13361230030340	-0.35376530893291	-0.99394252868669
O	3.92659763321594	-0.81871872366750	-2.12895553416302
N	1.09918085327283	-1.54547340193422	0.87674846300672
N	1.12417248901973	1.74425981877587	-0.32087526685900
C	3.57971341558528	0.22458031329546	0.68266043088615
C	2.76945664157340	-0.71765346838200	-1.90178621782480
C	-0.85287345014084	0.81244550783854	-1.19089205390919
C	-0.12918344492793	1.96483504176244	-0.83770286112267
C	-0.85666022720422	-1.38633118275297	-0.41896308764664
C	-2.17455328201468	0.75652269976645	-1.57961991932362
C	-0.14466673627002	-2.05267483967601	0.59518477515969
C	-2.76964224599018	-0.64111713683859	-1.82371666345553
C	-2.17604744299372	-1.58715533249011	-0.76517394487198
C	1.94590695320046	2.87490250837780	-0.07576951088329
C	-2.83695916836104	-2.64446023719993	-0.11058663408481
H	-3.88013049597119	-2.87023412926010	-0.33754212377573
C	1.82475101547408	-2.08631886329397	1.96847159071195
C	-2.15774781984627	-3.41921923333934	0.84347949087349
C	2.61011374052296	3.50044587174681	-1.15520345023762
C	2.95531384335442	-2.90127812383253	1.73398186522165
C	-0.81529880300331	3.18190866923932	-1.01828363478264
H	-0.31188137620021	4.11992307286250	-0.77435733954726
C	-4.30002281389546	-0.62105272247963	-1.76785870757761
H	-4.66443683069982	-0.28231192841808	-0.78600573017944
H	-4.70833399455422	-1.62450153715937	-1.96175318822262
H	-4.70906332806631	0.04898696422600	-2.53926574653954
C	-0.82906332487160	-3.12695244165297	1.19861332904818
H	-0.32887045530271	-3.71099550210102	1.97430683214885
C	-2.14910804247165	3.19189575415968	-1.46429154301109
C	2.10121355790115	3.36008500046219	1.24044402196472
C	-2.83203821666446	1.99318625197908	-1.72490110173294
H	-3.87646253985047	2.03011482982865	-2.03884221642484
C	3.67366229535657	-3.38722785752079	2.83642869000069
H	4.55285941685993	-4.01411489405113	2.65755700303535
C	1.42410231506306	-1.77977571313797	3.29166163887056
C	-2.85465510557636	-4.58678027947215	1.50349517518925
H	3.28690721279880	-3.09107047565765	4.14153646554807
H	3.86067105085097	-3.47954199462339	4.98812765641960
C	2.16243643940287	-2.29288404476990	4.36293988486525
H	1.85670614982915	-2.04837604696397	5.38517283965376
C	2.91101824030948	4.48148092040640	1.45817793488039
H	3.03260591760441	4.85814715477417	2.47850249836201
C	3.41298464726812	4.61912507493835	-0.89797041663090
H	3.93322673833648	5.10221941636160	-1.73095369708499
C	-2.84544450990290	4.51803564382901	-1.66594574272454
C	-2.31210699956023	-1.12726565737930	-3.22274884694751
H	-2.68818753784471	-0.44923439614070	-4.00637751722359
H	-2.69349163301742	-2.14286013662059	-3.41838852922453
H	-1.21430809356665	-1.15377049128346	-3.28989861200914
C	3.56349638519352	5.11297425733691	0.39824598998333
H	4.19520860643827	5.98669854742336	0.58349467045514
H	-2.69230162125717	-4.59052773713032	2.59440843181160
H	-3.94079222570355	-4.56587624828441	1.32200551654090
H	-2.47303052837470	-5.55057314581650	1.12107712157338
H	-2.64429955982393	5.21031108091879	-0.83156118558221
H	-2.49586026716226	5.01883906363699	-2.58680267805006
H	-3.93670350165373	4.39516700495917	-1.75046482704183
C	3.40406216615403	-3.23363452966957	0.33517604264920
H	4.08377981786927	-2.46228979721995	-0.06450993078879
H	3.94647618797887	-4.19260089466738	0.31964527484810
H	2.55377362095079	-3.30010767431964	-0.35775824826110
C	0.23235162798728	-0.89259588811827	3.53688776928668
H	0.28402415609344	0.01527084081015	2.91779251637245
H	-0.71302022114822	-1.39550887057389	3.27317936888774
H	0.17621050113425	-0.59098073543145	4.59410339904572
C	1.43115367704194	2.65252834333688	2.38515555921744
H	0.36906182750003	2.45288899784820	2.17404483335406
H	1.92153291629996	1.67615077753663	2.54983378652386
H	1.50305697959073	3.23860905043612	3.31449270768095
C	2.46455206903433	2.95559944214917	-2.55173988060877
H	3.05905051173112	3.54509094433245	-3.26649509727655
H	2.79904940131821	1.90732560029581	-2.61080801002559
H	1.41404273173400	2.96929443033587	-2.88529033320328

AlCOOC

Energy: -1931.11430461 Eh

Al	1.83571645679733	-0.36506951933054	-0.52622043570032
C	4.73299971071871	-0.44788061119305	-0.00588201751548
O	-0.10321428164843	-0.45692025556129	-1.17179808637725
O	3.99403479141590	-1.35672225405633	-2.01831533238362
N	1.06193498155377	-1.51647507803810	0.85058597292375
N	1.41412045427215	1.53900207888036	-0.64506151275628
O	3.62059224781634	-0.14955987874063	0.33153956908312
C	2.78695724242956	-1.26102428720562	-2.11260793209658
C	-0.68691014270415	0.78466219370053	-1.40277278398711
C	0.17135459072253	1.86402768942126	-1.13296288208526
C	-0.91079680593328	-1.31090521814239	-0.42428123235731
C	-2.02555042085906	0.85663669467205	-1.72809652136560
C	-0.24586544834540	-1.89285889463445	0.67026181913848
C	-2.78053893776243	-0.48091298144248	-1.83313416555490
C	-2.26273649202592	-1.37278979621796	-0.69041440336019
C	2.41028642989002	2.54690569974882	-0.60906302891580
C	-3.02474328353697	-2.21675096529626	0.13797531787854
H	-4.09880122674372	-2.32572494287509	-0.02006700828036
C	1.73065745147165	-1.91349969336673	2.03349197982585
C	-2.40673663867957	-2.91985255032781	1.18582850084638
C	3.01459442375268	2.97789591679689	-1.81421768480561
C	2.74416166228408	-2.89682497626604	1.97103974202669

C	-0.38542783981449	3.13891373365125	-1.36089372213661
H	0.22968085345927	4.02567588354626	-1.19222939018853
C	-4.29619621748362	-0.28202942475551	-1.75271336631666
H	-4.59158276973474	0.19361985317373	-0.80526636402119
H	-4.81846209088518	-1.24745816776034	-1.83310171048388
H	-4.64986499546104	0.34923353299625	-2.58215525659810
C	-1.03764738331956	-2.75570698137650	1.45647149945366
H	-0.58328953692265	-3.26572891049399	2.30896475865641
C	-1.72737833058009	3.27506095478946	-1.75625059907076
C	2.83379129929532	3.06858962234727	0.63134360285565
C	-2.55076026438236	2.14772171752194	-1.91646210390571
H	-3.59949843983621	2.28593293596164	-2.18451849954294
C	3.43227376690956	-3.22974566353080	3.14578781066475
H	4.22002349827422	-3.98794830187714	3.09987680432975
C	1.40666464013069	-1.29303506624832	3.26390631072300
C	-3.21815516847622	-3.86623585306542	2.04031587679813
C	3.12852583933986	-2.61622759382862	4.36063173525141
H	3.67998439019578	-2.88569211805335	5.26611378738837
C	2.11705508187137	-1.65548425698253	4.41448774490479
H	1.87514629983564	-1.16862303706467	5.36461128148758
C	3.84037621017810	4.04203376855809	0.65100995273034
H	4.16825259767870	4.44752379915236	1.61317674624388
C	4.01424341290581	3.95678680135190	-1.75366899175725
H	4.48665088429906	4.28935239345845	-2.68319619943533
C	-2.28248514784233	4.65674530363503	-2.01478363387002
C	-2.41972574752558	-1.14804785916818	-3.18475779797892
H	-2.74483974857254	-0.51175102986309	-4.02410148466057
H	-2.91601796275763	-2.12849861609633	-3.27081693558940
H	-1.33468821459639	-1.30426960168946	-3.27269673185176
C	4.42586199242807	4.49258262339582	-0.53261633246112
H	5.21253939938546	5.25204028496885	-0.50292209136573
H	-2.96749050623851	-3.76200422724911	3.10900556059701
H	-4.29933521617764	-3.68999643675110	1.92552109130959
H	-3.02413294717229	-4.91935253705854	1.76780510645422
H	-1.94731273147512	5.37708571350198	-1.25042934578157
H	-1.94516776611203	5.04743165609630	-2.99180516192217
H	-3.38388359962206	4.65675369127078	-2.02233899419788
C	2.61405814376038	2.36506890104483	-3.13076636234705
H	3.21131024862865	2.78569669214431	-3.95413213095353
H	2.76227824940755	1.27159856628788	-3.12877604705376
H	1.54967632262816	2.53780343840594	-3.35885421089910
C	3.07524581314547	-3.57758601298439	0.66968236316395
H	3.67490379618731	-2.93500617619419	0.00454627296691
H	3.65207461177233	-4.49841012332885	0.84780153544735
H	2.16365617286398	-3.83638055797345	0.11007371061371
C	0.31106414387067	-0.26182843296447	3.33223028884163
H	0.35811795025106	0.42918981512524	2.47909187381609
H	-0.68566393693798	-0.73349344478854	3.29215670142407
H	0.37436679660981	0.32274251860691	4.26294183861614
C	2.22365962195610	2.55745188049531	1.90751599965483
H	1.12383477325395	2.56986329639588	1.85961937243849
H	2.52411431534433	1.51238478281448	2.08873116003997
H	2.54573835699865	3.15806295146444	2.77203808034348

CO

Energy: -113.32506229 Eh

C	-2.09834715022359	-2.73860000000000	0.03590000000000
O	-0.97325284977641	-2.73860000000000	0.03590000000000

TS1

Energy: -1817.80663113 Eh

Al	-2.62348214297459	-0.80362553069939	-1.41111703645489
N	-3.46707620039230	-1.73527251008171	0.23894385669664
N	-3.12733345091661	1.16913878394736	-1.01097310311684
C	-4.77573642957118	-2.11659865326206	0.12551263036087
C	-2.81775273736767	-1.95654790707313	1.46432665498710
C	-4.38966368537333	1.58524590961204	-1.32219621046508
C	-2.13966066006608	2.17426462151443	-0.89187419612983
C	-5.52465421783726	-1.55481665108584	-0.92634342231041
C	-5.51506399766435	-2.97271527633851	0.97897441457336
C	-1.69541447667787	-2.81732242726111	1.53678668042270
C	-3.25013901214147	-1.27030216515220	2.63156736513043
C	-5.32083620875989	0.59670300576129	-1.69980362568820
C	-4.92111715040018	2.89878384551628	-1.28967636547393
C	-1.42649530177445	2.61525794646850	-2.03279614730471
C	-1.84231774897537	2.73110931853371	0.37677621812908
O	-4.80494364657683	-0.69475691780960	-1.75134701197449
C	-6.90480771076349	-1.55034603204028	-1.02039251251863
C	-6.90469804184546	-3.10685908944923	0.84680366009737
H	-4.99695239158994	-3.48274715847139	1.79492293647811
C	-0.99795020957108	-2.93806674587852	2.74488534132337
C	-2.52563664143769	-1.42071757613594	3.82013058192134
C	-6.68446603656086	0.76184324697709	-1.84160519715626
H	-4.25901548640220	3.73257347052372	-1.04398832991851
C	-6.28788874379223	3.13676876066458	-1.50767017843962
C	-0.39219015784134	3.54945660526289	-1.87394535510327
C	-0.81166275399301	3.67029456539842	0.49298584570434
C	-7.50748266594736	-0.53289799091758	-2.01093766861261
C	-7.60903250282426	-2.37161519666497	-0.12345566989644
C	-7.65353626237175	-4.04312145467061	1.76728022336602
H	-0.12731417405226	-3.60045433488625	2.78704450354327
C	-1.39827105523865	-2.24006318448185	3.88441840903588
H	-2.85033500481333	-0.86925152336543	4.70868823441353
C	-7.17724375000175	2.07659399749000	-1.75363570177241
C	-6.80170310252429	4.55817928366409	-1.47412166132534
H	0.17040358976705	3.87281275613379	-2.75596133913650
C	-0.07524770068797	4.07140776535965	-0.62208367694136
H	-0.58206617172445	4.08736769298074	1.47870909025269
C	-8.99433322630018	-0.29289955866391	-1.73747532974482
C	-7.33960371935968	-1.05865284553574	-3.45795856707450
H	-8.69847005810565	-2.42854968427387	-0.15580662829611
H	-7.16531188250611	-4.11849791516661	2.75238354619634
H	-8.69200607637502	-3.70918318003501	1.92591532487579
H	-7.70074448623720	-5.06623854402263	1.35086215045441
H	-0.83860808894893	-2.33686291457830	4.81935055481569
H	-8.24311906662447	2.28349341253666	-1.86376455266989
H	-6.33703274812722	5.13735903449900	-0.65892496979271
H	-6.57297925249503	5.09137005595800	-2.41507706201826
H	-7.89419325555405	4.59215268740254	-1.33499231426621
H	0.73933513376285	4.79387423626116	-0.51427129951068
H	-9.16288933856405	0.08321528743855	-0.71730501032853
H	-9.56747098391685	-1.22479670218645	-1.86166725255109
H	-9.40477433048675	0.44101997363085	-2.44815430255018
H	-7.72528626953691	-0.32001797986671	-4.17994279940168
H	-7.89489455143165	-2.00225819600971	-3.58874997382992
H	-6.28215423892494	-1.24696288891265	-3.68933721132479
C	-0.65566281222060	-0.03598687337363	0.34420055580958
O	0.48771427722812	-0.04421032459752	0.33565202174319
C	-1.80083542035729	2.15021782908495	-3.41734763618958
H	-0.91845512743559	2.10880783233633	-4.07517660932968
H	-2.26647981165496	1.15605329038328	-3.40136724489480
H	-2.52147372235204	2.85504476689228	-3.87204927553312
C	-2.62304274685011	2.29554269600754	1.58325518015749
H	-3.70642497877890	2.39576353519875	1.41768635003663
H	-2.42996601454796	1.23416064716332	1.79964302082731
H	-2.34627944531632	2.88736804759943	2.46975526360788
C	-4.46501656884761	-0.38050972653650	2.59604495170847
H	-4.53928364521752	0.14966075267140	1.63762855250162
H	-5.39314100763313	-0.96713885737444	2.70062356049293
H	-4.43516746060476	0.36040188236358	3.40994144263030
C	-1.26722530355831	-3.60887755561534	0.32720390977489
H	-0.53083519368966	-4.37889748093195	0.60405146548135
H	-2.13378077625805	-4.09727711082699	-0.14739136161846
H	-0.83058407520024	-2.96612591097465	-0.45463843538545

TS2

Energy: -1931.11325604 Eh

Al	0.63244013662136	0.52053186634206	1.44010928201872
O	3.52456999249042	0.75048955882265	2.12430013430894
O	-1.43822586938788	0.31327707217064	0.84148763571928
O	5.24377007047140	-1.18416956746561	-3.14142027890625
N	-0.10547587336738	-0.82154440670534	2.73526310162999
N	-0.10038866728784	2.38013559305828	1.61082609175239
C	2.38131999839925	0.85815952885228	2.40898007112355
C	4.06790988376200	-1.12589043630046	-3.01911954706723
C	-2.14030531630448	1.51108493604368	0.79857361393740
C	-1.38007833744437	2.62840386709094	1.19745348181999
C	-2.12372236250163	-0.69046725739121	1.51417788943932
C	-3.49387751821194	1.49462858653332	0.52970863402760
C	-1.36814219937830	-1.30808458509712	2.53008974249687
C	-4.13032443861923	0.11282521874553	0.28807948940025
C	-3.47583538068617	-0.85774332351963	1.28922053813361
C	0.75685372360415	3.49074919943952	1.79964977502504
C	-4.12284330227930	-1.85888967450662	2.03797828640296
H	-5.18709134729011	-2.05693447948646	1.90009742941727
C	0.58511371286999	-1.24619741251138	3.89244155601453
C	-3.39927868773014	-2.60468423591007	2.98271204805210
C	1.29532499931333	4.16243539681401	0.67548522274595
C	1.69676756765545	-2.11379758583069	3.78535635896311
C	-2.07179029718912	3.86016923082886	1.15565808591692
H	-1.54409134500021	4.77594379236949	1.43219085018889
C	-5.65164285601965	0.15693741010457	0.45792118349024
H	-5.93560631823661	0.48266849301499	1.46997561792078
H	-6.09191103055554	-0.83569940965629	0.27738848391283
H	-6.10327973962627	0.85001722382578	-0.26829195209401

C	-2.04530630121464	-2.32924464294249	3.23424883271010
H	-1.51572887161198	-2.87608712588150	4.01790700115516
C	-3.43526113515502	3.91141499639471	0.81967606461220
C	1.09341764815517	3.91298877566888	3.10590907896486
C	-4.15238251939052	2.73918036185854	0.53138870157850
H	-5.21995465529637	2.80396696580390	0.31468458633092
C	2.39056907081029	-2.47544791216917	4.94789926665866
H	3.25279696767629	-3.14460780179221	4.86302907605285
C	0.16834084083123	-0.77977889727863	5.16526817958864
C	-4.07860782826290	-3.71830513470350	3.74640503730859
C	1.99971913480175	-2.00304463920305	6.20045141823734
H	2.55733552161640	-2.29031472646947	7.09672960472639
C	0.88940554318905	-1.16321709295464	6.30155528425381
H	0.57532533409850	-0.78867246498867	7.28124739326954
C	1.96025620098238	5.00086587616436	3.26847624953963
H	2.21902027160104	5.32499315110129	4.28149902642016
C	2.15550244538464	5.24882083453208	0.87813705533785
H	2.57495522223393	5.76350066253264	0.00768746871672
C	-4.13109233170080	5.25281669139829	0.77723243623221
C	-3.79375145700141	-0.34888884036697	-1.15185640744383
H	-4.21466685446636	0.35513754071467	-1.88856322844071
H	-4.21278303707753	-1.35118864805158	-1.34038468499952
H	-2.70620947651076	-0.39670984142671	-1.30454780578950
C	2.49087235274630	5.67062088367809	2.16537580611234
H	3.16889438884322	6.51725975514337	2.30844612190009
H	-3.79925271219440	-3.70596533103473	4.81318319764893
H	-5.17581333290212	-3.64404356894331	3.68135564460871
H	-3.79093596737778	-4.71013552608106	3.35271537070807
H	-3.89465000684377	5.85909780254168	1.66790761937584
H	-3.81485216118920	5.84274487913864	-0.10199470618667
H	-5.22557028883424	5.14070902578305	0.72436423378493
C	0.94439264367921	3.70369977189179	-0.71560905903860
H	1.55483221419513	4.22431729052113	-1.46984955768929
H	1.10150062599888	2.61778612912926	-0.81971323971179
H	-0.11912839725716	3.89042138227558	-0.94502956235399
C	0.53059476936770	3.18586605369085	4.29358861459865
H	-0.56423084307777	3.09410871713929	4.22480266846642
H	0.93655999743094	2.16069262007173	4.33437341123817
H	0.78391426155676	3.70003244687705	5.23380287244476
C	-1.03537883413901	0.11672294699767	5.28670730904049
H	-1.07675449790120	0.82844094394653	4.45197335504263
H	-1.97275730735707	-0.46396837194111	5.24533523894360
H	-1.02134044299154	0.67751263367536	6.23415644425485
C	2.13456172287857	-2.64346576705599	2.44398003634765
H	2.73248643135581	-1.89794277043044	1.89536178391137
H	2.75307546909640	-3.54752083447568	2.56512111238398
H	1.27322005879638	-2.88240019601275	1.80294929364499

TS2A

Energy: -1931.10438658 Eh

Al	1.80372065174143	-0.23253375950592	-0.43261281731754
O	3.81536053774195	0.34086189198721	0.63036572908749
O	-0.07113464411187	-0.50327406431915	-1.21174920534001
O	3.86981681034758	0.61555994240211	-2.25488153205808
N	1.03392591384499	-1.57826474114143	0.85069913068873
N	1.06132714180411	1.59164930064315	-0.23283294210071
C	4.77884734002518	0.74323844929257	0.10875332212118
C	2.75108168077241	0.18688902542191	-2.28799518909509
C	-0.76778025554688	0.68929838014133	-1.42675204718938
C	-0.12668484822133	1.81471049990950	-0.88167016870762
C	-0.84898229073560	-1.45923054813256	-0.56487754871632
C	-2.07078107036468	0.63609448313396	-1.87980149263106
C	-0.21784195886096	-2.05297394870906	0.54071872987926
C	-2.65287800088265	-0.76649857917358	-2.12779595952514
C	-2.15634842330049	-1.64918189358280	-0.96740214922044
C	1.47269838275950	2.57502329267772	0.70070882017586
C	-2.89467748241942	-2.61072734788352	-0.25654882392756
H	-3.93356120789604	-2.81717390939389	-0.51902361381614
C	1.88365654169492	-2.37779216224366	1.65342655489714
C	-2.30083756387940	-3.31184315391804	0.80752743402111
C	2.51770864231347	3.47538941173501	0.39929942000506
C	2.33205915839655	-3.63777525049299	1.17914881978552
C	-0.84085941753181	3.02626539651098	-1.00373371325852
H	-0.39895060134080	3.94424863655290	-0.61001620028887
C	-4.18159691135980	-0.74205268896461	-2.20198024338183
H	-4.62663451527642	-0.35674843634860	-1.27213893563172
H	-4.57597605423992	-1.75393563677160	-2.38178055532756
H	-4.51961786808929	-0.10814941381768	-3.03590359423703
C	-0.98313468986514	-3.03403385733200	1.20607730517196
H	-0.55033857427832	-3.55348830329747	2.06433191234843
C	-2.12874971937095	3.04951944446020	-1.56213603410463
C	0.81217541762584	2.63832597432245	1.95343154713467
C	-2.75500731152517	1.86121354800216	-1.97429856106240
H	-3.78004517357063	1.89715339116335	-2.34639270523500
C	3.19813600905996	-4.39890286785168	1.97356352010704
H	3.54160931378122	-5.36947939401735	1.60157026045480
C	2.35634047065772	-1.88595946705050	2.89211265679471
C	-3.08383840603315	-4.38118724506947	1.53421891262234
C	3.64711076757277	-3.92791246451643	3.20725601404386
H	4.33067121399038	-4.52993813542286	3.81291019062214
C	3.23169170007323	-2.67303544402489	3.65129472458076
H	3.58931131815507	-2.28774068977537	4.61122087068698
C	1.26303378986286	3.54827508919784	2.91617831192127
H	0.76581360054850	3.58247015136873	3.89085189783428
C	2.93907824880165	4.37363381821481	1.39082444642373
H	3.75567156012478	5.06585499774204	1.16283251360541
C	-2.84586584549988	4.37098916706150	-1.71216538978661
C	-2.08580395967813	-1.32112326845711	-3.45863337479480
H	-2.40852007427291	-0.68876941541499	-4.30177726797063
H	-2.44532533268785	-2.34915958691078	-3.62927074897127
H	-0.98670467440436	-1.33520610224157	-3.44559626550543
C	2.33200123756998	4.40519958686480	2.64549505840450
H	2.68111008000667	5.10780563293670	3.40803542784022
H	-2.89312104812474	-4.35547445592315	2.61962968611206
H	-4.16808193875411	-4.26646003966260	1.37674943888087
H	-2.80529984034741	-5.39163085311096	1.18362024839828
H	-2.64752104205708	5.03689508443239	-0.85648270535953
H	-2.51212286241404	4.90666378048003	-2.61938489261709
H	-3.93605715744996	4.23477894437272	-1.79430898674936
C	3.14415033916207	3.49810539732449	-0.96832609405912
H	3.90509676500922	2.71176706472220	-1.09358489013844
H	2.39542576072080	3.31526599693791	-1.75254358432444
H	3.62903532602019	4.46950724478307	-1.15501216068138
C	-0.38060361470110	1.75720284623011	2.22113413756286
H	-1.26434111364478	2.11638908639089	1.66689207858715
H	-0.20232457182093	0.72688373889634	1.88499133591732
H	-0.63237311793879	1.74333691214406	3.29258890206621
C	1.92178699454864	-0.53584473859050	3.39148081197127
H	2.26481904370805	0.27345591864403	2.72874018114379
H	0.82544067466104	-0.46427065543666	3.43833768026865
H	2.32706768516196	-0.33901461213922	4.39574899731465
C	1.91934276964261	-4.13475749207582	-0.18124724885078
H	2.04378162926007	-3.34074195644254	-0.93589915455050
H	2.52741753482654	-5.00097287647462	-0.48361880793648
H	0.85800259552879	-4.43295316501880	-0.21078176145220

TS3

Energy: -1931.11400742 Eh

Al	1.89765398363898	-0.13600479857886	-0.37105907736485
O	3.45112200410847	0.13880293671686	0.77327902324441
O	0.05463851638652	-0.43017617686253	-1.29007184968390
O	3.66435003055940	-0.26106292352963	-2.88266199029368
N	1.45761039997270	-1.92582416501212	0.24852128696914
N	0.90684790337944	1.44457454586798	0.24595287967964
C	4.58134200172217	-0.15725799578465	0.40310499750486
C	3.26591495182284	-0.37080712530219	-1.76202100399850
C	-0.86849736452102	0.58290774524630	-1.04998862239226
C	-0.37073818133914	1.61229033202363	-0.23294727369687
C	-0.47023271342302	-1.70562735753179	-1.09885260183368
C	-2.16751099169425	0.44188105773033	-1.49559857885114
C	0.32285093186589	-2.50795402303469	-0.26025404501299
C	-2.50264047473099	-0.85681072320586	-2.25254436085236
C	-1.74593657862293	-1.99305937825874	-1.54078240184906
C	1.56004204990718	2.57766640101927	0.79655350869385
C	-2.23650396312618	-3.27691169191475	-1.24158897184165
H	-3.23191923767057	-3.58073249194111	-1.56906948336573
C	2.10246873655102	-2.59617936202496	1.32393105149982
C	-1.45250766582749	-4.17526897163157	-0.49869411691244
C	1.99116143036998	3.61941583524558	-0.06011515625594
C	3.30273585338233	-3.30779275381986	1.10276509554587
C	-1.27548734153887	2.66451208297761	0.01772784482193
H	-0.94962599311357	3.51172993208455	0.62527669548133
C	-4.01135114295855	-1.11642513458732	-2.28439213711256
H	-4.42751482830404	-1.20550294688648	-1.26960526364761
H	-4.23441477035002	-2.04436701781185	-2.83263364395648
H	-4.53505052458386	-0.29883519830850	-2.80280826013199
C	-0.19464402971389	-3.79436632933432	-0.00250003291325
H	0.37549869320979	-4.47903435492078	0.62922078436366
C	-2.59357659349604	2.60920720254162	-0.46571273424047
C	1.82204676717575	2.64307028821394	2.18199269116229
C	-3.04733480582737	1.49710961378651	-1.19488084749891
H	-4.08750781458350	1.46137168786337	-1.52281478633579
C	3.93641797115326	-3.91088094285592	2.19920074353493
H	4.87290671494029	-4.45251455870029	2.03463334637892
C	1.52834926515264	-2.53685345181287	2.61517715690915
C	-1.96224131235405	-5.57037797020827	-0.21982055155783
C	3.39375663903506	-3.83375236211517	3.48079941437143

H	3.90649588120241	-4.30628186856171	4.32397786060046
C	2.18993260322136	-3.15524502250156	3.68294354102104
H	1.75313683410033	-3.09937139193933	4.68512189047517
C	2.48408622009517	3.76469809929022	2.69692531741789
H	2.68473325289956	3.81346192491569	3.77168316577584
C	2.64475016274096	4.72735269995594	0.49298907233731
H	2.98077450676967	5.53061355007658	-0.17025557816252
C	-3.52671747633922	3.76723865858810	-0.19612873587878
C	-1.97536847803758	-0.73723504873095	-3.70435404609426
H	-2.47151957834988	0.09833705753007	-4.22473074021886
H	-2.17291286008952	-1.66810514240281	-4.26076530877815
H	-0.89133123932763	-0.55445114802424	-3.71854093875110
C	2.88960937018491	4.80786537080474	1.86432678745315
H	3.40745591375111	5.67653863544197	2.28117653252906
H	-1.77695726433551	-5.86616346306463	0.82615219231000
H	-3.04376551666158	-5.65318185359372	-0.41097987015975
H	-1.45535323992164	-6.31705090716199	-0.85724971142986
H	-3.40595598024386	4.15368920402751	0.82920362035827
H	-3.32699476786069	4.61088479535117	-0.88141101780850
H	-4.58132231352695	3.47835249412917	-0.32892367142855
C	1.41120629213026	1.51117955574813	3.08086575812915
H	0.35163229710536	1.24995756219827	2.93785007174067
H	2.00096677158048	0.60775994262731	2.85531051498074
H	1.56929365060704	1.76760367531455	4.13973505735819
C	0.20735340348425	-1.84467350023229	2.82837057107543
H	-0.62839074788742	-2.47041686919345	2.47076180098734
H	0.03844948141755	-1.62701501360931	3.89400431879876
H	0.15095313854873	-0.90499079531090	2.26345369750401
C	3.87466364333290	-3.41349064311659	-0.28003770763787
H	4.74680184412557	-4.08514389647820	-0.29862687844255
H	3.12317327663650	-3.79105588168618	-0.99296472953417
H	4.17909289687329	-2.41577495555809	-0.66054570166230
C	1.77477798442432	3.52113342897903	-1.54813130822343
H	2.15849281654882	2.56608518613386	-1.94228105830282
H	0.70395197537844	3.56100470085993	-1.81050577443247
H	2.28561286756104	4.34200352944556	-2.07402026964205

TS4

Energy: -3863.303209302529 Eh

Al	3.57554049153497	-0.25038549471990	-0.63874570655031
O	5.54232641696349	0.43002286140926	-1.04405452376590
O	1.97261695791571	-1.15276908841256	-0.20987878214390
O	1.69088014515823	1.16721974525180	-2.69802549477116
N	4.40333278617753	-1.78580822616309	-1.57358042145127
N	4.09734039330841	0.57225190033305	1.06662277208588
C	6.34463166742324	-0.46383016036916	-1.73462243411325
C	5.68773874112561	-1.67630392427399	-2.02690617519385
C	6.47240031943506	-2.62958391320286	-2.71166877150853
H	6.02472705084860	-3.58767950196345	-2.98493242711760
C	7.82554235671968	-2.37760429619542	-2.99484191255130
C	8.43672507637068	-1.18087687489196	-2.59029100813159
H	9.49907453531406	-1.02826307970749	-2.78803412236139
C	7.68352246012522	-0.19259015837751	-1.92619674054304
C	8.20861016763134	1.14495552382279	-1.37828580627915
C	7.49169033862805	1.40690327533247	-0.04234774101921
C	8.04717943586800	2.01054158907576	1.10284588468872
H	9.08957154489961	2.33389163820529	1.10941787500330
C	7.25869910413184	2.20549195409034	2.24858386484299
C	5.92345982543912	1.77218716509165	2.28945182016030
H	5.32685389678772	1.90179303929332	3.19549964515553
C	5.33588361041936	1.13272379615662	1.17731623411125
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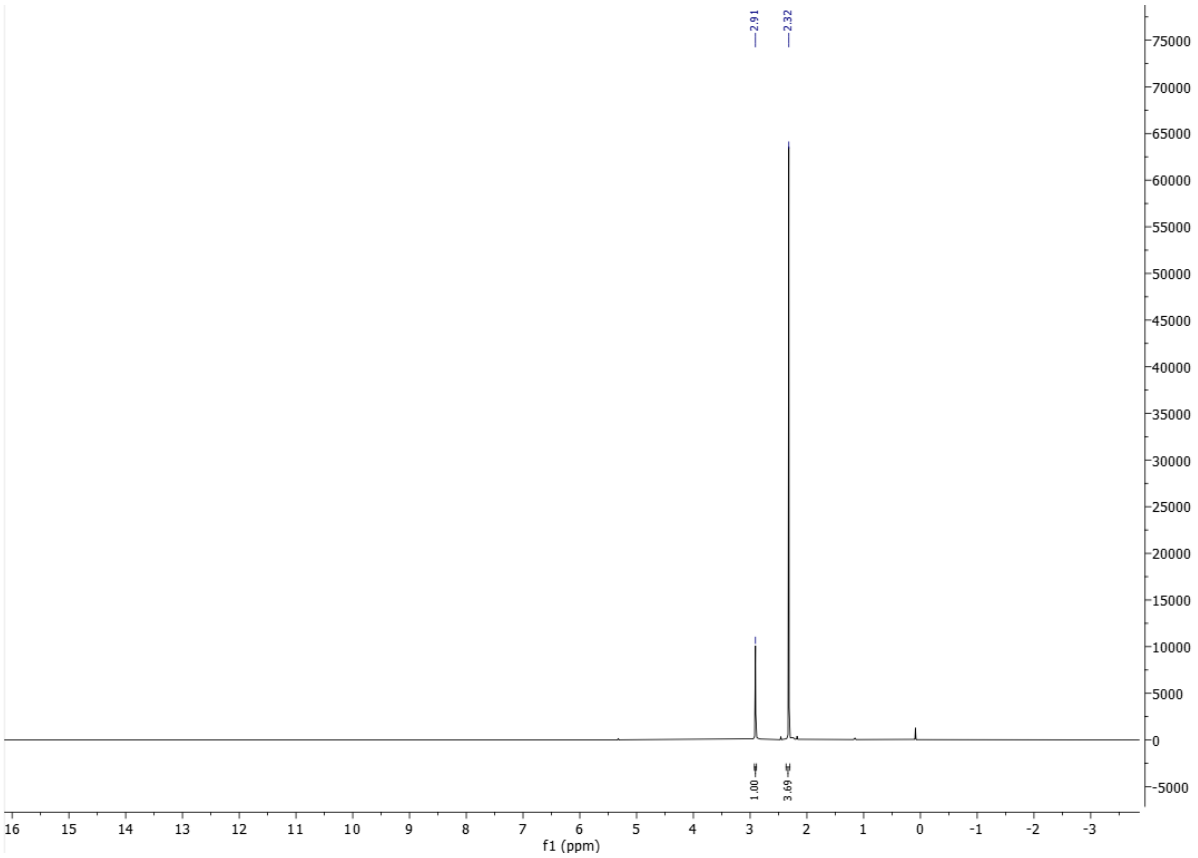
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H	3.91065083570597	3.55790133870560	-2.68959555877553
H	2.82760585444709	2.61506445298546	1.36392074353575

Chapter 7 - Modulating Hydrogen Shuttling in Ammonia by Neutral and Cationic Boron-containing Frustrated Lewis Pairs (FLPs)

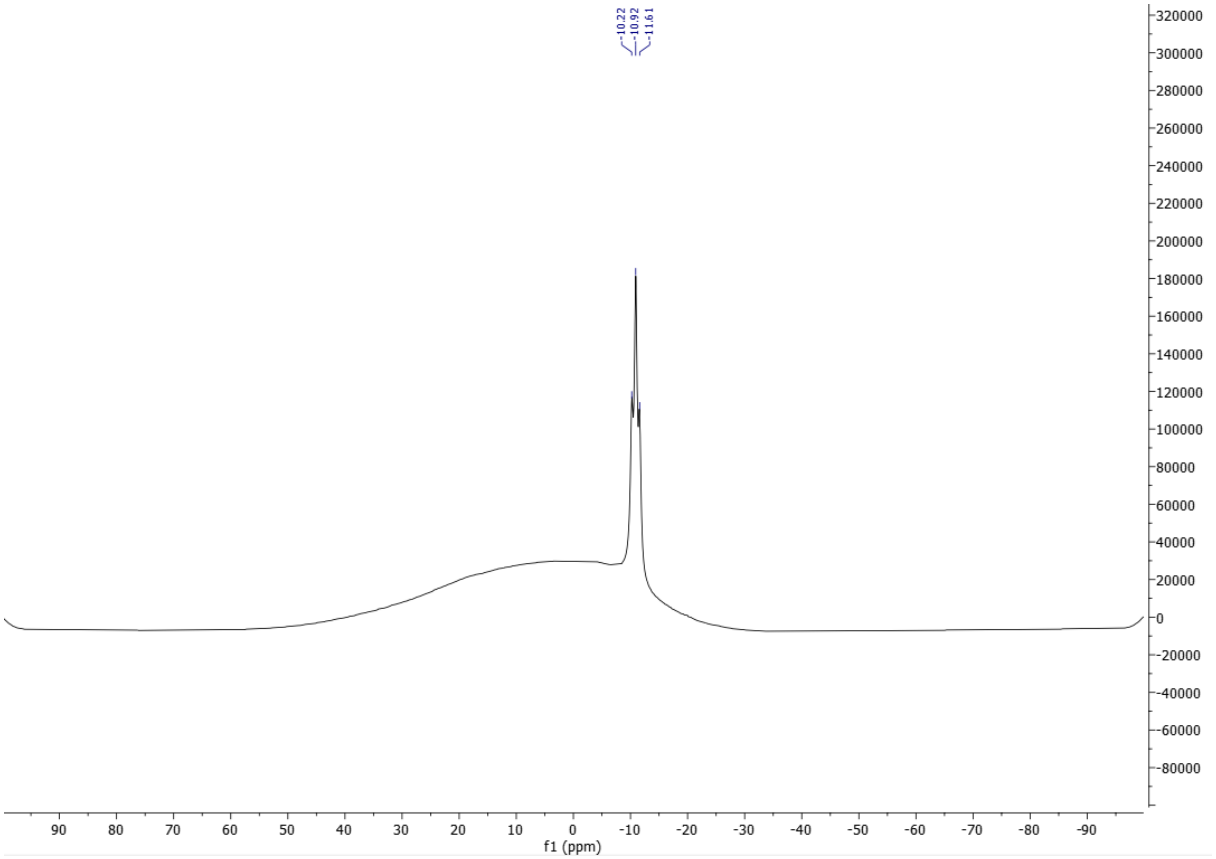
Spectra

NMR

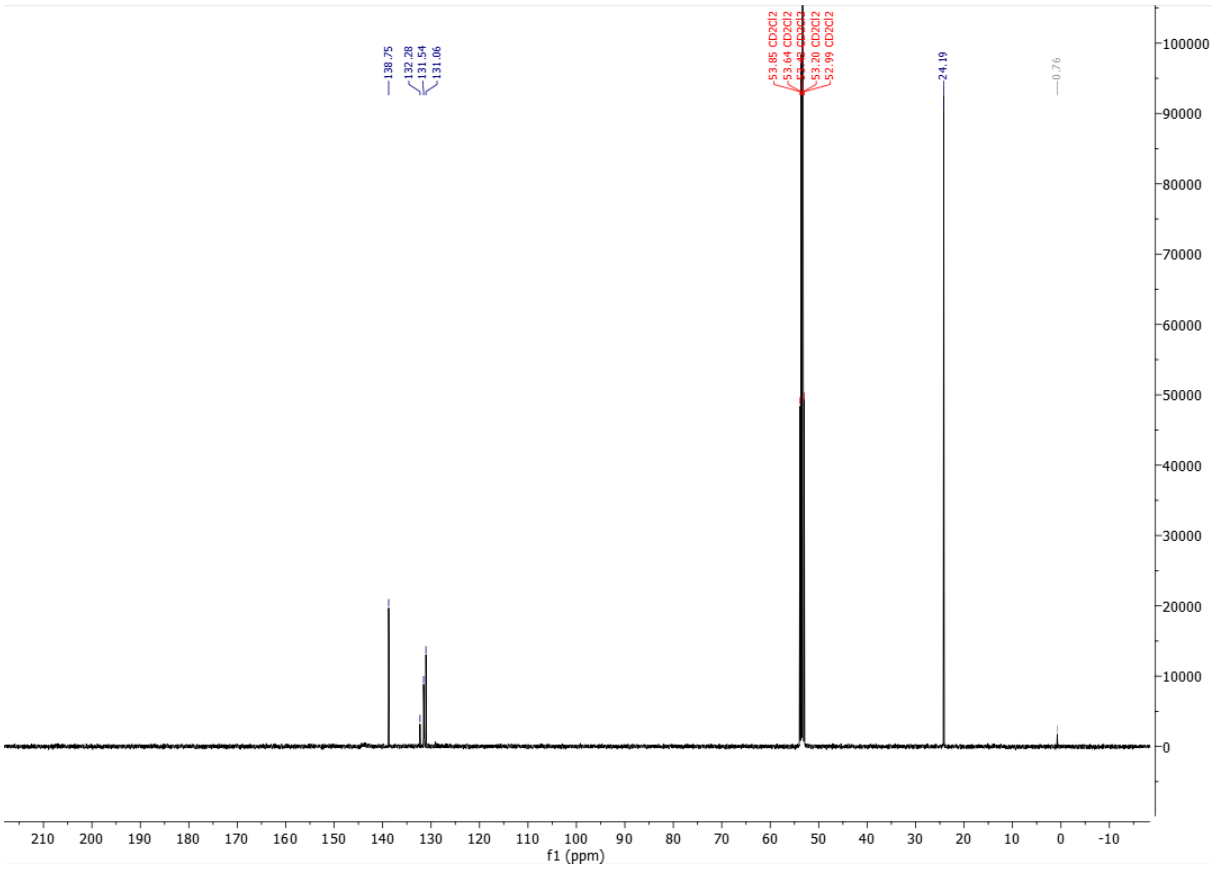
Precursors



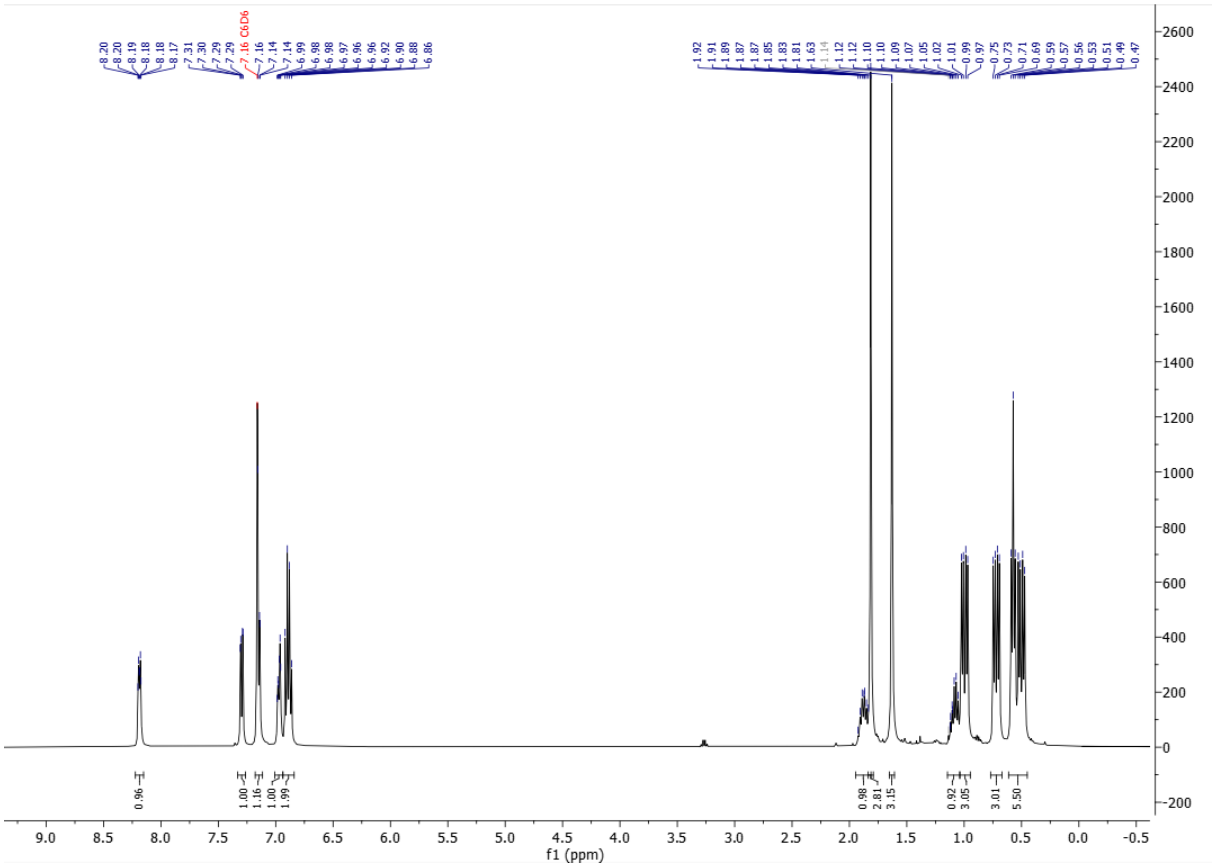
A 7.1: $^{1}H\{^{11}B\}$ NMR spectra of $Ar^{Cl}BH_2{\cdot}SMe_2$



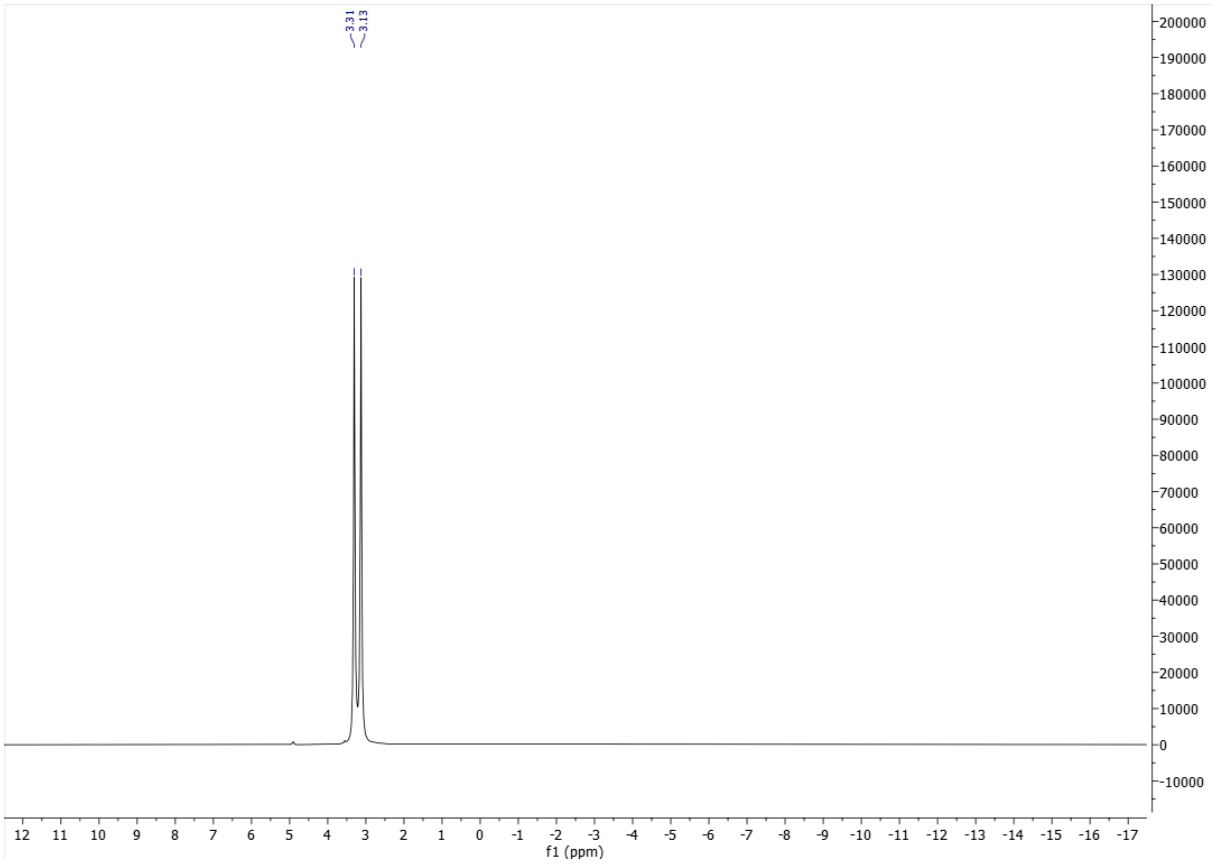
A 7.2: ^{11}B NMR spectra of $Ar^{Cl}BH_2{\cdot}SMe_2$



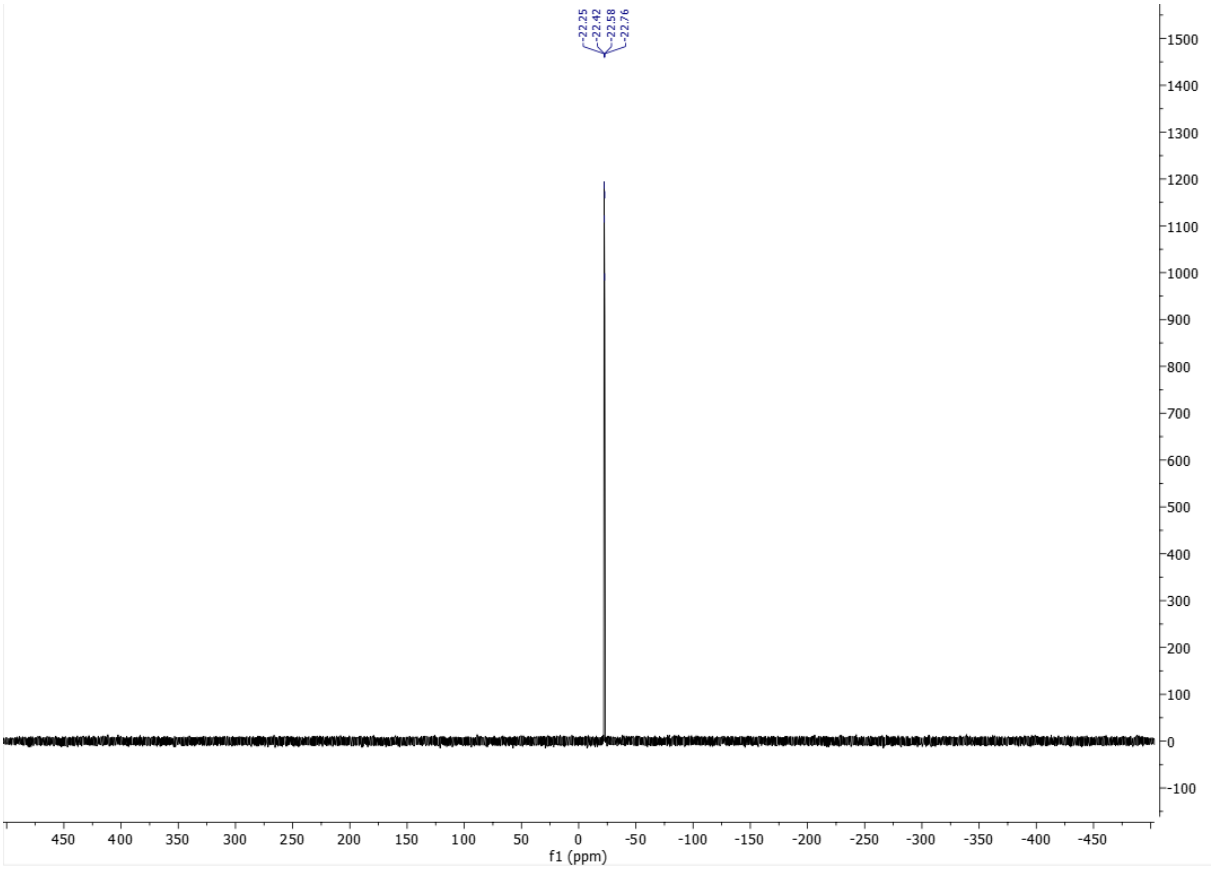
A 7.3: ^{13}C NMR spectra of $Ar^{Cl}BH_2{\cdot}SMe_2$



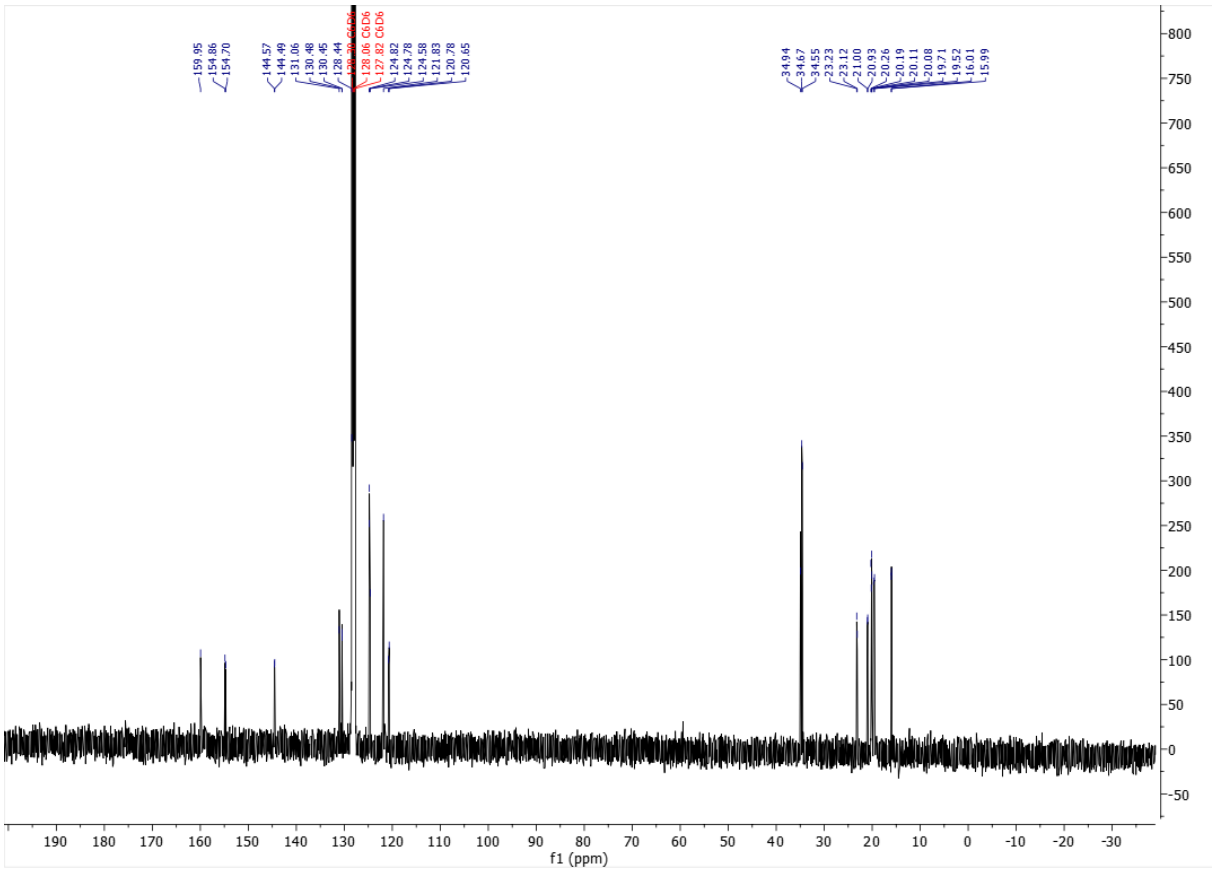
A 7.4: ^{1}H NMR spectra of $^{i}Pr_2$P-xan-Li



A 7.5: ^{7}Li NMR spectra of $^{i}Pr_2$P-xan-Li

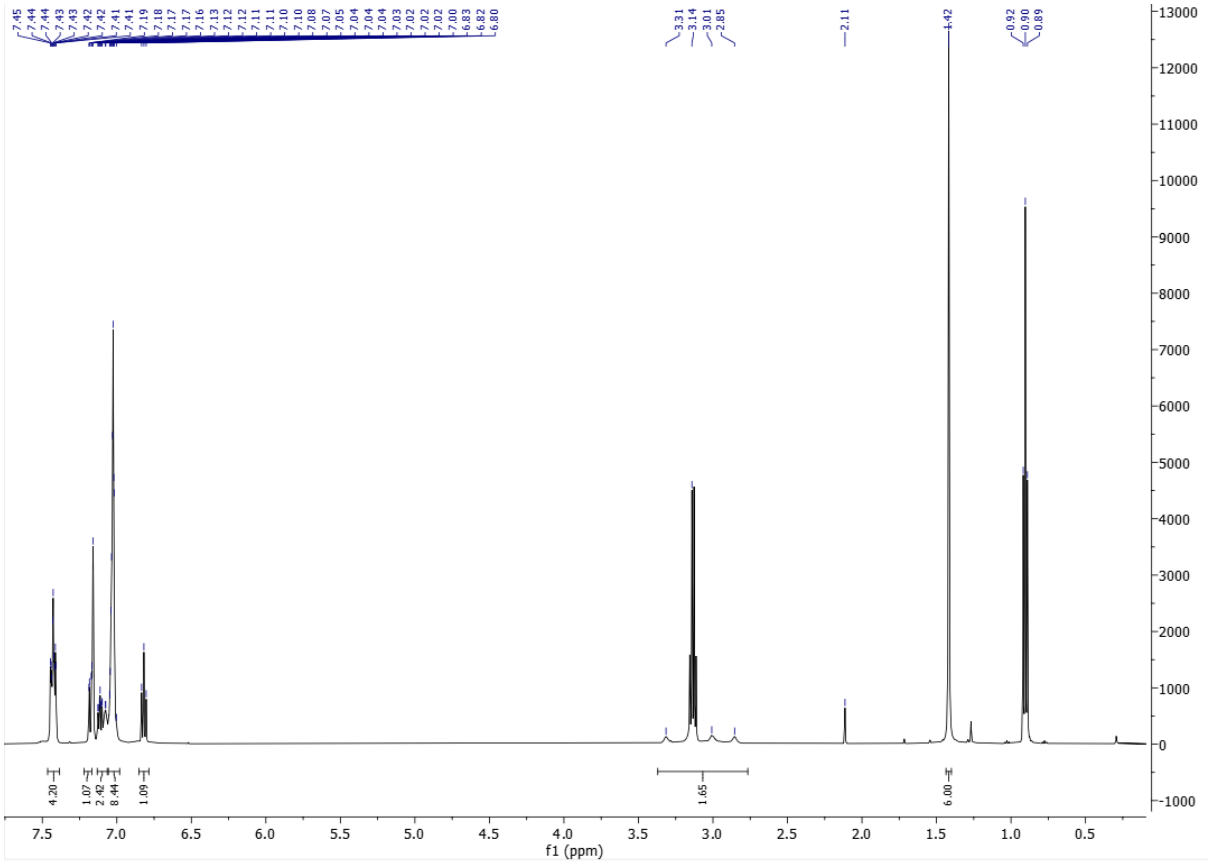


S 1 ^{31}P NMR spectra of $^{i}Pr_2$P-xan-Li

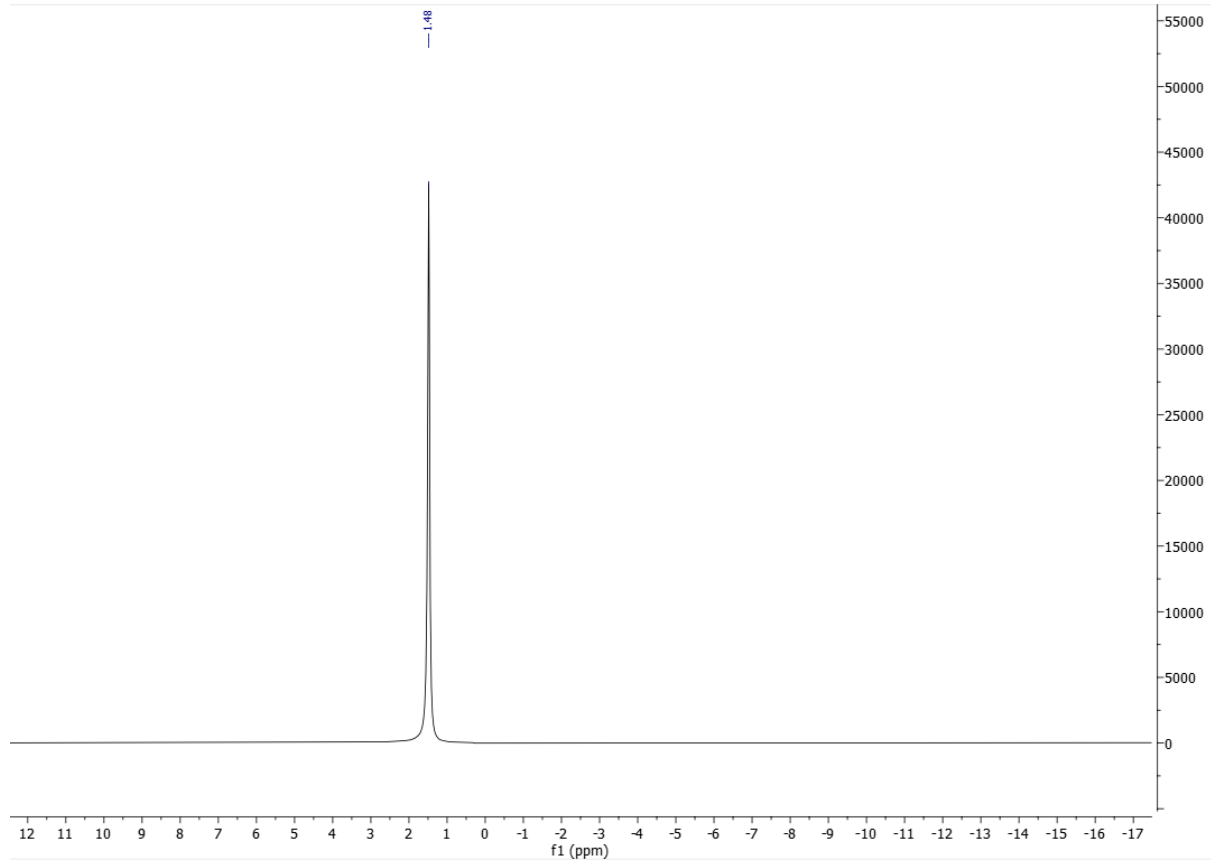


A 7.6: ^{13}C NMR spectra of $^{i}Pr_2$P-xan-Li

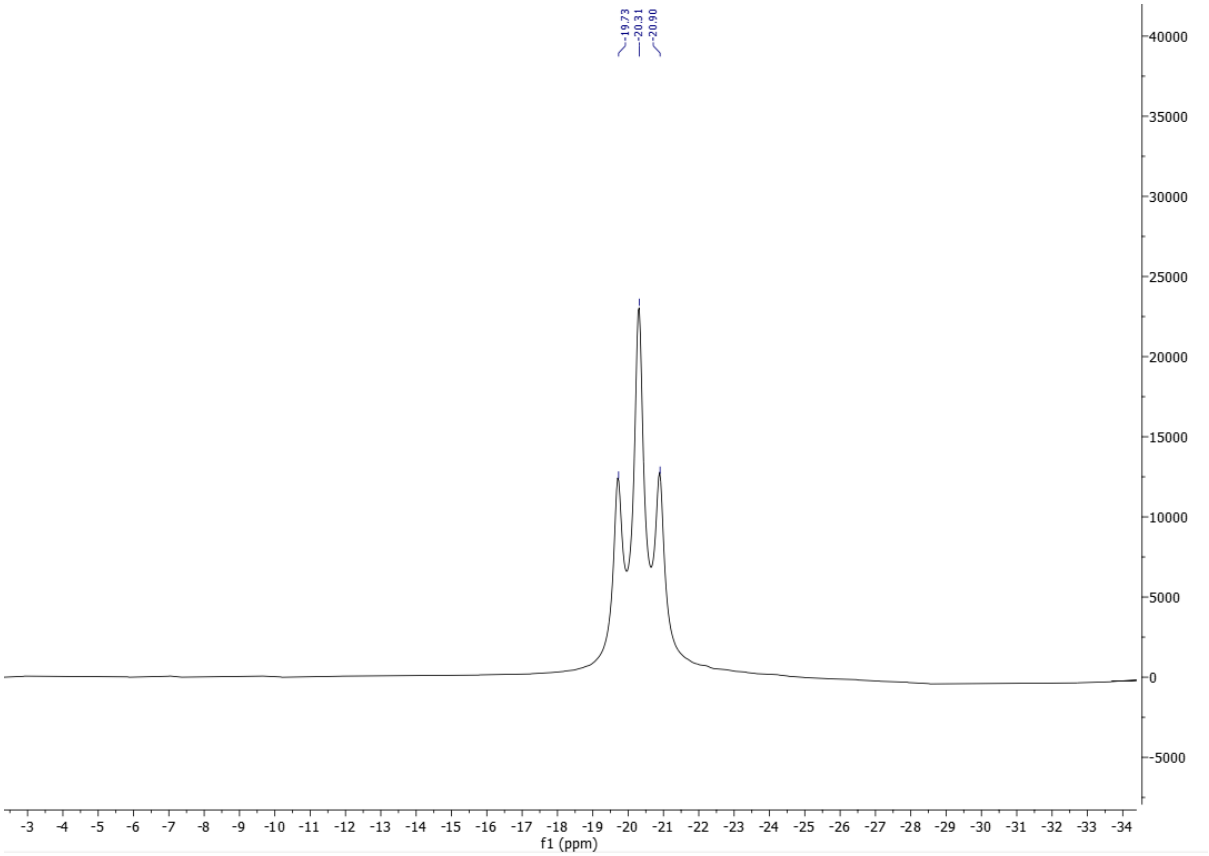
1a-d



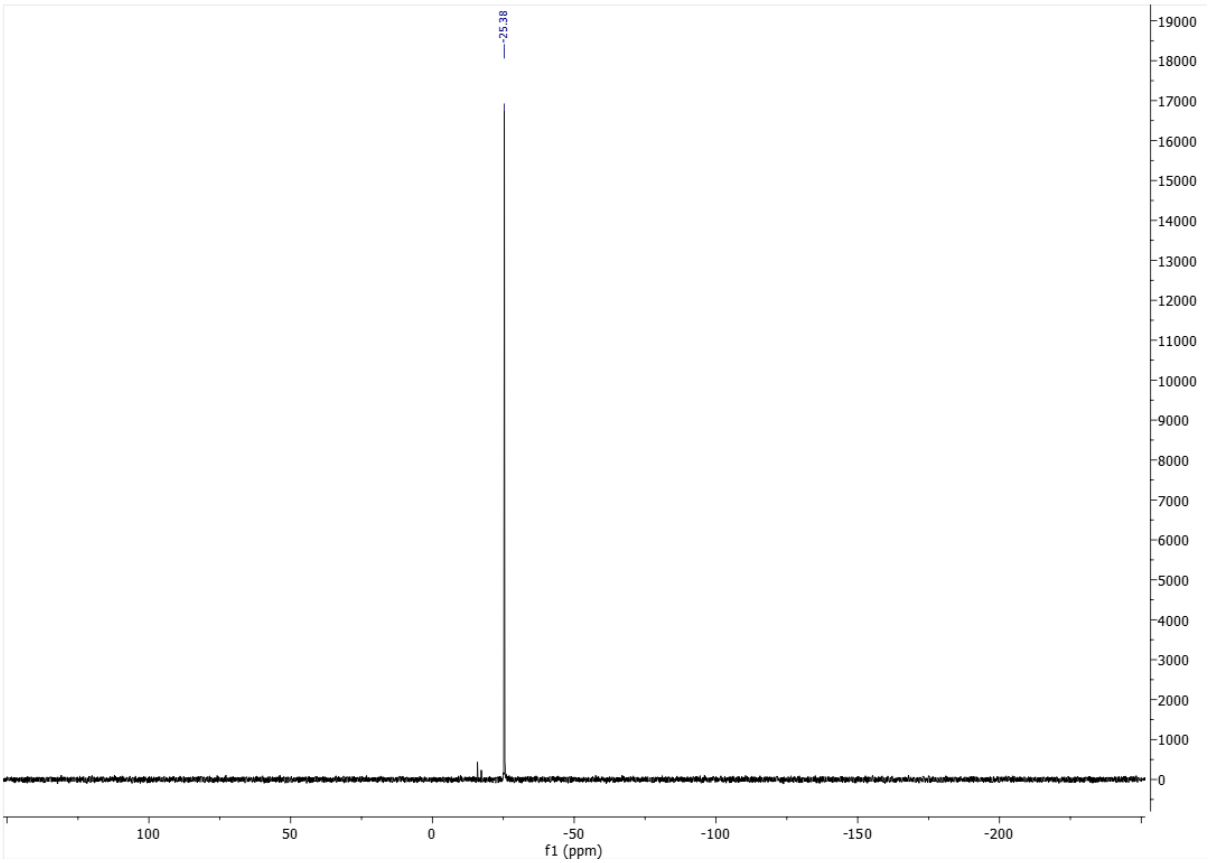
A 7.7: 1H NMR spectrum of 1a



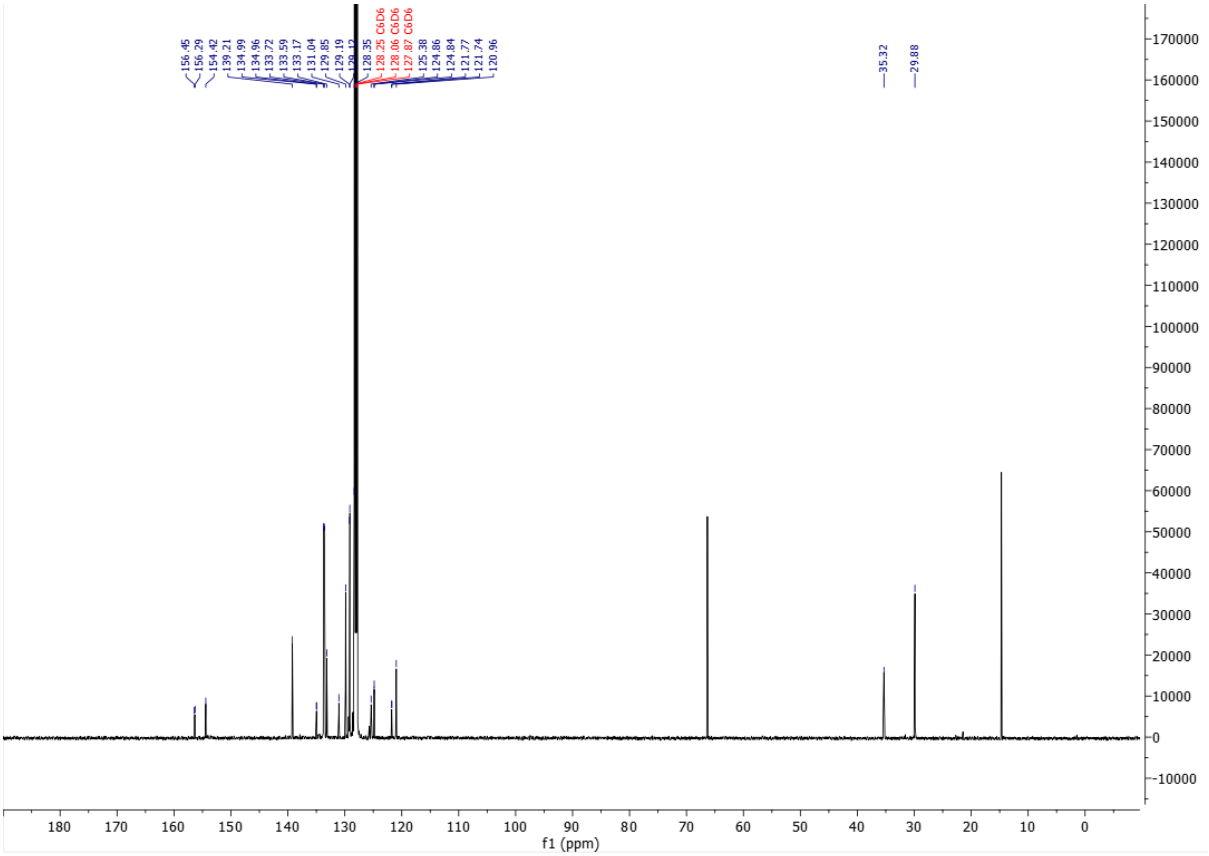
A 7.8: ^{7}Li NMR spectrum of **1a**



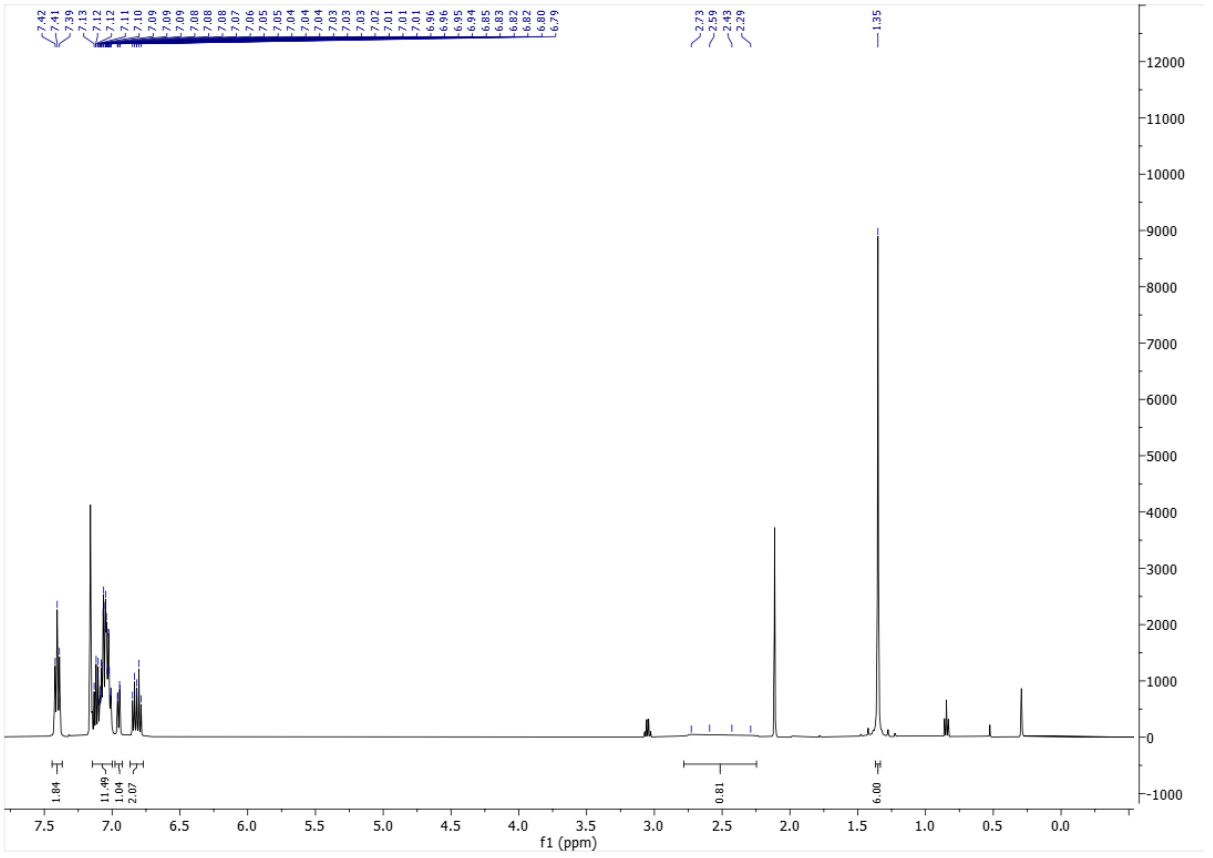
A 7.9: ^{11}B NMR spectrum of **1a**



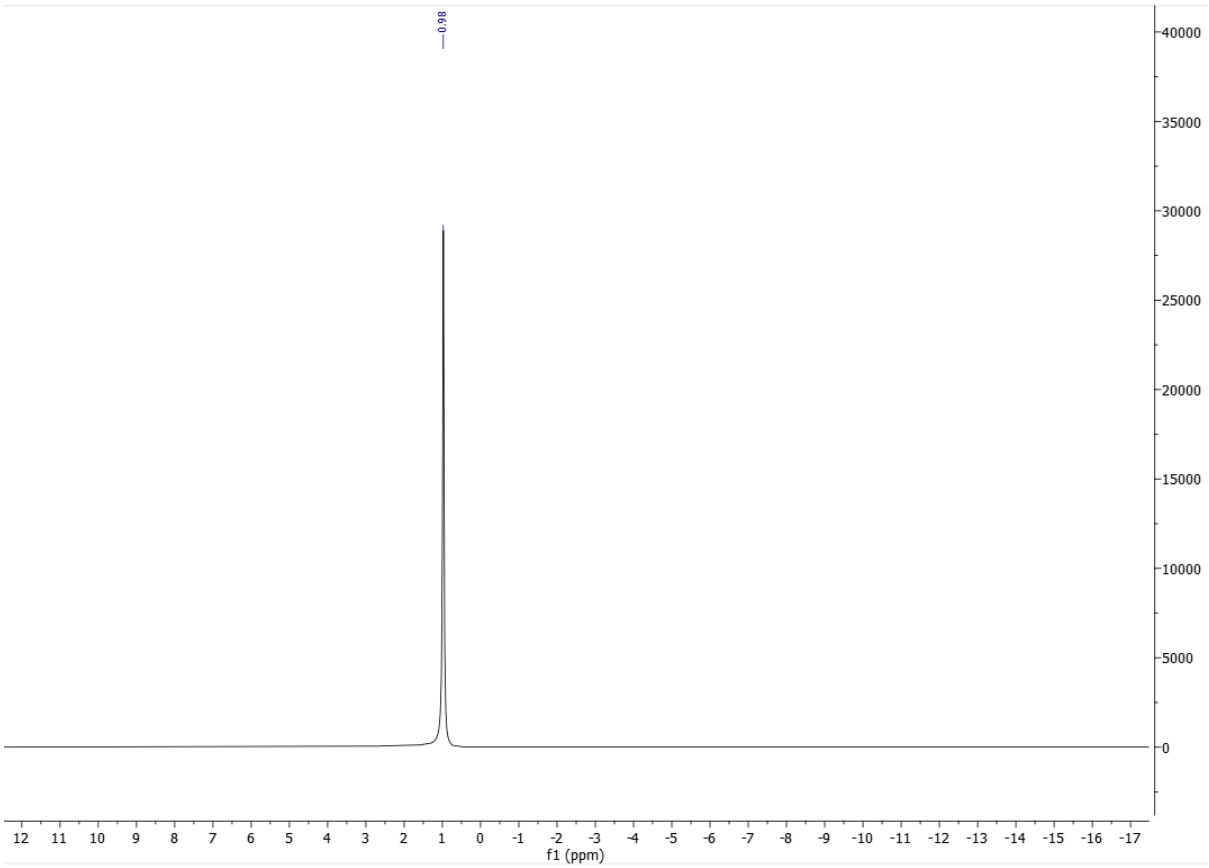
A 7.10: ^{31}P NMR spectrum of **1a**



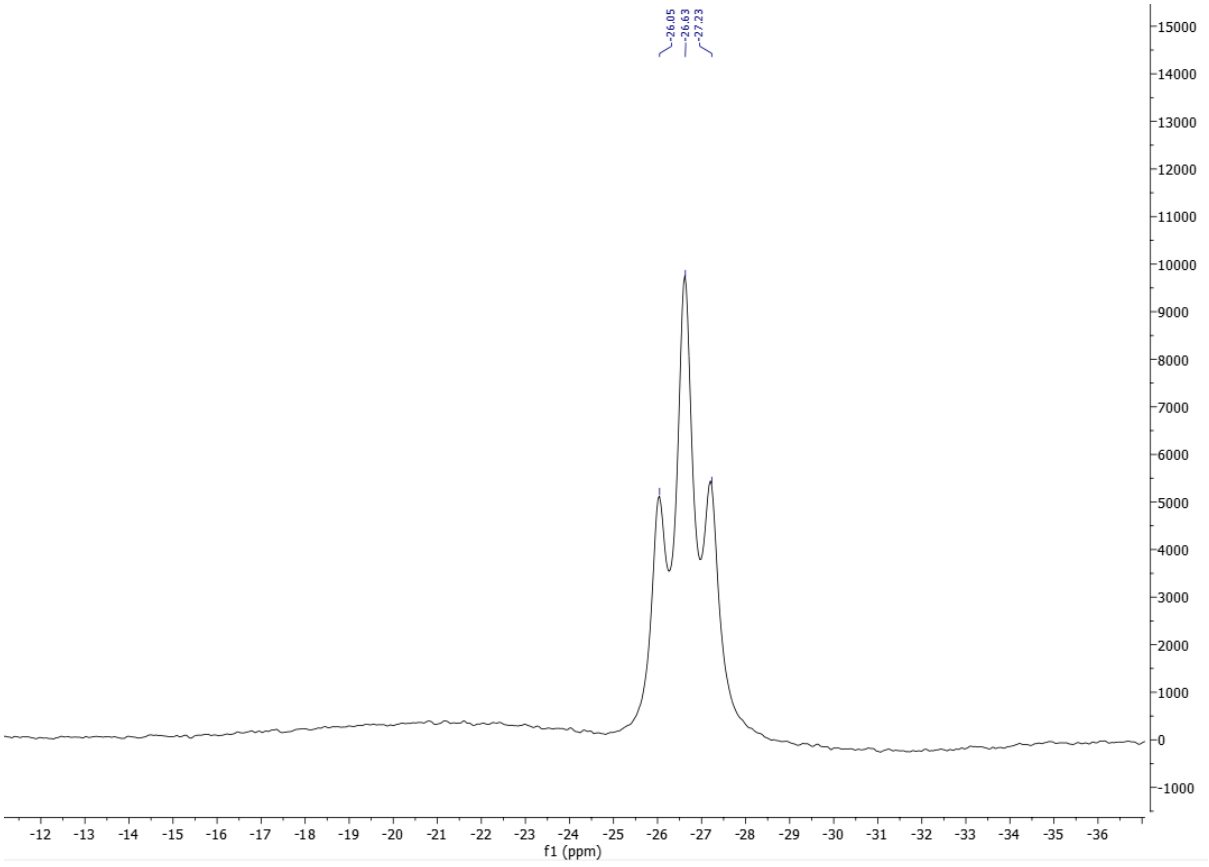
A 7.11: ^{13}C NMR spectrum of **1a**



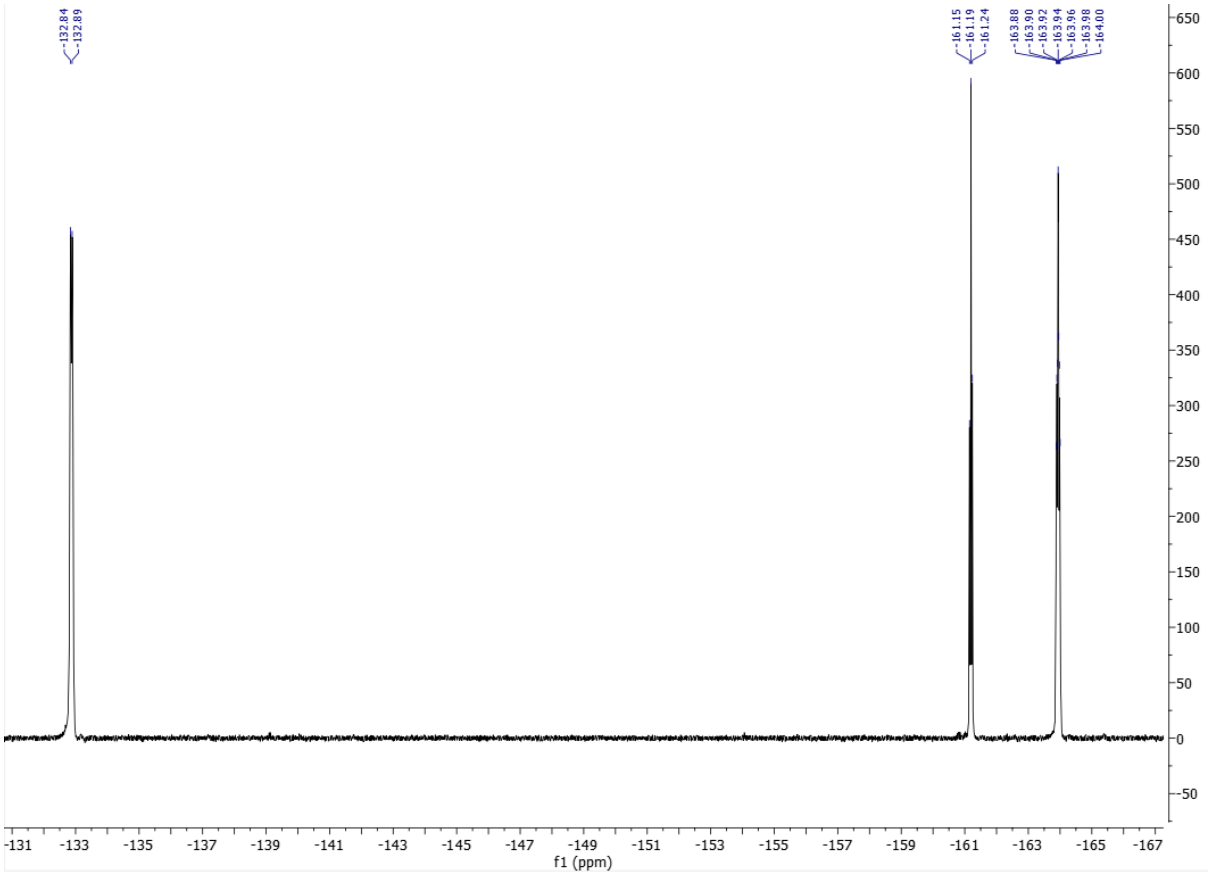
A 7.12: ^{1}H NMR spectrum of **1b**



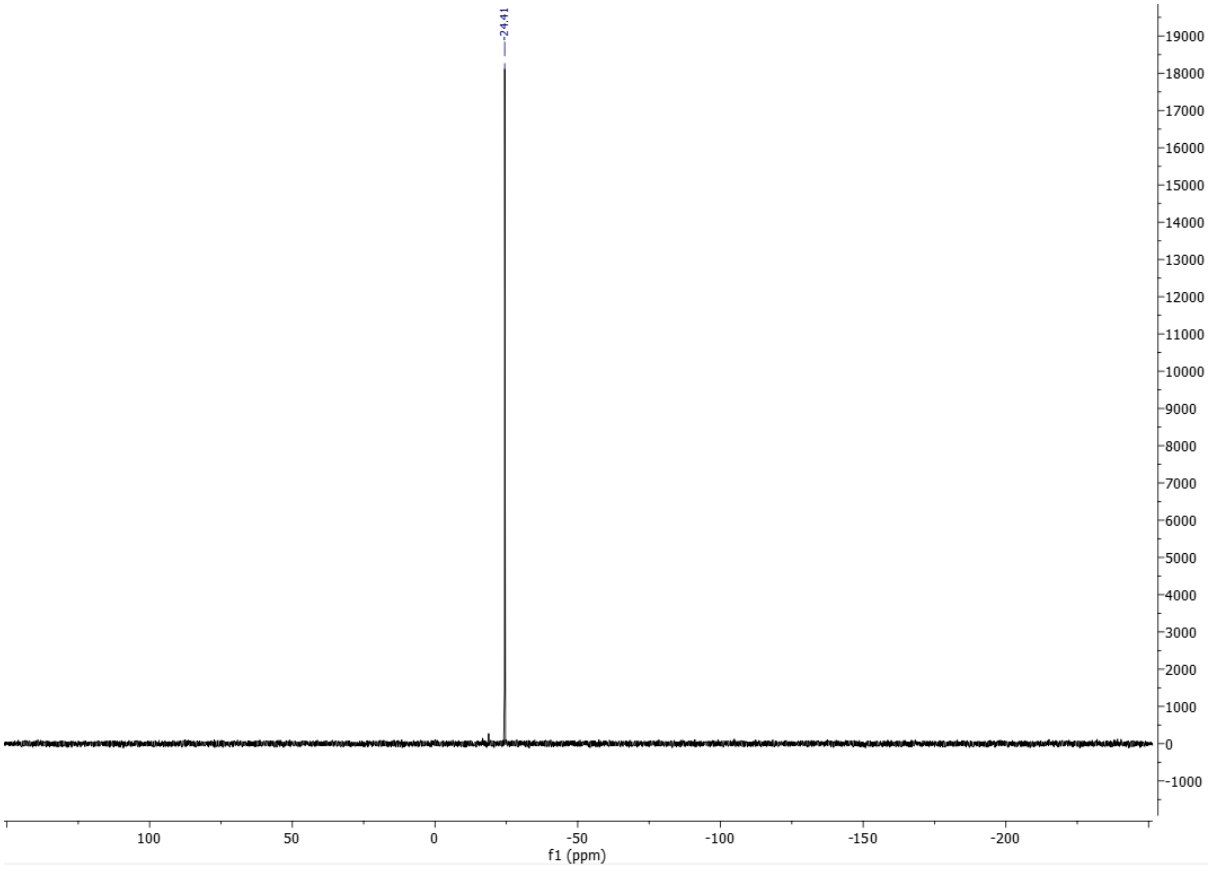
A 7.13: ^{7}Li NMR spectrum of **1b**



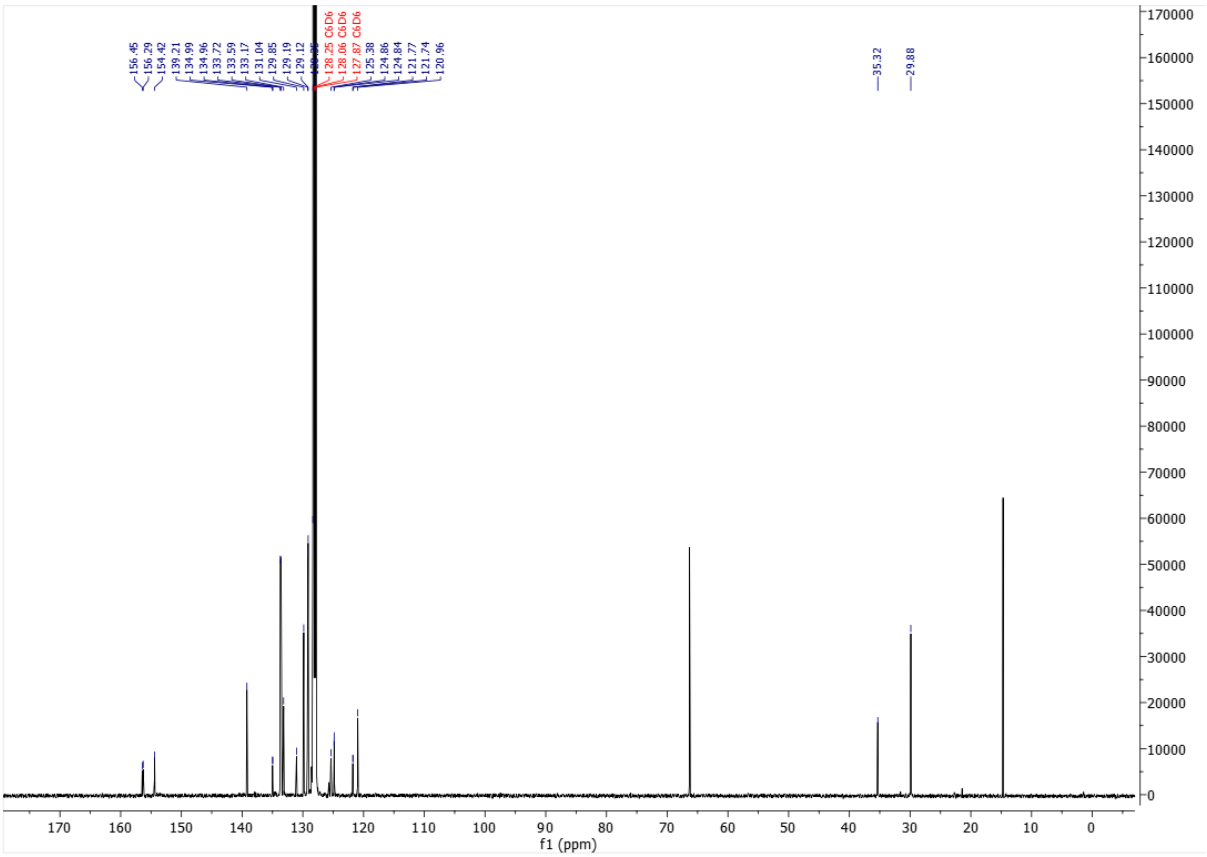
A 7.14: ^{11}B NMR spectrum of **1b**



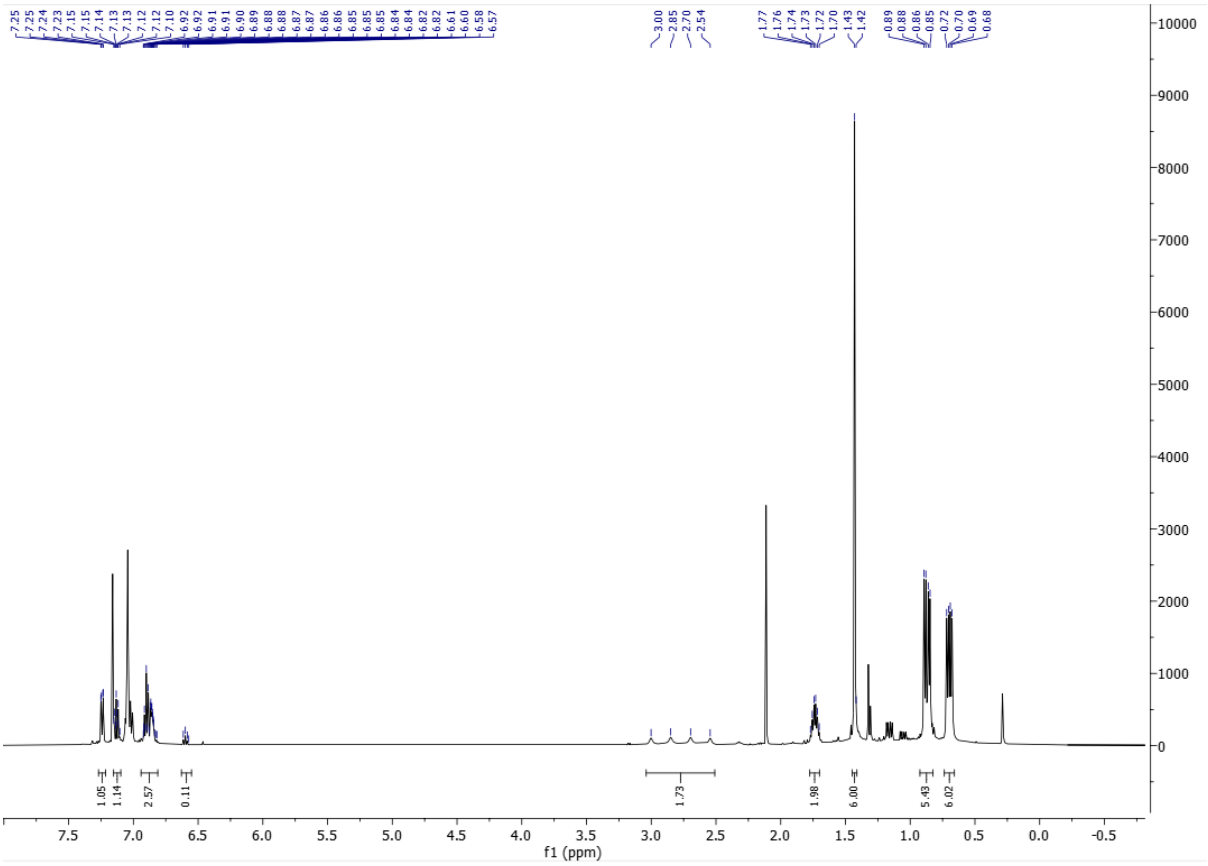
A 7.15: ^{19}F NMR spectrum of **1b**



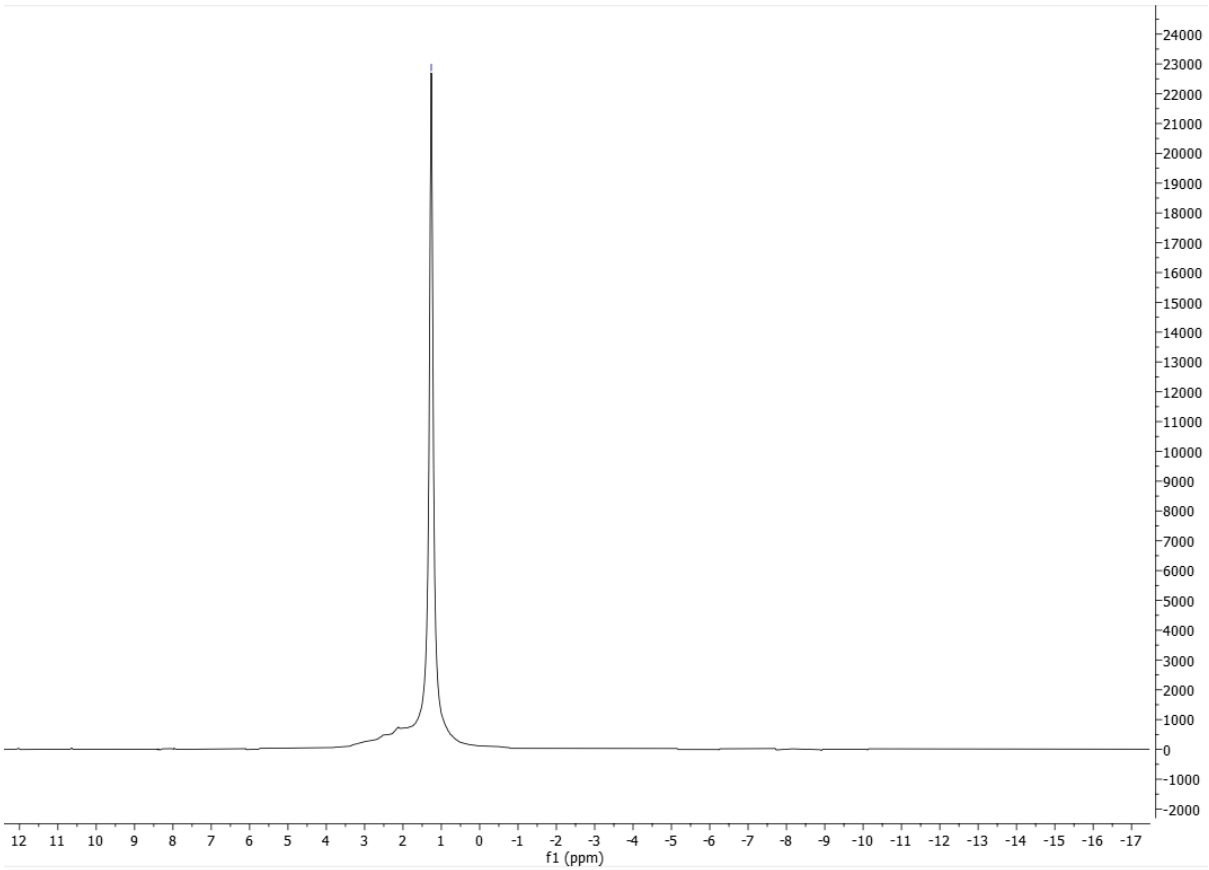
A 7.16: ^{31}P NMR spectrum of **1b**



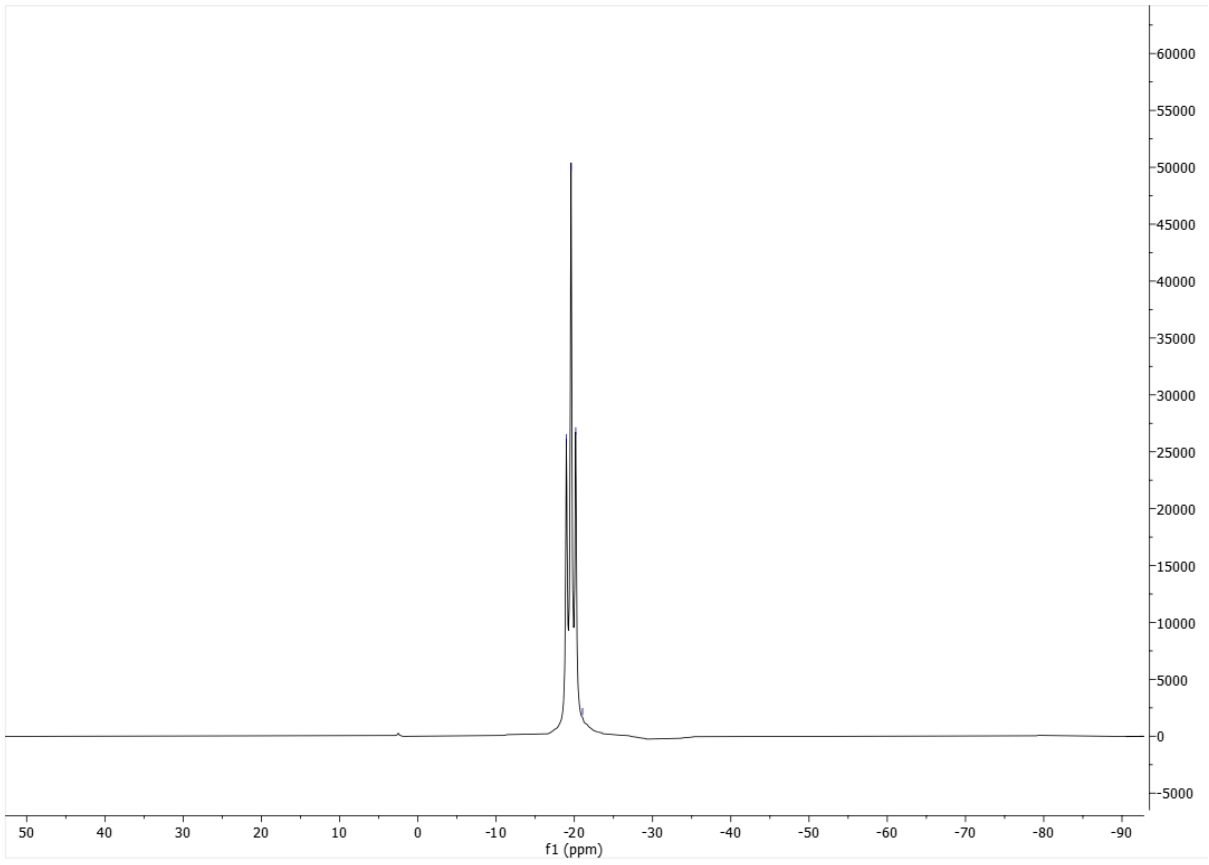
A 7.17: ^{13}C NMR spectrum of **1b**



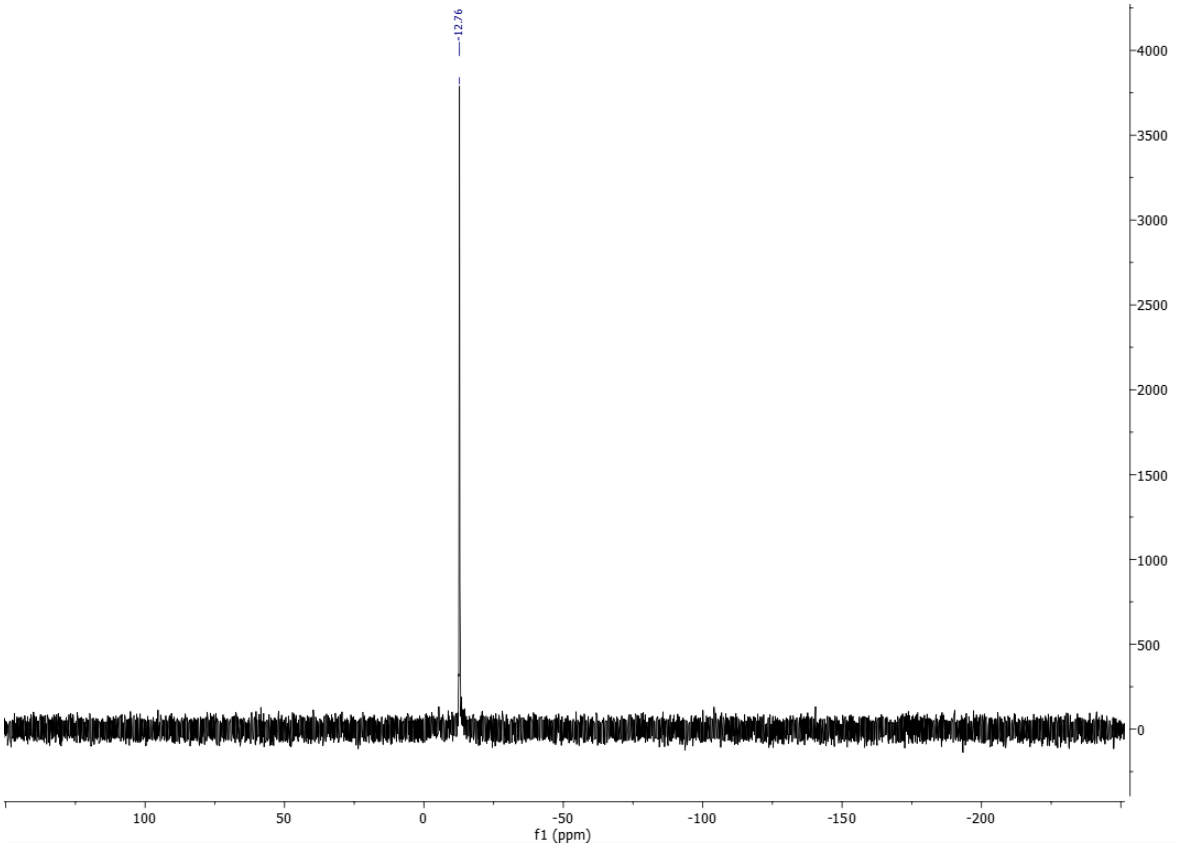
A 7.18: ^{1}H NMR spectrum of **1c**



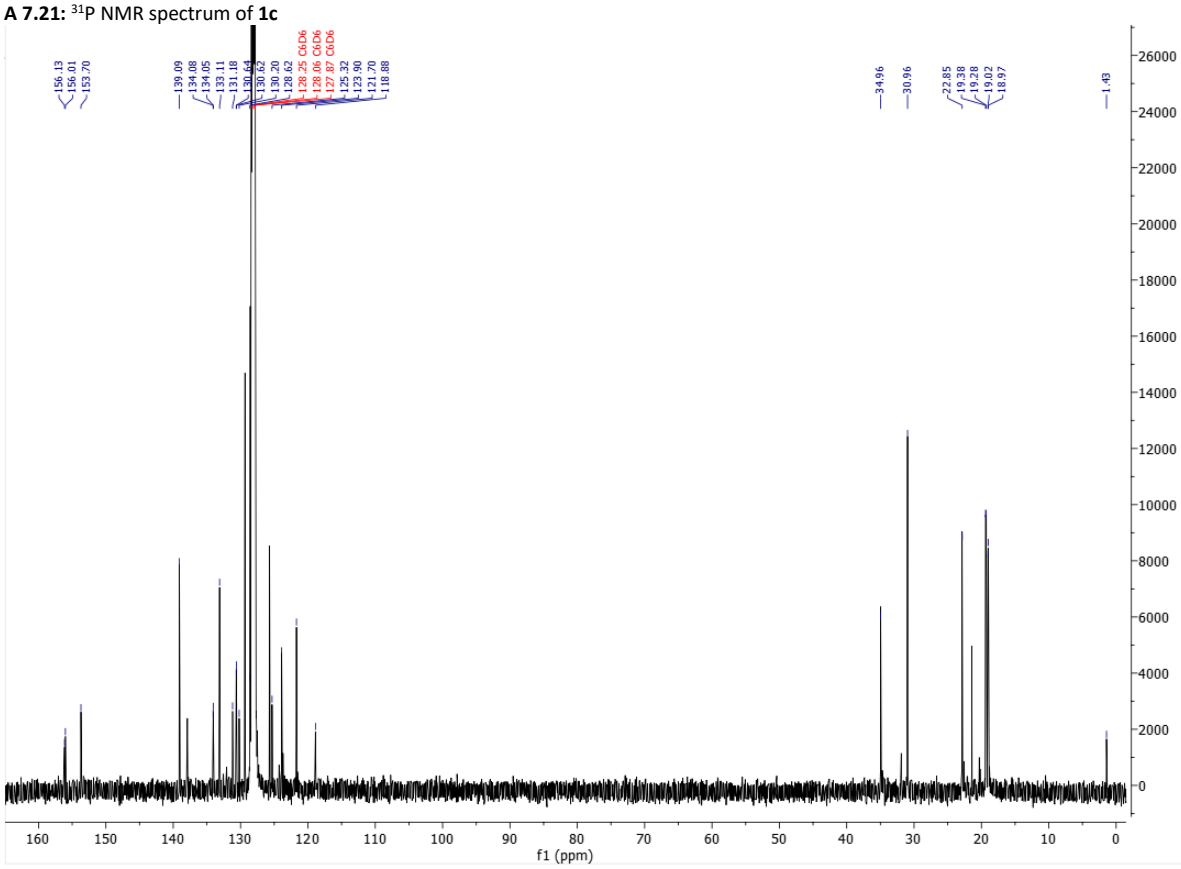
A 7.19: ^{7}Li NMR spectrum of **1c**



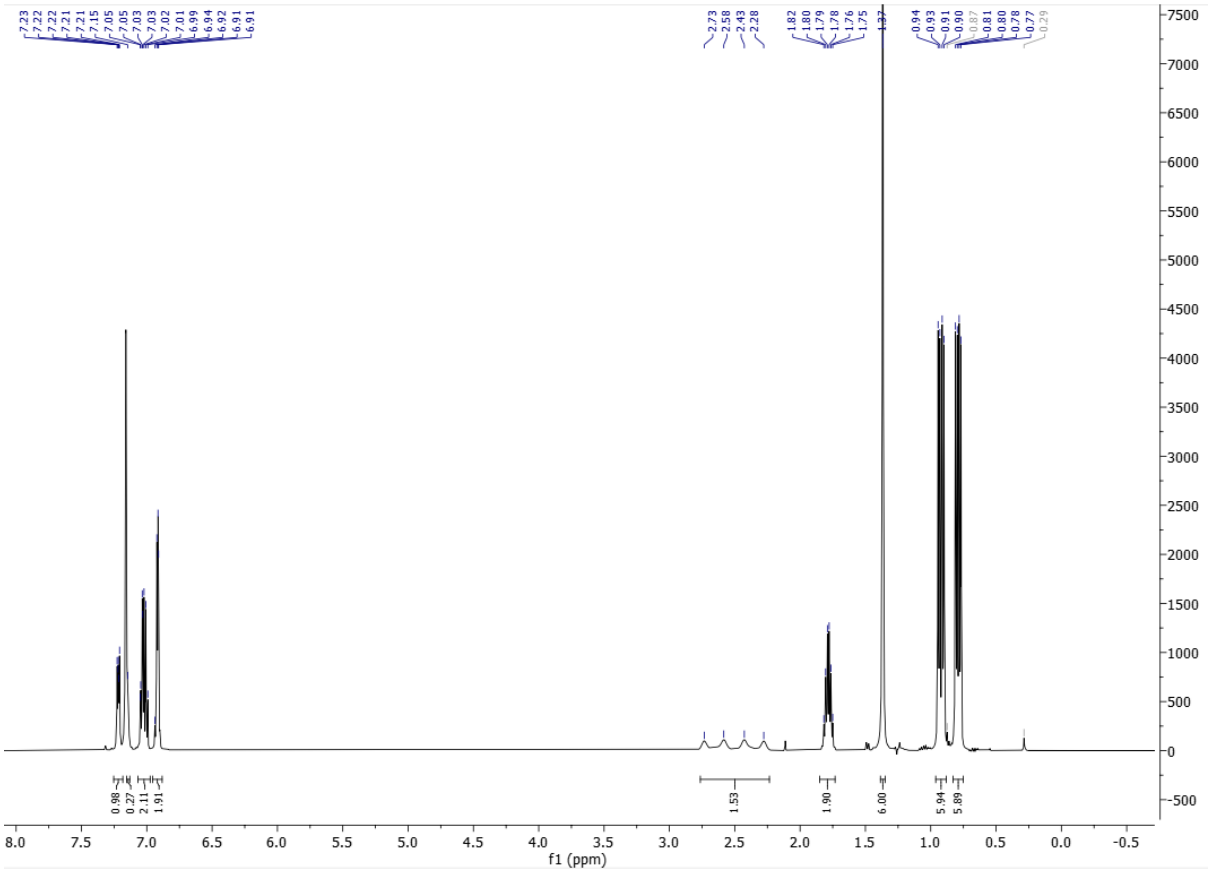
A 7.20: ^{11}B NMR spectrum of **1c**



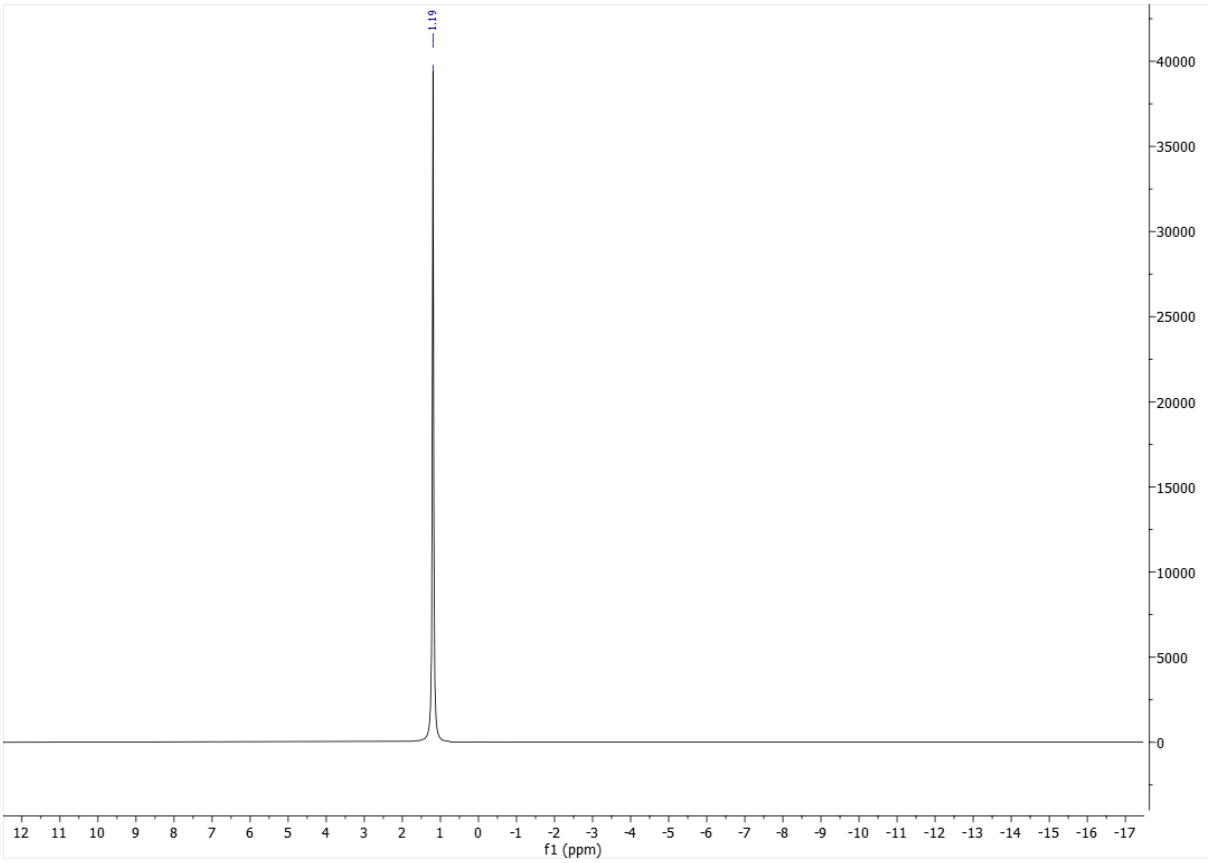
A 7.21: ^{31}P NMR spectrum of **1c**



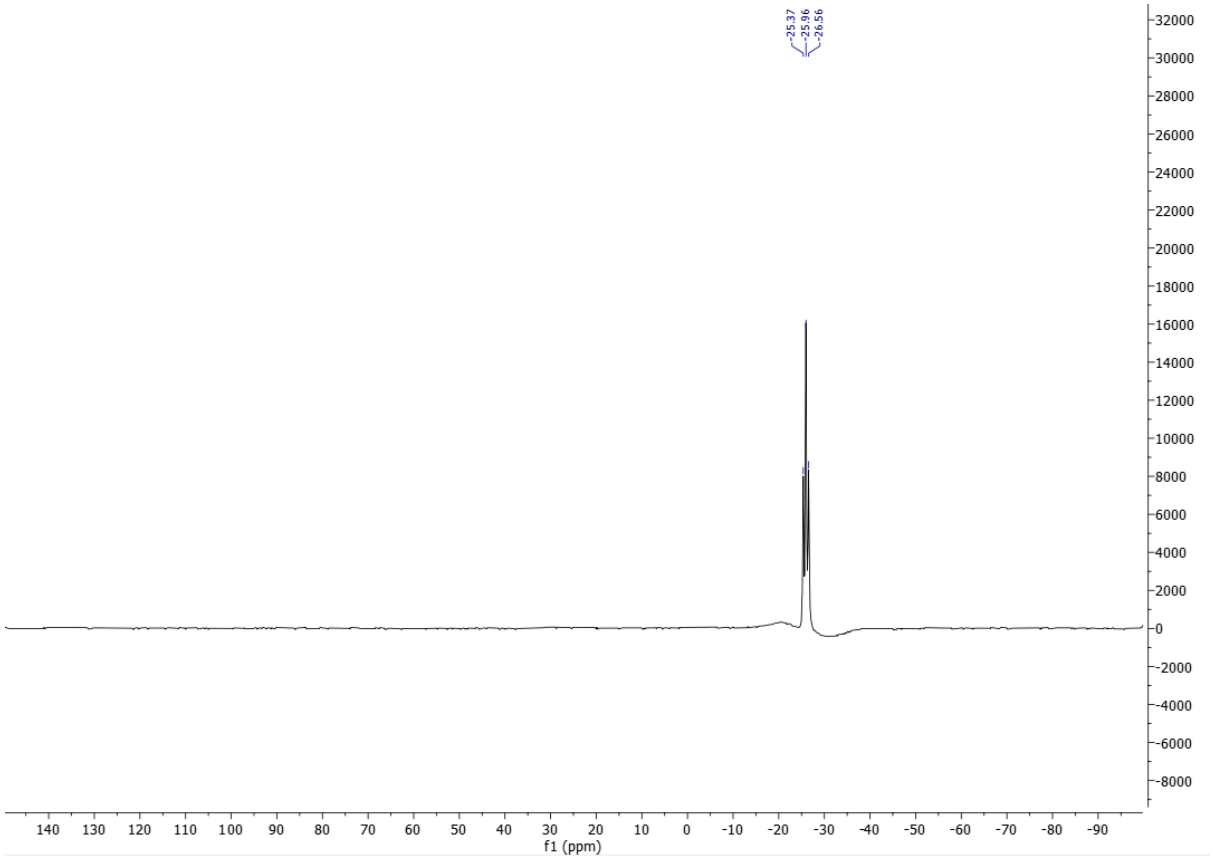
A 7.22: ^{13}C NMR spectrum of **1c**



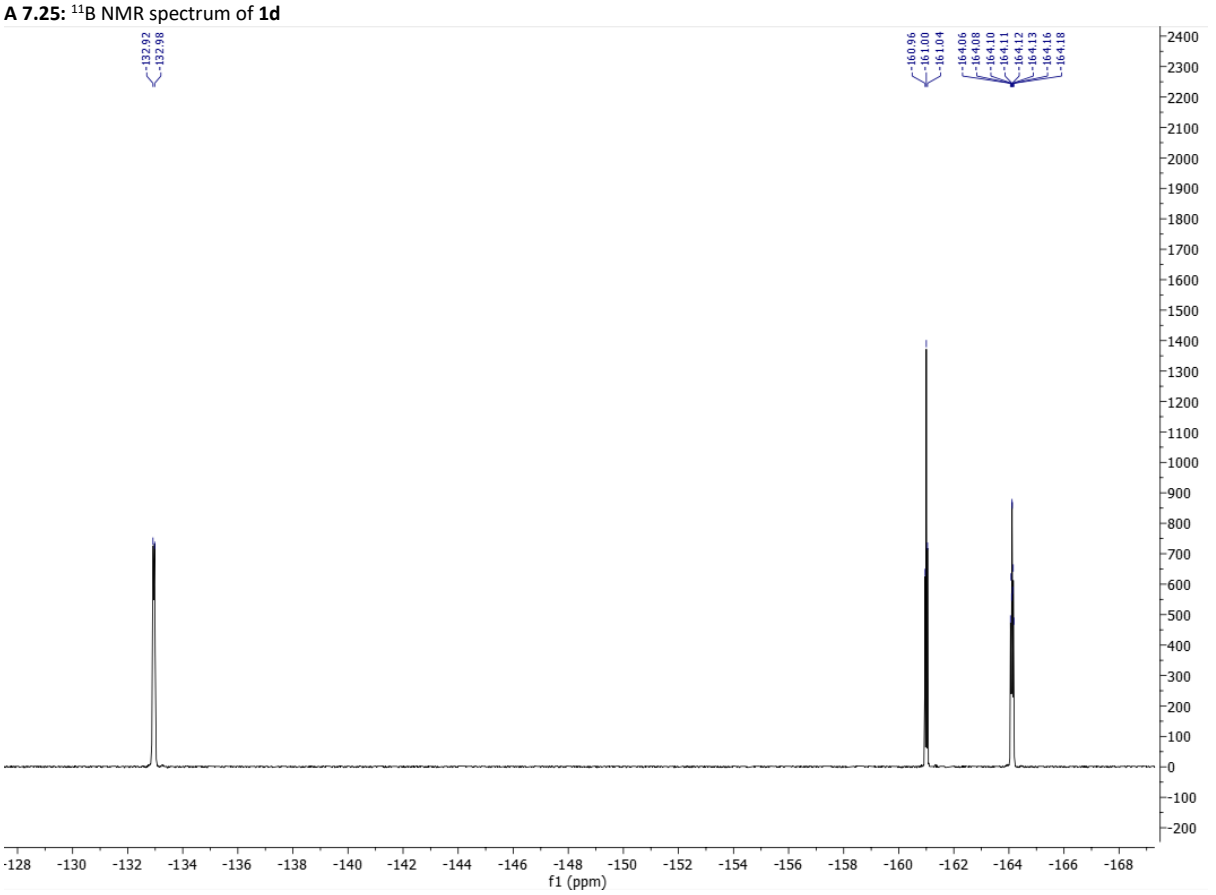
A 7.23: ^{1}H NMR spectrum of **1d**



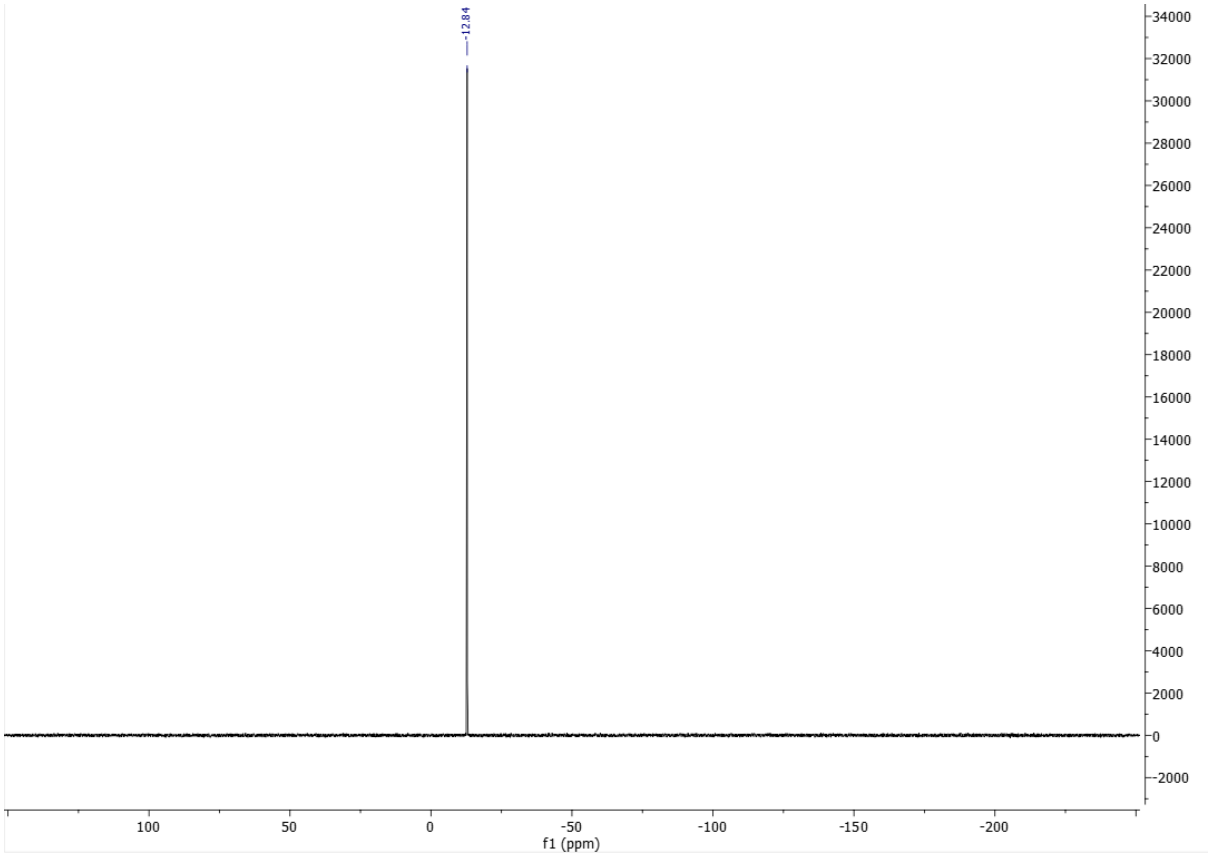
A 7.24: ^{7}Li NMR spectrum of **1d**



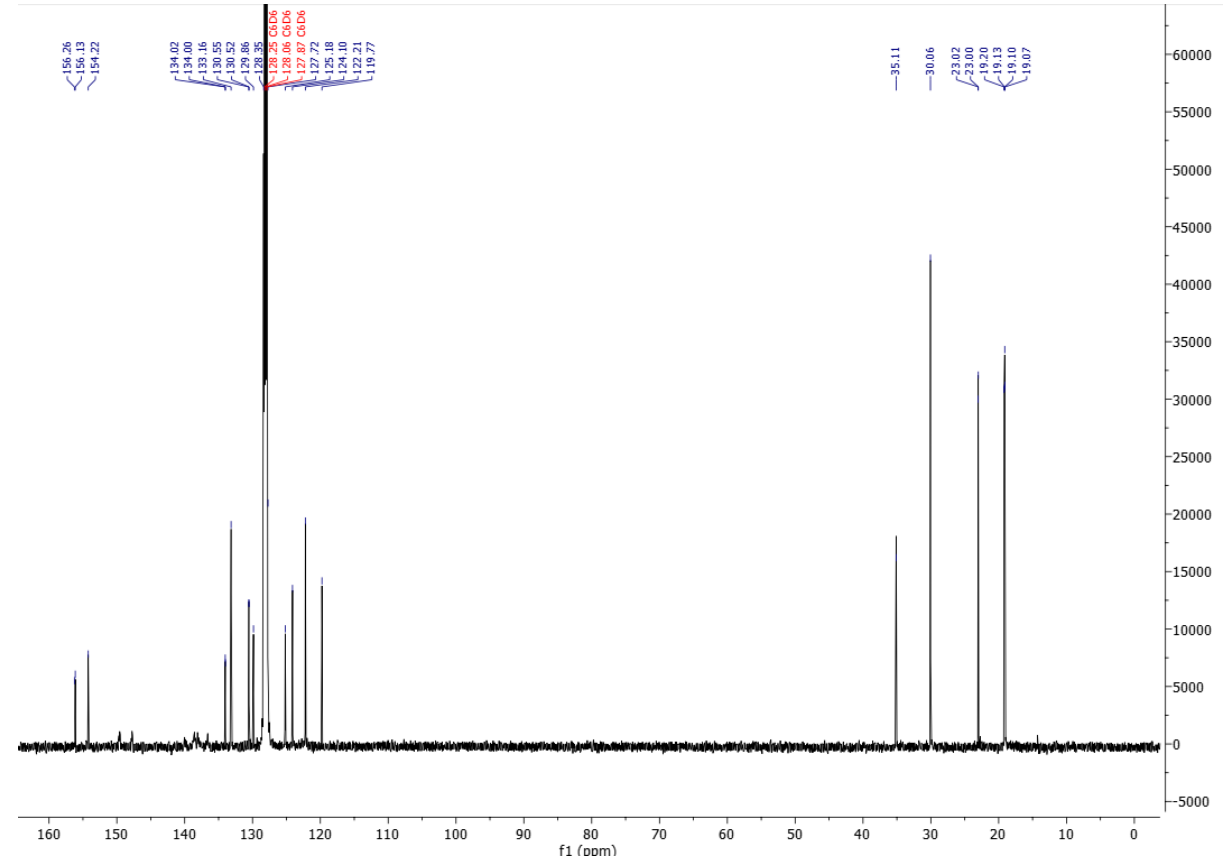
A 7.25: ^{11}B NMR spectrum of **1d**



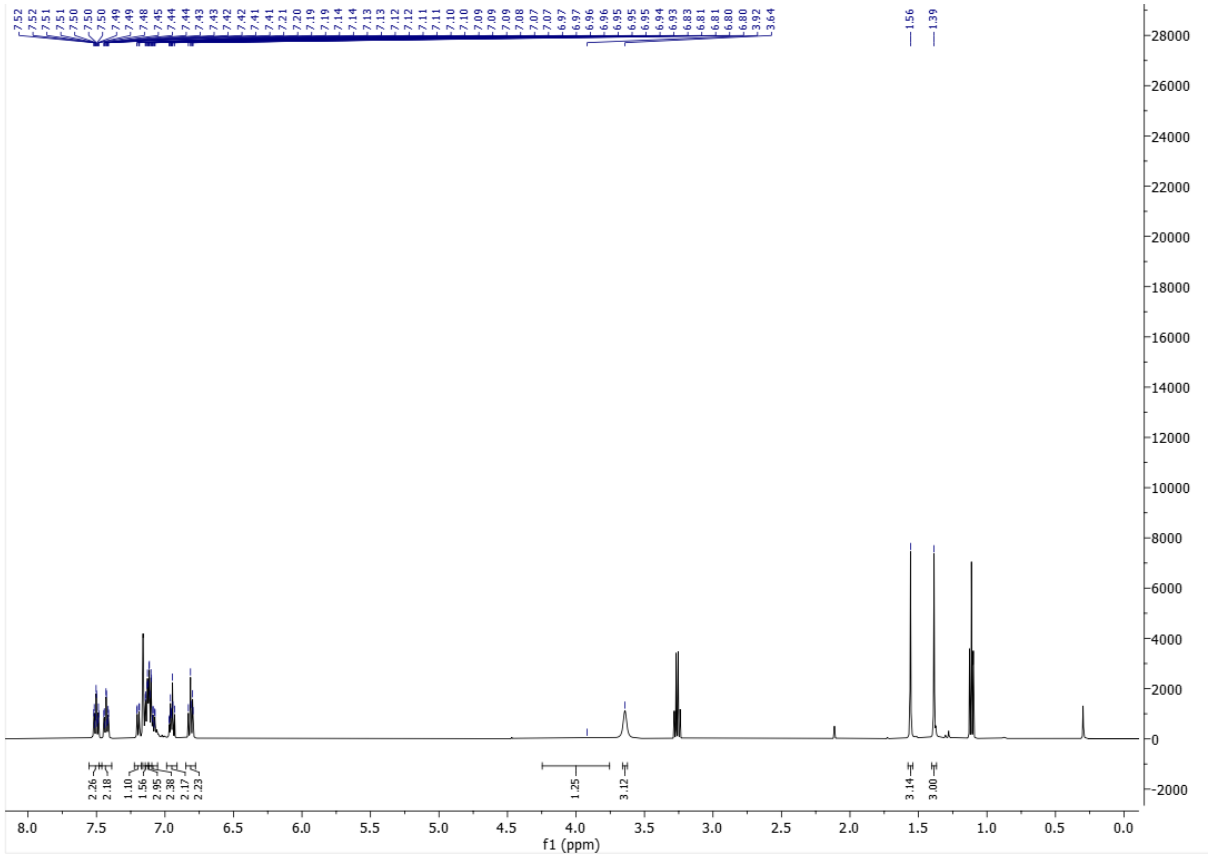
A 7.26: ^{19}F NMR spectrum of **1d**



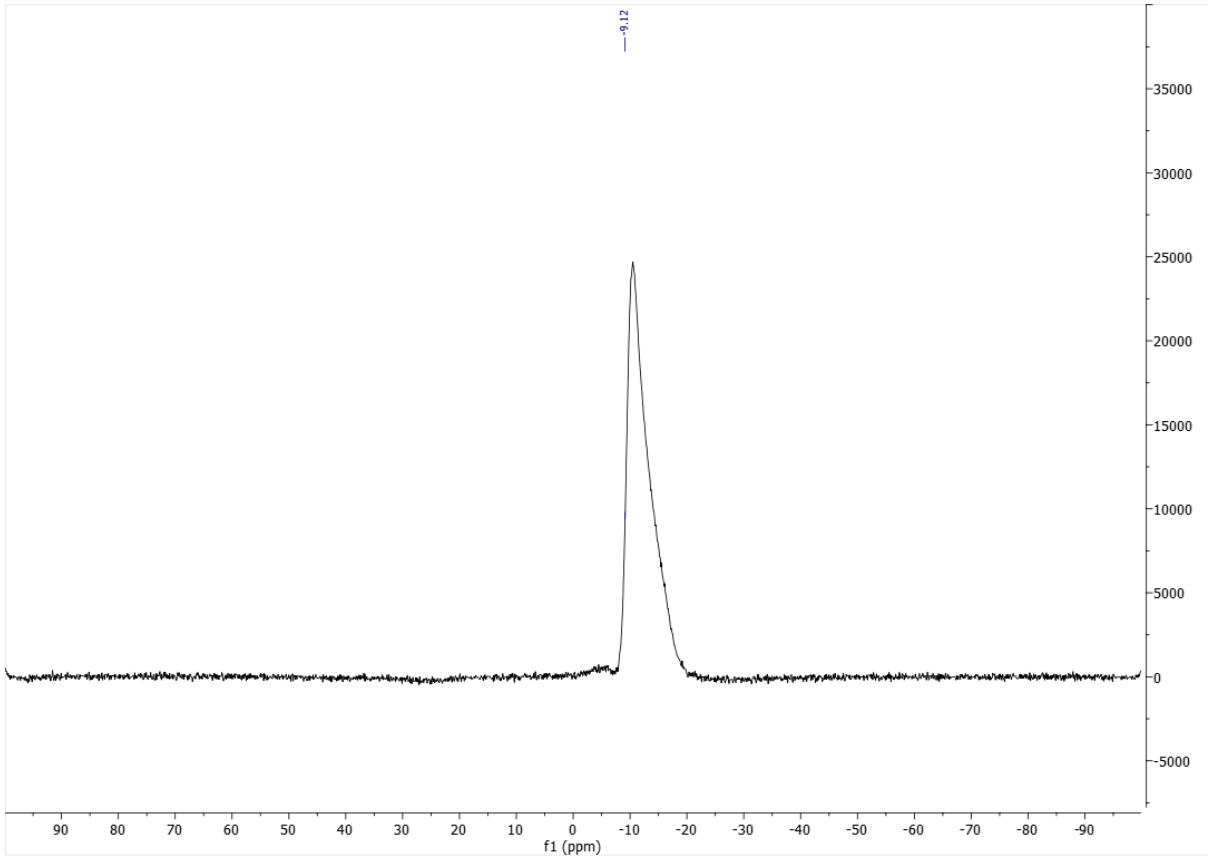
A 7.27: ^{31}P NMR spectrum of **1d**



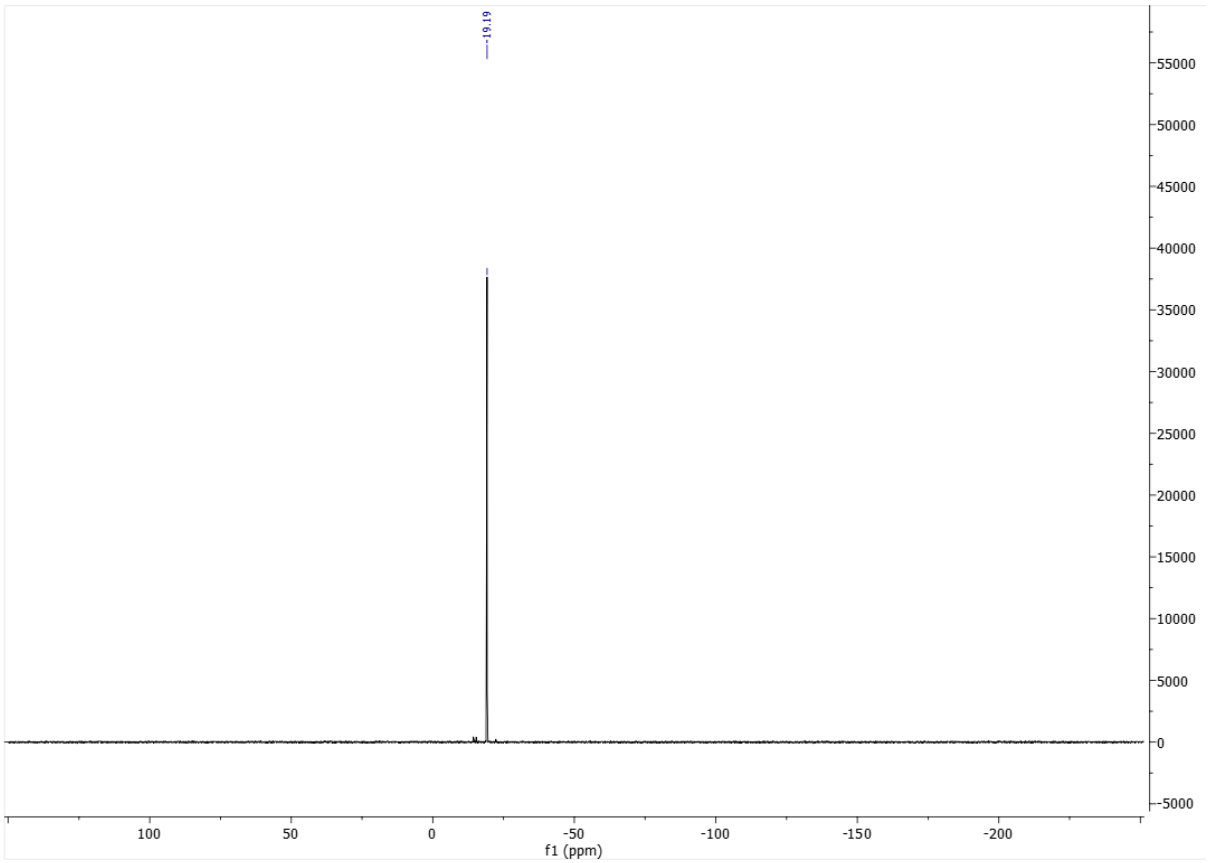
A 7.28: ^{13}C NMR spectrum of **1d**



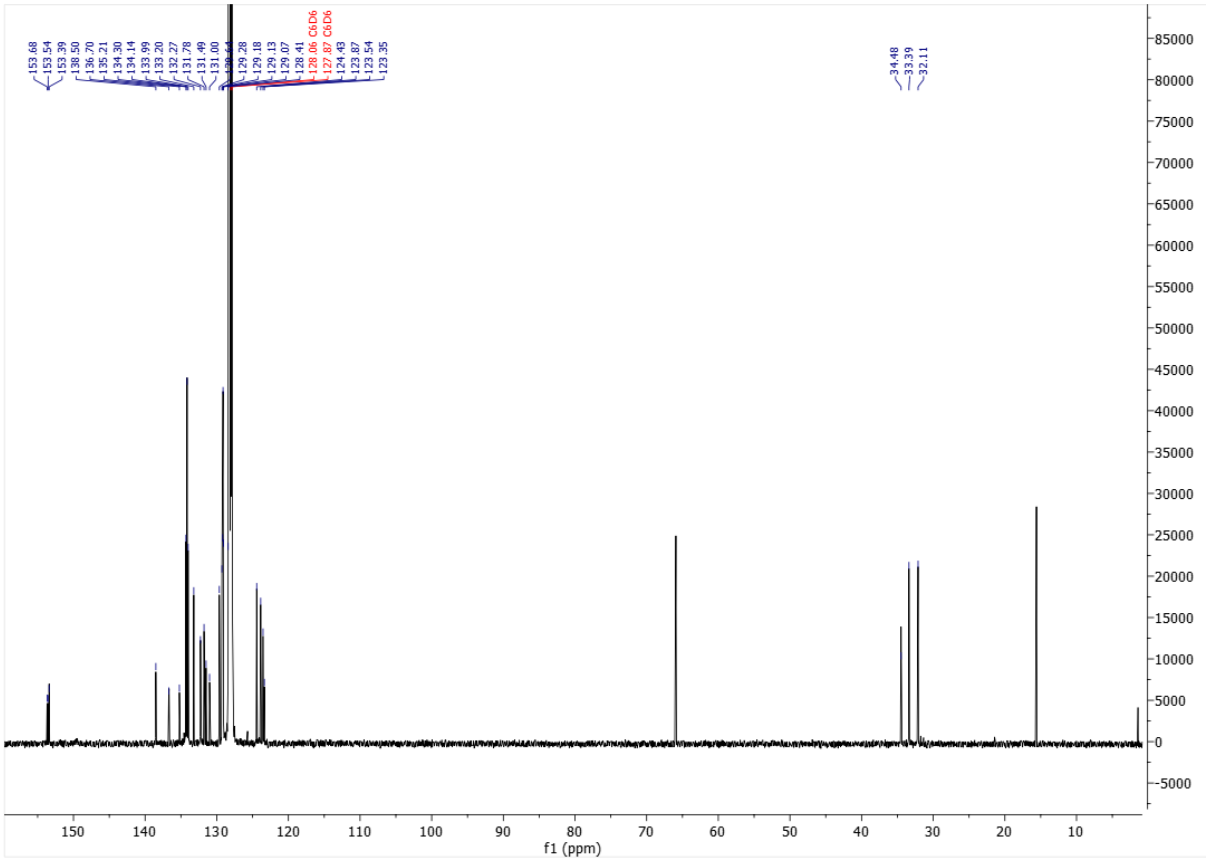
A 7.29: ^{1}H NMR spectrum of **4a**



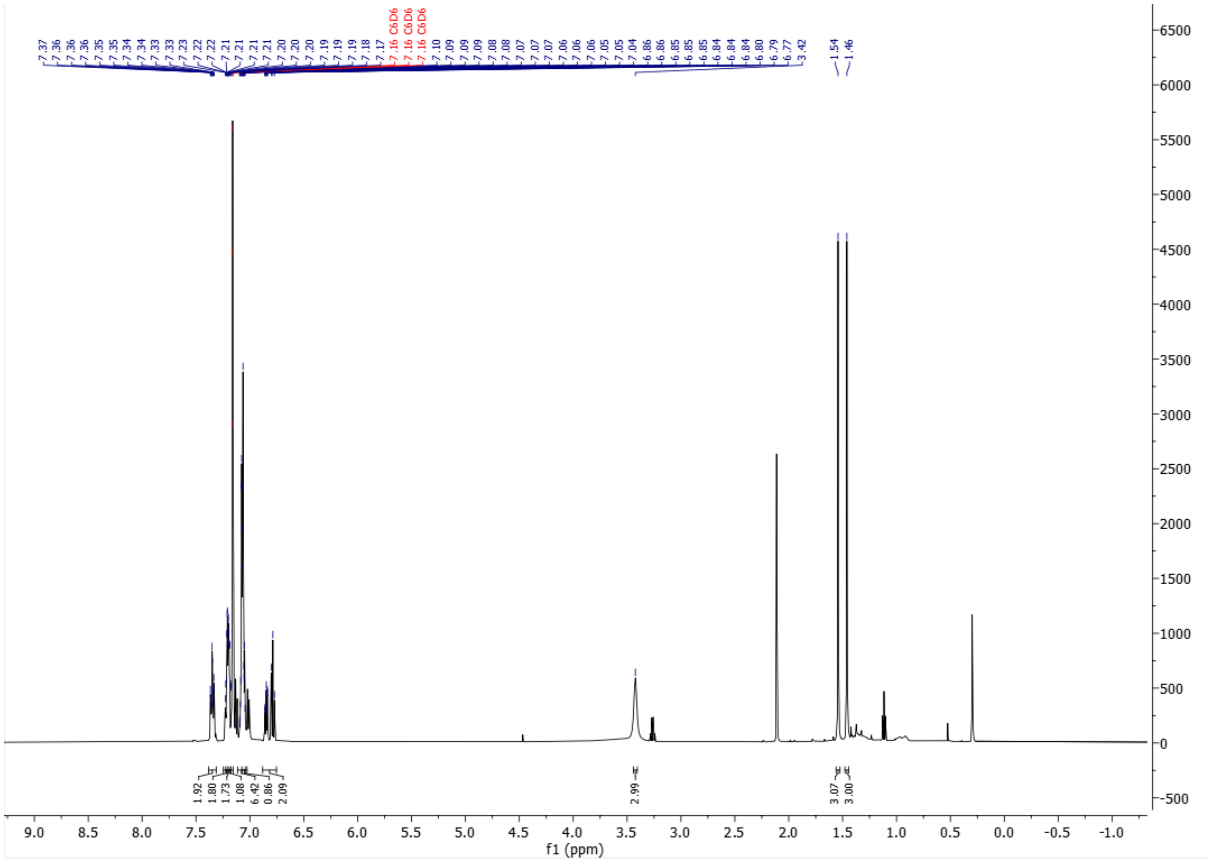
A 7.30: ^{11}B NMR spectrum of **4a**



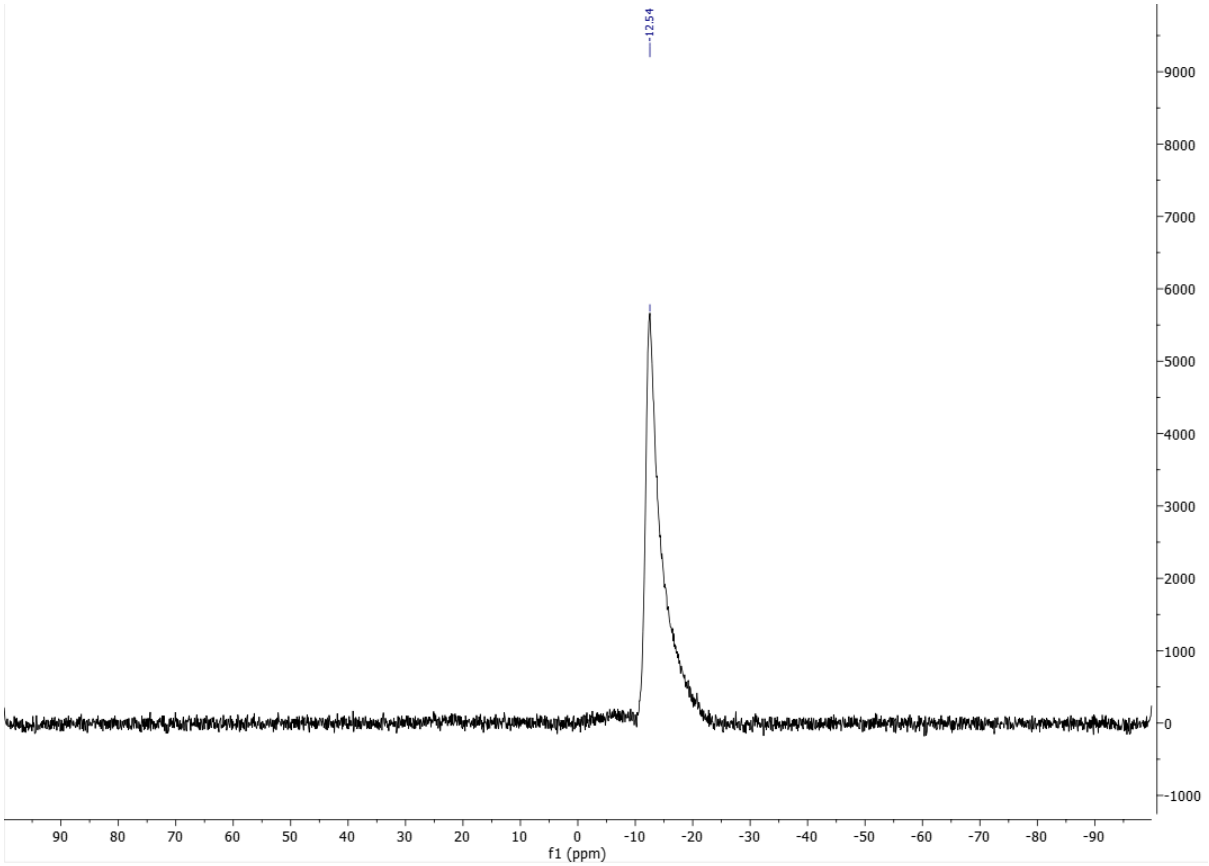
A 7.31: ^{31}P NMR spectrum of **4a**



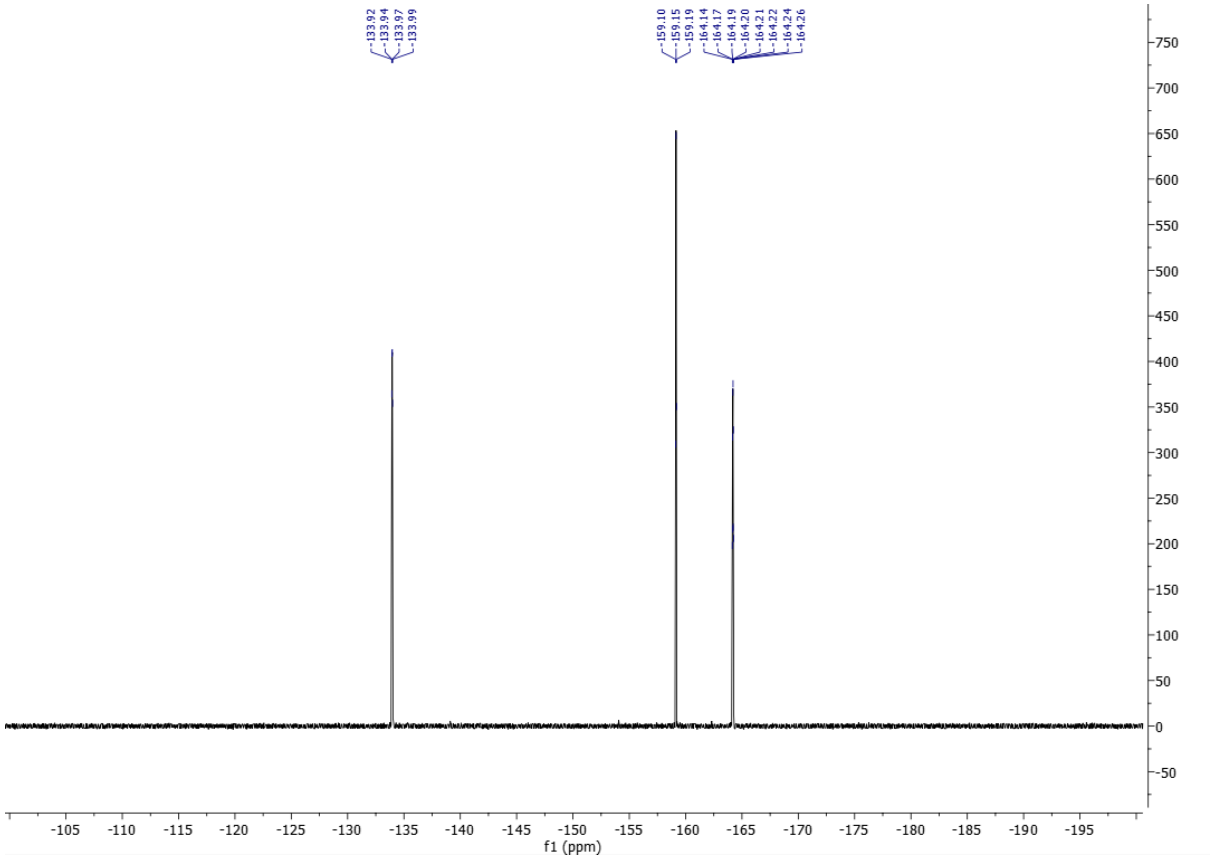
A 7.32: ^{13}C NMR spectrum of **4a**



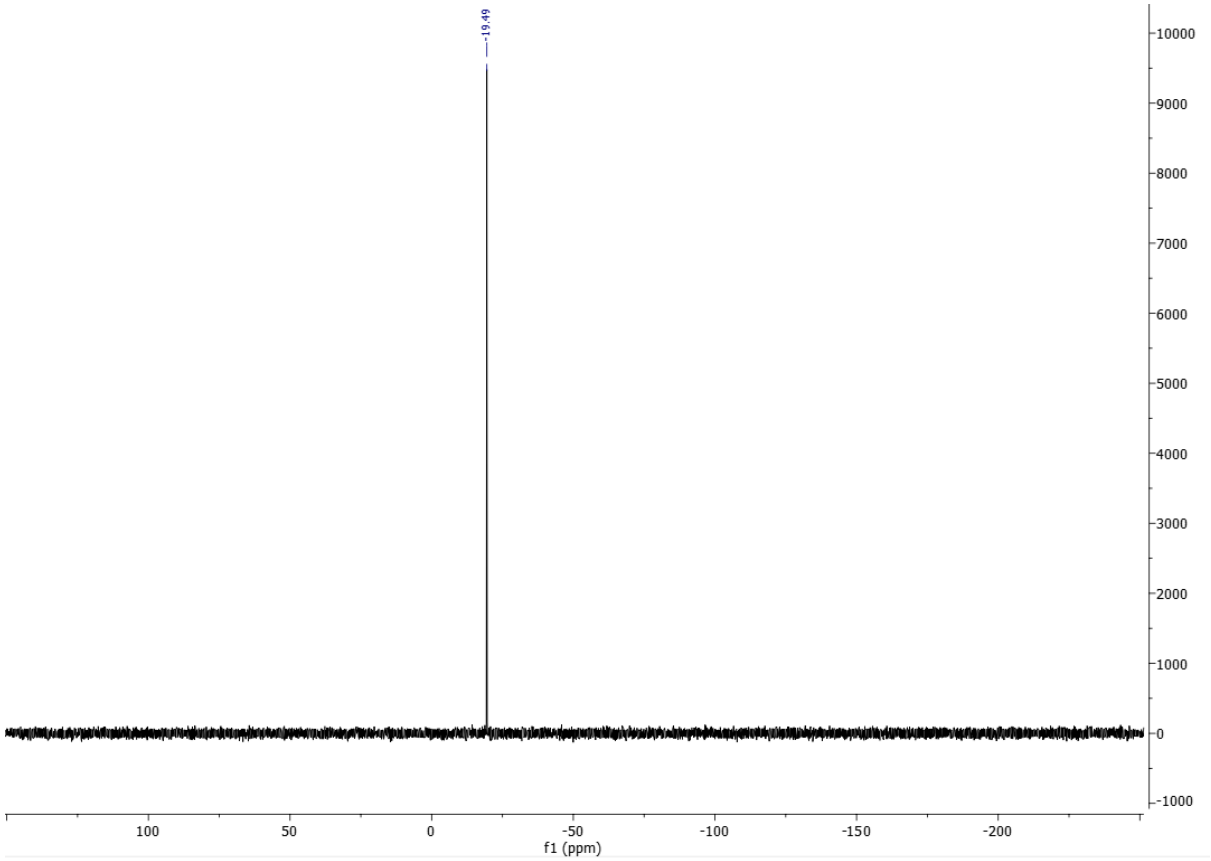
A 7.33: ^{1}H NMR spectrum of **4b**



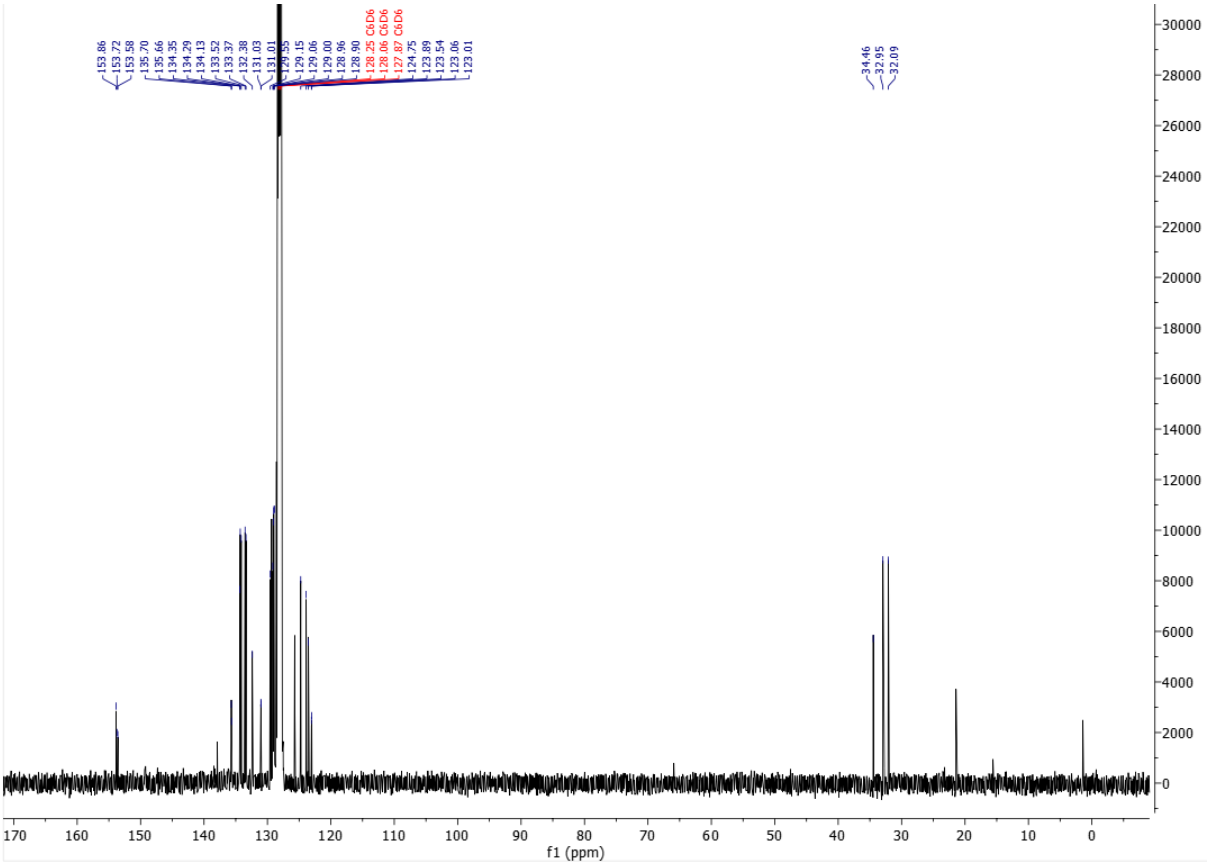
A 7.34: ^{11}B NMR spectrum of **4b**



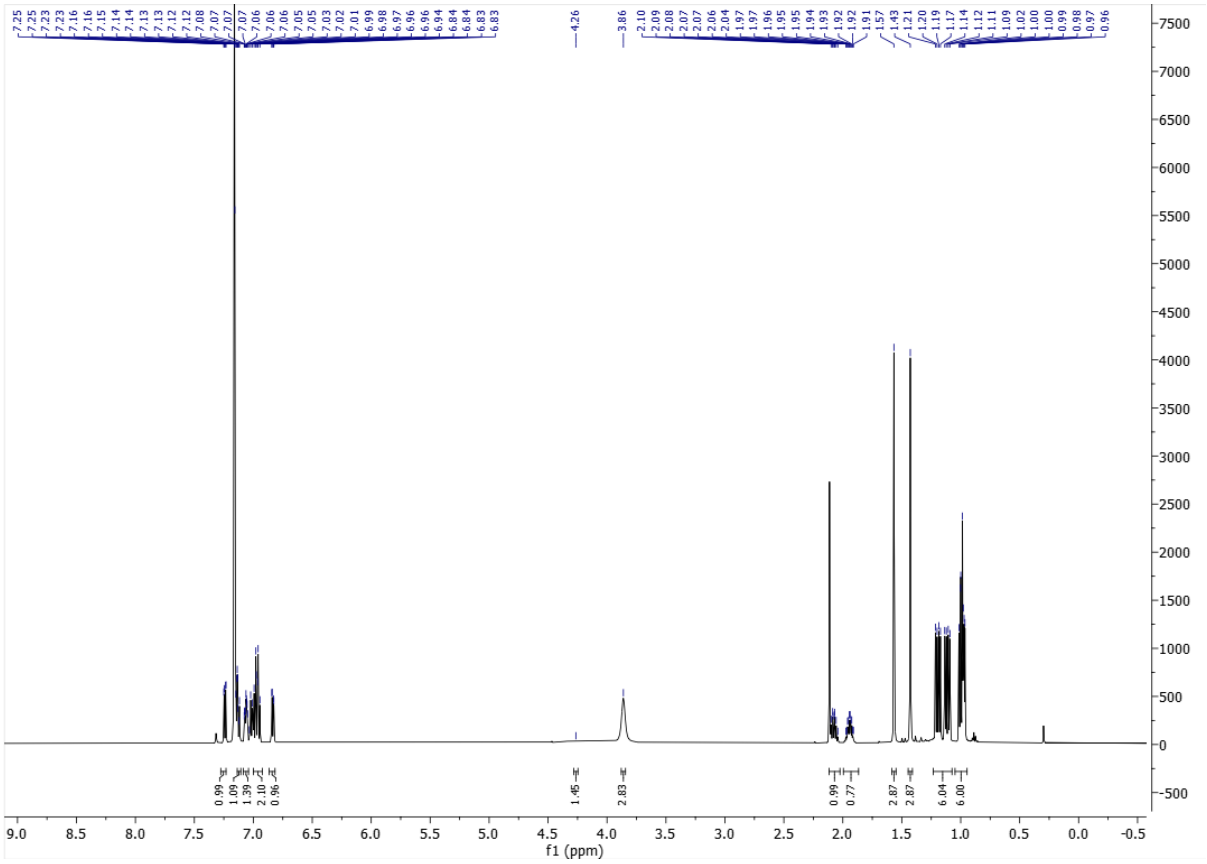
A 7.35: ^{19}F NMR spectrum of **4b**



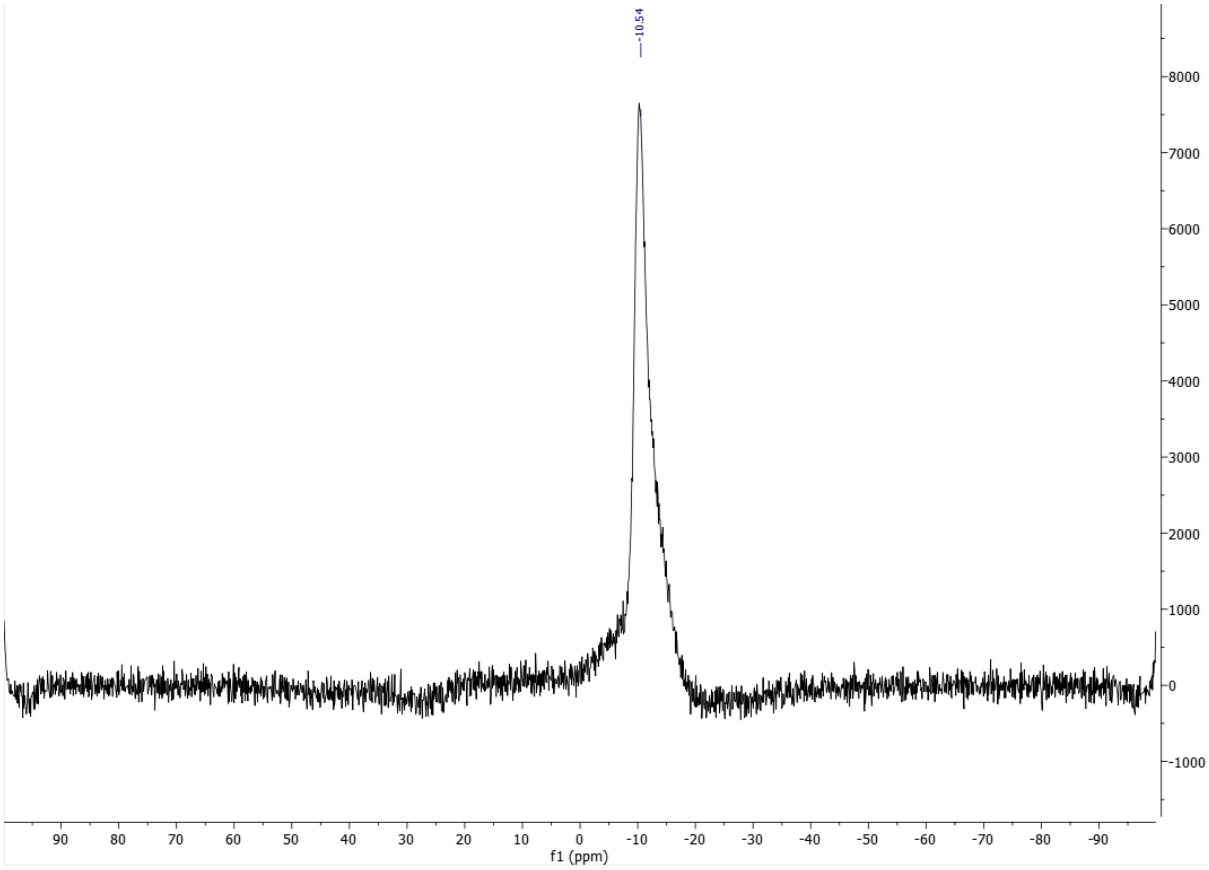
A 7.36: ^{31}P NMR spectrum of **4b**



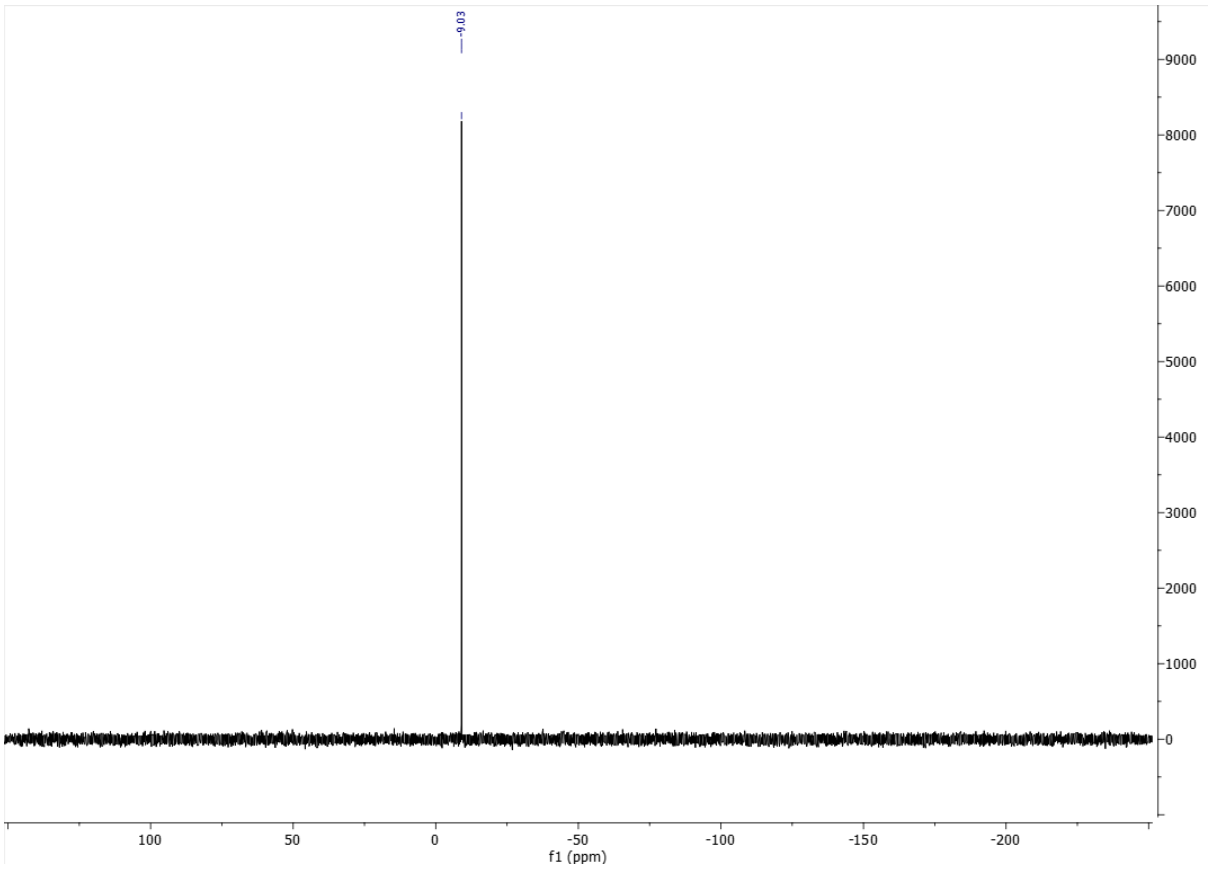
A 7.37: ^{13}C NMR spectrum of **4b**



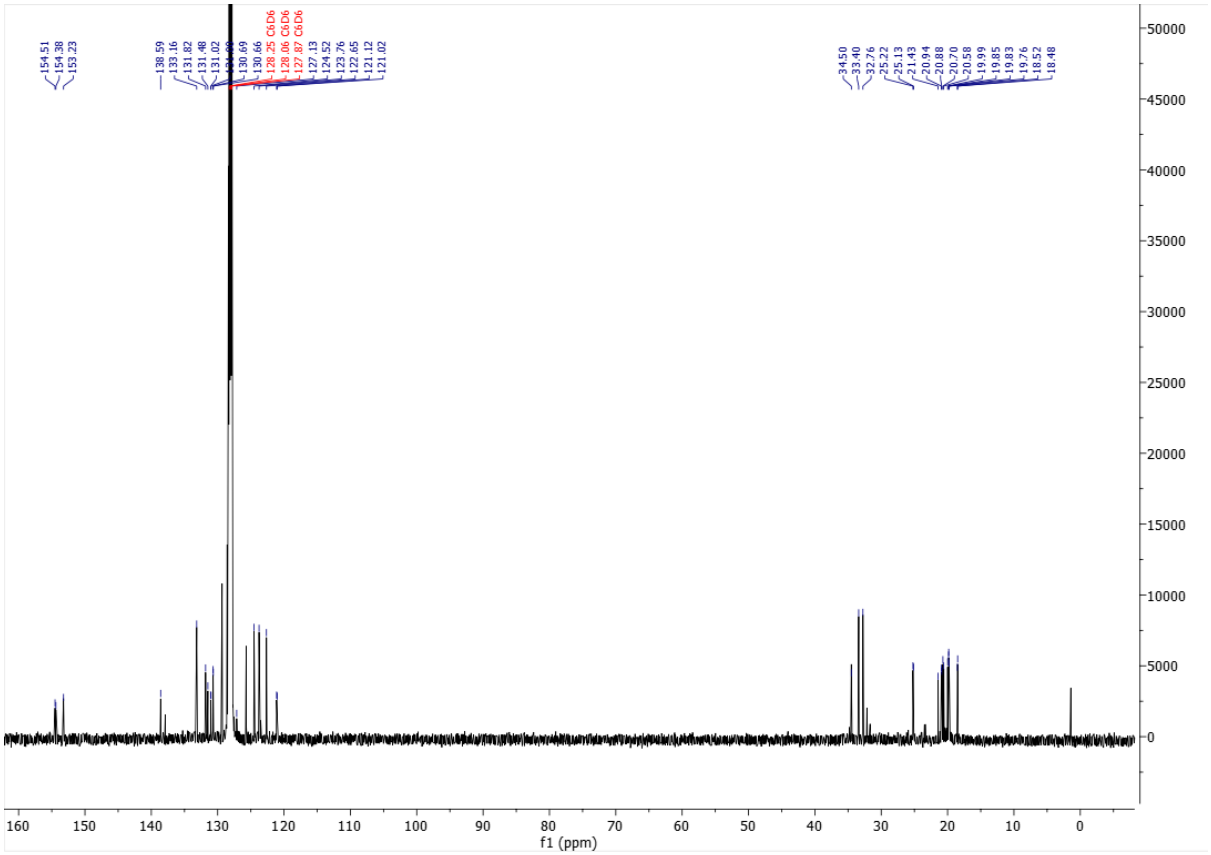
A 7.38: ^{1}H NMR spectrum of **4c**



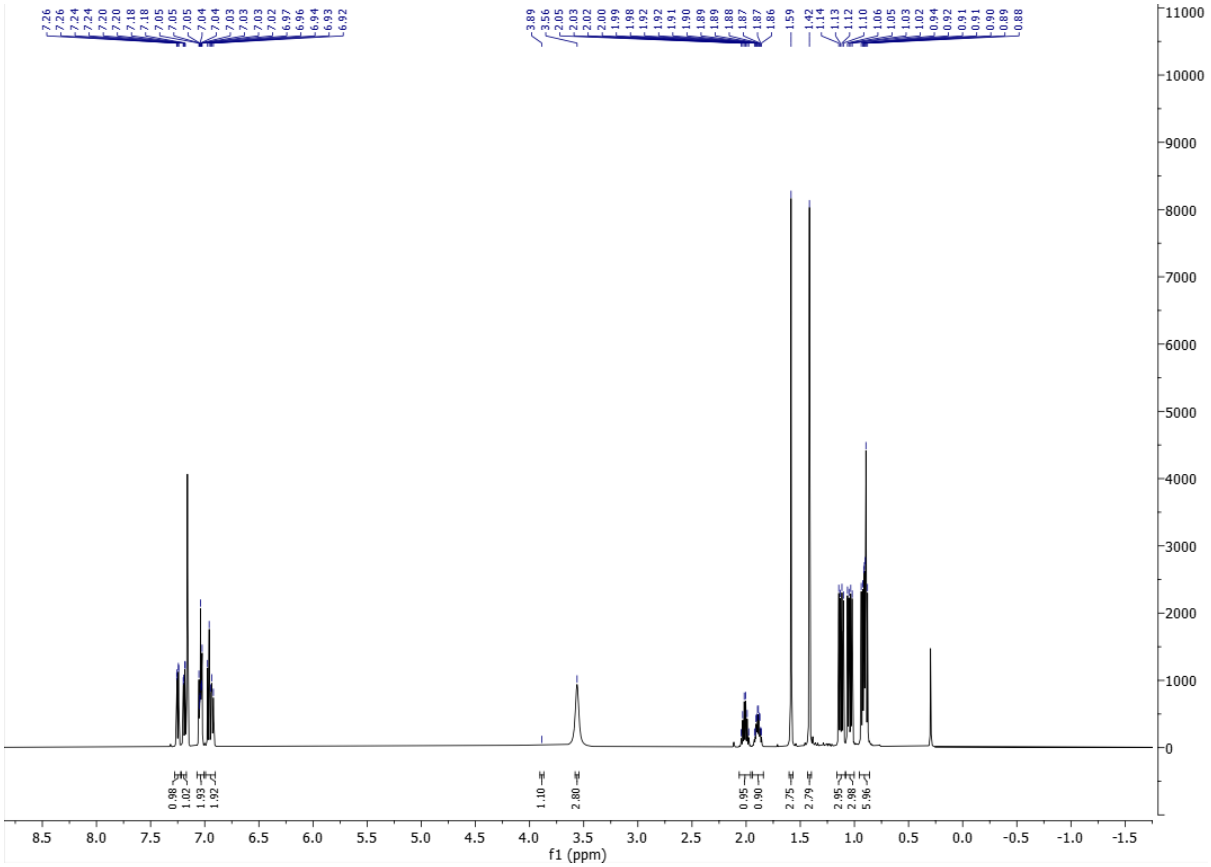
A 7.39: ^{11}B NMR spectrum of **4c**



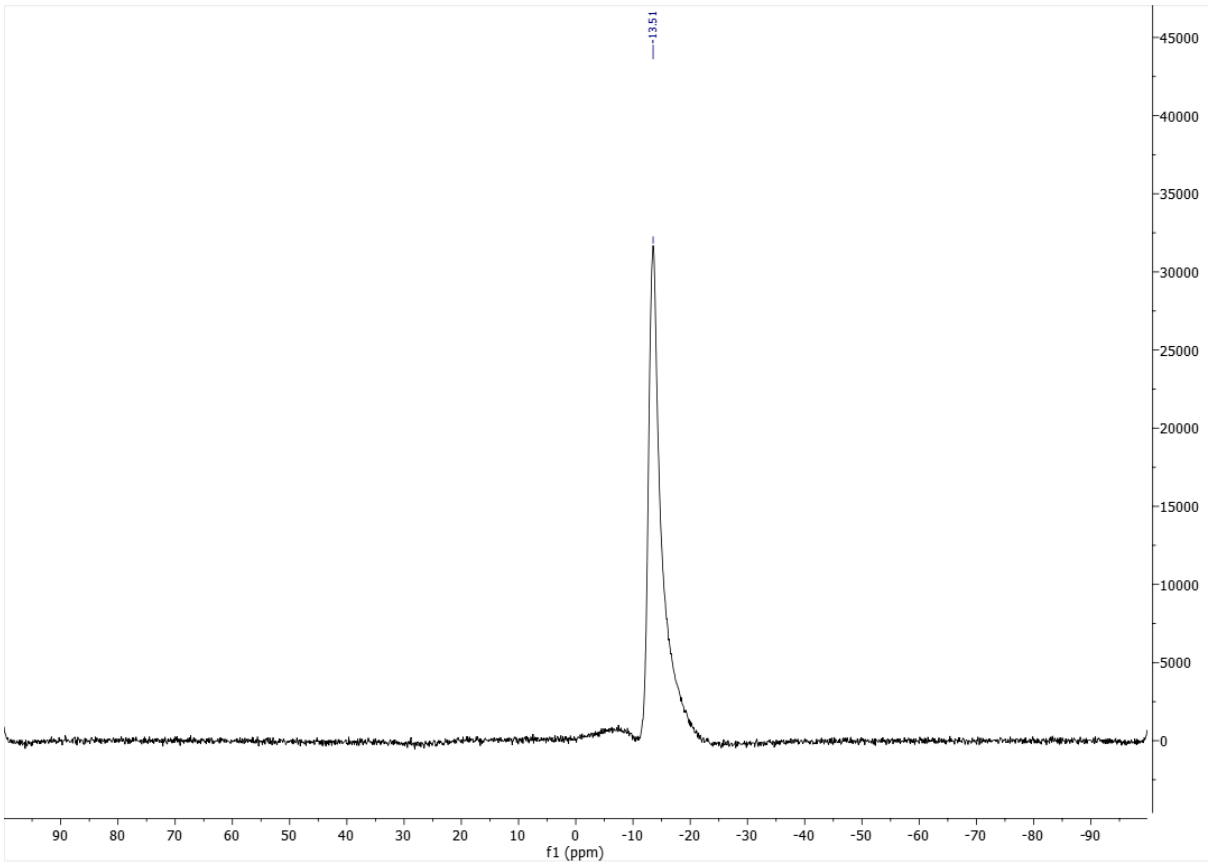
A 7.40: ^{31}P NMR spectrum of **4c**



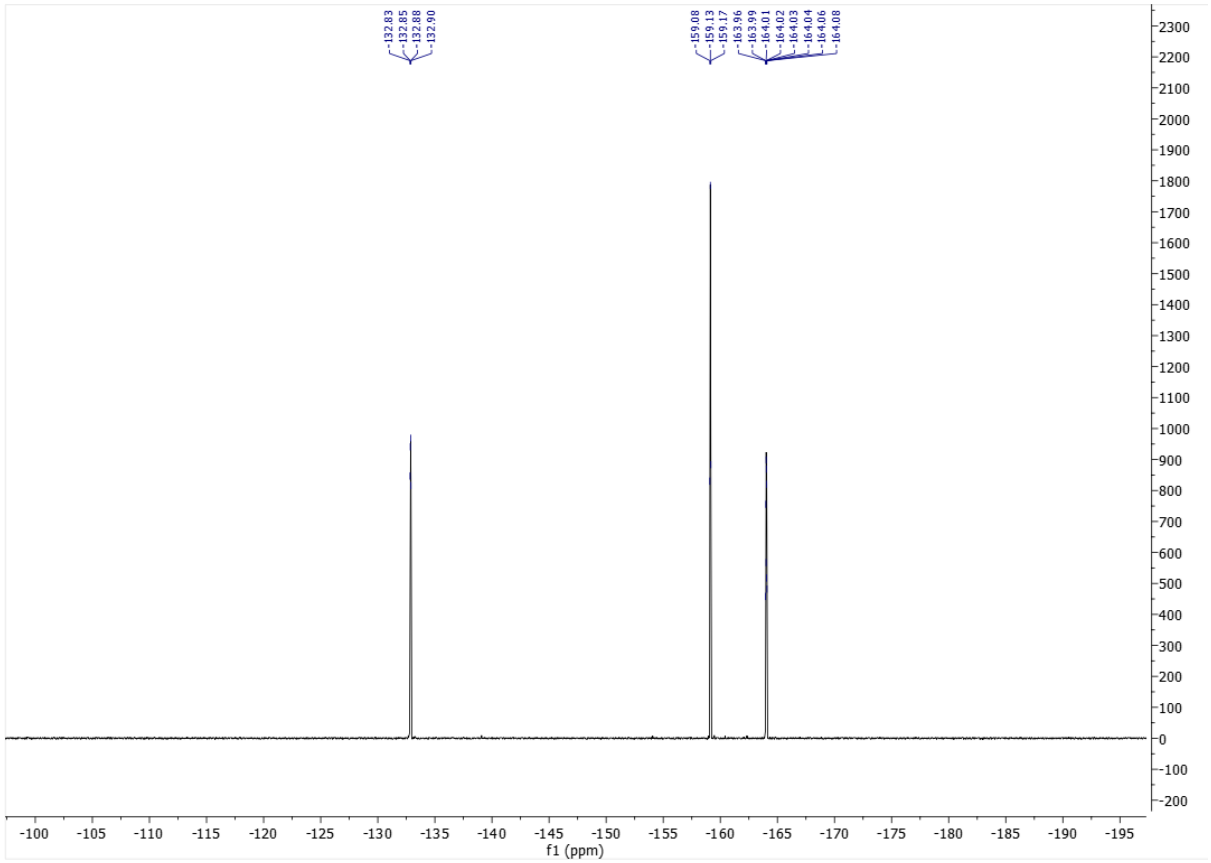
A 7.41: ^{13}C NMR spectrum of **4c**



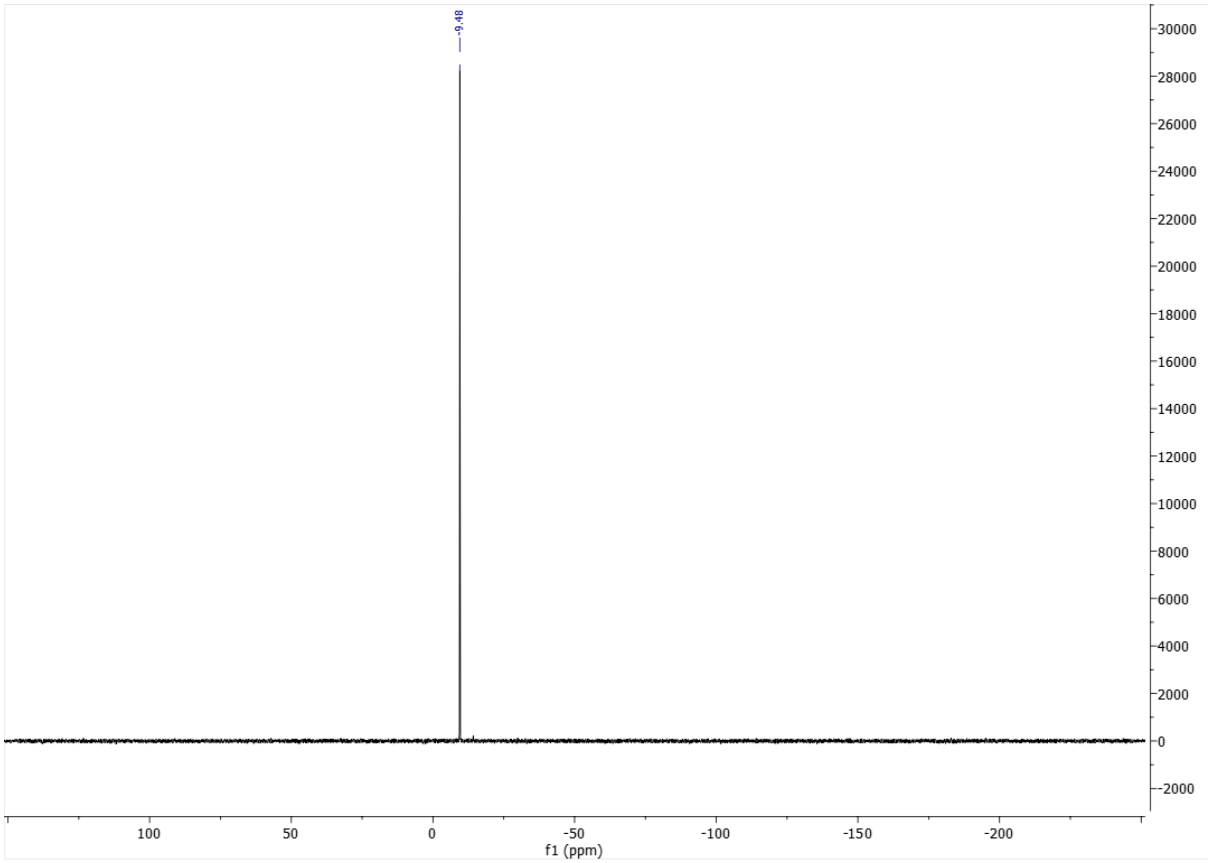
A 7.42: ^{1}H NMR spectrum of **4d**



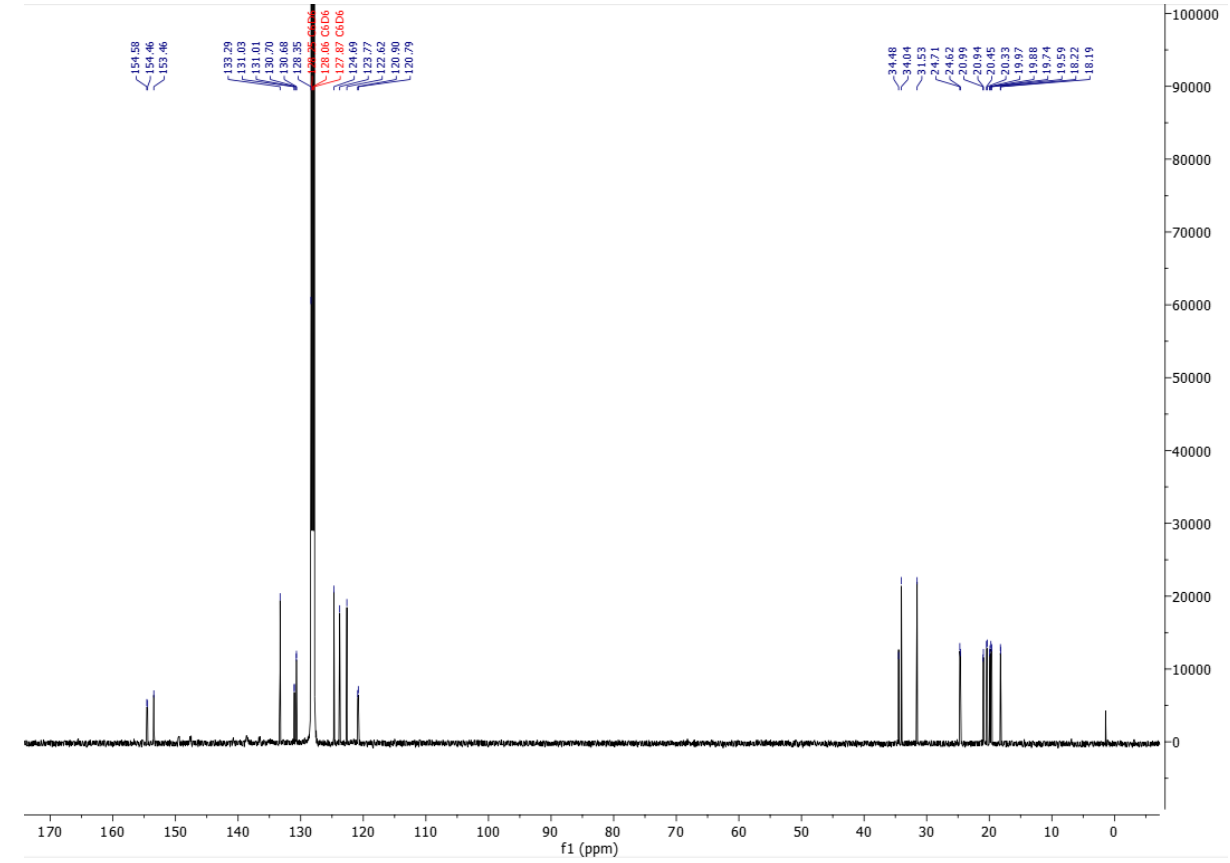
A 7.43: ^{11}B NMR spectrum of **4d**



A 7.44: ^{19}F NMR spectrum of **4d**

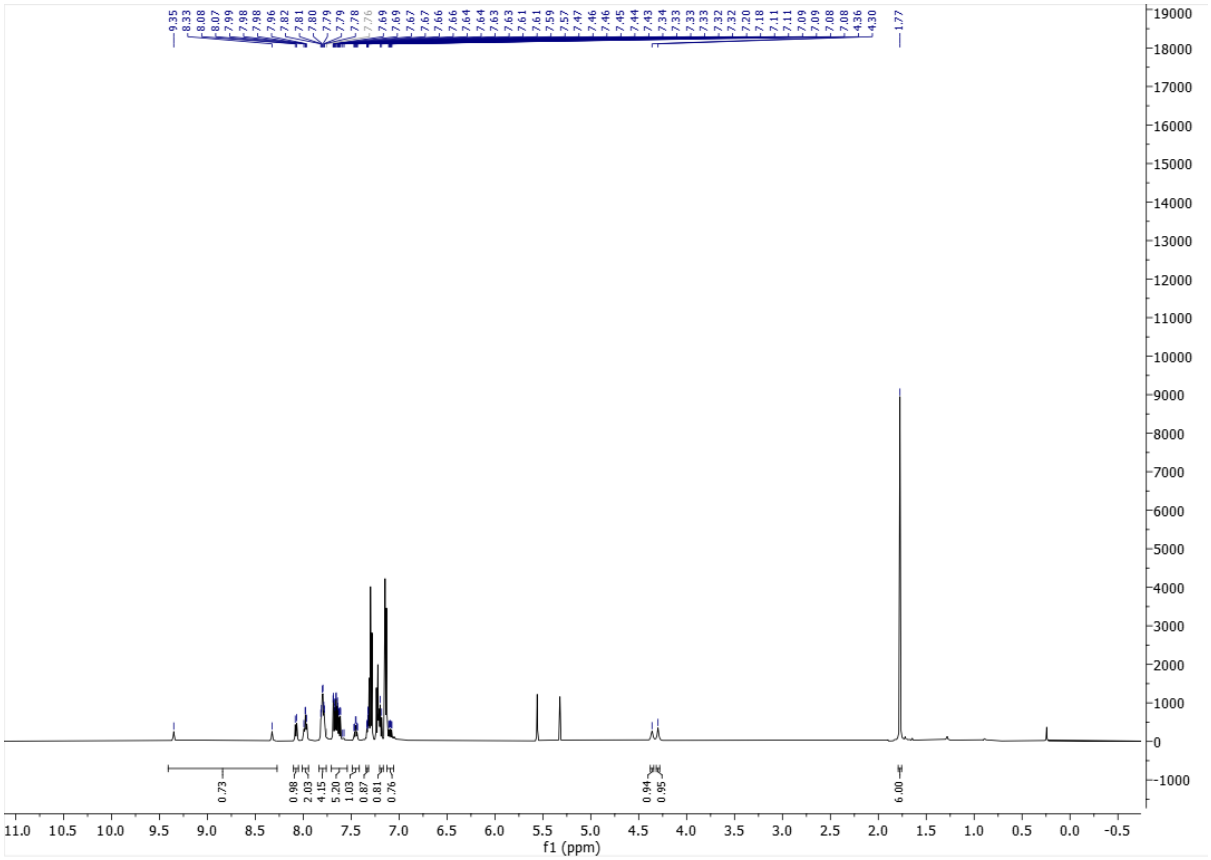


A 7.45: ^{31}P NMR spectrum of **4d**

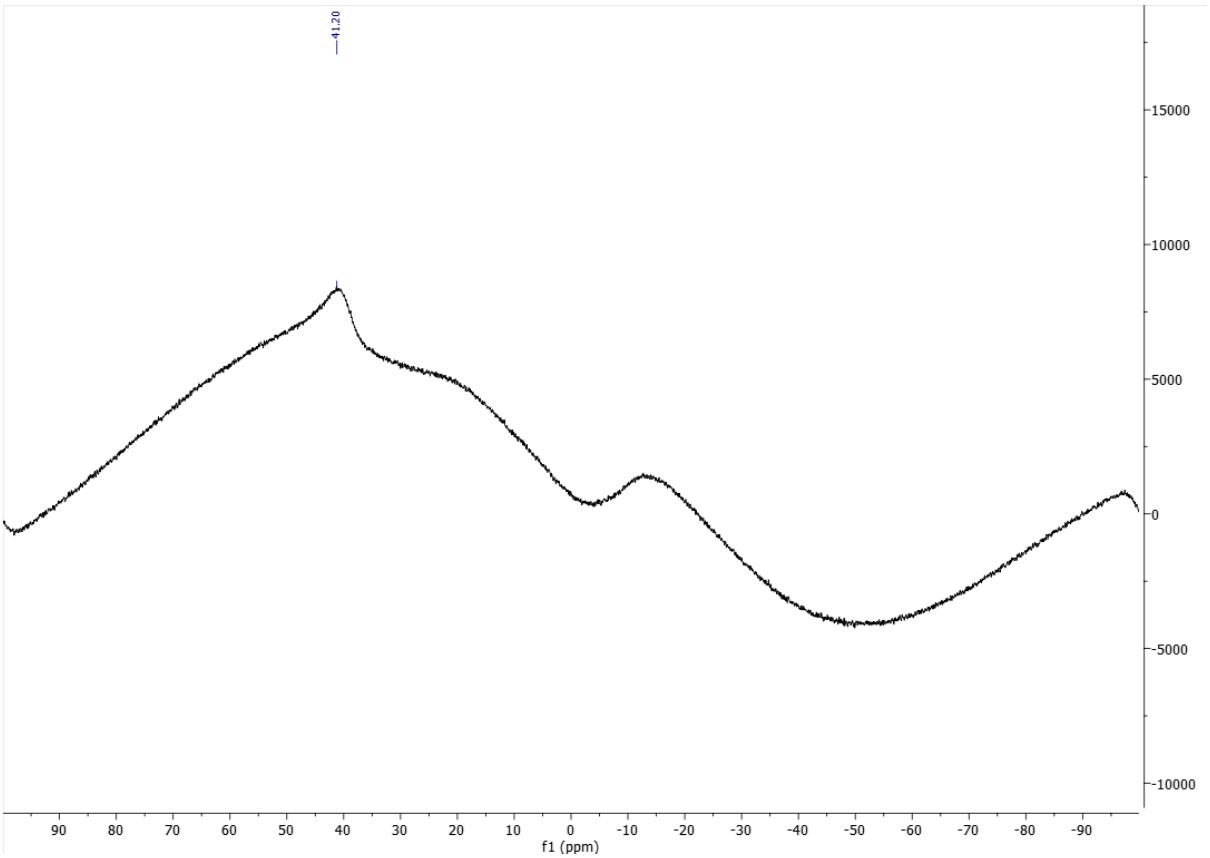


A 7.46: ^{13}C NMR spectrum of **4d**

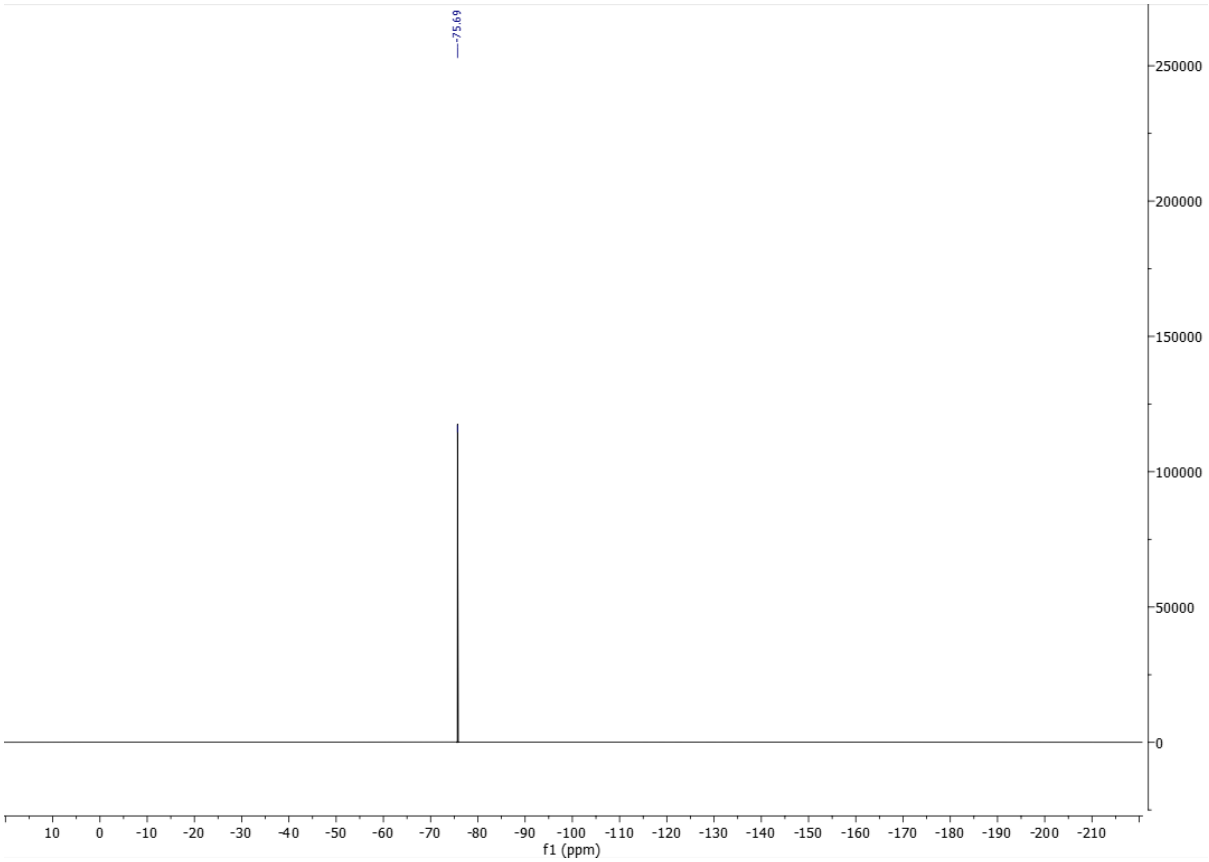
5a-d



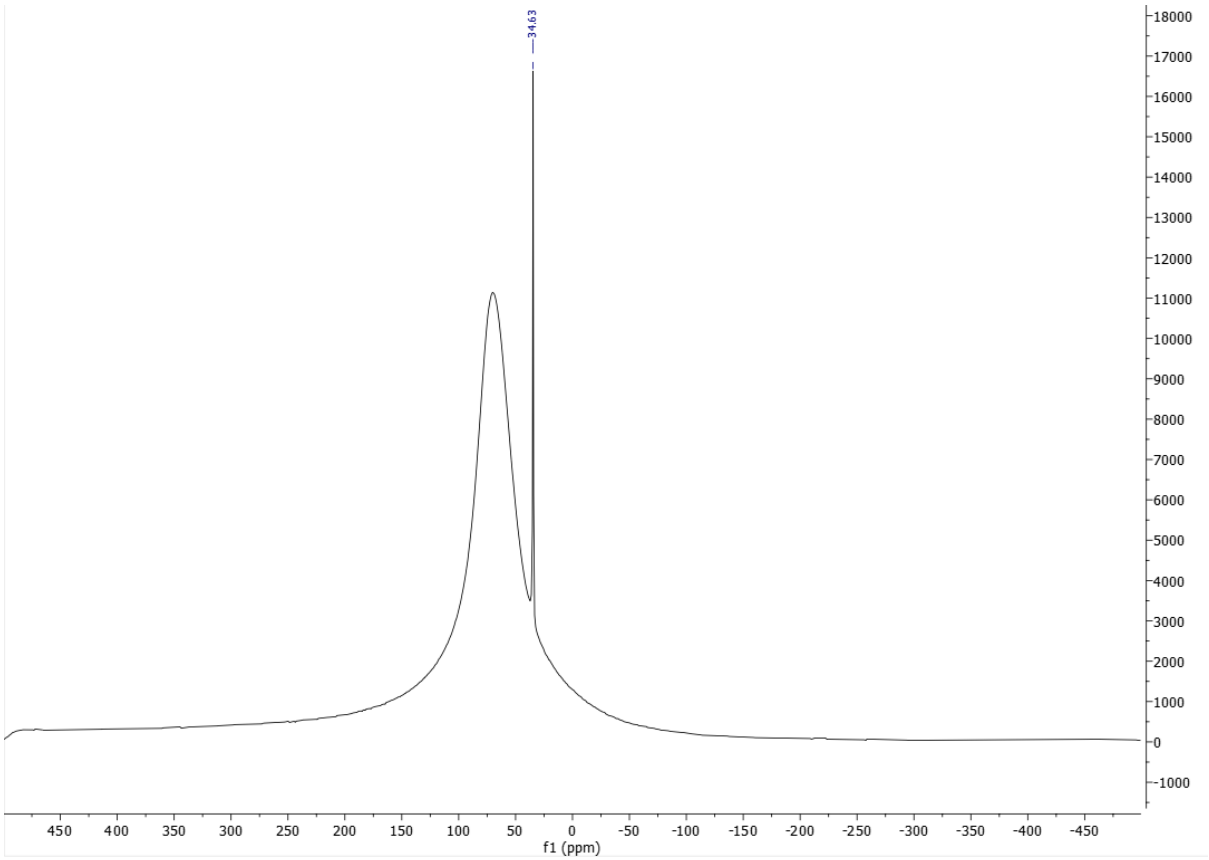
A 7.47: ^{1}H NMR spectrum of **5a**



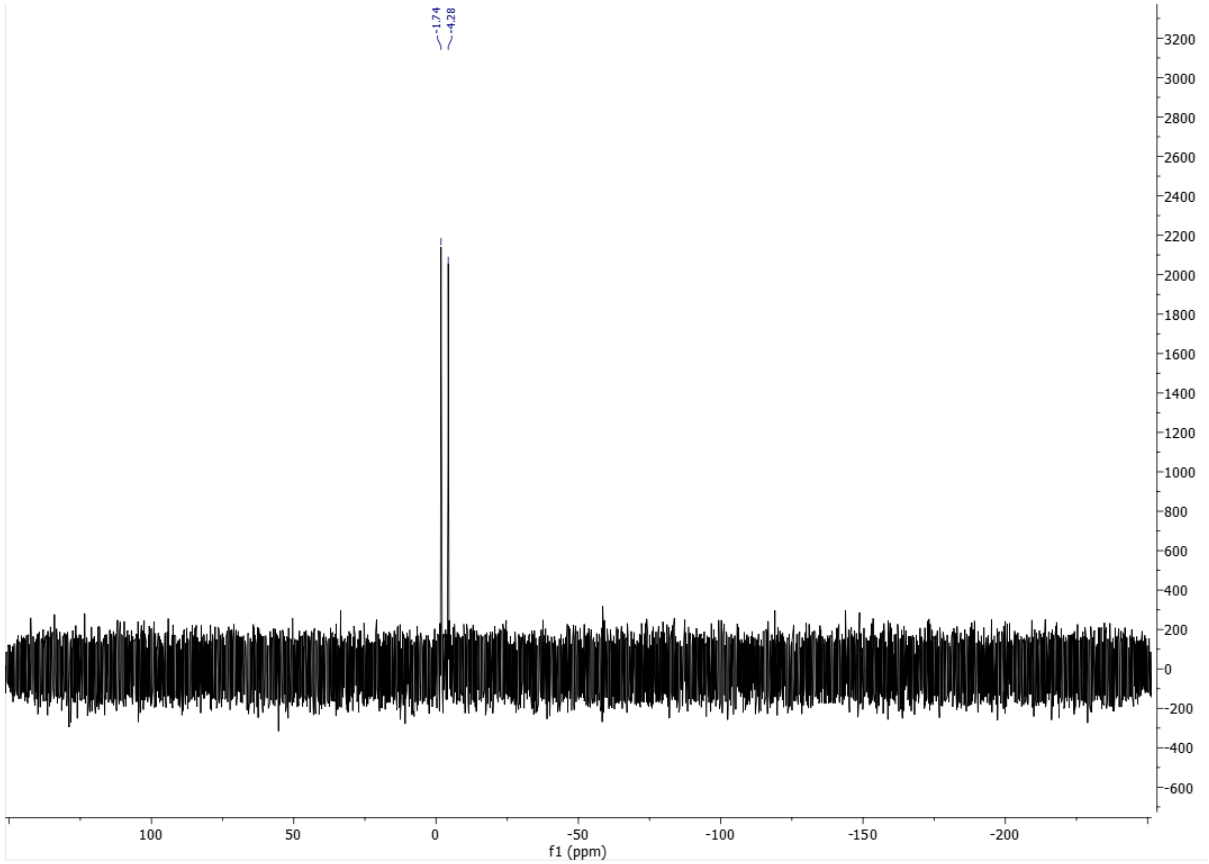
A 7.48: ^{11}B NMR spectrum of **5a**



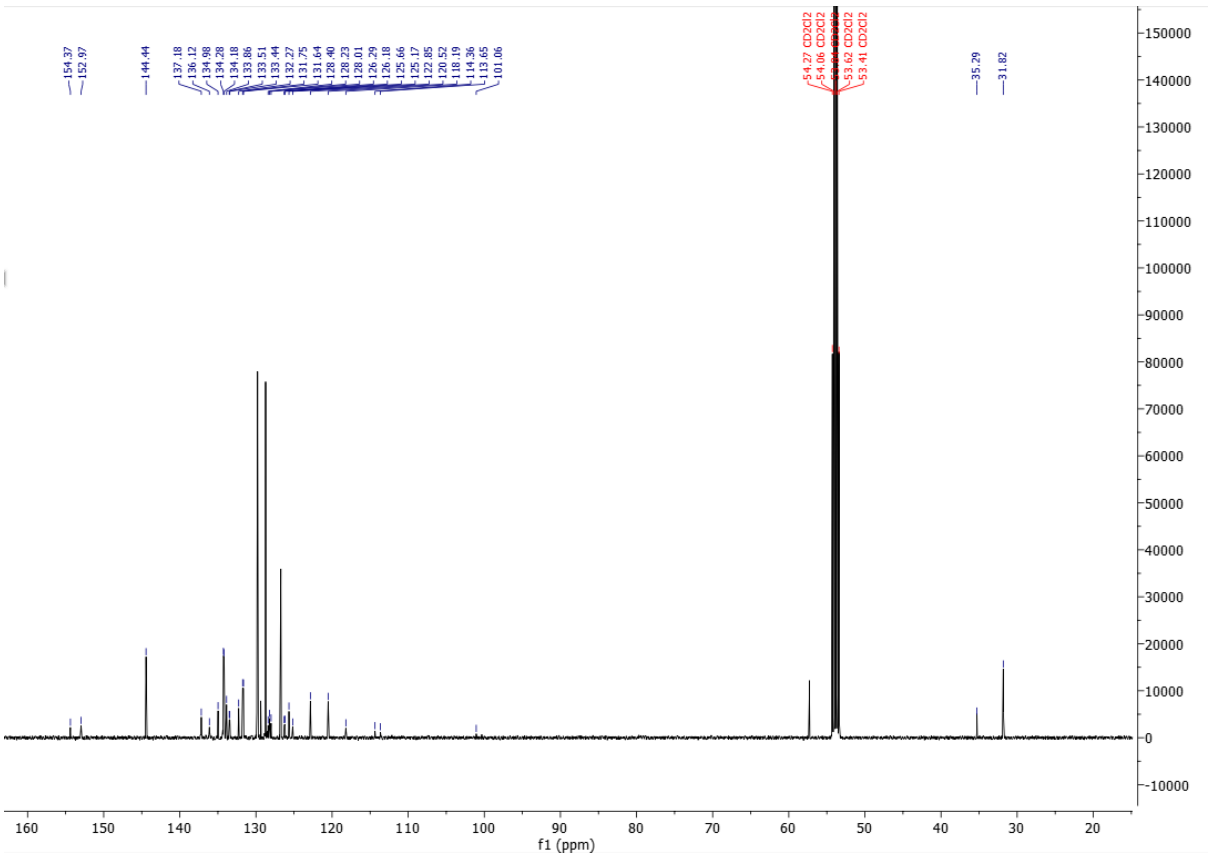
A 7.49: ^{19}F NMR spectrum of **5a**



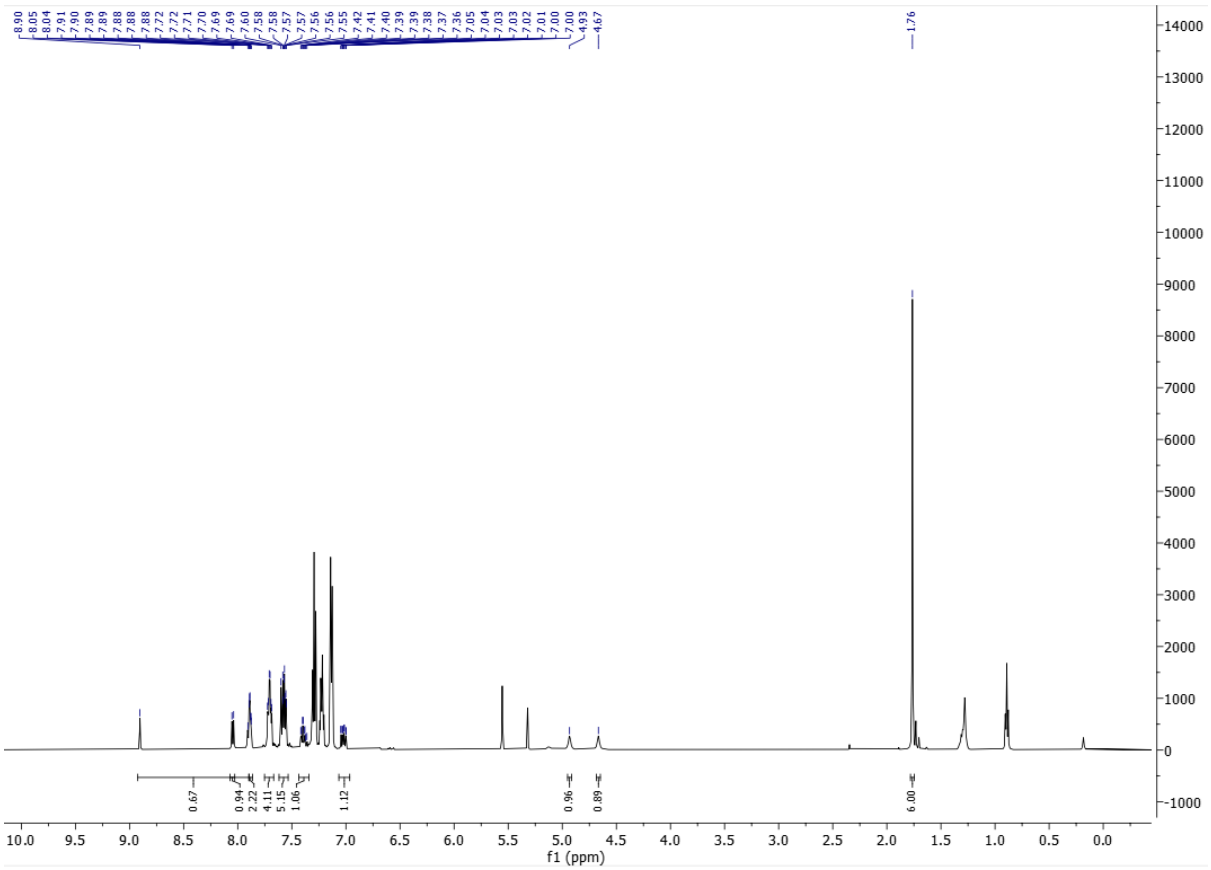
A 7.50: ^{27}Al NMR spectrum of **5a**



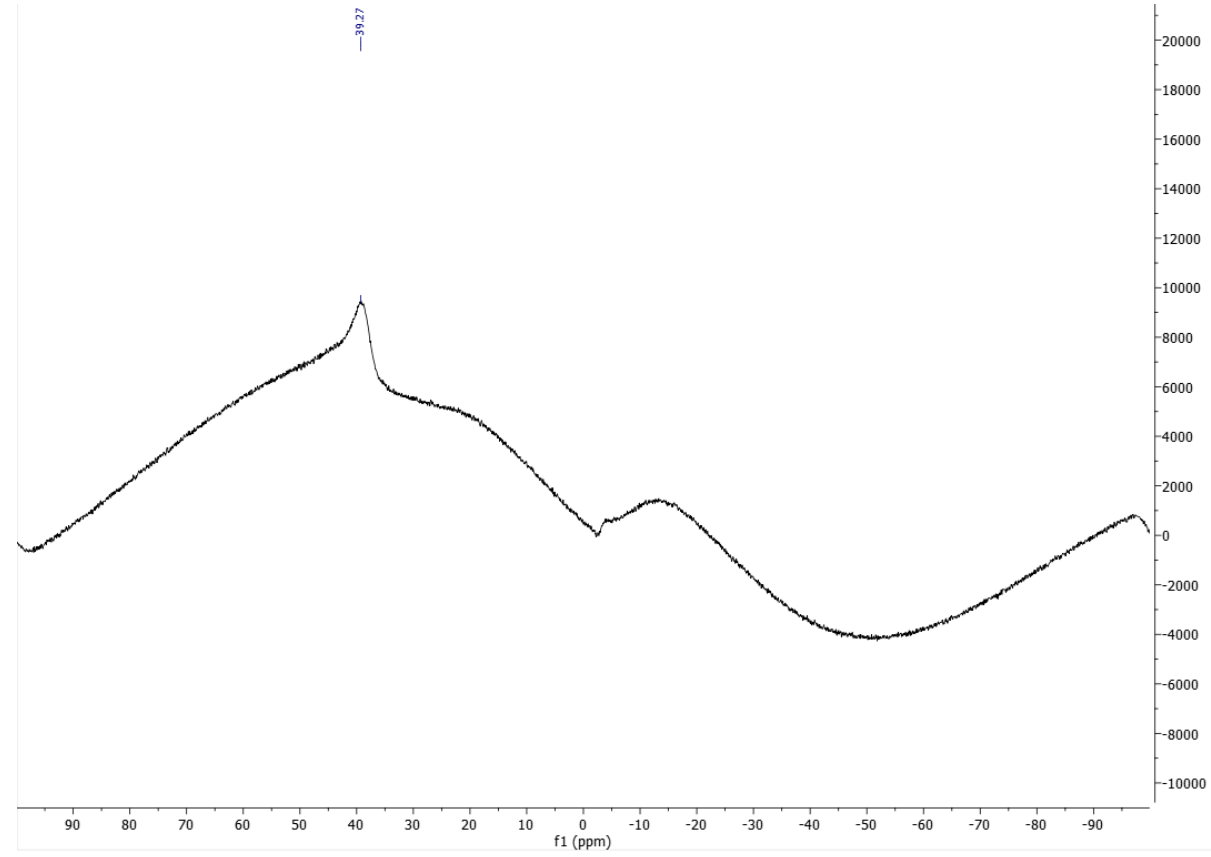
A 7.51: ^{31}P NMR spectrum of **5a**



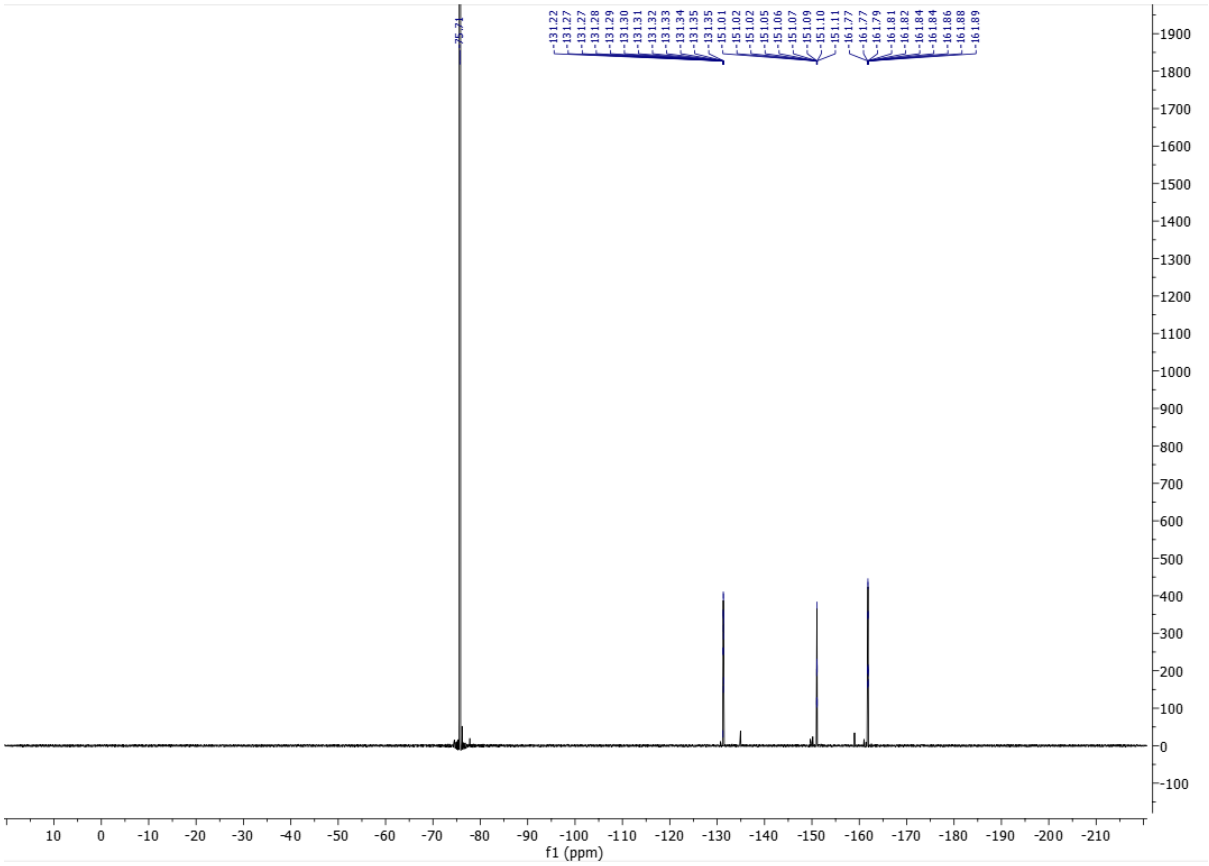
A 7.52: ^{13}C NMR spectrum of **5a**



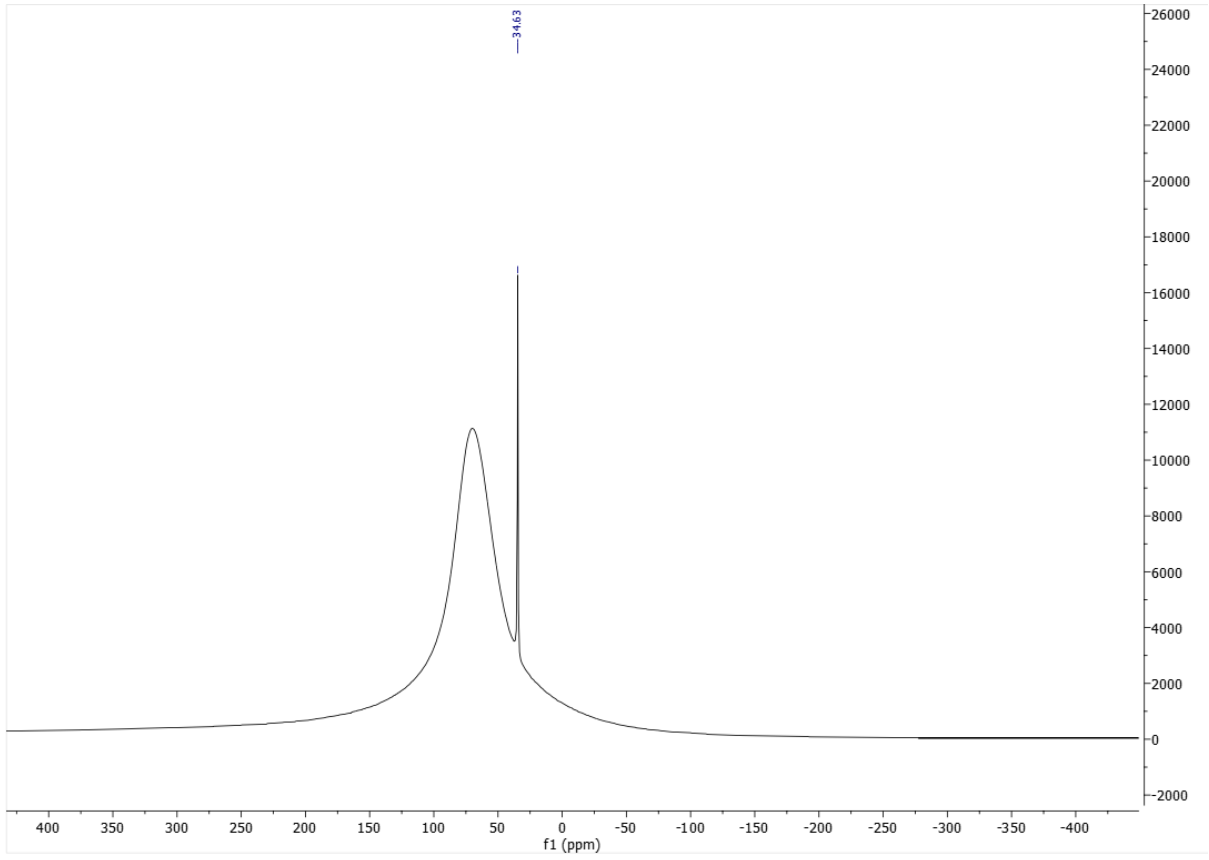
A 7.53: ^{1}H NMR spectrum of **5b**



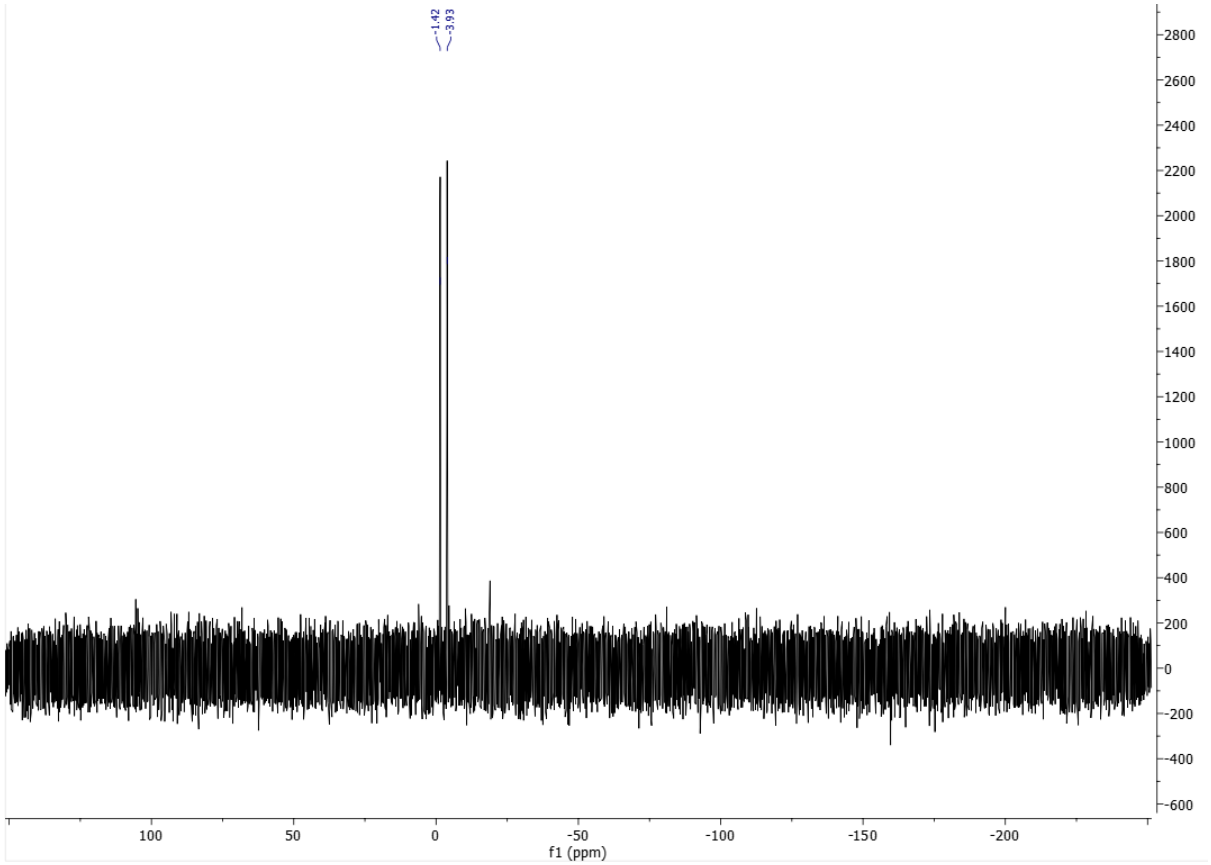
A 7.54: ^{11}B NMR spectrum of **5b**



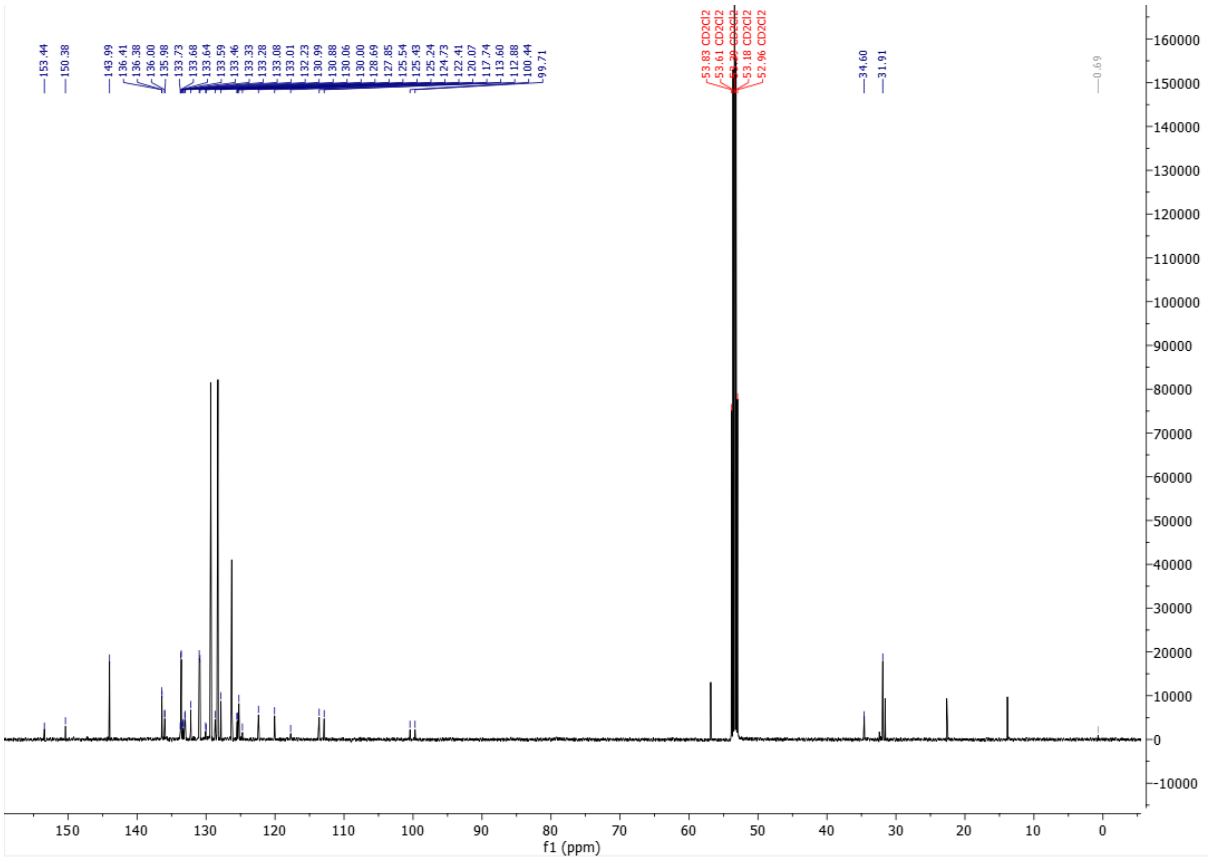
A 7.55: ^{19}F NMR spectrum of **5b**



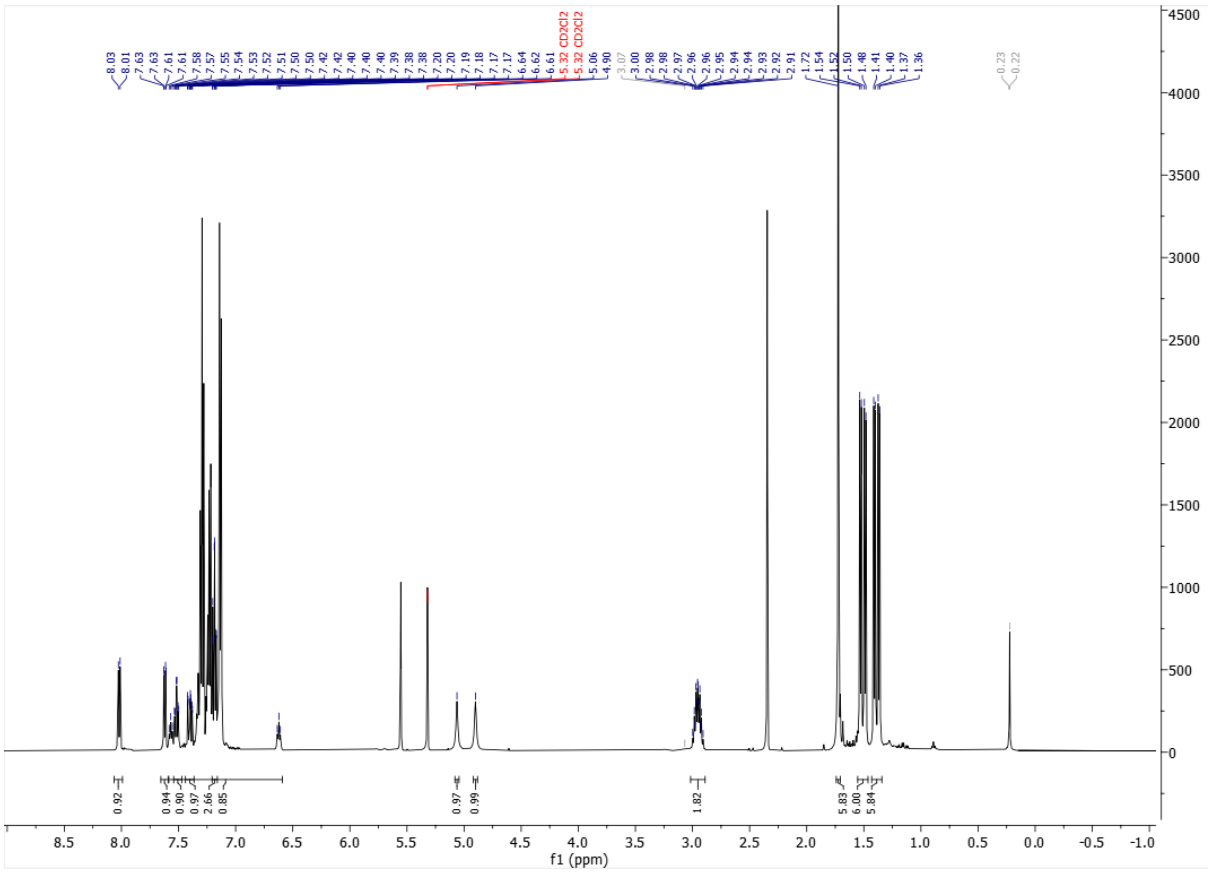
A 7.56: ^{27}Al NMR spectrum of **5b**



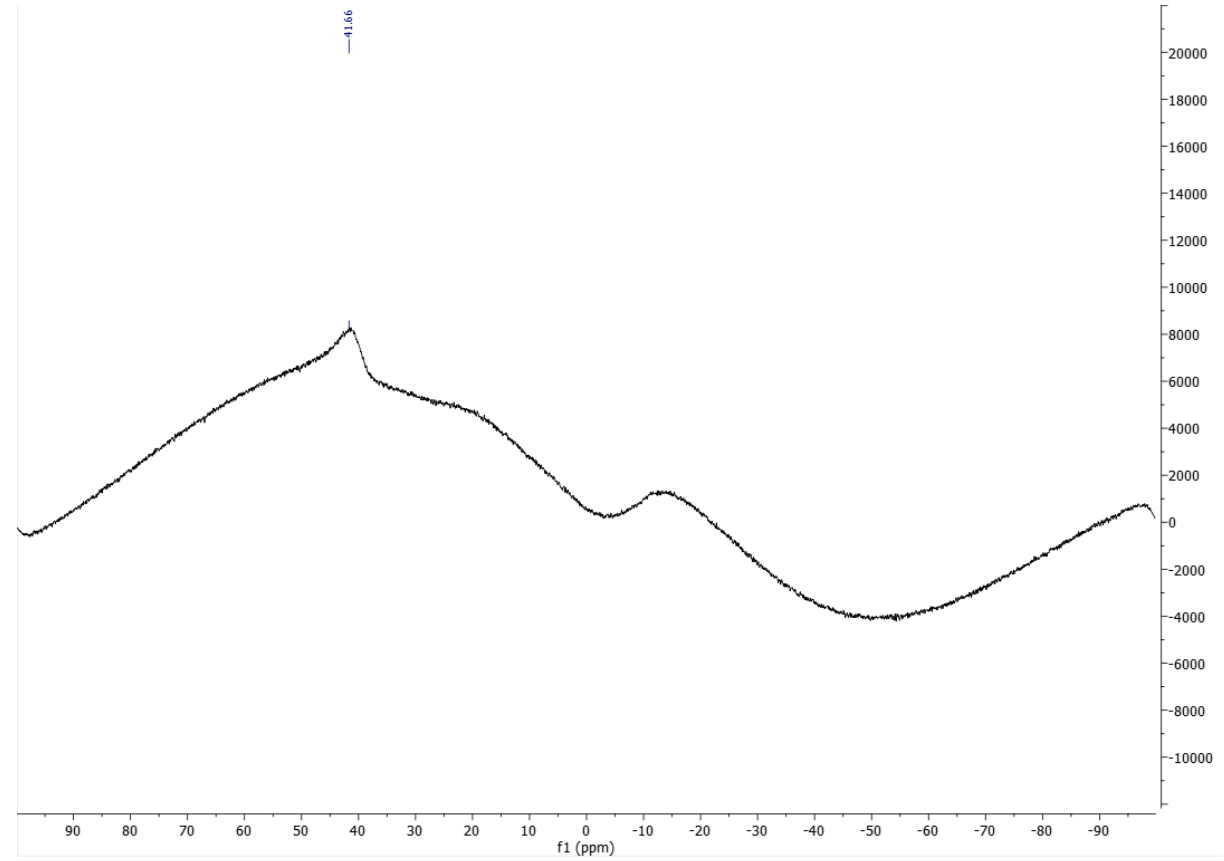
A 7.57: ^{31}P NMR spectrum of **5b**



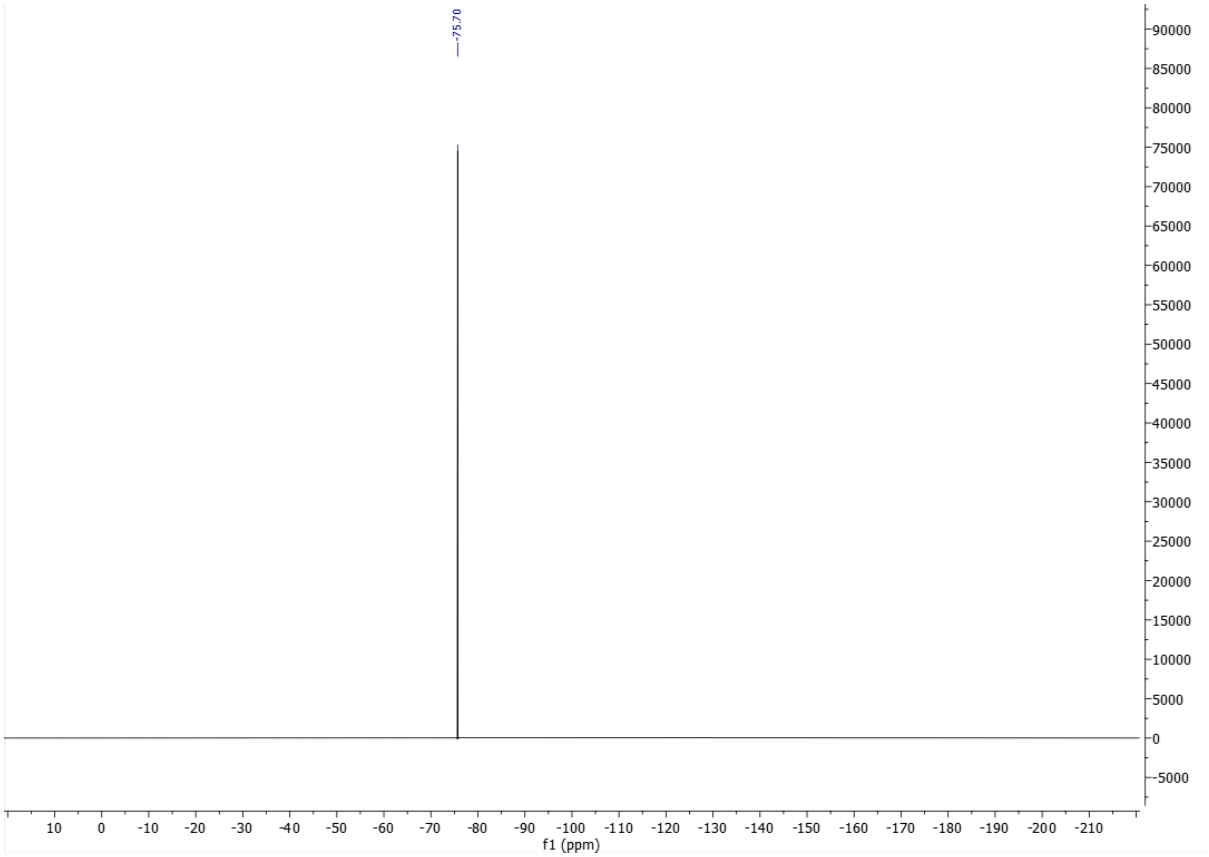
A 7.58: ^{13}C NMR spectrum of **5b**



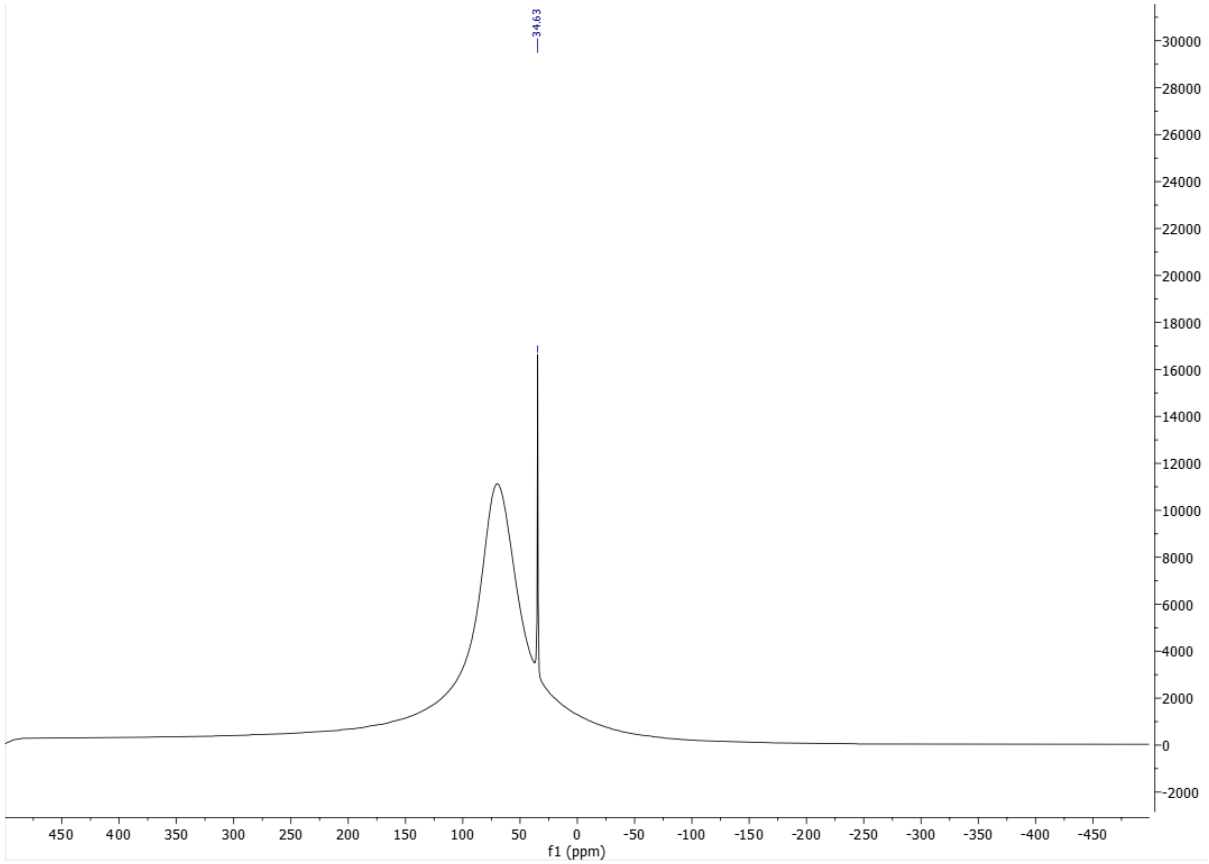
A 7.59: ^{1}H NMR spectrum of **5c**



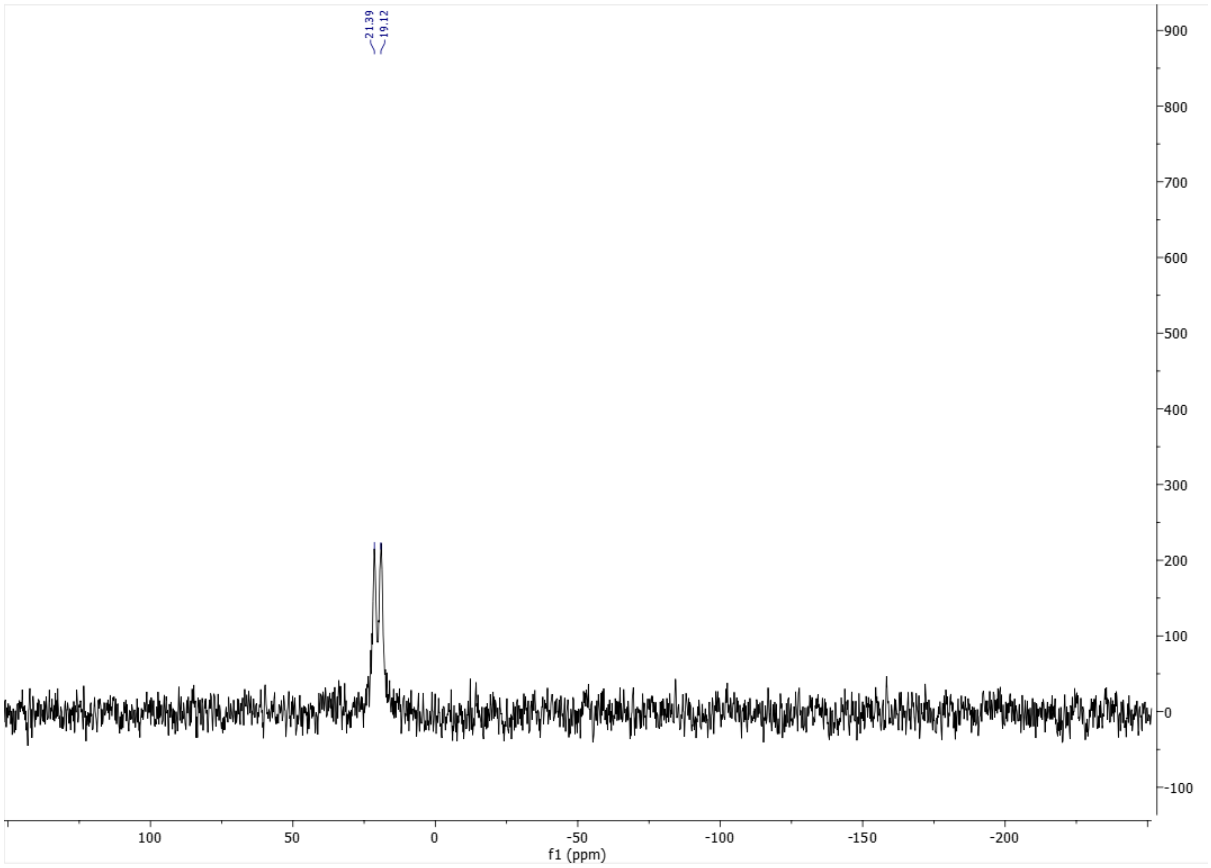
A 7.60: ^{11}B NMR spectrum of **5c**



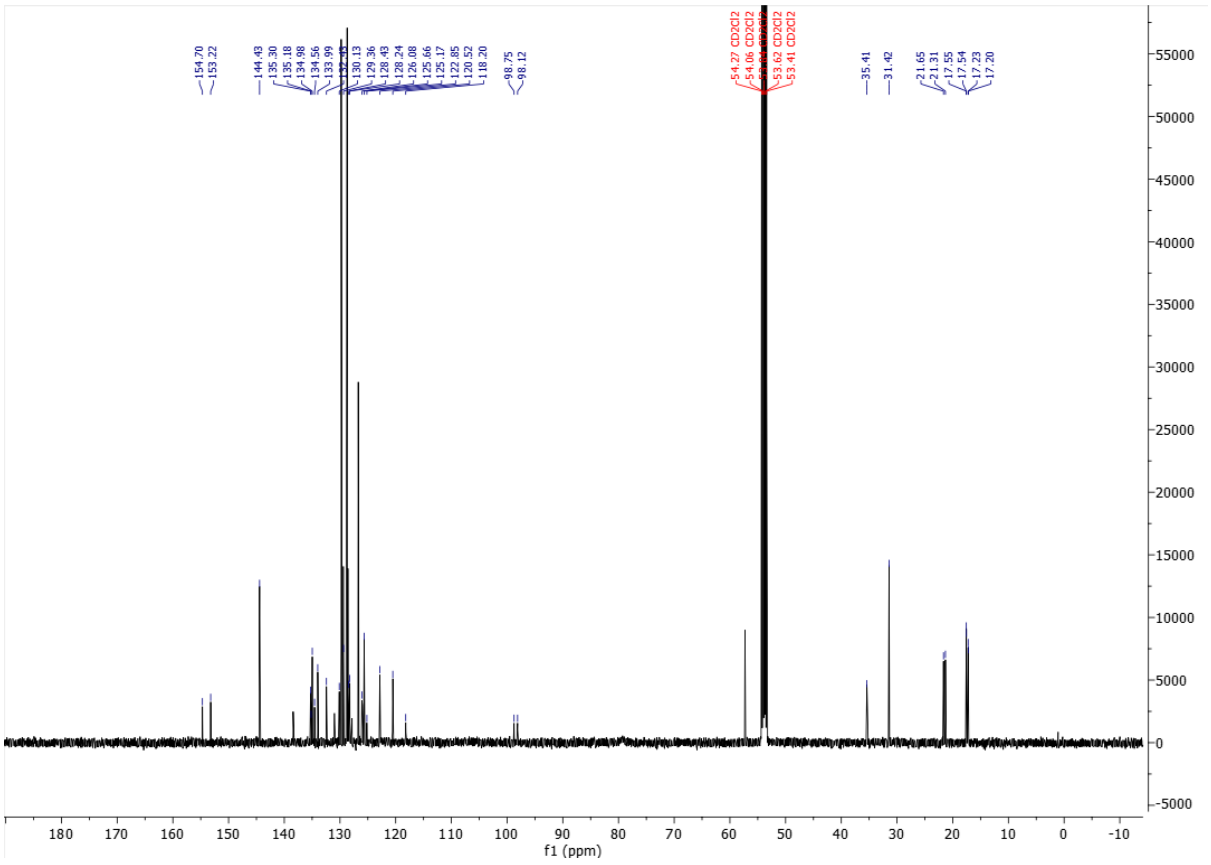
A 7.61: ^{19}F NMR spectrum of **5c**



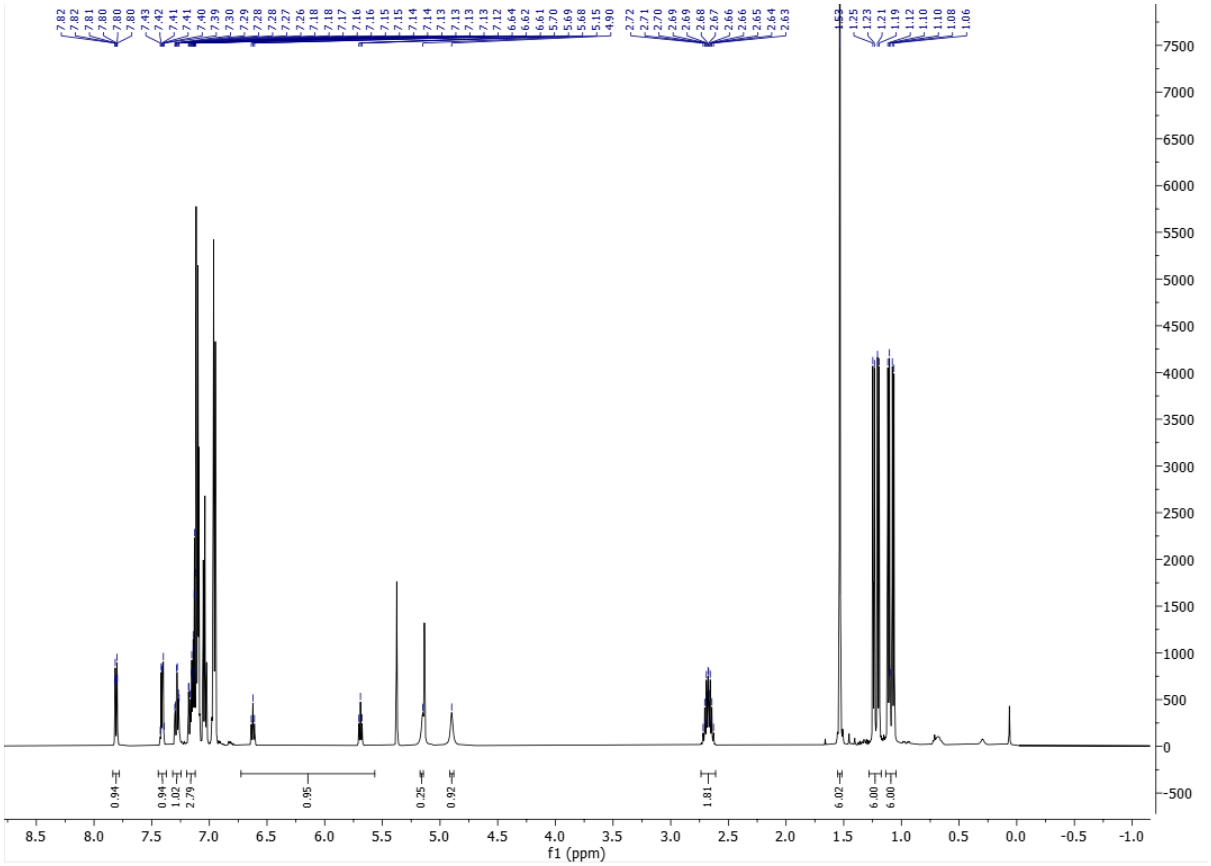
A 7.62: ^{27}Al NMR spectrum of **5c**



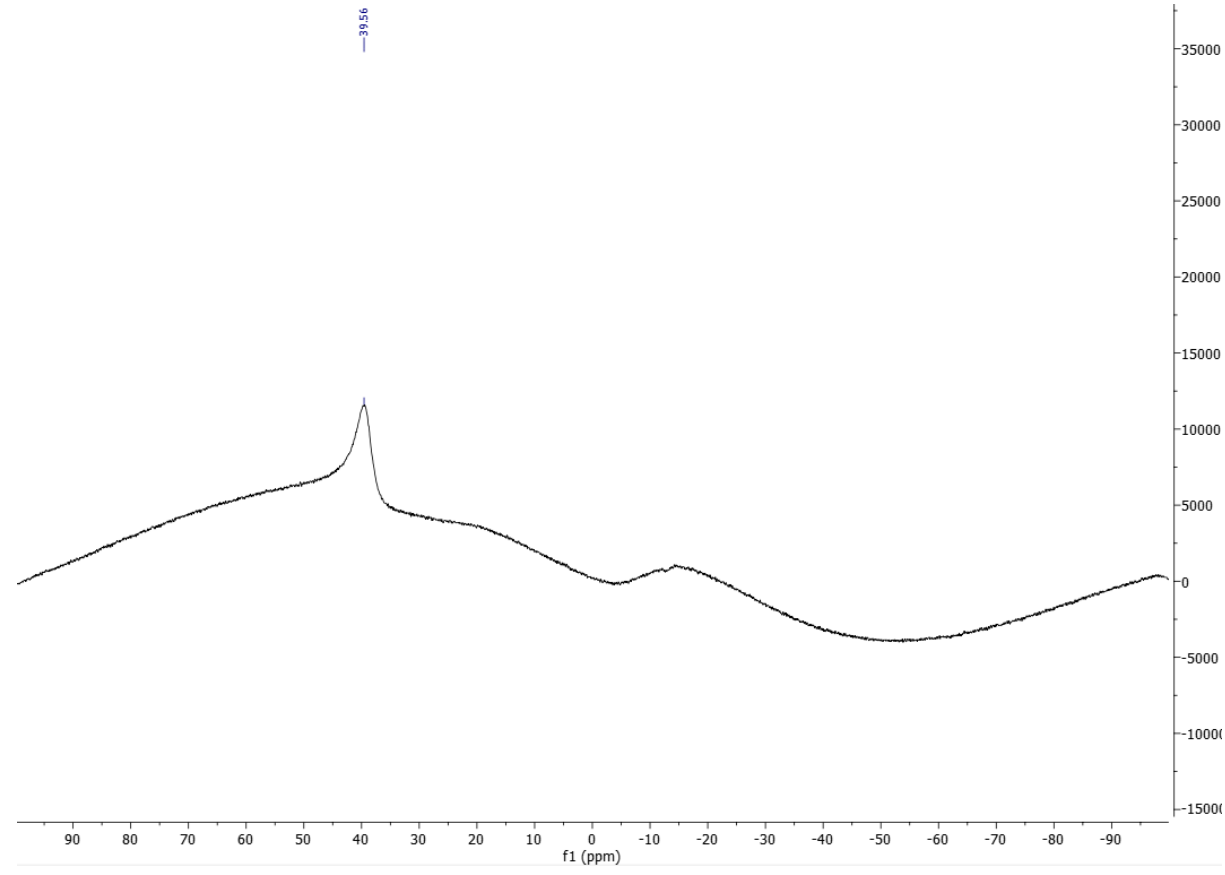
A 7.63: ^{31}P NMR spectrum of **5c**



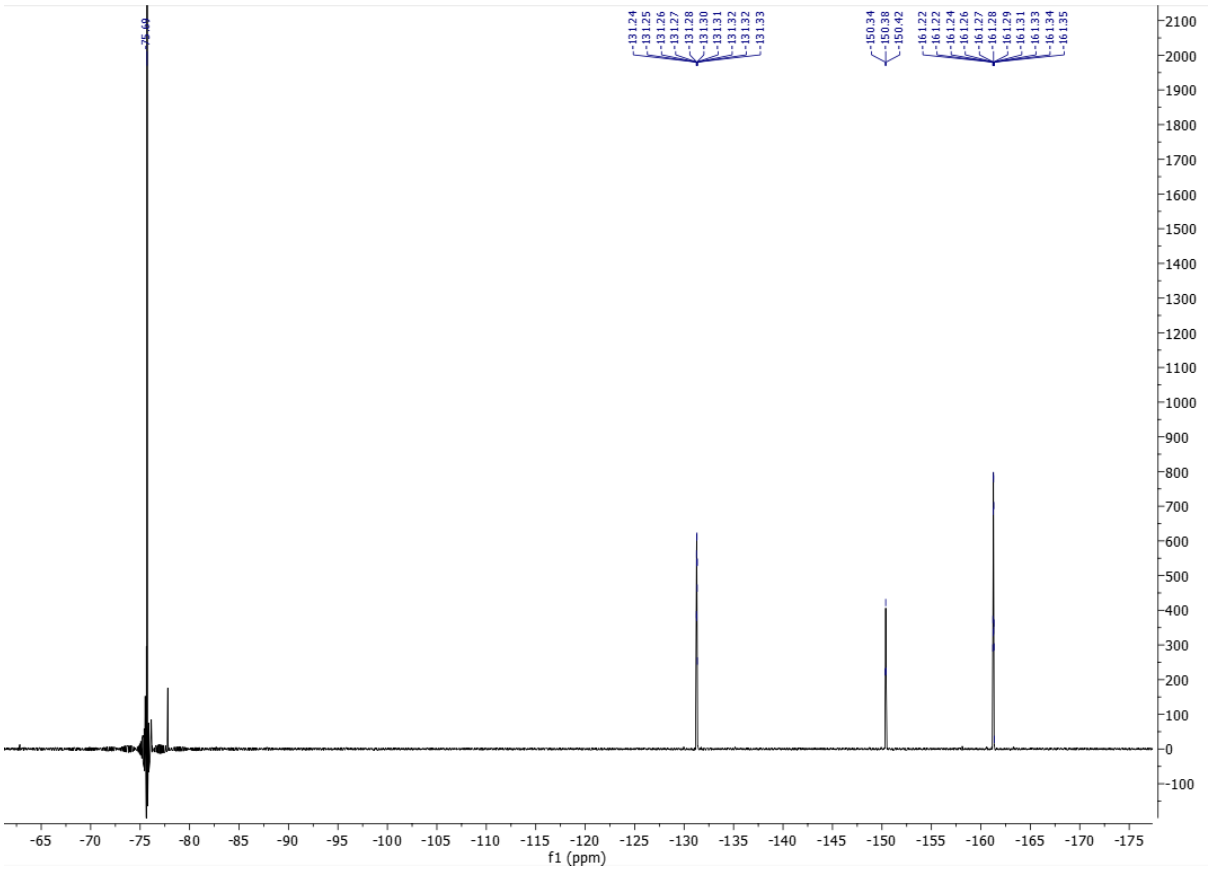
A 7.64: ^{13}C NMR spectrum of **5c**



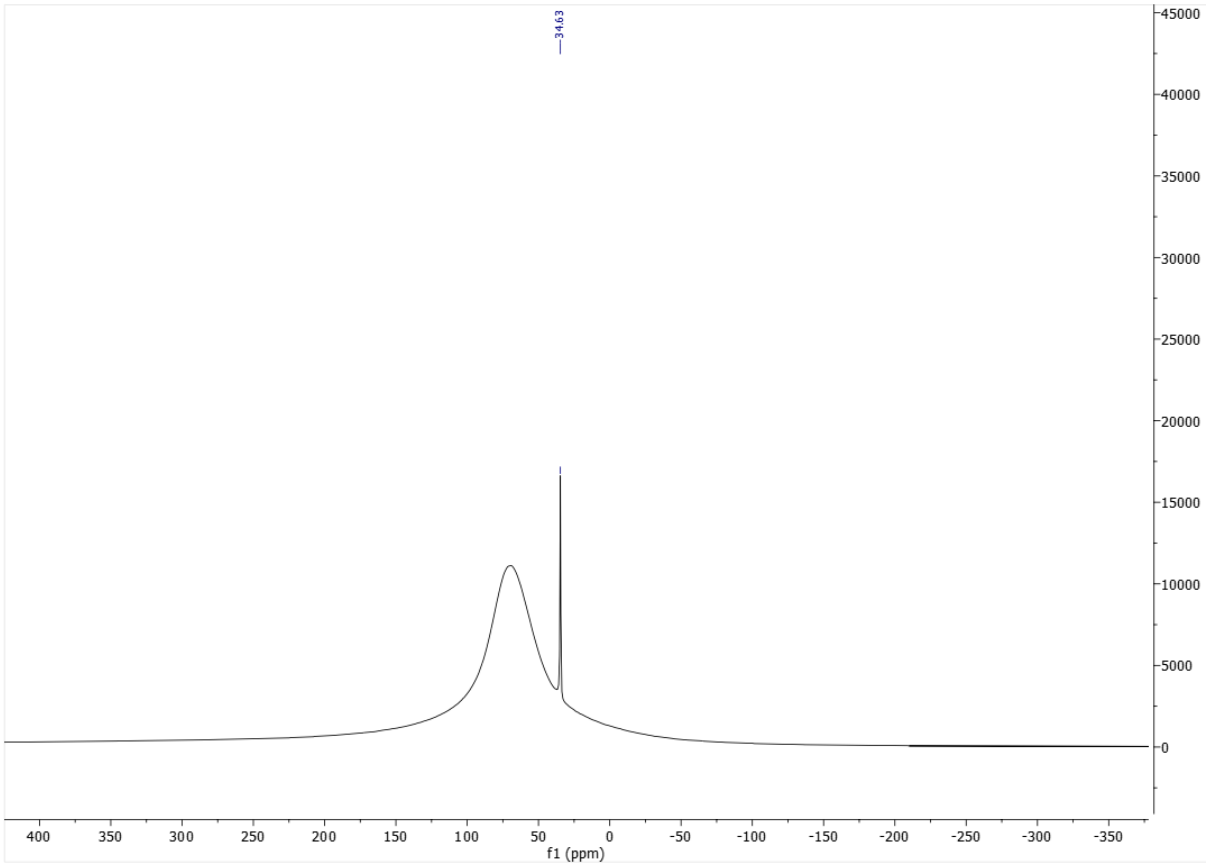
A 7.65: ^{1}H NMR spectrum of **5d**



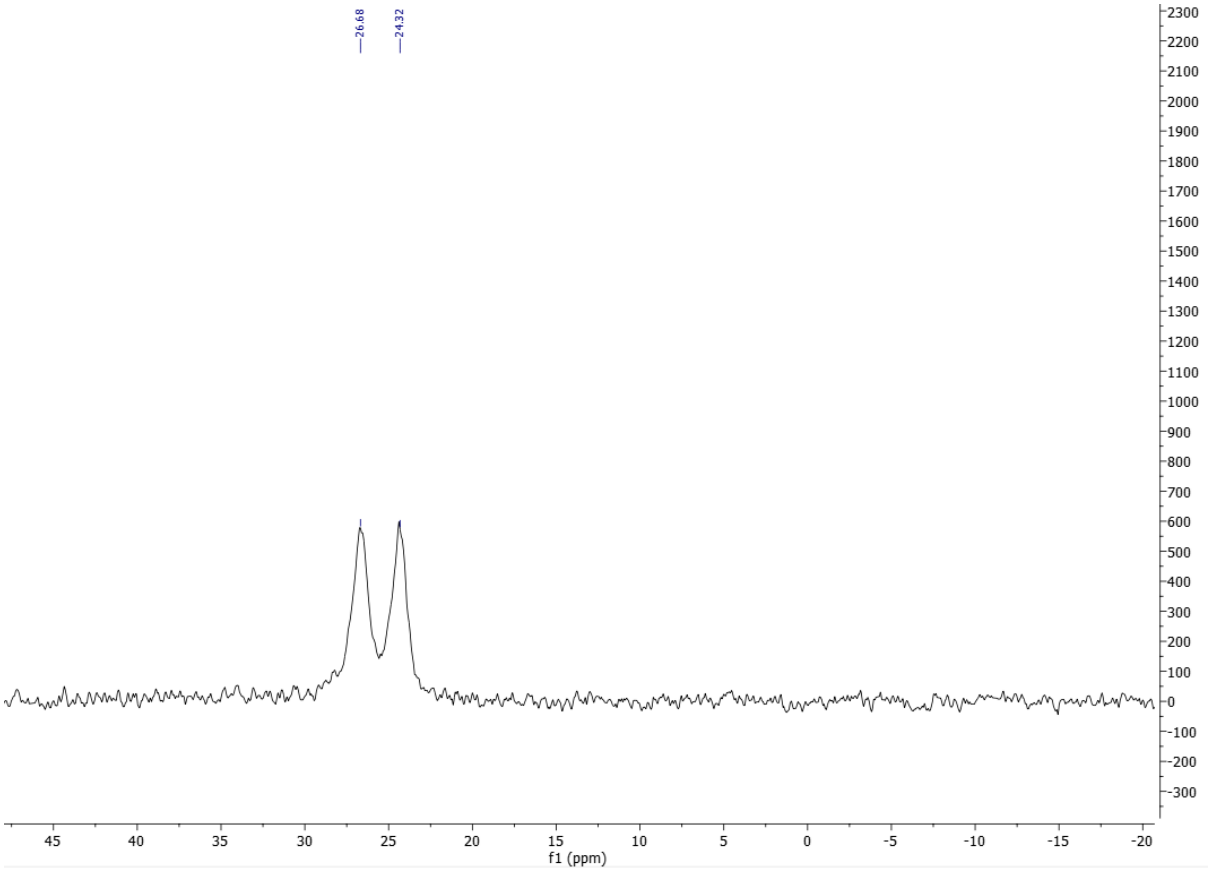
A 7.66: ^{11}B NMR spectrum of **5d**



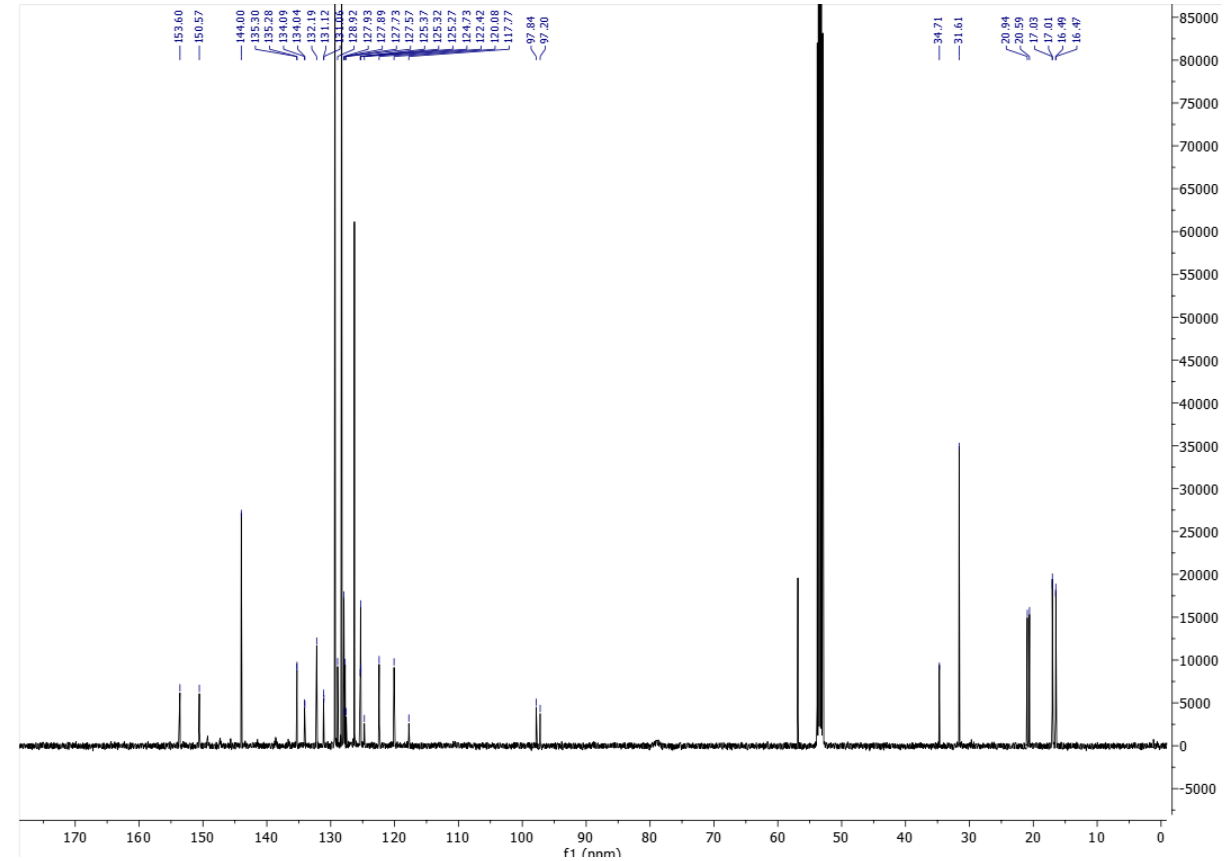
A 7.67: ^{19}F NMR spectrum of **5d**



A 7.68: ^{27}Al NMR spectrum of **5d**

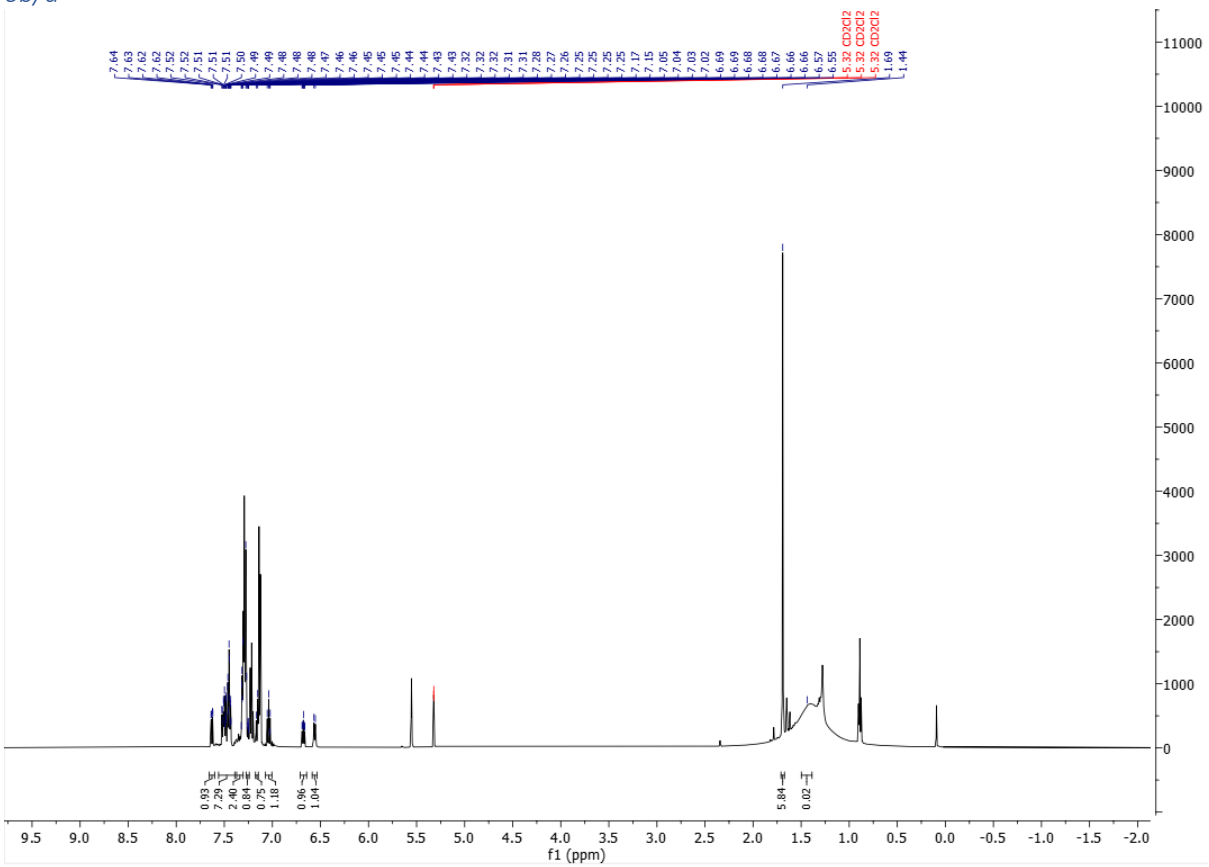


A 7.69: ^{31}P NMR spectrum of **5d**

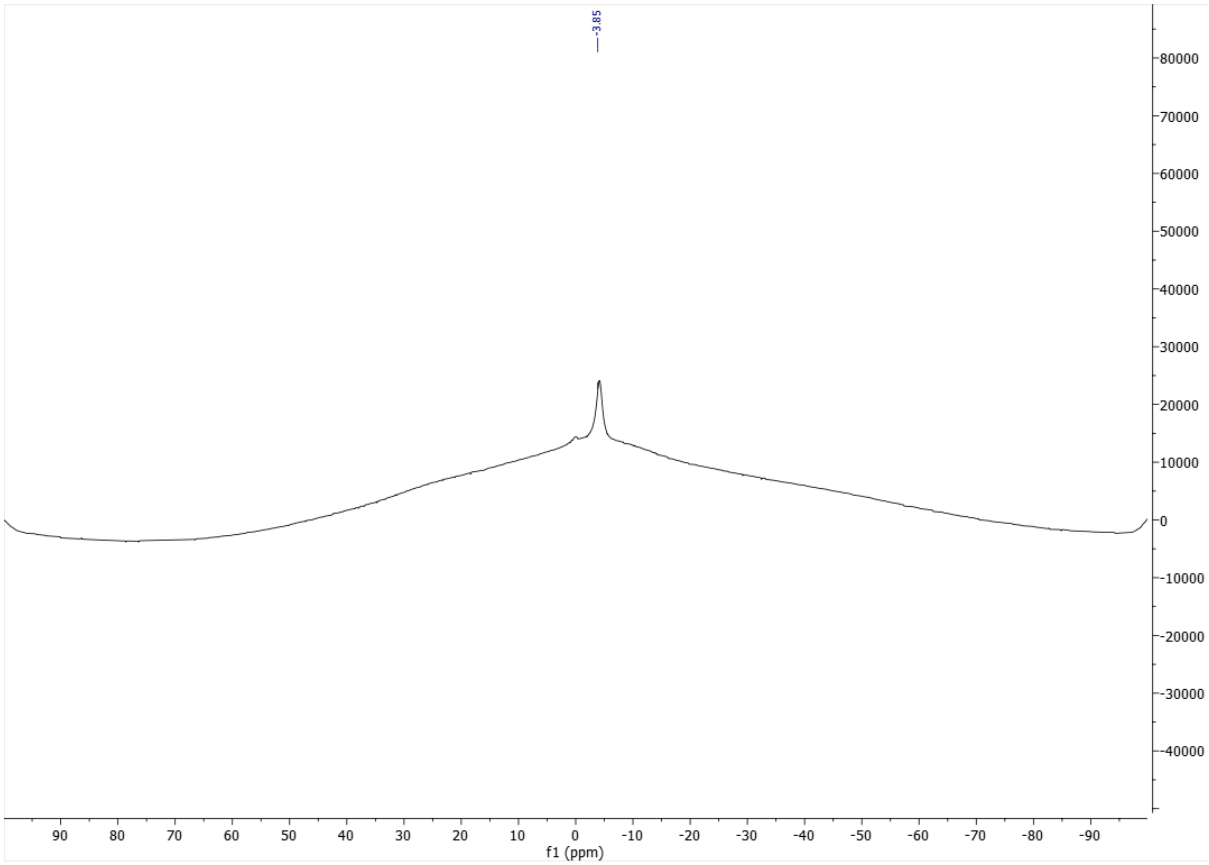


A 7.70: ^{13}C NMR spectrum of **5d**

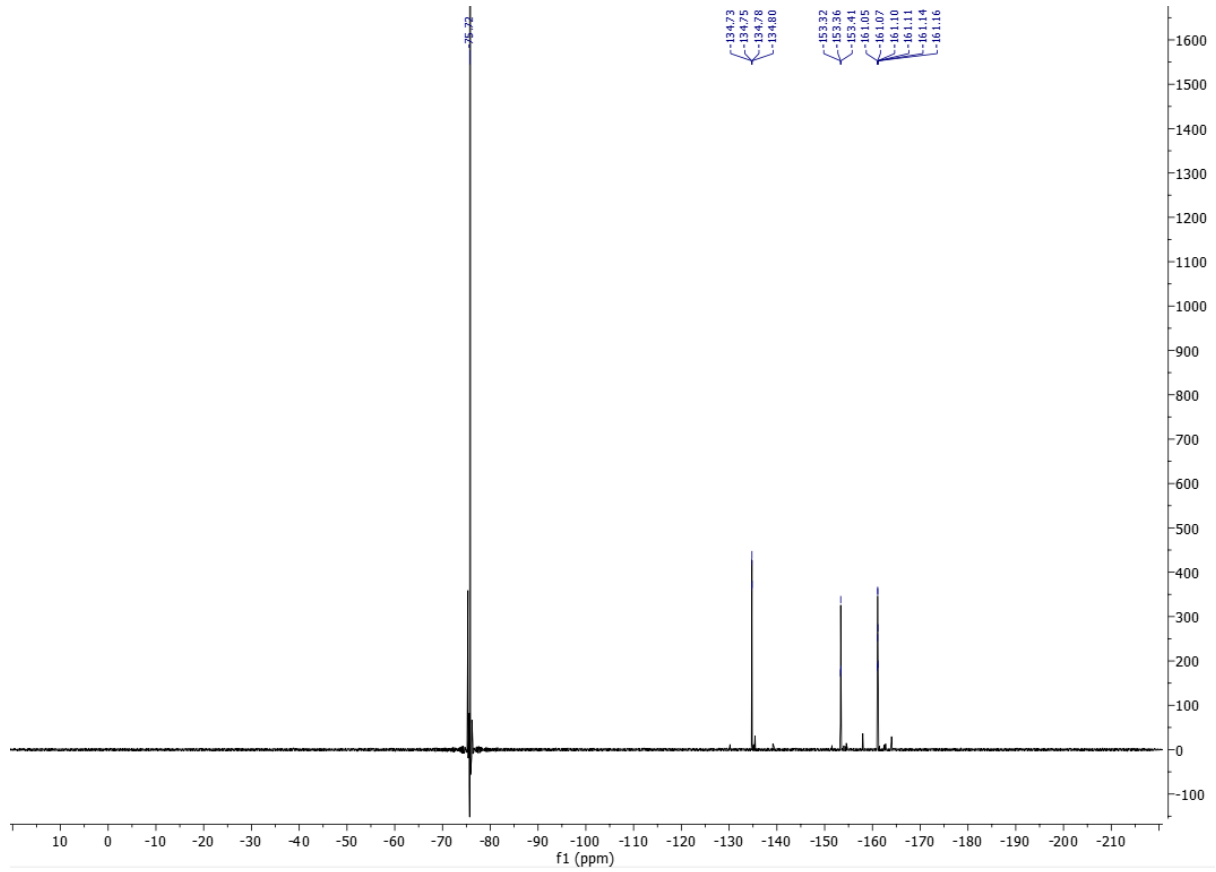
6b/d



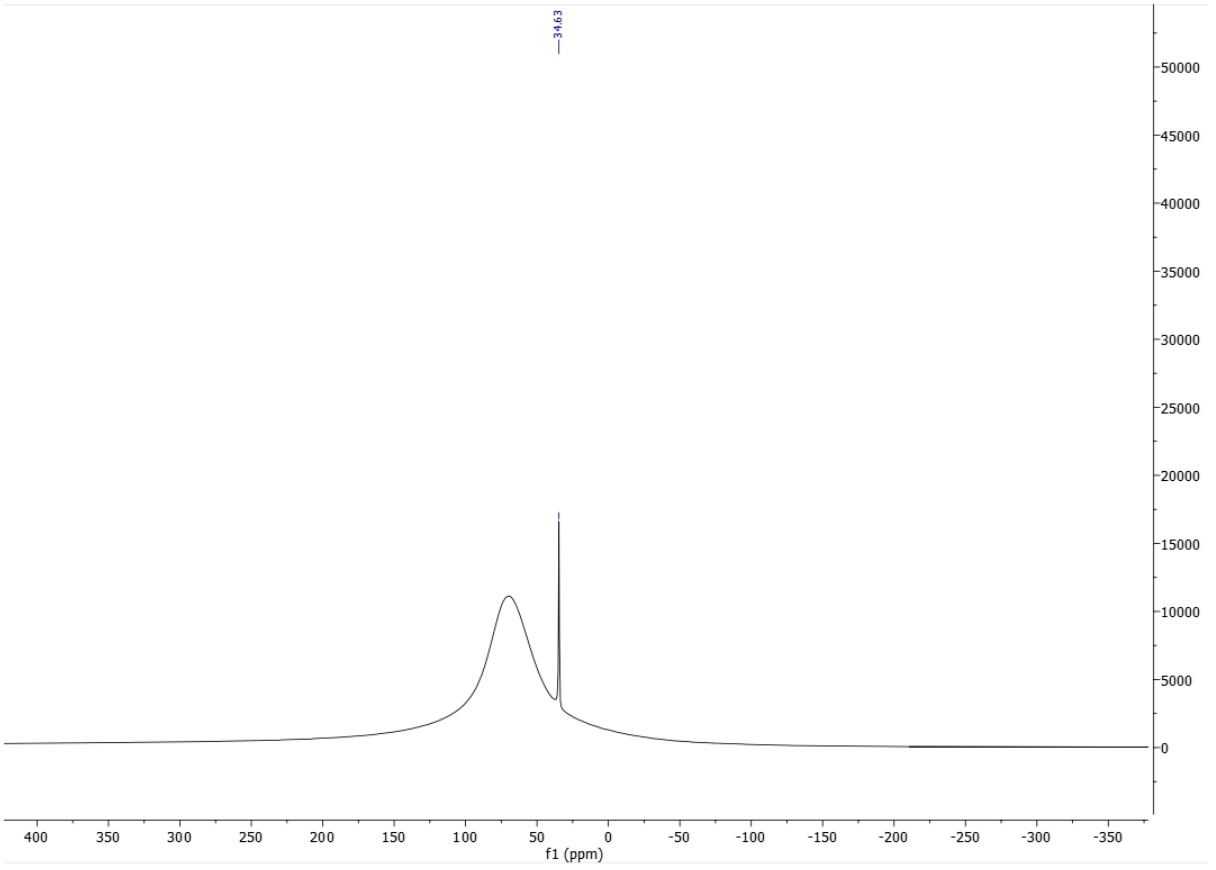
A 7.71: ^{1}H NMR spectrum of **6b**



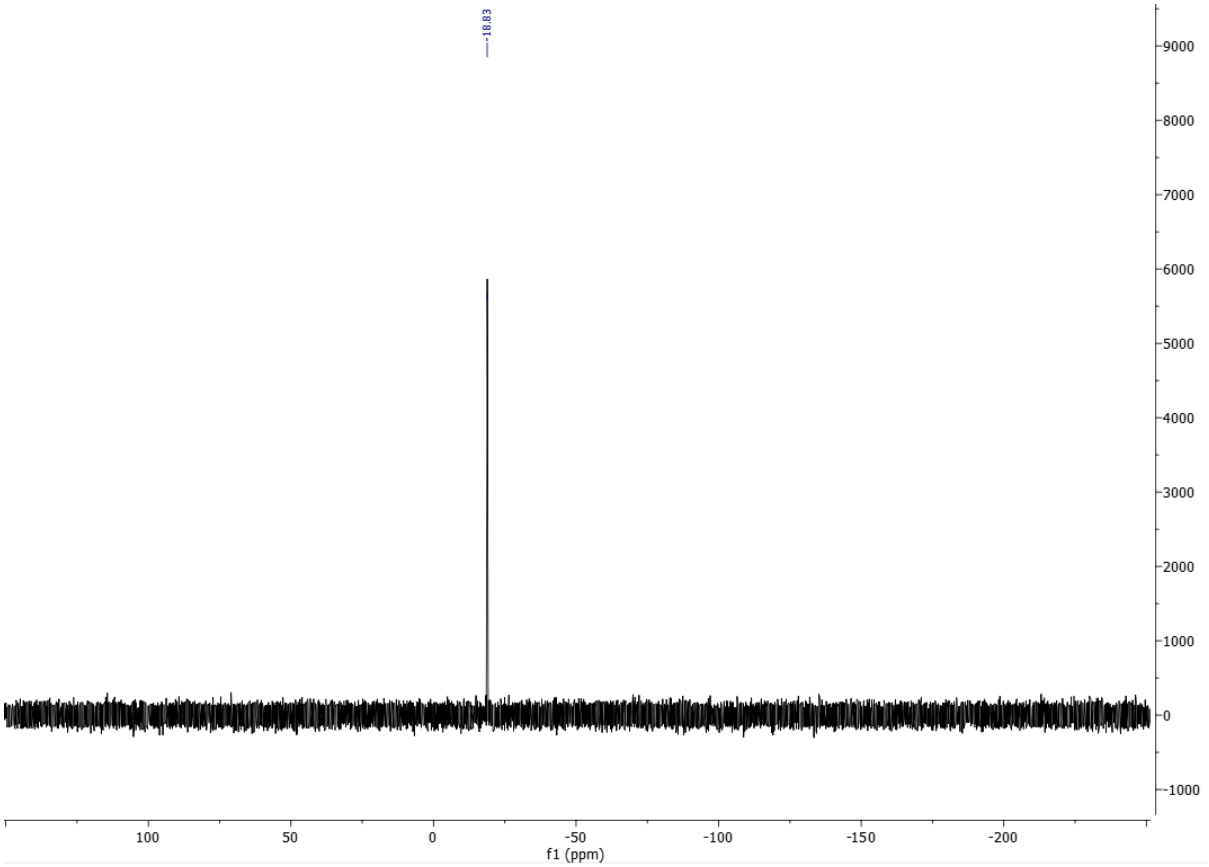
A 7.72: ^{11}B NMR spectrum of **6b**



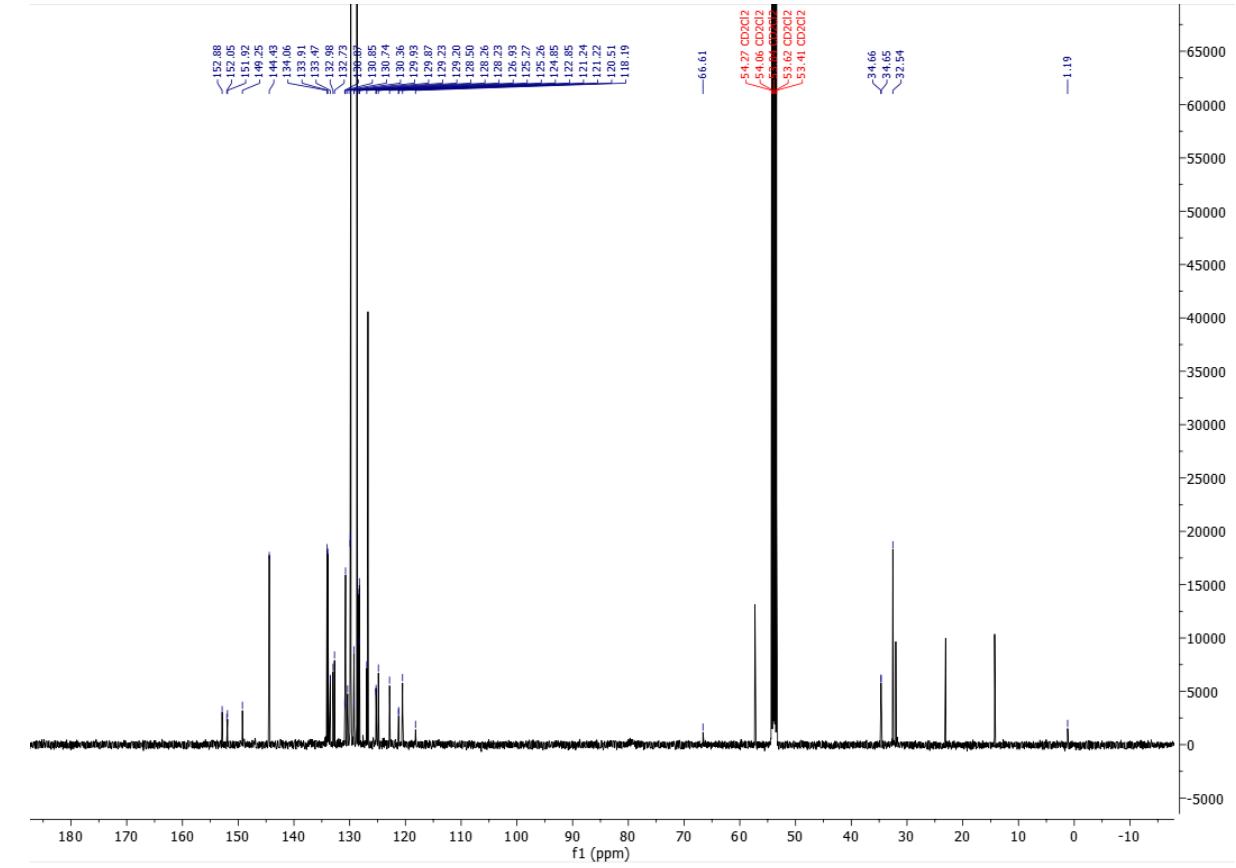
A 7.73: ^{19}F NMR spectrum of **6b**



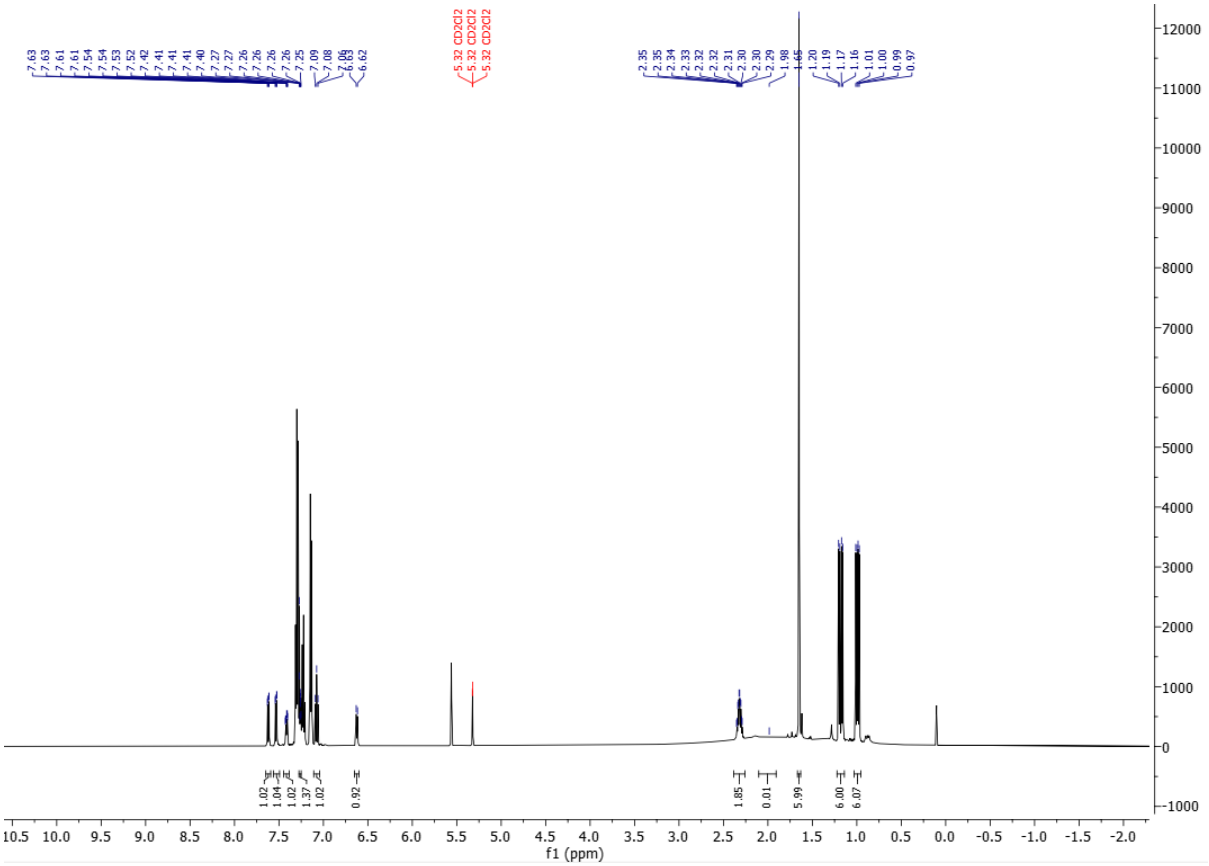
A 7.74: ^{27}Al NMR spectrum of **6b**



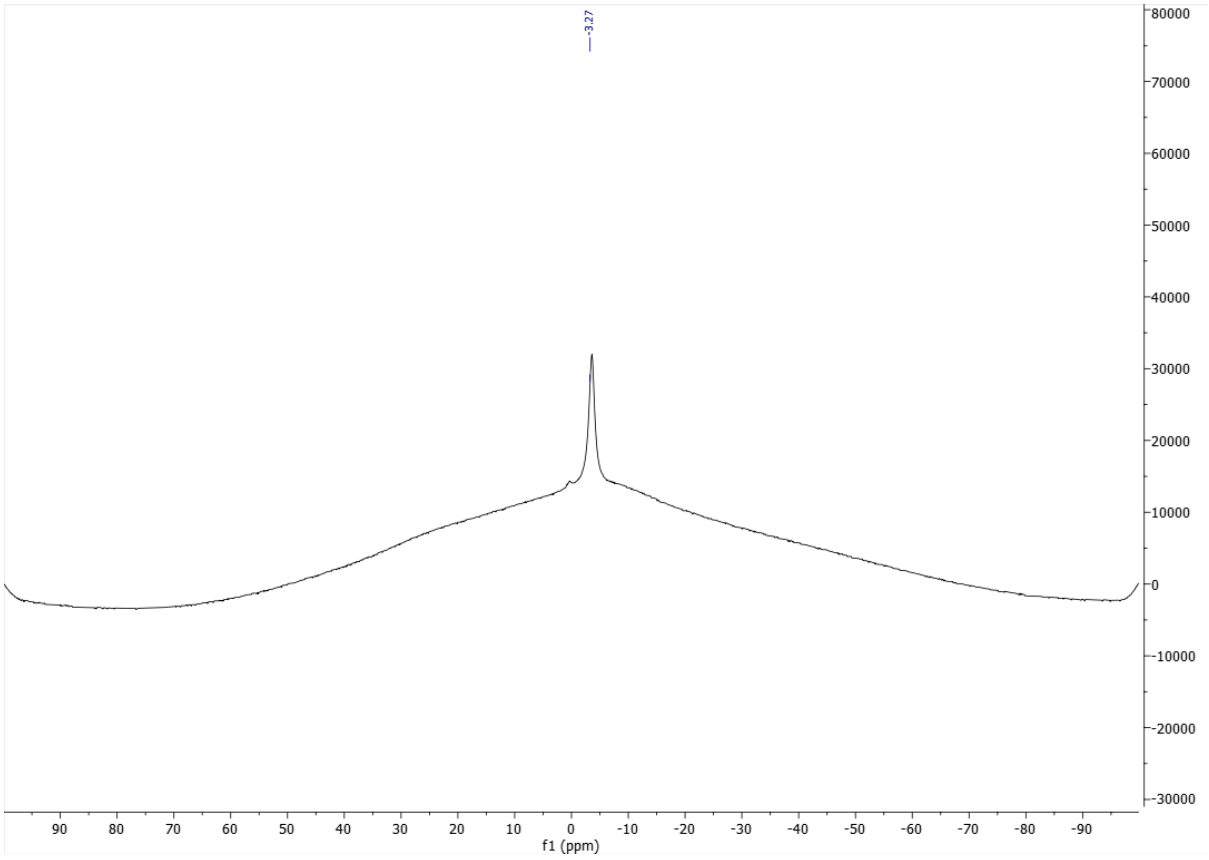
A 7.75: ^{31}P NMR spectrum of **6b**



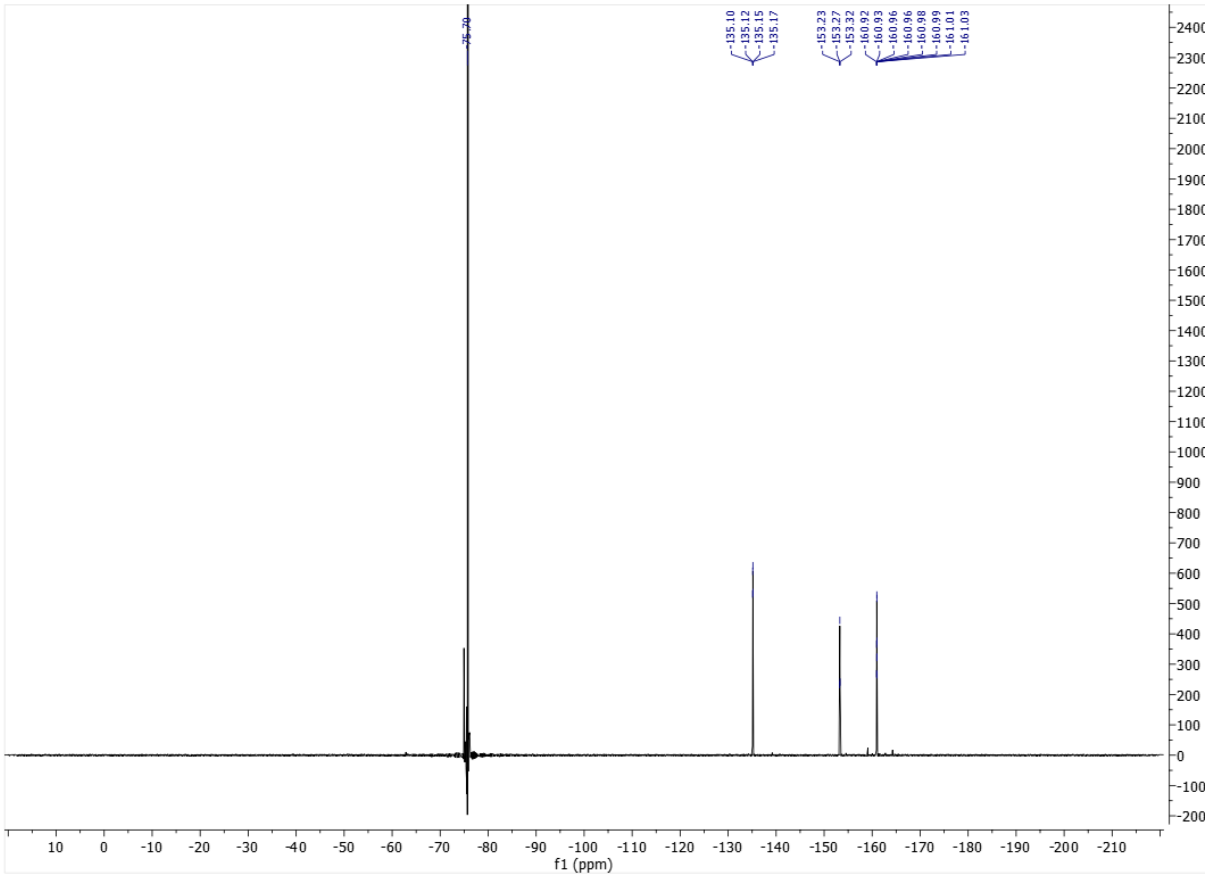
A 7.76: ^{13}C NMR spectrum of **6b**



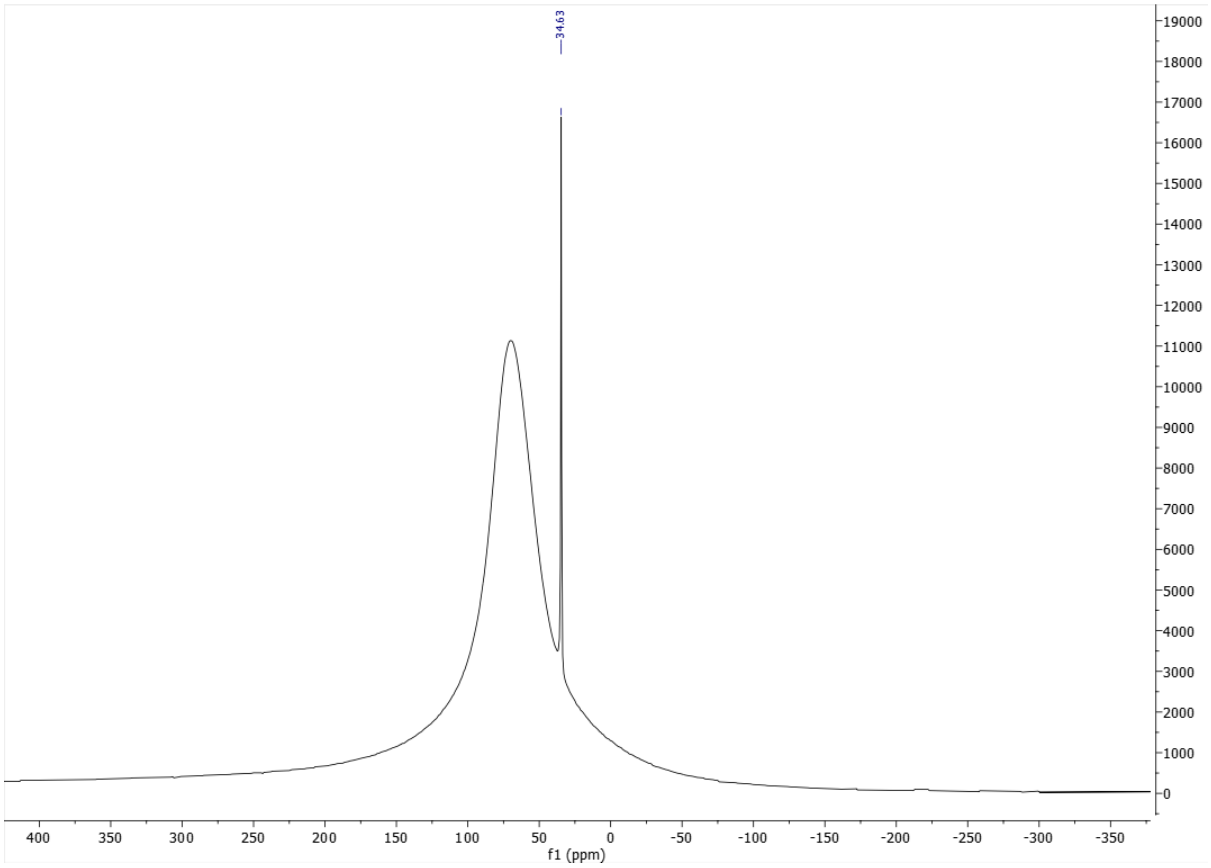
A 7.77: ^{1}H NMR spectrum of **6d**



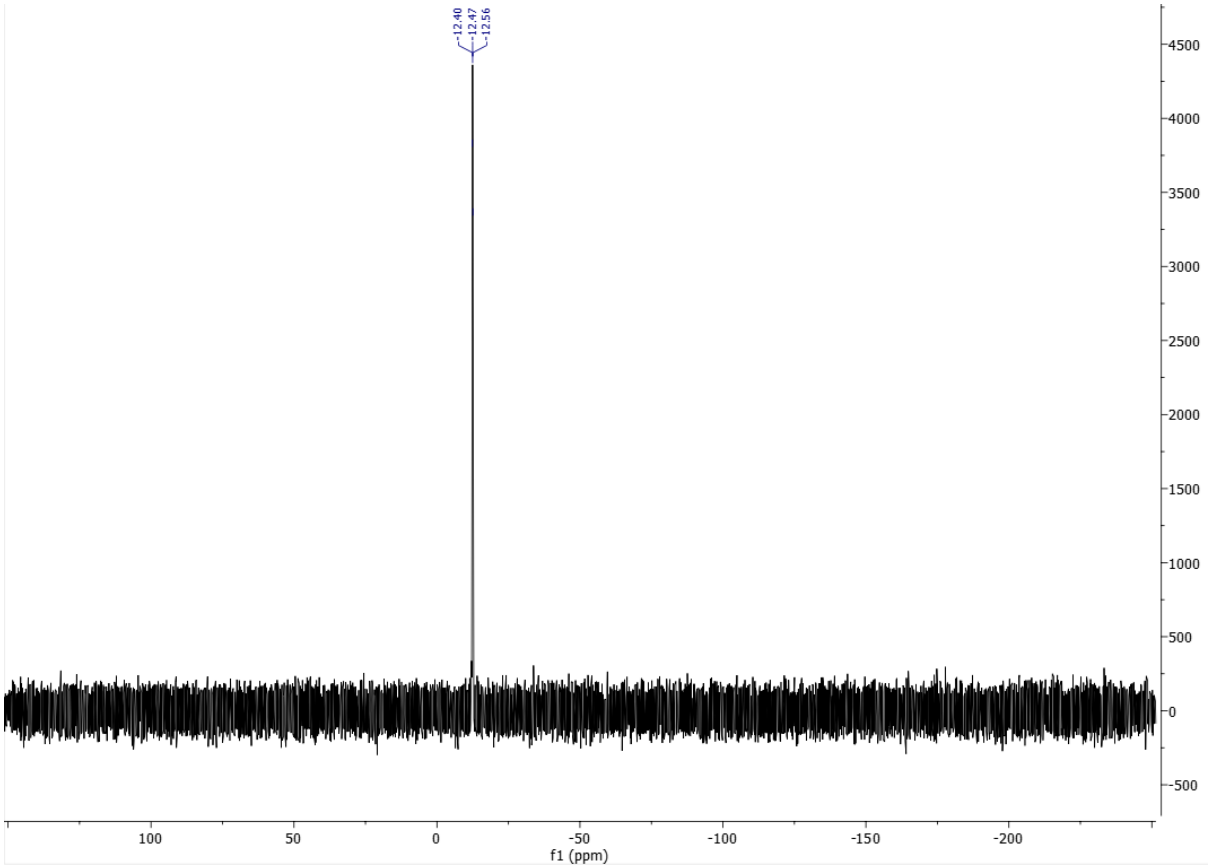
A 7.78: ^{11}B NMR spectrum of **6d**



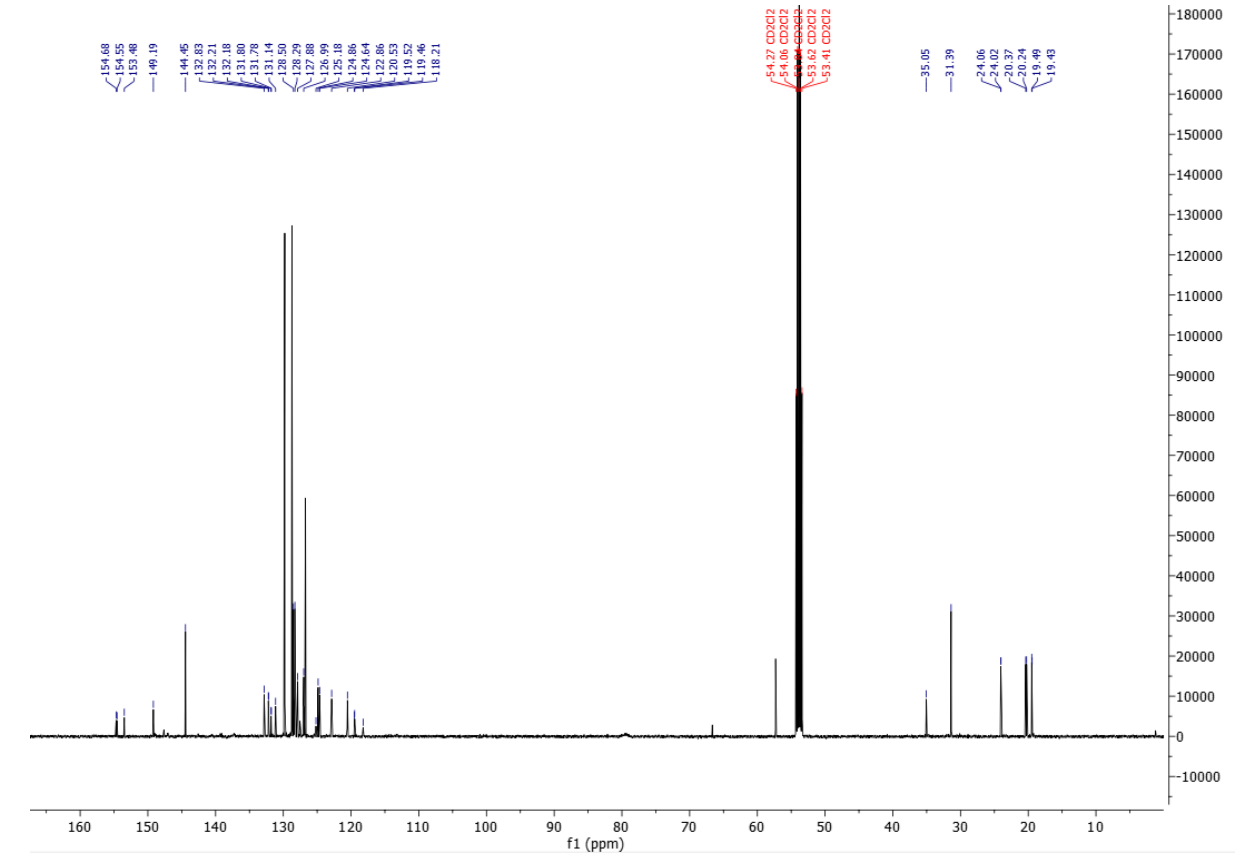
A 7.79: ^{19}F NMR spectrum of **6d**



A 7.80: ^{27}Al NMR spectrum of **6d**

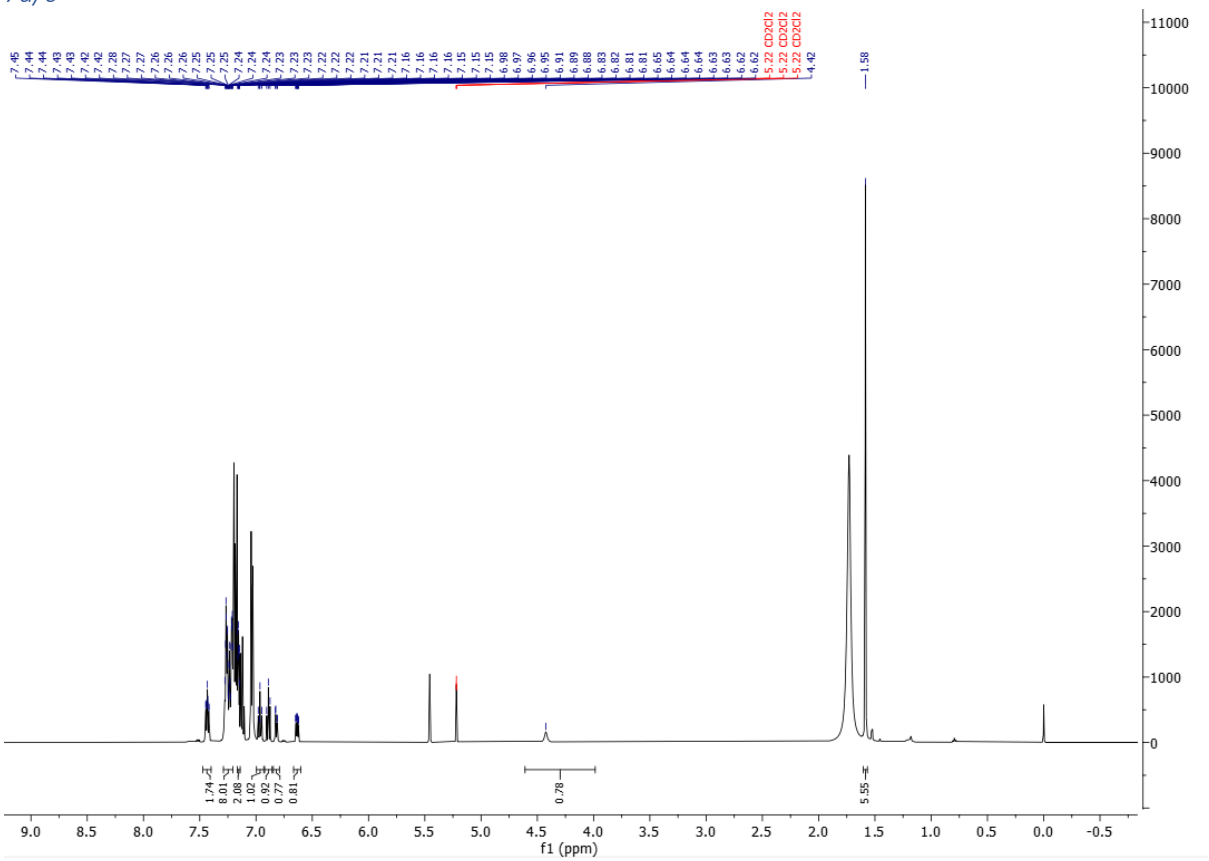


A 7.81: ^{31}P NMR spectrum of **6d**

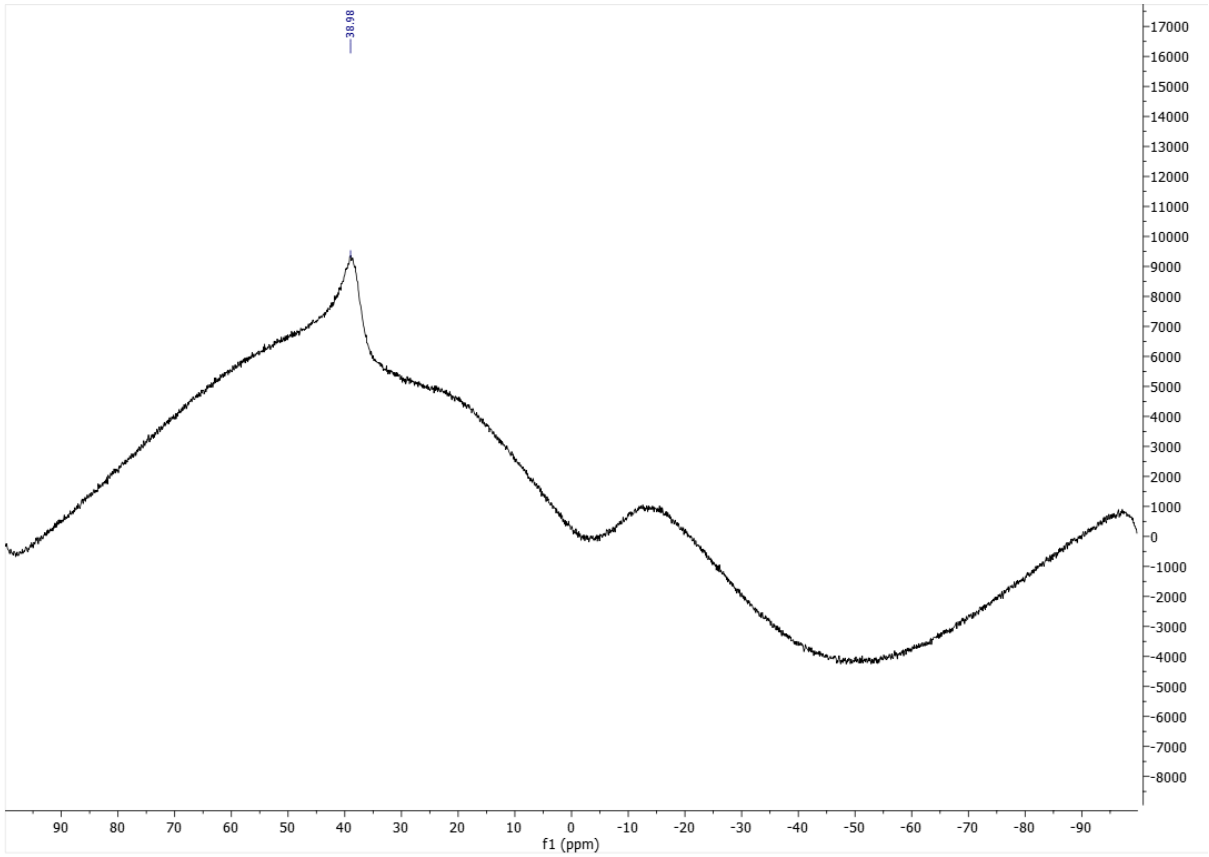


A 7.82: ^{13}C NMR spectrum of **6d**

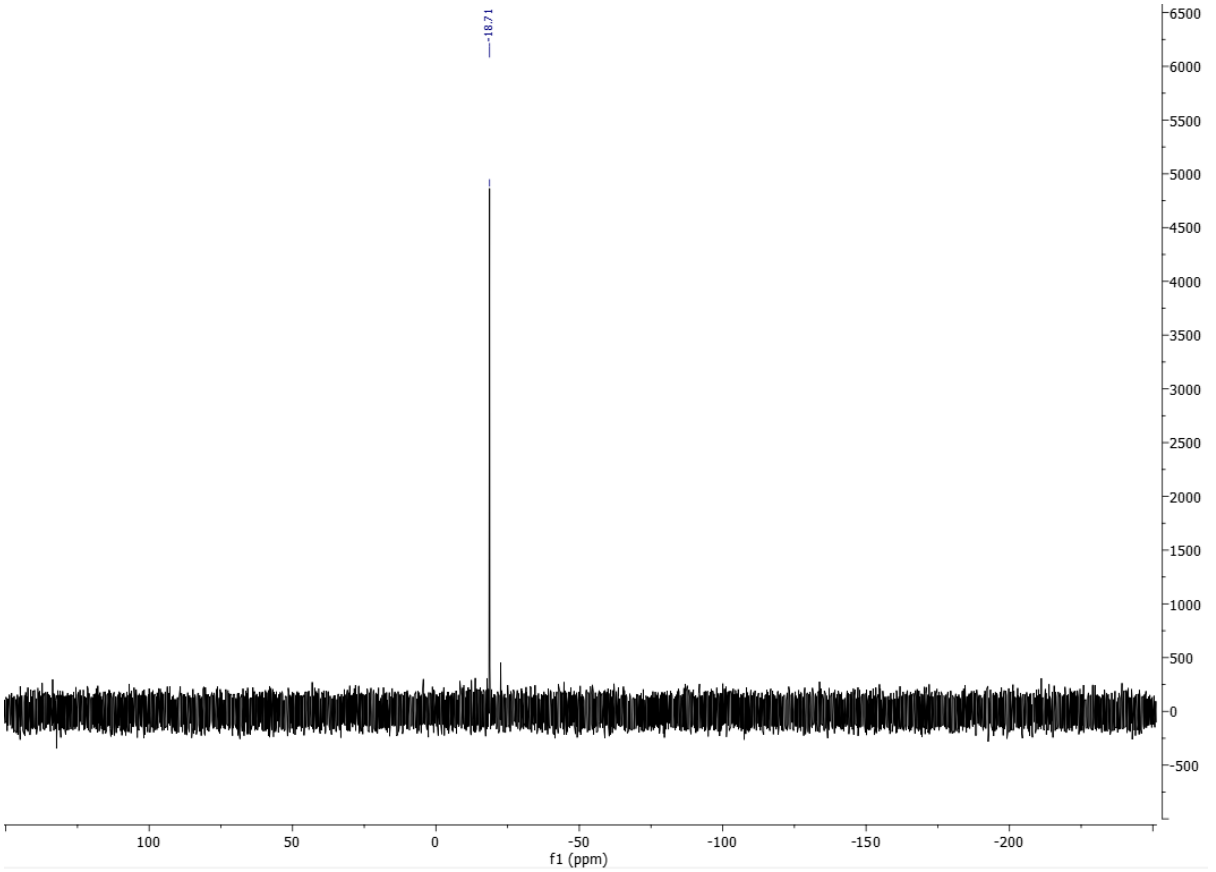
7a/c



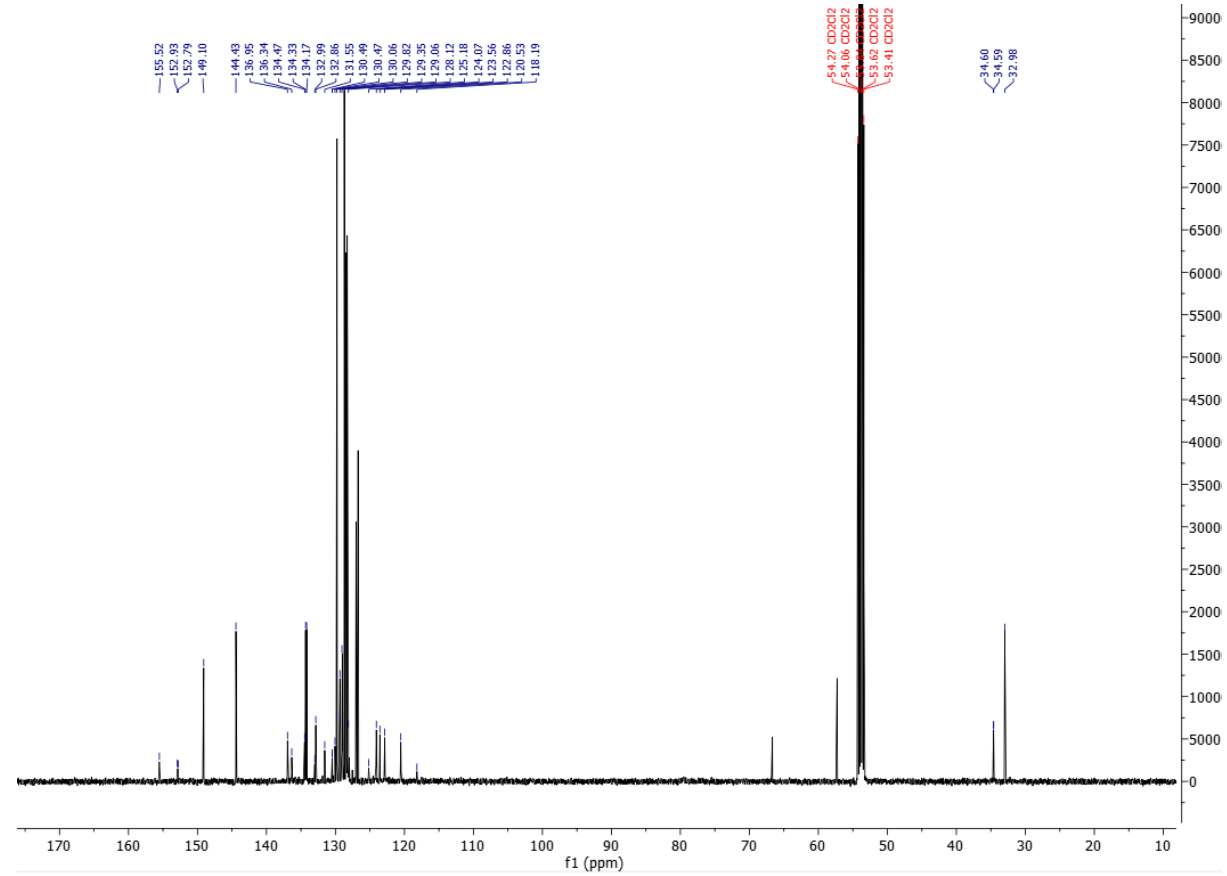
A 7.83: ^{1}H NMR spectrum of **7a**



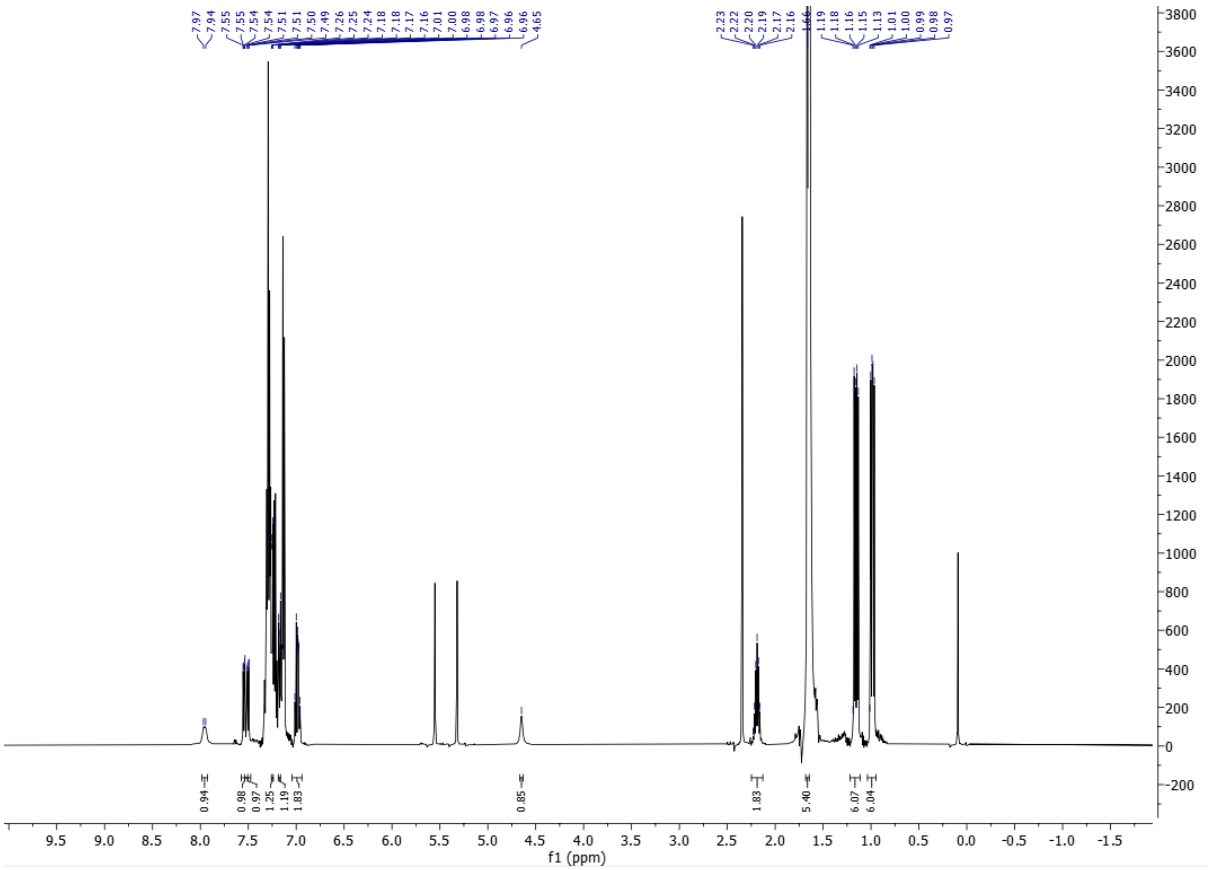
A 7.84: ^{11}B NMR spectrum of **7a**



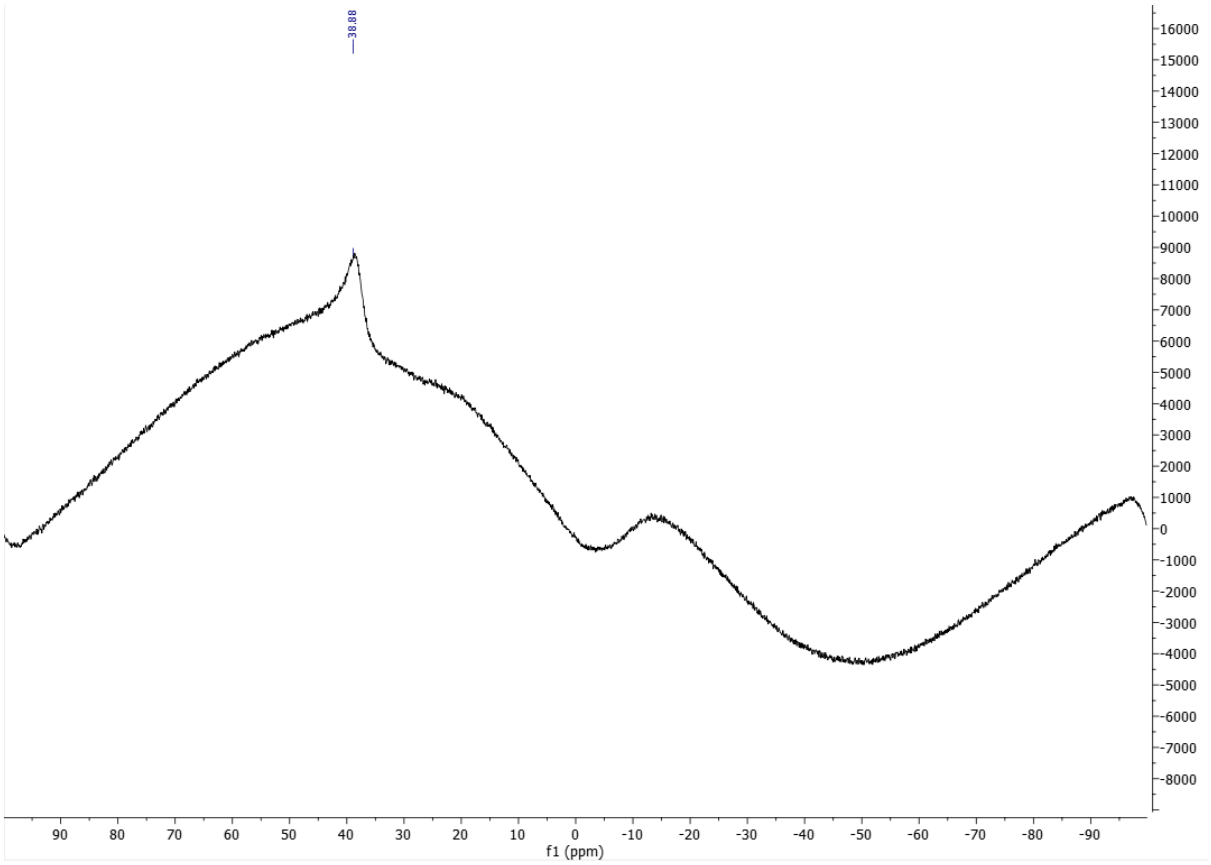
A 7.85: ^{31}P NMR spectrum of **7a**



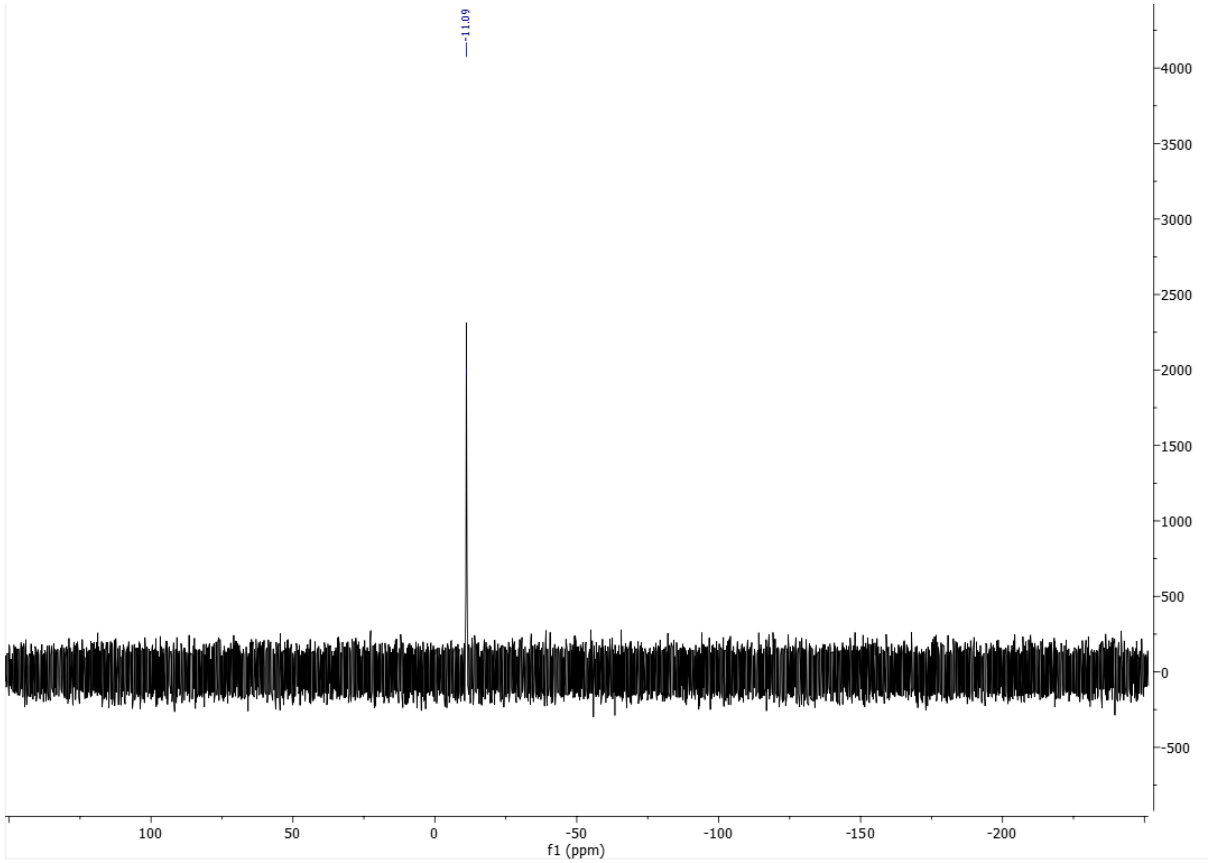
A 7.86: ^{13}C NMR spectrum of **7a**



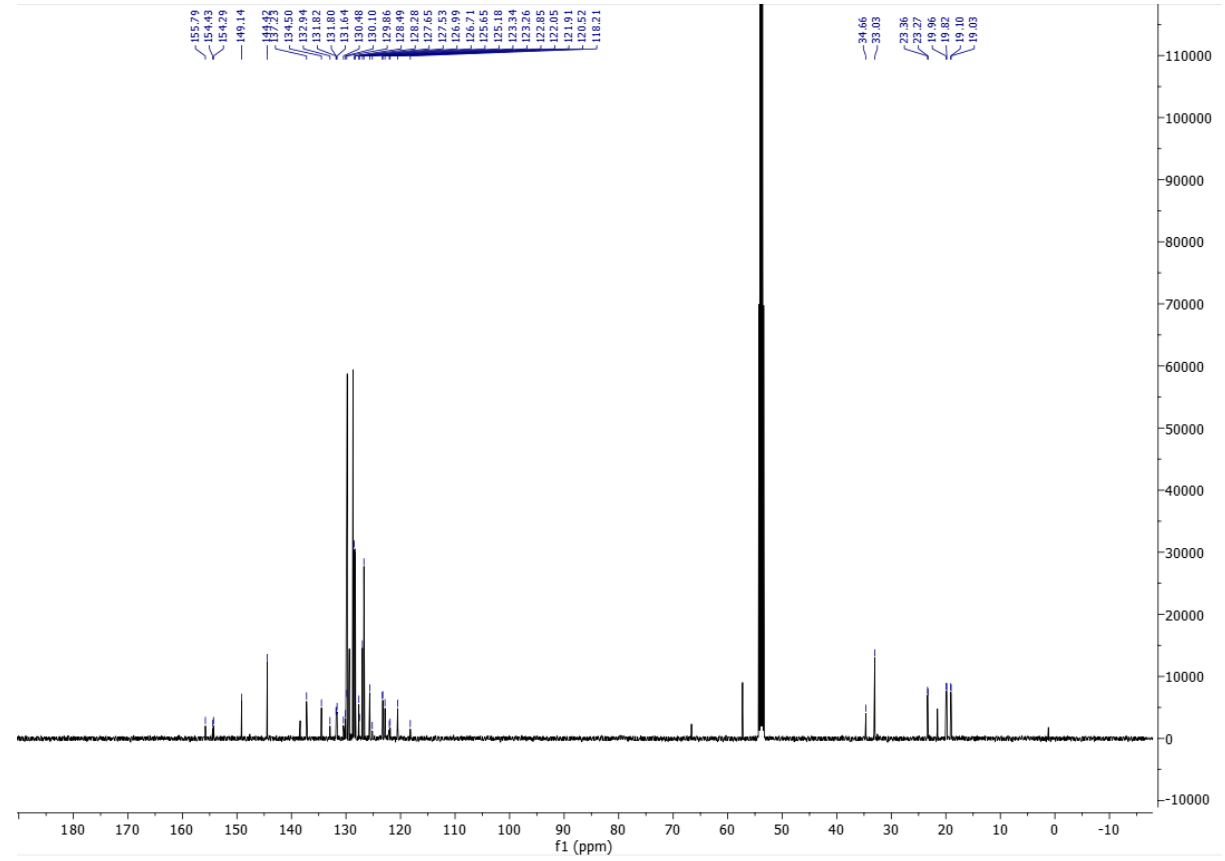
A 7.87: ^{1}H NMR spectrum of **7a**



A 7.88: ^{11}B NMR spectrum of **7a**

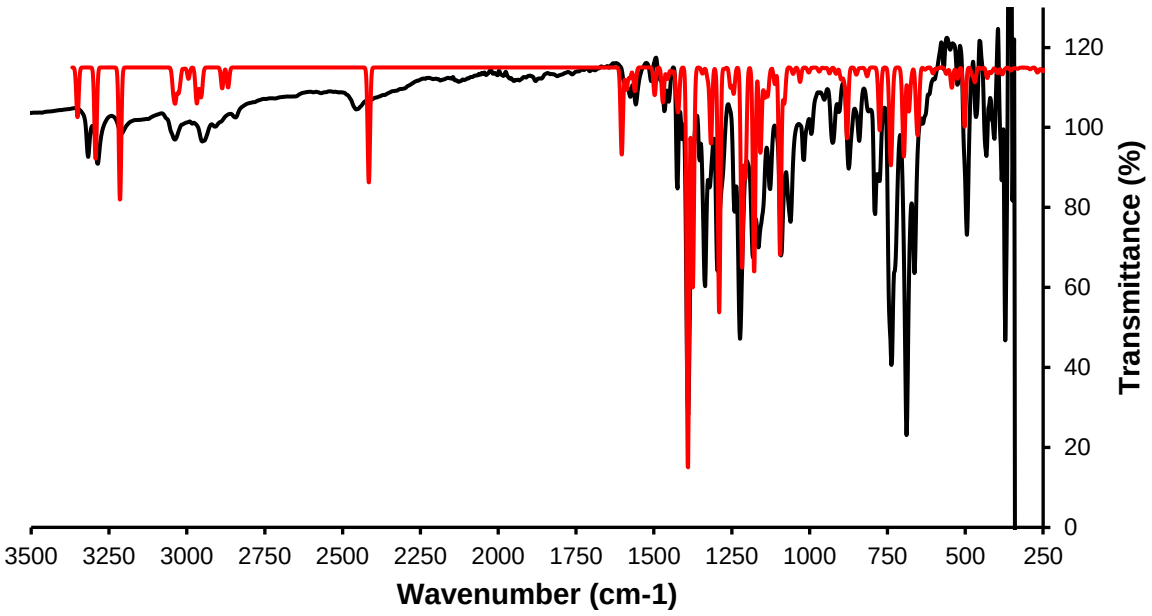


A 7.89: ^{31}P NMR spectrum of **7a**

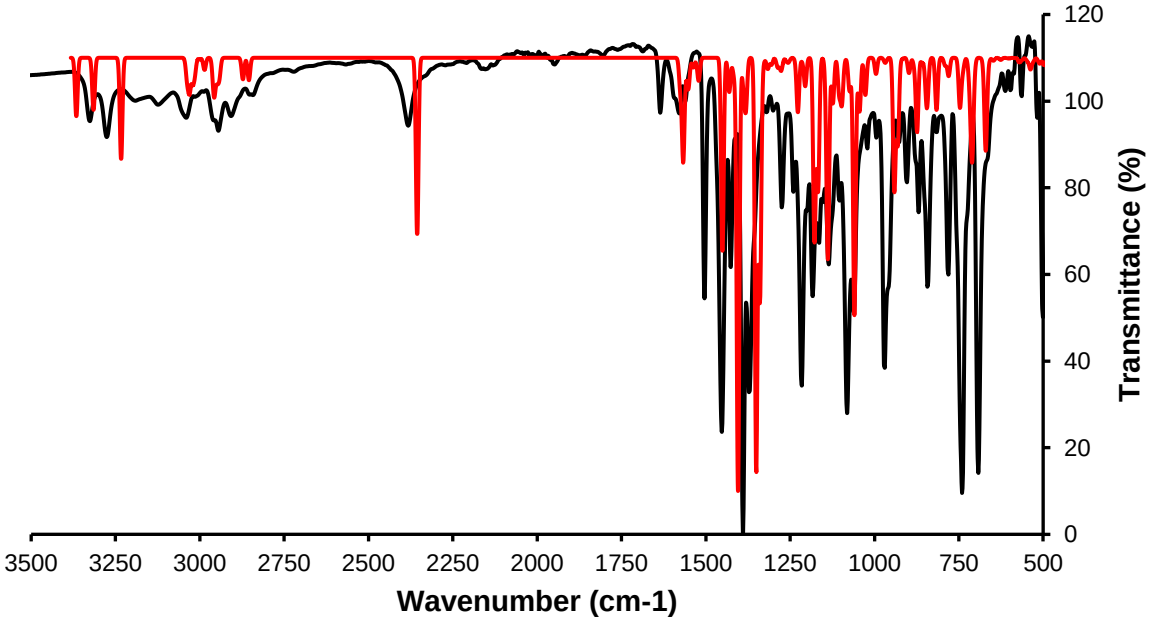


A 7.90: ^{13}C NMR spectrum of **7a**

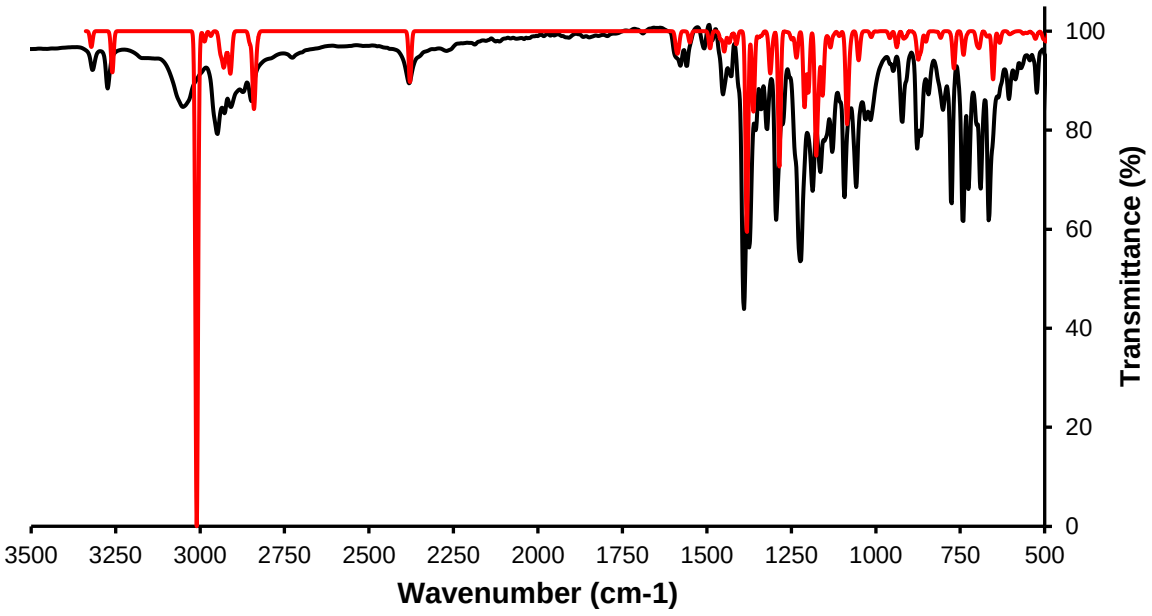
IR



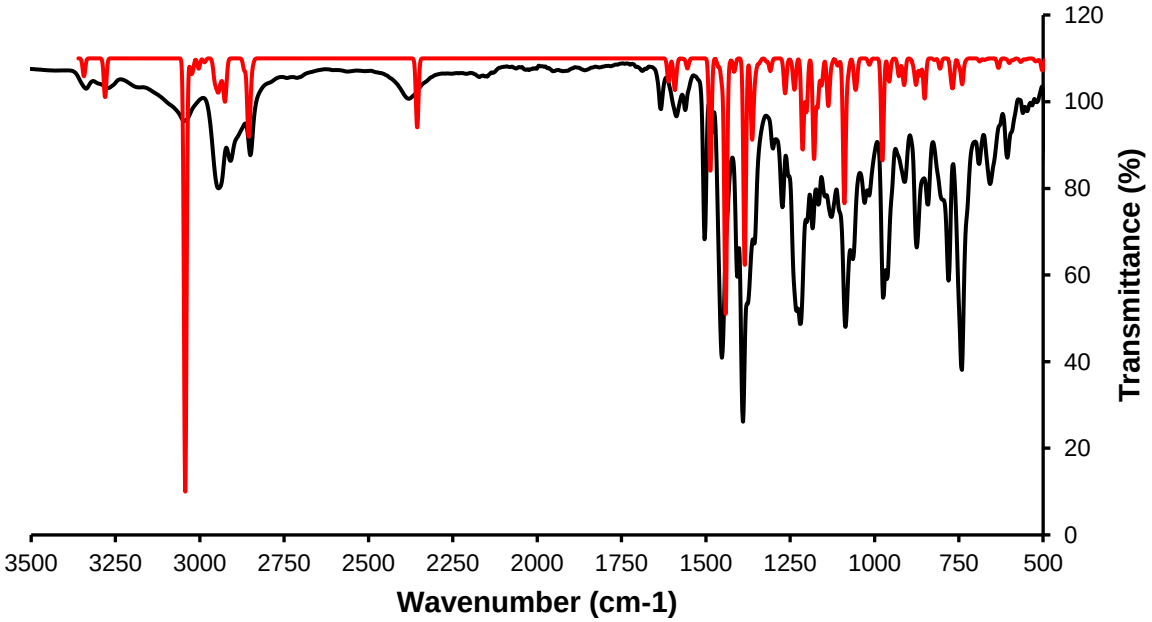
A 7.91: FT-IR spectra of **4a** in black and calculated spectra in red (R2-SCAN-3c see DFT methods, 0.965 linear scale factor applied)



A 7.92: FT-IR spectra of **4b** in black and calculated spectra in red (R2-SCAN-3c see DFT methods, 0.982 linear scale factor applied)



A 7.93: FT-IR spectra of **4c** in black and calculated spectra in red (R2-SCAN-3c see DFT methods, 0.984 linear scale factor applied)



A 7.94: FT-IR spectra of **4d** in black and calculated spectra in red (R2-SCAN-3c see DFT methods, 0.9803 linear scale factor applied)

Coordinates

1P_cip

Energy: -3844.333064

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C	-5.43095400	2.14596000	-3.62109400
C	-6.52558700	2.27536600	-4.49160000
C	-6.84022600	1.16523300	-5.28155600
C	-3.71366500	0.86774800	-2.32391900
C	-3.79711600	3.37987800	-2.41223000
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C	-1.74291200	2.38821700	-1.70163500
H	-1.12178000	1.51707700	-1.52332400
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C	-2.03077500	4.77020400	-1.61052400
C	-3.32939500	4.67582300	-2.13539300
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H	-7.66252200	1.21260100	-5.98640000
H	-0.22239600	3.75545000	-1.03897400
H	-1.63358800	5.75136600	-1.36335600
O	-5.08666000	3.27589300	-2.90235100
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H	-8.27826300	3.09275700	-6.63774200
C	-9.93181300	2.68468500	-5.32100500
H	-10.58063900	2.43365000	-6.16964900
H	-9.57917600	1.75083200	-4.87515300
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H	-8.52182500	5.54233600	-6.73478600
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C	-8.62743800	2.86680100	-2.16906700
H	-8.80095800	3.08644000	-1.10790400
H	-9.58097500	2.55513500	-2.60303200
H	-7.93388800	2.02195200	-2.22660500
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1P_cph

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C	-3.96606200	3.24509800	-1.86460400
C	-3.13751500	2.12137200	-1.82034700
C	-1.87198600	2.27406200	-1.25536500
H	-1.19221200	1.42940000	-1.21564000
C	-1.46756200	3.49691100	-0.72895700
C	-2.33964900	4.57655500	-0.74257100
C	-3.62492000	4.48396800	-1.30034800
H	-5.72791800	-0.22506100	-6.43693400
H	-4.13613200	-0.72495200	-4.62583200
H	-7.08526200	1.83685400	-6.37645400
H	-0.47670900	3.59940200	-0.29699200
H	-2.02189500	5.52175300	-0.30945100
O	-5.19644300	3.15920100	-2.49673700
B	-4.58505800	5.71844600	-1.20731300
P	-7.07085300	4.18788200	-4.50505100
C	-3.94223100	7.16330200	-1.00042600
C	-3.77266700	7.73818800	0.25643800
C	-3.51084800	7.89775300	-2.10312300
C	-3.19941700	9.00214200	0.42711900
C	-2.93595300	9.16495100	-1.97883300
C	-2.78099400	9.71753400	-0.70141400
C	-4.63176800	0.25015500	-1.16871800
H	-5.08747000	-0.69507300	-1.48353600
H	-4.05213100	0.08100300	-0.25473400
H	-5.43023700	0.96464700	-0.94571400
C	-2.61639900	-0.24870800	-2.56666900
H	-3.06405500	-1.19973600	-2.86729600
H	-1.93167600	0.08261900	-3.35448100
H	-2.03933800	-0.44791600	-1.65974400
N	-5.97130300	5.63599200	-1.24809800
H	-6.47322700	4.77732100	-1.42055100
H	-6.57236100	6.44214200	-1.16725700
Cl	-3.71104000	7.18446800	-3.68303900
Cl	-2.42190500	10.04447000	-3.37766000
Cl	-2.07100800	11.28473900	-0.51780000
Cl	-3.00478600	9.67996000	2.00801000
Cl	-4.27757800	6.82525300	1.65719600
C	-8.25671900	4.02815300	-3.10106300
C	-8.39650700	2.88162300	-2.31487600
C	-9.02150200	5.16083800	-2.78945500
C	-9.27911300	2.86999500	-1.23584600
H	-7.81855600	1.99069600	-2.54535100
C	-9.91313000	5.14170200	-1.72347300
H	-8.91318600	6.06393800	-3.38743000
C	-10.03966400	3.99635200	-0.93811700
H	-9.37428900	1.97267300	-0.63053200
H	-10.50329700	6.02561700	-1.49795400
H	-10.72722800	3.98482200	-0.09719400
C	-8.21164400	4.03672600	-5.94618400
C	-7.80622900	4.61783800	-7.15242800
C	-9.44289700	3.37489200	-5.88938800
C	-8.60867300	4.52511400	-8.28661200
H	-6.85663800	5.14615100	-7.20182200
C	-10.24902300	3.29327700	-7.02039500
H	-9.77178300	2.92304100	-4.95719800
C	-9.83268300	3.86495700	-8.22130400
H	-8.28184100	4.97852100	-9.21819500
H	-11.20486600	2.77950800	-6.96491900
H	-10.46436100	3.80003200	-9.10287200

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Energy: -2042.61409

C	-5.13597700	1.36891700	-5.88312500
C	-4.38003600	0.79834200	-4.86697500
C	-4.33474900	1.38437300	-3.60158100
C	-5.03583800	2.57653100	-3.41118900
C	-5.85918900	3.15153800	-4.39468600
C	-5.88162600	2.51718500	-5.64214100
C	-3.67340600	0.72792500	-2.39820900

C	-3.87502000	3.01600500	-1.38659700
C	-3.15467300	1.82436400	-1.48174400
C	-2.05427700	1.66743100	-0.63709300
H	-1.45879300	0.76236900	-0.69030100
C	-1.71958800	2.64364000	0.29456100
C	-2.49225200	3.79492400	0.39526100
C	-3.58161200	4.01976300	-0.45689200
H	-5.16396200	0.90447200	-6.86442200
H	-3.83462000	-0.11837500	-5.06187600
H	-6.48412500	2.92002100	-6.44789100
H	-0.86246500	2.50019600	0.94572700
H	-2.22742900	4.55561500	1.12626900
O	-4.96774100	3.24546900	-2.20344100
B	-4.39012000	5.36032700	-0.31982500
P	-6.71507600	4.74593100	-4.04153600
C	-4.64274500	6.34774600	-1.52918200
C	-5.71933600	7.23442900	-1.58093900
C	-3.78626000	6.39754200	-2.63069200
C	-5.94769800	8.10002000	-2.63839200
C	-3.96949200	7.26196600	-3.69966600
C	-5.06031400	8.11680800	-3.70399300
F	-6.62687600	7.26442500	-0.58182400
F	-2.71473400	5.59076300	-2.69387200
F	-3.12378900	7.26140700	-4.73639600
F	-7.01844000	8.90501700	-2.65122600
F	-5.27061300	8.93392300	-4.73762300
C	-7.79658700	4.30838000	-2.54741900
H	-7.08077100	4.40754800	-1.72000600
C	-7.83802600	4.94885600	-5.53988500
H	-7.13024300	4.83233200	-6.37394900
C	-8.98571700	3.95450100	-5.73217600
H	-9.42582700	4.08072000	-6.72982800
H	-8.66066900	2.91474400	-5.63512200
H	-9.78171400	4.12928700	-5.00177000
C	-8.34353500	6.39768600	-5.61888700
H	-9.06261400	6.62432900	-4.82648400
H	-7.51934500	7.11462400	-5.54223300
H	-8.84821500	6.56031700	-6.57895000
C	-8.37679800	2.89474500	-2.48530900
H	-8.83713500	2.73163300	-1.50215900
H	-9.14943200	2.73874000	-3.24326200
H	-7.60638600	2.13043000	-2.62451800
C	-8.88437600	5.36664400	-2.33602800
H	-9.69609300	5.25974800	-3.06228400
H	-9.31990200	5.25002100	-1.33660200
H	-8.49209900	6.38639600	-2.41117600
C	-4.77560100	-0.04454900	-1.62748800
H	-5.20630200	-0.82073100	-2.26983100
H	-4.34852100	-0.51516000	-0.73480300
H	-5.57854100	0.63018000	-1.31299200
C	-2.57737400	-0.26026700	-2.80448300
H	-2.99292300	-1.06004500	-3.42298700
H	-1.77406700	0.23423400	-3.36057800
H	-2.14872300	-0.74409300	-1.92319400
N	-4.82425000	5.71059900	0.96079500
H	-4.69095000	5.09642900	1.75047300
H	-5.30331300	6.56667800	1.19214500

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Energy: -2269.008318

C	-5.67392300	0.52090300	-5.68220500
C	-4.76449300	0.21975300	-4.67358200
C	-4.59412900	1.07884600	-3.58777900
C	-5.33457500	2.25996800	-3.57389200
C	-6.27171200	2.58434900	-4.56328300
C	-6.43156300	1.68510900	-5.62109200
C	-3.72885500	0.77106300	-2.37611200
C	-3.95436900	3.22541200	-1.91204000
C	-3.14523500	2.08702000	-1.88114300
C	-1.88321700	2.20714300	-1.30051200
H	-1.21820800	1.35047000	-1.26939800
C	-1.46479600	3.41152600	-0.74385000
C	-2.31634200	4.50738600	-0.74990500
C	-3.59387600	4.45134300	-1.33047500
H	-5.80130500	-0.16147500	-6.51724300
H	-4.19416800	-0.70105900	-4.73111700
H	-7.14553500	1.90687600	-6.40811200
H	-0.47898400	3.48689100	-0.29499300
H	-1.98965300	5.43778400	-0.29189100
O	-5.18639400	3.16868500	-2.54409500
B	-4.53182700	5.70168300	-1.21657700
P	-7.09877300	4.22713400	-4.49759000
C	-3.87697500	7.13452100	-0.99188300
C	-4.18024000	7.93792600	0.10242300
C	-2.94458200	7.65399200	-1.88496200
C	-3.59733000	9.18044400	0.31317900
C	-2.34533800	8.89448400	-1.71767600
C	-2.67496800	9.66051000	-0.60675100
C	-4.65872500	0.22109500	-1.26269900
H	-5.12743600	-0.71160700	-1.59531600
H	-4.07821500	0.02584400	-0.35444900
H	-5.44741800	0.94084500	-1.02213900
C	-2.65352200	-0.27322700	-2.67702700
H	-3.11301200	-1.21268900	-2.99551700
H	-1.96703700	0.06604900	-3.45990400
H	-2.07636900	-0.49835400	-1.77628700
N	-5.91983700	5.62101200	-1.22919000
H	-6.42392000	4.76193600	-1.39350700
H	-6.52203700	6.42490400	-1.13466100
C	-8.24809200	4.04578400	-3.06611000
C	-8.37305000	2.88527600	-2.29805800
C	-8.99761800	5.17620500	-2.71206200
C	-9.22477200	2.85817900	-1.19486200
H	-7.80733200	1.99568600	-2.56148500
C	-9.85876200	5.14206200	-1.62163100
H	-8.90087300	6.08992900	-3.29574400
C	-9.96943500	3.98305000	-0.85426800
H	-9.30836700	1.95013100	-0.60399100
H	-10.43692100	6.02481300	-1.36285500
H	-10.63232100	3.95957600	0.00599800
C	-8.27404700	4.09273800	-5.91206000
C	-7.89431700	4.68092900	-7.12344000
C	-9.50667000	3.43615600	-5.83135800
C	-8.72346900	4.60005400	-8.23899900
H	-6.94355600	5.20502900	-7.19164000
C	-10.33966100	3.36675000	-6.94367900
H	-9.81579900	2.97869000	-4.89518500
C	-9.94890900	3.94520000	-8.14979400
H	-8.41628200	5.05851000	-9.17479500
H	-11.29637700	2.85701600	-6.86930700
H	-10.60141800	3.88970800	-9.01671500
F	-2.60468800	6.94715400	-2.97752600
F	-1.46346900	9.36266700	-2.60851600
F	-2.10991600	10.85641000	-0.42667200
F	-3.91035300	9.91645600	1.38654600
F	-5.05834600	7.50899000	1.02940700

3T_cip

Energy: -3901.386304

C	-5.15078441	1.38583598	-6.34420405
C	-4.27089566	0.98247592	-5.35465422
C	-3.97405773	1.79196575	-4.25453983
C	-4.60292926	3.03276488	-4.16369531
C	-5.51059662	3.46204893	-5.15521607
C	-5.76431460	2.62727063	-6.24394018
C	-2.98821668	1.30708752	-3.21239018
C	-3.49226559	3.56984727	-2.10590497
C	-2.80576926	2.35349286	-2.12683183
C	-1.91306687	2.08213833	-1.08684703
H	-1.36970161	1.14231614	-1.08709170
C	-1.70593045	2.98307641	-0.05862492
C	-2.41489848	4.17392300	-0.05624367
C	-3.33235311	4.50883198	-1.06755745
H	-5.36031196	0.74007774	-7.19069288
H	-3.79434594	0.01062110	-5.43675697
H	-6.44469193	2.93876733	-7.02668527
H	-0.99708647	2.76232379	0.73321625
H	-2.22188969	4.88963622	0.73707442
O	-4.38707617	3.91023424	-3.12149523
B	-4.00731544	5.92265533	-0.86489861

P	-6.22298225	5.13243003	-5.04859421
C	-4.18549093	7.08719714	-1.94931282
C	-3.10636687	7.47498987	-2.75540752
C	-5.34023403	7.88252757	-2.04144374
C	-3.16100704	8.57388760	-3.61991314
C	-5.44515663	8.96066783	-2.92990301
C	-4.34909661	9.30229264	-3.72930468
C	-7.37134686	5.14839698	-3.57710969
H	-6.69342348	5.30848797	-2.72853558
C	-7.11856105	5.43797998	-6.65258643
H	-6.39754274	5.06292837	-7.39495521
C	-8.45521841	4.71614914	-6.85925829
H	-8.75880028	4.82368245	-7.90650294
H	-8.41109557	3.64918230	-6.62902753
H	-9.24322272	5.15865727	-6.24532448
C	-7.25924463	6.95052408	-6.88928950
H	-7.98188916	7.40392826	-6.20594577
H	-6.30537571	7.47639213	-6.77601587
H	-7.61795933	7.11980876	-7.91025236
C	-8.08924995	3.81157591	-3.37499899
H	-8.69193964	3.87538157	-2.46212467
H	-8.76365630	3.58445847	-4.20606363
H	-7.38873042	2.98002454	-3.26100723
C	-8.35821771	6.31640046	-3.64508299
H	-9.10439506	6.16850680	-4.42940916
H	-8.89320179	6.38251161	-2.69295884
H	-7.86285006	7.27628228	-3.81272928
C	-3.52701237	0.00544307	-2.57597945
H	-3.66913193	-0.77005045	-3.33459625
H	-2.82535760	-0.38125270	-1.83132747
H	-4.48695736	0.18936695	-2.08335999
C	-1.62878846	1.03283008	-3.89450346
H	-1.72940288	0.26916346	-4.67120524
H	-1.23897194	1.94671443	-4.35409772
H	-0.89517290	0.67164312	-3.16875851
N	-4.32851732	6.25887753	0.44943067
H	-4.26348337	5.59920747	1.21097959
H	-4.67736289	7.16025623	0.73699412
N	-3.54207719	6.23430231	-5.81949908
H	-3.42261282	5.67819986	-6.66279593
H	-3.41724339	7.21172576	-6.06984049
H	-4.80929587	5.95935876	-5.26470033
H	-2.80188930	5.97241137	-5.17162680
Cl	-1.60087430	6.59546473	-2.65632044
Cl	-1.78014693	9.04052548	-4.55787867
Cl	-4.45660459	10.62444596	-4.83435690
Cl	-6.89225877	9.90302949	-3.02824783
Cl	-6.71422211	7.56548343	-1.00981477

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Energy: -4127.776679

C	-5.56929081	1.25069145	-5.99567803
C	-4.57682676	0.85949859	-5.11030441
C	-4.08522088	1.71405306	-4.11908231
C	-4.64429235	2.98645457	-4.02282852
C	-5.63406278	3.41208922	-4.93093319
C	-6.08587379	2.53685118	-5.91636683
C	-2.96964350	1.25513933	-3.20199151
C	-3.24951374	3.59261644	-2.17012330
C	-2.57974306	2.36824433	-2.24176593
C	-1.52411647	2.14830992	-1.35351839
H	-0.98720405	1.20566301	-1.39234109
C	-1.15061187	3.10257837	-0.42337961
C	-1.86383817	4.28915270	-0.35102092
C	-2.94159316	4.57241947	-1.20701524
H	-5.92790448	0.56383805	-6.75518136
H	-4.16561404	-0.14206672	-5.19224324
H	-6.83279654	2.86627334	-6.63109169
H	-0.31595654	2.92044710	0.24627702
H	-1.55934887	5.03753966	0.37483183
O	-4.28696874	3.89623722	-3.05290996
B	-3.65539532	5.95345749	-0.92303900
P	-6.17443780	5.14362043	-4.88409542
C	-4.10360006	7.05338795	-1.99005783
C	-3.16720265	7.58748642	-2.87967814
C	-5.37289855	7.65003196	-1.98646288
C	-3.48064253	8.60053786	-3.79042395
C	-5.71397392	8.68739385	-2.86351996
C	-4.77053040	9.14016876	-3.79363258
C	-3.45156141	0.03378430	-2.38702223
H	-3.72942965	-0.78982884	-3.05177141
H	-2.65803510	-0.32241691	-1.72391211
H	-4.32108992	0.29709214	-1.77659684
C	-1.74861399	0.85878753	-4.06239370
H	-2.00987201	0.05977390	-4.76185512
H	-1.38675946	1.71803817	-4.63604398
H	-0.93092465	0.49208463	-3.43623474
N	-3.78014825	6.32194818	0.41508428
H	-3.55129116	5.70352375	1.17970715
H	-4.16357618	7.20413631	0.71973080
N	-3.30039425	5.74491463	-5.49696865
H	-3.24782031	5.08827035	-6.27168301
H	-2.95028526	6.64231818	-5.82238167
H	-4.70710040	5.77247012	-4.99484991
H	-2.67841901	5.41119543	-4.76492888
C	-6.98416769	5.52459381	-6.46215918
C	-6.31970240	6.34209753	-7.38210045
C	-8.26174823	5.03457411	-6.76182280
C	-6.92066099	6.65185238	-8.59868191
H	-5.34164143	6.75334271	-7.14891371
C	-8.85370393	5.34500179	-7.97944092
H	-8.79530075	4.42047210	-6.04099027
C	-8.18339515	6.15072455	-8.89876801
H	-6.40431109	7.29242935	-9.30713835
H	-9.84324976	4.96201707	-8.21001889
H	-8.65218055	6.39540953	-9.84740473
C	-7.48394658	5.26803252	-3.63031779
C	-7.62242490	4.29379377	-2.63801274
C	-8.40303687	6.31896266	-3.71614398
C	-8.68200778	4.37236861	-1.74080556
H	-6.92196926	3.46705684	-2.57209779
C	-9.45962440	6.38614241	-2.81686173
H	-8.30781347	7.07176181	-4.49350156
C	-9.60152139	5.41384820	-1.83047005
H	-8.79291020	3.61008818	-0.97539116
H	-10.17421514	7.20051534	-2.88922846
H	-10.43254576	5.46569709	-1.13309656
Cl	-6.57250000	7.12006882	-0.84141744
Cl	-7.26312002	9.45031910	-2.78321717
Cl	-5.18726962	10.37961419	-4.92174647
Cl	-2.29089583	9.19914379	-4.89988174
Cl	-1.51924380	7.00584429	-2.81458736

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Energy: -2099.675552

C	-5.22615900	1.22088300	-6.25008100
C	-4.26980600	0.88740800	-5.30307800
C	-3.93197800	1.75282200	-4.25847100
C	-4.60198700	2.97289400	-4.19416300
C	-5.55763800	3.35157200	-5.15856700
C	-5.86042400	2.45603400	-6.18489400
C	-2.84336100	1.37351600	-3.26749500
C	-3.49015100	3.59188700	-2.17136300
C	-2.71711600	2.43480100	-2.18555300
C	-1.81661600	2.25419100	-1.12984100
H	-1.18305600	1.37224000	-1.11683200
C	-1.72192900	3.16818100	-0.09270400
C	-2.55918600	4.27952700	-0.08132800
C	-3.45866400	4.52177600	-1.12420900
H	-5.47152600	0.52610200	-7.04670900
H	-3.76547300	-0.07112900	-5.37867000
H	-6.58930200	2.71386500	-6.94440500
H	-1.01460800	3.00562600	0.71458100
H	-2.50981400	4.97930700	0.74971200
O	-4.37608500	3.89426400	-3.20213500
B	-4.43066200	5.75370200	-0.97551700
P	-6.17102100	5.06709500	-5.13348600
C	-4.38036000	7.04458400	-1.89515100
C	-3.32800800	7.27972700	-2.78453600
C	-5.33791600	8.06478700	-1.85198700

C	-3.22705700	8.42087300	-3.56767800
C	-5.28014300	9.21430300	-2.62597100
C	-4.21231900	9.39516100	-3.49443500
F	-2.33659300	6.38134200	-2.92762300
F	-6.40664000	7.96428800	-1.04120300
F	-6.23868600	10.13878600	-2.54861200
F	-2.19671400	8.58207300	-4.41039700
F	-4.13733100	10.48502300	-4.25158800
C	-7.15611600	5.32694800	-3.57050000
H	-6.37118100	5.43163300	-2.81151300
C	-7.19401800	5.28901400	-6.66973200
H	-6.57841500	4.79544700	-7.43657800
C	-8.58020300	4.63628600	-6.65517100
H	-9.00627100	4.67688100	-7.66374100
H	-8.55482700	3.58972000	-6.34039500
H	-9.26175400	5.17352400	-5.98992900
C	-7.27403200	6.77572500	-7.04966600
H	-7.89435800	7.34307300	-6.35116200
H	-6.28470000	7.24317300	-7.08884200
H	-7.72786100	6.86537500	-8.04240100
C	-8.02610600	4.12797600	-3.18955900
H	-8.46747300	4.31342500	-2.20382100
H	-8.84364500	3.97649500	-3.89966300
H	-7.44219000	3.20485900	-3.13025800
C	-7.95289300	6.63415700	-3.61839200
H	-8.80017200	6.56554000	-4.30592700
H	-8.35402700	6.84098000	-2.62116300
H	-7.33522700	7.48829300	-3.91585500
C	-3.19862500	0.02153400	-2.60929700
H	-3.28722600	-0.76833600	-3.36061300
H	-2.41987700	-0.28065800	-1.90399200
H	-4.14694700	0.09526300	-2.06804400
C	-1.50239200	1.24553900	-4.02404100
H	-1.56660100	0.47350400	-4.79716700
H	-1.23587600	2.19448700	-4.50046200
H	-0.69860900	0.96757600	-3.33580400
N	-5.30985300	5.69213000	0.10551700
H	-5.33216500	4.88026500	0.70556600
H	-5.94549000	6.42007300	0.39062900
N	-3.42761100	6.08263100	-5.90701200
H	-3.27607900	5.52900200	-6.74672100
H	-3.27012500	7.05868000	-6.14435700
H	-4.70907000	5.82777200	-5.42718000
H	-2.72795600	5.80309200	-5.22264100

3T_fph

Energy: -2326.064242

C	-5.41800584	1.24118146	-6.08661650
C	-4.39784082	0.88804718	-5.21405823
C	-3.94830032	1.74943693	-4.20842060
C	-4.57238669	2.99035156	-4.10495319
C	-5.58167417	3.38586615	-5.00284344
C	-5.99969491	2.49956693	-5.99412624
C	-2.78198943	1.36282019	-3.31383787
C	-3.34188725	3.57173141	-2.14502610
C	-2.59279979	2.39962212	-2.21510683
C	-1.64722434	2.18452421	-1.20668214
H	-1.02432879	1.29576069	-1.24261789
C	-1.49068038	3.07613148	-0.15748284
C	-2.31418430	4.19401670	-0.08159816
C	-3.26051219	4.47340887	-1.07451448
H	-5.74508982	0.54581179	-6.85263796
H	-3.92922660	-0.08524230	-5.32342069
H	-6.76692563	2.80010888	-6.70068097
H	-0.74507891	2.88982921	0.60920096
H	-2.21468805	4.87535545	0.75987432
O	-4.25390659	3.91188694	-3.14202114
B	-4.20480391	5.71445567	-0.84567882
P	-6.09160947	5.12738861	-5.00839579
C	-4.34838398	6.92853234	-1.85148178
C	-3.36674212	7.22289983	-2.79803570
C	-5.43385419	7.80892992	-1.84258911
C	-3.45475310	8.28497952	-3.68610984
C	-5.57457495	8.86385869	-2.73224190
C	-4.57423739	9.10474695	-3.66406653
F	-2.25401306	6.46773617	-2.88210135
F	-6.42634696	7.65385242	-0.95220142
F	-6.65451170	9.64869915	-2.70051001
F	-2.47571572	8.52279321	-4.57207170
F	-4.68342057	10.11448877	-4.52378705
C	-3.05709002	-0.01511516	-2.67380033
H	-3.18004316	-0.78527804	-3.44014492
H	-2.22350746	-0.32151609	-2.03700669
H	-3.96508314	0.01805196	-2.06382222
C	-1.50206546	1.28792928	-4.17634880
H	-1.61560831	0.54269301	-4.97034265
H	-1.28945853	2.25812503	-4.63725224
H	-0.64289321	1.00239716	-3.56154828
N	-4.87340077	5.74730452	0.37771469
H	-4.79953946	4.98637013	1.03720239
H	-5.46593154	6.49769999	0.69635021
N	-3.24076880	5.81496416	-5.76347552
H	-3.14222428	5.10718441	-6.48690107
H	-2.98534156	6.71293068	-6.16527297
H	-4.62649237	5.75906998	-5.26208076
H	-2.57331025	5.59914650	-5.02691553
C	-7.07616188	5.38554175	-6.50958058
C	-6.47840716	5.98190497	-7.62417136
C	-8.41572179	4.98283068	-6.56699567
C	-7.21433352	6.16723194	-8.79064429
H	-5.44377368	6.31135603	-7.58582457
C	-9.14370721	5.17024059	-7.73542273
H	-8.88720954	4.52825538	-5.69963602
C	-8.54428454	5.76115260	-8.84645701
H	-6.74990056	6.63602205	-9.65283304
H	-10.18243206	4.85681903	-7.77842230
H	-9.11845637	5.90989004	-9.75622604
C	-7.22006310	5.45940178	-3.62513515
C	-7.38434570	4.54897748	-2.57966241
C	-7.97702249	6.63763117	-3.65739057
C	-8.31264814	4.81444733	-1.57661450
H	-6.80999104	3.62810056	-2.55343094
C	-8.90485545	6.88912642	-2.65521441
H	-7.85937981	7.34595748	-4.47420467
C	-9.07562533	5.97667992	-1.61591679
H	-8.44511275	4.10126469	-0.76845739
H	-9.49487686	7.80008458	-2.68683931
H	-9.80523314	6.17432764	-0.83608157

I1_cip

Energy: -3844.750456

C	-7.07368300	-0.59906600	-0.72059600
C	-5.71718600	-0.61626000	-0.40319300
C	-5.07013200	0.54527800	0.01351400
C	-5.83311000	1.70859500	0.08201900
C	-7.19526200	1.76738400	-0.22136300
C	-7.80881900	0.57611000	-0.62623500
C	-3.60496900	0.63649500	0.42608600
C	-3.93287900	3.06960000	-0.04798300
C	-3.08561000	1.96544000	-0.11126600
C	-1.81301400	2.17025700	-0.64063400
H	-1.12036700	1.33824700	-0.71410700
C	-1.40608800	3.42909200	-1.08807500
C	-2.28017700	4.49884200	-1.03707700
C	-3.58171900	4.35283500	-0.50844900
H	-7.56178500	-1.51350000	-1.04298800
H	-5.16587700	-1.54669600	-0.48519800
H	-8.86227800	0.56515800	-0.88383800
H	-0.40732100	3.55854000	-1.49212000
H	-1.96709400	5.46941900	-1.41232300
O	-5.21560500	2.90502100	0.42733500
B	-4.55177900	5.52912100	-0.56363500
P	-8.02979500	3.39230000	-0.10947300
C	-4.33623200	6.75312500	-1.52601500
C	-3.65903900	7.89970200	-1.12868500
C	-4.83910600	6.70397500	-2.82116600
C	-3.45224400	8.97251500	-1.99832800
C	-4.66248600	7.75255600	-3.72444100
C	-3.95803500	8.89180300	-3.30520500
C	-8.55728700	3.47244600	1.69011200

H	-7.57727200	3.53017400	2.19280300
C	-9.49044400	3.32662400	-1.27873900
H	-9.09818800	2.73589700	-2.12005100
C	-10.78198500	2.67420300	-0.77605300
H	-11.49409700	2.61491500	-1.60704500
H	-10.63524400	1.66390600	-0.38816900
H	-11.24774900	3.27562700	0.01017400
C	-9.77024300	4.74911300	-1.78817000
H	-10.12975800	5.39619900	-0.98031500
H	-8.87758900	5.20758500	-2.22472300
H	-10.54940100	4.71713300	-2.55768800
C	-9.29184700	2.25581500	2.25475000
H	-9.33114400	2.33529500	3.34735700
H	-10.32025200	2.20078500	1.89106000
H	-8.78437800	1.31952700	2.00421300
C	-9.31016200	4.77940300	1.96359500
H	-10.30151000	4.77147300	1.50005300
H	-9.45228400	4.90627300	3.04232400
H	-8.76960200	5.65607400	1.58840900
C	-3.53340600	0.67603900	1.97418700
H	-3.93266400	-0.25606000	2.38697800
H	-2.49182700	0.78705600	2.29303000
H	-4.11202300	1.51073300	2.38052500
C	-2.78619500	-0.55256100	-0.07476200
H	-3.17834800	-1.48416500	0.34159900
H	-2.79751200	-0.62346600	-1.16740300
H	-1.74944500	-0.47223300	0.26296700
N	-5.82048100	5.55826800	0.26033800
H	-5.66699900	5.24269100	1.22019000
H	-6.26181300	6.47805600	0.29175800
H	-6.62315500	4.82543800	-0.09398100
Cl	-3.07030900	7.94870700	0.51338100
Cl	-2.59423400	10.37245200	-1.47309100
Cl	-3.71759200	10.20050800	-4.39983300
Cl	-5.29982400	7.64875100	-5.32295300
Cl	-5.72278100	5.26596400	-3.27013000

I1_cph

Energy: -4071.145061

C	-7.19313800	-0.67821600	-0.65054100
C	-5.83677400	-0.65725000	-0.33665100
C	-5.18496600	0.54527300	-0.06197700
C	-5.94225000	1.70871900	-0.14537700
C	-7.30545300	1.72592600	-0.44502800
C	-7.92810700	0.50089000	-0.69595000
C	-3.73703500	0.66832800	0.39226500
C	-4.02108500	3.06883400	-0.27117500
C	-3.18364300	1.95619200	-0.20455100
C	-1.86641100	2.12613200	-0.62645800
H	-1.18341900	1.28326100	-0.60364500
C	-1.39381900	3.36176600	-1.07440200
C	-2.24026200	4.45168100	-1.10922100
C	-3.59140400	4.34195500	-0.70515100
H	-7.68265800	-1.62510100	-0.85573800
H	-5.28811800	-1.59207600	-0.29933400
H	-8.98610400	0.47610400	-0.93874000
H	-0.36069900	3.45975500	-1.39111800
H	-1.86939100	5.41326900	-1.45309600
O	-5.34490700	2.94663900	0.07241400
B	-4.47091500	5.57535900	-0.78536200
P	-8.14754400	3.34748600	-0.56741600
C	-4.03627500	6.90156600	-1.50340400
C	-3.40854700	7.92994600	-0.81068900
C	-4.27930300	7.07484200	-2.86114500
C	-2.99524500	9.10204600	-1.44606100
C	-3.88674500	8.22961400	-3.53915800
C	-3.23560500	9.24545900	-2.82173700
C	-3.73343400	0.82243600	1.93527800
H	-4.15580000	-0.07580500	2.39737500
H	-2.70727400	0.95717800	2.29315100
H	-4.32736600	1.68642300	2.25033400
C	-2.90349900	-0.55545700	0.01371000
H	-3.31785500	-1.45382400	0.47800700
H	-2.86944000	-0.70332500	-1.07062000
H	-1.88180800	-0.45622500	0.38955300
N	-5.87337800	5.60568200	-0.15817500
H	-5.88209200	5.23683800	0.79801700
H	-6.28637600	6.53983100	-0.13727000
H	-6.56140400	4.96998700	-0.66129300
Cl	-3.15461800	7.69532500	0.89977400
Cl	-2.20759200	10.34974000	-0.55535300
Cl	-2.73535100	10.68003900	-3.63317100
Cl	-4.20043300	8.40369700	-5.22471100
Cl	-5.11746900	5.78471200	-3.68388600
C	-9.80913200	2.92832700	-1.20428500
C	-10.00478800	2.97290600	-2.58924400
C	-10.86568300	2.55562600	-0.36723100
C	-11.24016000	2.63284500	-3.13105000
H	-9.18977800	3.27283600	-3.24395900
C	-12.10208300	2.22706100	-0.91427200
H	-10.72308900	2.52148000	0.70949400
C	-12.28992600	2.26265700	-2.29414300
H	-11.38570200	2.66687800	-4.20673100
H	-12.92029200	1.93975600	-0.26028700
H	-13.25680400	2.00574500	-2.71709600
C	-8.44128900	3.80550000	1.18888800
C	-8.02107200	3.02825400	2.27124700
C	-9.06047200	5.04024200	1.43252700
C	-8.22189500	3.47639100	3.57541200
H	-7.54671800	2.06567100	2.10035600
C	-9.27204800	5.47626300	2.73539900
H	-9.39584900	5.65414200	0.59784900
C	-8.84791400	4.69648800	3.81059700
H	-7.89534800	2.86220000	4.40977500
H	-9.76690800	6.42688000	2.91242300
H	-9.00822800	5.03987400	4.82842500

I1_fip

Energy: -2043.028661

C	-7.16082400	-0.60618000	-0.76629400
C	-5.80209600	-0.62619700	-0.46041900
C	-5.14415100	0.54016200	-0.07420100
C	-5.89865000	1.70921600	-0.02896400
C	-7.26767400	1.76822400	-0.30025600
C	-7.89052900	0.57322600	-0.67744000
C	-3.68238400	0.62358300	0.34862000
C	-3.97746600	3.05420900	-0.17530600
C	-3.13907400	1.94062700	-0.19252700
C	-1.84118900	2.12781000	-0.66272700
H	-1.15497200	1.28800100	-0.69702900
C	-1.39431700	3.38131400	-1.08626100
C	-2.25634600	4.46002000	-1.08293600
C	-3.59279500	4.33078500	-0.63806500
H	-7.65718100	-1.52320100	-1.06817200
H	-5.25803700	-1.56211500	-0.52554100
H	-8.94838800	0.56067100	-0.91573800
H	-0.37144300	3.50010800	-1.42846300
H	-1.90386700	5.42920600	-1.42426000
O	-5.27136200	2.91528900	0.26781700
B	-4.52318800	5.53597000	-0.71727700
P	-8.09404300	3.39750200	-0.16274100
C	-4.26236600	6.76485100	-1.63897800
C	-4.40063700	8.07846200	-1.18127400
C	-3.87116900	6.62402000	-2.97589400
C	-4.15018900	9.18839000	-1.96927900
C	-3.62951000	7.71138700	-3.80216300
C	-3.76379000	8.99878700	-3.29277000
F	-4.75506700	8.29487600	0.10182000
F	-3.75988500	5.40589500	-3.51806100
F	-3.27914900	7.53705400	-5.07428900
F	-4.27029000	10.42051800	-1.47983100
F	-3.52543200	10.04633900	-4.06850200
C	-8.41924300	3.51261400	1.68804500
H	-7.39198600	3.61664700	2.07560100
C	-9.69061600	3.25074000	-1.13159900
H	-9.38859100	2.65408200	-2.00542800
C	-10.87934300	2.56527300	-0.45114900
H	-11.68803800	2.44847100	-1.18188800
H	-10.64094200	1.57615700	-0.05406900
H	-11.26748400	3.17560200	0.36954700

C	-10.09205500	4.64622500	-1.63362100
H	-10.35942100	5.30725600	-0.80185100
H	-9.28696100	5.12023900	-2.20338300
H	-10.96897200	4.56381200	-2.28531800
C	-9.03772200	2.29148900	2.37083600
H	-8.95017500	2.40528900	3.45774800
H	-10.09917200	2.18815400	2.13513200
H	-8.52907800	1.36493800	2.08826600
C	-9.17939800	4.80270200	2.01633500
H	-10.21921400	4.74967300	1.67926900
H	-9.19389700	4.95877000	3.10062700
H	-8.72104200	5.68451900	1.55360000
C	-3.62898200	0.68032200	1.89727700
H	-4.04454600	-0.24200000	2.31592500
H	-2.59031300	0.78365500	2.22820700
H	-4.20356900	1.52645000	2.28598900
C	-2.87001300	-0.57976000	-0.12880600
H	-3.27953600	-1.50264100	0.28997400
H	-2.86608300	-0.66036200	-1.22079300
H	-1.83770500	-0.50983600	-0.62032600
C	-5.86059100	-0.62555200	-0.43600900
C	-5.19324100	0.56015900	-0.12721400
C	-5.93618300	1.73424300	-0.18016300
C	-7.30138900	1.77672700	-0.46698100
C	-7.93972000	0.56771700	-0.75275300
C	-3.74957900	0.65019900	0.34849300
C	-3.99498100	3.07408600	-0.25379500
C	-3.16901300	1.95268100	-0.18853100
C	-1.83469100	2.12471800	-0.55077100
H	-1.15735800	1.27765200	-0.52060400
C	-1.33664500	3.37049900	-0.93839400
C	-2.17832700	4.46269600	-0.99525200
C	-3.54991700	4.35106800	-0.66513900
H	-7.71851500	-1.55470100	-0.98232500
H	-5.32463200	-1.56836100	-0.42435900
H	-8.99994400	0.56226300	-0.98719300
H	-0.28731200	3.47452700	-1.19409000
H	-1.78103100	5.43033600	-1.28747500
O	-5.32495000	2.95856900	0.06410700
B	-4.43191100	5.58611800	-0.76416200
P	-8.12736700	3.41166200	-0.49698000
C	-4.07189300	6.85699700	-1.58567000
C	-4.23866800	8.14668800	-1.07173800
C	-3.56687300	6.78147500	-2.89004100
C	-3.91061900	9.29309400	-1.77363300
C	-3.24391600	7.90786700	-3.63160600
C	-3.41176700	9.16819100	-3.06710700
C	-3.76821800	0.74356700	1.89643200
H	-4.20872200	-0.16659000	2.31644300
H	-2.74650500	0.85164800	2.27556300
H	-4.35753800	1.60171100	2.23553500
C	-2.92456200	-0.56835900	-0.06581400
H	-3.35838400	-1.47970500	0.35310100
H	-2.87298100	-0.67150200	-1.15461800
H	-1.90865900	-0.49896700	0.33145800
N	-5.78469700	5.62779600	-0.03080300
H	-5.73812500	5.24082900	0.91618800
H	-6.19745800	6.55925000	0.03454100
H	-6.50475500	5.00987500	-0.51032000
C	-9.79634700	3.03565300	-1.14340500
C	-9.98923000	3.11018500	-2.52763800
C	-10.86064600	2.66577300	-0.31533200
C	-11.22912200	2.80165800	-3.07744900
H	-9.16815200	3.40736200	-3.17606400
C	-12.10189700	2.36940000	-0.87028400
H	-10.72064900	2.60809100	0.76066000
C	-12.28686700	2.43402800	-2.24925900
H	-11.37192600	2.85815200	-4.15257100
H	-12.92596900	2.08402300	-0.22282700
H	-13.25723500	2.20169800	-2.67838600
C	-8.40305900	3.77044400	1.28510000
C	-8.02592500	2.90604600	2.31600900
C	-8.96775200	5.01340600	1.60586900
C	-8.21616900	3.27721100	3.64566100
H	-7.59311900	1.93638800	2.08510600
C	-9.16919400	5.37320900	2.93349900
H	-9.26828000	5.69501600	0.81139800
C	-8.78863000	4.50661000	3.95718100
H	-7.92325100	2.59621800	4.43968800
H	-9.62133900	6.33208800	3.17022200
H	-8.94048500	4.79006900	4.99457500
F	-4.70449100	8.29806800	0.18469000
F	-4.06285000	10.49896400	-1.23163300
F	-3.10021500	10.25163700	-3.76259100
F	-2.78475000	7.79689600	-4.87547700
F	-3.42201100	5.59294900	-3.48604000

I2_cip

Energy: -3844.789847

C	-5.46505554	1.15352161	-5.74201252
C	-4.66216367	0.65392741	-4.72760223
C	-4.44525432	1.35239094	-3.53775948
C	-5.05599733	2.59591428	-3.39233023
C	-5.94017540	3.08290632	-4.37693949
C	-6.12355309	2.35969086	-5.55757347
C	-3.61956226	0.73553788	-2.42672623
C	-4.01129864	2.99896624	-1.28223658
C	-3.47384858	1.71235575	-1.27061455
C	-2.72246436	1.33312069	-0.15623028
H	-2.30650225	0.33121224	-0.11116528
C	-2.48458280	2.21212431	0.88644446
C	-2.96277412	3.50993485	0.79835668
C	-3.73412854	3.95763443	-0.28657582
H	-5.59860659	0.59511428	-6.66222301
H	-4.18937814	-0.31388137	-4.86381012
H	-6.78230797	2.72550477	-6.33594490
H	-1.89707000	1.89975403	1.74383108
H	-2.68789592	4.20020942	1.58883767
O	-4.85906506	3.40834194	-2.31040861
B	-4.04618707	5.49940313	-0.35070671
P	-6.96559807	4.51744552	-4.03744219
C	-4.45430165	6.33618070	-1.65026644
C	-5.58759230	7.15720838	-1.66971226
C	-3.60112594	6.41494666	-2.75529208
C	-5.85981474	8.03699788	-2.72523620
C	-3.85048748	7.26380234	-3.83986799
C	-4.97899392	8.09333190	-3.81296945
Cl	-6.72329064	7.07916755	-0.34274951
Cl	-2.14940256	5.45322300	-2.76305036
Cl	-2.77735092	7.31072020	-5.19207388
Cl	-7.26231239	9.04941675	-2.69966756
Cl	-5.28378198	9.18113753	-5.11987692
C	-7.97181124	4.22138639	-2.51673528
H	-7.22207059	4.31468188	-1.71763729
C	-7.91033952	4.99046474	-5.54942812
H	-7.17834383	4.83468369	-6.35524841
C	-9.14191160	4.11038626	-5.80155629
H	-9.53105370	4.34226598	-6.79782159
H	-8.92612091	3.03947320	-5.76466959
H	-9.93409874	4.32542232	-5.07972383
C	-8.27018767	6.48233274	-5.53316351
H	-9.01030218	6.71888829	-4.76512819
H	-7.39221736	7.11580426	-5.38163378
H	-8.70357103	6.73866938	-6.50512184
C	-8.55652569	2.80630131	-2.48054471
H	-9.05538235	2.66838355	-1.51613689
H	-9.30200127	2.65425755	-3.26644715
H	-7.78577850	2.03626402	-2.57537243
C	-9.04237649	5.30052577	-2.32255099
H	-9.86531441	5.17930990	-3.03193858
H	-9.45390371	5.19720864	-1.31373470
H	-8.64321866	6.31413010	-2.41241474
C	-4.33331037	-0.54669478	-1.94268099
H	-4.44231547	-1.26206462	-2.76359434
H	-3.75725297	-1.03228668	-1.14986505
H	-5.32820017	-0.30950036	-1.55256566
C	-2.21454431	0.38456298	-2.96447816
H	-2.28059450	-0.33097274	-3.78921120
H	-1.70453181	1.28444645	-3.32211421
H	-1.60327835	-0.07128265	-2.18113967

H	-6.13884209	5.61124358	-3.74778757
N	-3.84200244	6.29470216	0.77766934
H	-3.61260094	5.94558862	1.69527894
H	-3.96884886	7.29542266	0.76795593

I2_cph

Energy: -4071.173432

C	-5.66673300	0.36565900	-5.49301700
C	-4.71015500	0.10781400	-4.51110700
C	-4.54187100	0.95030400	-3.41298500
C	-5.35457000	2.07995100	-3.34589500
C	-6.31261500	2.36117800	-4.32621200
C	-6.47564400	1.48889900	-5.40656400
C	-3.60189300	0.69127100	-2.24559300
C	-3.98862400	3.12459200	-1.73986100
C	-3.10584700	2.04635200	-1.75101200
C	-1.82996900	2.26489600	-1.23052800
H	-1.10370300	1.45947800	-1.22257500
C	-1.47188600	3.50703800	-0.71613700
C	-2.38864200	4.54936900	-0.71246500
C	-3.68825300	4.38671100	-1.21794700
H	-5.77610400	-0.31402900	-6.33150400
H	-4.09073300	-0.77766200	-4.60650200
H	-7.21208100	1.70172400	-6.17573300
H	-0.47314000	3.65819100	-0.31869400
H	-2.09546100	5.51612500	-0.31131000
O	-5.25502600	2.97363600	-2.31689100
B	-4.69029200	5.59008900	-1.16287800
P	-7.26616900	3.86880700	-4.17422600
C	-4.10667600	7.06756100	-1.24317600
C	-3.87412400	7.84329400	-0.10956400
C	-3.79026100	7.63030700	-2.47643800
C	-3.34946100	9.13728100	-0.18764400
C	-3.27067000	8.91978600	-2.60459000
C	-3.05025900	9.67658100	-1.44587500
C	-4.43141300	0.04113900	-1.10809300
H	-4.83221300	-0.92257500	-1.44021300
H	-3.79195200	-0.12178300	-0.23451700
H	-5.26671900	0.68198400	-0.80752900
C	-2.45861400	-0.25060400	-2.62467800
H	-2.85137600	-1.21910200	-2.94497600
H	-1.84090900	0.16438700	-3.42772500
H	-1.82328300	-0.44635200	-1.75754300
H	-6.37648800	4.91454600	-3.87948500
N	-6.07059000	5.44567700	-1.03575700
H	-6.52909200	4.55308600	-0.92823600
H	-6.69171100	6.23326500	-0.92291400
Cl	-4.06111900	6.66177200	-3.91140500
Cl	-2.90346700	9.57719400	-4.16018100
Cl	-2.40756700	11.27412100	-1.57031600
Cl	-3.07046100	10.06370900	1.24324500
Cl	-4.23122400	7.14840600	1.45134200
C	-8.46617600	3.77265600	-2.83754500
C	-8.64668100	2.58417300	-2.12768900
C	-9.20425700	4.91950200	-2.51938400
C	-9.57175700	2.54687700	-1.08855200
H	-8.07294100	1.69697500	-2.38092800
C	-10.12292800	4.86871400	-1.47993200
H	-9.06290100	5.84187800	-3.07801400
C	-10.30473800	3.68469000	-0.76527700
H	-9.71808500	1.62626400	-0.53235300
H	-10.69867000	5.75347300	-1.22636400
H	-11.02424800	3.65093400	0.04742100
C	-8.06879700	4.27751100	-5.72566300
C	-7.35183200	4.99823800	-6.68749100
C	-9.37446800	3.84529000	-5.97734900
C	-7.95073400	5.28270200	-7.90824000
H	-6.33899200	5.33760400	-6.48438400
C	-9.96042900	4.13540200	-7.20403100
H	-9.92906200	3.29409800	-5.22260400
C	-9.25058400	4.85118500	-8.16523800
H	-7.40410500	5.84706700	-8.65723700
H	-10.97449000	3.80571200	-7.40728000
H	-9.71511300	5.07951200	-9.11991300

I2_fip

Energy: -2043.072186

C	-5.72174300	0.88988800	-5.59628300
C	-4.78387800	0.48271200	-4.65628300
C	-4.46604400	1.25451800	-3.53618600
C	-5.13143300	2.46919300	-3.38838900
C	-6.09802300	2.89437600	-4.32027700
C	-6.38550700	2.09682900	-5.42898700
C	-3.43535500	0.77634700	-2.52667900
C	-3.97984800	2.99285300	-1.36659000
C	-3.28317900	1.79067100	-1.40186000
C	-2.39525200	1.54102400	-0.34934800
H	-1.82840200	0.61482300	-0.34100200
C	-2.22031700	2.44908900	0.68292900
C	-2.93289900	3.64340600	0.67535300
C	-3.82606400	3.95287700	-0.35690400
H	-5.93703200	0.26668500	-6.45755600
H	-4.27909700	-0.46771000	-4.80133500
H	-7.11860300	2.40832600	-6.16438200
H	-1.52283700	2.23163800	1.48570900
H	-2.77015200	4.36624000	1.47096500
O	-4.90626800	3.32589500	-2.35305300
B	-4.54376900	5.35188300	-0.32585000
P	-6.97371800	4.43576800	-4.02325300
C	-4.59150600	6.32196500	-1.58108500
C	-5.56632700	7.30908000	-1.75018900
C	-3.64993500	6.24306800	-2.61271400
C	-5.64281600	8.12979000	-2.86721300
C	-3.68280800	7.05367800	-3.74043300
C	-4.68915500	8.00250000	-3.86941500
F	-6.52337500	7.48838200	-0.81915600
F	-2.64449800	5.36045500	-2.54964900
F	-2.76200500	6.93065800	-4.69773300
F	-6.62079700	9.03128000	-2.99198500
F	-4.74348400	8.78036000	-4.94718300
C	-7.93617500	4.35033300	-2.45073800
H	-7.14092100	4.36136900	-1.69151200
C	-7.90914600	4.94183200	-5.52857200
H	-7.24140100	4.63378500	-6.34648600
C	-9.25947900	4.23097700	-5.68104700
H	-9.66287200	4.46804200	-6.67029400
H	-9.18671300	3.14324800	-5.59854900
H	-9.97855400	4.58427400	-4.93730900
C	-8.05334500	6.46946900	-5.59217500
H	-8.69918900	6.85550000	-4.79952000
H	-7.08530200	6.97626800	-5.53581000
H	-8.51156900	6.72955400	-6.55156200
C	-8.71179400	3.03617000	-2.32509100
H	-9.16003300	2.99634100	-1.32742600
H	-9.52104300	2.96965700	-3.05775500
H	-8.06283300	2.16314300	-2.43931800
C	-8.82316200	5.58382300	-2.25227800
H	-9.69078100	5.56751600	-2.91720100
H	-9.19285600	5.57914200	-1.22220300
H	-8.28303500	6.52222900	-2.40422800
C	-3.89537100	-0.57718000	-1.94223900
H	-4.00651600	-1.32493100	-2.73310400
H	-3.15993200	-0.95735900	-1.22779100
H	-4.85495400	-0.46875500	-1.42717500
C	-2.07606400	0.60413500	-3.24054300
H	-2.15174700	-0.13389700	-4.04502300
H	-1.74250100	1.55462900	-3.66840600
H	-1.31470900	0.25470100	-2.53742000
H	-6.01153600	5.43802400	-3.82983800
N	-5.09956500	5.75911700	0.88630700
H	-5.09481200	5.15880600	1.69822300
H	-5.51074000	6.66275800	1.06096400

I2_fph

Energy: -2269.451937

C	-5.68167200	0.42917200	-5.57603600
C	-4.73089400	0.14210600	-4.59661800
C	-4.55685200	0.95968800	-3.48032500

C	-5.35809600	2.09600300	-3.39311100
C	-6.30930500	2.40710000	-4.37152800
C	-6.47930100	1.55889100	-5.46961500
C	-3.62703700	0.66128800	-2.31422200
C	-4.00082600	3.08354600	-1.74207200
C	-3.12922100	1.99651700	-1.76981500
C	-1.86290800	2.18521000	-1.21485700
H	-1.14453500	1.37273500	-1.21701900
C	-1.50443200	3.40583400	-0.65185500
C	-2.41097400	4.45749800	-0.63415900
C	-3.69908600	4.32430100	-1.17486400
H	-5.79566200	-0.23284000	-6.42792400
H	-4.12084200	-0.74795000	-4.70818100
H	-7.21193700	1.79493500	-6.23554200
H	-0.51365000	3.53263700	-0.22678100
H	-2.12107400	5.40796000	-0.19270300
O	-5.25833800	2.96847500	-2.34757600
B	-4.69655400	5.53061300	-1.07093600
P	-7.23966600	3.92568400	-4.19414300
C	-4.12862100	7.00262000	-1.21224800
C	-4.33787800	7.99639800	-0.26013300
C	-3.34994500	7.36531800	-2.30814600
C	-3.80006400	9.27168700	-0.37015300
C	-2.80448800	8.63069300	-2.46426600
C	-3.02972500	9.58840300	-1.48229000
C	-4.46973800	-0.02200700	-1.20632200
H	-4.87297300	-0.97168400	-1.57415300
H	-3.83988300	-0.21775000	-0.33247700
H	-5.30455200	0.61348800	-0.89277900
C	-2.48374800	-0.27205800	-2.71494600
H	-2.87647700	-1.22794900	-3.07090200
H	-1.85841100	0.16827400	-3.49827600
H	-1.85596100	-0.49916700	-1.85000600
H	-6.32869900	4.96264100	-3.93573000
N	-6.05513300	5.35911900	-0.81312600
H	-6.48252600	4.45581000	-0.67088600
H	-6.69372800	6.12885600	-0.67800400
C	-8.39932100	3.85299100	-2.82184200
C	-8.59340600	2.66209400	-2.11996000
C	-9.09431800	5.01644200	-2.47039800
C	-9.48739600	2.63975200	-1.05361400
H	-8.05370100	1.76153700	-2.39940100
C	-9.98256900	4.98066800	-1.40413400
H	-8.94240400	5.94089200	-3.02273300
C	-10.17664000	3.79474200	-0.69598900
H	-9.64385000	1.71748600	-0.50290700
H	-10.52459400	5.87874700	-1.12429700
H	-10.87173500	3.77264400	0.13809200
C	-8.08411200	4.33404700	-5.72385600
C	-7.38255600	5.01269700	-6.72684000
C	-9.40966900	3.93442000	-5.91903300
C	-8.01771800	5.28919600	-7.93098300
H	-6.35305400	5.32472400	-6.56954800
C	-10.03184000	4.21618700	-7.12983100
H	-9.95157800	3.41463800	-5.13355700
C	-9.33800200	4.89099800	-8.13129200
H	-7.48278700	5.82088000	-8.71168600
H	-11.06158300	3.91183400	-7.28895700
H	-9.83060000	5.11290100	-9.07331600
F	-3.12804300	6.46887800	-3.28911200
F	-2.07822300	8.94130500	-3.54180600
F	-2.51416900	10.80908700	-1.61149400
F	-4.01130500	10.19182400	0.57451900
F	-5.06898600	7.72923700	0.83800400

I3_cip

Energy: -3901.406823

C	-7.07367700	-0.92753100	0.21230000
C	-5.69658300	-0.71710400	0.26201500
C	-5.15011200	0.55846900	0.13939200
C	-6.02748800	1.62172500	-0.08051600
C	-7.41736500	1.43598100	-0.09660600
C	-7.93725300	0.14664900	0.05757100
C	-3.68335600	0.90169200	0.33008100
C	-4.29660200	3.02899900	-0.86663800
C	-3.34952700	2.02398300	-0.64437400
C	-2.10865400	2.15101800	-1.26538700
H	-1.35070200	1.38756100	-1.12923900
C	-1.82553600	3.26526000	-2.04608000
C	-2.78187900	4.25952500	-2.20015600
C	-4.05843200	4.18167500	-1.61900800
H	-7.47216300	-1.93160700	0.31323000
H	-5.04214200	-1.56873200	0.41363900
H	-9.00913800	-0.02186000	0.04405100
H	-0.85291700	3.36369000	-2.51879000
H	-2.52905900	5.14100300	-2.78835600
O	-5.56717400	2.89416900	-0.27958300
B	-5.08650300	5.39465900	-1.98492000
P	-8.46208200	2.89038400	-0.22116200
C	-4.27308000	6.84332400	-1.82989400
C	-3.80369700	7.16104000	-0.53901400
C	-4.01669500	7.82938400	-2.79162800
C	-3.11720600	8.33803600	-0.22671900
C	-3.33692100	9.02715700	-2.52263600
C	-2.87918400	9.28162600	-1.22990500
C	-8.36960500	3.81223100	1.37492200
H	-7.29661400	4.05766100	1.41435200
C	-10.14963600	2.45411600	-0.82711100
H	-9.96113900	1.60387400	-1.49911900
C	-11.12631900	2.01937400	0.27123800
H	-12.04202600	1.65589900	-0.20567800
H	-10.73551600	1.21785700	0.90332300
H	-11.40039100	2.86191800	0.91240800
C	-10.71499700	3.61511600	-1.65908100
H	-10.89290500	4.50214300	-1.04398200
H	-10.05185200	3.89005600	-2.48442200
H	-11.67545200	3.30508800	-2.08284800
C	-8.70736400	2.95269800	2.59526400
H	-8.43347700	3.50943200	3.49700800
H	-9.77578000	2.73140000	2.65200600
H	-8.15162400	2.01000700	2.60052500
C	-9.17220800	5.11564400	1.31847400
H	-10.24918500	4.92337200	1.32842600
H	-8.93498200	5.71394000	2.20388600
H	-8.93130700	5.71364600	0.43347900
C	-3.51800600	1.45832800	1.76924300
H	-3.78923200	0.69106400	2.50243200
H	-2.47626600	1.75365000	1.93087200
H	-4.15288100	2.33527600	1.92928000
C	-2.77520700	-0.31705000	0.16865000
H	-3.03500000	-1.08539900	0.90184300
H	-2.84649900	-0.74811700	-0.83542500
H	-1.73484100	-0.04385500	0.36064700
N	-6.44926100	5.44968000	-1.29922200
H	-6.35804700	5.37244200	-0.29320000
H	-6.90133800	6.34808800	-1.45476900
Cl	-4.07047000	6.05133100	0.79625400
Cl	-2.55539700	8.65316700	1.38078400
Cl	-2.03687200	10.74696800	-0.87098700
Cl	-3.05313600	10.20013400	-3.76532100
Cl	-4.54808600	7.63129400	-4.46290500
N	-5.48860000	5.01409900	-3.53947800
H	-6.17573400	5.63835700	-3.95885400
H	-4.69659500	4.96076400	-4.17784800
H	-7.86564800	3.77612900	-1.15285700
H	-5.90732100	4.08554800	-3.49531700

I3_cph

Energy: -4127.791112

C	-7.16131100	-0.94336900	0.02828000
C	-5.78136300	-0.75403900	0.09089300
C	-5.20494200	0.50760200	-0.05055100
C	-6.05807400	1.57951400	-0.31325100
C	-7.45005100	1.41166200	-0.34136800
C	-8.00408900	0.14130000	-0.16219200
C	-3.74121100	0.82626800	0.19557600
C	-4.27671600	2.99259000	-0.98452400
C	-3.34787900	1.98131400	-0.71730500
C	-2.05476200	2.14283500	-1.21162100
H	-1.30681500	1.37743400	-1.03722900

C	-1.70329700	3.29595500	-1.90258200
C	-2.64771100	4.29376600	-2.09955700
C	-3.97654800	4.17826600	-1.65993400
H	-7.57734200	-1.93799500	0.14907100
H	-5.14593600	-1.61379500	0.27460000
H	-9.08171700	0.00918900	-0.18264700
H	-0.68839300	3.42190700	-2.26757700
H	-2.34083300	5.20883400	-2.60584300
O	-5.59334000	2.84291300	-0.52077600
B	-4.96315200	5.41529900	-2.05877300
P	-8.47976800	2.86095500	-0.54051400
C	-4.24403000	6.84116800	-1.56464400
C	-4.10399900	7.02021600	-0.17297500
C	-3.79150300	7.92508200	-2.32898500
C	-3.57385700	8.17192200	0.41567700
C	-3.25648700	9.10103600	-1.78110300
C	-3.14745100	9.22605800	-0.39629000
C	-3.62549100	1.33203600	1.65868600
H	-3.93067300	0.54391100	2.35585800
H	-2.58885500	1.61431800	1.86926700
H	-4.26001200	2.20970400	1.82124900
C	-2.84346800	-0.39996600	0.02406800
H	-3.14322000	-1.19274400	0.71427800
H	-2.87928600	-0.78844500	-0.99895700
H	-1.80824700	-0.15306200	0.27031200
N	-6.43004000	5.35640200	-1.65346000
H	-6.53593100	5.15704800	-0.66680900
H	-6.88568700	6.25615100	-1.78990500
Cl	-4.61074600	5.75643300	0.93659500
Cl	-3.43618400	8.32141200	2.13664300
Cl	-2.49662900	10.66483000	0.30619700
Cl	-2.72550500	10.40534700	-2.79039300
Cl	-3.85319200	7.88527000	-4.09249000
C	-10.19347000	2.38763000	-0.79863700
C	-10.61387300	2.04260100	-2.08820200
C	-11.07891700	2.33284100	0.28157300
C	-11.92758600	1.63858400	-2.29045500
H	-9.92322800	2.09064300	-2.92643100
C	-12.39084700	1.92628400	0.06540100
H	-10.74951900	2.61029200	1.27925600
C	-12.81290000	1.58010100	-1.21577200
H	-12.26227800	1.37406600	-3.28867700
H	-13.08485300	1.88365800	0.89902100
H	-13.83982000	1.26712300	-1.37957100
C	-8.31958900	3.95670900	0.88000900
C	-7.64524100	3.54150100	2.02990900
C	-8.86295600	5.24429500	0.79396500
C	-7.51028700	4.42429100	3.09652100
H	-7.22369400	2.54206200	2.09219100
C	-8.71976600	6.11636500	1.86492400
H	-9.38511400	5.56533700	-0.10465400
C	-8.04200800	5.70746900	3.01258000
H	-6.98261400	4.10897700	3.99130800
H	-9.13231700	7.11852200	1.80249200
H	-7.92541200	6.39611200	3.84409700
N	-5.06089100	5.24605500	-3.69674800
H	-5.65259100	5.94067600	-4.14998700
H	-4.16655500	5.24437100	-4.18341200
H	-8.03578900	3.59730300	-1.65792900
H	-5.49504600	4.33570200	-3.84586800

I3_fip

Energy: -2099.696763

C	-7.14267200	-0.91068700	-0.25088100
C	-5.76772500	-0.74581500	-0.08953800
C	-5.18882500	0.51951000	-0.01451100
C	-6.03225600	1.62279100	-0.15419600
C	-7.42381500	1.48097300	-0.26345100
C	-7.97604200	0.19658900	-0.30951700
C	-3.73419900	0.79277900	0.33334400
C	-4.21867900	3.07902400	-0.61335800
C	-3.30133300	2.04204400	-0.42468900
C	-2.00206600	2.24195500	-0.88913800
H	-1.25587200	1.46398100	-0.77152500
C	-1.64762800	3.44233300	-1.49213300
C	-2.59370000	4.44767900	-1.64860200
C	-3.92323200	4.30432500	-1.22271500
H	-7.56518500	-1.90846600	-0.30562000
H	-5.14207200	-1.62792800	-0.00519400
H	-9.04855100	0.05852400	-0.40016500
H	-0.63011000	3.59242600	-1.84055600
H	-2.29570600	5.37759000	-2.12697500
O	-5.54242200	2.89671700	-0.17633600
B	-5.00953000	5.45624300	-1.60562900
P	-8.43304300	2.96602600	-0.20516200
C	-4.26710900	6.89881900	-1.86087700
C	-3.68702500	7.51697000	-0.75205500
C	-4.14383100	7.61752300	-3.04288800
C	-3.04330400	8.74442000	-0.79630700
C	-3.51215100	8.85206700	-3.14164600
C	-2.95493500	9.42083400	-2.00690300
F	-3.73169300	6.90385100	0.44942900
F	-4.65064900	7.12553400	-4.20622500
F	-3.43460800	9.49103000	-4.31481000
F	-2.50696100	9.28151600	0.30472300
F	-2.34397100	10.60428800	-2.07587300
C	-8.41653300	3.62192400	1.51835900
H	-7.34378500	3.83420000	1.64823800
C	-10.08957800	2.68116300	-0.96684700
H	-9.88149400	1.94542300	-1.75765000
C	-11.13364800	2.10380900	-0.00364500
H	-12.02831500	1.84452600	-0.57834900
H	-10.79322500	1.20297100	0.51311900
H	-11.42556000	2.84300800	0.74734200
C	-10.58687400	3.97701400	-1.62454700
H	-10.78931000	4.75346300	-0.88091400
H	-9.87184600	4.37004100	-2.35323800
H	-11.52423900	3.76494000	-2.14852100
C	-8.83281200	2.59317100	2.57184100
H	-8.59595100	2.99679100	3.56136500
H	-9.90643200	2.39222300	2.54327600
H	-8.29436600	1.64746000	2.45701500
C	-9.19094500	4.94012400	1.62005300
H	-10.27053500	4.77975100	1.54486400
H	-8.99162500	5.38936600	2.59823200
H	-8.88623200	5.65773800	0.85141000
C	-3.67576400	1.10820500	1.85104700
H	-4.01864000	0.24253600	2.42809500
H	-2.64545400	1.34165900	2.13872100
H	-4.30592400	1.96752800	2.10166200
C	-2.83585300	-0.41125000	0.04639800
H	-3.16033800	-1.27801600	0.62812100
H	-2.83950000	-0.67647400	-1.01592800
H	-1.80823600	-0.20207000	0.35241400
N	-6.21476100	5.60552900	-0.68565200
H	-6.00117100	5.34126800	0.26868000
H	-6.55326600	6.56154600	-0.64164400
N	-5.63422000	4.91925700	-3.05114700
H	-6.34682400	5.54044200	-3.43195700
H	-4.92778500	4.78981800	-3.77377400
H	-7.76779900	3.98340800	-0.93078100
H	-6.07339500	4.01473500	-2.88811200

I3_fph

Energy: -2326.079141

C	-7.17259700	-0.92127400	0.03909900
C	-5.79208300	-0.73670200	0.10617800
C	-5.21385000	0.52568600	-0.01775300
C	-6.06439800	1.60370200	-0.26200200
C	-7.45562400	1.43902600	-0.30420800
C	-8.01237700	0.16693700	-0.14463200
C	-3.74663800	0.84011800	0.21196800
C	-4.28954500	3.01101100	-0.95330300
C	-3.36610400	1.98454600	-0.71981300
C	-2.09735700	2.11479000	-1.27904800
H	-1.35618800	1.33668700	-1.13414900
C	-1.76029400	3.25373800	-2.00108000
C	-2.69229200	4.26947900	-2.15614000
C	-4.00157900	4.18617100	-1.65221600
H	-7.59141000	-1.91635000	0.14596300

H	-5.15814900	-1.60025900	0.27696500
H	-9.08983300	0.03582600	-0.17788500
H	-0.76344800	3.35577000	-2.41940600
H	-2.38917900	5.17559900	-2.67996100
O	-5.59163400	2.86928600	-0.44340100
B	-4.97167500	5.45936300	-1.96185600
P	-8.48194900	2.88981100	-0.51271200
C	-4.17934600	6.83558900	-1.51960200
C	-3.93450200	7.00955500	-0.15760500
C	-3.72795400	7.87736000	-2.31813800
C	-3.30239100	8.11916100	0.38124700
C	-3.08925300	9.01202700	-1.83069300
C	-2.87486000	9.13416400	-0.46639700
C	-3.60902900	1.35562500	1.66936100
H	-3.90560200	0.57191000	2.37503800
H	-2.56842800	1.63529300	1.86310700
H	-4.23842500	2.23550400	1.83723200
C	-2.85555000	-0.39001400	0.03825300
H	-3.14763800	-1.17473000	0.74102200
H	-2.90810400	-0.78919500	-0.97998500
H	-1.81597900	-0.14276800	0.26578700
N	-6.39559200	5.41479600	-1.42923200
H	-6.41310900	5.13157000	-0.45617700
H	-6.82690000	6.33599900	-1.44335600
C	-10.17802700	2.41441600	-0.86772200
C	-10.53268000	2.09809400	-2.18402700
C	-11.11463400	2.32555100	0.16638100
C	-11.83160800	1.68985900	-2.45987600
H	-9.80260300	2.17148000	-2.98613400
C	-12.41096200	1.91465800	-0.12320600
H	-10.83650700	2.57894400	1.18579900
C	-12.76756800	1.59791400	-1.43148200
H	-12.11515000	1.44781200	-3.47941700
H	-13.14385300	1.84532400	0.67457900
H	-13.78255700	1.28141100	-1.65279100
C	-8.40843600	3.94356700	0.94549600
C	-7.77256200	3.51043900	2.11029700
C	-8.98976500	5.21548300	0.87631500
C	-7.71615700	4.35954400	3.21110700
H	-7.32173100	2.52304600	2.15889300
C	-8.92683400	6.05300100	1.98168500
H	-9.48200500	5.54964100	-0.03424200
C	-8.28905100	5.62597900	3.14599600
H	-7.21993900	4.03025800	4.11868200
H	-9.37215800	7.04195200	1.93469400
H	-8.23770900	6.28697200	4.00609700
F	-4.32506500	6.05317400	0.71477700
F	-3.09945900	8.22609100	1.69979300
F	-2.26883800	10.21481000	0.02907900
F	-2.68029200	9.98032900	-2.65939400
F	-3.89068600	7.82799600	-3.66936500
N	-5.15577100	5.44933900	-3.60138900
H	-5.71664800	6.22879300	-3.94322200
H	-4.27758800	5.46640400	-4.11727600
H	-7.97800900	3.66425400	-1.57857200
H	-5.64420400	4.59109200	-3.85297000

P1_cip

Energy: -3901.422868

C	-7.14631000	-0.78686800	-0.45881300
C	-5.78588100	-0.67231000	-0.18750900
C	-5.19867200	0.57894300	-0.00418200
C	-6.02090200	1.69700800	-0.13649700
C	-7.40377700	1.61939200	-0.34196500
C	-7.95250900	0.34442500	-0.51300900
C	-3.75226600	0.80528900	0.41638800
C	-4.15078000	3.10473600	-0.49642500
C	-3.26052200	2.04637400	-0.31474100
C	-1.95838700	2.22043500	-0.78244100
H	-1.23137600	1.42283900	-0.67320300
C	-1.57404500	3.41424600	-1.38453500
C	-2.49229500	4.44536600	-1.54024400
C	-3.81813700	4.31989900	-1.10440400
H	-7.58601700	-1.76850000	-0.60589900
H	-5.18298400	-1.57073400	-0.11298900
H	-9.01464100	0.22676400	-0.69718700
H	-0.55440700	3.53684900	-1.73665200
H	-2.17660200	5.36789200	-2.02135800
O	-5.47201900	2.97071900	-0.06685900
B	-4.91188900	5.43719300	-1.47113800
P	-8.34443400	3.19548100	-0.35012200
C	-4.24300800	6.87738000	-1.88550200
C	-3.60588500	7.62288800	-0.87256100
C	-4.19152300	7.46235900	-3.16041300
C	-3.03494800	8.88329600	-1.07957200
C	-3.63176500	8.72426700	-3.40945500
C	-3.06149700	9.44542800	-2.35865700
C	-8.40347300	3.58289000	1.49888100
H	-7.35014400	3.83725900	1.69952000
C	-10.05308000	2.75015000	-0.98358600
H	-9.82856900	2.07045700	-1.81983400
C	-11.01881200	2.04540500	-0.02650800
H	-11.90171000	1.71603500	-0.58697000
H	-10.58316300	1.17029600	0.46054200
H	-11.36684700	2.72851500	0.75406100
C	-10.70847600	4.00722400	-1.57542700
H	-10.92194400	4.74950400	-0.79868300
H	-10.07390300	4.47856600	-2.33241700
H	-11.66105600	3.74011400	-2.04669500
C	-8.77471600	2.44199600	2.44832000
H	-8.52329000	2.73426000	3.47489900
H	-9.84421600	2.22281600	2.42182600
H	-8.22763300	1.52280500	2.21808100
C	-9.24825400	4.83601900	1.75360300
H	-10.31432500	4.63307000	1.61166800
H	-9.11379300	5.17127400	2.78807700
H	-8.97341900	5.66426200	1.08972600
C	-3.74460200	1.10468300	1.93783400
H	-4.13391000	0.24178900	2.48842600
H	-2.72136100	1.30661600	2.27174800
H	-4.36433500	1.97518200	2.17465100
C	-2.87087000	-0.41547400	0.15248200
H	-3.23981600	-1.27913000	0.71190500
H	-2.83991600	-0.67223700	-0.91152900
H	-1.85084100	-0.23199400	0.49969200
N	-6.00102300	5.71580100	-0.29015100
H	-5.59266200	5.58430900	0.63328700
H	-6.37173600	6.66625100	-0.31315900
H	-6.80848000	5.06573900	-0.35305900
Cl	-3.44701700	6.96401500	0.74557000
Cl	-2.28744900	9.75017700	0.21404200
Cl	-2.38033600	11.00397600	-2.63842300
Cl	-3.62724700	9.40114200	-4.99911100
Cl	-4.79504700	6.61501000	-4.57573400
N	-5.86204400	4.74451700	-2.59097300
H	-6.54904700	5.35546300	-3.03415100
H	-5.30495700	4.33410500	-3.33849000
H	-6.39042200	3.98146800	-2.14738600

P1_cph

Energy: -4127.819589

C	-7.21663000	-0.90859900	-0.37364000
C	-5.85164800	-0.78036100	-0.13765200
C	-5.25051300	0.47695600	-0.05966800
C	-6.06506100	1.58797900	-0.26043500
C	-7.44121100	1.49371200	-0.49420000
C	-8.01116300	0.21971400	-0.54185300
C	-3.79526200	0.71246700	0.31598400
C	-4.19551300	3.01976500	-0.58974300
C	-3.31721200	1.94584100	-0.43852000
C	-2.01769700	2.11528000	-0.91491200
H	-1.30239900	1.30349700	-0.83927800
C	-1.61836500	3.32285700	-1.47795700
C	-2.50648000	4.38889700	-1.54064300
C	-3.82799700	4.27428600	-1.08924600
H	-7.66532200	-1.89585900	-0.42203700
H	-5.25299600	-1.67418300	-0.00061900
H	-9.07570400	0.11374200	-0.72681500
H	-0.60394200	3.43719400	-1.84728000
H	-2.16685300	5.33772600	-1.94854700

O	-5.53342700	2.86897400	-0.21603800
B	-4.84589900	5.51185400	-1.20128900
P	-8.36098700	3.02913700	-0.88047500
C	-4.08799300	6.95180700	-1.46536900
C	-3.30428700	7.51149200	-0.43351700
C	-4.11382500	7.71332500	-2.64633000
C	-2.69881700	8.77084600	-0.51246000
C	-3.52763100	8.98252000	-2.76368000
C	-2.83268600	9.52437200	-1.68130800
C	-3.74892200	1.03875600	1.83157900
H	-4.12126800	0.18455100	2.40708300
H	-2.71882500	1.25140800	2.13677400
H	-4.36720600	1.91144600	2.06684700
C	-2.91967400	-0.51245700	0.04973700
H	-3.26821900	-1.36601500	0.63642500
H	-2.92080100	-0.78923800	-1.00958600
H	-1.89015200	-0.32119800	0.36284800
N	-5.75000000	5.69208000	0.13856800
H	-5.16757100	5.91265500	0.94722900
H	-6.44226400	6.43983400	0.06828100
H	-6.25577800	4.83428300	0.38303500
Cl	-2.97210200	6.60414100	1.03580600
Cl	-1.77746000	9.40665200	0.80321200
Cl	-2.12140000	11.09007600	-1.79536800
Cl	-3.63942300	9.88622200	-4.23210700
Cl	-4.83543000	7.08674100	-4.12062400
C	-10.07096600	2.44411000	-1.17030300
C	-10.47572300	2.23330700	-2.49265700
C	-10.96423100	2.18600200	-0.12509600
C	-11.75454800	1.75680600	-2.76544200
H	-9.78900800	2.44010600	-3.31018300
C	-12.24486600	1.71984900	-0.40344200
H	-10.65921400	2.34835200	0.90530900
C	-12.64026200	1.50251700	-1.72179300
H	-12.06157100	1.59258400	-3.79417000
H	-12.93503800	1.52254600	0.41173300
H	-13.64095400	1.13808700	-1.93526800
C	-8.47870200	3.89285800	0.73979200
C	-7.88423200	3.42431500	1.91542200
C	-9.12635400	5.13799100	0.75226200
C	-7.92859100	4.19203400	3.07888700
H	-7.39191100	2.45548900	1.92850500
C	-9.18214900	5.89238400	1.91818400
H	-9.59851800	5.51134900	-0.15515200
C	-8.57423200	5.42453300	3.08355600
H	-7.46485400	3.81640600	3.98660800
H	-9.69934200	6.84775600	1.91909500
H	-8.61161100	6.01734200	3.99283100
N	-5.97491300	5.11783100	-2.28619100
H	-6.58197500	5.88426700	-2.57897700
H	-5.54649400	4.75125000	-3.13475300
H	-6.60660400	4.37328500	-1.93124000

P1_fip

Energy: -2099.714522

C	-7.11867300	-0.81735200	-0.50006800
C	-5.76021100	-0.69223700	-0.22638900
C	-5.18712700	0.56222500	-0.02163200
C	-6.02035100	1.67432900	-0.13214000
C	-7.39951100	1.58548600	-0.35619000
C	-7.93412000	0.30721900	-0.54589300
C	-3.73981400	0.79417400	0.38939500
C	-4.16376800	3.11192900	-0.46292800
C	-3.26748800	2.05247500	-0.32481600
C	-1.97166800	2.24438900	-0.80364000
H	-1.24257000	1.44466300	-0.73026300
C	-1.59571400	3.45863700	-1.36684200
C	-2.51477200	4.49667300	-1.46505100
C	-3.83692800	4.35417300	-1.02264900
H	-7.54832400	-1.80116000	-0.66162200
H	-5.14696600	-1.58470000	-0.16727000
H	-8.99329700	0.18283200	-0.74195500
H	-0.58125300	3.59497000	-1.72859900
H	-2.20286300	5.43737700	-1.91085200
O	-5.47995700	2.95216900	-0.02131100
B	-4.91435000	5.52958200	-1.21668000
P	-8.35245500	3.15170400	-0.40840300
C	-4.26499400	6.91844800	-1.74806200
C	-3.48695800	7.70332000	-0.89770700
C	-4.32168500	7.37935000	-3.06085200
C	-2.83861400	8.86550300	-1.28667100
C	-3.69051400	8.53561700	-3.50186000
C	-2.94281800	9.28697300	-2.60617400
F	-3.31488400	7.32394400	0.39188300
F	-5.00649400	6.68541500	-4.00029900
F	-3.79121000	8.92321900	-4.77397400
F	-2.11451200	9.57036000	-0.41676200
F	-2.33026900	10.39653800	-3.00644100
C	-8.49774000	3.54814900	1.43356600
H	-7.45225800	3.78318800	1.69348300
C	-10.03039800	2.69159700	-1.11159300
H	-9.76471100	2.00888400	-1.93300900
C	-11.03942100	1.98947900	-0.19816600
H	-11.89158400	1.65086500	-0.79928200
H	-10.62551100	1.12037000	0.31760600
H	-11.42985700	2.67747400	0.55786300
C	-10.66158300	3.94389300	-1.73939300
H	-10.90900200	4.69040500	-0.97685100
H	-9.99578300	4.41141100	-2.47158000
H	-11.59256700	3.67248900	-2.24972700
C	-8.92983700	2.41522400	2.36734600
H	-8.71637400	2.70296800	3.40371300
H	-10.00113600	2.21754400	2.29571100
H	-8.39141300	1.48588800	2.15870600
C	-9.33492100	4.81390600	1.64484900
H	-10.39474000	4.62493700	1.44727900
H	-9.25101900	5.14875100	2.68483000
H	-9.01486600	5.63582600	0.99367800
C	-3.71795300	1.06816800	1.91557600
H	-4.09215500	0.19180300	2.45518500
H	-2.69310200	1.27453300	2.24179600
H	-4.34411600	1.92760300	2.17463500
C	-2.84953400	-0.41354100	0.09693100
H	-3.20443000	-1.28940200	0.64631700
H	-2.82692900	-0.65309200	-0.97124400
H	-1.82791200	-0.22570600	0.43713000
N	-5.66697800	5.82192700	0.19245000
H	-4.98637500	6.06289900	0.91262000
H	-6.34294200	6.58624000	0.15621200
H	-6.15638700	4.98340900	0.51410700
N	-6.10443500	5.02716600	-2.17776700
H	-6.67282600	5.78139100	-2.56392300
H	-5.72884100	4.51459700	-2.97529500
H	-6.77122300	4.38902600	-1.68267500

P1_fph

Energy: -2326.111779

C	-7.20848000	-0.91709800	-0.48629400
C	-5.84830800	-0.78650200	-0.22631400
C	-5.25374300	0.47183400	-0.11529700
C	-6.07057500	1.58212100	-0.30955900
C	-7.44312000	1.48551200	-0.56520100
C	-8.00616000	0.21035800	-0.64506100
C	-3.80751300	0.70119400	0.29844500
C	-4.20009400	3.03589400	-0.54571500
C	-3.31627600	1.96839700	-0.38903000
C	-1.99414300	2.17630300	-0.78342900
H	-1.27110300	1.37235000	-0.69854000
C	-1.58124400	3.41116300	-1.27034100
C	-2.48236600	4.46661300	-1.34720300
C	-3.82656400	4.31316700	-0.98465500
H	-7.65122100	-1.90547900	-0.55987300
H	-5.24820100	-1.68021600	-0.09550100
H	-9.06757600	0.10318800	-0.84674100
H	-0.54833700	3.55460100	-1.57200100
H	-2.13586100	5.43271200	-1.70445200
O	-5.55008700	2.86595000	-0.23474600
B	-4.86794000	5.53333900	-1.07916900
P	-8.36447900	3.02121700	-0.94450100
C	-4.16134600	6.96443500	-1.38478300

C	-3.34644400	7.55193400	-0.41644400
C	-4.21650900	7.66560500	-2.58630400
C	-2.65643500	8.74110500	-0.59491400
C	-3.54508700	8.86017100	-2.81629400
C	-2.75829100	9.40421200	-1.81132600
C	-3.79578700	0.96379400	1.82697600
H	-4.17455200	0.08429700	2.35854700
H	-2.77412400	1.17050200	2.16314900
H	-4.42560600	1.82232800	2.08356200
C	-2.91936400	-0.50745400	-0.00155000
H	-3.27509900	-1.38749000	0.53973700
H	-2.89694500	-0.73701800	-1.07179800
H	-1.89778200	-0.32648000	0.34155800
N	-5.67778400	5.67740100	0.31967400
H	-5.02297800	5.87165200	1.07747600
H	-6.36698700	6.43144700	0.33004000
H	-6.17223500	4.81618700	0.57707100
C	-10.07904400	2.44068200	-1.21593300
C	-10.50402600	2.24457000	-2.53420000
C	-10.95831500	2.17698100	-0.16023600
C	-11.78935400	1.77754600	-2.79269100
H	-9.82821300	2.45604400	-3.35954000
C	-12.24528400	1.72027400	-0.42410800
H	-10.63765600	2.32812200	0.86716100
C	-12.66114100	1.51815300	-1.73865400
H	-12.11239900	1.62498200	-3.81829400
H	-12.92467800	1.51903100	0.39912000
H	-13.66700900	1.16166800	-1.94093100
C	-8.46619100	3.88875000	0.67487600
C	-7.90225400	3.40018400	1.85744800
C	-9.06995000	5.15561900	0.68047300
C	-7.93188600	4.16942600	3.02051600
H	-7.44466400	2.41445600	1.87527500
C	-9.11099800	5.91288600	1.84562900
H	-9.51892400	5.54482200	-0.23202900
C	-8.53245700	5.42486300	3.01766900
H	-7.49208100	3.77788000	3.93343600
H	-9.59419800	6.88593600	1.84072500
H	-8.55836200	6.01918400	3.92637900
F	-3.18453200	6.93892500	0.78085900
F	-1.89704300	9.24555200	0.37806300
F	-2.10970300	10.54724600	-2.00978400
F	-3.64968000	9.48278100	-3.99118000
F	-4.94537100	7.19258900	-3.62528300
N	-5.99897100	5.19759800	-2.17367000
H	-6.61174300	5.98230100	-2.39899900
H	-5.56193700	4.91821400	-3.05195600
H	-6.62459500	4.41643300	-1.89635300

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Energy: -3845.525335

C	-7.13694100	-0.79751100	-0.53361200
C	-5.78408800	-0.66844900	-0.23363900
C	-5.21249500	0.59024500	-0.05490900
C	-6.03314300	1.70704100	-0.22702400
C	-7.41608600	1.61065800	-0.44132900
C	-7.94896300	0.32894300	-0.60887000
C	-3.78537300	0.83487100	0.41248100
C	-4.15620200	3.11405100	-0.56721800
C	-3.27095700	2.06051600	-0.32912700
C	-1.94981800	2.21680100	-0.74773300
H	-1.22999800	1.42028200	-0.59242400
C	-1.54519900	3.39822800	-1.35870100
C	-2.45952100	4.42448900	-1.56574700
C	-3.80662700	4.31773400	-1.18942200
H	-7.56694600	-1.78349600	-0.68240900
H	-5.17521700	-1.56048300	-0.13290400
H	-9.00695900	0.20049600	-0.80924500
H	-0.51299700	3.51658100	-1.67627700
H	-2.12355600	5.33543900	-2.05608300
O	-5.49349400	2.97469800	-0.17312700
B	-4.85840800	5.45245700	-1.64565000
P	-8.37704800	3.17485600	-0.46565800
C	-4.12984700	6.89025500	-1.93040500
C	-3.56264900	7.65437000	-0.90120400
C	-4.00005200	7.43412600	-3.21763000
C	-2.95639600	8.89870700	-1.10136400
C	-3.39824400	8.67629500	-3.46334500
C	-2.88114900	9.41606400	-2.39682800
C	-8.36542600	3.59650500	1.38000900
H	-7.31540100	3.89733400	1.52053900
C	-10.10942700	2.65799700	-0.98063700
H	-9.91258900	1.97866400	-1.82401200
C	-10.99290500	1.93000000	0.03689700
H	-11.89264100	1.55419000	-0.46596700
H	-10.49186400	1.08359600	0.51208400
H	-11.32419600	2.61214600	0.82610400
C	-10.84537400	3.88111600	-1.54873900
H	-11.04608500	4.62404400	-0.76899000
H	-10.26720900	4.36804900	-2.33969500
H	-11.81058500	3.57269700	-1.96769900
C	-8.64223500	2.47066900	2.37854900
H	-8.35990600	2.80207800	3.38572200
H	-9.70060700	2.20129800	2.40550100
H	-8.06382800	1.57093700	2.14688300
C	-9.24177200	4.82398100	1.65014600
H	-10.30584000	4.57787200	1.57282000
H	-9.06432200	5.19471700	2.66647400
H	-9.03290200	5.64014300	0.94881800
C	-3.83780800	1.16883600	1.92629100
H	-4.24227900	0.31726200	2.48483300
H	-2.82942400	1.38947900	2.29306300
H	-4.47236400	2.04027200	2.11489700
C	-2.89003300	-0.38868200	0.21619700
H	-3.27920400	-1.24082900	0.78053600
H	-2.81433200	-0.66982300	-0.83947700
H	-1.88542200	-0.19084200	0.59915800
H	-5.45124400	5.07602800	-2.62841600
N	-6.05524600	5.69464500	-0.57046800
H	-5.75615300	5.68175700	0.40231600
H	-6.51609900	6.58866900	-0.73106700
H	-6.77316900	4.96176000	-0.69107600
Cl	-3.56327900	7.02892600	0.74193000
Cl	-2.29038600	9.80021300	0.22230800
Cl	-2.14414600	10.95791000	-2.67652000
Cl	-3.28110500	9.31351300	-5.07201000
Cl	-4.57165700	6.54484100	-4.61104500

S_cph

Energy: -4071.922686

C	-7.21212600	-0.86547800	-0.72500400
C	-5.86433100	-0.77725800	-0.39151000
C	-5.25998500	0.46207700	-0.17929900
C	-6.04531800	1.60291700	-0.34744100
C	-7.40478700	1.54803300	-0.68452700
C	-7.97902100	0.28628500	-0.86165200
C	-3.82904500	0.64783100	0.30239600
C	-4.14616700	3.01891100	-0.45048500
C	-3.28946500	1.92396400	-0.33022100
C	-1.95907900	2.11026900	-0.70798200
H	-1.25597300	1.28584700	-0.65181500
C	-1.51875000	3.35506300	-1.14624500
C	-2.39538900	4.43536000	-1.17703600
C	-3.74396500	4.30635400	-0.82368200
H	-7.66929200	-1.83871500	-0.87664500
H	-5.28402700	-1.68755600	-0.28527600
H	-9.02920200	0.20801500	-1.12551700
H	-0.48197000	3.48606300	-1.44296400
H	-2.02611500	5.40847800	-1.49280000
O	-5.50483000	2.85783300	-0.16824100
B	-4.79097000	5.52861600	-0.85216200
P	-8.28146700	3.11413500	-1.08713100
C	-4.12600700	6.94673100	-1.31233600
C	-3.31170700	7.74227200	-0.49538600
C	-4.32218900	7.44159600	-2.61346400
C	-2.80093200	8.98676100	-0.88209900
C	-3.82374400	8.67772200	-3.04429000
C	-3.07192200	9.46307300	-2.16623000
C	-3.87474000	0.86544700	1.83722600
H	-4.28332600	-0.02352400	2.33076900

H	-2.86458400	1.05283100	2.21757700
H	-4.50467200	1.72427200	2.09134100
C	-2.95298100	-0.56959500	0.00590600
H	-3.34774900	-1.45780400	0.50665100
H	-2.89084300	-0.76910200	-1.06896400
H	-1.94224700	-0.41538300	0.39296100
H	-5.74395800	5.27906800	-1.54693700
N	-5.47583200	5.66340000	0.62665600
H	-4.81352700	5.70318000	1.39838400
H	-6.08013500	6.48024200	0.69931600
H	-6.07105700	4.84582400	0.77301200
Cl	-2.82942400	7.15859700	1.09453800
Cl	-1.82822800	9.93632500	0.19581000
Cl	-2.46525900	11.00455500	-2.67042300
Cl	-4.12228600	9.25370000	-4.65230500
Cl	-5.18779200	6.48314300	-3.79122500
C	-10.01816600	2.52195500	-1.27426700
C	-10.49683600	2.33514300	-2.57541800
C	-10.86408000	2.25346300	-0.19293700
C	-11.79252400	1.87319100	-2.79224100
H	-9.85022600	2.55386000	-3.42226900
C	-12.16226700	1.80310000	-0.41124800
H	-10.50742200	2.39775400	0.82358700
C	-12.62800000	1.60939400	-1.71047800
H	-12.15175800	1.72945700	-3.80738300
H	-12.81203800	1.60055600	0.43575900
H	-13.64220100	1.25786400	-1.87843400
C	-8.38142000	3.96861300	0.54441900
C	-7.96155800	3.40886700	1.75570700
C	-8.87064000	5.28244500	0.53999300
C	-8.02001900	4.15122700	2.93429800
H	-7.58605200	2.38899900	1.77866800
C	-8.94581100	6.01518900	1.71992200
H	-9.18847800	5.73358500	-0.39809100
C	-8.51167100	5.45393800	2.92046000
H	-7.68600600	3.70488600	3.86701900
H	-9.33401200	7.02988800	1.70114200
H	-8.55868400	6.02962800	3.84051500

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Energy: -2043.81072

C	-7.14624800	-0.79573500	-0.55904500
C	-5.79350400	-0.66598900	-0.25877900
C	-5.22202300	0.59297200	-0.08075200
C	-6.04315600	1.70862600	-0.25586300
C	-7.42675000	1.61195900	-0.46569800
C	-7.95937300	0.33015000	-0.63253100
C	-3.79812800	0.83759800	0.39673000
C	-4.16421600	3.12020000	-0.58124600
C	-3.27850000	2.07028900	-0.32975600
C	-1.94905900	2.23743500	-0.71753400
H	-1.22807300	1.44439500	-0.55017800
C	-1.53691400	3.42515900	-1.30995700
C	-2.45374900	4.44577000	-1.53616600
C	-3.80961100	4.32692900	-1.19719200
H	-7.57577100	-1.78198000	-0.70747000
H	-5.18481000	-1.55793800	-0.15637200
H	-9.01787300	0.20108800	-0.82992200
H	-0.49783700	3.55234600	-1.60053900
H	-2.11358900	5.35954900	-2.01767200
O	-5.50565200	2.97710400	-0.20658500
B	-4.85923300	5.45530400	-1.68523600
P	-8.38776400	3.17668600	-0.47890700
C	-4.13481200	6.89042900	-1.93155400
C	-3.64808400	7.65932800	-0.88021700
C	-3.91481900	7.42436800	-3.19678900
C	-3.00389000	8.87713600	-1.04079900
C	-3.26904000	8.63736900	-3.41159600
C	-2.81159900	9.36897200	-2.32493100
F	-3.79692800	7.21383300	0.39281900
F	-4.32057000	6.76167300	-4.29670800
F	-3.08424100	9.11127500	-4.65184300
F	-2.56659700	9.57905500	0.01480600
F	-2.19469100	10.54071700	-2.51166500
C	-8.35898800	3.59419600	1.36793400
H	-7.30826200	3.89658100	1.49944400
C	-10.12464300	2.65844300	-0.97724200
H	-9.93506000	1.98142800	-1.82411300
C	-10.99526000	1.92616900	0.04824200
H	-11.89833700	1.54689200	-0.44596200
H	-10.48561400	1.08170300	0.51766900
H	-11.32159400	2.60621800	0.84131400
C	-10.86916400	3.88097900	-1.53504900
H	-11.06339700	4.62217900	-0.75202900
H	-10.30058800	4.37077200	-2.33120400
H	-11.83801200	3.57108900	-1.94443700
C	-8.62513900	2.46661900	2.36748800
H	-8.32895800	2.79477800	3.37171700
H	-9.68376400	2.19988100	2.40754300
H	-8.05218400	1.56591700	2.12614700
C	-9.23438400	4.82011600	1.64827000
H	-10.29882500	4.57227400	1.58231100
H	-9.04665000	5.19047300	2.66290000
H	-9.03464000	5.63709800	0.94520600
C	-3.86233600	1.15982300	1.91267100
H	-4.26998700	0.30361900	2.46176400
H	-2.85706100	1.37916700	2.28867500
H	-4.49960100	2.02908400	2.10263500
C	-2.89943800	-0.38320400	0.19708800
H	-3.29230500	-1.24083400	0.75034400
H	-2.81452400	-0.65450100	-0.86044800
H	-1.89839300	-0.18834100	0.59055500
H	-5.43002500	5.09242100	-2.69204700
N	-6.04722300	5.70033000	-0.60224900
H	-5.71764700	5.72334600	0.36100500
H	-6.52842900	6.58037000	-0.77829000
H	-6.75386800	4.95220100	-0.68009500

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Energy: -2270.205349

C	-7.09605577	-0.84896299	0.01628021
C	-5.71892881	-0.65878734	0.05185389
C	-5.16327878	0.60274156	-0.15929106
C	-6.02764596	1.65825547	-0.45774125
C	-7.42212653	1.50075408	-0.46682956
C	-7.94209290	0.22724818	-0.22137417
C	-3.69074063	0.92714814	0.01717659
C	-4.24371225	3.01881451	-1.25576463
C	-3.32738103	1.98884831	-1.00987019
C	-2.08370949	2.05949543	-1.63283369
H	-1.35398563	1.27127171	-1.48291464
C	-1.76080324	3.14984835	-2.43478630
C	-2.67027188	4.18656771	-2.58492175
C	-3.94553722	4.16558816	-1.99639268
H	-7.51263926	-1.83647555	0.19019560
H	-5.07293617	-1.50395589	0.26329805
H	-9.01721886	0.07798555	-0.22862846
H	-0.79088817	3.19696703	-2.92175605
H	-2.39415700	5.05350198	-3.18312158
O	-5.53642726	2.91983475	-0.71602108
B	-4.80502672	5.52137700	-2.18880076
P	-8.47893484	2.92777117	-0.92826420
C	-4.12184147	6.71247989	-1.30648854
C	-4.09622192	6.66865077	0.08371017
C	-3.47025370	7.80541961	-1.86766299
C	-3.49098890	7.62738874	0.88149972
C	-2.84013770	8.78868038	-1.11230965
C	-2.85175707	8.69899852	0.27215944
C	-3.51863662	1.55811169	1.42481738
H	-3.81016012	0.83722501	2.19700568
H	-2.47242144	1.84402039	1.57854739
H	-4.13920612	2.45370574	1.53063021
C	-2.80277990	-0.31387682	-0.07160295
H	-3.07237638	-1.03183718	0.70775249
H	-2.88724310	-0.80406868	-1.04724566
H	-1.75677378	-0.04561606	0.09766972
H	-4.85284521	5.83400541	-3.35684372
N	-6.33722206	5.40732568	-1.70356772
H	-6.43087378	5.21040839	-0.70651496
H	-6.83947240	6.27392341	-1.88665636
H	-6.84730802	4.65758489	-2.17563398

F	-4.69636787	5.63448482	0.72533104
F	-3.51010378	7.53405079	2.21918436
F	-2.25454772	9.63811631	1.01398267
F	-2.22432467	9.82284011	-1.70272155
F	-3.41742920	7.95736210	-3.20622087
C	-10.17439955	2.24740073	-0.72179190
C	-10.81749198	2.16539710	0.51771549
C	-10.83534553	1.78948324	-1.86658874
C	-12.09882505	1.63084653	0.60805744
H	-10.31446459	2.52057237	1.41325182
C	-12.11273183	1.24421650	-1.77186484
H	-10.34658090	1.86014032	-2.83567772
C	-12.74723779	1.16711377	-0.53491818
H	-12.59144606	1.57338640	1.57472026
H	-12.61601334	0.88889971	-2.66658824
H	-13.74768724	0.75003457	-0.46150375
C	-8.33610816	4.04568665	0.53203991
C	-7.52681127	3.78456120	1.64040946
C	-9.02830954	5.26416449	0.46896456
C	-7.40622779	4.72535018	2.66130850
H	-6.98678252	2.84445529	1.70999451
C	-8.91818899	6.19418850	1.49602710
H	-9.65901585	5.48261061	-0.39144461
C	-8.09841017	5.92993253	2.59278417
H	-6.76554494	4.51296432	3.51258569
H	-9.46505184	7.13108408	1.43659179
H	-7.99890008	6.66271387	3.38836820

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Energy: -4579.04001

C	-7.19187400	-0.51029900	1.98565200
C	-5.99228800	-0.39086400	1.29762200
C	-5.64965900	0.78871500	0.63266500
C	-6.58426500	1.82355800	0.64448700
C	-7.71696100	1.80191500	1.48096400
C	-8.01853300	0.60002200	2.12139800
C	-4.25081800	0.98884700	0.06897800
C	-5.26084900	3.15433800	-0.84214100
C	-4.15727900	2.32057900	-0.66085200
C	-2.94483300	2.73085100	-1.22032700
H	-2.05999000	2.11485900	-1.08799700
C	-2.84796700	3.91997500	-1.92740300
C	-3.99568400	4.65912700	-2.18007600
C	-5.25439600	4.27671000	-1.69533700
H	-7.44820800	-1.44344000	2.47795200
H	-5.29854000	-1.22654200	1.29245700
H	-8.89042800	0.53090700	2.75952800
H	-1.88882300	4.24938500	-2.31478200
H	-3.91456900	5.55262200	-2.79237500
O	-6.44188400	2.93604300	-0.15620700
B	-6.57609900	5.09221600	-2.12353000
P	-8.52437700	3.41797400	1.84135300
C	-6.31772200	6.16174900	-3.32534100
C	-6.52564600	7.55146600	-3.30503900
C	-5.83010300	5.66115600	-4.55513200
C	-6.28380600	8.38870100	-4.40379300
C	-5.54741500	6.47018400	-5.66049600
C	-5.78957000	7.84348800	-5.59038900
C	-3.26856400	0.97679200	1.26445200
H	-3.31710300	0.01751400	1.78900600
H	-2.23945300	1.12584900	0.92391200
H	-3.51968700	1.77231100	1.97333400
C	-3.87178000	-0.14251100	-0.90878500
H	-3.95179900	-1.12178200	-0.42786400
H	-4.52040900	-0.13062200	-1.78921000
H	-2.83839300	-0.02478500	-1.24770800
N	-7.24033500	5.64699000	-0.77733300
H	-6.59550400	6.26064600	-0.28015600
H	-8.10889900	6.16622500	-0.89922500
H	-7.44708300	4.86326100	-0.13906800
C	-9.05057200	3.70949200	-3.20059000
H	-7.53707700	4.33993500	-2.61128500
C	-8.79302200	3.83166500	-4.63490000
C	-8.69166200	5.09831900	-5.24765900
C	-8.73390900	2.68455700	-5.45150900
C	-8.52883000	5.20946100	-6.61805900
H	-8.71537800	5.99478200	-4.63772300
C	-8.58096500	2.80479500	-6.82269400
H	-8.85221300	1.70205000	-5.00937100
C	-8.46827800	4.06402600	-7.40930100
H	-8.43540600	6.19174400	-7.07152500
H	-8.55688300	1.91227700	-7.44025100
H	-8.33829800	4.15407900	-8.48381500
C	-8.91326200	2.37833500	-2.57792900
C	-7.73643700	1.62645900	-2.72559600
C	-10.01215900	1.79465500	-1.92514000
C	-7.66040900	0.33813300	-2.22532300
H	-6.87419800	2.07677700	-3.20725300
C	-9.93401800	0.49456200	-1.44221900
H	-10.94450400	2.34305200	-1.84262100
C	-8.75853000	-0.23404900	-1.58225500
H	-6.74077300	-0.22738200	-2.32993100
H	-10.79843200	0.05127100	-0.95741400
H	-8.69287200	-1.24514300	-1.19157300
C	-10.01614700	4.64090600	-2.59157300
C	-10.10529200	4.72431800	-1.19179100
C	-10.93375100	5.38400200	-3.35890800
C	-11.01694200	5.56658800	-0.57893300
H	-9.44478800	4.12214400	-0.57348200
C	-11.85949000	6.21422500	-2.74129700
H	-10.96052300	5.27306600	-4.43645900
C	-11.89393200	6.32563000	-1.35401400
H	-11.04731100	5.62477300	0.50579500
H	-12.56814200	6.76782900	-3.34956600
H	-12.61461800	6.98414200	-0.87798400
C	-10.19506700	3.08170800	2.64858900
H	-10.60353600	4.10504700	2.66750000
C	-7.44689600	4.03126600	3.27575800
H	-8.14352900	4.63575300	3.87606600
C	-10.26374500	2.56451700	4.08935500
H	-11.30886700	2.59038500	4.42139100
H	-9.91885300	1.53245400	4.19053400
H	-9.68656300	3.18486000	4.77978100
C	-11.08698200	2.26216800	1.70971200
H	-12.11946500	2.27051900	2.07723700
H	-11.08615900	2.66676800	0.69249800
H	-10.76123300	1.21892000	1.65348500
C	-6.83246400	2.94491100	4.15844300
H	-6.34123700	3.40838000	5.02257400
H	-7.56993800	2.23020600	4.53041500
H	-6.07395700	2.38043400	3.60466700
C	-6.35277600	4.96081400	2.73809500
H	-5.68625700	4.43070600	2.04621100
H	-6.77874500	5.82524700	2.21797800
H	-5.73747000	5.33633300	3.56410200
Cl	-7.09979100	8.36915500	-1.85794800
Cl	-6.57556200	10.09183000	-4.31636400
Cl	-5.48441400	8.85428000	-6.95565100
Cl	-4.93748600	5.79388200	-7.13055900
Cl	-5.56112100	3.95079400	-4.77362200

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Energy: -4805.436768

C	-7.23799300	-0.80782100	2.05001500
C	-6.03567500	-0.66271100	1.37509200
C	-5.71254200	0.52020300	0.70181500
C	-6.67229200	1.52829100	0.67689000
C	-7.83736700	1.45907800	1.46169800
C	-8.11694600	0.26742400	2.12839800
C	-4.33359100	0.71342400	0.09492100
C	-5.29729000	2.95893000	-0.65871200
C	-4.19619100	2.12380600	-0.45936100
C	-2.94909800	2.59306700	-0.87982200
H	-2.06973900	1.97112900	-0.74430900
C	-2.81300100	3.84290600	-1.46273700
C	-3.94847700	4.59109200	-1.74057900
C	-5.23637000	4.15038800	-1.40529100
H	-7.47153200	-1.73942700	2.55601100
H	-5.32368700	-1.48267400	1.37871400
H	-9.02208900	0.18469700	2.72173200

H	-1.83138000	4.21335800	-1.74167700
H	-3.83338600	5.53537400	-2.26493000
O	-6.53512600	2.65745800	-0.10364600
B	-6.51875000	5.01792800	-1.86427000
P	-8.96804000	2.89787300	1.52551700
C	-6.16406800	6.08719800	-3.03655000
C	-6.38596300	7.47352200	-3.03776600
C	-5.56508600	5.58481200	-4.21511800
C	-5.99767600	8.31829200	-4.08739300
C	-5.13973600	6.39977300	-5.26837500
C	-5.35868200	7.77812800	-5.20583800
C	-3.27989600	0.46508500	1.19681000
H	-3.36218500	-0.55141500	1.59055200
H	-2.26603000	0.57980600	0.80514900
H	-3.41620100	1.16912000	2.02384400
C	-4.11139100	-0.28566300	-1.06199400
H	-4.22928100	-1.31641600	-0.71185200
H	-4.82864700	-0.10666300	-1.86943600
H	-3.10168500	-0.17590500	-1.47066600
N	-7.14820400	5.58415800	-0.50676100
H	-6.51870900	6.23616600	-0.03744100
H	-8.05306900	6.04770000	-0.59029000
H	-7.26516000	4.79718000	0.13817700
C	-9.02979800	3.90225200	-3.13340900
H	-7.51519100	4.34502800	-2.39495300
C	-8.62976300	3.97186900	-4.53880500
C	-8.35341600	5.20942700	-5.15807900
C	-8.60543000	2.80743100	-5.33480800
C	-8.05566700	5.27517800	-6.50890400
H	-8.35343900	6.11885000	-4.56906900
C	-8.31263200	2.88246800	-6.68573200
H	-8.86271000	1.85020600	-4.89682200
C	-8.02667900	4.11275200	-7.27567300
H	-7.83230900	6.23555900	-6.96387200
H	-8.31720600	1.97820500	-7.28642900
H	-7.78967600	4.16686500	-8.33424000
C	-9.10870100	2.57128000	-2.50256800
C	-8.01857700	1.68624900	-2.54764500
C	-10.31937700	2.12821700	-1.94458700
C	-8.13410200	0.40355700	-2.04117400
H	-7.07168500	2.03225100	-2.95278300
C	-10.43384200	0.83326400	-1.45517600
H	-11.18324600	2.78431000	-1.93494900
C	-9.34272000	-0.02811800	-1.49315600
H	-7.27938500	-0.26525500	-2.05890000
H	-11.38160700	0.49669600	-1.04588400
H	-9.42770800	-1.03460100	-1.09398500
C	-9.92066700	4.95519300	-2.61201300
C	-10.12461100	5.06847200	-1.22441600
C	-10.66766100	5.79438000	-3.46093500
C	-10.97691900	6.02756600	-0.70304500
H	-9.62673200	4.37244900	-0.55169100
C	-11.52788500	6.74818900	-2.93423700
H	-10.61976000	5.66657200	-4.53561600
C	-11.67119800	6.88481600	-1.55697800
H	-11.11378000	6.09906100	0.37200000
H	-12.10290600	7.37694700	-3.60700100
H	-12.34226000	7.63558900	-1.15010300
C	-7.95613900	4.19388400	2.36349900
C	-8.59064300	5.42750900	2.57927100
C	-6.60010300	4.07178900	2.68098100
C	-7.88721400	6.50897900	3.09512600
H	-9.64841800	5.53583200	2.34575000
C	-5.89194100	5.16313600	3.18283200
H	-6.08778500	3.12361400	2.54399400
C	-6.52883100	6.38333000	3.38691700
H	-8.39732700	7.45289500	3.26584400
H	-4.83780700	5.05200600	3.42111000
H	-5.97410800	7.23074400	3.77919500
C	-10.15197300	2.42529100	2.84599200
C	-9.82824800	2.47031600	4.20646200
C	-11.42738100	2.00331000	2.45747300
C	-10.76740600	2.09410100	5.16051800
H	-8.84074600	2.80086100	4.51808300
C	-12.36258400	1.61737100	3.41446500
H	-11.68842400	1.97999400	1.40172500
C	-12.03368200	1.66451300	4.76611500
H	-10.51057200	2.13363200	6.21529600
H	-13.35055400	1.28932500	3.10443400
H	-12.76477200	1.37132800	5.51408800
Cl	-5.35713000	3.86595700	-4.43958200
Cl	-4.38846700	5.72488100	-6.67195800
Cl	-4.86501800	8.79906000	-6.50681100
Cl	-6.29416300	10.02148800	-4.02423600
Cl	-7.20563700	8.26457900	-1.69856400

T1_fip

Energy: -2777.331023

C	-7.35924000	-0.37027900	2.22200000
C	-6.18069200	-0.35746400	1.48895300
C	-5.78920400	0.76679600	0.76085100
C	-6.64971200	1.86527900	0.75747700
C	-7.76507300	1.94281900	1.61272200
C	-8.11503700	0.79055100	2.31962300
C	-4.40578600	0.85291000	0.14007600
C	-5.34967800	2.97605300	-0.92796800
C	-4.33523000	2.02166300	-0.83095900
C	-3.20265800	2.20052000	-1.62723000
H	-2.38104700	1.49483800	-1.55366100
C	-3.09002800	3.28518600	-2.48325900
C	-4.14724400	4.17478800	-2.60087800
C	-5.33222700	4.04030600	-1.86009600
H	-7.65233600	-1.26025400	2.77033600
H	-5.54124100	-1.23415200	1.50324300
H	-8.97074100	0.80399500	2.98173500
H	-2.18339400	3.43340900	-3.06171400
H	-4.03885700	5.01342700	-3.27985600
O	-6.43790700	2.94812000	-0.07362900
B	-6.55643300	5.04077700	-2.12716400
P	-8.52377700	3.59491000	1.90565200
C	-6.28823700	6.17764400	-3.23874600
C	-6.35044000	7.55638000	-3.04557500
C	-5.97398000	5.79727900	-4.54723100
C	-6.12594500	8.49111000	-4.04735700
C	-5.72743800	6.69277700	-5.57642100
C	-5.81272300	8.05519200	-5.32748800
C	-3.40086500	1.10666900	1.29177600
H	-3.44377200	0.28829800	2.01841100
H	-2.38001900	1.17289700	0.90047300
H	-3.63564800	2.04301800	1.80920400
C	-4.03100500	-0.46475400	-0.56523500
H	-3.97413500	-1.28783700	0.15152900
H	-4.76655600	-0.72359400	-1.33130900
H	-3.04883600	-0.39281900	-1.03762900
N	-7.12107800	5.65037100	-0.75928300
H	-6.41092600	6.21423500	-0.29179200
H	-7.93543900	6.25169800	-0.88330200
H	-7.39413900	4.91349500	-0.09132900
C	-8.99656200	3.62409800	-3.29582100
H	-7.57627800	4.37806800	-2.62520400
C	-8.76736700	3.90663900	-4.71382900
C	-8.80332400	5.23639800	-5.18206200
C	-8.60527800	2.86820800	-5.65076800
C	-8.66510500	5.51462800	-6.53149000
H	-8.91843600	6.05004700	-4.47298200
C	-8.47611300	3.15444700	-7.00058500
H	-8.63158100	1.83544100	-5.32205700
C	-8.49494900	4.47536300	-7.44431600
H	-8.67946200	6.54498800	-6.87425700
H	-8.37211100	2.34225300	-7.71339200
H	-8.38549300	4.69512100	-8.50224600
C	-8.65066200	2.30400000	-2.75964800
C	-7.43700600	1.69059000	-3.12533300
C	-9.53641900	1.60575200	-1.92034800
C	-7.13596100	0.41464200	-2.68456200
H	-6.72482700	2.23643800	-3.73643500
C	-9.22377100	0.32788000	-1.47798700
H	-10.49095100	2.04764600	-1.65583400
C	-8.02641100	-0.27162600	-1.85837700
H	-6.19836300	-0.04393200	-2.98161100

H	-9.92262500	-0.20572300	-0.84093800
H	-7.78330100	-1.27043500	-1.50764700
C	-10.05767200	4.40899600	-2.63760400
C	-10.06764000	4.56943500	-1.24521100
C	-11.11965000	4.95772100	-3.38033600
C	-11.05793000	5.30764500	-0.61903800
H	-9.28888700	4.11004600	-0.64344400
C	-12.12911800	5.66983700	-2.74591700
H	-11.17657900	4.79095900	-4.45012900
C	-12.09258800	5.86697200	-1.36868800
H	-11.02529400	5.44089400	0.45865300
H	-12.94957900	6.07129700	-3.33285800
H	-12.87327300	6.44145100	-0.87879200
C	-10.22861100	3.30917000	2.66517800
H	-10.63756300	4.33067900	2.61204600
C	-7.46787000	4.22077400	3.34890500
H	-8.15664000	4.87325400	3.90642700
C	-10.35450800	2.87921100	4.13122800
H	-11.41010800	2.93887000	4.42320500
H	-10.02992900	1.85075200	4.30703600
H	-9.79265900	3.53253600	4.80379200
C	-11.08544900	2.43469100	1.74199200
H	-12.13102400	2.46465700	2.06914000
H	-11.04852100	2.78087800	0.70437000
H	-10.76091600	1.38990400	1.75709800
C	-6.91824800	3.14668300	4.28734000
H	-6.43034000	3.62418800	5.14561000
H	-7.69265600	2.47672300	4.66723900
H	-6.16993900	2.53303800	3.77366400
C	-6.32511800	5.08660400	2.80585600
H	-5.66421400	4.50372800	2.15175300
H	-6.70379100	5.94663800	2.24353500
H	-5.71544400	5.46877000	3.63296900
F	-5.90028300	4.49074600	-4.86549800
F	-5.44521900	6.25843000	-6.80805900
F	-5.60074000	8.93453400	-6.30479100
F	-6.19650000	9.79988400	-3.78947200
F	-6.62366200	8.06717100	-1.81960000

T1_fph

Energy: -3003.727459

C	-7.51231200	-0.35320000	2.40746300
C	-6.34462600	-0.40015700	1.65793500
C	-5.93711200	0.67618400	0.86482400
C	-6.77179000	1.78956400	0.82010000
C	-7.88742800	1.91415900	1.66469600
C	-8.25953000	0.81874700	2.44195100
C	-4.56778200	0.69329600	0.20972900
C	-5.43515700	2.85294800	-0.86595300
C	-4.45981400	1.85906500	-0.76415100
C	-3.32225500	1.98988300	-1.56239800
H	-2.53230500	1.24850700	-1.49171300
C	-3.16353000	3.07084500	-2.41569000
C	-4.17768800	4.01009500	-2.52526900
C	-5.37004000	3.92424500	-1.78830600
H	-7.80939500	-1.20727000	3.00803600
H	-5.72183400	-1.28768900	1.71009200
H	-9.12468400	0.89511700	3.09381200
H	-2.25198800	3.18092200	-2.99494000
H	-4.02666200	4.84983900	-3.19391900
O	-6.53537900	2.85406400	-0.02452000
B	-6.54508900	4.98445900	-2.05544500
P	-8.67260900	3.56439700	1.81818500
C	-6.19403800	6.16218900	-3.10315200
C	-6.19787100	7.53047400	-2.83627900
C	-5.87364700	5.84086400	-4.42574400
C	-5.91555100	8.50721100	-3.78192400
C	-5.57218500	6.77889600	-5.40112200
C	-5.60188200	8.12828600	-5.07966400
C	-3.51959300	0.89264700	1.33285000
H	-3.57941300	0.07445400	2.05839100
H	-2.50840400	0.91057500	0.91299200
H	-3.69399900	1.83727300	1.85866800
C	-4.28602600	-0.64191300	-0.50651900
H	-4.27518800	-1.47026400	0.20649900
H	-5.04699700	-0.84799800	-1.26314400
H	-3.30743700	-0.62965900	-0.99200800
N	-7.14381600	5.56187400	-0.68687300
H	-6.43659300	6.06275100	-0.14772300
H	-7.92278100	6.20631600	-0.81998400
H	-7.48387700	4.80464000	-0.08077100
C	-8.96139300	3.64153900	-3.35857400
H	-7.57233700	4.38722900	-2.61703800
C	-8.69642400	4.00155600	-4.75272600
C	-8.72011100	5.35513100	-5.14532800
C	-8.51253700	3.01606700	-5.74040800
C	-8.54762700	5.70796900	-6.47312000
H	-8.84973100	6.12705600	-4.39305300
C	-8.35149000	3.37670000	-7.06910400
H	-8.54637800	1.96695700	-5.46860600
C	-8.35791700	4.72027100	-7.43828700
H	-8.55100800	6.75576700	-6.75862800
H	-8.23114400	2.60539600	-7.82356200
H	-8.22244800	4.99848400	-8.47931900
C	-8.60410200	2.30269900	-2.87805300
C	-7.37291400	1.72873900	-3.24812600
C	-9.48716200	1.55246100	-2.07991900
C	-7.04554600	0.44644700	-2.84389200
H	-6.66519100	2.30998400	-3.83029000
C	-9.14849100	0.26979300	-1.67373000
H	-10.45693800	1.96044500	-1.81636100
C	-7.92877100	-0.28606200	-2.05156000
H	-6.09102200	0.02281200	-3.13963800
H	-9.84392700	-0.30282700	-1.06759500
H	-7.66579500	-1.28856800	-1.72616200
C	-10.05920100	4.36814500	-2.69626000
C	-10.12821900	4.43511000	-1.29797700
C	-11.10664400	4.93879200	-3.44368800
C	-11.16887700	5.08900000	-0.66127200
H	-9.35362700	3.96848700	-0.69865100
C	-12.16415600	5.57111800	-2.80278600
H	-11.11527600	4.84764500	-4.52402300
C	-12.19286500	5.66452400	-1.41416300
H	-11.18414500	5.14089300	0.42416700
H	-12.97328000	5.98907900	-3.39398900
H	-13.01523800	6.17226800	-0.91874000
F	-5.84549100	4.55137900	-4.81471100
F	-5.28599300	6.39927600	-6.64986000
F	-5.33766100	9.04842200	-6.00526000
F	-5.93483800	9.80196700	-3.45349100
F	-6.47217600	7.98762400	-1.58965300
C	-7.55325500	4.39645200	3.01650200
C	-7.67557900	5.78703100	3.13792400
C	-6.58756900	3.72757400	3.77398600
C	-6.86186600	6.49292500	4.01794300
H	-8.42106100	6.31738900	2.54732500
C	-5.76381200	4.43954800	4.64231800
H	-6.48034800	2.64955200	3.69003200
C	-5.90053200	5.81935600	4.76862600
H	-6.97261500	7.56941900	4.11223100
H	-5.01536200	3.91188800	5.22680400
H	-5.25747700	6.37006600	5.44908300
C	-10.18169800	3.19598200	2.79317700
C	-10.31995300	3.51870600	4.14517900
C	-11.25452100	2.59848100	2.11749400
C	-11.51282900	3.24384400	4.81093400
H	-9.49624400	3.98099800	4.68171600
C	-12.43700700	2.31274800	2.78922900
H	-11.15963900	2.34867000	1.06196300
C	-12.57017000	2.63940000	4.13813800
H	-11.61090800	3.49835200	5.86245500
H	-13.25911800	1.84123700	2.25833900
H	-13.49710100	2.42355700	4.66144800

T2_cip

Energy: -3844.749887

C	-7.03352763	-0.59203648	-0.73585114
C	-5.67820476	-0.60589184	-0.41175802
C	-5.03895659	0.55357463	0.02209767
C	-5.80884768	1.71162228	0.10107068

C	-7.16894671	1.76688160	-0.21088311
C	-7.77565314	0.57801364	-0.63289657
C	-3.57553825	0.65069003	0.44106219
C	-3.92026208	3.08526244	-0.01333760
C	-3.06399102	1.98872043	-0.08246505
C	-1.79279673	2.20831112	-0.60955112
H	-1.09160720	1.38380290	-0.68637348
C	-1.39963222	3.47330730	-1.05145443
C	-2.28680112	4.53313723	-1.00134837
C	-3.58620290	4.37161834	-0.47408247
H	-7.51496540	-1.50524574	-1.07136321
H	-5.12175479	-1.53249371	-0.50260863
H	-8.82746768	0.56473944	-0.89711968
H	-0.40185744	3.61530439	-1.45384124
H	-1.98516482	5.50693391	-1.37780573
O	-5.20125275	2.90534263	0.46546518
B	-4.58356910	5.52839980	-0.54245661
P	-8.00856446	3.38580634	-0.08374653
C	-4.39827012	6.73046681	-1.54003076
C	-3.75062558	7.90451171	-1.17472816
C	-4.89972221	6.63400338	-2.83305450
C	-3.57373174	8.95957959	-2.07229914
C	-4.75319429	7.66343234	-3.76341336
C	-4.07964022	8.83191586	-3.37526507
C	-8.56175053	3.45287613	1.70546306
H	-7.58915779	3.50292782	2.22308546
C	-9.44241456	3.35584318	-1.28388156
H	-9.03555719	2.78197122	-2.12988875
C	-10.74427470	2.69598147	-0.81874942
H	-11.43976754	2.65432356	-1.66466268
H	-10.60675998	1.67786738	-0.44823670
H	-11.22445405	3.28280239	-0.03023364
C	-9.70803037	4.79060412	-1.76545659
H	-10.08077919	5.42046672	-0.95019944
H	-8.80675308	5.25555159	-2.17650793
H	-10.47321721	4.77748390	-2.54927212
C	-9.30757420	2.23104870	2.24358058
H	-9.36865776	2.30085201	3.33573005
H	-10.32848350	2.17972938	1.85867080
H	-8.79480978	1.29718269	1.99492774
C	-9.31616646	4.75868655	1.98029799
H	-10.30321137	4.75451554	1.50780189
H	-9.46778097	4.87739768	3.05856086
H	-8.77122306	5.63765890	1.61720578
C	-3.50946532	0.67457137	1.98962959
H	-3.90326636	-0.26456186	2.39160720
H	-2.46964957	0.78951397	2.31270078
H	-4.09484590	1.50111543	2.40277253
C	-2.74745153	-0.52762060	-0.06970901
H	-3.13495503	-1.46625924	0.33514290
H	-2.75459137	-0.58661756	-1.16309196
H	-1.71233669	-0.44398654	0.27222007
N	-5.84260198	5.54730720	0.28009275
H	-5.68964625	5.23543865	1.24062595
H	-6.29949478	6.45923739	0.30519327
H	-6.66580327	4.77727675	-0.07090835
Cl	-3.15822973	8.01195745	0.46336964
Cl	-2.75205071	10.39500734	-1.58579682
Cl	-3.87687447	10.11822725	-4.50389819
Cl	-5.38968770	7.50125627	-5.35765173
Cl	-5.74125499	5.16005316	-3.24643634

T2_cph

Energy: -4071.139053

C	-7.09687300	-0.59126100	-0.65654900
C	-5.72549200	-0.63100000	-0.40051400
C	-5.03576600	0.51242300	-0.00107100
C	-5.77631800	1.68490800	0.11631500
C	-7.14162500	1.76444000	-0.15221200
C	-7.80734400	0.59641400	-0.53735800
C	-3.55307100	0.58346700	0.35058200
C	-3.88138900	3.03543600	-0.04485700
C	-3.04467600	1.92846000	-0.16403600
C	-1.78843600	2.14585300	-0.72720700
H	-1.09828500	1.31672500	-0.84358000
C	-1.39783000	3.41657000	-1.15378800
C	-2.27188900	4.48523100	-1.05347000
C	-3.55482800	4.32679300	-0.48981700
H	-7.61177200	-1.49709200	-0.96047000
H	-5.19599500	-1.57069700	-0.51667000
H	-8.87012700	0.62696100	-0.76017100
H	-0.41200600	3.55772000	-1.58503300
H	-1.97104700	5.46273300	-1.42095000
O	-5.14878000	2.86023800	0.47788400
B	-4.55798400	5.49109800	-0.50510200
P	-7.93906600	3.39365800	-0.03644300
C	-4.37056200	6.71193600	-1.48479200
C	-3.68853000	7.86202900	-1.10468500
C	-4.89203100	6.65867000	-2.77218500
C	-3.50174200	8.93419700	-1.98005100
C	-4.73598700	7.70618900	-3.68090700
C	-4.03045700	8.84973500	-3.27701100
C	-3.41851200	0.56971200	1.89468900
H	-3.80547100	-0.37430500	2.29210100
H	-2.36418200	0.66532300	2.17390500
H	-3.97461600	1.39310500	2.35238700
C	-2.76624000	-0.59288900	-0.22645400
H	-3.14736200	-1.53661700	0.17260400
H	-2.82434100	-0.62354400	-1.31945300
H	-1.71554100	-0.53079300	0.06903600
N	-5.79101900	5.49595400	0.32011000
H	-5.66029000	5.12903800	1.26310300
H	-6.25250300	6.40249500	0.37954600
H	-6.70468400	4.66612400	-0.06683500
C	-8.58472700	3.54075600	1.65877500
C	-8.98466600	4.81020100	2.09659700
C	-8.66249900	2.44896600	2.52679400
C	-9.47513200	4.97841200	3.38637600
H	-8.92956300	5.66477800	1.42446600
C	-9.14593700	2.62698900	3.81983200
H	-8.34787100	1.46347700	2.19529700
C	-9.55348000	3.88700800	4.24913400
H	-9.79252200	5.96199300	3.71955200
H	-9.20603000	1.77673500	4.49268200
H	-9.93134300	4.02028100	5.25856800
C	-9.36855800	3.32685300	-1.15890800
C	-9.12087900	3.20209300	-2.53195600
C	-10.68172800	3.41591800	-0.69117100
C	-10.18302900	3.15807200	-3.42573100
H	-8.10075200	3.12432200	-2.90053400
C	-11.73996800	3.37767600	-1.59544300
H	-10.88107900	3.50826500	0.37241600
C	-11.49342500	3.24908000	-2.95874600
H	-9.98793600	3.05563500	-4.48898900
H	-12.76020500	3.44358900	-1.22936600
H	-12.32210900	3.21836700	-3.65998600
Cl	-5.77233500	5.21532600	-3.21358100
Cl	-5.39841300	7.59634700	-5.26974700
Cl	-3.81564800	10.15807200	-4.37868200
Cl	-2.63841200	10.33887800	-1.47420700
Cl	-3.06228000	7.91940600	0.52342400

T2_fip

Energy: -2043.026506

C	-7.12681208	-0.59113608	-0.69482123
C	-5.75904990	-0.63000927	-0.42720218
C	-5.08027679	0.51660305	-0.02016877
C	-5.82619381	1.68725808	0.08931613
C	-7.19632524	1.76802865	-0.16601943
C	-7.84367201	0.59169887	-0.56178554
C	-3.60174543	0.58710253	0.34907962
C	-3.91987128	3.03164844	-0.08689832
C	-3.08059145	1.92314446	-0.17270370
C	-1.80953306	2.13133210	-0.70420487
H	-1.11810477	1.29968887	-0.79164860
C	-1.40109765	3.39789673	-1.12743120
C	-2.27687627	4.46654516	-1.06959640
C	-3.58330365	4.31507374	-0.55579024
H	-7.63788149	-1.49570684	-1.00915358
H	-5.22531777	-1.56749729	-0.54010094

H	-8.90617246	0.59770906	-0.78041795
H	-0.39922425	3.53466913	-1.52147284
H	-1.95875932	5.44173399	-1.42831772
O	-5.18808635	2.86871429	0.42978290
B	-4.57025111	5.48854112	-0.59779434
P	-7.99097664	3.40469866	-0.00255864
C	-4.41533949	6.68176176	-1.59574866
C	-4.57086775	8.01166545	-1.19573627
C	-4.11282894	6.48601265	-2.94768106
C	-4.41787945	9.08697607	-2.05483692
C	-3.96987700	7.53565066	-3.84304922
C	-4.11796305	8.84255138	-3.39110558
F	-4.84594291	8.28647711	0.09522804
F	-3.99538344	5.24494901	-3.43700231
F	-3.70311343	7.30598973	-5.12757936
F	-4.55096475	10.33875040	-1.61963850
F	-3.97822435	9.85551695	-4.23539554
C	-8.50882010	3.48178785	1.79452957
H	-7.52655982	3.50227668	2.29541165
C	-9.43910685	3.43609301	-1.18410653
H	-9.06683476	2.84675011	-2.03516519
C	-10.75869297	2.82694008	-0.70082491
H	-11.46891409	2.81963821	-1.53536573
H	-10.65559223	1.80088238	-0.34097496
H	-11.20166196	3.42633774	0.09985805
C	-9.65213184	4.88107007	-1.66096723
H	-9.98548539	5.52597831	-0.84050131
H	-8.73878818	5.30837093	-2.08662768
H	-10.42896256	4.90008576	-2.43300027
C	-9.27982256	2.27835017	2.33827974
H	-9.33025229	2.34983759	3.43077116
H	-10.30468784	2.25163880	1.96137903
H	-8.79117596	1.33262241	2.08597227
C	-9.22110314	4.80770794	2.08655807
H	-10.21566276	4.83363855	1.63109238
H	-9.35075975	4.92521388	3.16772999
H	-8.65737778	5.67272641	1.71889410
C	-3.48623687	0.59003202	1.89499382
H	-3.88369830	-0.34710646	2.29817408
H	-2.43492960	0.68302946	2.18646245
H	-4.04363909	1.42147859	2.33625097
C	-2.81046658	-0.59821981	-0.20325162
H	-3.20165170	-1.53608032	0.19979021
H	-2.85180324	-0.64040701	-1.29662256
H	-1.76426864	-0.53755076	0.10801370
N	-5.77515141	5.50850038	0.29464817
H	-5.57967679	5.17163356	1.23817727
H	-6.23472080	6.41499981	0.36701567
H	-6.64816178	4.73136402	-0.02913309

T2_fph

Energy: -2269.416077

C	-7.18757671	-0.56092714	-0.65581052
C	-5.81271044	-0.63471889	-0.42502300
C	-5.08869906	0.48948193	-0.03151336
C	-5.80054686	1.67707889	0.10483287
C	-7.16974061	1.78889225	-0.12787116
C	-7.86966056	0.64078943	-0.51069219
C	-3.60046269	0.52455564	0.30315869
C	-3.87782149	2.98557864	-0.08640557
C	-3.06332411	1.86175123	-0.20410363
C	-1.79798867	2.05639251	-0.75446190
H	-1.12211312	1.21503661	-0.86688574
C	-1.37707226	3.32254432	-1.16589980
C	-2.23476864	4.40506249	-1.07991246
C	-3.53324438	4.26834281	-0.54526176
H	-7.72813766	-1.45205840	-0.95858272
H	-5.30824194	-1.58614112	-0.55652703
H	-8.93631745	0.69669421	-0.70963133
H	-0.38022285	3.44875585	-1.57599977
H	-1.90813912	5.37862036	-1.43565677
O	-5.14043217	2.83715901	0.45400203
B	-4.51772785	5.45188829	-0.56888367
P	-7.92229280	3.43533890	0.03515272
C	-4.35826819	6.63743312	-1.58055148
C	-4.47350584	7.97214809	-1.18536747
C	-4.08958432	6.42674741	-2.93636256
C	-4.31231884	9.03848487	-2.05492422
C	-3.93916674	7.46666905	-3.84172456
C	-4.04589122	8.77931559	-3.39519260
F	-4.71763601	8.26134292	0.10823502
F	-4.01185222	5.17877854	-3.41914878
F	-3.70354444	7.22287470	-5.13036011
F	-4.40731034	10.29620064	-1.62566761
F	-3.89873275	9.78404450	-4.24915765
C	-3.45130954	0.49310705	1.84561196
H	-3.85828933	-0.44432377	2.23864127
H	-2.39223845	0.55937008	2.11537796
H	-3.98161981	1.32637914	2.31610769
C	-2.84771327	-0.66462435	-0.29328021
H	-3.24867927	-1.60308025	0.09874704
H	-2.91607939	-0.68135190	-1.38595102
H	-1.79333988	-0.63184829	-0.00663150
N	-5.70482033	5.48547297	0.32211297
H	-5.53604762	5.11742342	1.25826924
H	-6.15946877	6.39265532	0.40510945
H	-6.65436839	4.67283017	-0.02294131
C	-8.54339905	3.55859058	1.74110181
C	-9.01759500	4.80482265	2.17218828
C	-8.52380245	2.47748318	2.62519553
C	-9.48406759	4.95853090	3.47205518
H	-9.03688324	5.65108540	1.48785160
C	-8.98471341	2.64193429	3.92875432
H	-8.15406224	1.50999362	2.29754414
C	-9.46582261	3.87737703	4.35175253
H	-9.85889064	5.92336637	3.80040176
H	-8.97007128	1.79937375	4.61372754
H	-9.82632541	4.00028972	5.36882225
C	-9.36674810	3.44473040	-1.06729417
C	-9.14282945	3.61797416	-2.43864890
C	-10.66744922	3.27500076	-0.58537281
C	-10.21656659	3.60978996	-3.32063209
H	-8.13180369	3.75392410	-2.81665772
C	-11.73720723	3.27451305	-1.47582507
H	-10.84480018	3.14177271	0.47803397
C	-11.51366363	3.43998278	-2.83977624
H	-10.04172705	3.74185937	-4.38414924
H	-12.74767889	3.14149119	-1.10096967
H	-12.35158987	3.43914263	-3.53067251

T3_cip

Energy: -3901.3921

C	-7.08748501	-0.87428615	-0.20904355
C	-5.71139360	-0.73621061	-0.03497951
C	-5.11861818	0.51574091	0.10839590
C	-5.94603992	1.63921239	0.04520948
C	-7.33289649	1.52139441	-0.12929286
C	-7.90090454	0.24713296	-0.24678624
C	-3.64564049	0.75487300	0.39415895
C	-4.13331597	3.08864883	-0.39437378
C	-3.24811736	2.00804562	-0.37619512
C	-2.02816553	2.16520275	-1.02959100
H	-1.31264849	1.35088039	-1.05341645
C	-1.72071269	3.36777182	-1.65785242
C	-2.61298495	4.42859398	-1.60729823
C	-3.85171277	4.33981687	-0.95148009
H	-7.52434003	-1.86207022	-0.31167825
H	-5.09497876	-1.62819260	-0.00194391
H	-8.97106310	0.12964212	-0.38311955
H	-0.77384891	3.47901549	-2.17752162
H	-2.34336790	5.36191806	-2.09479893
O	-5.42467245	2.90122592	0.14305623
B	-4.87583467	5.56809032	-0.97608044
P	-8.34234442	3.00439362	-0.16841595
C	-4.33914222	7.00124584	-1.51252534
C	-3.20648182	7.55234069	-0.88789037
C	-4.94005233	7.81896694	-2.47709171
C	-2.58820330	8.72833558	-1.32426135
C	-4.35164313	9.00074585	-2.94835623
C	-3.14780219	9.43883445	-2.39051078

C	-8.60397141	3.62740645	1.54641563
H	-7.56719792	3.80068324	1.87517868
C	-9.85061084	2.76477028	-1.20776770
H	-9.52090845	2.02942955	-1.95623826
C	-11.06448568	2.20614781	-0.45667310
H	-11.84527221	1.98206400	-1.19007355
H	-10.84890514	1.28698453	0.09380314
H	-11.47060797	2.94159309	0.24319868
C	-10.19031233	4.07915004	-1.92706335
H	-10.48600332	4.86101458	-1.22140459
H	-9.35357969	4.44927009	-2.52695971
H	-11.03547893	3.89831717	-2.59849407
C	-9.22458847	2.58179946	2.47671388
H	-9.16153636	2.95483848	3.50366359
H	-10.27923703	2.41092053	2.24904182
H	-8.69391439	1.62573369	2.43414500
C	-9.35629895	4.96157927	1.54799036
H	-10.40821315	4.82776543	1.27941137
H	-9.32441370	5.38122182	2.55838669
H	-8.90849198	5.69045183	0.86461900
C	-3.49388048	1.04436311	1.91010436
H	-3.81221568	0.17225056	2.49116638
H	-2.44479562	1.25843718	2.13822449
H	-4.09460999	1.90634645	2.21546053
C	-2.78340045	-0.45574753	0.03894636
H	-3.07994604	-1.32372044	0.63409211
H	-2.85825556	-0.71296728	-1.02280549
H	-1.73566683	-0.25776668	0.27847864
N	-5.93807982	5.68476073	-0.02362664
H	-6.01533781	5.03623001	0.74238987
H	-6.31029574	6.59496744	0.20062551
N	-5.69197918	4.60676281	-2.83554754
H	-6.65207608	4.77229136	-3.11780080
H	-5.10071577	4.88257805	-3.61473589
H	-7.58284318	4.00652658	-0.79490538
H	-5.55955449	3.60766660	-2.71065984
Cl	-2.57333585	6.79700132	0.55623477
Cl	-1.15700941	9.32044360	-0.55474706
Cl	-2.38390118	10.87262570	-2.97707072
Cl	-5.10215750	9.93684182	-4.19647031
Cl	-6.54862701	7.45367526	-3.07530559

T3_cph

Energy: -4127.775956

C	-7.13763054	-0.92246277	-0.34520243
C	-5.76352697	-0.78018035	-0.15520402
C	-5.16789407	0.47295267	-0.02346200
C	-5.99271249	1.59386247	-0.12056559
C	-7.37527104	1.46814229	-0.31393639
C	-7.95130832	0.19753241	-0.41652586
C	-3.70466818	0.71459241	0.30395978
C	-4.17072571	3.06123656	-0.47392414
C	-3.28374833	1.98148066	-0.43163504
C	-2.02903497	2.15976567	-1.00867824
H	-1.31036665	1.34791951	-1.01431675
C	-1.68720884	3.38192631	-1.57952023
C	-2.58008585	4.44202851	-1.54029552
C	-3.85631328	4.33136347	-0.96385386
H	-7.57191474	-1.91252998	-0.43537981
H	-5.14903627	-1.67231505	-0.09656133
H	-9.02175440	0.09401897	-0.56707934
H	-0.71126478	3.50956299	-2.03809513
H	-2.28083949	5.39557301	-1.96860844
O	-5.49254809	2.86027914	-0.02365028
B	-4.85858830	5.57929690	-0.98946805
P	-8.37844715	2.94512356	-0.42400615
C	-4.22997356	7.04140344	-1.30597806
C	-3.15109267	7.48267548	-0.52034030
C	-4.71040921	7.97596453	-2.23118477
C	-2.46309863	8.67507616	-0.76683344
C	-4.05018840	9.17990069	-2.51244693
C	-2.89726366	9.51393623	-1.79745636
C	-3.60317192	0.98671057	1.82754392
H	-3.93910110	0.10754173	2.38797769
H	-2.56304552	1.20118406	2.09347395
H	-4.21634064	1.84477691	2.12068590
C	-2.82839392	-0.48956191	-0.03963427
H	-3.14192378	-1.36632539	0.53333209
H	-2.86887418	-0.73150551	-1.10678009
H	-1.78940929	-0.29399188	0.23674642
N	-6.02993207	5.62989255	-0.17640289
H	-6.26156829	4.90162426	0.47811926
H	-6.45075617	6.51498701	0.06030393
N	-5.45270180	4.84868695	-3.02195354
H	-6.39713523	5.04223019	-3.33679142
H	-4.81984955	5.20857156	-3.73084163
H	-7.75098287	3.84513474	-1.30133110
H	-5.31979819	3.84248591	-2.99448858
C	-8.52916187	3.76532269	1.16849530
C	-8.04130980	3.15765251	2.32723617
C	-9.14227586	5.02376938	1.21899434
C	-8.16778024	3.81838992	3.54530690
H	-7.56668878	2.18130396	2.28142580
C	-9.26067457	5.67162736	2.44047952
H	-9.51926049	5.49336709	0.31341398
C	-8.77323436	5.06995880	3.60075767
H	-7.78987988	3.35329533	4.45035175
H	-9.73160576	6.64854958	2.48841851
H	-8.86614608	5.58303088	4.55334214
C	-9.99597120	2.56642961	-1.10530863
C	-10.13598151	2.45298504	-2.49333066
C	-11.08330432	2.34750368	-0.25441769
C	-11.37390615	2.11736026	-3.02627638
H	-9.28848661	2.62609596	-3.15206826
C	-12.31633986	2.01063940	-0.80155575
H	-10.97074098	2.44461469	0.82195166
C	-12.46039323	1.89604160	-2.18179170
H	-11.49224008	2.03309132	-4.10201657
H	-13.16622638	1.84146613	-0.14783752
H	-13.42689944	1.63687653	-2.60368707
Cl	-2.67930995	6.55716181	0.88600423
Cl	-1.09758680	9.13108513	0.19281419
Cl	-2.04389230	10.97439899	-2.14983828
Cl	-4.65180207	10.26871834	-3.71698090
Cl	-6.25551627	7.72578931	-3.02299020

T3_fip

Energy: -2099.681251

C	-7.11129300	-0.84281500	-0.36967900
C	-5.73913200	-0.73138400	-0.14978200
C	-5.13356800	0.50594500	0.05464600
C	-5.94418800	1.64176200	0.00197600
C	-7.32808600	1.55073500	-0.20660800
C	-7.90978700	0.29001900	-0.38552700
C	-3.66962300	0.71404900	0.40632600
C	-4.09863500	3.07412900	-0.33611400
C	-3.22353300	1.98814400	-0.30047100
C	-1.96566500	2.15850500	-0.87656500
H	-1.25385600	1.34047500	-0.88332800
C	-1.61413200	3.37621100	-1.44763800
C	-2.50806300	4.43866300	-1.43219400
C	-3.78606600	4.33319500	-0.86161900
H	-7.55774800	-1.81993100	-0.52140800
H	-5.13705200	-1.63348000	-0.12876700
H	-8.97763400	0.19153500	-0.55156600
H	-0.63554000	3.49661500	-1.90237600
H	-2.21060900	5.37743100	-1.89029800
O	-5.41008900	2.89376300	0.14578600
B	-4.79861400	5.55724000	-0.90288000
P	-8.31120200	3.05155300	-0.18334800
C	-4.32726500	6.94309200	-1.57488600
C	-3.23450100	7.59554500	-1.00212500
C	-4.96158100	7.65320700	-2.58900600
C	-2.74895400	8.81974400	-1.43854700
C	-4.50977900	8.88073500	-3.06066700
C	-3.39284100	9.46714900	-2.48437400
F	-2.60423500	7.03387400	0.04901900
F	-6.08886400	7.18499200	-3.16885600
F	-5.15362500	9.50944500	-4.05066900
F	-1.68900800	9.38730100	-0.85547900

F	-2.95169100	10.64704500	-2.91997000
C	-8.54470300	3.60755600	1.55865400
H	-7.50165200	3.75387500	1.88040800
C	-9.83398000	2.87712000	-1.21277100
H	-9.52313900	2.17385500	-1.99933300
C	-11.04111000	2.29635900	-0.46750800
H	-11.83488400	2.10813200	-1.19696100
H	-10.82373000	1.35417600	0.04199500
H	-11.43010100	3.00536400	0.26846400
C	-10.17109100	4.22569200	-1.86659600
H	-10.45304000	4.97586000	-1.12199800
H	-9.33829900	4.61682700	-2.45840200
H	-11.02528400	4.08238600	-2.53566500
C	-9.16680900	2.53287500	2.45427800
H	-9.08145000	2.86112000	3.49481500
H	-10.22748400	2.38732000	2.23737500
H	-8.65183100	1.57175900	2.36254000
C	-9.27904000	4.95014400	1.62611900
H	-10.33592600	4.84197800	1.36575000
H	-9.22889000	5.32570900	2.65300300
H	-8.82996700	5.70182900	0.96880800
C	-3.57798600	0.94689000	1.93673100
H	-3.93664400	0.06107500	2.47173200
H	-2.53623600	1.13284100	2.21724300
H	-4.17643500	1.80894100	2.24657800
C	-2.80989900	-0.49597000	0.04272800
H	-3.14581400	-1.38100800	0.58986700
H	-2.84107200	-0.71054600	-1.03057400
H	-1.77114600	-0.32531900	0.33628000
N	-5.81378000	5.72380300	0.07955500
H	-5.93044000	5.07804100	0.84285500
H	-6.21928600	6.62930100	0.25825900
N	-5.74437800	4.52814500	-2.78583400
H	-6.65229500	4.80211400	-3.14701600
H	-5.06747200	4.72685400	-3.51676500
H	-7.53907600	4.06264500	-0.77882200
H	-5.74230600	3.52045800	-2.66122700

T3_fph

Energy: -2326.065146

C	-7.15617752	-0.88588512	-0.47291333
C	-5.78492988	-0.77860329	-0.24058551
C	-5.16879156	0.45659455	-0.04698485
C	-5.97096500	1.59454256	-0.12890978
C	-7.35085273	1.50489276	-0.35538651
C	-7.94829889	0.25104342	-0.51976759
C	-3.71343873	0.65867179	0.34114498
C	-4.11393728	3.03632285	-0.37721093
C	-3.24251016	1.94760568	-0.32294801
C	-1.95491514	2.13522557	-0.82320793
H	-1.24216734	1.31803113	-0.81432458
C	-1.57282603	3.37000536	-1.33561292
C	-2.46443260	4.43445285	-1.33076703
C	-3.77222359	4.31293636	-0.83642010
H	-7.60586889	-1.86332390	-0.61217935
H	-5.19052927	-1.68516843	-0.19747454
H	-9.01691576	0.17363194	-0.69710369
H	-0.57047757	3.50283034	-1.73142485
H	-2.14073608	5.38924344	-1.73532696
O	-5.45206722	2.84782746	0.01850799
B	-4.78282985	5.54158183	-0.89010463
P	-8.31579050	3.01042784	-0.40588449
C	-4.24499945	6.97378191	-1.39703612
C	-3.17741915	7.55945014	-0.71600362
C	-4.82400811	7.78086808	-2.37118633
C	-2.66334368	8.81302491	-1.01688664
C	-4.34289262	9.04100756	-2.70787354
C	-3.25152481	9.56055997	-2.02802119
F	-2.60153442	6.90309394	0.31089793
F	-5.92454952	7.37865854	-3.04501780
F	-4.93445558	9.76275061	-3.66692644
F	-1.62830139	9.31379056	-0.33517909
F	-2.78228357	10.77090149	-2.33188614
C	-3.66457864	0.86437337	1.87758361
H	-4.03660190	-0.03076133	2.38765858
H	-2.63169244	1.04839327	2.19044432
H	-4.27364746	1.72114232	2.18319034
C	-2.84635146	-0.54612791	-0.02323274
H	-3.19818478	-1.44129479	0.49654368
H	-2.84989013	-0.73812465	-1.10119195
H	-1.81545996	-0.38487261	0.30125605
N	-5.89210279	5.64189209	-0.00699778
H	-6.13360368	4.92774981	0.66009542
H	-6.33748950	6.52672481	0.17873240
N	-5.53006032	4.69550028	-2.90274897
H	-6.41086648	5.02512836	-3.28342197
H	-4.81018671	4.91881791	-3.58369855
H	-7.64253864	3.94314544	-1.21169359
H	-5.56461964	3.68288937	-2.83980145
C	-8.47964754	3.74334184	1.22789826
C	-8.01930778	3.06566128	2.35868645
C	-9.07146483	5.00809274	1.33807780
C	-8.15201749	3.66196248	3.60882272
H	-7.56066840	2.08502129	2.26628558
C	-9.19707637	5.59110019	2.59123721
H	-9.42847968	5.53184142	0.45426435
C	-8.73699223	4.91921212	3.72378933
H	-7.79547591	3.14203309	4.49245753
H	-9.65271359	6.57190819	2.68551712
H	-8.83557867	5.38156151	4.70145229
C	-9.92608965	2.71553515	-1.14229220
C	-10.03910915	2.69745705	-2.53728817
C	-11.03627978	2.46847642	-0.32936622
C	-11.27306400	2.42900092	-3.11555496
H	-9.17403101	2.89261728	-3.16632764
C	-12.26496968	2.19948920	-0.92173010
H	-10.94394921	2.49161004	0.75307580
C	-12.38223965	2.18006656	-2.30918331
H	-11.37059253	2.41924518	-4.19664264
H	-13.13242582	2.00909735	-0.29761395
H	-13.34548378	1.97408302	-2.76636274

T4_cip

Energy: -3901.400669

C	-7.08719027	-0.85206771	0.07155576
C	-5.70209801	-0.71406743	0.16197212
C	-5.10297940	0.54373872	0.18004180
C	-5.94219686	1.65297341	0.07601447
C	-7.33473432	1.54660935	0.00050015
C	-7.90441304	0.26867521	0.00500153
C	-3.61603430	0.81293020	0.36836474
C	-4.18778235	3.04630531	-0.62645406
C	-3.26268321	2.00587280	-0.51414186
C	-2.05273134	2.14862367	-1.19105153
H	-1.30320236	1.36621037	-1.14147816
C	-1.79260896	3.29903747	-1.92946227
C	-2.74533616	4.30749889	-2.01053671
C	-3.98722221	4.21404019	-1.36327720
H	-7.53007919	-1.84280932	0.06286870
H	-5.08763229	-1.60591888	0.22633500
H	-8.98084830	0.14549713	-0.05578390
H	-0.84280732	3.40561098	-2.44490201
H	-2.52180577	5.19751282	-2.59644579
O	-5.41575980	2.91912226	0.03108417
B	-5.11379942	5.33954709	-1.68638203
P	-8.27717215	3.09009087	-0.08392742
C	-4.40033372	6.82822679	-1.82590796
C	-3.72298661	7.30886368	-0.68631091
C	-4.38492405	7.70384943	-2.91964657
C	-3.05055751	8.53397734	-0.64147869
C	-3.72458712	8.94174673	-2.91784220
C	-3.04687683	9.35711736	-1.77114109
C	-8.55466724	3.64240762	1.66703857
H	-7.51831841	3.83740018	1.98880328
C	-9.82598631	2.81160161	-1.07276691
H	-9.51103675	2.06097774	-1.81265856
C	-11.03406877	2.26670985	-0.30422550
H	-11.83131129	2.04210179	-1.02097246
H	-10.81410841	1.35092872	0.24936927
H	-11.42455330	3.00690235	0.39969074

C	-10.18345225	4.10728160	-1.81710788
H	-10.46492671	4.90394901	-1.12087448
H	-9.35409558	4.46680708	-2.43465302
H	-11.04002901	3.92145329	-2.47344552
C	-9.14966028	2.58454740	2.59678595
H	-9.08075318	2.94212651	3.62983480
H	-10.20469972	2.40189594	2.37885268
H	-8.60990775	1.63503666	2.53327149
C	-9.32724963	4.96574565	1.70554407
H	-10.37475972	4.82714007	1.42155803
H	-9.31299892	5.36055924	2.72670942
H	-8.88818646	5.72290185	1.04709379
C	-3.38705689	1.21825128	1.84743942
H	-3.66965427	0.39303322	2.50975853
H	-2.32886236	1.45174622	2.00376584
H	-3.97703246	2.09969084	2.11636783
C	-2.76439580	-0.41798009	0.05856625
H	-3.03289327	-1.24397803	0.72285146
H	-2.88671839	-0.74568267	-0.97907929
H	-1.70731402	-0.20524687	0.23664240
N	-6.35703385	5.42642412	-0.76152952
H	-6.08128561	5.50366783	0.21372374
H	-6.89733741	6.26882026	-0.95455274
N	-5.75488865	4.74732612	-3.08196462
H	-6.54879480	5.26881792	-3.45158522
H	-5.06869447	4.67321849	-3.83167849
H	-7.35072826	4.24176740	-0.63999238
H	-6.07203567	3.79882936	-2.87900312
Cl	-5.22775840	7.30495607	-4.41594155
Cl	-3.73421283	9.96680494	-4.31255089
Cl	-2.22217671	10.87370077	-1.74391177
Cl	-2.22221000	9.05194712	0.78620986
Cl	-3.69372906	6.35900362	0.78831384

T4_cph

Energy: -4127.787015

C	-7.11154179	-0.86059610	0.08621096
C	-5.72311965	-0.72570953	0.13653175
C	-5.11190387	0.52670334	0.10316055
C	-5.94390604	1.63921617	-0.01341452
C	-7.33667375	1.52850244	-0.05699368
C	-7.92437862	0.26139284	0.00146007
C	-3.62204904	0.78989369	0.26574686
C	-4.19090338	3.02503786	-0.73919909
C	-3.27145355	1.97916251	-0.62344261
C	-2.05467306	2.11874782	-1.28885561
H	-1.31021990	1.33179355	-1.23645857
C	-1.77880320	3.27298427	-2.01472852
C	-2.72202672	4.29043342	-2.09002490
C	-3.97228268	4.20058435	-1.45824457
H	-7.55782952	-1.84914633	0.11963390
H	-5.11291727	-1.61965257	0.21280825
H	-9.00546800	0.16003983	-0.03552187
H	-0.82305730	3.37768864	-2.51945150
H	-2.48279676	5.18881738	-2.65752929
O	-5.42618980	2.90236131	-0.09211289
B	-5.05881442	5.37222589	-1.76645609
P	-8.28817659	3.05185499	-0.15823778
C	-4.30105271	6.85009722	-1.73598971
C	-3.69806971	7.22045413	-0.51646907
C	-4.19499695	7.81375063	-2.74757212
C	-3.01355454	8.42398322	-0.32160883
C	-3.52063817	9.03473577	-2.59500282
C	-2.92005133	9.33971093	-1.37331561
C	-3.37337345	1.20228302	1.73999698
H	-3.65101787	0.38181799	2.41040716
H	-2.31261020	1.43330858	1.88189690
H	-3.95741952	2.08757134	2.01027131
C	-2.78187147	-0.44790324	-0.04891485
H	-3.04795821	-1.26948748	0.62168334
H	-2.91873535	-0.77848269	-1.08380390
H	-1.72140576	-0.24266164	0.11661463
N	-6.36102802	5.41507689	-0.93922487
H	-6.16242706	5.44026341	0.05705801
H	-6.88528138	6.26806851	-1.12756231
N	-5.59597113	4.91489153	-3.25349322
H	-6.35344714	5.48275630	-3.63075013
H	-4.85830943	4.89071730	-3.95599902
H	-7.45670613	4.12811344	-0.82426865
H	-5.94311101	3.96086235	-3.15499738
C	-8.57061674	3.69094319	1.50870670
C	-8.39921497	2.88470637	2.63627899
C	-8.95403344	5.03069473	1.64742209
C	-8.61990893	3.41984674	3.90130807
H	-8.09152779	1.84825861	2.52823100
C	-9.17504913	5.55445633	2.91530142
H	-9.08516538	5.66083173	0.77033691
C	-9.00723776	4.74984658	4.04075691
H	-8.48633869	2.79584347	4.77970750
H	-9.47330992	6.59256387	3.02549360
H	-9.17595934	5.16344915	5.03066624
C	-9.87609777	2.69174254	-0.94388324
C	-9.87523758	2.27459454	-2.28110718
C	-11.07995093	2.83162922	-0.24942525
C	-11.07887871	1.99567851	-2.91506621
H	-8.93814524	2.15702995	-2.82075397
C	-12.28080389	2.55229039	-0.89567203
H	-11.08178714	3.15298720	0.78805831
C	-12.28131749	2.13574765	-2.22324122
H	-11.07999481	1.66889988	-3.95049151
H	-13.21727386	2.65787285	-0.35653865
H	-13.22082086	1.91801651	-2.72247517
Cl	-3.79004992	6.15166337	0.87157834
Cl	-4.93111284	7.55808369	-4.32996534
Cl	-3.41933948	10.17431932	-3.89456550
Cl	-2.08125659	10.83398353	-1.15885461
Cl	-2.28049908	8.80368858	1.19934373

T4_fip

Energy: -2099.690123

C	-7.11976900	-0.83852100	-0.19794800
C	-5.73733600	-0.72620200	-0.04559000
C	-5.12553300	0.51951300	0.07852400
C	-5.95038100	1.64140500	0.01011500
C	-7.34138200	1.56149400	-0.11070600
C	-7.92430800	0.29386000	-0.21186700
C	-3.64858300	0.75971800	0.36723500
C	-4.14935900	3.05784200	-0.51632000
C	-3.23338100	2.01042100	-0.40244300
C	-1.97790200	2.19730600	-0.97836800
H	-1.22934600	1.41421200	-0.92309200
C	-1.66993400	3.39247200	-1.62105800
C	-2.62496100	4.39736100	-1.72730000
C	-3.91438700	4.25897800	-1.19086800
H	-7.57234100	-1.82059500	-0.29038200
H	-5.13712400	-1.62952700	-0.01415300
H	-8.99966800	0.18684000	-0.31141300
H	-0.68295000	3.53336900	-2.05140000
H	-2.36982000	5.31261900	-2.25710900
O	-5.41336100	2.90116100	0.05774200
B	-5.06453100	5.33964400	-1.56775500
P	-8.25429300	3.12631100	-0.07149700
C	-4.42048500	6.81080800	-1.87529300
C	-3.81272300	7.47670200	-0.81060800
C	-4.39622500	7.50746800	-3.07657700
C	-3.22592000	8.72867000	-0.91335700
C	-3.82402700	8.76440100	-3.23315300
C	-3.23178200	9.38033000	-2.14091700
F	-3.77520600	6.88717100	0.40362300
F	-4.94828800	6.96777000	-4.19615500
F	-3.83971000	9.38118700	-4.41919400
F	-2.65710800	9.31218100	0.14528900
F	-2.67848100	10.58592300	-2.26583100
C	-8.51367300	3.53557500	1.72145800
H	-7.47213700	3.68516400	2.05030700
C	-9.81253300	2.95751700	-1.06904500
H	-9.51656900	2.26691400	-1.87266700
C	-11.02115300	2.36853300	-0.33472700
H	-11.82904700	2.21303400	-1.05780400
H	-10.80792300	1.40866400	0.14147100

H	-11.39267600	3.05516800	0.43107800
C	-10.15651800	4.31603000	-1.69877200
H	-10.42087900	5.05525400	-0.93579900
H	-9.32710800	4.71502500	-2.29147700
H	-11.02089000	4.19815900	-2.36063800
C	-9.12120700	2.41575500	2.56685000
H	-9.03380400	2.68439000	3.62513600
H	-10.18212000	2.27240600	2.34776200
H	-8.60180400	1.46454400	2.41750000
C	-9.25993600	4.86586500	1.87399700
H	-10.31254500	4.77085300	1.59091700
H	-9.22832700	5.17674800	2.92340400
H	-8.81091700	5.66451700	1.27383800
C	-3.50660100	1.05139200	1.88350000
H	-3.83884600	0.18398000	2.46381300
H	-2.45786200	1.25664700	2.12189900
H	-4.10360000	1.91924500	2.17990700
C	-2.78931300	-0.45492000	0.01635700
H	-3.10411000	-1.32506900	0.59880500
H	-2.85122200	-0.70226300	-1.04857600
H	-1.74315800	-0.27060600	0.27323300
N	-6.25658600	5.45640500	-0.58259900
H	-5.92765600	5.46172500	0.37954300
H	-6.75988000	6.33354100	-0.70308600
N	-5.73441600	4.72784300	-2.94436600
H	-6.49000500	5.29418200	-3.32960300
H	-5.04338800	4.61317400	-3.68467300
H	-7.30215600	4.30359100	-0.52531800
H	-6.11196100	3.80141300	-2.74623000

T4_fph

Energy: -2326.077134

C	-7.10956820	-0.83015180	-0.10554179
C	-5.72041742	-0.71948311	-0.01608875
C	-5.09238799	0.52268752	0.05447784
C	-5.90903610	1.65154607	-0.00281451
C	-7.30336916	1.56624439	-0.06851851
C	-7.90734481	0.30552874	-0.11566505
C	-3.60528838	0.75339528	0.28805304
C	-4.11406356	3.06016678	-0.58040207
C	-3.20597266	2.00321751	-0.49172139
C	-1.95987004	2.18343514	-1.09005112
H	-1.21790202	1.39306263	-1.05539699
C	-1.65212691	3.38135829	-1.72668458
C	-2.59654649	4.39919159	-1.79811441
C	-3.87657481	4.27068583	-1.23785512
H	-7.56879082	-1.81204081	-0.15550278
H	-5.12458038	-1.62595238	0.00979594
H	-8.98901503	0.22028023	-0.17364171
H	-0.67276962	3.51607997	-2.17606740
H	-2.34023107	5.31965261	-2.31807356
O	-5.37537937	2.90739256	0.00697285
B	-5.01513598	5.38579049	-1.55859136
P	-8.23997713	3.10231211	-0.01168627
C	-4.34130954	6.84566051	-1.87163306
C	-3.68778167	7.48390677	-0.81699923
C	-4.33913733	7.55963264	-3.06275594
C	-3.08194060	8.72691796	-0.91997953
C	-3.74969465	8.80871186	-3.21889227
C	-3.11335695	9.39743393	-2.13682509
F	-3.62124688	6.87616865	0.38626495
F	-4.93339035	7.04714769	-4.17413572
F	-3.79068096	9.44407901	-4.39517781
F	-2.47137734	9.28587093	0.12946354
F	-2.54258358	10.59569233	-2.26085125
C	-3.40953704	1.04418497	1.79887243
H	-3.72189105	0.17736627	2.39113901
H	-2.35272064	1.24873880	1.99887430
H	-3.99480269	1.91303437	2.11539036
C	-2.76800769	-0.46776293	-0.09293424
H	-3.06865647	-1.33608089	0.49955748
H	-2.86840346	-0.71327324	-1.15534150
H	-1.71232872	-0.29242093	0.12824095
N	-6.16796582	5.50965295	-0.54677582
H	-5.84017189	5.40956804	0.40914506
H	-6.62081296	6.41920033	-0.59078630
N	-5.73277599	4.81060917	-2.93387226
H	-6.49333201	5.39635299	-3.27774946
H	-5.07181717	4.69798954	-3.70125169
H	-7.38123934	4.23032183	-0.49147746
H	-6.12062974	3.88925154	-2.73483847
C	-8.61766713	3.52153906	1.70316302
C	-8.68756365	2.53760381	2.69290968
C	-8.84510242	4.86578803	2.02075193
C	-8.99586846	2.90213070	3.99882901
H	-8.49576820	1.49648010	2.44841722
C	-9.15550345	5.21850882	3.32899465
H	-8.78404588	5.63214497	1.25166461
C	-9.23056727	4.23799033	4.31568466
H	-9.04923376	2.14107604	4.77126718
H	-9.33250242	6.26004697	3.57914611
H	-9.46810082	4.51739472	5.33791967
C	-9.77496880	2.87712660	-0.93962756
C	-9.69288929	2.46426207	-2.27579919
C	-11.01683052	3.14332182	-0.35833390
C	-10.85469909	2.31802242	-3.02233529
H	-8.72799225	2.24150677	-2.72580665
C	-12.17466431	2.99462599	-1.11662618
H	-11.08219787	3.45876907	0.67893041
C	-12.09498709	2.58438401	-2.44375367
H	-10.79371369	1.99277756	-4.05646559
H	-13.14108290	3.19647371	-0.66489880
H	-13.00142528	2.46788368	-3.03029438

3

Energy: -4011.43824

B	6.11153365	4.60680711	3.34430332
C	6.26802540	4.31690677	4.88850757
C	5.59867441	3.25979636	5.49318517
C	5.71593331	2.99457787	6.85832013
C	6.53986502	3.81563787	7.64042264
C	7.23020588	4.88499487	7.05341581
C	7.07832140	5.11635623	5.68568639
C	5.24083069	5.82075621	2.90125696
C	4.13143676	6.25223784	3.63920308
C	3.37565633	7.35909969	3.28597174
C	3.73919265	8.10048632	2.16887912
C	4.84545586	7.72450886	1.41455402
C	5.56538875	6.60161142	1.78424292
C	6.82839254	3.66935936	2.32864414
C	6.27267250	3.35964630	1.07971056
C	6.85493384	2.46791890	0.19552704
C	8.05124370	1.84986651	0.54273758
C	8.64406140	2.12389042	1.76909231
C	8.02434726	3.00803862	2.63812652
Cl	4.55552238	2.28760384	4.48783218
Cl	4.85598121	1.67842295	7.57448499
Cl	6.70501404	3.50875443	9.33213616
Cl	8.25490544	5.89718035	8.00734109
Cl	7.95001505	6.40925610	4.90253035
F	3.73278349	5.57126771	4.72096454
F	2.30947214	7.71910497	4.00293123
F	3.03186378	9.16998708	1.82191056
F	5.19939820	8.45029120	0.35215739
F	6.63801686	6.29806250	1.04085729
F	5.10521522	3.90106095	0.70787209
F	6.28197667	2.18958278	-0.97696090
F	8.62438253	0.99569532	-0.29738593
F	9.79505983	1.53329133	2.09547237
F	8.64224482	3.23815898	3.80330356

4T_cip

Energy: -3901.380669

C	-5.11251400	1.57702000	-5.84232500
C	-4.40032400	0.96938800	-4.82165900
C	-4.33449900	1.54568700	-3.54962300
C	-4.99977800	2.75034300	-3.35409000
C	-5.81863500	3.34508300	-4.33203100
C	-5.82860500	2.74311600	-5.59237200

C	-3.61003300	0.82922100	-2.42328600
C	-4.19074800	2.95108900	-1.11776800
C	-3.62759600	1.67224400	-1.15874200
C	-3.02796200	1.19159200	0.00381900
H	-2.60672200	0.19043600	0.00332300
C	-2.95156300	1.95131200	1.16704500
C	-3.42821600	3.24757400	1.15293800
C	-4.03463400	3.80871900	0.00698400
H	-5.13888600	1.12806300	-6.83049000
H	-3.88936800	0.03075900	-5.01326800
H	-6.41329700	3.17283600	-6.39651600
H	-2.49681200	1.53784600	2.06124100
H	-3.30188400	3.83995300	2.05472700
O	-4.90877600	3.44943800	-2.15383800
B	-4.25620100	5.32277900	-0.03738400
P	-6.77535600	4.86645700	-3.91869800
C	-4.57361400	6.25008400	-1.27206500
C	-5.70908000	7.05948600	-1.26577900
C	-3.67881800	6.41394600	-2.32840900
C	-5.96571100	7.99916600	-2.26407200
C	-3.90221500	7.33353800	-3.35438600
C	-5.05042300	8.13472700	-3.31444800
C	-7.89059200	4.22218200	-2.52418500
H	-7.22477400	4.29680300	-1.65237300
C	-7.83729800	5.11581100	-5.45356900
H	-7.08570900	5.09725600	-6.25713600
C	-8.92527400	4.08686000	-5.77569900
H	-9.32097700	4.27278500	-6.78207800
H	-8.56154500	3.05661200	-5.74268300
H	-9.76347800	4.17167900	-5.07809600
C	-8.41861800	6.53811800	-5.44950300
H	-9.20119300	6.65503700	-4.69404500
H	-7.64639600	7.28914600	-5.25537800
H	-8.86801900	6.75515800	-6.42568500
C	-8.37264100	2.77290800	-2.61322400
H	-8.89379000	2.50531300	-1.68517200
H	-9.07233900	2.62818800	-3.44024500
H	-7.54457300	2.07008900	-2.74559900
C	-9.06222900	5.18132700	-2.28895600
H	-9.83051000	5.07134300	-3.06006100
H	-9.53242600	4.95883400	-1.32388300
H	-8.74530300	6.22903100	-2.27333800
C	-4.31750900	-0.51824600	-2.15902000
H	-4.30240900	-1.14138300	-3.05778100
H	-3.81711000	-1.07276000	-1.35895400
H	-5.36035400	-0.35383300	-1.87010200
C	-2.13898600	0.57899900	-2.82302000
H	-2.08288200	-0.03825400	-3.72386400
H	-1.62881200	1.52713900	-3.02094700
H	-1.60308500	0.05379500	-2.02629800
N	-3.89053700	6.11866000	1.18434400
H	-4.15284100	5.70089400	2.07616000
H	-4.25172500	7.07097000	1.17426100
H	-0.89163100	6.59140500	2.07040300
H	-0.97312200	6.94197600	0.46835600
H	-0.88414500	5.38215800	0.95949000
H	-2.65441500	6.21478800	1.20367100
N	-1.28703900	6.28951600	1.18341200
Cl	-2.21034300	5.46665100	-2.33043800
Cl	-2.78047800	7.48772500	-4.65681000
Cl	-5.34416100	9.28000600	-4.56902800
Cl	-7.39131900	8.97033300	-2.21701300
Cl	-6.84881900	6.85104100	0.04605400

4T_cph

Energy: -4127.77899

C	-5.58444000	1.18333900	-5.59457400
C	-4.72903500	0.63205200	-4.65439800
C	-4.42759700	1.30121000	-3.46432900
C	-5.00653900	2.54907600	-3.26377500
C	-5.92240300	3.11053900	-4.16900500
C	-6.18717000	2.41135700	-5.34578400
C	-3.52908300	0.65018600	-2.42952300
C	-3.90948500	2.84782900	-1.16571300
C	-3.34396800	1.57031800	-1.23370900
C	-2.56454600	1.14650500	-0.15836300
H	-2.12435100	0.15403900	-0.18573000
C	-2.33168600	1.95087300	0.95100000
C	-2.86700400	3.22354100	0.97879900
C	-3.65687700	3.72856400	-0.07730200
H	-5.79829700	0.65038500	-6.51579800
H	-4.28667200	-0.34110100	-4.84529400
H	-6.87601100	2.83050300	-6.07156500
H	-1.72848700	1.58524800	1.77545000
H	-2.64308700	3.84175900	1.84323200
O	-4.73293000	3.31971200	-2.13876400
B	-4.05725000	5.20699200	-0.04101200
P	-6.66368200	4.75732000	-3.80686300
C	-4.64671900	6.13640800	-1.16842800
C	-5.87828500	6.76148300	-0.97588400
C	-3.89793400	6.52020800	-2.27709900
C	-6.35620500	7.74993100	-1.83645600
C	-4.35296000	7.47949400	-3.18272600
C	-5.58831200	8.09940600	-2.95518900
C	-4.18213800	-0.67095600	-1.96368400
H	-4.31532700	-1.35094300	-2.80964000
H	-3.55479300	-1.17800900	-1.22455100
H	-5.16243400	-0.47816400	-1.51668300
C	-2.14710400	0.35742300	-3.05490700
H	-2.24847900	-0.31294500	-3.91297600
H	-1.67380800	1.28442700	-3.39357200
H	-1.48600300	-0.12798400	-2.33030500
N	-3.65937400	6.00996200	1.16698600
H	-3.74107300	5.52983100	2.06209800
H	-4.16288000	6.89196500	1.24766300
H	-0.69354000	6.94575400	1.72842600
H	-1.03133100	7.35271500	0.17357600
H	-0.62248100	5.81088300	0.54343600
H	-2.46272400	6.31126100	1.04508300
N	-1.14001700	6.62243200	0.87382300
C	-7.63423400	5.09098400	-5.33233800
C	-7.08264900	5.99001400	-6.25106700
C	-8.87521500	4.50646800	-5.61053900
C	-7.75275000	6.29200700	-7.43392600
H	-6.12419900	6.45835600	-6.03629700
C	-9.54758800	4.81647700	-6.78778400
H	-9.31588000	3.80876700	-4.90324700
C	-8.98735800	5.70793100	-7.70154800
H	-7.31471600	6.99151200	-8.14015200
H	-10.51111900	4.35928000	-6.99506300
H	-9.51616600	5.94927600	-8.61930000
C	-7.98767900	4.33264200	-2.59694200
C	-7.97495000	3.18469300	-1.80011200
C	-9.00341300	5.27826200	-2.39906700
C	-8.95253100	2.99043100	-0.82602500
H	-7.21415800	2.42325200	-1.94418700
C	-9.98340400	5.07647800	-1.43551500
H	-9.03644300	6.17342200	-3.01551300
C	-9.95799300	3.93351400	-0.63853000
H	-8.93175200	2.08855200	-0.22020900
H	-10.76843800	5.81629000	-1.30496400
H	-10.72242600	3.77615100	0.11700300
Cl	-2.33110500	5.78248100	-2.50868000
Cl	-3.41610600	7.88932400	-4.57352600
Cl	-6.17598700	9.28187900	-4.06382200
Cl	-7.85450800	8.54463700	-1.52014400
Cl	-6.83154800	6.25698300	0.39738300

4T_fip

Energy: -2099.661815

C	-5.49217900	1.28666800	-5.82520300
C	-4.64572700	0.72611000	-4.88200300
C	-4.39908500	1.36679800	-3.66369700
C	-5.03352400	2.58360400	-3.44506600
C	-5.93962300	3.16375900	-4.35206400
C	-6.13787400	2.49081600	-5.55928300
C	-3.48215300	0.73012100	-2.62966400
C	-3.99308000	2.86029300	-1.31702000
C	-3.37469200	1.61323700	-1.39545900
C	-2.61501000	1.20665600	-0.29693500

H	-2.12060300	0.23991700	-0.32580900
C	-2.47565100	1.99596300	0.83995500
C	-3.08683000	3.23813600	0.88259100
C	-3.83523400	3.72414600	-0.20641100
H	-5.66376900	0.78026200	-6.77007500
H	-4.16594600	-0.22433900	-5.09538500
H	-6.80632900	2.89779400	-6.30854800
H	-1.88436300	1.64280600	1.67849900
H	-2.94131800	3.85667600	1.76558400
O	-4.81950700	3.32156800	-2.29252400
B	-4.35451900	5.17054100	-0.17521800
P	-6.68301100	4.80293500	-3.94615400
C	-4.43523700	6.15304100	-1.38426300
C	-5.38148800	7.17876700	-1.47906300
C	-3.53346900	6.07620100	-2.45385100
C	-5.46242700	8.04807500	-2.55206300
C	-3.56385900	6.94609800	-3.53101000
C	-4.53999000	7.93212900	-3.58391800
F	-6.31517600	7.32435900	-0.51226400
F	-2.56392300	5.15290300	-2.45452000
F	-2.68238000	6.83240900	-4.52372100
F	-6.42124500	8.97275500	-2.61659400
F	-4.60726600	8.74680900	-4.62867600
C	-7.68502600	4.40965400	-2.38394500
H	-6.91205800	4.45995500	-1.60214600
C	-7.88597400	5.08123500	-5.36584800
H	-7.24372300	4.91300300	-6.24340900
C	-9.11250000	4.17127200	-5.47962800
H	-9.59928000	4.32787800	-6.45036900
H	-8.86233800	3.11025000	-5.39590100
H	-9.85052200	4.40635400	-4.70714000
C	-8.29356500	6.56189700	-5.41341200
H	-8.94877900	6.83030100	-4.57946400
H	-7.41988800	7.22179700	-5.38520000
H	-8.84241800	6.76295500	-6.34080800
C	-8.33499600	3.02863800	-2.29292000
H	-8.75625600	2.88706400	-1.28932200
H	-9.15041700	2.91687700	-3.01229600
H	-7.61463400	2.22453000	-2.47103000
C	-8.69629900	5.52473600	-2.09599300
H	-9.56146400	5.46276000	-2.76223500
H	-9.06801500	5.42927300	-1.06897500
H	-8.25872700	6.52310600	-2.20380900
C	-4.05502600	-0.64733500	-2.22981600
H	-4.12774600	-1.30055900	-3.10379000
H	-3.40799600	-1.14169000	-1.49899100
H	-5.05366500	-0.53810000	-1.79538900
C	-2.07112100	0.55234400	-3.23311700
H	-2.10871100	-0.09005400	-4.11769800
H	-1.65282500	1.52069000	-3.52534900
H	-1.39644200	0.08542600	-2.50851200
N	-4.61903200	5.76164200	1.17721000
H	-4.89553400	5.07833600	1.88088800
H	-5.30765900	6.51222300	1.18060300
H	-2.24737900	6.78231500	2.98608800
H	-2.48409000	7.93075300	1.84001100
H	-1.62546100	6.58098800	1.48182800
H	-3.58030400	6.30385200	1.58299800
N	-2.43277600	6.92672200	1.99642700

4T_fph

Energy: -2326.059476

C	-6.12548100	0.83004500	-5.50430400
C	-5.09683000	0.32454800	-4.71462000
C	-4.46346900	1.12933100	-3.76558600
C	-4.91987200	2.43741500	-3.64212900
C	-5.97341500	2.96861200	-4.38995500
C	-6.56219200	2.14250000	-5.34842300
C	-3.26606200	0.70448200	-2.92426800
C	-3.83706900	2.73870800	-1.57483200
C	-3.36171800	1.42758600	-1.58543500
C	-2.91858400	0.90207700	-0.37192600
H	-2.54608100	-0.11602800	-0.32946900
C	-2.93667900	1.66316100	0.79549900
C	-3.40414300	2.96939300	0.76572200
C	-3.85609300	3.55123100	-0.43165600
H	-6.59680900	0.19200100	-6.24559400
H	-4.78227800	-0.70434700	-4.85218600
H	-7.37515300	2.52120000	-5.96020600
H	-2.57885000	1.23256100	1.72535800
H	-3.39499500	3.55370300	1.68435400
O	-4.35718200	3.29610700	-2.71495600
B	-4.40111500	5.00076600	-0.44876600
P	-6.43630700	4.72517600	-4.08521600
C	-4.05210700	6.10752500	-1.48992000
C	-4.76327000	7.31187000	-1.61343600
C	-3.00855500	5.95023600	-2.41974100
C	-4.54509600	8.23481400	-2.61981600
C	-2.75384000	6.85733800	-3.43581500
C	-3.53304800	8.00241300	-3.54325700
F	-5.73447800	7.62905600	-0.73222000
F	-2.18185000	4.90511300	-2.34746500
F	-1.76132100	6.65143800	-4.29949400
F	-5.27822500	9.34577000	-2.69904000
F	-3.29986500	8.88062500	-4.50704400
C	-3.18329100	-0.81382700	-2.76043600
H	-3.09443400	-1.29731000	-3.73631200
H	-2.29030500	-1.09237600	-2.19453600
H	-4.06523500	-1.21379600	-2.24938500
C	-1.98289800	1.20673400	-3.63469700
H	-1.89304000	0.73138300	-4.61713200
H	-2.01047000	2.29167300	-3.77609300
H	-1.10101200	0.95541400	-3.03555300
N	-5.25562000	5.38280000	0.72056000
H	-5.55636500	4.57046500	1.25748300
H	-6.10315900	5.88596000	0.44611200
H	-4.23523200	6.91627800	3.27163700
H	-4.39366000	8.03771800	2.08599200
H	-3.05511600	7.09345400	2.14682600
H	-4.68158400	6.18072100	1.47648000
N	-4.06304600	7.09641100	2.28557500
C	-7.89945900	4.91531700	-5.18379600
C	-7.71667200	5.60958300	-6.38411100
C	-9.16171800	4.39120100	-4.88214400
C	-8.77522700	5.76749000	-7.27529500
H	-6.74147500	6.02872000	-6.62132400
C	-10.21980000	4.55948900	-5.76871800
H	-9.31689600	3.84861000	-3.95317400
C	-10.02798100	5.24566800	-6.96689700
H	-8.62218000	6.30638800	-8.20583600
H	-11.19684900	4.15111700	-5.52609800
H	-10.85642500	5.37521000	-7.65749000
C	-7.25619900	4.62134000	-2.42903000
C	-7.31529400	3.46887700	-1.63818900
C	-7.84594300	5.79777300	-1.94556100
C	-7.95594800	3.49004700	-0.40010900
H	-6.88644400	2.53780000	-1.99760500
C	-8.49532600	5.81610000	-0.71545400
H	-7.81096800	6.70482200	-2.54656200
C	-8.55168300	4.65967100	0.06423600
H	-8.00422700	2.58009200	0.19215600
H	-8.96517500	6.73281400	-0.36924900
H	-9.06791000	4.66977600	1.02034700

5

Energy: -5813.154684

B	7.33537045	3.23273035	8.96123477
C	8.31388028	2.52444849	9.98098585
C	8.79048213	3.18887849	11.11403206
C	9.66023312	2.58419259	12.02519095
C	10.07510113	1.26696413	11.80075473
C	9.60946629	0.56847019	10.67931716
C	8.73132358	1.20055744	9.79697885
C	7.76287072	4.57981821	8.25307732
C	6.98759772	5.74131199	8.35679657
C	7.36430644	6.94297966	7.75389742
C	8.54435191	6.99168494	7.00041344
C	9.33084443	5.84320225	6.85963316
C	8.92889325	4.66117211	7.48714624
C	5.94705682	2.60193802	8.65527748

C	5.24658874	1.84880063	9.60586373
C	4.00518680	1.28923392	9.35498825
C	3.42647348	1.45661951	8.10186192
C	4.08763711	2.18725554	7.12082235
C	5.31832199	2.75095731	7.41265395
Cl	8.22789057	4.80544303	11.43332852
Cl	10.21728684	3.44445654	13.41612554
Cl	11.15824658	0.50294555	12.90571225
Cl	10.12305905	-1.05803072	10.40049576
Cl	8.18607990	0.32620328	8.39166950
Cl	5.53456438	5.70957913	9.31802289
Cl	6.39290179	8.36165267	7.92938626
Cl	9.02572822	8.46600925	6.24404166
Cl	10.77688992	5.89205164	5.91517646
Cl	9.87878150	3.22060281	7.25454406
F	5.75475115	1.67104264	10.83225013
F	3.35933285	0.59786840	10.29564927
F	2.24020201	0.91861284	7.84253642
F	3.53079768	2.33525800	5.91743006
F	5.92140517	3.43259717	6.43009401

5T_cip

Energy: -3901.379018

C	-7.14823100	-0.80521400	-0.48667900
C	-5.78889000	-0.70411700	-0.20868500
C	-5.18791800	0.54240600	-0.03967300
C	-5.99217400	1.67070000	-0.19345100
C	-7.37531700	1.60681600	-0.39870500
C	-7.93787600	0.33628200	-0.55592700
C	-3.74333300	0.75133500	0.39024800
C	-4.10443800	3.04353500	-0.55727500
C	-3.22884200	1.97786200	-0.34774500
C	-1.91067100	2.13206300	-0.77606700
H	-1.20335200	1.32050800	-0.64241200
C	-1.47523300	3.31941600	-1.35784300
C	-2.36204700	4.36923000	-1.52758200
C	-3.71492600	4.25601900	-1.15210000
H	-7.60006000	-1.78254100	-0.62532300
H	-5.19745700	-1.60848500	-0.11807100
H	-9.00059800	0.23088900	-0.74184800
H	-0.44187800	3.42053600	-1.67371600
H	-2.01658300	5.29131100	-1.98715000
O	-5.42230300	2.94143100	-0.14579000
B	-4.66870000	5.39775700	-1.56835900
P	-8.31146200	3.18612300	-0.41805700
C	-4.11188300	6.83597700	-1.94833900
C	-3.41332400	7.62807000	-1.01832900
C	-4.23359900	7.37242900	-3.23982600
C	-2.97839800	8.92495000	-1.31523700
C	-3.80445300	8.66015800	-3.57443600
C	-3.19166500	9.44947500	-2.59535900
C	-8.44961000	3.54366100	1.43115900
H	-7.41487500	3.83377900	1.67257000
C	-9.99621600	2.74831600	-1.12415600
H	-9.73943700	2.07641100	-1.95728700
C	-11.00937800	2.03946100	-0.21949300
H	-11.87055100	1.72814900	-0.82259300
H	-10.60670500	1.15175100	0.27242100
H	-11.38513400	2.71275500	0.55650100
C	-10.62037100	4.01573300	-1.72812700
H	-10.86200000	4.74955600	-0.95153000
H	-9.95233000	4.49287900	-2.45202600
H	-11.55376500	3.76000100	-2.24219100
C	-8.80796900	2.37301900	2.34891800
H	-8.65448800	2.67621300	3.39164100
H	-9.85379300	2.07670200	2.24326500
H	-8.18043100	1.49735000	2.15865400
C	-9.35638700	4.75466900	1.68041600
H	-10.40975600	4.49596100	1.53693800
H	-9.24097600	5.09892500	2.71415000
H	-9.13154500	5.59742400	1.01605600
C	-3.74315700	1.06917700	1.90831200
H	-4.14995000	0.21839400	2.46489300
H	-2.71978900	1.25972100	2.24861100
H	-4.35237300	1.95105600	2.12984800
C	-2.87656500	-0.48437800	0.14787000
H	-3.26551700	-1.33675300	0.71070400
H	-2.83706300	-0.75182500	-0.91321900
H	-1.85827900	-0.31486200	0.50691400
N	-5.96468800	6.04520200	0.48489200
H	-5.53598600	5.53751900	1.25052200
H	-5.91046700	7.03489200	0.69894300
H	-6.94402800	5.78171900	0.44443600
N	-6.04769000	4.97830300	-2.15543200
H	-6.61057200	5.76913600	-2.47032800
H	-5.92462600	4.36752800	-2.96624000
H	-6.65452700	4.43810600	-1.48595800
Cl	-3.03379800	7.00036600	0.56129500
Cl	-2.17009600	9.88136700	-0.12699600
Cl	-2.67683000	11.04848900	-2.97373900
Cl	-4.00633600	9.27632600	-5.17397200
Cl	-4.86120000	6.37691800	-4.53795100

5T_cph

Energy: -4127.775365

C	-7.22829100	-0.88047300	-0.29260900
C	-5.85221500	-0.78104300	-0.11614200
C	-5.21875300	0.46211600	-0.08705700
C	-6.01204800	1.59034100	-0.28159000
C	-7.40168200	1.52584800	-0.42701700
C	-8.00254400	0.26553500	-0.42908800
C	-3.75058000	0.66514800	0.25230300
C	-4.12384000	2.95481200	-0.71276300
C	-3.25739700	1.87688400	-0.52491300
C	-1.94712200	2.01827500	-0.98148200
H	-1.24857100	1.19566900	-0.87273200
C	-1.50478900	3.20697700	-1.55458400
C	-2.37052200	4.28210500	-1.66185700
C	-3.71576400	4.18412100	-1.25829200
H	-7.70154200	-1.85722700	-0.30939900
H	-5.27018200	-1.68679100	0.01371900
H	-9.07836500	0.18422200	-0.55026600
H	-0.47834300	3.29486100	-1.89580600
H	-2.01264000	5.21678100	-2.08537400
O	-5.44521000	2.85926900	-0.31137100
B	-4.63001600	5.40240200	-1.52247800
P	-8.32528900	3.09025500	-0.66762600
C	-4.01744500	6.85465700	-1.71934400
C	-3.25792200	7.47274500	-0.70730500
C	-4.14391600	7.57699600	-2.91673300
C	-2.76073500	8.77507700	-0.83214000
C	-3.65349900	8.87627700	-3.07899000
C	-2.97409700	9.48564600	-2.01902000
C	-3.66402800	1.00948300	1.76229000
H	-4.05181700	0.17473700	2.35575200
H	-2.62181500	1.19294600	2.04467200
H	-4.24985400	1.90422800	1.99816200
C	-2.91160500	-0.58489500	-0.01699200
H	-3.27345700	-1.42306600	0.58331200
H	-2.93790700	-0.87090700	-1.07354700
H	-1.87228200	-0.42168700	0.27857500
N	-5.87100600	5.81554400	0.62318500
H	-5.45512000	5.17800000	1.29359500
H	-5.72634000	6.75919900	0.96539900
H	-6.87116600	5.63215200	0.62308700
N	-6.02671700	5.11313400	-2.14524600
H	-6.59901400	5.94947300	-2.26818700
H	-5.93047600	4.68735200	-3.07003700
H	-6.60043300	4.44202000	-1.59031500
C	-8.51395200	3.73761700	1.04238400
C	-7.85750000	3.19036700	2.14744700
C	-9.27864900	4.90223500	1.20991000
C	-7.96237400	3.79783300	3.39750600
H	-7.27015500	2.28258400	2.03939100
C	-9.39135500	5.49655600	2.46152800
H	-9.79724500	5.33918800	0.35821800
C	-8.72696200	4.94905700	3.55839700
H	-7.45013000	3.36089200	4.25007700

H	-9.99644500	6.39074900	2.58074700
H	-8.80997500	5.41723200	4.53480900
C	-10.01384700	2.52573100	-1.09700300
C	-10.34144600	2.41905500	-2.45306600
C	-10.96561800	2.18570100	-0.12979300
C	-11.59929100	1.96466900	-2.83689600
H	-9.61009100	2.69041400	-3.21101500
C	-12.22564800	1.74187900	-0.51817700
H	-10.72143300	2.26598200	0.92600400
C	-12.54328500	1.62867600	-1.86989500
H	-11.84541200	1.88224800	-3.89150400
H	-12.96047000	1.48011700	0.23767200
H	-13.52812200	1.28205800	-2.16930400
Cl	-2.88545400	6.61566100	0.76228100
Cl	-1.87694400	9.51329400	0.45394700
Cl	-2.38065800	11.09346000	-2.18528400
Cl	-3.86105100	9.72515700	-4.56744800
Cl	-4.86091400	6.81750700	-4.32360500

5T_fip

Energy: -2099.666199

C	-7.12884600	-0.84002200	-0.43073300
C	-5.77108000	-0.72007900	-0.15237200
C	-5.18122300	0.53544100	-0.01063300
C	-5.99600300	1.65157200	-0.19045400
C	-7.37670300	1.57053700	-0.40522800
C	-7.92862000	0.29235400	-0.53285400
C	-3.73929600	0.76771200	0.41672700
C	-4.12357700	3.04293700	-0.56434600
C	-3.23683600	1.99067200	-0.33647900
C	-1.91730600	2.15758000	-0.75638200
H	-1.20034600	1.35693500	-0.60908400
C	-1.49381500	3.34435600	-1.34706100
C	-2.39330500	4.38115000	-1.53529500
C	-3.74673600	4.25617500	-1.16693900
H	-7.57133500	-1.82461600	-0.54606400
H	-5.17204300	-1.61690200	-0.03945600
H	-8.98950900	0.17344100	-0.72227800
H	-0.45981500	3.45572300	-1.65741000
H	-2.05505000	5.29874000	-2.00838200
O	-5.44247500	2.92932400	-0.16206200
B	-4.72090900	5.38994000	-1.56624400
P	-8.31398200	3.14579100	-0.48870400
C	-4.19779500	6.82664800	-1.92846300
C	-3.33863100	7.52180300	-1.07191500
C	-4.50276500	7.47698100	-3.12455600
C	-2.83492500	8.77992500	-1.36399000
C	-4.01141000	8.72922700	-3.46092500
C	-3.17122500	9.38565900	-2.57003200
F	-2.98864600	6.98390200	0.10639200
F	-5.29414200	6.86888000	-4.03473600
F	-4.32800400	9.29973500	-4.62270100
F	-2.03411900	9.41129800	-0.50632300
F	-2.69173300	10.58649800	-2.86839200
C	-8.45733100	3.57616600	1.34233600
H	-7.41414200	3.83829600	1.57902800
C	-9.99435900	2.68653300	-1.18794900
H	-9.73543300	1.98518400	-1.99569100
C	-11.01036800	2.01185500	-0.26074300
H	-11.86795900	1.67447400	-0.85480400
H	-10.60713800	1.14583400	0.26831100
H	-11.39068500	2.71576300	0.48553200
C	-10.61438700	3.93341300	-1.83709600
H	-10.85270600	4.69486800	-1.08654600
H	-9.94543200	4.38221200	-2.57809200
H	-11.54892700	3.66248200	-2.34113400
C	-8.86126900	2.45481800	2.30213800
H	-8.66855300	2.77793500	3.33222600
H	-9.92434300	2.21675400	2.22620000
H	-8.28871800	1.53957300	2.12486400
C	-9.32420700	4.82599300	1.53418800
H	-10.38367800	4.59858000	1.38079200
H	-9.21508300	5.20335500	2.55711500
H	-9.05794500	5.63321100	0.84119100
C	-3.74464900	1.10698600	1.93026000
H	-4.14132800	0.25919900	2.49858800
H	-2.72443200	1.31591300	2.26927600
H	-4.36624000	1.98362700	2.13805000
C	-2.85741700	-0.46086100	0.19239600
H	-3.23661900	-1.31016000	0.76631000
H	-2.81331200	-0.74209900	-0.86490600
H	-1.84183600	-0.27411800	0.55053000
N	-5.74084900	6.00230500	0.64720200
H	-5.27480400	5.39542800	1.31293100
H	-5.52991700	6.96177900	0.89860100
H	-6.74067100	5.86389800	0.74330600
N	-6.10032900	4.99626300	-2.15485900
H	-6.66570200	5.79923700	-2.43102900
H	-5.97806000	4.42765600	-2.99734500
H	-6.71496000	4.41684400	-1.51543800

5T_fph

Energy: -2326.062946

C	-7.21815200	-0.90591000	-0.33063800
C	-5.84652700	-0.79378100	-0.12952400
C	-5.22348600	0.45498400	-0.09687500
C	-6.02279700	1.57428600	-0.31256700
C	-7.40867700	1.49726400	-0.48502400
C	-7.99962600	0.23259400	-0.48979800
C	-3.76390900	0.67190000	0.27042600
C	-4.13994400	2.95989600	-0.70213000
C	-3.26627500	1.89253700	-0.49080100
C	-1.94382100	2.05310400	-0.90497200
H	-1.23814400	1.23958400	-0.77596000
C	-1.49968000	3.24874300	-1.46067200
C	-2.37713300	4.31179400	-1.59675900
C	-3.73250700	4.19666600	-1.23437400
H	-7.68266700	-1.88682500	-0.34888400
H	-5.25973700	-1.69377600	0.01752100
H	-9.07248700	0.14222800	-0.62982600
H	-0.46429600	3.35121300	-1.76928900
H	-2.01880500	5.24788200	-2.01592800
O	-5.47006100	2.84920200	-0.33884600
B	-4.66038000	5.40587200	-1.49574700
P	-8.33200700	3.05417700	-0.76492600
C	-4.08703700	6.85628200	-1.68106300
C	-3.19635200	7.40528100	-0.75320900
C	-4.38496100	7.66758800	-2.77629900
C	-2.65049200	8.67238100	-0.88884900
C	-3.85234300	8.93492600	-2.95575400
C	-2.97841700	9.44033300	-2.00111400
F	-2.85688600	6.70867100	0.34129000
F	-5.21308600	7.21229900	-3.74130300
F	-4.16366600	9.66290800	-4.02753300
F	-1.81755800	9.15983200	0.02985000
F	-2.45894100	10.65240800	-2.14963900
C	-3.71048000	1.01011000	1.78333800
H	-4.09795300	0.16729400	2.36551000
H	-2.67667200	1.20699600	2.08690100
H	-4.31414300	1.89505400	2.01130300
C	-2.90737100	-0.56864900	0.01122300
H	-3.27265100	-1.41362100	0.59969200
H	-2.91041200	-0.84894900	-1.04715300
H	-1.87573000	-0.39743700	0.32816200
N	-5.64819600	5.75172300	0.78881400
H	-4.97927100	5.28040800	1.38778700
H	-5.67341400	6.72917700	1.05850000
H	-6.56277100	5.34605800	0.96654100
N	-6.05736800	5.15182100	-2.12509400
H	-6.65265100	5.98123800	-2.12837200
H	-5.96333400	4.86242000	-3.10298800
H	-6.61086200	4.39938200	-1.66040400
C	-8.49201600	3.76003700	0.92512300
C	-7.91992300	3.18220000	2.06179200
C	-9.16308900	4.98604800	1.04607500
C	-8.01619100	3.82060300	3.29713800

H	-7.40334900	2.22911700	1.98739000
C	-9.26937900	5.61189000	2.28305100
H	-9.61256500	5.44720600	0.16820300
C	-8.68977600	5.03288900	3.41152700
H	-7.56893600	3.36132200	4.17409900
H	-9.80158800	6.55517100	2.36610700
H	-8.76619000	5.52548600	4.37640500
C	-10.02782400	2.47844900	-1.14718700
C	-10.37132100	2.31018000	-2.49324700
C	-10.96934000	2.18891600	-0.15426100
C	-11.63516800	1.84364400	-2.84074800
H	-9.64757400	2.54222700	-3.27128800
C	-12.23579100	1.73331400	-0.50711700
H	-10.71303400	2.31790600	0.89381900
C	-12.56922100	1.55764900	-1.84821400
H	-11.89368400	1.71267300	-3.88744700
H	-12.96306800	1.51153300	0.26856700
H	-13.55874100	1.20156400	-2.11984100

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Energy: -7614.873922

B	1.32641879	2.54043436	4.05962693
C	1.72863085	1.95704418	2.64768519
C	1.46062234	0.62718895	2.30230411
C	1.80275748	0.09750278	1.05632648
C	2.44370220	0.91514216	0.11770690
C	2.73050197	2.24889226	0.43271594
C	2.36669138	2.74816562	1.68502221
C	1.78143675	1.79952018	5.37896822
C	3.12314223	1.47251993	5.60745991
C	3.54365161	0.81946778	6.76802167
C	2.59612770	0.46796606	7.73696908
C	1.24521271	0.77788827	7.53846394
C	0.86107112	1.43970955	6.37032691
C	0.46816586	3.86374096	4.15276846
C	0.88323131	4.95194970	4.92922463
C	0.13804793	6.12946273	5.02013151
C	-1.07036968	6.23091677	4.32031429
C	-1.51666300	5.15932822	3.53744427
C	-0.74220561	3.99972152	3.46265158
Cl	0.59779279	-0.38072580	3.42891765
Cl	1.43590652	-1.54516033	0.66486939
Cl	2.87914920	0.27987850	-1.42599515
Cl	3.53143801	3.25614908	-0.72047006
Cl	2.79603510	4.38626155	2.08739444
Cl	4.32246182	1.96723872	4.44695741
Cl	5.21336685	0.45116398	7.01759000
Cl	3.09281972	-0.34686901	9.17424874
Cl	0.07293754	0.33539489	8.72848202
Cl	-0.83074548	1.75139833	6.10558603
Cl	2.41813373	4.87062846	5.74589616
Cl	0.69562627	7.45494058	5.97848620
Cl	-2.00863052	7.67501951	4.42268489
Cl	-3.01339531	5.27812004	2.68206076
Cl	-1.34712620	2.65050752	2.54411430

7

Energy: -2209.71742

B	1.33169632	2.54603386	4.06384231
C	1.72719247	1.96844976	2.66836946
C	1.76259240	0.59263551	2.41458264
C	2.09156892	0.06129476	1.17826733
C	2.42833663	0.92041265	0.13892339
C	2.42020132	2.29525740	0.34411565
C	2.06287591	2.79107449	1.58710872
C	1.78337309	1.81296105	5.36562432
C	3.03168267	1.18947407	5.47574579
C	3.45143605	0.53844177	6.62406310
C	2.59543266	0.47168618	7.71726504
C	1.34053109	1.06591561	7.65384922
C	0.96409604	1.72856524	6.49715608
C	0.48027403	3.85107385	4.15384709
C	0.67911357	4.80682706	5.15700999
C	-0.05947604	5.97555543	5.24338482
C	-1.06336042	6.21403847	4.31196865
C	-1.30859771	5.28951641	3.30362677
C	-0.53461032	4.14301605	3.23484097
F	1.43730493	-0.27925639	3.38046884
F	2.09113173	-1.25762828	0.97435541
F	2.75891873	0.42819699	-1.05021572
F	2.75326487	3.11537360	-0.65474056
F	2.07907317	4.12396405	1.73474361
F	3.89787928	1.23169971	4.45275173
F	4.65986852	-0.02370770	6.69439716
F	2.97633322	-0.16066276	8.82207191
F	0.51906221	0.99275406	8.70315135
F	-0.26098973	2.27407485	6.48403121
F	1.64064565	4.63011864	6.07477223
F	0.17676377	6.86996345	6.20553289
F	-1.78833939	7.32509606	4.38495543
F	-2.28018997	5.51709745	2.41726505
F	-0.81914165	3.28119464	2.24782310

I4_cip

Energy: -3900.951426

C	-7.11949000	-0.85676200	-0.05788300
C	-5.75495100	-0.65414700	0.11990900
C	-5.21529800	0.63046200	0.07554000
C	-6.07944200	1.69485400	-0.19180800
C	-7.46963300	1.53360800	-0.29454800
C	-7.96930000	0.22860000	-0.23738100
C	-3.76639500	0.96710500	0.38465500
C	-4.27667500	3.08080200	-0.86349700
C	-3.35096700	2.07420000	-0.57188200
C	-2.07339300	2.18108000	-1.11930200
H	-1.33296400	1.41195900	-0.92748200
C	-1.73558100	3.27966300	-1.90074900
C	-2.67402100	4.27904700	-2.12725300
C	-3.98052600	4.21523700	-1.62156100
H	-7.52652600	-1.86314400	-0.03122400
H	-5.11019700	-1.50727000	0.30116800
H	-9.03346000	0.04936200	-0.34186000
H	-0.73760900	3.36018400	-2.32224100
H	-2.38915900	5.14166600	-2.72768000
O	-5.57588800	2.97176600	-0.35017700
B	-4.98973700	5.39005200	-2.11609100
P	-8.49455600	3.04074900	-0.50729000
C	-4.18432300	6.86876900	-1.87381300
C	-3.75400500	7.21955400	-0.58151500
C	-3.83706100	7.79650300	-2.86716200
C	-3.05503200	8.39157100	-0.27584900
C	-3.13354200	8.98357000	-2.60678100
C	-2.74215000	9.28461200	-1.30227400
C	-8.33278200	3.79613000	1.22136800
H	-7.29005500	4.14872300	1.20184100
C	-10.24377200	2.39499300	-0.74416600
H	-10.10209600	1.59247700	-1.48381000
C	-10.98667100	1.82196400	0.46628400
H	-11.91425800	1.34142600	0.13103600
H	-10.40180000	1.08165600	1.01715600
H	-11.26666000	2.61727200	1.16414300
C	-11.08753800	3.48629600	-1.42121500
H	-11.24187500	4.34152800	-0.75455900
H	-10.61365600	3.85133000	-2.33735600
H	-12.07490900	3.08575300	-1.67994900
C	-8.45776300	2.86221400	2.42719900
H	-8.10090800	3.38127000	3.32569900
H	-9.49317000	2.56463700	2.60836000
H	-7.85591000	1.95692300	2.30132900
C	-9.23993300	5.02317100	1.35531700
H	-10.29269800	4.73260200	1.43239300
H	-8.98649000	5.58063300	2.26471800
H	-9.14043100	5.70313200	0.50114600
C	-3.70923000	1.53434200	1.82765300
H	-4.03939500	0.77370000	2.54400800
H	-2.68250900	1.83037600	2.06862100
H	-4.35453400	2.41228700	1.93065200
C	-2.85249800	-0.25557200	0.30777100

H	-3.17279300	-1.01588500	1.02562300
H	-2.84852900	-0.69663500	-0.69458900
H	-1.82810100	0.01725400	0.57484200
N	-6.35886100	5.56526100	-1.24087500
H	-6.21671200	5.73178300	-0.24688200
H	-6.90054400	6.34917700	-1.60206900
H	-6.95405800	4.72646800	-1.33426500
Cl	-4.06381800	6.14657700	0.78565700
Cl	-2.56081500	8.75909900	1.34725200
Cl	-1.87736700	10.74470300	-0.95811400
Cl	-2.73450400	10.09436200	-3.87953000
Cl	-4.24657200	7.52684200	-4.55600200
N	-5.51607800	4.98527100	-3.46726100
H	-6.02680300	5.69032500	-3.98466600
H	-4.80531100	4.62234600	-4.08908400

I4_cph

Energy: -4127.348195

C	-7.20208300	-0.86501500	-0.14137000
C	-5.83101300	-0.68287700	0.00571200
C	-5.25911800	0.58485700	-0.10142500
C	-6.09918700	1.65491100	-0.41568500
C	-7.49046300	1.50785500	-0.51687100
C	-8.02914400	0.22697400	-0.37574100
C	-3.80861000	0.89797200	0.22096100
C	-4.25980500	3.04453200	-1.00363500
C	-3.35711200	2.01978600	-0.70191400
C	-2.05062300	2.14331500	-1.17264600
H	-1.32547300	1.36143600	-0.97475900
C	-1.65985500	3.27691500	-1.87562000
C	-2.57274500	4.30210100	-2.08928800
C	-3.90675400	4.22243100	-1.66515100
H	-7.63024900	-1.85862400	-0.05012300
H	-5.20421700	-1.54041900	0.22514300
H	-9.10239000	0.08603900	-0.45756900
H	-0.63882000	3.36816000	-2.23494200
H	-2.24411500	5.20135700	-2.60851400
O	-5.59258100	2.92336100	-0.59086100
B	-4.84750000	5.47880400	-2.08388700
P	-8.50572500	2.98420900	-0.90916600
C	-4.07695200	6.88583800	-1.52570200
C	-3.86275800	7.06605100	-0.14689600
C	-3.57481600	7.92371200	-2.32594300
C	-3.25826400	8.19621900	0.41317500
C	-2.96082400	9.07481600	-1.80652200
C	-2.80948500	9.21631200	-0.42721400
C	-3.76598600	1.44501200	1.67293800
H	-4.11970400	0.68074500	2.37426000
H	-2.73982400	1.72493100	1.93476000
H	-4.40091900	2.33156800	1.77379200
C	-2.91079300	-0.33677000	0.13701900
H	-3.24817000	-1.10359300	0.83949500
H	-2.90166400	-0.76196700	-0.87208600
H	-1.88606900	-0.08363200	0.42073600
N	-6.30847400	5.52695000	-1.35113900
H	-6.30526400	5.42835100	-0.33759000
H	-6.78942700	6.39898200	-1.56675900
H	-6.88590700	4.76671100	-1.72430900
Cl	-4.33640800	5.81484200	1.00298600
Cl	-3.04536100	8.35671000	2.12866300
Cl	-2.06616100	10.63276300	0.23563500
Cl	-2.37774600	10.33519900	-2.84790900
Cl	-3.64471700	7.84324400	-4.08125000
C	-10.21482500	2.31091900	-0.85882600
C	-10.79782400	1.93248700	-2.07323200
C	-10.94126700	2.15621500	0.32634600
C	-12.08005000	1.39165200	-2.10024000
H	-10.24375400	2.06081700	-3.00038400
C	-12.22802900	1.62746800	0.29482500
H	-10.49888800	2.44926000	1.27475300
C	-12.79800100	1.24135000	-0.91657000
H	-12.52199900	1.09738100	-3.04795300
H	-12.78591200	1.51306900	1.22007200
H	-13.80246900	0.82804000	-0.93795300
C	-8.42045300	3.96052100	0.65361000
C	-7.70130500	3.56748900	1.78496100
C	-9.05490200	5.21080800	0.65444800
C	-7.61313500	4.41022200	2.89141000
H	-7.20761700	2.59979900	1.80693500
C	-8.97903700	6.04314600	1.76545400
H	-9.61272200	5.53271200	-0.22368800
C	-8.24930000	5.64767300	2.88560600
H	-7.04464600	4.09416800	3.76180500
H	-9.48073200	7.00674700	1.75344700
H	-8.17514700	6.30391300	3.74796700
N	-5.22812100	5.31355600	-3.53266000
H	-5.64756400	6.11891500	-3.98210000
H	-4.46449700	5.01432700	-4.12470000

I4_fip

Energy: -2099.240943

C	-7.15472300	-0.83966400	-0.30411300
C	-5.79561100	-0.66245100	-0.06645400
C	-5.24622800	0.61746400	-0.00641100
C	-6.09350000	1.70386700	-0.23452500
C	-7.48166900	1.56439400	-0.38369300
C	-7.99169400	0.26316300	-0.43199600
C	-3.81079700	0.92270500	0.38942000
C	-4.25624100	3.11414300	-0.75127100
C	-3.34605400	2.08883700	-0.46988000
C	-2.04405000	2.22158300	-0.94797100
H	-1.31336800	1.44200900	-0.76089300
C	-1.66898500	3.35787200	-1.65524300
C	-2.59813700	4.36387900	-1.88777400
C	-3.93030500	4.27800400	-1.45560800
H	-7.56920000	-1.84178600	-0.36058800
H	-5.16394200	-1.53185500	0.08032200
H	-9.05380200	0.10111000	-0.57795300
H	-0.65086800	3.45846200	-2.02055300
H	-2.28813900	5.24675100	-2.44323100
O	-5.57562800	2.98247900	-0.29909500
B	-4.94905500	5.44002900	-1.96589400
P	-8.48995600	3.09479400	-0.49233100
C	-4.16334600	6.90727300	-1.88453500
C	-3.72043000	7.39428900	-0.65683900
C	-3.82077600	7.70885100	-2.96929900
C	-3.00908900	8.57182900	-0.48668600
C	-3.10706900	8.89855200	-2.85405700
C	-2.69779400	9.33438100	-1.60387100
F	-3.97708000	6.68832900	0.47545300
F	-4.15774900	7.36193900	-4.23095700
F	-2.80670100	9.62735900	-3.93886100
F	-2.61618300	8.98047200	0.72865200
F	-2.01472700	10.47643600	-1.47445200
C	-8.35788700	3.69634300	1.29879100
H	-7.31278400	4.04035000	1.32651700
C	-10.23904900	2.48244500	-0.81278400
H	-10.08980400	1.73802700	-1.60943500
C	-11.00691900	1.82594000	0.33804500
H	-11.93307100	1.38091400	-0.04666600
H	-10.43686900	1.04090000	0.84029300
H	-11.29065200	2.57006500	1.08873000
C	-11.06251900	3.62980100	-1.41807700
H	-11.22253800	4.43269800	-0.69022700
H	-10.56984600	4.06034700	-2.29499200
H	-12.04819000	3.25897100	-1.72343500
C	-8.51352600	2.66875600	2.42204200
H	-8.16226700	3.10740600	3.36458000
H	-9.55561700	2.37440600	2.56547300
H	-7.92390100	1.76652500	2.23210600
C	-9.25544200	4.91851400	1.51841800
H	-10.31219800	4.63456400	1.55523700
H	-9.01127700	5.39638600	2.47449400
H	-9.13515900	5.66457300	0.72432300
C	-3.81918900	1.38670700	1.86974900
H	-4.19473000	0.58291700	2.51285700
H	-2.80257900	1.64864300	2.18260100
H	-4.45878700	2.26458000	2.00277300
C	-2.89931600	-0.29864400	0.26946700
H	-3.25618200	-1.10501800	0.91620900

H	-2.85025200	-0.66800300	-0.76027500
H	-1.88740700	-0.05362700	0.60284900
N	-6.22537300	5.63787400	-0.94676500
H	-5.96477300	5.68664300	0.03586500
H	-6.73508400	6.49194200	-1.16656000
H	-6.88526300	4.85408200	-1.06744700
N	-5.56783400	5.03146800	-3.27941900
H	-5.92283500	5.78495700	-3.85593900
H	-4.94593700	4.48626900	-3.86249000

I4_fph

Energy: -2325.636812

C	-7.21485100	-0.83674900	-0.14589600
C	-5.84311700	-0.66323300	0.00719200
C	-5.26625900	0.60407000	-0.07574100
C	-6.10229000	1.68313200	-0.36658400
C	-7.49282600	1.54411800	-0.47831900
C	-8.03683800	0.26269800	-0.36430400
C	-3.81175200	0.90678800	0.23954900
C	-4.26417000	3.07405600	-0.95217700
C	-3.36535300	2.03556600	-0.67857800
C	-2.07225100	2.14368000	-1.18516800
H	-1.35138100	1.35262600	-1.00937100
C	-1.68877900	3.27300500	-1.90015000
C	-2.59459600	4.30822700	-2.08762200
C	-3.91816700	4.24861400	-1.62505900
H	-7.64727200	-1.83014800	-0.07523500
H	-5.21952600	-1.52723800	0.20986800
H	-9.10988800	0.12691000	-0.45712500
H	-0.67791400	3.35148900	-2.28999400
H	-2.27173900	5.20168000	-2.61972500
O	-5.59015300	2.95283900	-0.51486900
B	-4.85039600	5.52956200	-1.99788000
P	-8.49373100	3.03307600	-0.86059700
C	-4.03406600	6.90284900	-1.52667200
C	-3.67768400	7.06521300	-0.18932600
C	-3.58571300	7.92149100	-2.36132300
C	-2.94605800	8.13355900	0.30522200
C	-2.84623600	9.01397500	-1.91665200
C	-2.52367900	9.12191600	-0.57341800
C	-3.75239300	1.43526100	1.69746500
H	-4.10425800	0.66390200	2.39181700
H	-2.72212100	1.70499000	1.95368300
H	-4.38092100	2.32368300	1.81619100
C	-2.92059400	-0.33078700	0.13219400
H	-3.25451100	-1.10408100	0.82925000
H	-2.92311700	-0.74444200	-0.88174100
H	-1.89204900	-0.08508200	0.40882500
N	-6.22587200	5.58864000	-1.09569200
H	-6.09365400	5.46528500	-0.09310000
H	-6.70366000	6.47790700	-1.23185300
H	-6.86601200	4.85522900	-1.41577400
C	-10.20102200	2.35584400	-0.93127000
C	-10.71752800	2.02910900	-2.18932800
C	-10.98912700	2.15241200	0.20638900
C	-11.99646700	1.49210500	-2.30745800
H	-10.11485600	2.19676500	-3.07941700
C	-12.27160200	1.62698400	0.08421200
H	-10.59867400	2.40612100	1.18828700
C	-12.77622000	1.29300800	-1.17120100
H	-12.38711800	1.23953100	-3.28913600
H	-12.87789500	1.47422100	0.97278800
H	-13.77778900	0.88235900	-1.26337200
C	-8.50105100	3.94034600	0.74487300
C	-7.81926300	3.51510400	1.88721800
C	-9.17546300	5.16938900	0.77499000
C	-7.81157300	4.30335100	3.03683200
H	-7.29426100	2.56371100	1.88532500
C	-9.18048700	5.94550700	1.92781300
H	-9.70361100	5.51657300	-0.11180900
C	-8.49089400	5.51722500	3.06178600
H	-7.27360800	3.96192100	3.91699800
H	-9.71465200	6.89160600	1.93928700
H	-8.48280000	6.12922200	3.95922000
F	-4.04765600	6.12741200	0.72014200
F	-2.63949700	8.22567200	1.60753500
F	-1.81575500	10.16521900	-0.12814900
F	-2.44075400	9.96312200	-2.77272700
F	-3.84104700	7.90319400	-3.68874800
N	-5.32791100	5.43131000	-3.42146200
H	-5.53777300	6.30004200	-3.89558100
H	-4.71734700	4.89757100	-4.02506700

Kross

Energy: -4750.609225

Al	18.07730267	18.96015742	17.41305065
F	21.76702897	20.99098867	19.08811848
F	22.19888057	19.17269505	17.99311538
F	19.18356205	21.19496711	20.02901061
F	20.46636312	20.29693274	21.53785637
F	20.66437345	17.53232297	21.17912453
F	20.33064785	17.39645015	15.80392023
F	18.53864579	19.40654490	21.06994302
F	19.08812667	17.09018527	19.74426260
F	18.38866068	17.75805640	13.92609733
F	20.17844622	15.48133530	16.80961946
F	16.37643109	17.42201354	14.66043976
F	16.16171053	15.08099217	16.10231393
F	22.57843958	19.25926136	20.13118503
O	19.58859451	19.26370907	18.23850408
F	21.16714960	16.93585343	19.14852837
F	17.67426461	14.81000189	17.62910353
F	17.99383677	13.99802791	15.63892270
F	17.44711544	15.81693326	13.65754863
O	17.86212232	17.31218315	16.87093086
F	20.05481150	15.57717574	14.64018816
C	20.25809135	19.14644469	19.40294275
C	18.15399357	16.41274730	15.90989683
C	20.29904628	17.65250422	19.88581122
C	19.60371802	20.02803367	20.53209876
C	21.72944521	19.64613929	19.15474659
C	17.58027147	16.85607249	14.51179491
C	17.48988903	15.04722831	16.32394214
C	19.70581942	16.20863887	15.78046740
O	16.79599363	19.29678968	18.55096660
C	15.48786674	19.15901435	18.84309925
C	15.31150708	18.06035126	19.95422066
F	16.05578861	16.98443457	19.66668999
F	14.02833663	17.65688780	20.08193365
F	15.71323855	18.52311596	21.15325398
C	14.96273599	20.53846590	19.38792259
F	14.78355003	21.40652683	18.37293667
F	15.85033944	21.08255398	20.23015435
F	13.78805366	20.42497699	20.04456041
C	14.63253798	18.74970993	17.58707628
F	15.06144382	19.41359979	16.50317708
F	13.31926208	19.01803206	17.74454204
F	14.75093862	17.43465378	17.33125081
O	18.06860008	19.97439070	15.99091811
C	18.34160455	21.19115801	15.48042758
C	18.56310835	22.27557273	16.59924910
F	17.67949850	22.09643248	17.59281733
F	18.41666387	23.53491284	16.13667679
F	19.79554073	22.17681744	17.12837824
C	19.63828848	21.10816860	14.59421578
F	19.38232524	20.48957706	13.42578212
F	20.58832704	20.40469186	15.22404587
F	20.14483528	22.32729266	14.30633780
C	17.12593057	21.62786436	14.58261289
F	16.69382330	20.59989689	13.84099720
F	17.43556564	22.63988134	13.74356840
F	16.09650717	22.03273385	15.35200411

KrossNH4

Energy: -4977.578426

Al	17.79287389	18.95519230	17.63012489
F	21.60136203	21.13973212	18.76379076
F	21.92585896	19.44588098	17.45198262
F	19.22977824	21.08891734	20.13252039

F	20.79855595	20.18460122	21.33568385
F	21.12216065	17.49348601	20.75493404
F	19.76821920	17.33384725	15.79509959
F	18.87256101	19.19506123	21.12520074
F	19.36000843	16.99970534	19.57711323
F	17.57800189	17.63765728	14.17204463
F	19.75378535	15.43569600	16.84728196
F	15.68440806	17.30484171	15.17253286
F	15.68274766	15.02382972	16.70448212
F	22.69773491	19.40346526	19.48462115
O	19.41686866	19.27909202	18.16987730
F	21.31303860	17.05802515	18.63294518
F	17.37547817	14.83193774	18.04296206
F	17.45587472	13.93647364	16.06363357
F	16.63604288	15.67964220	14.08913099
O	17.45419566	17.30134020	17.15940880
F	19.33662600	15.49413484	14.71363223
N	14.96566833	18.64177846	12.34545228
N	12.74984539	18.83182838	14.24341903
N	12.61829115	16.48110401	15.94431535
C	20.29769872	19.16298967	19.18851173
C	17.62818448	16.35831541	16.21285037
C	20.53430564	17.65369495	19.55408961
C	19.79678539	19.92416427	20.47083120
N	12.53913526	21.22206264	15.89442577
C	21.66010491	19.79519519	18.71777879
C	16.87317629	16.74200467	14.88784964
C	17.03625095	15.00769386	16.76390988
C	19.15090668	16.14557183	15.88026609
O	16.71226401	19.32141584	18.95471421
C	15.47650796	19.18837959	19.46942753
C	15.52163084	18.23367305	20.72074265
F	16.28558068	17.16558809	20.45940629
F	14.29175418	17.79424844	21.06891752
F	16.04544477	18.86463066	21.78479900
C	14.97415480	20.60872843	19.92127702
F	14.60202854	21.33502794	18.84075688
F	15.94947013	21.28090626	20.53656171
F	13.91565045	20.54631432	20.75347876
C	14.46097747	18.59700477	18.42505627
F	14.69612929	19.11897274	17.20600432
F	13.17055260	18.85400090	18.73115391
F	14.59359499	17.26233551	18.32128270
O	17.50468283	19.93489068	16.20473657
C	17.69016226	21.14225808	15.63456610
C	18.31949499	22.19063312	16.62519109
F	17.76681774	22.05289124	17.84049055
F	18.12167027	23.46183993	16.22041218
F	19.64179726	21.99969486	16.74918709
C	18.63761258	20.98856458	14.38864501
F	17.97424240	20.41646447	13.35652410
F	19.67391549	20.19947861	14.68663743
F	19.11583152	22.17008938	13.95321990
C	16.29469661	21.68395897	15.15523570
F	15.56421900	20.69182596	14.61041000
F	16.39358903	22.66480249	14.23822588
F	15.58812222	22.16451300	16.19796792
H	13.58208822	18.79593691	13.59878303
H	12.73812667	19.71055808	14.82601757
H	12.73022743	17.98399906	14.87164489
H	11.90858366	18.82190344	13.67092141
H	15.81070986	19.02815748	12.75569252
H	12.19574888	16.64798525	16.85274917
H	15.18518015	17.67822438	12.10996851
H	13.55780409	16.14446125	16.13166355
H	14.83298841	19.12684520	11.46329382
H	12.11321065	15.70127937	15.53464013
H	13.15795060	21.13485549	16.69495405
H	12.80590865	22.08552386	15.43115516
H	11.60854371	21.37547545	16.27068516

NH3

Energy: -56.61348004

N	-0.38489920	-3.18536907	-0.03727692
H	0.01086750	-4.11987492	-0.03727692
H	0.01087661	-2.71814632	0.77204277
H	0.01087661	-2.71814632	-0.84659660

NH4

Energy: -57.02302959

H	-4.51173922	-0.75991992	-0.00000000
H	-4.51188495	0.68591483	0.83442816
H	-4.51188495	0.68591483	-0.83442816
H	-5.87399519	0.20414082	-0.00000000
N	-4.85209898	0.20363956	0.00000000

NH4NH3

Energy: -226.9245366

N	14.92622156	18.69462939	12.43456422
N	12.60231948	18.74969433	14.19185372
N	12.60427435	16.42318266	15.94611255
N	12.59429894	21.19677261	15.77304546
H	13.44591218	18.72994821	13.55966901
H	12.60100030	19.63450550	14.76544748
H	12.60540326	17.90764839	14.82642785
H	11.76157073	18.72725517	13.61877042
H	15.79867989	18.87855646	12.92110226
H	12.22758008	16.62606553	16.86738767
H	15.04641406	17.79753467	11.97343751
H	13.53392297	16.04439495	16.10112909
H	14.86904632	19.38510968	11.69168923
H	12.04757767	15.65668876	15.57934149
H	13.29323428	21.19529235	16.51009770
H	12.77837760	22.02498995	15.21444881
H	11.70345634	21.36200139	16.23240553

T4_1_cip

Energy: -3958.013335

C	-5.56994700	1.08230100	-5.92635200
C	-4.52537500	0.76710100	-5.07258800
C	-4.02480900	1.68611100	-4.14711700
C	-4.62023600	2.94683300	-4.08514700
C	-5.64429500	3.31225900	-4.98797600
C	-6.11163200	2.36003800	-5.89543400
C	-2.81980800	1.32622200	-3.29954500
C	-3.27617900	3.60310800	-2.21021100
C	-2.52552800	2.42965500	-2.29641700
C	-1.47438000	2.25636700	-1.39135400
H	-0.86204100	1.36166100	-1.44749200
C	-1.20312600	3.20830000	-0.42677100
C	-2.02238700	4.32703200	-0.32647400
C	-3.09214600	4.56659800	-1.19599600
H	-5.94630800	0.34670000	-6.62965300
H	-4.07651700	-0.21960400	-5.13261800
H	-6.89893600	2.61220500	-6.59553400
H	-0.37318100	3.07256800	0.26012200
H	-1.77920900	5.03761700	0.45776100
O	-4.24700700	3.90138500	-3.17345800
B	-4.16894900	5.75154300	-0.89259700
P	-6.15897200	5.05215000	-5.10631800
C	-4.19666000	7.11634700	-1.87775900
C	-3.19907700	7.44877300	-2.81070000
C	-5.22920300	8.06680300	-1.78496900
C	-3.27971800	8.55573800	-3.66922600
C	-5.35769100	9.17541900	-2.63097600
C	-4.38634400	9.40340000	-3.60724500
C	-7.14498500	5.51254900	-3.60921000
H	-6.37817300	5.56745500	-2.82183100
C	-7.11535900	5.23254200	-6.69352700
H	-6.54764300	4.60405000	-7.39528200
C	-8.57245100	4.75823000	-6.66820400
H	-8.96707600	4.76289500	-7.69029400
H	-8.69226000	3.74937700	-6.26510800
H	-9.19476800	5.43248800	-6.07378300
C	-7.01579900	6.68119500	-7.19837700
H	-7.57033100	7.37336600	-6.55926000
H	-5.97902900	7.02687400	-7.25955200
H	-7.44916400	6.73858000	-8.20267600
C	-8.14692600	4.43909000	-3.17902900

H	-8.56557000	4.72685900	-2.20780900
H	-8.97584600	4.33709400	-3.88517400
H	-7.66742100	3.46274100	-3.06068100
C	-7.79867200	6.88688700	-3.77757400
H	-8.64429200	6.85390900	-4.47038200
H	-8.18289000	7.21974100	-2.80796000
H	-7.09116500	7.64242000	-4.13300200
C	-3.09771000	0.01309700	-2.53407500
H	-3.29777400	-0.80986800	-3.22589700
H	-2.23536100	-0.27255200	-1.92615200
H	-3.96272200	0.13036200	-1.87385900
C	-1.60330300	1.13512300	-4.23399300
H	-1.79836600	0.34307300	-4.96389700
H	-1.38661500	2.06116700	-4.77641800
H	-0.71499000	0.85496100	-3.66004800
N	-5.49059900	5.07166800	-0.72596700
H	-5.44907100	4.08416600	-0.51875500
H	-6.25768900	5.49712900	-0.23069700
N	-3.39983500	5.94987100	-5.97465000
H	-3.25452800	5.33021800	-6.76749800
H	-3.24202600	6.90284300	-6.29135700
H	-4.72053400	5.73281300	-5.43140200
H	-2.69008600	5.73286500	-5.27822400
N	-3.70940700	6.44831100	0.58002500
H	-4.41596700	7.11909300	0.87951700
H	-3.65259100	5.73763800	1.30878700
H	-2.81943600	6.94630300	0.55603200
Cl	-1.71640600	6.51747000	-2.91076400
Cl	-2.00734900	8.92239000	-4.79440400
Cl	-4.53612800	10.73692800	-4.69606100
Cl	-6.68642200	10.27609000	-2.48646800
Cl	-6.43510100	7.95779800	-0.50569400

T4_1_cph

Energy: -4184.401806

C	-5.64569400	1.08254400	-5.79411800
C	-4.54675800	0.77536600	-5.00484400
C	-3.98806900	1.69783000	-4.11571300
C	-4.57907000	2.95765500	-4.03024900
C	-5.65118400	3.31300700	-4.87594200
C	-6.18398500	2.36104300	-5.74549000
C	-2.73067200	1.35569700	-3.33892600
C	-3.16128500	3.62160800	-2.21147400
C	-2.41123300	2.45128400	-2.33212200
C	-1.33434000	2.27773900	-1.45851800
H	-0.71503500	1.38993800	-1.54090600
C	-1.04793500	3.22177300	-0.48939500
C	-1.87272100	4.33229000	-0.35360000
C	-2.96437700	4.57748600	-1.19459000
H	-6.06302100	0.33915500	-6.46531300
H	-4.10140800	-0.21118400	-5.08924800
H	-7.00848900	2.63111400	-6.39808000
H	-0.19963700	3.08471400	0.17443500
H	-1.61508200	5.03649200	0.43194200
O	-4.16485100	3.91939600	-3.14687600
B	-4.02656700	5.77659600	-0.86816200
P	-6.15637700	5.04953100	-4.99292600
C	-3.98717500	7.18033600	-1.80019200
C	-3.00440600	7.49371900	-2.75371500
C	-4.99737300	8.15403400	-1.68779400
C	-3.09153500	8.58701200	-3.62907900
C	-5.14480100	9.23643600	-2.56204000
C	-4.19545700	9.43791800	-3.56617600
C	-2.93034000	0.02207700	-2.58570200
H	-3.15191400	-0.79221600	-3.28104400
H	-2.02515700	-0.25428600	-2.03939300
H	-3.75470800	0.10416600	-1.87056700
C	-1.56343400	1.21513800	-4.34245400
H	-1.77817300	0.42855400	-5.07310800
H	-1.40327400	2.15508900	-4.88074200
H	-0.63720500	0.95317700	-3.82201600
N	-5.37725300	5.13595500	-0.70943100
H	-5.49856000	4.29747900	-1.25698400
H	-6.21308100	5.69198300	-0.81778800
N	-3.38424500	5.97431700	-5.78140000
H	-3.18156300	5.31243900	-6.52592100
H	-3.26144900	6.91271700	-6.15275600
H	-4.71821100	5.74972400	-5.27487000
H	-2.69458600	5.83058000	-5.04651000
N	-3.62901300	6.34552000	0.65186300
H	-4.36463800	6.96683000	0.98537700
H	-3.58674900	5.56563400	1.30753700
H	-2.75164700	6.86123100	0.70730700
C	-7.13442000	5.19204600	-6.52113100
C	-6.46017700	5.23611400	-7.74800500
C	-8.53034100	5.25432600	-6.49476000
C	-7.17797400	5.33532700	-8.93364400
H	-5.37547700	5.17978200	-7.78519700
C	-9.24228800	5.35755600	-7.68615400
H	-9.06237700	5.22347600	-5.54847000
C	-8.56962100	5.39801800	-8.90375900
H	-6.65033000	5.36770200	-9.88216000
H	-10.32683200	5.40525500	-7.66009100
H	-9.12881300	5.47977300	-9.83115600
C	-7.29268700	5.46143600	-3.64555500
C	-7.85352000	4.45848600	-2.85227200
C	-7.67271500	6.79649500	-3.47165500
C	-8.79292400	4.79429300	-1.88181000
H	-7.56193700	3.42108700	-2.99488200
C	-8.62069200	7.12034100	-2.50893300
H	-7.24289200	7.57720800	-4.09545600
C	-9.17819300	6.12136600	-1.71270200
H	-9.22710800	4.01583300	-1.26150700
H	-8.91841700	8.15558300	-2.37472900
H	-9.91560900	6.37958900	-0.95824500
Cl	-1.52674400	6.55066100	-2.85900900
Cl	-1.83561400	8.92685400	-4.78217100
Cl	-4.36516200	10.74570800	-4.68355200
Cl	-6.46903900	10.34429900	-2.41484800
Cl	-6.13440600	8.11069400	-0.34304300

T4_1_fip

Energy: -2156.304381

C	-5.51076400	1.09314900	-5.97527500
C	-4.47795800	0.77928100	-5.10608900
C	-4.00366500	1.69323800	-4.16163600
C	-4.62018400	2.94277000	-4.09405700
C	-5.62712000	3.31047400	-5.01461000
C	-6.06609200	2.36565800	-5.94320800
C	-2.81055100	1.33947100	-3.29345100
C	-3.29646200	3.61259700	-2.21153100
C	-2.51566600	2.46090600	-2.30972200
C	-1.44354000	2.32249000	-1.42253200
H	-0.80955800	1.44307900	-1.48299100
C	-1.17720600	3.28841000	-0.47080300
C	-2.03112100	4.38159800	-0.35312300
C	-3.13240400	4.57481800	-1.19267700
H	-5.86685200	0.36047000	-6.69205300
H	-4.01904400	-0.20293800	-5.16681800
H	-6.84154700	2.61886500	-6.65658300
H	-0.32762300	3.18100700	0.19673200
H	-1.80630900	5.09541500	0.43406300
O	-4.28935600	3.88587500	-3.15619600
B	-4.23374800	5.72820400	-0.89499200
P	-6.14343900	5.05085200	-5.11531700
C	-4.25371300	7.03233200	-1.90729700
C	-3.31899900	7.28165100	-2.90608200
C	-5.20781700	8.03542900	-1.75970500
C	-3.34386400	8.40941900	-3.71879600
C	-5.27839900	9.17761800	-2.54375500
C	-4.33365600	9.36436200	-3.54308700
F	-2.30508700	6.41839200	-3.13855800
F	-6.14631700	7.92665300	-0.78532000
F	-6.24090300	10.08656100	-2.35744400
F	-2.41402400	8.58820400	-4.67224200
F	-4.37364900	10.44688100	-4.32062300
C	-7.11711000	5.48238600	-3.60329700
H	-6.34480200	5.48802500	-2.82062300
C	-7.10915300	5.25325200	-6.69231800
H	-6.54513000	4.64101400	-7.41132000

C	-8.56372500	4.77298800	-6.66013700
H	-8.96988700	4.79366900	-7.67748100
H	-8.67420700	3.75675500	-6.27290100
H	-9.18099500	5.43567400	-6.04712400
C	-7.02101200	6.71265200	-7.16706400
H	-7.57213600	7.38746900	-6.50640700
H	-5.98646000	7.06443300	-7.23174000
H	-7.46567900	6.79085400	-8.16498200
C	-8.13949200	4.41638000	-3.20272800
H	-8.53736300	4.67427200	-2.21461700
H	-8.98043800	4.36089400	-3.89929300
H	-7.68133700	3.42548400	-3.12871300
C	-7.73772000	6.87881300	-3.70339400
H	-8.60433300	6.89401800	-4.37119700
H	-8.08500400	7.18466900	-2.71032400
H	-7.02096700	7.62868500	-4.05345400
C	-3.11362000	0.04869700	-2.49985800
H	-3.31512400	-0.78733200	-3.17602200
H	-2.26212800	-0.22985800	-1.87285400
H	-3.98607300	0.19209900	-1.85479000
C	-1.58745000	1.11066000	-4.21012500
H	-1.78413500	0.30407200	-4.92303900
H	-1.35254400	2.02060800	-4.77167800
H	-0.70859800	0.83099100	-3.62206300
N	-5.57538800	5.10289100	-0.69815400
H	-5.58161900	4.17482100	-0.29770400
H	-6.33597000	5.64758100	-0.31597500
N	-3.38650300	5.94579800	-5.99001300
H	-3.26718600	5.34977800	-6.80498300
H	-3.20987200	6.90419100	-6.27891700
H	-4.70453700	5.73099000	-5.43944700
H	-2.67246800	5.68869000	-5.31270900
N	-3.77941400	6.48048700	0.56840400
H	-4.51048000	7.13444600	0.84404500
H	-3.70519800	5.79418400	1.31860600
H	-2.90592100	7.00618500	0.53567100

T4_1_fph

Energy: -2382.693323

C	-5.60606400	1.04138500	-5.80529600
C	-4.50684400	0.75116700	-5.00900900
C	-3.96660800	1.68334100	-4.11849100
C	-4.58374800	2.93034500	-4.03491900
C	-5.64585300	3.27461900	-4.89720400
C	-6.15887100	2.31465100	-5.76968700
C	-2.70127600	1.36871500	-3.34064700
C	-3.18039700	3.62650900	-2.22229000
C	-2.38605500	2.48909300	-2.35943800
C	-1.27985400	2.36915300	-1.51247400
H	-0.62568000	1.50735900	-1.60442500
C	-1.00635300	3.33300700	-0.55911000
C	-1.88388800	4.40134000	-0.39529200
C	-3.01554500	4.57837700	-1.19736800
H	-6.01003500	0.28963700	-6.47536300
H	-4.04705400	-0.22937000	-5.08830600
H	-6.97743800	2.57409300	-6.43398900
H	-0.13131100	3.23973200	0.07696800
H	-1.65464600	5.11162400	0.39437400
O	-4.20832100	3.89210700	-3.13726800
B	-4.13032200	5.71301300	-0.85902600
P	-6.13437600	5.01337000	-5.03792300
C	-4.09073600	7.08368300	-1.78426900
C	-3.18160300	7.34783800	-2.80096300
C	-5.02085500	8.10020900	-1.58009100
C	-3.21526200	8.49234700	-3.58979700
C	-5.10171000	9.25827500	-2.33843900
C	-4.18631000	9.45560400	-3.36339800
F	-2.18101800	6.47788500	-3.07991600
F	-5.92527000	7.98363200	-0.57516100
F	-6.04565400	10.17690700	-2.10234500
F	-2.31241000	8.67862400	-4.56827200
F	-4.23653000	10.55555400	-4.11647800
C	-2.88575500	0.05326300	-2.55263600
H	-3.10228000	-0.78042700	-3.22675900
H	-1.97538400	-0.19784900	-2.00201200
H	-3.70848500	0.14603000	-1.83686500
C	-1.54026200	1.21079100	-4.34857600
H	-1.75407900	0.40459000	-5.05751500
H	-1.39029400	2.13777200	-4.91147400
H	-0.60856300	0.96718600	-3.82937000
N	-5.48978600	5.09170300	-0.69083800
H	-5.62635600	4.23874900	-1.21307600
H	-6.29214600	5.68165900	-0.86894500
N	-3.38103500	6.01101900	-5.83421100
H	-3.17195300	5.39769000	-6.61731900
H	-3.27454900	6.97071900	-6.15215800
H	-4.70639400	5.72832300	-5.33422500
H	-2.68677200	5.83776600	-5.11113600
N	-3.77366300	6.30703900	0.66894100
H	-4.54867100	6.88892700	0.98348200
H	-3.70807600	5.53240300	1.32883700
H	-2.92434700	6.86545300	0.74258600
C	-7.13140800	5.14819400	-6.55398600
C	-6.47747900	5.11898800	-7.79251900
C	-8.52036700	5.29390300	-6.50632800
C	-7.20965500	5.22697800	-8.96845300
H	-5.39854300	4.99650100	-7.84522300
C	-9.24648400	5.40547700	-7.68853600
H	-9.03596300	5.32105300	-5.55089400
C	-8.59465700	5.37240700	-8.91752000
H	-6.69828100	5.20098100	-9.92600500
H	-10.32567800	5.51800400	-7.64621700
H	-9.16475800	5.46110000	-9.83757200
C	-7.23360200	5.48012400	-3.67807600
C	-7.89300100	4.50613300	-2.92532200
C	-7.47504300	6.83742100	-3.44499400
C	-8.79011300	4.89394400	-1.93491200
H	-7.70696100	3.45157800	-3.11244400
C	-8.37526900	7.21636100	-2.45571300
H	-6.97070300	7.59493700	-4.04057600
C	-9.02977000	6.24565100	-1.69952100
H	-9.30135600	4.13830300	-1.34600100
H	-8.56263300	8.27006600	-2.27199500
H	-9.72990200	6.54483500	-0.92503900

T4_2_cip

Energy: -3958.040699

C	-6.82376000	-0.18506500	-0.03318400
C	-5.45386400	-0.04643200	0.16645900
C	-4.86486000	1.21672300	0.21167300
C	-5.68911200	2.32567300	0.01220100
C	-7.08434400	2.22639200	-0.11305300
C	-7.63343100	0.93896100	-0.14592700
C	-3.40596000	1.47897200	0.54836000
C	-3.82973800	3.67777000	-0.57980600
C	-2.94541800	2.62085300	-0.34489600
C	-1.66576500	2.70908300	-0.89182100
H	-0.95391400	1.90489300	-0.74098900
C	-1.28637200	3.83330500	-1.61564000
C	-2.18469200	4.87857500	-1.79125000
C	-3.49067500	4.83802600	-1.28079500
H	-7.26747400	-1.17515800	-0.07165000
H	-4.84376400	-0.93339400	0.29741300
H	-8.70323400	0.80665100	-0.26244800
H	-0.28505400	3.89845900	-2.03073000
H	-1.86305700	5.76114900	-2.34191000
O	-5.13646100	3.59370300	-0.07843900
B	-4.46815200	6.05956200	-1.71428700
P	-8.04798600	3.78430600	-0.23401000
C	-3.65616000	7.50100900	-1.52903800
C	-3.09877500	7.79491900	-0.26858400
C	-3.40999900	8.47184200	-2.51174800
C	-2.31279600	8.92104800	-0.00563300
C	-2.62102600	9.61209200	-2.29311900
C	-2.06133500	9.83331700	-1.03387800
C	-7.85789100	4.45090100	1.52496000
H	-6.80169100	4.76085900	1.52796100
C	-9.81896000	3.23820600	-0.52895900
H	-9.70775400	2.47346600	-1.31309900
C	-10.58974400	2.62931700	0.64592300

H	-11.53327900	2.20744600	0.27981000
H	-10.03967900	1.83552000	1.15654300
H	-10.84151400	3.39578800	1.38496500
C	-10.60814700	4.40437400	-1.14354700
H	-10.73411600	5.22335400	-0.42782000
H	-10.11527600	4.80384800	-2.03522800
H	-11.60849600	4.06077400	-1.43006100
C	-8.02950100	3.45825200	2.67668300
H	-7.65832900	3.91620400	3.60146100
H	-9.07719500	3.19576500	2.83758500
H	-7.46394200	2.53652300	2.50937100
C	-8.71770100	5.70432500	1.71706400
H	-9.78025600	5.45101500	1.78313400
H	-8.44155500	6.20367000	2.65250200
H	-8.59278900	6.42316200	0.89881900
C	-3.33826700	1.96337100	2.02050800
H	-3.70415900	1.17758700	2.69000100
H	-2.30249300	2.20123900	2.28422800
H	-3.94787100	2.85948400	2.17178400
C	-2.53763300	0.22958100	0.40574800
H	-2.88967300	-0.55715700	1.07832300
H	-2.54109000	-0.15582000	-0.61933800
H	-1.50630100	0.44843400	0.69390200
N	-5.81727400	6.22521100	-0.84140700
H	-5.60875100	6.31340400	0.15298500
H	-6.31925800	7.07289700	-1.10677300
H	-6.48510400	5.43505900	-0.93374300
N	-4.99282900	5.65203700	-3.12953400
H	-5.69668100	6.27281000	-3.52465000
H	-4.22944300	5.65339900	-3.80283600
H	-4.91811200	2.54340800	-3.08024200
H	-6.41444200	2.88142200	-2.48825200
H	-5.42060200	4.34593100	-3.14701400
H	-6.14912100	2.89817600	-4.11685700
N	-5.74098800	3.12875200	-3.21404800
Cl	-1.64411800	9.20599400	1.56412400
Cl	-1.08322400	11.22534600	-0.74340000
Cl	-2.33250000	10.75881400	-3.55622200
Cl	-4.10459400	8.33768800	-4.12139200
Cl	-3.37809700	6.72302800	1.09834300

T4_2_cph

Energy: -4184.436992

C	-6.86803800	-0.29081800	0.15732900
C	-5.48585500	-0.15855500	0.23619000
C	-4.87544300	1.09224500	0.13585000
C	-5.69550800	2.19692900	-0.09574500
C	-7.09381600	2.09840200	-0.14011900
C	-7.66931000	0.83196700	-0.00895300
C	-3.39652000	1.34166000	0.37588200
C	-3.84122800	3.54917700	-0.73798900
C	-2.96383100	2.47920700	-0.53665800
C	-1.68750800	2.57479400	-1.09042300
H	-0.98247200	1.75938000	-0.97193700
C	-1.29593100	3.72174800	-1.77064600
C	-2.17321800	4.79357400	-1.87521200
C	-3.47700500	4.74620700	-1.36078900
H	-7.32411500	-1.27188100	0.24621400
H	-4.87880300	-1.04266500	0.39698000
H	-8.74930400	0.72818900	-0.04479900
H	-0.29701100	3.78912600	-2.19089600
H	-1.83359200	5.70623000	-2.36319300
O	-5.15518000	3.46036700	-0.26123300
B	-4.38912000	6.05880100	-1.63422900
P	-8.07863900	3.60453700	-0.48312200
C	-3.53461200	7.41479700	-1.18451100
C	-3.06899800	7.50243000	0.14300700
C	-3.17000500	8.49812400	-1.99920600
C	-2.28194000	8.55247700	0.62644800
C	-2.37416800	9.56658600	-1.55658900
C	-1.92381100	9.59173800	-0.23591000
C	-3.23867600	1.83531700	1.83849900
H	-3.57351700	1.05853500	2.53447300
H	-2.18763300	2.06703800	2.04054400
H	-3.83066200	2.73956700	2.01491000
C	-2.55240300	0.08028400	0.19138700
H	-2.87080500	-0.69730100	0.89024800
H	-2.62368500	-0.31178800	-0.82858900
H	-1.50307100	0.28682200	0.41571200
N	-5.77120400	6.13505700	-0.79291600
H	-5.63169700	5.99436200	0.20857200
H	-6.21897000	7.04596100	-0.89736400
H	-6.45726100	5.42662800	-1.07877900
N	-4.88034000	5.91391500	-3.10949500
H	-5.50043400	6.65481800	-3.43126600
H	-4.09192700	5.92789000	-3.75243600
H	-5.24661300	2.80780600	-3.22590900
H	-6.72460800	3.41357300	-2.80276600
H	-5.44675600	4.67615200	-3.30008300
H	-6.26925700	3.36351500	-4.39365100
N	-5.93624200	3.52387100	-3.44608600
C	-7.93540500	4.58900900	1.06462700
C	-7.13231600	4.21987500	2.14610900
C	-8.60671500	5.81973800	1.09983800
C	-6.99644100	5.07194600	3.24089100
H	-6.61519800	3.26449100	2.14320500
C	-8.48115700	6.65909900	2.20065000
H	-9.23802600	6.11773200	0.26412700
C	-7.66657300	6.29086200	3.27085900
H	-6.36785900	4.77512900	4.07571200
H	-9.01543900	7.60467100	2.22204300
H	-7.55867500	6.95156600	4.12599700
C	-9.80776100	3.00482800	-0.44490200
C	-10.50952700	2.81527900	0.75041800
C	-10.43047100	2.71414100	-1.66321500
C	-11.81502400	2.33654200	0.72260200
H	-10.03480900	3.04204200	1.70131100
C	-11.73333900	2.22532100	-1.68611800
H	-9.89541800	2.87175800	-2.59711000
C	-12.42692500	2.03870000	-0.49345400
H	-12.35581000	2.19330800	1.65358100
H	-12.21021700	2.00026100	-2.63558400
H	-13.44679800	1.66551100	-0.51092800
Cl	-3.69954500	8.60490800	-3.67258200
Cl	-1.94180400	10.86285200	-2.61787600
Cl	-0.94370400	10.89486700	0.32971000
Cl	-1.73935600	8.58835400	2.26872200
Cl	-3.46645000	6.24861200	1.31102000

T4_2_fip

Energy: -2156.329312

C	-6.85801000	-0.15964000	-0.26274000
C	-5.49232000	-0.05477000	-0.01589000
C	-4.88797000	1.19472000	0.12421000
C	-5.69459000	2.32317000	-0.02940000
C	-7.08861000	2.25422000	-0.18592000
C	-7.65259000	0.97947000	-0.31645000
C	-3.43999000	1.41792000	0.53303000
C	-3.80130000	3.68548000	-0.48385000
C	-2.93096000	2.61536000	-0.25674000
C	-1.62320000	2.73448000	-0.72540000
H	-0.91804000	1.92351000	-0.57913000
C	-1.20650000	3.89621000	-1.36413000
C	-2.09959000	4.94460000	-1.54884000
C	-3.43567000	4.87299000	-1.12816000
H	-7.31324000	-1.13901000	-0.37686000
H	-4.89886000	-0.95757000	0.07612000
H	-8.72092000	0.86930000	-0.46775000
H	-0.18226000	3.98409000	-1.71419000
H	-1.75478000	5.84689000	-2.04900000
O	-5.12779000	3.58409000	-0.04423000
B	-4.43708000	6.06268000	-1.59029000
P	-8.02268000	3.83768000	-0.20178000
C	-3.66468000	7.50836000	-1.58360000
C	-3.17685000	8.00534000	-0.37551000
C	-3.38817000	8.30983000	-2.68697000
C	-2.47109000	9.19114000	-0.24671000
C	-2.67895000	9.50404000	-2.61289000
C	-2.21605000	9.94833000	-1.38338000
F	-3.39782000	7.30729000	0.76486000

F	-3.79887000	7.95078000	-3.92564000
F	-2.43992000	10.22521000	-3.71222000
F	-2.03956000	9.61287000	0.94509000
F	-1.54081000	11.09259000	-1.29199000
C	-7.83146000	4.35686000	1.60485000
H	-6.77097000	4.64748000	1.63329000
C	-9.80146000	3.34782000	-0.54410000
H	-9.69959000	2.62644000	-1.36944000
C	-10.59916000	2.69517000	0.58818000
H	-11.55089000	2.32265000	0.19106000
H	-10.07686000	1.85851000	1.05840000
H	-10.83550000	3.42704000	1.36675000
C	-10.55556000	4.56856000	-1.09437000
H	-10.66260000	5.34831000	-0.33247000
H	-10.04787000	5.00615000	-1.95848000
H	-11.56360000	4.27017000	-1.40427000
C	-8.02801000	3.28519000	2.67856000
H	-7.64446000	3.66201000	3.63449000
H	-9.08278000	3.03953000	2.82173000
H	-7.48763000	2.36368000	2.44113000
C	-8.67165000	5.60573000	1.88455000
H	-9.73973000	5.36699000	1.91631000
H	-8.40011000	6.02463000	2.86016000
H	-8.52237000	6.38373000	1.12632000
C	-3.43150000	1.79047000	2.03816000
H	-3.83692000	0.96255000	2.62941000
H	-2.40536000	1.99096000	2.36394000
H	-4.03593000	2.68239000	2.23044000
C	-2.57615000	0.17230000	0.33438000
H	-2.96030000	-0.65746000	0.93344000
H	-2.54175000	-0.13806000	-0.71529000
H	-1.55542000	0.35782000	0.67834000
N	-5.70150000	6.25688000	-0.59589000
H	-5.40225000	6.26624000	0.37923000
H	-6.17876000	7.14312000	-0.76245000
H	-6.41124000	5.50833000	-0.68573000
N	-5.04850000	5.64782000	-2.97040000
H	-5.77371000	6.28014000	-3.30542000
H	-4.31664000	5.69462000	-3.68152000
H	-4.80962000	2.56502000	-3.08343000
H	-6.33383000	2.69971000	-2.50230000
H	-5.43001000	4.32900000	-3.03652000
H	-6.05352000	2.91555000	-4.11010000
N	-5.67329000	3.10027000	-3.17688000

T4_2_fph

Energy: -2382.725583

C	-6.87441800	-0.28093300	0.07089900
C	-5.49253700	-0.15841200	0.16927600
C	-4.87473800	1.09152000	0.11047900
C	-5.68672500	2.20582300	-0.10160500
C	-7.08539800	2.11727400	-0.15866200
C	-7.66842100	0.85069400	-0.06934900
C	-3.39866700	1.32834500	0.38053000
C	-3.81717600	3.56460200	-0.69128000
C	-2.94679700	2.48617700	-0.49673000
C	-1.66577800	2.58248100	-1.03767100
H	-0.96590800	1.76205000	-0.92339400
C	-1.26226500	3.73526600	-1.70112200
C	-2.13464800	4.81027500	-1.80660100
C	-3.44623300	4.76369900	-1.31039500
H	-7.33631600	-1.26169600	0.12668600
H	-4.89207900	-1.04988800	0.31330100
H	-8.74875500	0.75425200	-0.11560400
H	-0.25861700	3.80265300	-2.10994500
H	-1.78872600	5.72352500	-2.28786300
O	-5.13750800	3.46921900	-0.23066800
B	-4.36537000	6.07019400	-1.58604900
P	-8.05905200	3.64445300	-0.43918000
C	-3.51859200	7.43290000	-1.25673200
C	-3.02849000	7.62224300	0.03456600
C	-3.18270100	8.44049500	-2.15467000
C	-2.26280700	8.70899100	0.42592700
C	-2.41561100	9.54925300	-1.81368500
C	-1.95176000	9.68471200	-0.51337400
F	-3.30218000	6.69832200	0.98706300
F	-3.59152300	8.38278700	-3.44359500
F	-2.12639300	10.48439100	-2.72350000
F	-1.82448500	8.82917200	1.68200900
F	-1.22004000	10.74207700	-0.16659400
C	-3.26288100	1.77958800	1.85877700
H	-3.61502000	0.98542500	2.52597500
H	-2.21376100	1.99652500	2.08565400
H	-3.85109900	2.68264900	2.05201500
C	-2.55717800	0.06827800	0.17502900
H	-2.89148000	-0.72715700	0.84573700
H	-2.61203200	-0.29416700	-0.85686700
H	-1.51098200	0.26258400	0.42379400
N	-5.67081300	6.14544400	-0.62937000
H	-5.43555700	5.98641400	0.35053400
H	-6.12103300	7.05973600	-0.67620800
H	-6.38118000	5.44255900	-0.86685400
N	-4.92858300	5.96456700	-3.03971700
H	-5.55062000	6.72736400	-3.30506400
H	-4.16148600	6.00781800	-3.70789700
H	-5.27244900	2.86574100	-3.20557600
H	-6.75881500	3.44796400	-2.78197500
H	-5.49851000	4.73291700	-3.25750500
H	-6.29708300	3.42114300	-4.37117100
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C	-7.93781000	4.53431300	1.16681200
C	-7.21308200	4.05913500	2.26215200
C	-8.56043400	5.78782400	1.24938400
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H	-6.73398700	3.08491300	2.21988300
C	-8.46808500	6.54453600	2.41175100
H	-9.13000300	6.16806000	0.40264500
C	-7.73537400	6.06841600	3.49831600
H	-6.54493800	4.44844700	4.26653200
H	-8.96505400	7.50879000	2.46927500
H	-7.65527200	6.66318300	4.40351100
C	-9.79029900	3.04844800	-0.46252900
C	-10.52557100	2.82826100	0.70680300
C	-10.38064600	2.79596000	-1.70542200
C	-11.83195300	2.35683900	0.62895600
H	-10.07703700	3.02516000	1.67679400
C	-11.68393800	2.31375800	-1.77855300
H	-9.82001000	2.97875500	-2.61963400
C	-12.41114600	2.09660000	-0.61123200
H	-12.39885500	2.18976900	1.54021000
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H	-13.43167200	1.72908300	-0.66750700

Trit

Energy: -733.4967482

C	-1.22912828	0.31700451	-0.00119239
C	-0.50254821	1.55695490	0.10222208
C	-1.06317239	2.76086450	-0.38491653
C	0.78199120	1.58828968	0.69365599
C	-0.35333558	3.94422860	-0.29612313
H	-2.02775819	2.73892769	-0.88218009
C	1.46742349	2.78393645	0.80555010
H	1.19982845	0.67828763	1.11236025
C	0.90652497	3.96007092	0.30492741
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H	1.45434395	4.89465542	0.38355378
C	-2.66636857	0.31358701	0.10057705
C	-3.32966337	1.23725075	0.94193945
C	-3.43538550	-0.61384588	-0.64075481
C	-4.70831312	1.21708275	1.04620693
H	-2.74650277	1.92160346	1.54997900
C	-4.81516922	-0.60168300	-0.55254984
H	-2.93756635	-1.29451194	-1.32403777
C	-5.45278454	0.30578338	0.29514979
H	-5.21006018	1.90616616	1.71818812
H	-5.40154090	-1.29363857	-1.14870236
H	-6.53631163	0.30297400	0.37091205
C	-0.51905602	-0.91976988	-0.20581365
C	-1.00069621	-2.12502591	0.35670454

C	0.67026339	-0.94746636	-0.97124537
C	-0.30521521	-3.30576911	0.17224644
H	-1.88634611	-2.10554770	0.98384993
C	1.33836024	-2.14066456	-1.17551295
H	1.02155742	-0.03682843	-1.44601458
C	0.85834074	-3.31788088	-0.59882985
H	-0.66157479	-4.22124796	0.63378093
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H	1.39413259	-4.25028090	-0.75138635

Trit_H

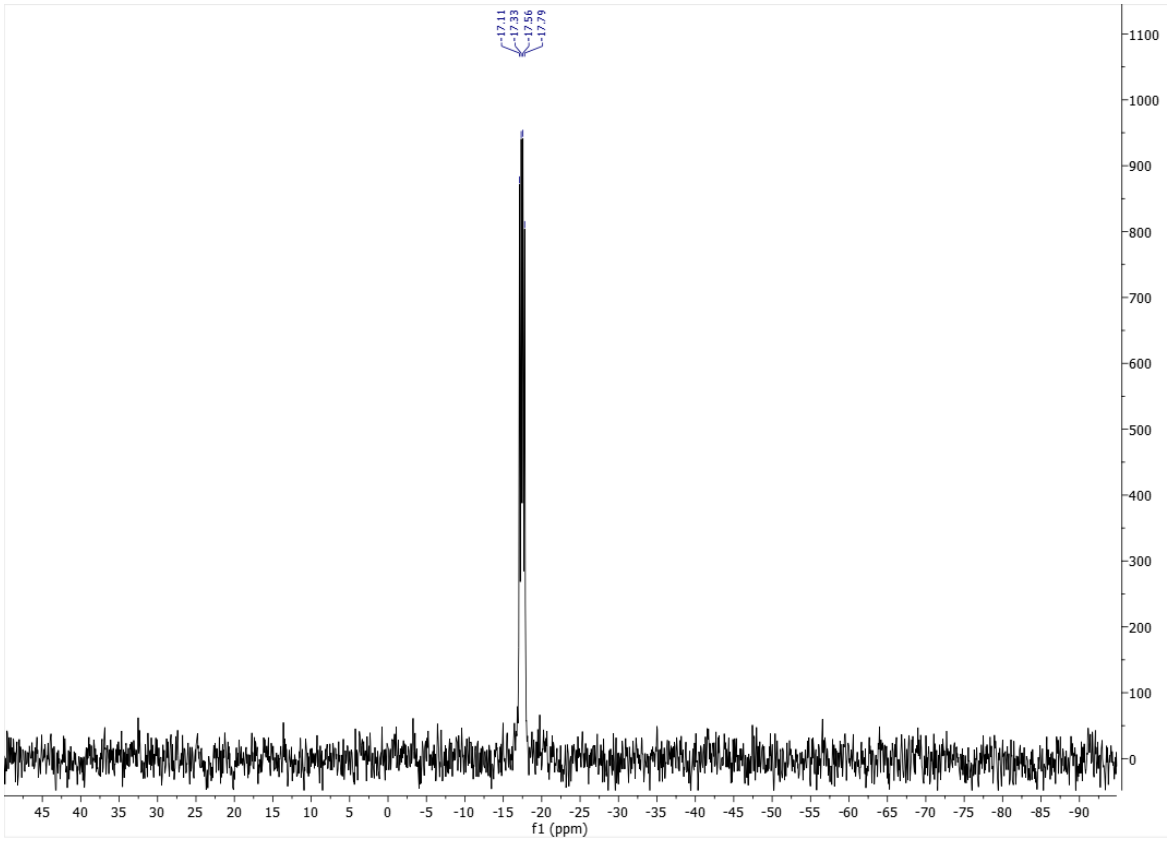
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H	0.53740595	1.55044272	0.67821698
C	-1.33146153	0.86958870	-0.03871711
C	-2.06741156	-0.27893032	-0.33088418
C	-2.01699999	2.03192377	0.32678001
C	-3.45946660	-0.26486317	-0.26394665
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C	-3.40537775	2.04741674	0.39836021
H	-1.45183658	2.93401449	0.55257944
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H	-4.01737583	-1.16834174	-0.49446421
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H	-5.21801007	0.90539234	0.15881829
C	0.82119165	-0.45363510	0.06646342
C	1.27857493	-1.23899907	-0.99162036
C	0.91054153	-0.95982978	1.36679741
C	1.80994517	-2.50592786	-0.75575746
H	1.22268991	-0.85734890	-2.00751973
C	1.44319046	-2.22145489	1.60500982
H	0.55284591	-0.35624423	2.19867955
C	1.89449794	-3.00152418	0.54133658
H	2.16180107	-3.10481429	-1.59136243
H	1.50934801	-2.59666208	2.62261494
H	2.31308202	-3.98708284	0.72470574
C	0.65877102	1.57846746	-1.43302471
C	-0.12274040	1.61375061	-2.58756266
C	1.93932062	2.13929984	-1.47108249
C	0.36643207	2.19306662	-3.75747301
H	-1.12249675	1.18842287	-2.57364478
C	2.42780110	2.72107566	-2.63504738
H	2.55829192	2.11286448	-0.57636389
C	1.64131045	2.74860062	-3.78592074
H	-0.25597105	2.21221859	-4.64794192
H	3.42325925	3.15656248	-2.64499674
H	2.02014247	3.20464873	-4.69622356

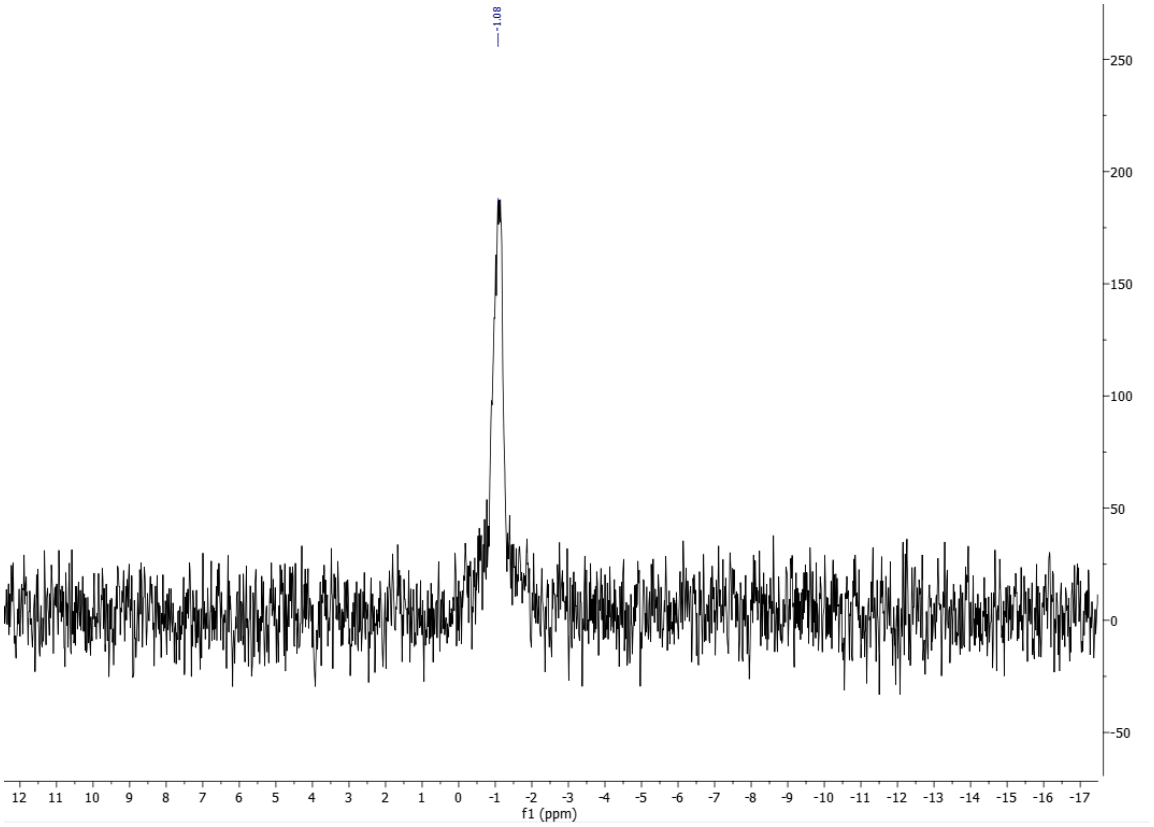
Chapter 8

Spectra

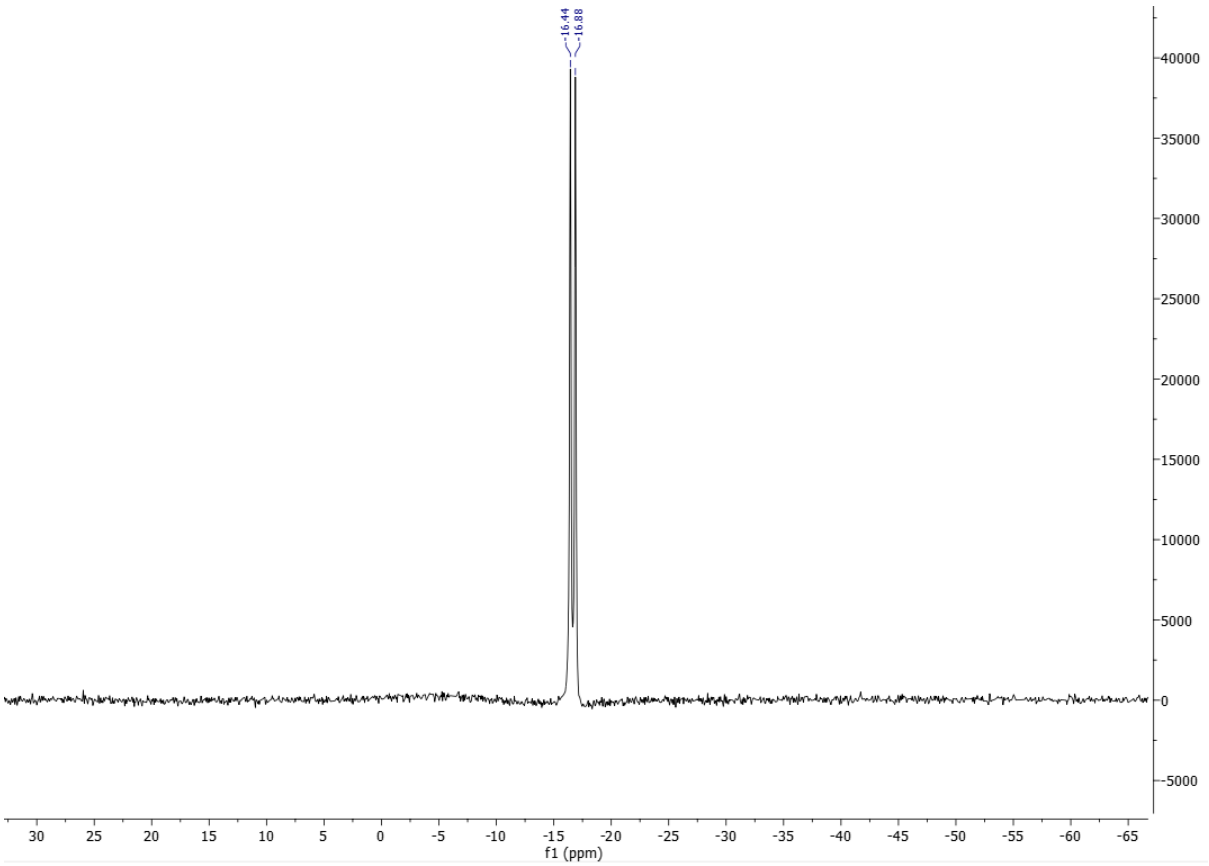
NMR



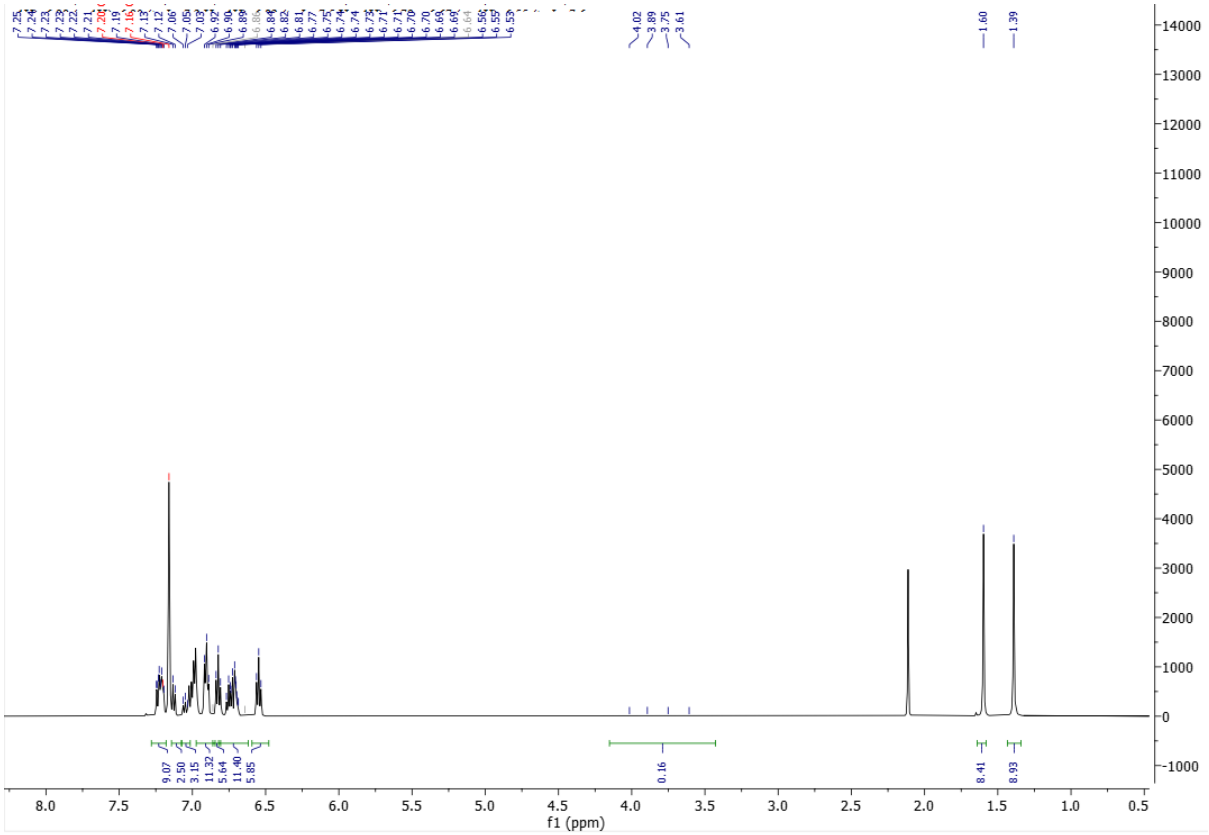
A 8.1: 31P NMR of (Ph_2P-xan)3BH-Li



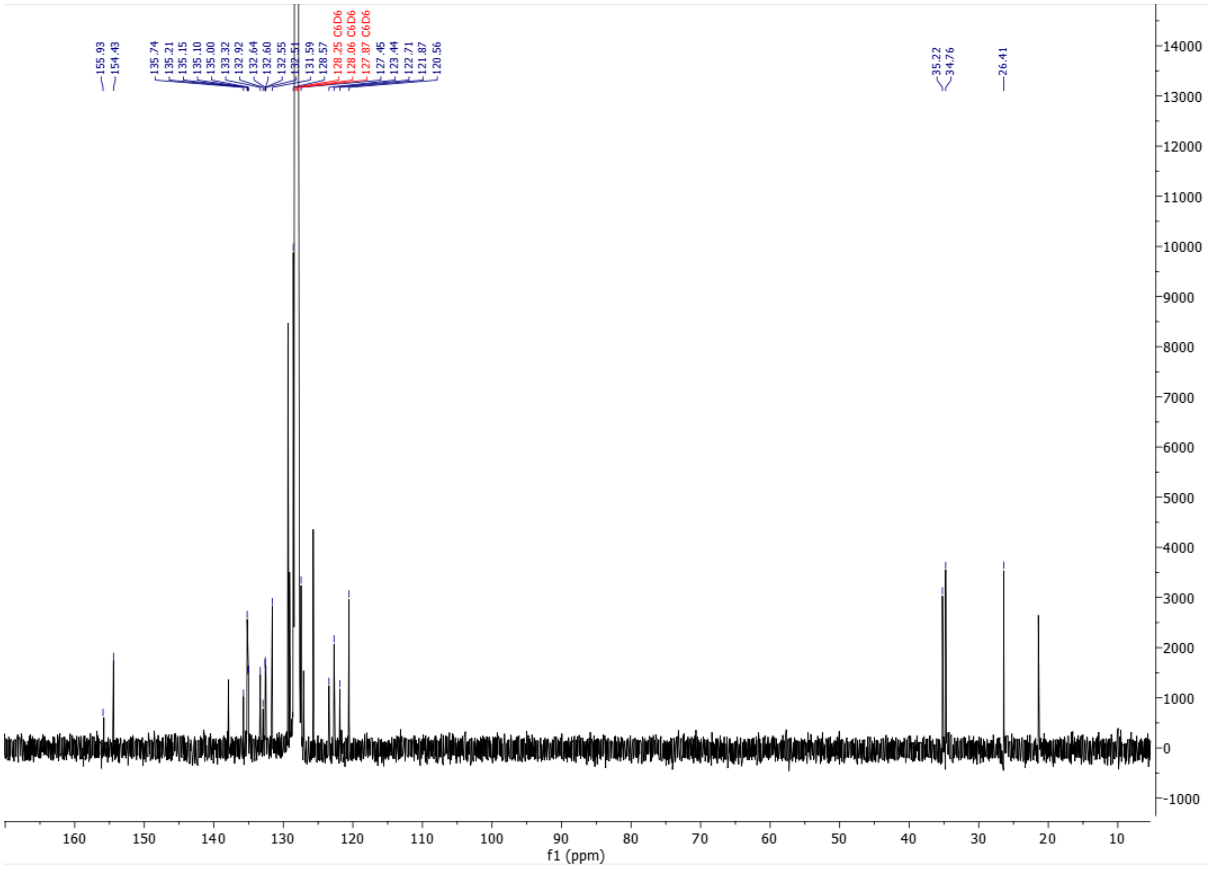
A 8.2: ^{7}Li NMR of $(Ph_2P\text{-xan})_3BH\text{-Li}$



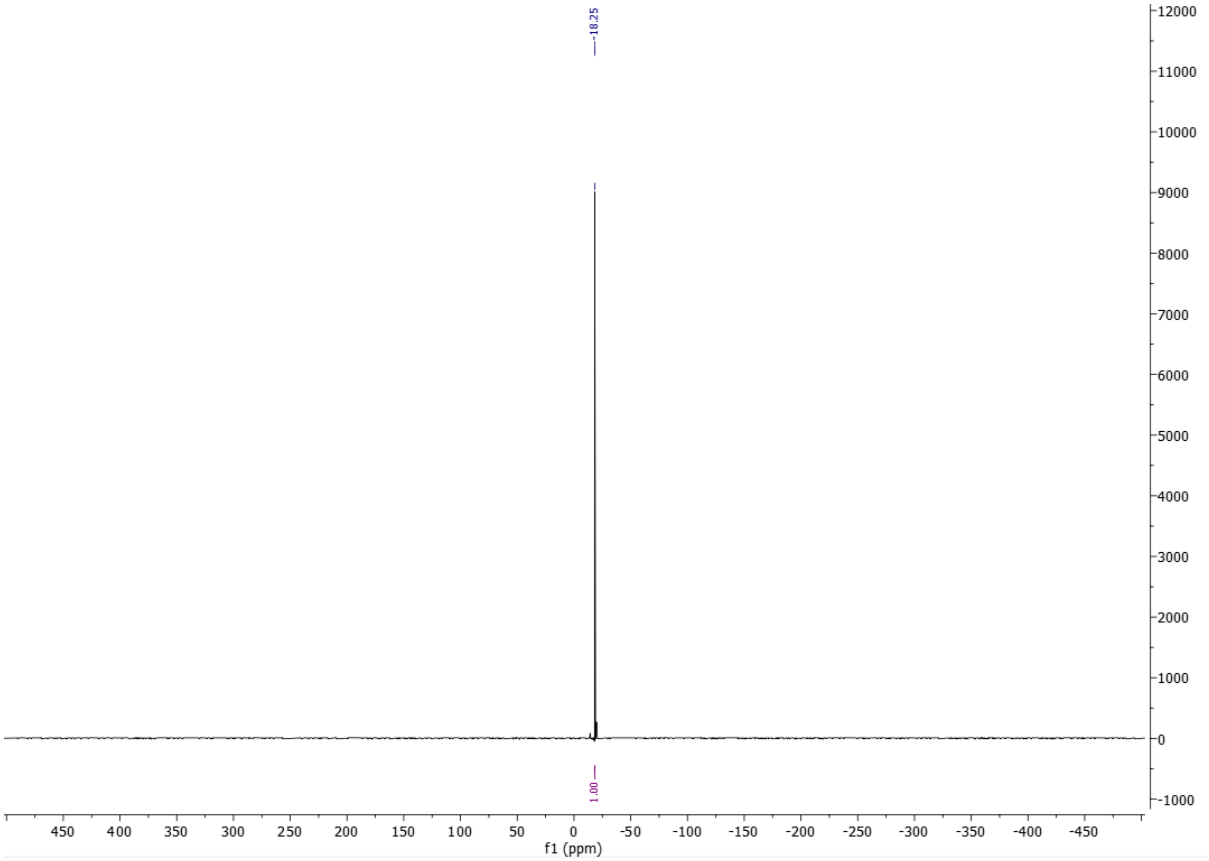
A 8.3: ^{11}B NMR of $(Ph_2P\text{-xan})_3BH\text{-Li}$



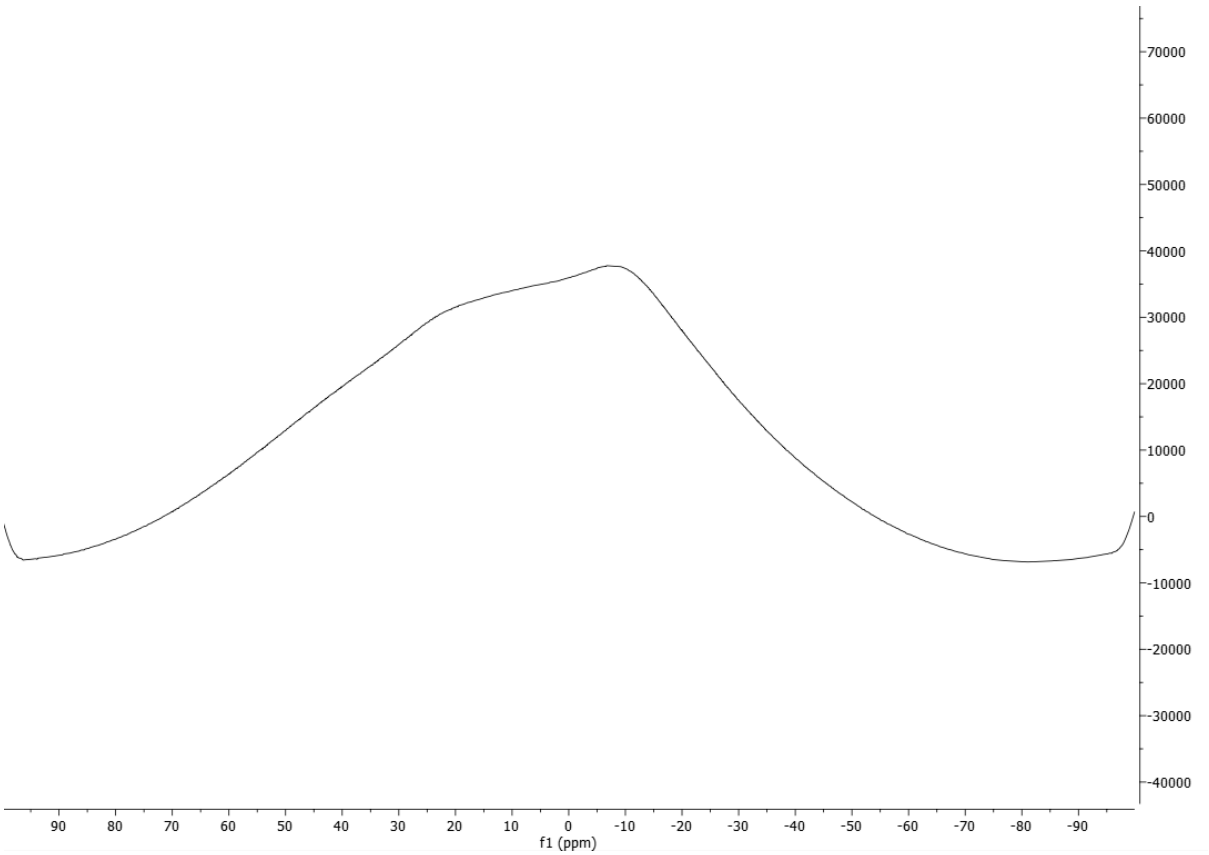
A 8.4: ^{1}H NMR of $(Ph_2P\text{-xan})_3BH\text{-}Li$



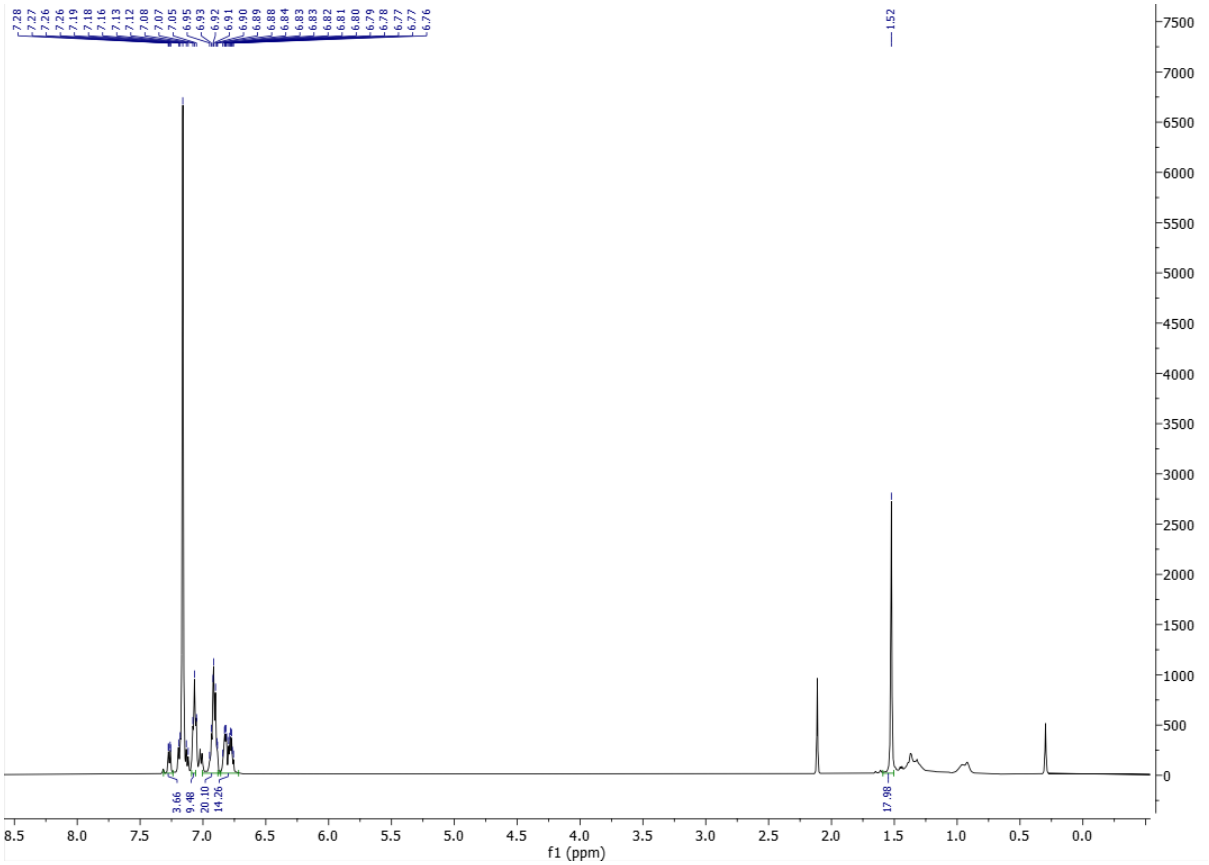
A 8.5: ^{13}C NMR of $(Ph_2P\text{-xan})_3BH\text{-}Li$



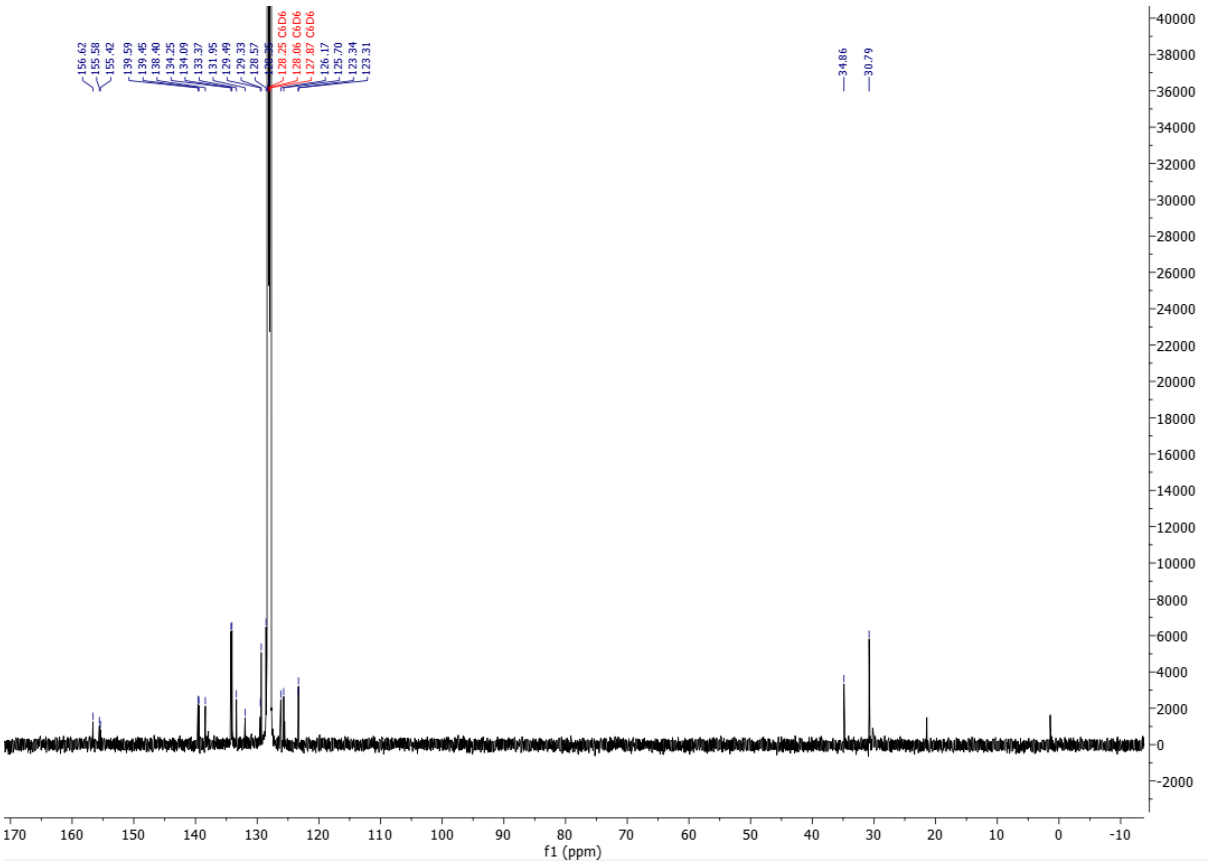
A 8.6: ^{31}P NMR of $(Ph_2P\text{-xan})_3B$



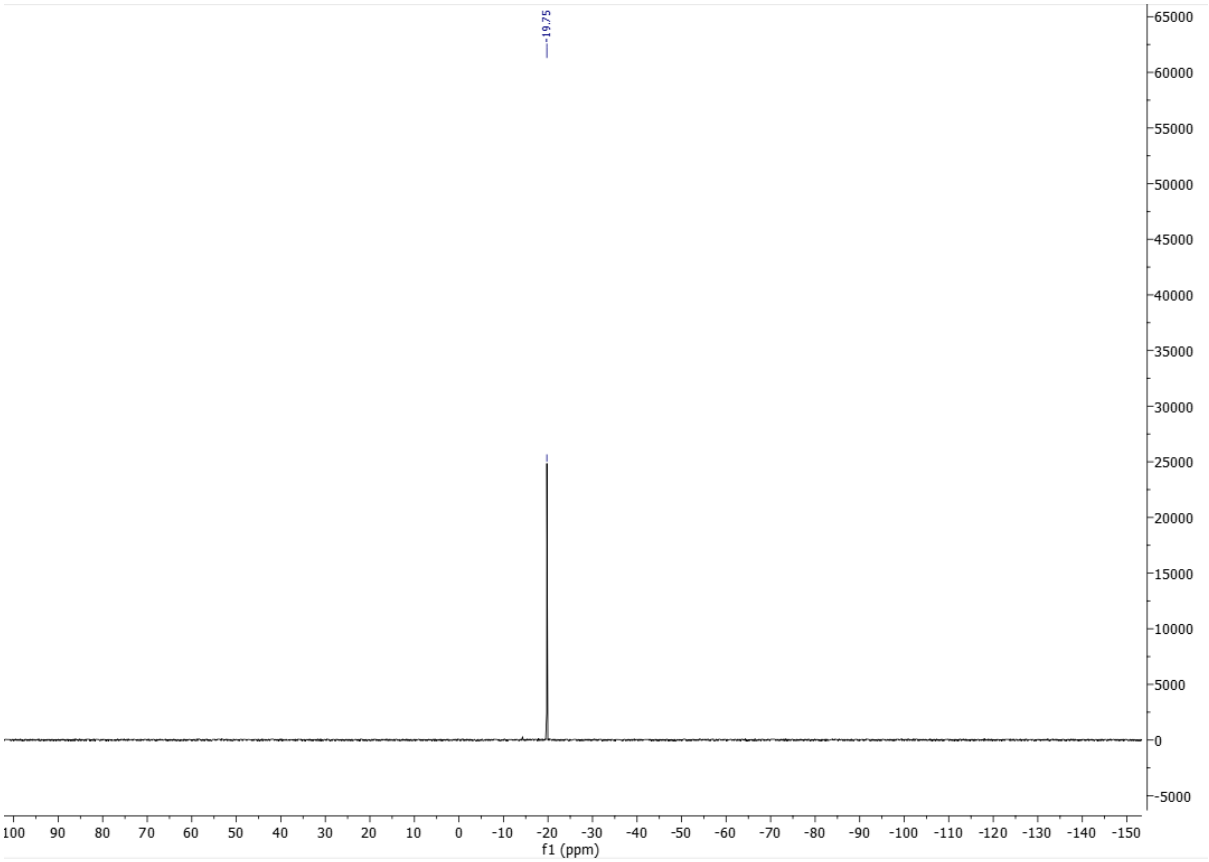
A 8.7: ^{11}B NMR of $(Ph_2P\text{-xan})_3B$, no clear resonance could be observed, possible very broad shoulder at 25 ppm



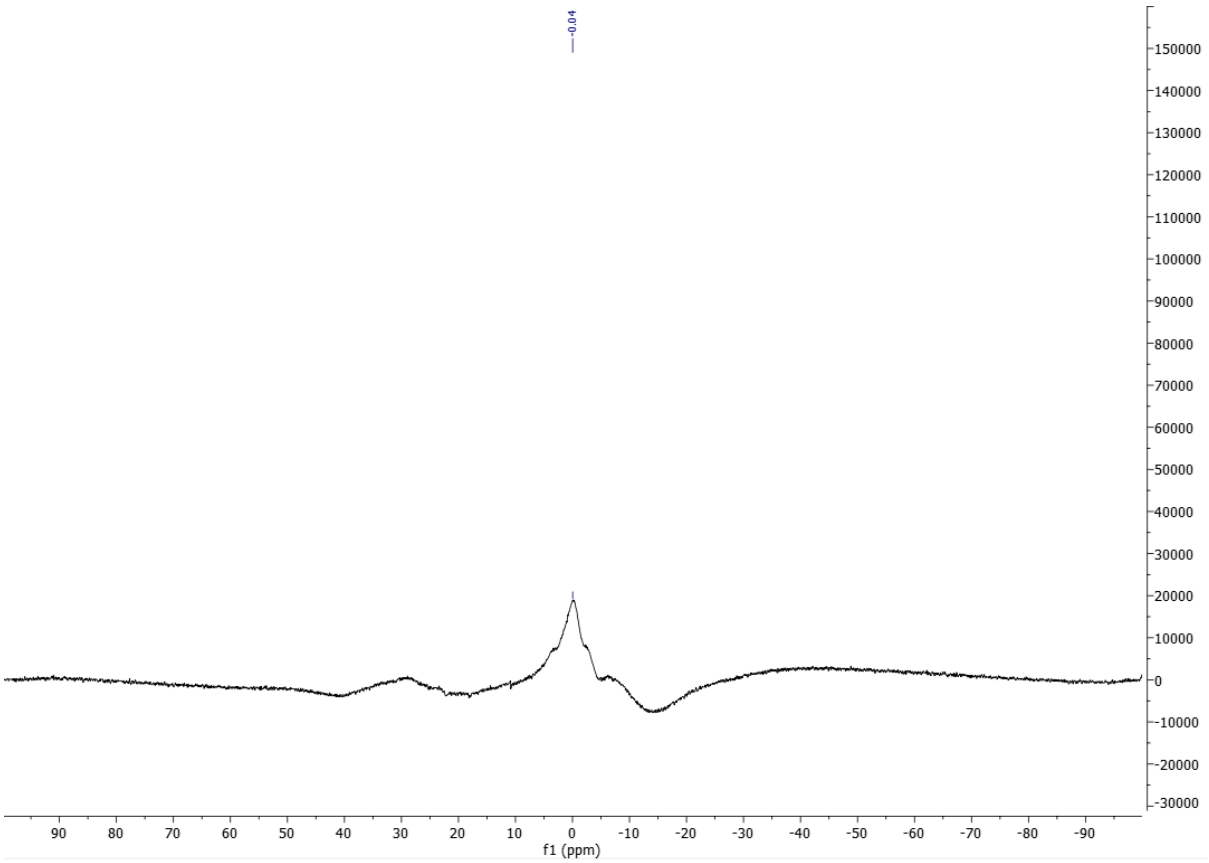
A 8.8: ^{1}H NMR of $(Ph_2P\text{-xan})_3B$



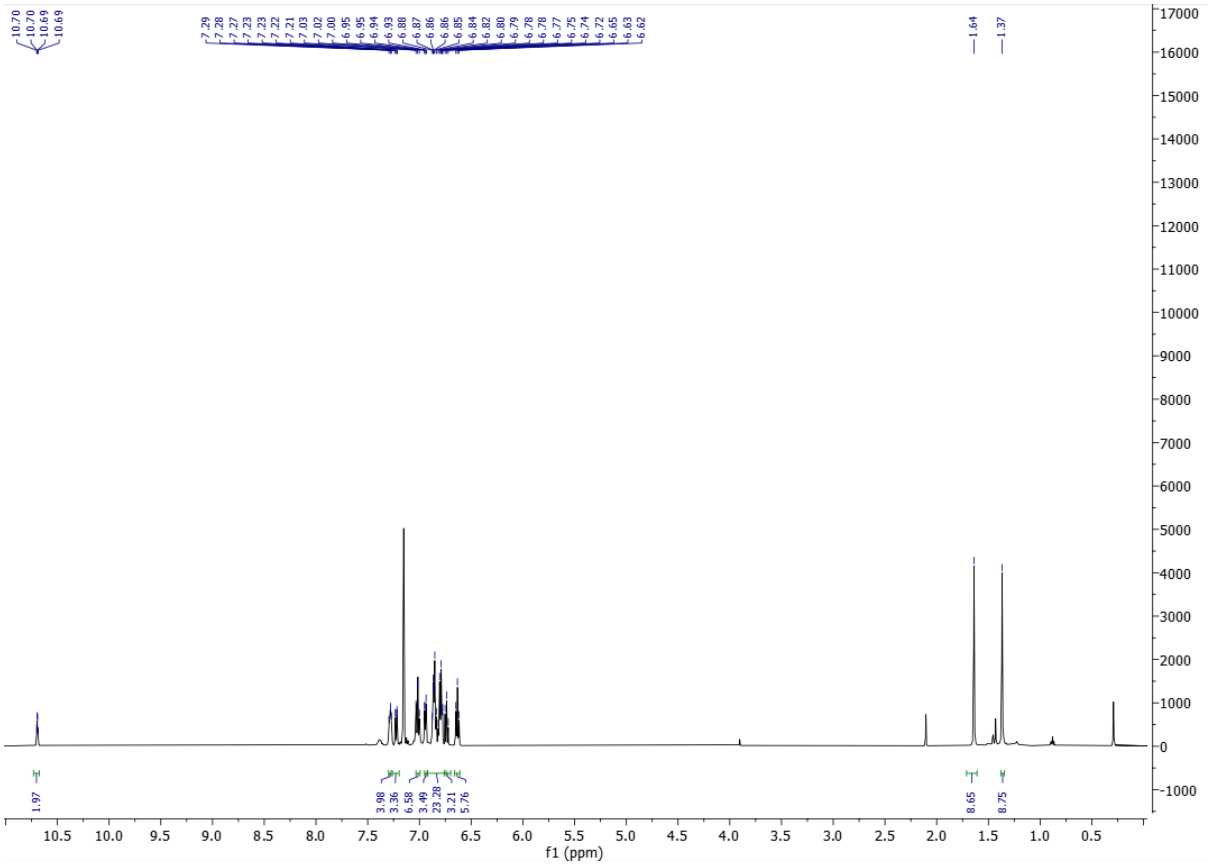
A 8.9: ^{13}C NMR of $(Ph_2P\text{-xan})_3B$



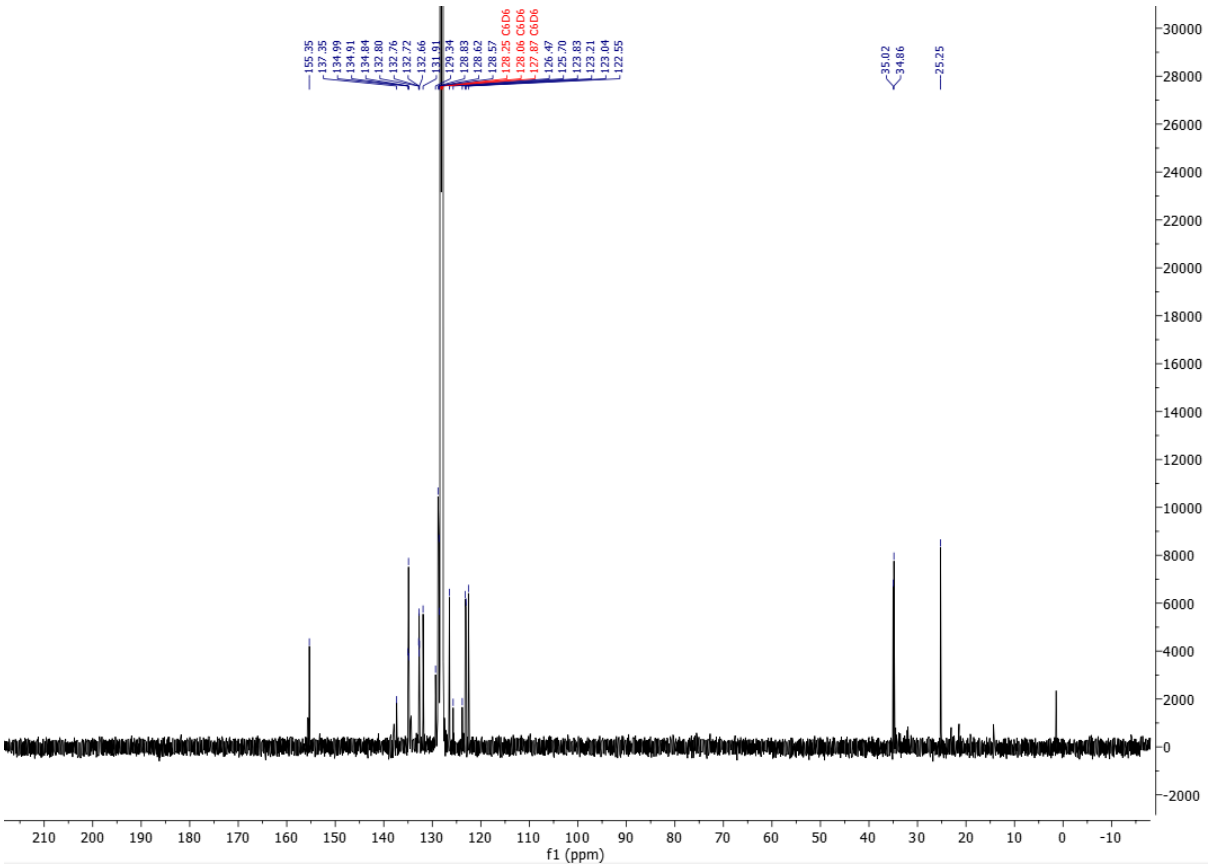
A 8.10: ^{31}P NMR of $(Ph_2P\text{-xan})_3B\text{-}OH_2$



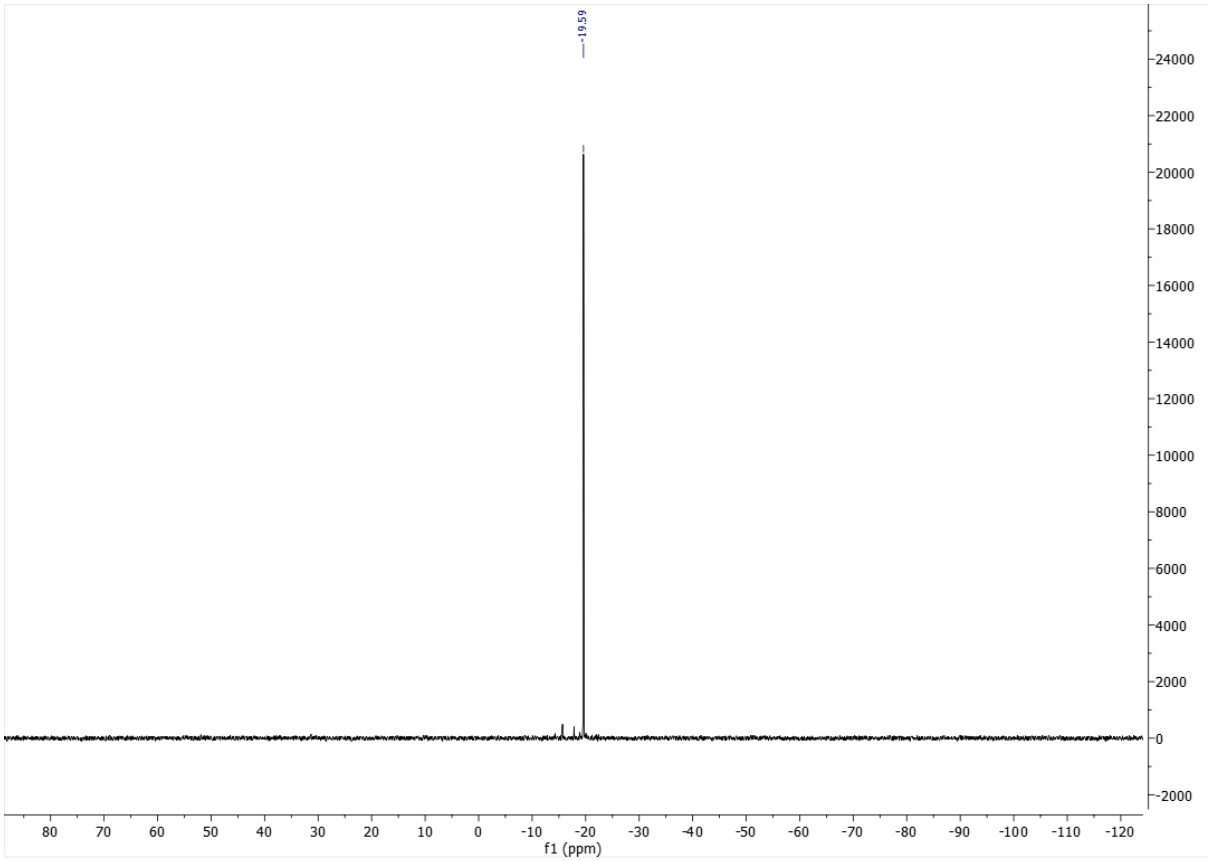
A 8.11: ^{11}B NMR of $(Ph_2P\text{-xan})OH_2$



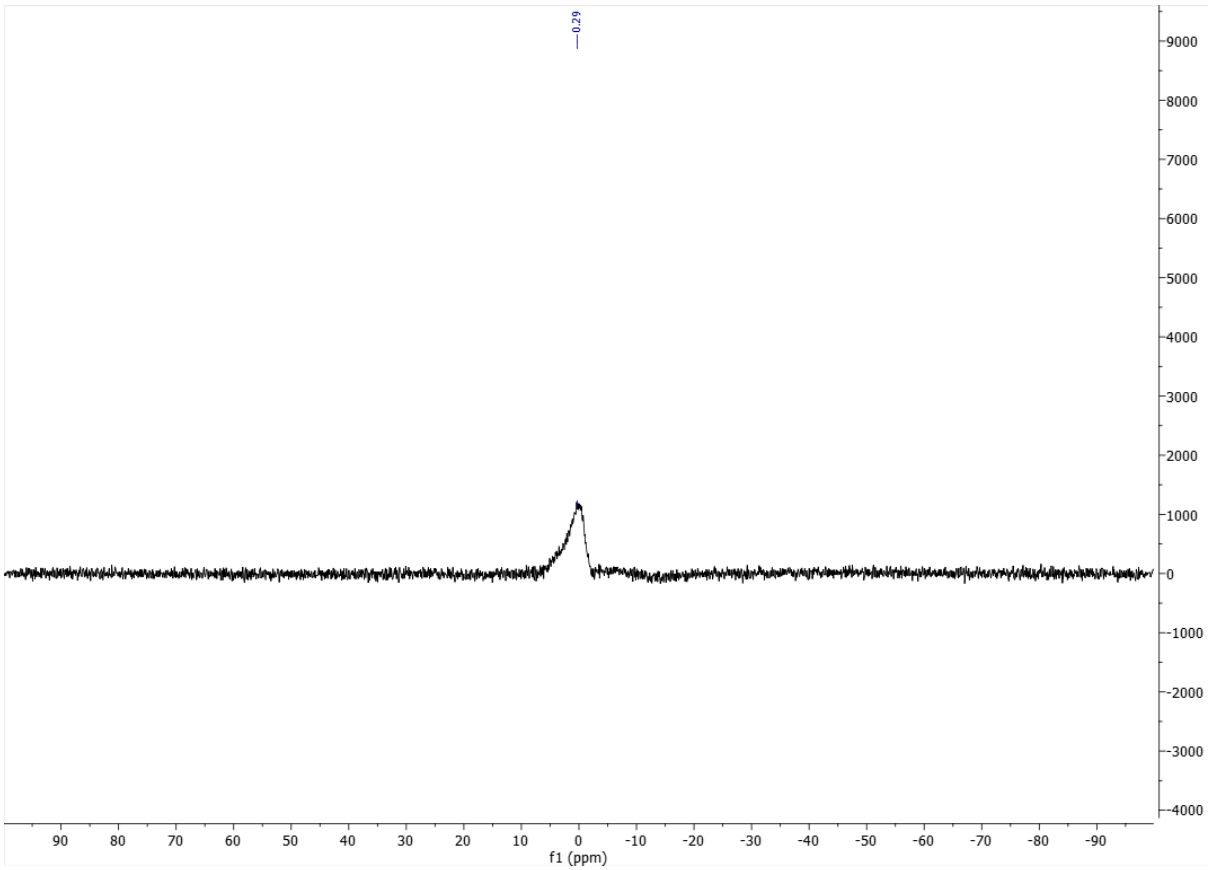
A 8.12: ^{1}H NMR of $(Ph_2P\text{-}xan)_3B\text{-}OH_2$



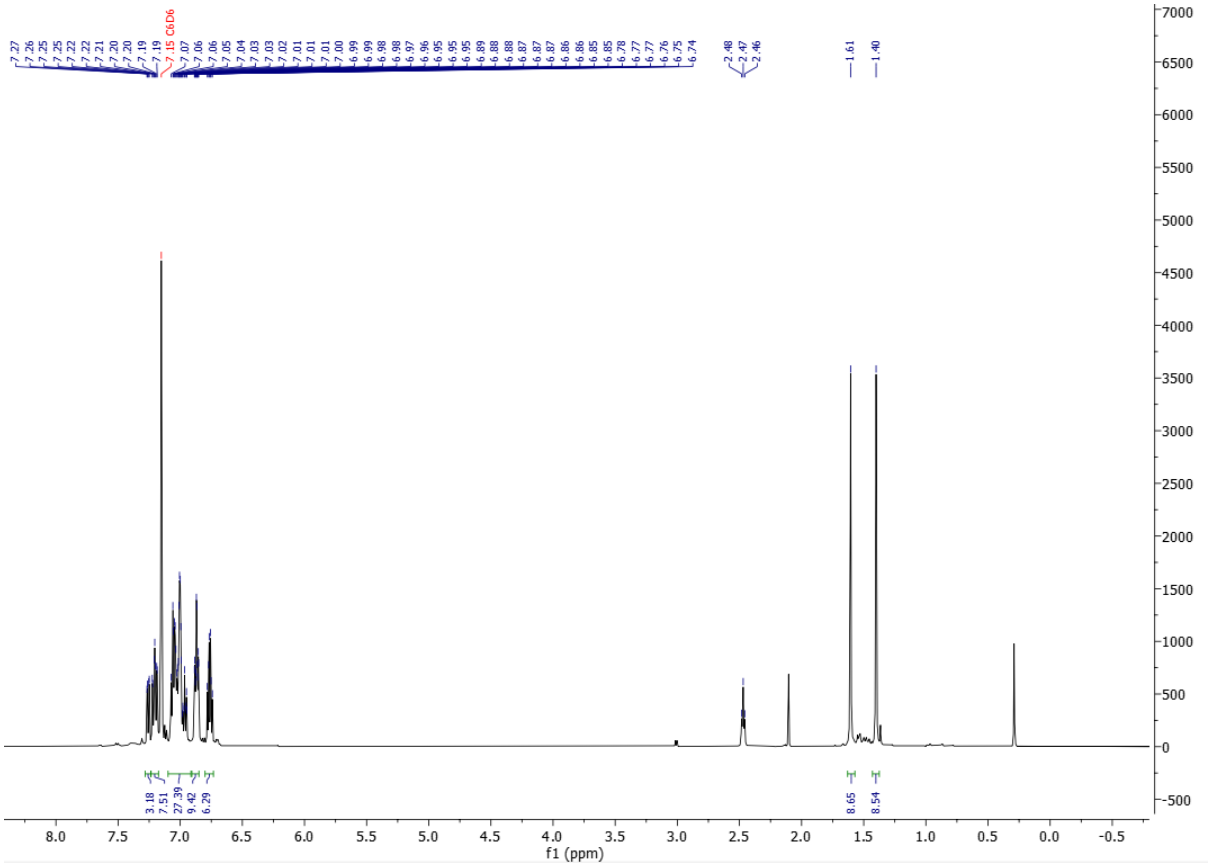
A 8.13: ^{13}C NMR of $(Ph_2P\text{-}xan)_3B\text{-}OH_2$



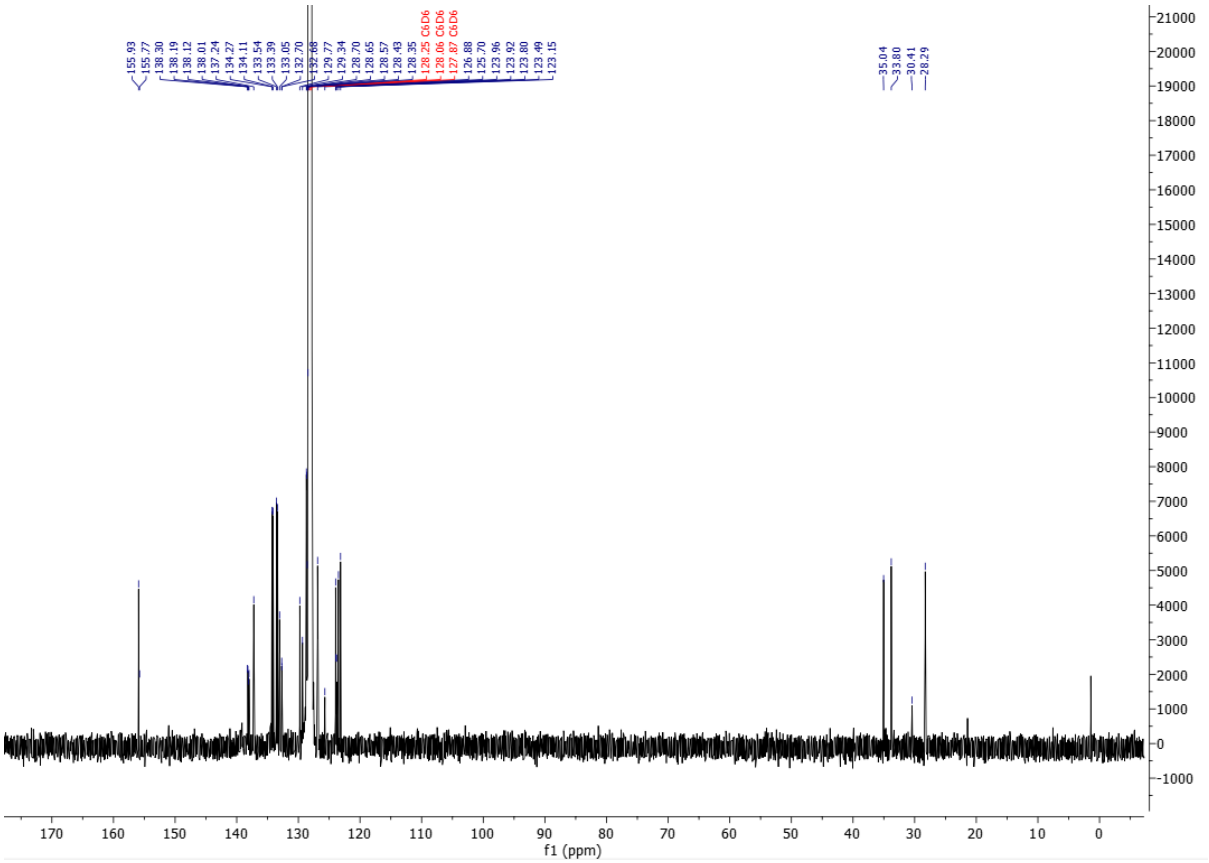
A 8.14: ^{31}P NMR of $(Ph_2P\text{-}xan)_3B\text{-}NH_2CH_3$



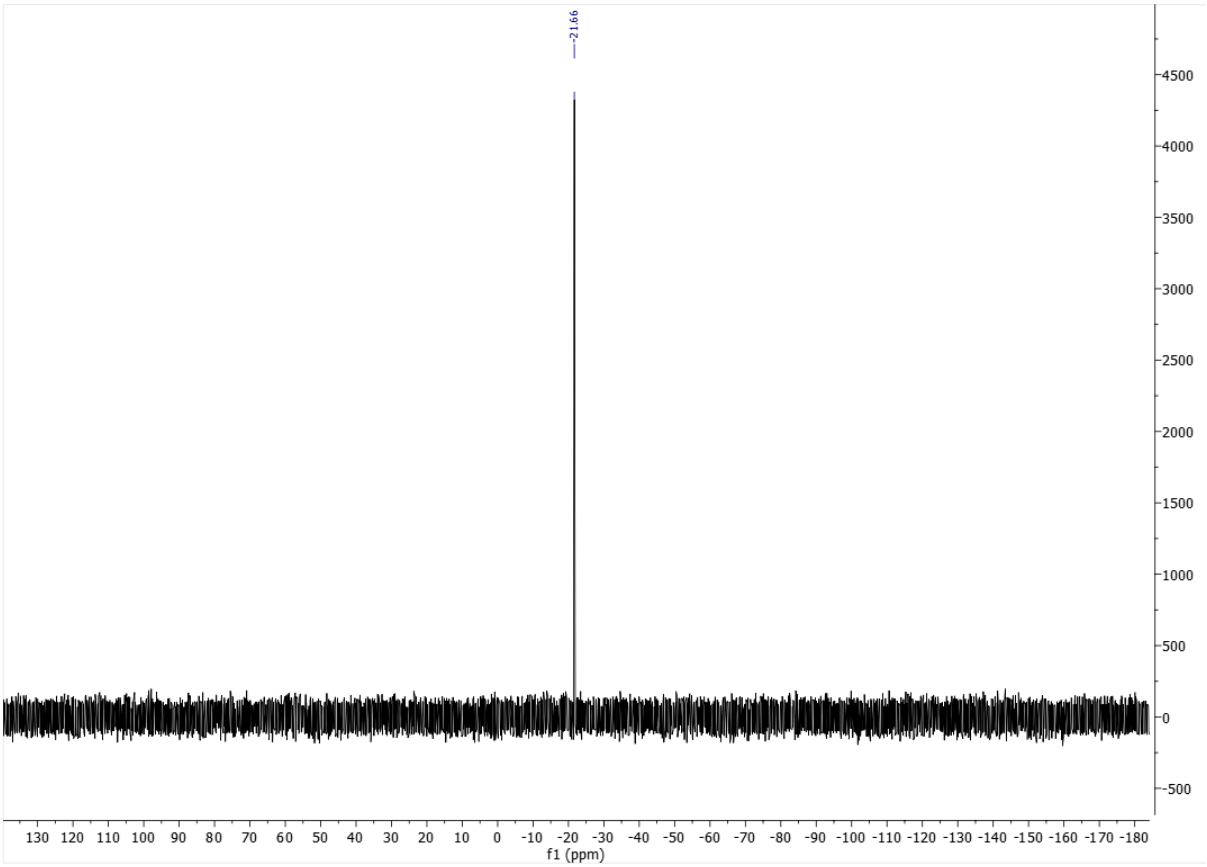
A 8.15: ^{11}B NMR of $(Ph_2P\text{-}xan)_3B\text{-}NH_2CH_3$



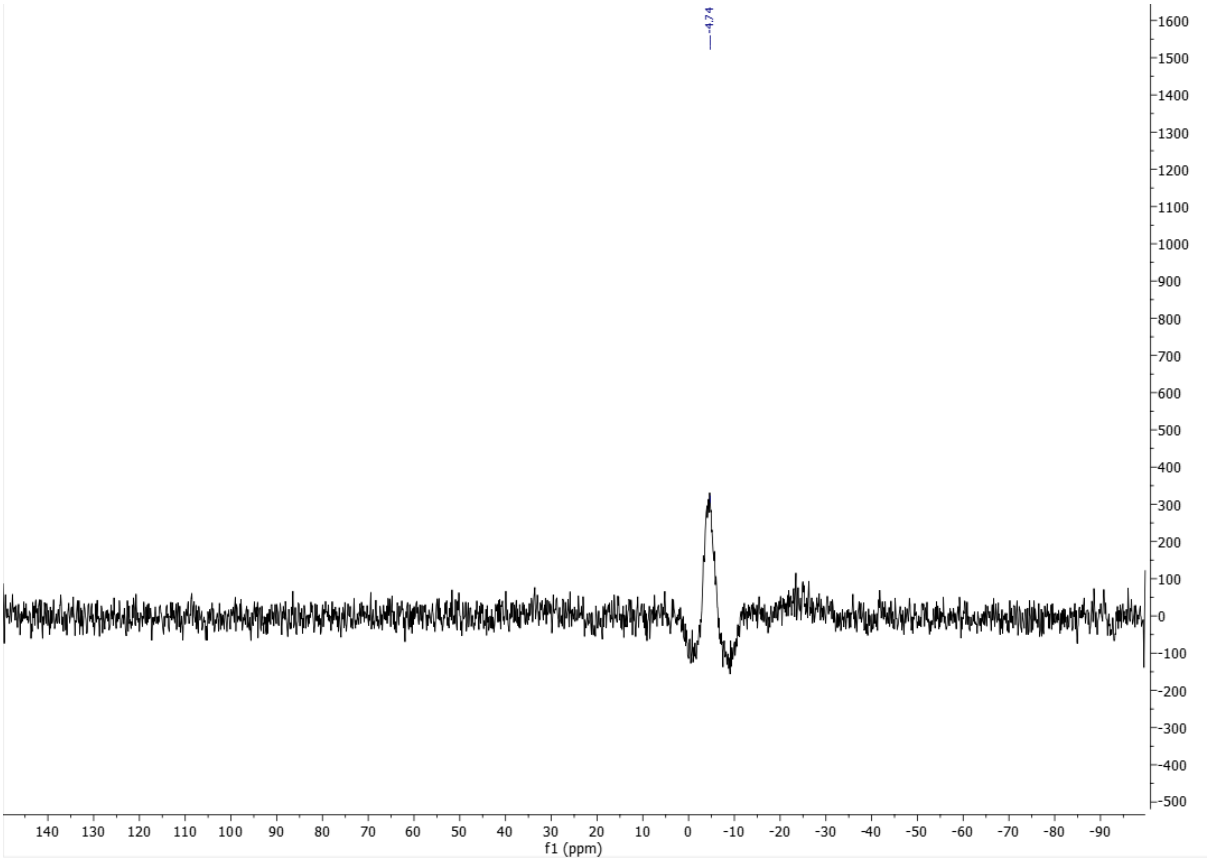
A 8.16: ^{1}H NMR of $(Ph_2P\text{-}xan)_3B\text{-}NH_2CH_3$



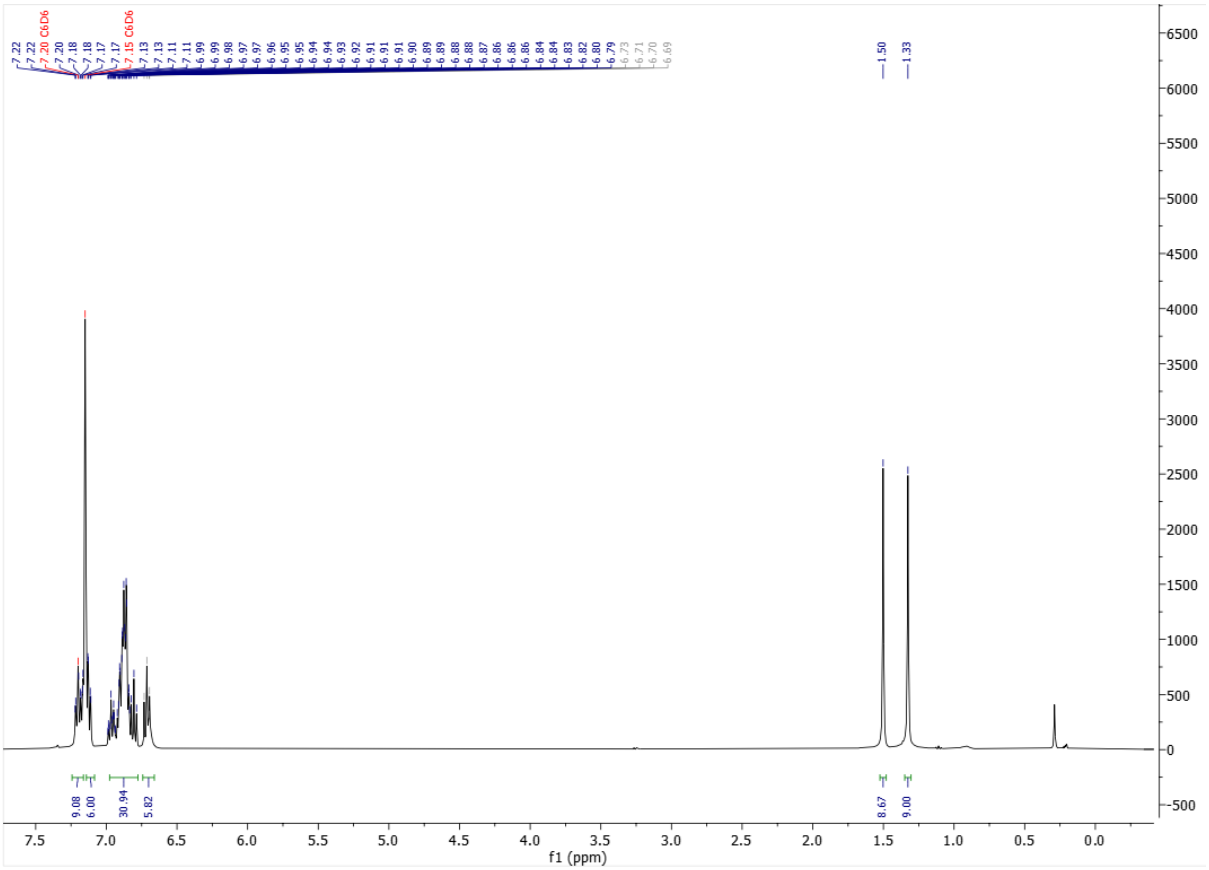
A 8.17: ^{13}C NMR of $(Ph_2P\text{-}xan)_3B\text{-}NH_2CH_3$



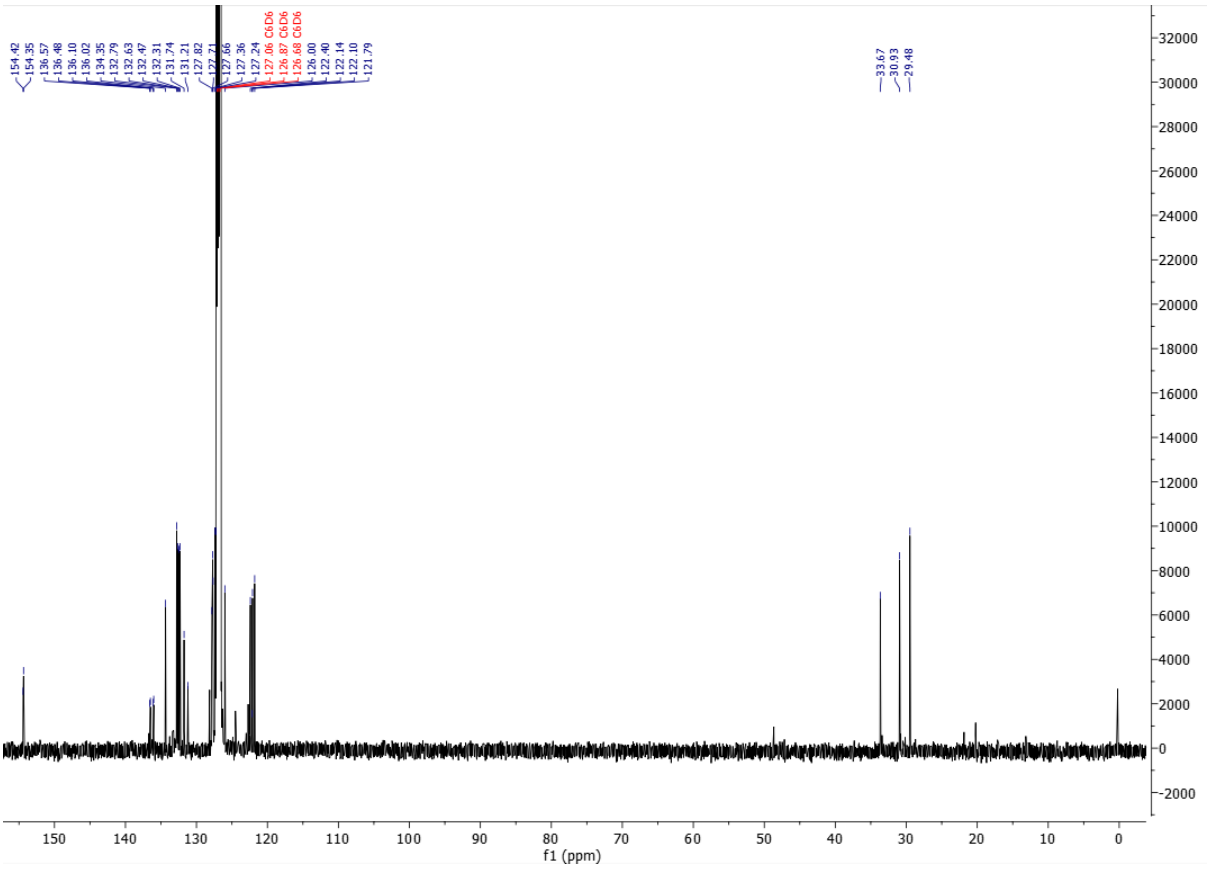
A 8.18: ^{31}P NMR of $(Ph_2P\text{-xan})_3B\text{-}NH_3$



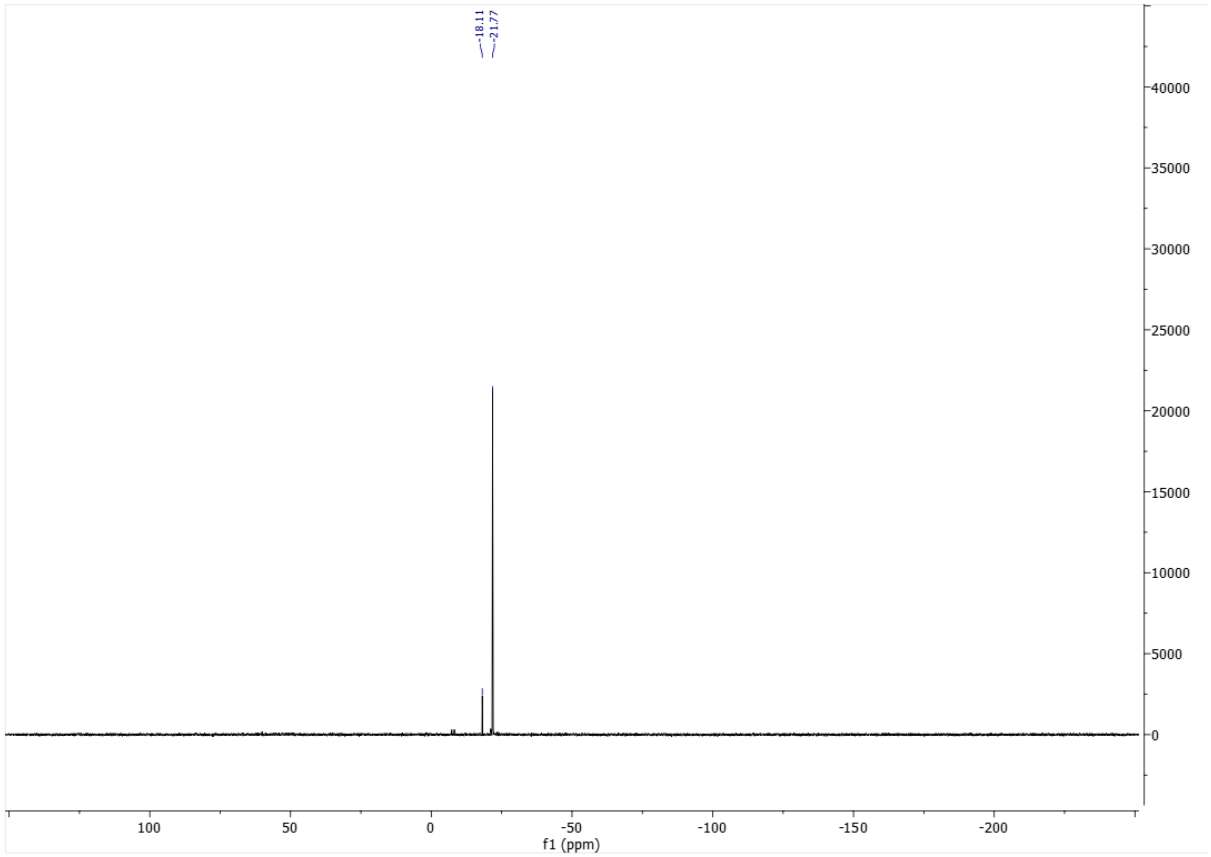
A 8.19: ^{11}B NMR of $(Ph_2P\text{-xan})_3B\text{-}NH_3$



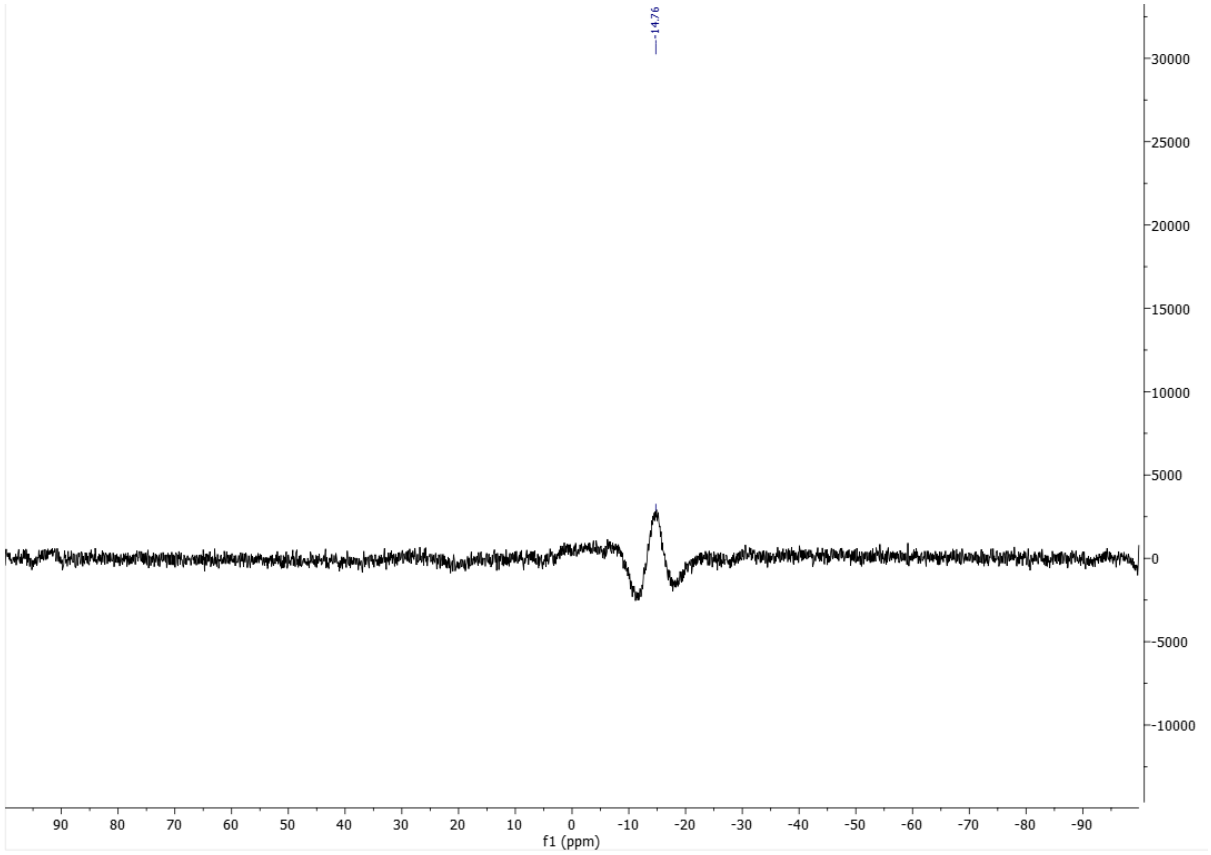
A 8.20: ^{1}H NMR of $(Ph_2P\text{-}xan)_3B\text{-}NH_3$



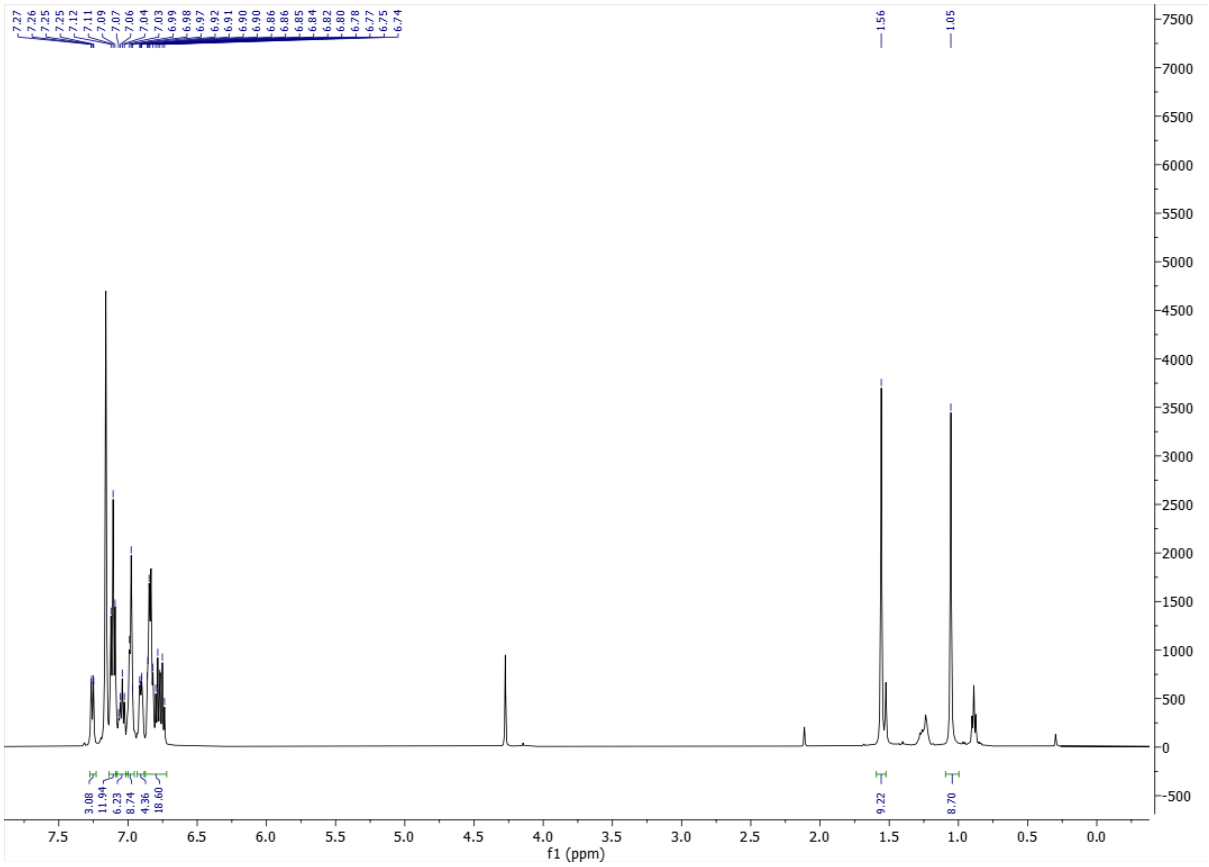
A 8.21: ^{13}C NMR of $(Ph_2P\text{-}xan)_3B\text{-}NH_3$



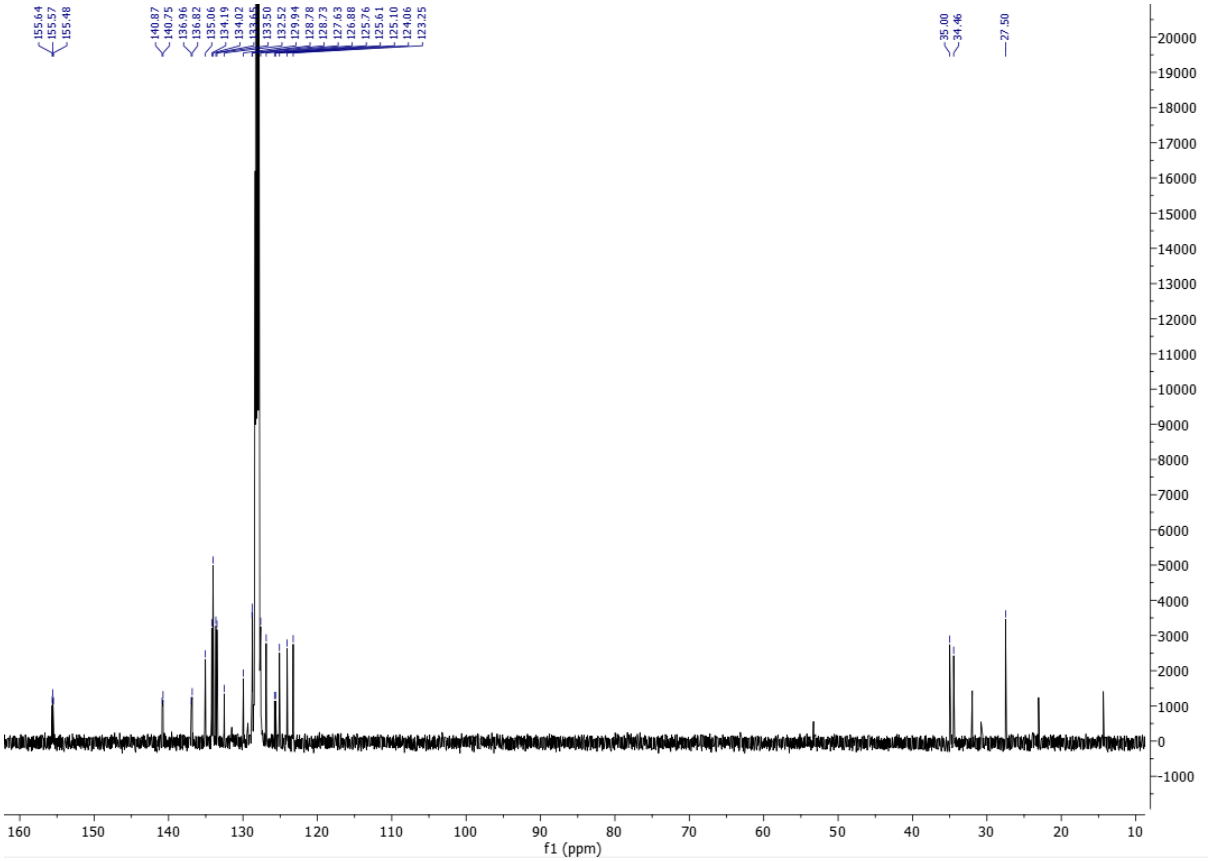
A 8.22: ^{31}P NMR of $(Ph_2P\text{-xan})_3B\text{-CO}$ with a trace $(Ph_2P\text{-xan})_3B$



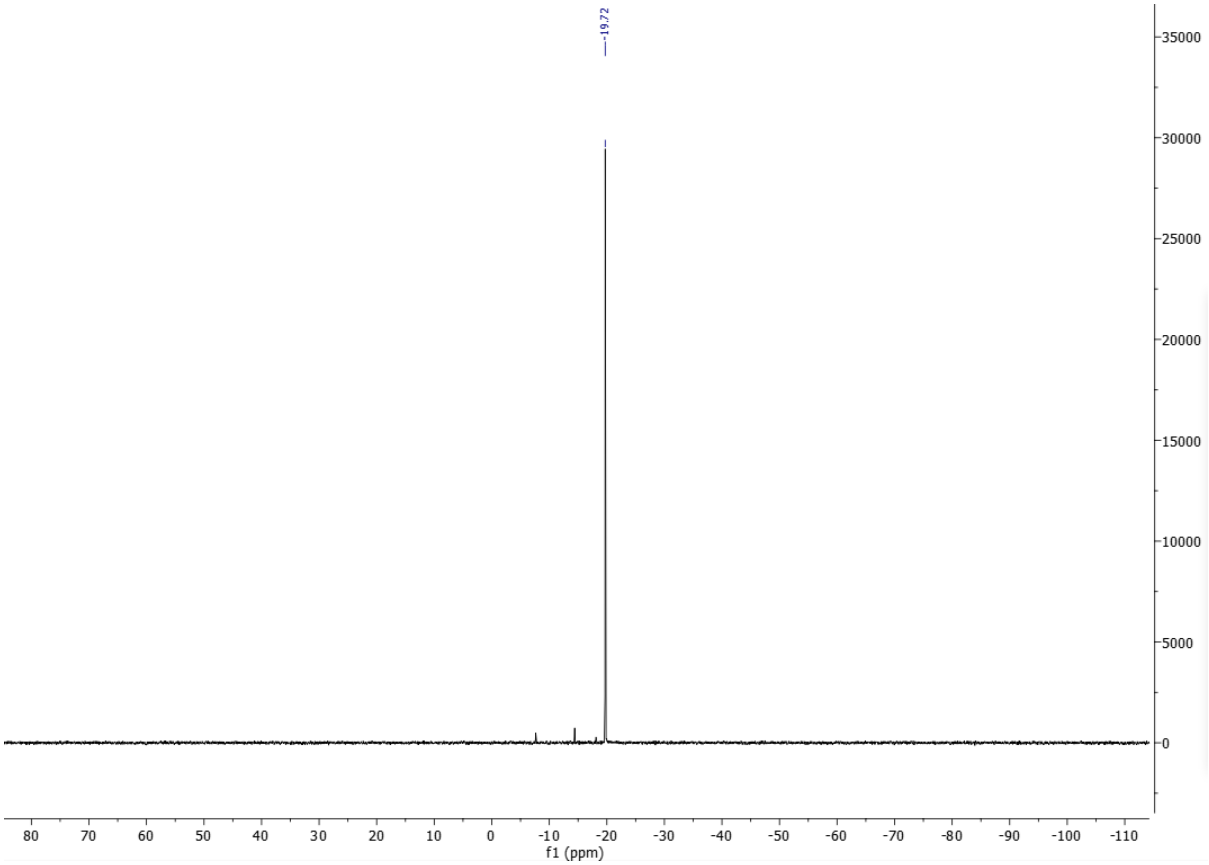
A 8.23: ^{11}B NMR of $(Ph_2P\text{-xan})_3B\text{-CO}$



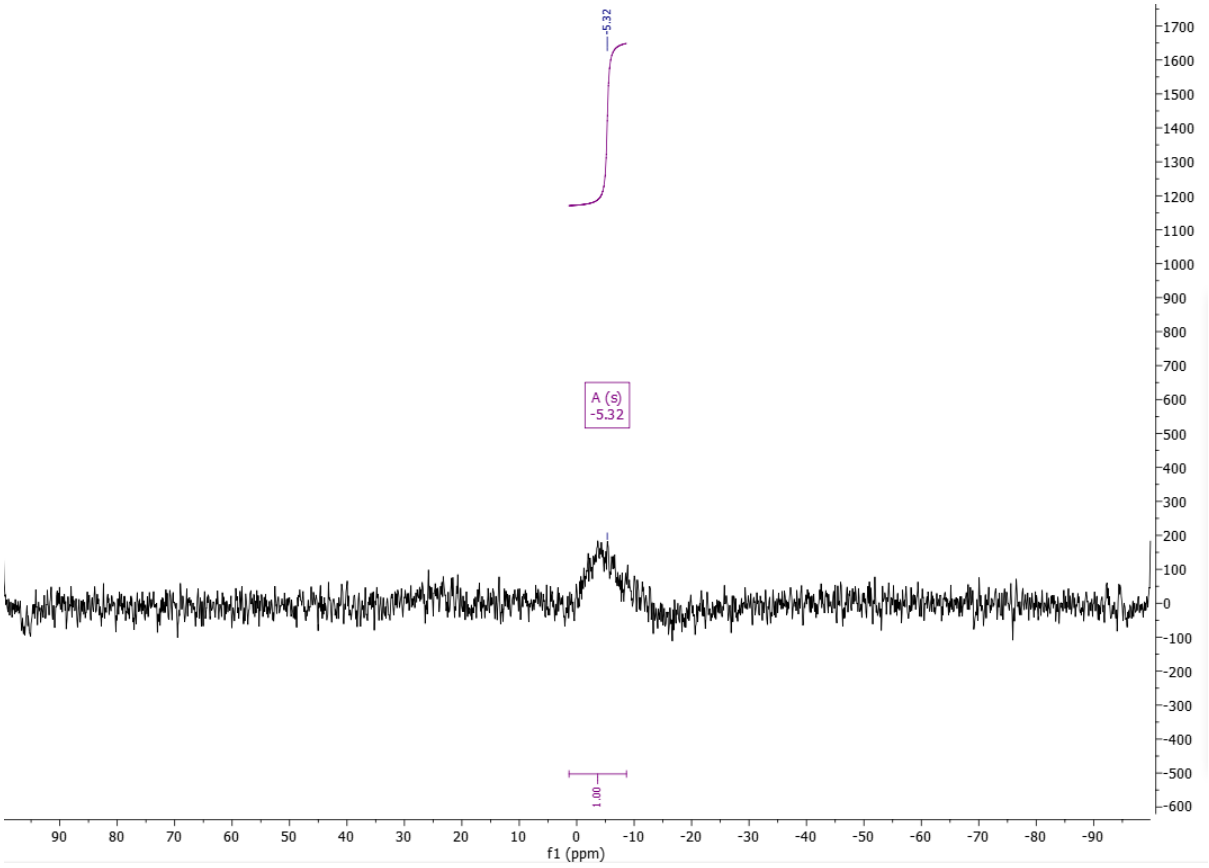
A 8.24: ^{1}H NMR of $(Ph_2P\text{-xan})_3B\text{-CO}$



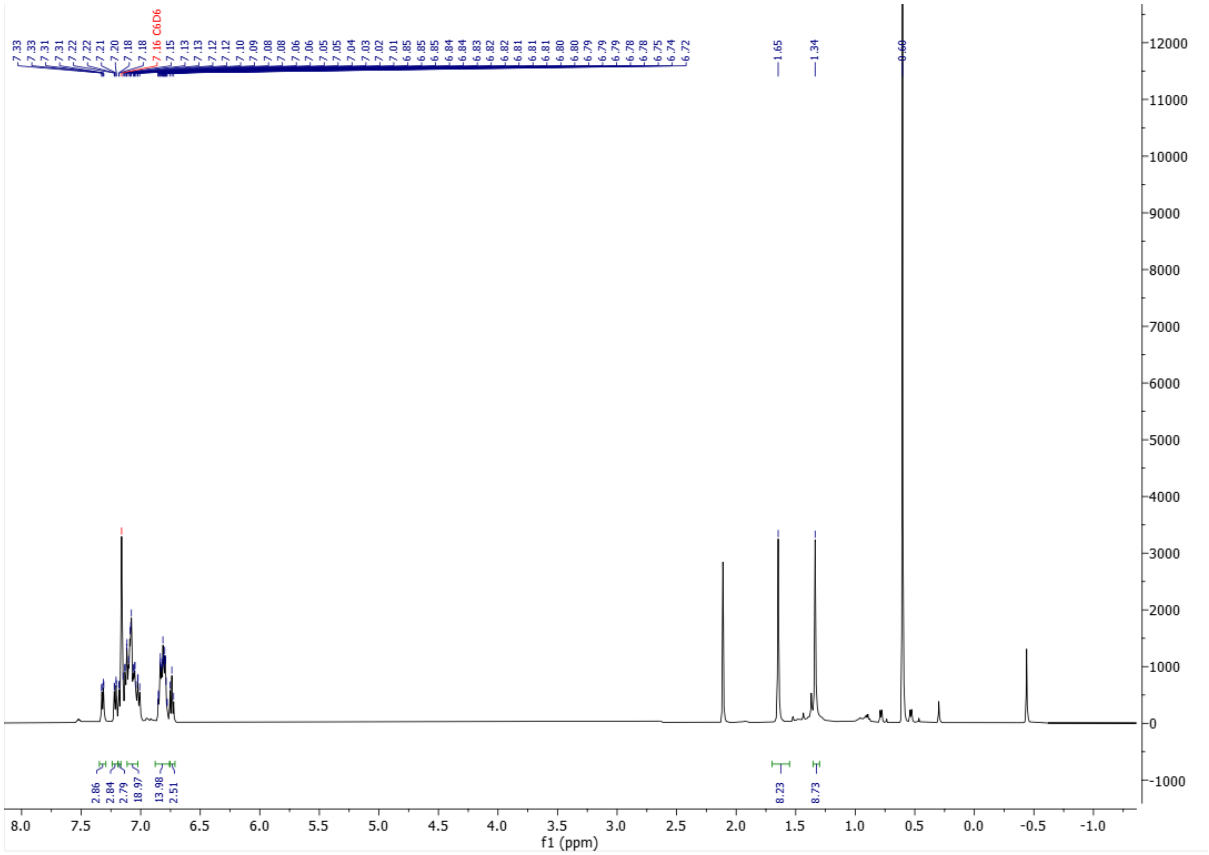
A 8.25: ^{13}C NMR of $(Ph_2P\text{-xan})_3B\text{-CO}$



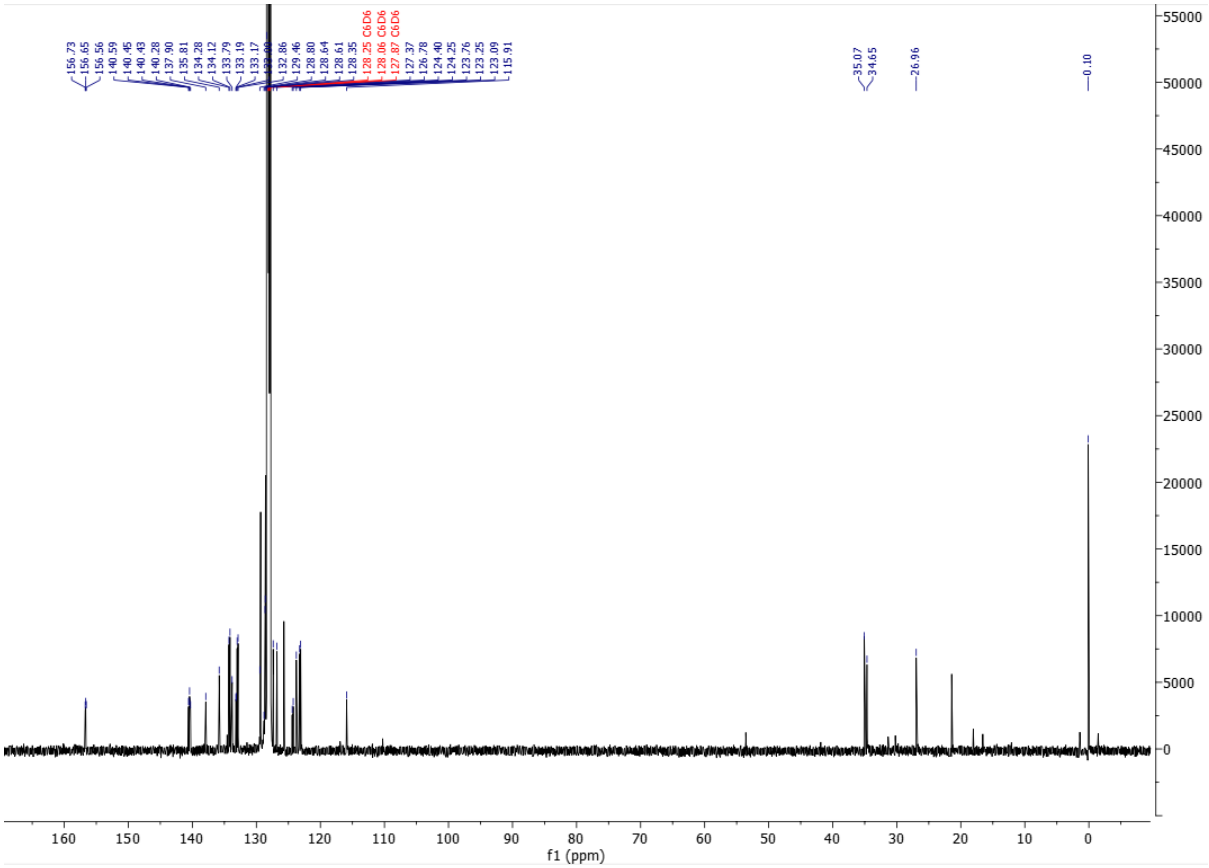
A 8.26: ^{31}P NMR of $(Ph_2P\text{-xan})_3B\text{-}NCCH_3$



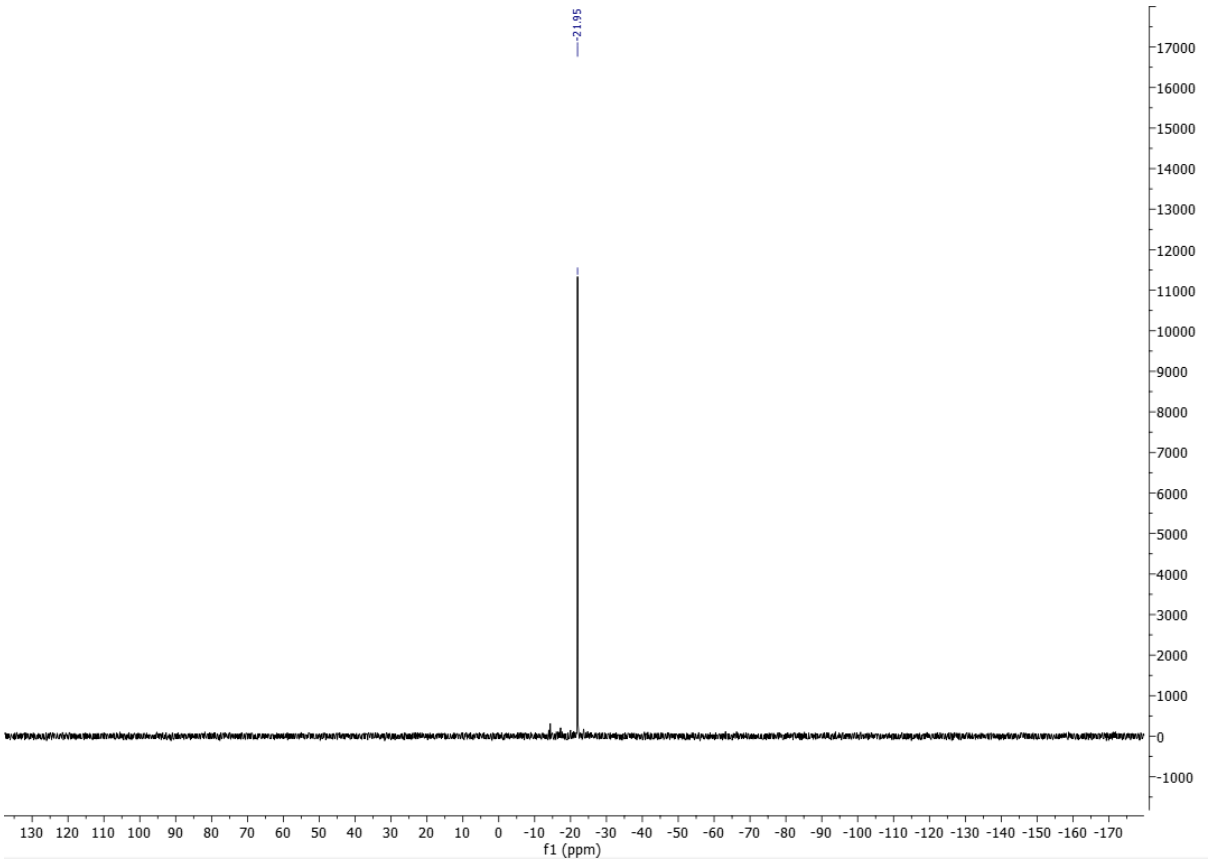
A 8.27: ^{11}B NMR of $(Ph_2P\text{-xan})_3B\text{-}NCCH_3$



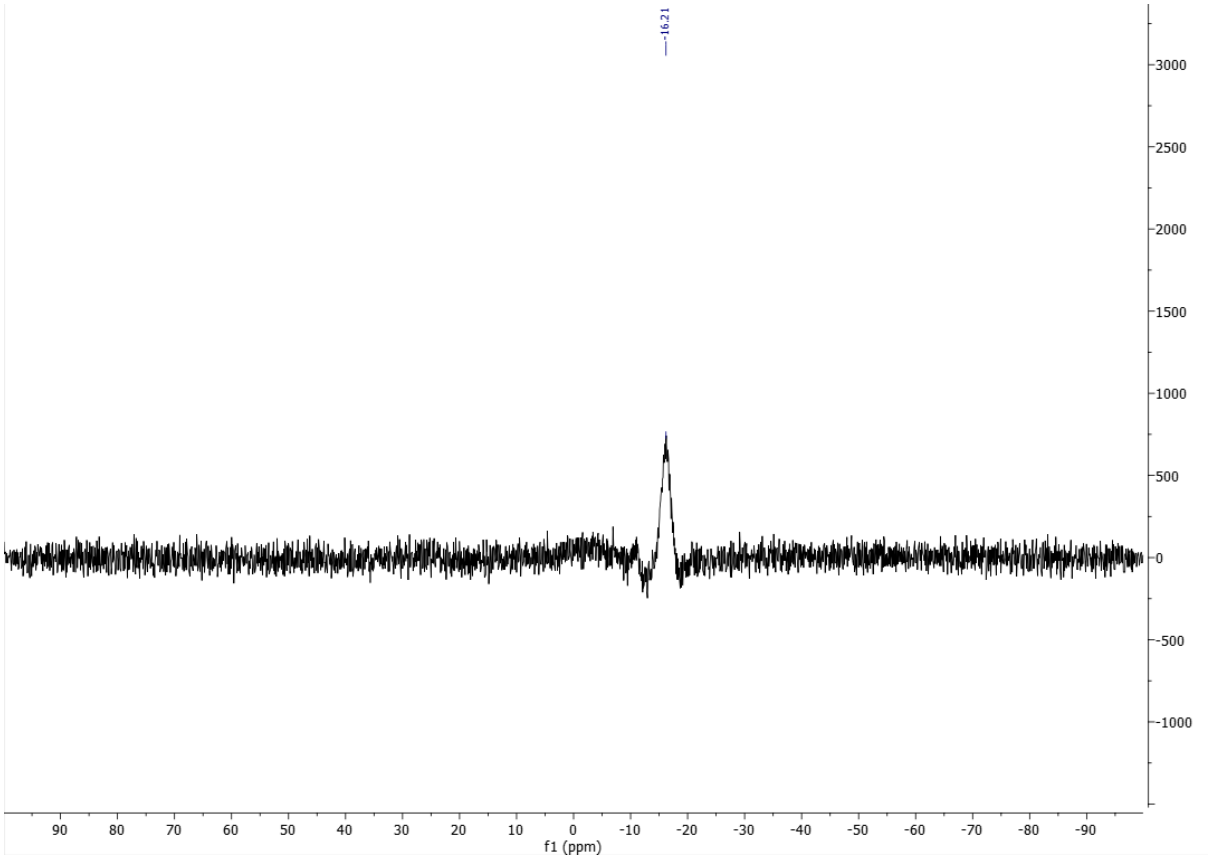
A 8.28: ^{1}H NMR of $(Ph_2P\text{-}xan)_3B\text{-}NCCH_3$



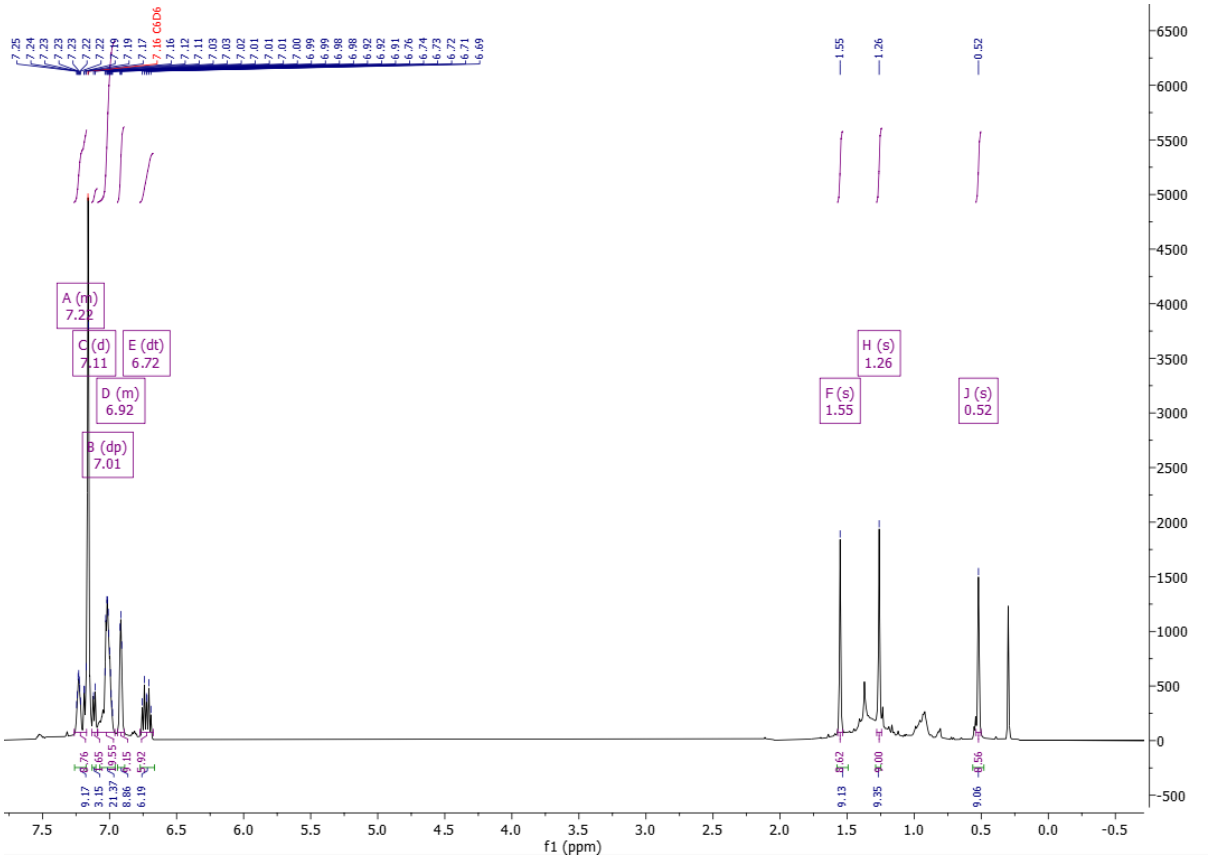
A 8.29: ^{13}C NMR of $(Ph_2P\text{-}xan)_3B\text{-}NCCH_3$



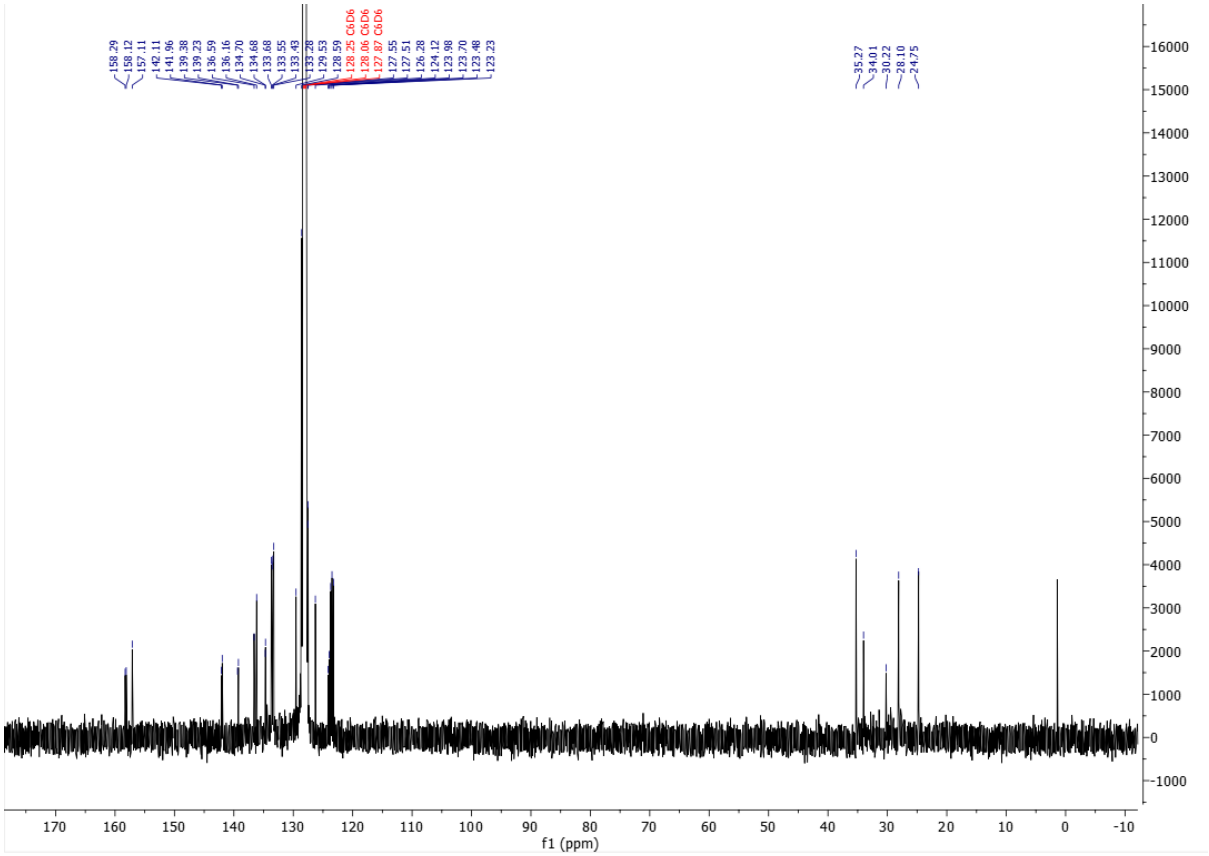
A 8.30: ^{31}P NMR of $(Ph_2P\text{-xan})_3B\text{-}CN^tBu$



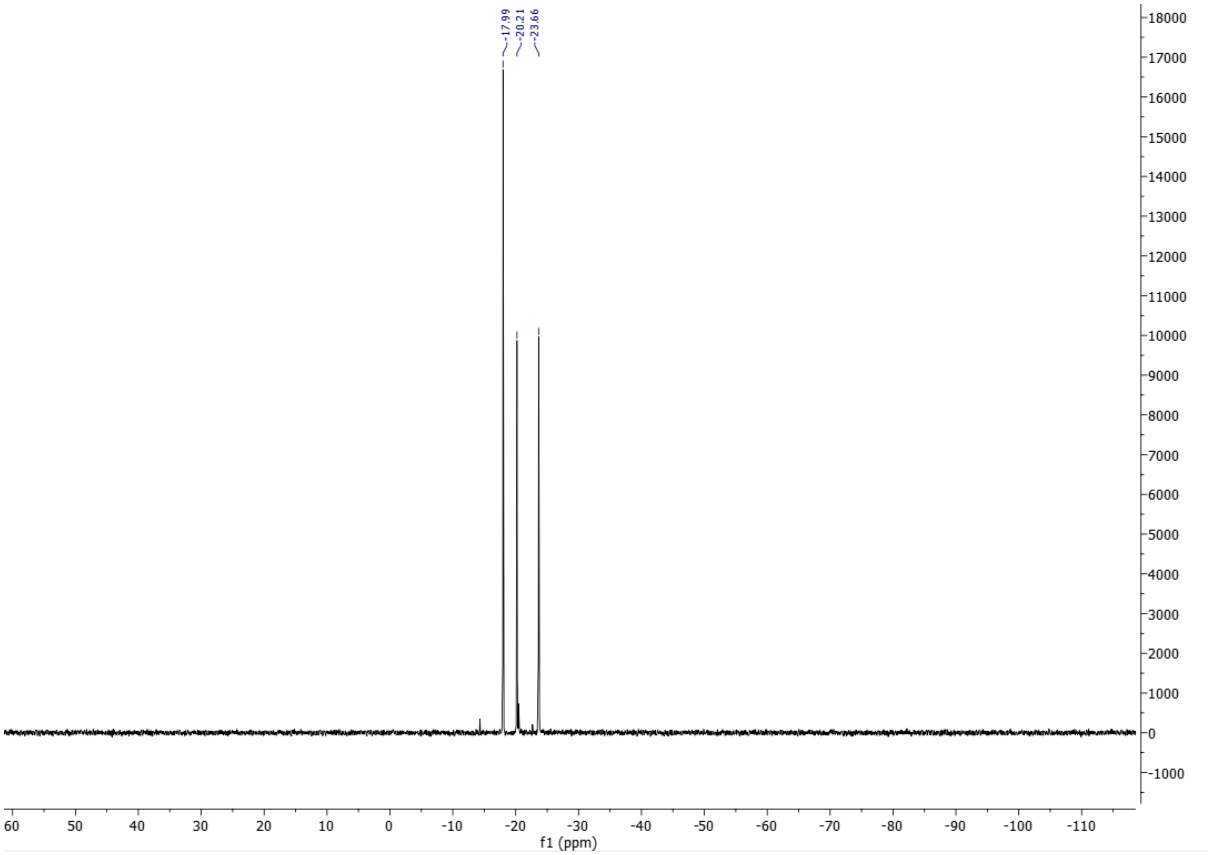
A 8.31: ^{11}B NMR of $(Ph_2P\text{-xan})_3B\text{-}CN^tBu$



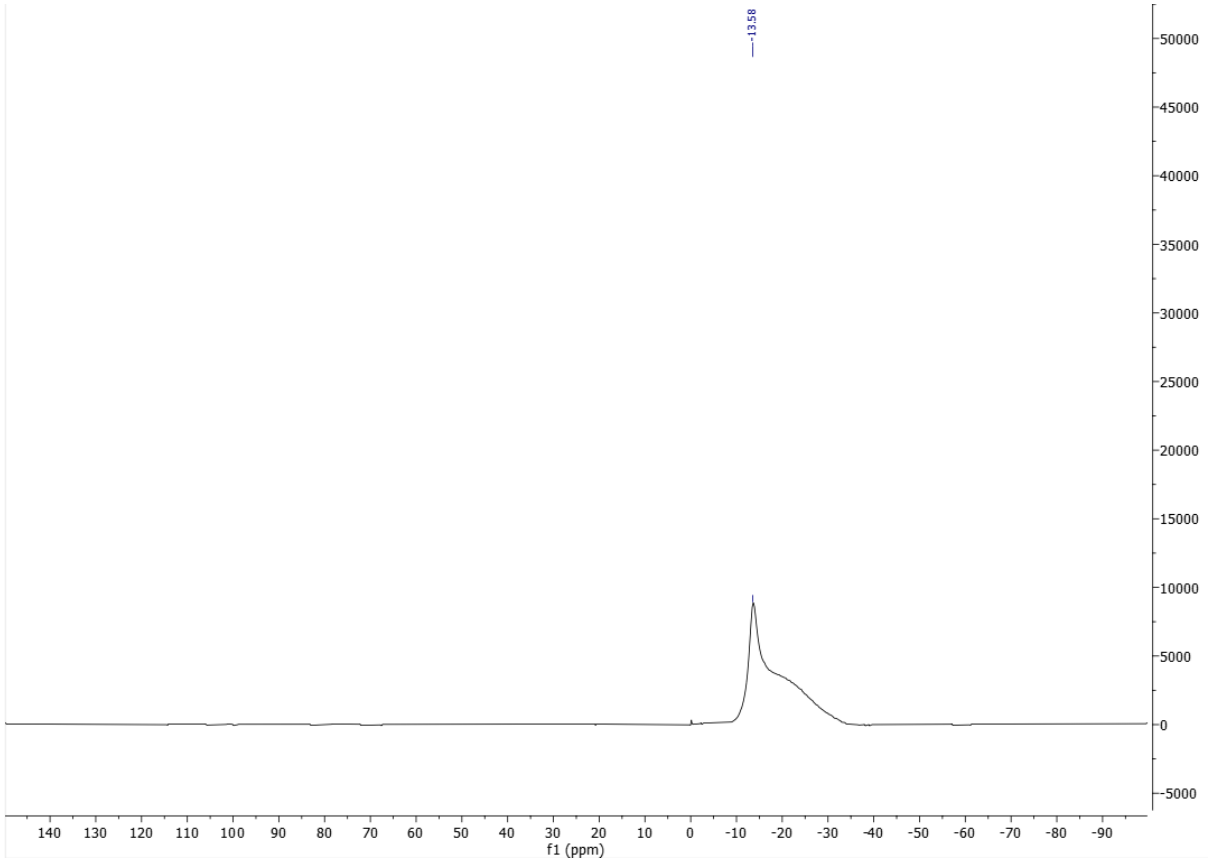
A 8.32: ^{1}H NMR of $(Ph_2P\text{-}xan)_3B\text{-}CN^tBu$



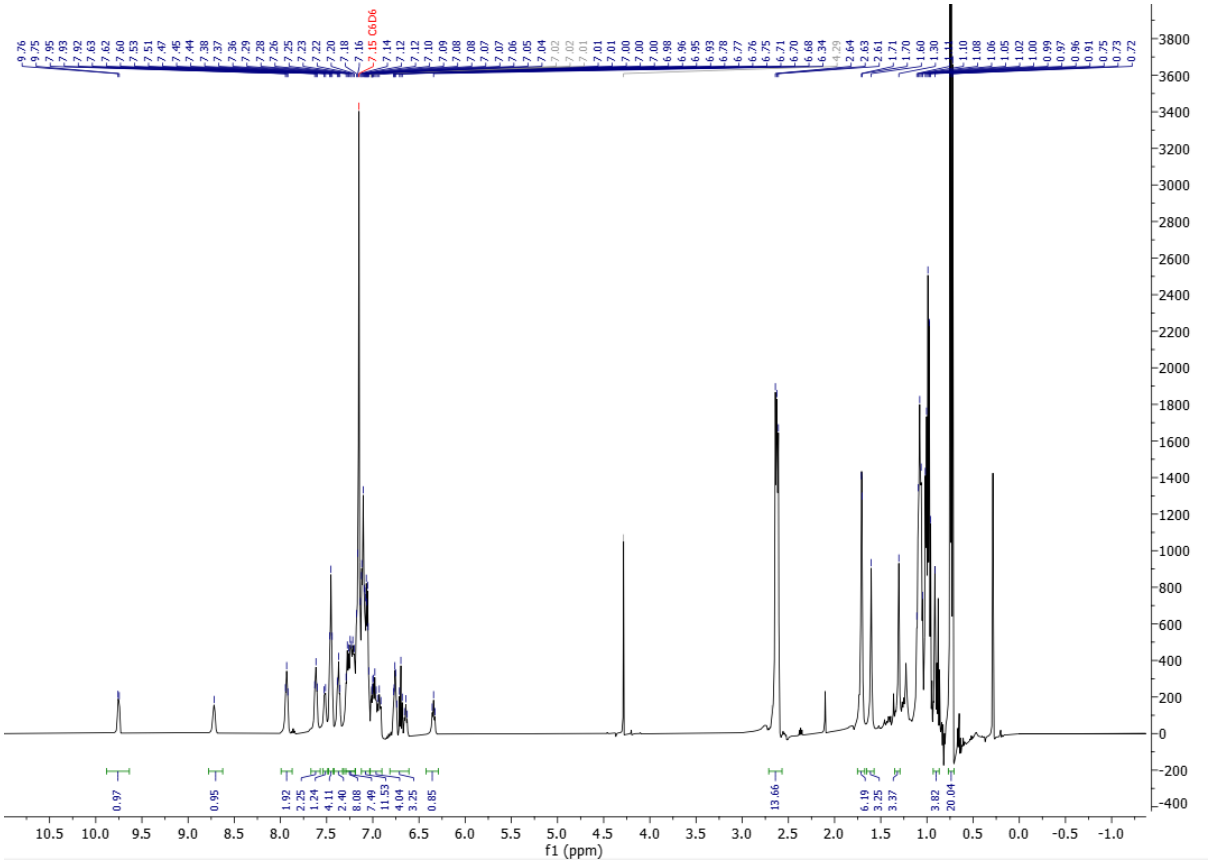
A 8.33: ^{13}C NMR of $(Ph_2P\text{-}xan)_3B\text{-}CN^tBu$



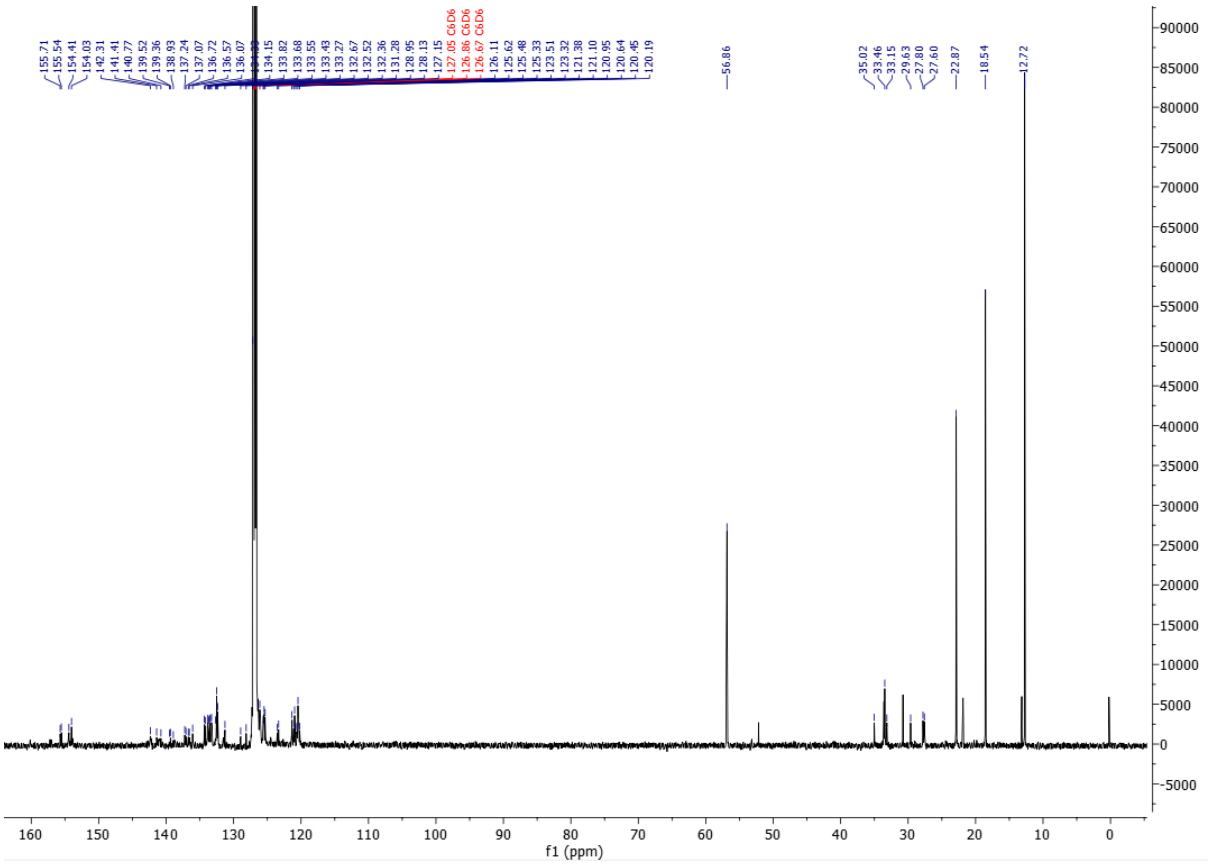
A 8.34: ^{31}P NMR of $(Ph_2P\text{-xan})_3B\text{-CN}$



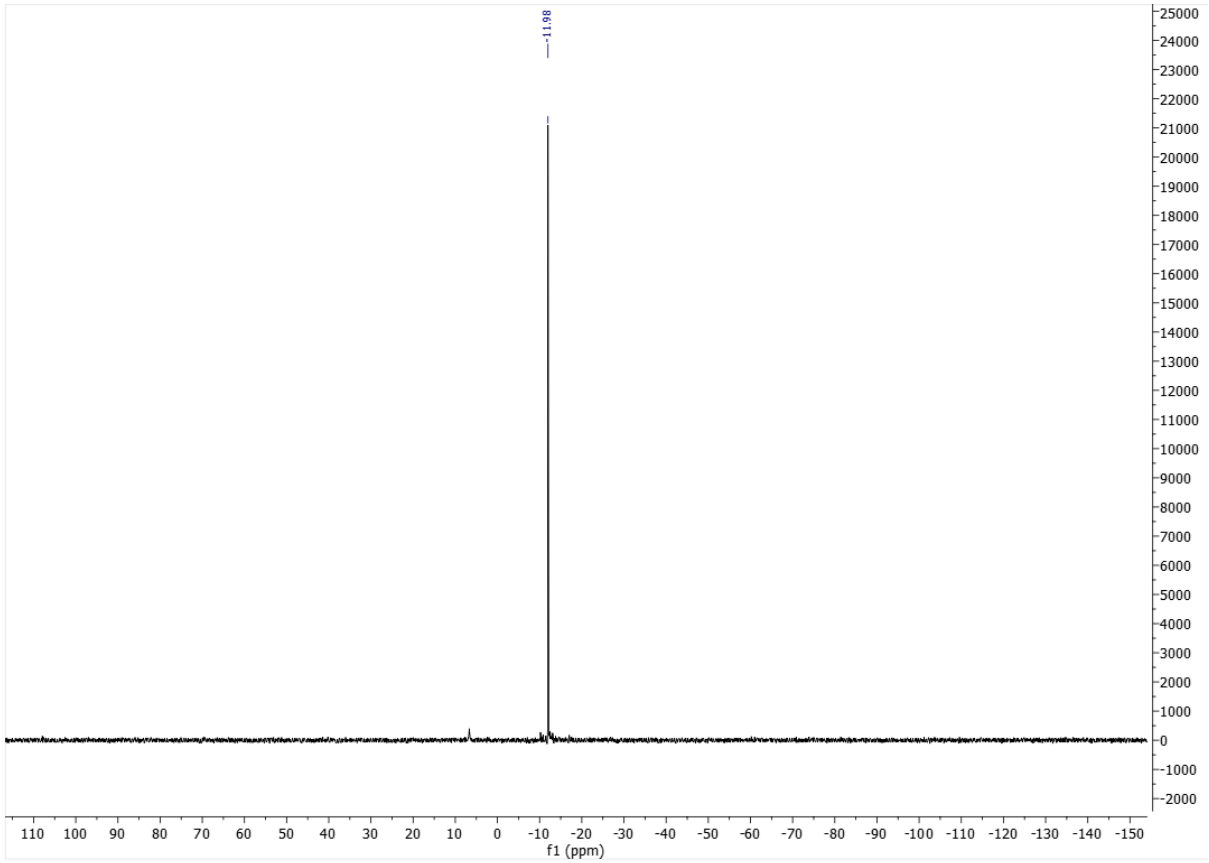
A 8.35: ^{11}B NMR of $(Ph_2P\text{-xan})_3B\text{-CN}$



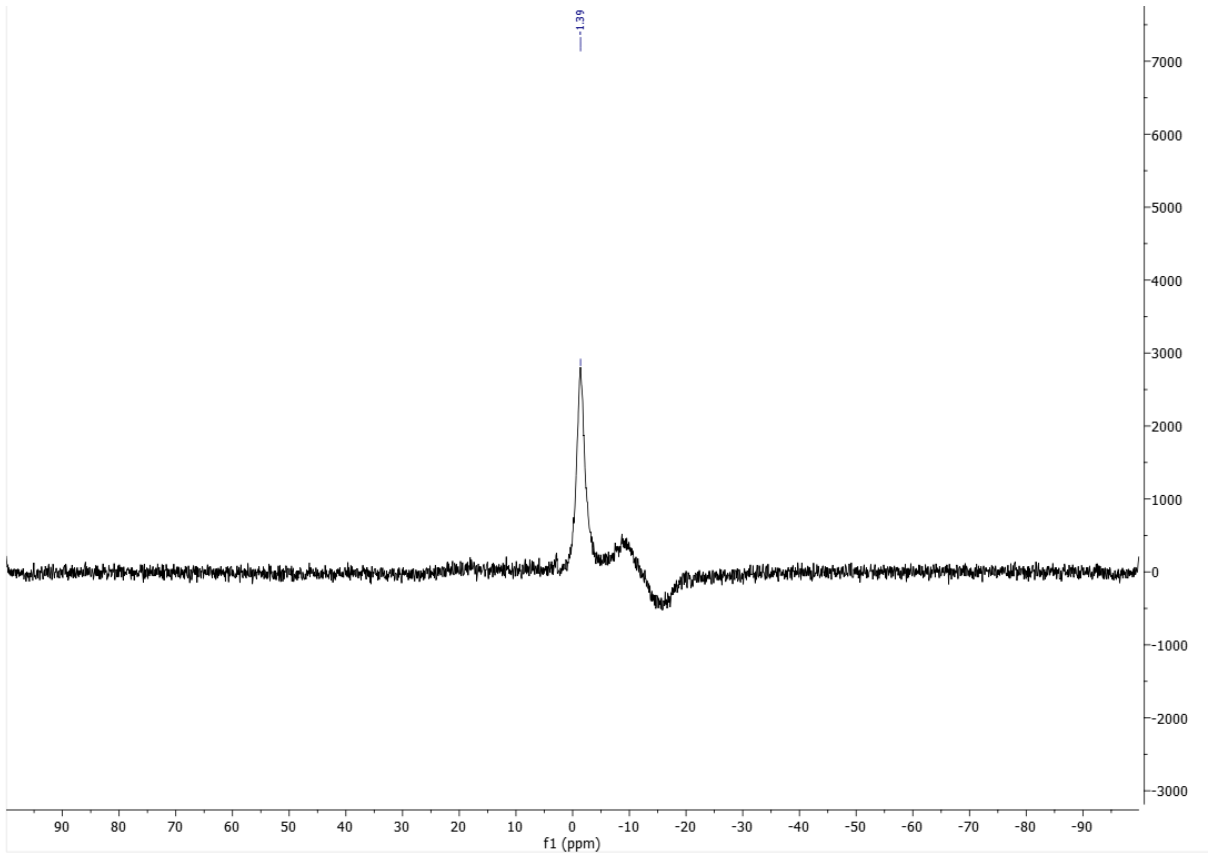
A 8.36: ^{1}H NMR of $(Ph_2P\text{-}xan)_3B\text{-}CN$



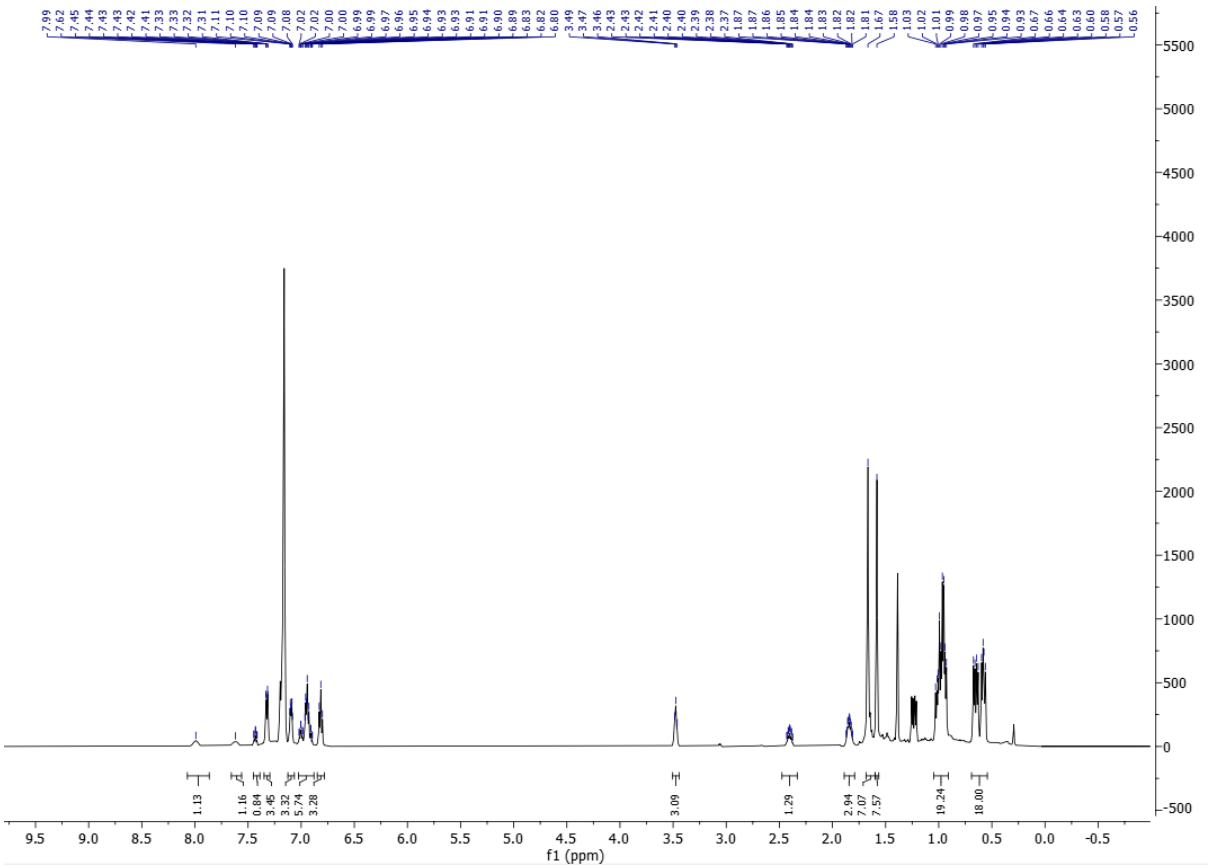
A 8.37: ^{13}C NMR of $(Ph_2P\text{-}xan)_3B\text{-}CN$



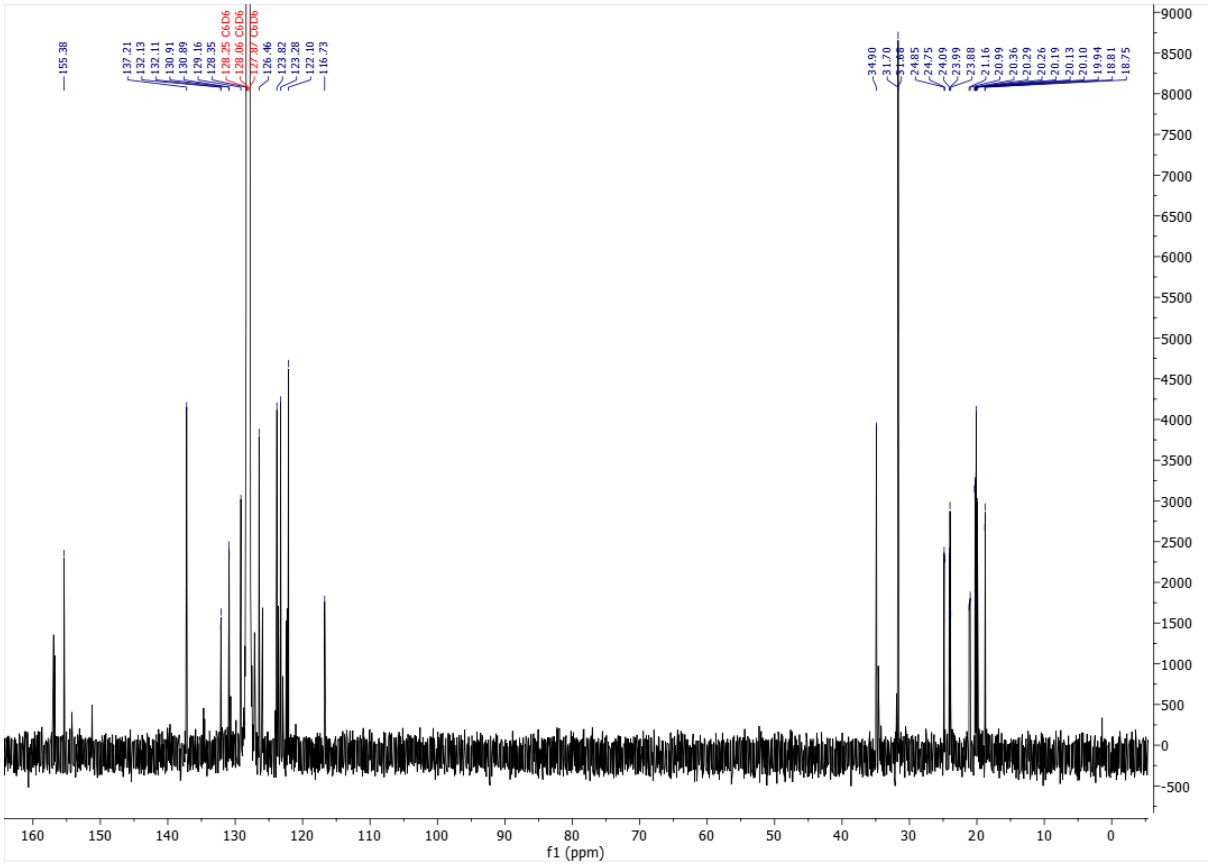
A 8.38: ^{31}P NMR of ($^{i}Pr_2P$-xan)$_3$B- NH_2CH_3



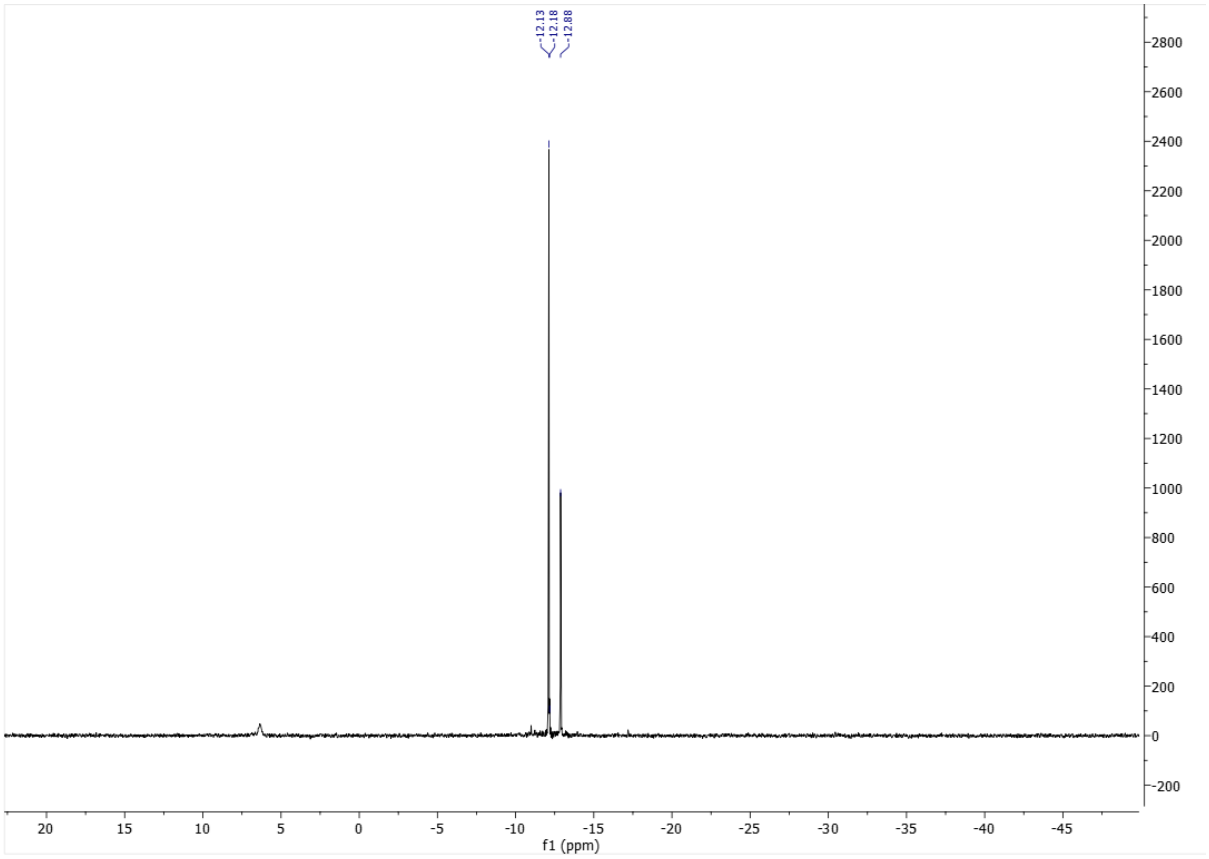
A 8.39: ^{11}B NMR of ($^{i}Pr_2P$-xan)$_3$B- NH_2CH_3



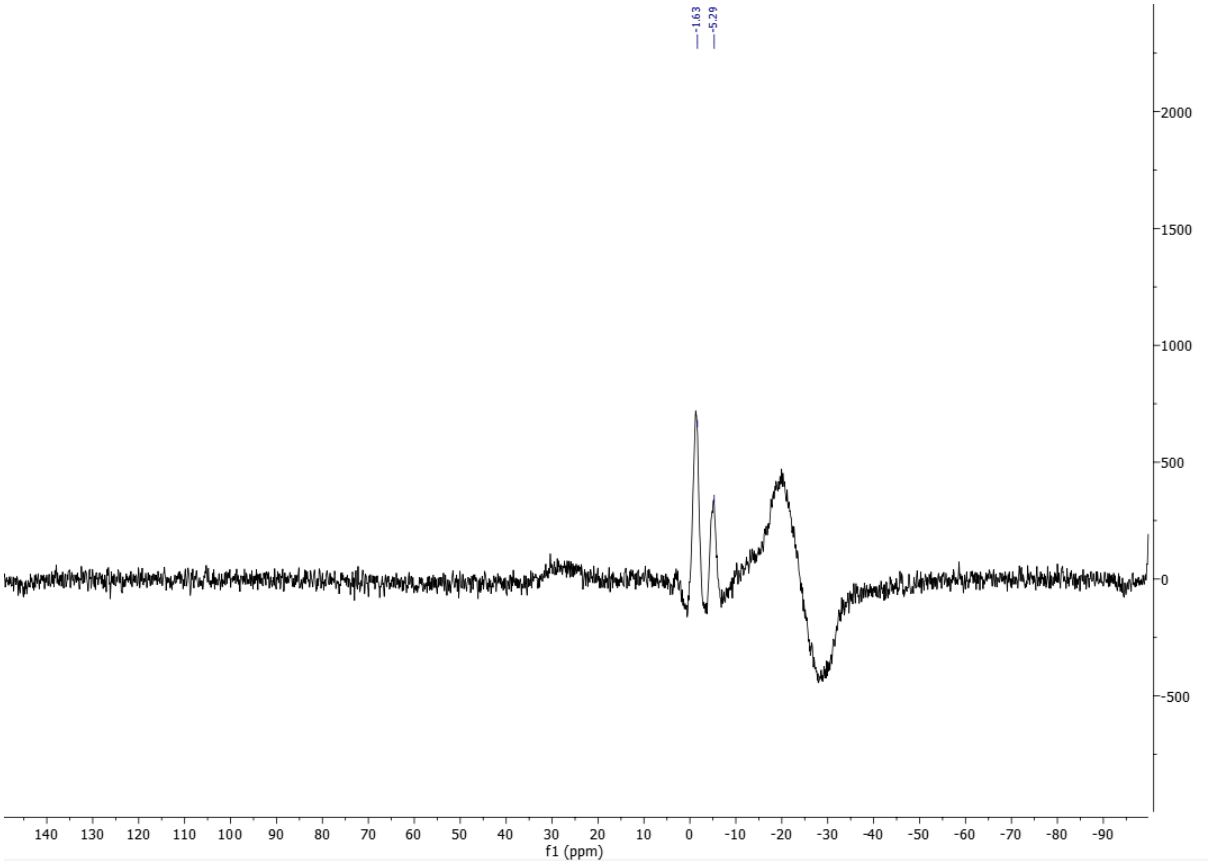
A 8.40: ^{1}H NMR of ($^{i}Pr_2P$-xan)$_3$B- NH_2CH_3



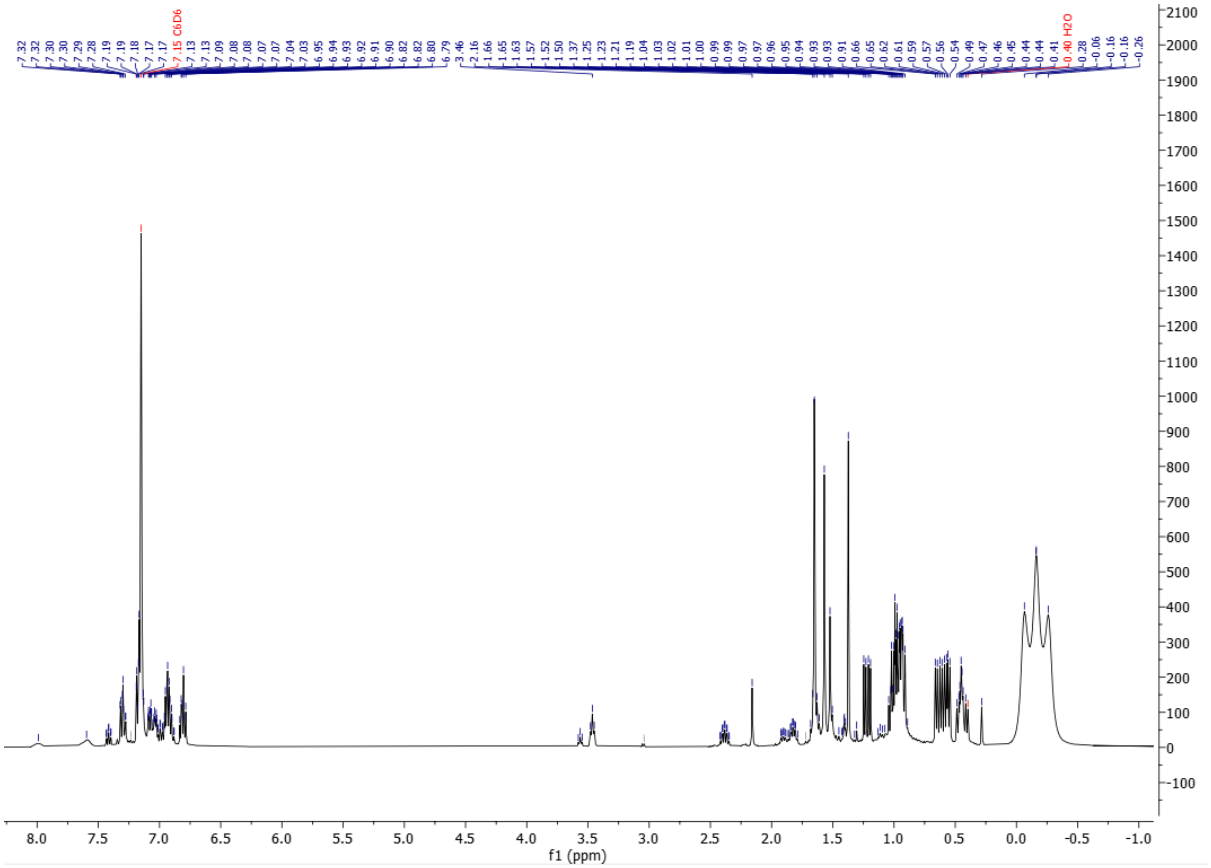
A 8.41: ^{13}C NMR of ($^{i}Pr_2P$-xan)$_3$B- NH_2CH_3



A 8.42: ^{31}P NMR of $(^{i}Pr_2P\text{-xan})_3B\text{-}NH_2CH_3$/$(^{i}Pr^{2}P\text{-xan})_3B\text{-}NH_3$

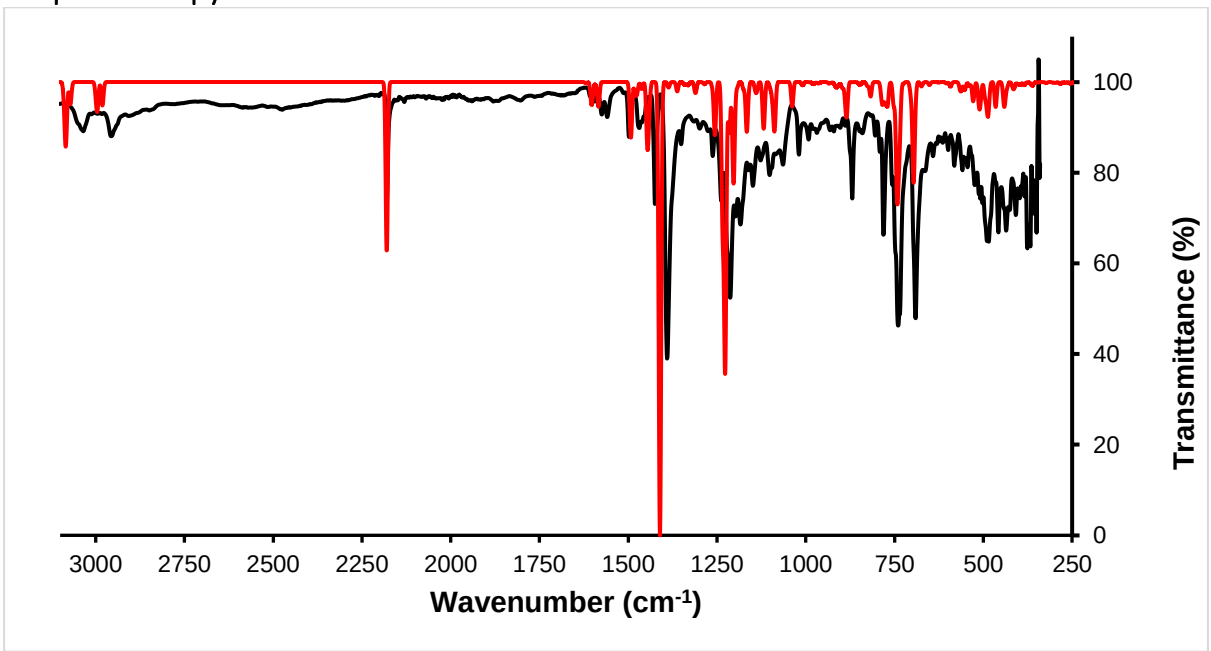


A 8.43: ^{11}B NMR of $(^{i}Pr_2P\text{-xan})_3B\text{-}NH_2CH_3$/$(^{i}Pr^{2}P\text{-xan})_3B\text{-}NH_3$

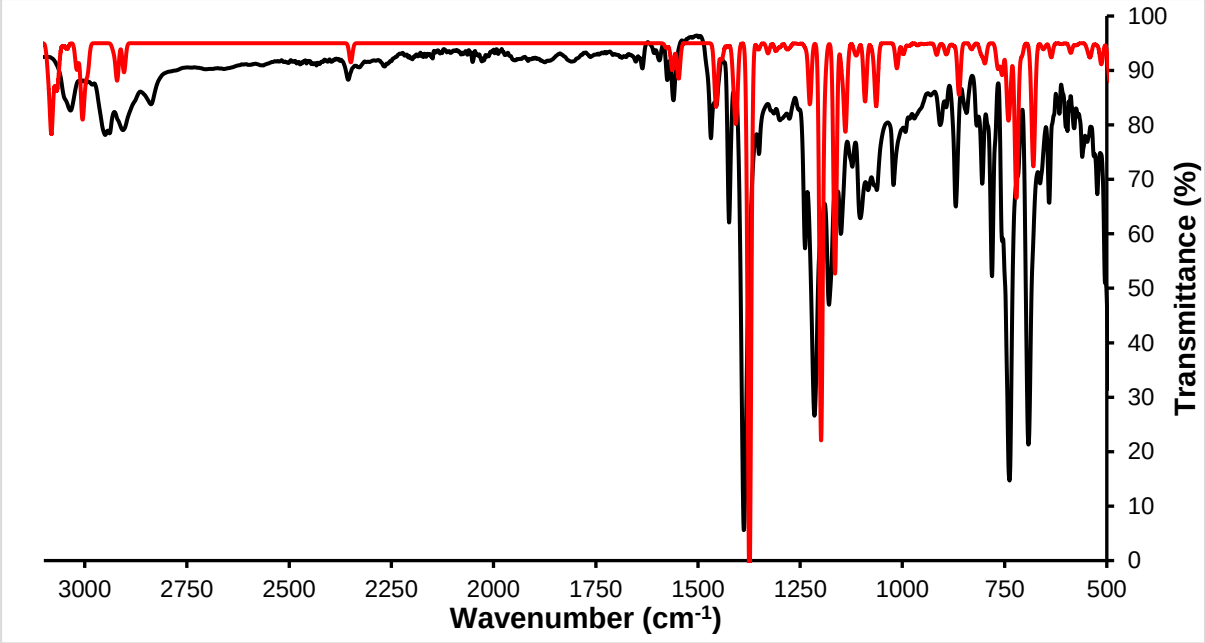


A 8.44: ^{1}H NMR of ($^{i}Pr_2$P-xan)$_3$B-NH_2CH_3/($^{i}Pr^2$P-xan)$_3$B-NH_3

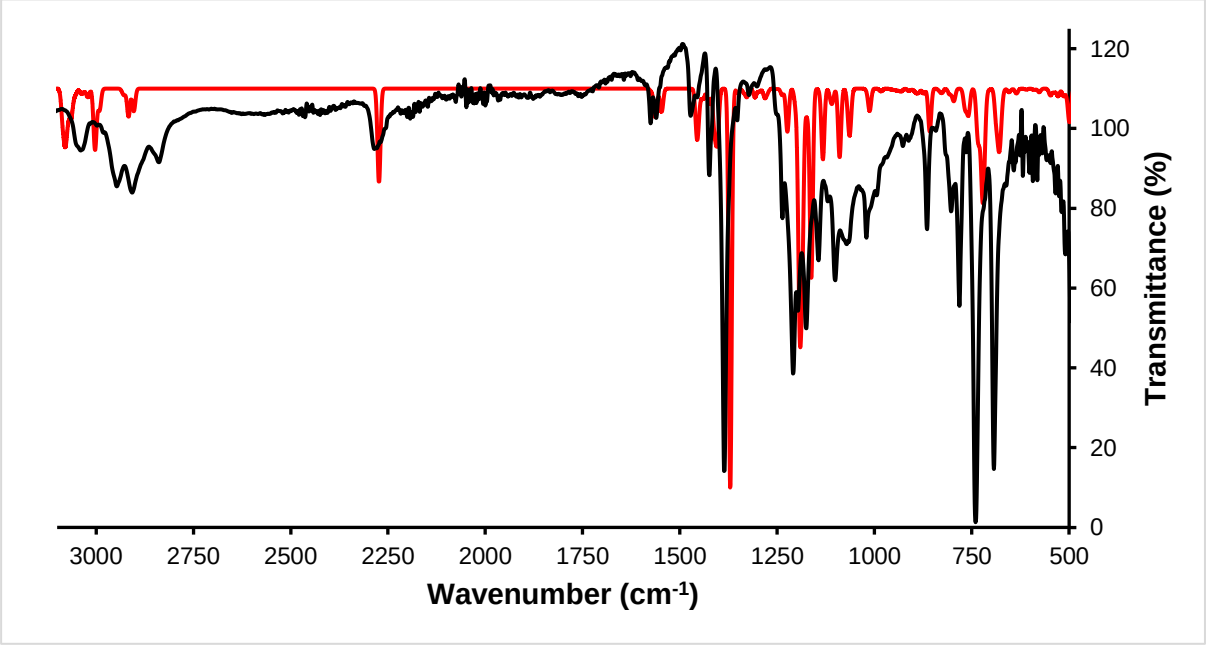
IR spectroscopy



A 8.45: FT-IR spectra of (Ph_2P-xan)$_3$B-CO complex in black and calculated spectra in red (R2scan functional details below, 0.990 linear scale factor applied). C-O stretch at 2178.7 cm^{-1}.



A 8.46: FT-IR spectra of $(Ph_2P\text{-xan})_3B\text{-}NCMe$ complex in black and calculated spectra in red (R2scan functional details below, 0.975 linear scale factor applied). C-N stretch at 2356.0 cm^{-1}.



A 8.47: FT-IR spectra of $(Ph_2P\text{-xan})_3B\text{-}CN^tBu$ complex in black and calculated spectra in red (R2scan functional details below, 0.965 linear scale factor applied). C-N stretch at 2284.5 cm^{-1}.

Coordinates

AcN

Energy: -132.8614743

C	8.54863607	11.25006612	16.21551116
H	8.91755462	10.58463537	17.00079088
H	8.77593108	10.81176141	15.23987396
H	9.05405682	12.21605790	16.29900984
N	5.97627990	11.56653528	16.46500637
C	7.11782369	11.42844533	16.35372500

CO

Energy: -113.3860758

O	6.97995094	11.42400442	16.42674429
C	5.85733906	11.54945558	16.46408571

Cage

Energy: -4404.017809

P	6.57410736	12.88251814	13.23258515
P	6.99463127	13.57496747	19.38885877
P	5.65971008	7.73766833	16.66481810
O	5.57217954	14.21807436	16.89201615
O	5.17325378	9.91546791	18.55134917
O	4.82289733	10.70234202	14.12747133
C	4.54013695	14.25946952	15.96962098
C	5.85509118	15.38064983	17.57731934
C	5.14140423	16.66835670	15.55325727
C	4.27780103	15.44546265	15.27908455
C	5.16552876	8.71574476	19.23474711
C	5.55485351	16.62566987	17.01525648
C	4.46036698	10.96687930	19.10185779
C	3.95700386	11.93035600	18.21095490
C	6.47529334	15.25269703	18.82778072
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C	4.30756433	11.04768093	20.48837442
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C	3.82660108	9.97724067	14.74283438
C	5.00553091	10.58899397	12.77299468
C	5.38907083	7.55655620	18.47742069
C	5.81275591	11.57318086	12.17578899
C	7.31643284	13.88005746	21.17963985
C	6.71039807	16.42037169	19.55958444
H	7.18682880	16.35054803	20.53274473
C	5.78048306	17.76196159	17.79015347
H	5.53912638	18.74265432	17.39451747
C	3.48388462	10.40871105	16.03824295
C	6.63753279	14.27140583	12.02074502
C	8.35396139	12.38597557	13.28596299
C	5.36314266	6.32937631	19.14389470
H	5.53829496	5.41554412	18.58495447
C	6.33773265	17.66204006	19.06113956
H	6.51147234	18.55785456	19.64991764
C	3.30223694	13.03145994	18.78811257
H	2.90373175	13.80356946	18.13465545
C	4.92689361	7.43566704	21.23940941
H	4.76585208	7.37027397	22.31009775
C	6.23042078	14.24044221	21.99103851
H	5.26423569	14.44344142	21.53581526
C	4.42536998	9.55301816	12.03553741
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C	3.60549110	12.13912330	20.99777070
H	3.46052770	12.23455339	22.06866616
C	8.72228660	13.50279223	18.73700549
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H	3.25015966	9.60617956	22.65570671
H	4.36984942	10.84176200	23.27898851
C	5.10869042	6.26652084	20.50901563
H	5.07709334	5.30361235	21.01032234
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H	3.03618424	16.32736850	13.76049785
C	3.25283381	8.86752204	14.12682463
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H	4.19221691	17.98987949	14.11876832
H	5.08021804	18.83080779	15.37044724
H	3.50243008	18.10243983	15.75536457
C	5.99527942	11.52395512	10.79255924
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C	7.81230191	14.95349797	11.69420840
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C	2.58084068	9.60641586	16.74879800
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C	5.42513386	10.50917656	10.03485475
H	5.58087545	10.47552884	8.96078828
C	6.45543043	10.41302910	21.58516737
H	6.50687112	11.36448545	22.12468878
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C	8.99516042	11.61359057	12.31184811
H	8.42602823	11.19724347	11.48601349
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H	1.90646149	7.22261370	14.45142294
C	7.76778183	16.09569125	10.89557504
H	8.69108175	16.61465919	10.65209365
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H	11.04530015	13.06102197	15.25781944
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H	3.66684706	5.71600231	16.32464209
C	10.36412965	11.37278600	12.39013066
H	10.84901525	10.76984636	11.62691484
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C	7.60055993	14.05453946	23.96964909
H	7.71032938	14.11966734	25.04847642
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C	2.02134017	8.46742769	16.18510921
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H	8.69745014	11.34555764	18.78849786
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C	9.65739738	8.47356843	17.50786224
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H	2.61258902	7.77300324	10.90039136
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CageAcN

Energy: -4536.914784

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P	6.01740745	7.61934466	16.70938173
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O	5.33903968	9.79446747	18.60149412
O	5.04011235	10.77290091	13.89951640
C	4.69222001	14.35598663	16.11180323
C	5.91205706	15.49222643	17.78742001
C	5.19679785	16.78996472	15.78138805
C	4.34753544	15.56113618	15.49492896
C	5.23914334	8.57669215	19.23143134
C	5.57712222	16.74036433	17.25108261
C	4.55590543	10.83637578	19.10693881
C	4.12086452	11.80380066	18.19401202
C	6.48368049	15.35663648	19.06050284
C	4.06240587	13.13410783	15.85026973
C	4.25801320	10.85899991	20.47158139
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C	4.06376174	10.04399697	14.58527526
C	4.90885157	10.85434287	12.53315147
C	5.50895398	7.43023862	18.47064421
C	5.44442558	11.98304790	11.89733430
C	7.36264501	14.03548248	21.41375454
C	6.63825334	16.51144182	19.83300465
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C	3.75792720	10.45822405	15.88616277
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C	8.02598842	12.53973527	12.97405963
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H	5.57358199	5.28207057	18.52676663
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C	2.96420175	12.85866646	20.06841771
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C	6.50924106	16.68593770	14.96117249
H	7.03934807	15.75365467	15.18222793
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H	6.28362567	16.70299289	13.88948949
C	5.44490875	15.47437797	11.52247933
H	4.55482207	15.32915128	12.13210356
C	4.13628913	9.97281898	10.44477729
H	3.64787565	9.19550153	9.86647272
C	7.67025083	14.80145838	10.88920568
H	8.51699579	14.12689862	10.97894700
C	2.75448654	9.73055562	16.53361546
H	2.47393711	10.01603916	17.54440012
C	6.46342581	14.22137043	23.65898417
H	5.61437209	14.16971706	24.33519641
C	3.01045289	13.17937363	14.92993579
H	2.48336031	12.25787238	14.69603980
C	10.64129605	11.55081115	13.24849221
H	11.65277563	11.16829849	13.35323022
C	4.60959790	11.10946417	9.79573378
H	4.47570072	11.21831664	8.72357147
C	6.37126702	10.22331590	21.63336518
H	6.40507752	11.16918710	22.18463120
H	6.91383439	10.35746566	20.69187530
H	6.87523203	9.44809231	22.22217567
C	9.03330372	13.32464934	13.55536645
H	8.79833048	14.32713646	13.90952272
C	8.34734040	11.24769747	12.54619779
H	7.58475350	10.62142824	12.09096110
C	2.44946512	8.28296460	14.63310775
H	1.94042183	7.44548500	14.16687529
C	7.73074747	15.86554084	9.99154521
H	8.62680616	16.01392621	9.39486098
C	10.33116898	12.84179070	13.67506820
H	11.10027855	13.46966563	14.11688287
C	4.64190464	5.43360316	15.72086858
H	3.80225590	6.12584994	15.75193693
C	9.64418566	10.75579497	12.68996105
H	9.87466575	9.74844337	12.35312160
C	3.98227785	8.54123395	12.58234874
C	7.73205940	14.52506215	24.14944786
H	7.87747138	14.71190882	25.20978391
C	2.60994180	14.36320527	14.31924691
H	1.77909691	14.36190738	13.61882261
B	4.44994913	11.74484030	16.60210799
C	8.63000515	14.34913153	21.91288986
H	9.47907793	14.41425675	21.23835254
C	6.64762745	16.72835754	9.84927874
H	6.69701934	17.55571322	9.14685087
C	2.09711780	8.66837103	15.92153633
H	1.31181695	8.13524937	16.45071927
C	9.44593504	12.42300949	19.30521778
H	9.04705601	11.71430579	20.02902469
C	9.20171742	14.41908689	17.97896513
H	8.62606169	15.28752265	17.67017438
C	5.50017419	16.52547598	10.61406972
H	4.64991793	17.19429791	10.51118578
C	8.81270712	14.58592319	23.27371789
H	9.80383385	14.82725082	23.64844382
C	4.45241051	4.13248429	15.26919546
H	3.46343289	3.80938232	14.95561515
C	10.71619177	12.22345916	18.77792355
H	11.30141484	11.36421213	19.09443071
C	5.31691925	7.77737543	12.78542798
H	5.14170786	6.86397516	13.36363089
H	6.03736943	8.39368919	13.33281532
H	5.74771240	7.51137605	11.81321124
C	11.23099358	13.11178091	17.83423291
H	12.21981398	12.95083068	17.41380241
C	6.98081708	4.97640544	16.07810618
H	7.96822999	5.29025642	16.40445169
C	10.46727079	14.20473427	17.43396778
H	10.85909276	14.90445122	16.70037622
C	5.53043726	3.25124823	15.20547385
H	5.38675779	2.23745252	14.84222075
C	6.79259411	3.67770210	15.60896346
H	7.63665792	2.99444922	15.56751236
C	8.48110365	8.07953890	18.10189435
H	7.90971558	8.06307301	19.02619185
C	7.83978825	7.84917536	16.88068450
C	8.60515078	7.87427232	15.70482388
H	8.12025956	7.71463279	14.74314330
C	9.97700407	8.09228931	15.75349182
H	10.55426554	8.09672269	14.83276507
C	10.60711206	8.32423611	16.97577255
H	11.67747319	8.50662748	17.01346925
C	9.85359223	8.32216884	18.14638948
H	10.33409604	8.50087128	19.10476292
C	3.01287125	7.63068482	11.82923692
H	3.43724209	7.33373189	10.86592171
H	2.04903530	8.12037439	11.65323256
H	2.84029791	6.70961787	12.39321787
C	8.54519720	11.25038327	16.21638071
H	8.90703305	10.58383306	17.00418590
H	8.76425638	10.81234512	15.23839957
H	9.04342087	12.22026951	16.29992269
N	5.99893279	11.56363609	16.46229683
C	7.13144189	11.42703436	16.35273152

CageCO

Energy: -4517.432834

P	6.61904141	12.83254565	13.22115502
P	7.12116320	13.58180129	19.28235070
P	5.86186832	7.75912763	16.72096145
O	5.70454397	14.28281085	16.80221885
O	5.29142048	9.93021305	18.60926691
O	5.02278709	10.52416889	14.09074973
O	6.98007685	11.42399065	16.42673982
C	4.61243412	14.30880567	15.94176253
C	5.85721008	11.54947162	16.46408623
C	5.93797453	15.42212542	17.54301588
C	5.10094651	16.74215577	15.59178053
C	4.24771665	15.50888861	15.33015421
C	5.24267713	8.72083664	19.27185449
C	5.56767487	16.67248579	17.03751177
C	4.50591589	10.96109076	19.11312631
C	4.04340992	11.90064155	18.18683279
C	6.57226106	15.26725671	18.78068998
C	3.94393797	13.09693814	15.74814687
C	4.23909888	11.01943101	20.48170378
C	4.96491148	8.67789636	20.64009725
C	3.91903078	9.93817385	14.69478640
C	5.05111961	10.56447512	12.71685463
C	5.51229661	7.57057899	18.51873256
C	5.79032058	11.59888598	12.12911849
C	7.37795975	13.82478733	21.09076758
C	6.77940789	16.41453643	19.55289481
H	7.27028014	16.32443666	20.51723293
C	5.76384945	17.78594783	17.85153814
H	5.47115677	18.76996592	17.50087125
C	3.58783695	10.43116228	15.95880971
C	6.66387013	14.28315738	12.08663571
C	8.37985340	12.28338188	13.20812255
C	5.45548039	6.33736757	19.17367726
H	5.66234280	5.42847952	18.61749410
C	6.35555578	17.65917301	19.10557827
H	6.50882249	18.53849232	19.72415664
C	3.27133832	12.94801479	18.69378034
H	2.89419151	13.70467894	18.01066028
C	4.88610806	7.42520652	21.24767292
H	4.65656334	7.35099729	22.30536189
C	6.25041636	14.12267802	21.86984607
H	5.29051153	14.28906125	21.38587106
C	4.36983282	9.60021905	11.96660786
C	4.89730734	9.99561938	21.39654187
C	3.43693890	12.06743882	20.93311812
H	3.19754475	12.15192773	21.98796301
C	8.85463490	13.55834909	18.65002208
C	4.17357615	9.86646437	22.73798193
H	4.68679648	9.14875790	23.38364455
H	3.13428762	9.54562522	22.60935966
H	4.18437086	10.82370288	23.26624818
C	5.12323915	6.26283244	20.52094319
H	5.06788208	5.29581705	21.01205305
C	3.14470812	15.48479638	14.47646554
H	2.81978974	16.39450494	13.98231829
C	3.23370791	8.91104181	14.05001714
C	4.35670251	18.04034573	15.27670086
H	4.07224593	18.06666092	14.22125981
H	5.00442103	18.90488343	15.44669096
H	3.45444258	18.14887791	15.88797013
C	5.82160095	11.66627659	10.73309238
H	6.37735833	12.46613548	10.25220994
C	5.89571290	5.99694720	16.18714386
C	2.95713391	13.02615966	20.04712661
H	2.33893011	13.84059845	20.41458482
C	6.36880161	16.67414372	14.70194089
H	6.92093744	15.74476515	14.87298710
H	7.02691461	17.51905865	14.93376919
H	6.08998660	16.71416775	13.64436006
C	5.43154693	14.82430582	11.69299605
H	4.50720222	14.33630406	11.99546694
C	4.41478346	9.71741968	10.57810159
H	3.89433009	8.99478973	9.95869412
C	7.83861966	14.93972522	11.71396429
H	8.80372176	14.53856416	12.01117347
C	2.52730441	9.80616923	16.61419449
H	2.24120473	10.15081042	17.60470398
C	6.34455068	14.19581328	23.25351999
H	5.46166375	14.43492475	23.84053859
C	2.86509459	13.11961593	14.86038932
H	2.31686289	12.20024922	14.67320092
C	11.10812763	11.65069672	13.27685587
H	12.16691998	11.40686857	13.30046547
C	5.13152203	10.74015256	9.96270351
H	5.15567684	10.80858241	8.87919958
C	6.35768246	10.43901044	21.66762714
H	6.36875086	11.38709420	22.21469759
H	6.90545589	10.58049716	20.73017427
H	6.87153928	9.67506843	22.26211941
C	9.20229222	12.78599981	14.22461221
H	8.77723972	13.42167262	15.00005000
C	8.93498204	11.43553959	12.24458351
H	8.30812420	11.02380081	11.45839621
C	2.17026461	8.32712618	14.74176441
H	1.60952516	7.51522967	14.29030665
C	7.78252713	16.11241320	10.96106555
H	8.70539391	16.61251471	10.67959843
C	10.56010654	12.48130023	14.25089083
H	11.18308656	12.88443633	15.04373346
C	4.65480677	5.36986989	16.00690995
H	3.73963653	5.92456230	16.20930580
C	10.29094949	11.12071767	12.28050284
H	10.71051625	10.46163221	11.52501088
C	3.72303877	8.42616156	12.69045090
C	7.56248188	13.95042038	23.88819459
H	7.63430829	13.99727629	24.97116068
C	2.46245108	14.29724260	14.23691648
H	1.60974934	14.29018694	13.56368038
B	4.30345436	11.74713886	16.58634580
C	8.59565398	13.58872819	21.73287284
H	9.48232541	13.35730548	21.14925395
C	6.55660645	16.63635556	10.56395653
H	6.51585903	17.54811647	9.97467023
C	1.82589175	8.76222207	16.01681060
H	1.00025914	8.29143063	16.54302037
C	9.48063071	12.30875054	18.55970237
H	8.92638414	11.40670377	18.81315394
C	9.56725182	14.70157385	18.27535783
H	9.09241661	15.67753190	18.32564071
C	5.37911143	15.98304460	10.92962268
H	4.41535120	16.38492209	10.62806080
C	8.68376277	13.64619577	23.12344293
H	9.63831835	13.45767005	23.60742780
C	4.58319221	4.05303181	15.56965647
H	3.61385766	3.57844192	15.44318650
C	10.80708291	12.21060632	18.15180288
H	11.28140240	11.23549320	18.09830006
C	4.81970073	7.35573051	12.91295131
H	4.40510614	6.49470344	13.44741806
H	5.64262236	7.75850943	13.51120936
H	5.21849197	7.02236123	11.94813256
C	11.51485357	13.35613411	17.79648335
H	12.54944377	13.27964290	17.47236648
C	7.06098283	5.28467228	15.89472594
H	8.03150674	5.75513281	16.02592890
C	10.88787898	14.59884485	17.84539193
H	11.43113147	15.49495097	17.55737412
C	5.75132462	3.34920046	15.27769562
H	5.69672285	2.32334396	14.92423815
C	6.98641254	3.96994785	15.43660659
H	7.90081613	3.42814195	15.21019829
C	8.47767802	8.13052599	17.83991740
H	8.07521946	7.78498491	18.78875386
C	7.64878204	8.20252979	16.71687443
C	8.18413127	8.66171640	15.50693976
H	7.54093039	8.76519111	14.63495802
C	9.52639236	9.00844838	15.41146620
H	9.92433655	9.36645470	14.46654841
C	10.34755774	8.92612263	16.53357598
H	11.39513742	9.20596273	16.46088287
C	9.81924229	8.49550950	17.74794619
H	10.45340846	8.43678692	18.62897530
C	2.59008177	7.80248635	11.86821258
H	2.96686500	7.42394457	10.91443915
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CageH2O

Energy: -4480.534438

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O	5.64107341	14.34204915	16.94767739
O	5.23377955	9.83470273	18.53994870
O	5.07110766	10.39008225	14.07790123
C	4.62756463	14.32999130	15.99109827
C	5.74212538	15.47376885	17.72512600

C	5.05754800	16.78492236	15.72712346
C	4.26604395	15.53392436	15.37775902
C	5.13261259	8.63660592	19.21423985
C	5.35985519	16.71643068	17.21393483
C	4.50401785	10.91426684	19.05509159
C	4.06414560	11.86828465	18.13308722
C	6.28830205	15.32583988	19.00587854
C	4.01637254	13.09570200	15.72440933
C	4.27810206	10.98227883	20.43041074
C	4.89381245	8.61628605	20.58999980
C	3.88882368	9.92457181	14.64877902
C	5.13988229	10.45925650	12.71491800
C	5.32403153	7.46671592	18.46722631
C	6.00160660	11.42345941	12.18010354
C	7.47096498	13.98918698	21.21361235
C	6.34771665	16.45864122	19.82129803
H	6.76679115	16.37661357	20.81931128
C	5.40581051	17.81794372	18.06646510
H	5.09226938	18.79312549	17.70886147
C	3.57447182	10.45914870	15.90166221
C	6.91332674	14.08281548	12.42312829
C	8.69591755	11.93931207	13.13706174
C	5.20298576	6.24212726	19.12878755
H	5.34488019	5.31887533	18.57582243
C	5.87763597	17.68679142	19.36935499
H	5.91384037	18.55324525	20.02315853
C	3.31637243	12.92269222	18.66652137
H	2.93854397	13.68876704	17.99330054
C	4.74987380	7.37456294	21.20834420
H	4.54309921	7.32132937	22.27197715
C	6.45842133	14.03615068	22.18327449
H	5.41907355	13.93039685	21.87641507
C	4.37630108	9.59795319	11.91995940
C	4.92993610	9.94247962	21.33060541
C	3.51652163	12.05096776	20.90334854
H	3.30282917	12.13946909	21.96353222
C	8.56643454	13.70576374	18.59077805
C	4.27007784	9.86348782	22.70779519
H	4.78052823	9.12815107	23.33602803
H	3.21152525	9.59184641	22.63528950
H	4.35208826	10.82512963	23.22194706
C	4.89287443	6.19598587	20.48307334
H	4.78538023	5.23664939	20.98052298
C	3.21424836	15.50801648	14.46315253
H	2.89028806	16.42399212	13.98000831
C	3.12776061	8.98002603	13.96461182
C	4.33259017	18.07007495	15.32948256
H	4.17537643	18.09678958	14.24729061
H	4.93992534	18.94442120	15.58040792
H	3.36171948	18.16111453	15.82835892
C	6.05990966	11.55261342	10.78925611
H	6.69888737	12.31372885	10.34924737
C	5.90232638	5.86474110	16.19269104
C	3.03420484	13.01542995	20.02552527
H	2.44301995	13.84477912	20.40448857
C	6.41796016	16.74008183	14.98351690
H	6.97294011	15.82748269	15.22380834
H	7.02749647	17.60340747	15.27440870
H	6.25470910	16.76434253	13.90189013
C	5.65760235	14.60550996	12.08991441
H	4.75433034	14.06260701	12.35765567
C	4.46000478	9.76448452	10.53918316
H	3.87895161	9.12587232	9.88212839
C	8.06099578	14.80849367	12.09780709
H	9.04369579	14.41967124	12.34961608
C	2.43283176	9.92521965	16.50749116
H	2.13858736	10.29745474	17.48607900
C	6.76852157	14.21159658	23.52630008
H	5.97026596	14.25514096	24.26247350
C	2.98953833	13.12994431	14.77029125
H	2.47245910	12.20488267	14.52979913
C	11.39269113	11.19993300	12.99460602
H	12.43870143	10.91142327	12.93852449
C	5.28781833	10.73496938	9.97529385
H	5.33131296	10.84673375	8.89615505
C	6.42204293	10.31928097	21.52331234
H	6.50253265	11.27515972	22.05129899
H	6.92978617	10.41934489	20.55866318
H	6.92832441	9.54310096	22.10873505
C	9.60770943	12.38615380	14.10261638
H	9.26564087	13.00963743	14.92755709
C	9.14540555	11.10007312	12.11379016
H	8.44804370	10.72553809	11.37042784
C	1.99139388	8.49385648	14.61508165
H	1.36492824	7.74857065	14.13578522
C	7.95399602	16.02898528	11.43271943
H	8.85493295	16.58109727	11.17953921
C	10.94971344	12.02955682	14.02194371
H	11.64531218	12.38712333	14.77501698
C	4.75850188	5.13712617	15.84029656
H	3.78571610	5.62587923	15.85968453
C	10.48670665	10.73056951	12.04665836
H	10.82324314	10.07280032	11.24993506
C	3.60166245	8.47771248	12.60354898
C	8.09956161	14.31659603	23.92943282
H	8.34419040	14.44186878	24.98050958
C	2.58236106	14.30942856	14.15483231
H	1.76758874	14.29547390	13.43588247
B	4.33665803	11.73471747	16.54861026
C	8.80118407	14.10075547	21.62608006
H	9.60203449	14.06838437	20.89289416
C	6.70483426	16.53244186	11.08281057
H	6.62488821	17.48029838	10.55802160
C	1.65660718	8.95063035	15.88542308
H	0.77590216	8.55589901	16.38455644
C	9.26206998	12.49643346	18.47410132
H	8.81484237	11.57835928	18.85142002
C	9.13940039	14.86755561	18.06330582
H	8.60992746	15.81360919	18.13709953
C	5.55617320	15.81561282	11.41559648
H	4.57446444	16.20382638	11.15750197
C	9.11150886	14.25681412	22.97658906
H	10.15146736	14.33899405	23.28131224
C	4.85602182	3.79986296	15.47105669
H	3.95940993	3.24538068	15.20791867
C	10.52509334	12.46032909	17.89050105
H	11.06038484	11.51796207	17.82458773
C	4.58269985	7.30087756	12.82900610
H	4.06438419	6.46927576	13.31800772
H	5.41334679	7.60226339	13.47390241
H	4.98737022	6.95649821	11.87049298
C	11.09581268	13.62621935	17.38559890
H	12.08438491	13.60050285	16.93497997
C	7.14835946	5.23382834	16.14507951
H	8.04606385	5.78450051	16.41246041
C	10.39283111	14.82600186	17.45840099
H	10.82697485	15.73771806	17.05669285
C	6.10254266	3.17844947	15.42483642
H	6.18174642	2.13702061	15.12564108
C	7.24625791	3.89914805	15.75803082
H	8.22090694	3.41995070	15.72215246
C	8.19780747	8.33660594	17.78897249
H	7.80846141	8.03414575	18.75757404
C	7.38048118	8.26270034	16.65552667
C	7.90203298	8.66634958	15.41807648
H	7.26977619	8.64535540	14.53269221
C	9.22345856	9.08554888	15.30804304
H	9.61672820	9.38319759	14.34090633
C	10.03343897	9.13742129	16.43896973
H	11.06471381	9.46781632	16.35048849
C	9.51451608	8.77623580	17.67978207
H	10.13911407	8.82578581	18.56814271
C	2.43666144	7.98473990	11.73935775
H	2.80177267	7.58847494	10.78781182
H	1.71997649	8.78743052	11.53611763
H	1.91155098	7.16450693	12.23462454
O	5.96640795	11.53681835	16.41142215
H	6.24302325	10.61743792	16.57319021
H	6.27644639	11.79150647	15.50317728

CageMeNH

Energy: -4500.020826

P	10.43843551	2.38084628	9.23601670
P	8.78540744	1.61528806	2.23663517
P	9.73236509	7.51109088	5.67977257
O	10.57770573	1.27978246	6.53990819
O	11.47398516	5.80782981	7.30994153
O	10.25331449	4.19507639	2.58381781
N	10.09600469	4.00540917	5.86690759
C	12.59866991	3.85793545	6.54397895
C	10.62019103	0.24956773	7.44915761
C	12.54130736	4.91656377	7.46147415
C	11.19607326	1.07334091	5.29993459
C	11.67659134	2.21017085	4.64255505
C	12.34590782	1.95997699	3.43815202
H	12.76011829	2.80298359	2.89055323
C	11.28243877	-0.22770561	4.79824296
C	11.96719445	4.85375363	4.13221706
C	10.54623732	0.59780488	8.80506283
C	10.68696834	-1.07753999	7.01913977
C	11.97447883	-0.41339789	3.60250385

H	12.08646493	-1.40980251	3.18752943
C	11.66367209	7.11582661	7.66344783
C	13.65721865	2.96561446	6.74360483
H	13.76215621	2.12192605	6.06566335
C	11.31400405	5.05349230	2.90447592
C	13.45270205	5.13800110	8.49251256
C	12.51462190	0.67711749	2.92986337
H	13.05547374	0.52612135	1.99935999
C	13.21894824	6.30314498	9.44944997
C	9.74306274	8.95539325	4.53694100
C	9.39485628	2.73343013	0.90576711
C	11.66229289	6.05212689	1.98575209
C	8.69334322	2.77782519	8.78787417
C	10.54396509	-1.33887036	5.52920820
C	10.36201853	2.31274575	11.07300799
C	8.20071055	0.16456458	1.26236121
C	7.19017175	2.43714263	2.67746171
C	12.57859481	7.44430661	8.66841340
C	10.35078382	4.90042027	0.28420298
C	10.02207822	3.94231823	1.24947393
C	10.60696766	-0.43029168	9.74875511
H	10.55281994	-0.18978820	10.80612048
C	13.49761547	6.64412051	3.42703330
H	14.37601710	7.24935635	3.63541831
C	14.58900171	3.13399800	7.76465531
H	15.39998079	2.42054651	7.88357583
C	13.07453040	5.69103926	4.34556540
H	13.64463480	5.57051831	5.26146999
C	14.49430387	4.21860670	8.62931111
H	15.23332748	4.34106871	9.41450978
C	8.85163650	3.55242951	5.19962745
H	8.67926682	4.15731955	4.31124427
H	8.00674576	3.66146674	5.88677575
H	8.95405504	2.51042295	4.90052054
C	10.77488632	-2.07349097	7.99132166
H	10.85012969	-3.11406676	7.69341729
C	8.58455032	9.61912739	4.12567843
H	7.62281465	9.35938757	4.55878488
C	10.89431507	8.07571639	6.99102498
C	6.77412361	3.66815096	2.16281164
H	7.35171451	4.15273888	1.38031672
C	9.17359234	2.29210525	11.80802602
H	8.21684998	2.30098381	11.29289663
C	10.74494961	-1.75382411	9.34541101
H	10.80685810	-2.54193988	10.08991383
C	9.13244395	-0.85678929	1.03673743
H	10.14195154	-0.75362088	1.43029288
C	5.62219261	4.28633535	2.64724135
H	5.31749269	5.24604152	2.23775194
C	4.86243168	3.67788385	3.64159324
H	3.96300373	4.15919944	4.01581855
C	12.78414848	6.83320284	2.25210032
H	13.09356262	7.59985044	1.54968713
C	9.22433156	2.44992958	-0.45230304
H	8.75320351	1.51677544	-0.74507092
C	7.75714219	1.83263839	8.35832992
H	8.03117025	0.78200143	8.30898091
C	6.90052172	0.01508372	0.76990965
H	6.16606238	0.79869951	0.93486459
C	6.42027514	1.83550431	3.68344589
H	6.73741623	0.88456112	4.10843086
C	10.75813977	6.27329132	0.78536732
C	7.47822331	-2.13632262	-0.16489798
H	7.19609528	-3.02875531	-0.71664824
C	8.06805917	7.63646997	6.45854011
C	10.18650859	4.57021546	-1.05962266
H	10.46276840	5.28345730	-1.82892335
C	9.64836129	3.34213916	-1.42928214
H	9.52582045	3.09495027	-2.47961483
C	9.03693090	-1.21908271	5.17912871
H	8.89279998	-1.34686127	4.10019638
H	8.65025293	-0.23467655	5.46252494
H	8.46473861	-1.98681385	5.71277511
C	8.77727574	-1.99399792	0.31878695
H	9.51239324	-2.77537290	0.14601556
C	5.26141939	2.44269371	4.15169261
H	4.67525334	1.95803240	4.92777833
C	6.54189077	-1.13158099	0.06538298
H	5.52768677	-1.23648848	-0.31059792
C	9.20937853	2.25802933	13.20010801
H	8.27915005	2.24462664	13.76164165
C	11.58515826	2.30304407	11.75558550
H	12.51491664	2.33299587	11.18987153
C	9.47796866	7.00289411	1.27276983
H	8.97960000	6.44034295	2.06906473
H	8.77633394	7.12548482	0.43953699
H	9.74180743	7.98997718	1.66766170
C	10.97010575	9.31264584	3.96185462
H	11.87687629	8.79033657	4.25628336
C	8.65303590	10.62184919	3.15951990
H	7.74351066	11.13025129	2.85112087
B	11.59308615	3.71170197	5.25248264
C	11.03586511	10.32053401	3.00838338
H	11.99662789	10.58818802	2.57652858
C	7.79954529	8.28944623	7.66468217
H	8.60722827	8.76084430	8.21792574
C	8.31841640	4.12787934	8.83822044
H	9.04433702	4.87900416	9.14588383
C	11.40757125	7.12809133	-0.30226816
H	11.65220158	8.11934205	0.09005148
H	10.71012727	7.28066799	-1.13089442
H	12.32221435	6.66851785	-0.69223178
C	7.03113548	4.52024012	8.49039645
H	6.75794717	5.57022048	8.53357362
C	7.01475523	7.01536671	5.77295672
H	7.21526810	6.47378193	4.84979701
C	11.02706240	-2.73196887	5.12635759
H	10.45425347	-3.50343182	5.64857124
H	12.09046805	-2.87122572	5.34818913
H	10.86749205	-2.89210416	4.05640870
C	6.10497214	3.57094183	8.06154591
H	5.10459936	3.88032078	7.77085654
C	10.42925724	2.23425059	13.87098699
H	10.45392679	2.20556640	14.95676698
C	14.50609689	6.74007150	10.15334585
H	14.91593386	5.91797627	10.74555059
H	14.30506506	7.55659440	10.85212682
H	15.26521540	7.06800363	9.43545740
C	9.87565736	10.97716475	2.59877570
H	9.92634367	11.76042560	1.84771648
C	6.47217822	2.22967347	7.99392902
H	5.75647297	1.48470580	7.65664923
C	12.19850532	5.84559225	10.52207304
H	11.26465787	5.51623262	10.05606304
H	11.97614472	6.66906213	11.21039751
H	12.60727443	5.00344869	11.09033103
C	11.61862402	2.25197881	13.14487451
H	12.57406623	2.23746861	13.66200864
C	12.75572090	8.79612695	8.95637067
H	13.46489313	9.09805283	9.71996131
C	5.71337043	7.08764519	6.25824999
H	4.90735362	6.60848947	5.70907016
C	11.08961859	9.41904087	7.32608106
H	10.51841979	10.18518592	6.80869477
C	6.49801203	8.34348008	8.15933589
H	6.30112781	8.85308247	9.09867940
C	5.45147287	7.75412319	7.45350829
H	4.43737135	7.80361460	7.84044667
C	12.02241853	9.77759151	8.29061305
H	12.17520199	10.82456874	8.53475013
H	10.10181283	3.61827169	6.81056952
H	10.03417961	5.02075671	5.98373983

CageMeNH_ipr

Energy: -4460.688154

P	2.14022237	30.95218813	14.89361817
P	4.45558016	37.37697215	17.22979588
P	6.48570807	32.28072799	12.47707687
O	1.60853528	33.77977190	15.59788355
O	3.83889548	32.96128063	11.32149360
O	5.23072317	36.82027811	14.30616718
N	3.93824130	33.85202804	14.03568512
C	2.46399584	33.22769873	11.36025413
C	1.36610627	35.14470441	15.40626335
C	5.06278910	36.75810907	12.92266190
C	2.11329446	35.78146978	14.40867515
C	3.98386790	35.99902576	12.43589895
C	2.02375033	34.15295696	12.32039796
C	1.63517115	32.59963489	10.42747445
C	5.97736364	37.84547991	14.84236148
C	0.64017834	34.37733802	12.32360798
H	0.22938989	35.08628565	13.03670870
C	0.54575031	32.99141790	15.97045740
C	3.75323436	36.13559079	11.05745454
H	2.90612019	35.61392998	10.62215095
C	5.45830514	31.21902938	11.37243390
C	6.97122266	38.47503261	14.07573709
C	4.23679657	31.71673425	10.89042623
C	3.44682414	31.00920334	9.97622818
C	0.38502620	35.76750390	16.18007249
C	5.68363414	37.52637981	10.73655435

H	6.34931044	38.06758866	10.07275472
C	-0.50670495	33.54739242	16.70650018
C	1.83008566	37.14098773	14.23018564
H	2.37556578	37.68534620	13.46233174
C	5.97209692	37.43319289	12.09621921
C	4.55051376	36.90982607	10.22339209
H	4.31203195	36.99729840	9.16683602
C	0.58784583	31.63320137	15.62125581
C	4.70567597	34.12273658	15.27651750
H	5.64790291	34.61054272	15.02669568
H	4.92417056	33.17475734	15.77956041
H	4.13443573	34.77811166	15.93636723
C	2.27678972	31.74527199	9.34539752
C	5.73568276	38.21094487	16.17676016
C	-0.22999306	33.73388496	11.44857526
H	-1.29701208	33.93290834	11.49957421
C	0.26595137	32.85487765	10.49589475
H	-0.41523430	32.37250310	9.80287952
C	-1.61087502	32.74203369	16.97477438
H	-2.45676290	33.14667113	17.52073081
C	5.82795578	29.92914419	10.97430781
H	6.75911963	29.50064557	11.33153574
C	7.68614551	39.52520062	14.64403770
H	8.44450427	40.03801429	14.06247242
C	-0.30618387	34.94989464	17.26077527
C	0.84681253	37.79958285	14.96128582
H	0.63723652	38.84922625	14.77295040
C	7.28161405	37.90346665	12.70608469
C	3.84175061	29.71954807	9.63006375
H	3.23717421	29.13406735	8.94558961
C	0.11980133	37.11332445	15.92769687
H	-0.65016024	37.63256622	16.48890656
C	7.73172371	32.99873553	11.26357351
H	8.39856107	33.59630628	11.90283535
C	-0.53533566	30.85737147	15.92759743
H	-0.55453739	29.80703534	15.65368446
C	1.55257973	29.47171589	13.91245251
H	0.97879614	28.79671143	14.56068955
C	6.50998291	39.24524380	16.71503037
H	6.34448147	39.54980260	17.74496924
C	2.85259448	32.69795268	8.26470496
H	3.35930065	32.11919427	7.48410866
H	3.57136862	33.39861731	8.70165107
H	2.03983571	33.27535480	7.81047883
C	3.65104072	38.87344434	18.06687819
H	4.34392209	39.27791647	18.82055347
C	-1.63804181	31.41065524	16.56724310
H	-2.50869768	30.79655336	16.77759052
C	2.91224402	30.16799462	16.43952775
H	3.91236579	29.85977238	16.10042942
C	0.66442855	29.93081051	12.75565518
H	-0.22396216	30.46666825	13.10451159
H	0.33417497	29.06383004	12.17008025
H	1.21453323	30.60109254	12.08684072
C	5.01794326	29.17384730	10.13637121
H	5.31426279	28.16720530	9.85659953
C	7.46846529	31.03844542	13.47272525
H	7.96396060	30.31480684	12.81240956
C	7.46068755	39.91463009	15.96018580
H	8.03244200	40.72930510	16.39488850
C	5.63278567	36.75738305	18.57619675
H	6.26893695	37.59854491	18.88753891
C	2.78106945	28.72121750	13.38465129
H	3.38261300	29.37077767	12.73715058
H	2.46382601	27.85711939	12.78859045
H	3.42497674	28.35326961	14.19101373
C	1.28286451	30.79494330	8.67688271
H	0.47843462	31.35945198	8.19822044
H	0.84131854	30.09835630	9.39789350
H	1.77513424	30.21987693	7.88748890
C	8.56542235	31.98038693	10.48953031
H	9.13987101	31.32268901	11.14978515
H	9.27777236	32.50212522	9.83812547
H	7.92838166	31.35656460	9.85308187
B	3.02933798	34.99665308	13.32361685
C	0.65262872	34.83664305	18.47469770
H	0.83581016	35.83034846	18.89606625
H	1.61554061	34.40797559	18.17865001
H	0.20822785	34.19720999	19.24618979
C	6.99485654	33.95420062	10.32071330
H	6.32110631	33.40068897	9.65521643
H	7.71411306	34.49292293	9.69192143
H	6.39732655	34.69098370	10.86779138
C	8.54523118	31.78140063	14.27095916
H	8.09852947	32.56123489	14.90056715
H	9.28924009	32.25398236	13.62178053
H	9.07282747	31.08060125	14.92867506
C	8.17944664	36.65354670	12.90783484
H	8.40325912	36.19834917	11.93651368
H	7.67667228	35.90551311	13.53047731
H	9.11892699	36.93891829	13.39514004
C	2.18852337	28.95075094	17.01237484
H	1.17125757	29.21082527	17.32583821
H	2.72477270	28.59018931	17.89934274
H	2.13103420	28.12103212	16.30207631
C	-1.61438870	35.58353710	17.73389632
H	-2.06314745	34.98303102	18.53037258
H	-2.33641861	35.68024635	16.91609135
H	-1.42693829	36.57538642	18.15447475
C	3.08319635	31.23816456	17.52271514
H	3.55689457	32.14740717	17.14056127
H	3.70044950	30.84846871	18.34061360
H	2.11032225	31.52047738	17.94129784
C	3.30852098	39.96552708	17.04843770
H	4.19646407	40.42823154	16.61167237
H	2.71528471	40.75060012	17.53343698
H	2.70715414	39.54962138	16.23133041
C	2.35896405	38.42204880	18.76218717
H	1.63154599	38.08793105	18.01390974
H	1.91922277	39.26170143	19.31482248
H	2.51404984	37.60057564	19.46591116
C	6.52583207	35.66023548	17.98933166
H	5.93298069	34.77644557	17.72673814
H	7.27745377	35.35272386	18.72633740
H	7.05094276	35.99829463	17.08932305
C	8.03150109	38.89163715	11.81163153
H	8.99345918	39.15958906	12.25711937
H	7.45328844	39.80660068	11.64455467
H	8.25268132	38.43455582	10.84337512
C	6.51410581	30.29071654	14.40863707
H	7.06611466	29.55755961	15.00906520
H	5.73157140	29.76089811	13.85574362
H	6.02427659	30.99050900	15.09729090
C	4.87738160	36.23340052	19.79906103
H	4.38216041	37.03612057	20.35220040
H	5.57717915	35.74182467	20.48630409
H	4.11894762	35.49517150	19.50866336
H	4.61442245	33.48760211	13.35006223
H	3.31355435	33.05643231	14.22762223

CageNH3

Energy: -4460.688154

P	6.68786648	12.76838265	13.19077210
P	7.27124324	13.58953079	19.18019879
P	5.67513677	7.64801792	16.74635111
O	5.76278389	14.31198593	16.77632469
O	5.21205833	9.84985730	18.61659453
O	5.02077228	10.52474547	14.05142965
C	4.63024542	14.33455018	15.95523550
C	6.02099770	15.44077421	17.51320861
C	5.12536162	16.77169974	15.60351061
C	4.25431608	15.54392368	15.36716977
C	5.13859816	8.65416435	19.29459212
C	5.63617190	16.69719207	17.03359757
C	4.46263328	10.92062057	19.11818589
C	4.02394975	11.86865809	18.18471851
C	6.69733782	15.27523268	18.72669670
C	3.95158636	13.12053287	15.79615854
C	4.21109166	10.98471313	20.49081237
C	4.88402501	8.63097052	20.66734290
C	3.89780826	9.96574163	14.66311406
C	5.07510367	10.53880416	12.68476822
C	5.36827501	7.48673153	18.55211371
C	5.85899193	11.54194934	12.09684647
C	7.43200108	13.74966164	21.00672957
C	6.93038579	16.41147327	19.50789310
H	7.44956557	16.30747917	20.45629037
C	5.86057982	17.80058688	17.85312834
H	5.55748932	18.78901325	17.52366272
C	3.58577634	10.47257984	15.92977467
C	6.65548477	14.25077954	12.10245945
C	8.46353045	12.27897019	13.15772708
C	5.28307284	6.26210865	19.21910497
H	5.45627887	5.34156821	18.67045781
C	6.49264235	17.66053333	19.08753221
H	6.66397762	18.53329555	19.71052984
C	3.25161970	12.91081045	18.70943375
H	2.87750259	13.67316726	18.02980778
C	4.77519963	7.38751875	21.28966785
H	4.55913652	7.33146870	22.35134867
C	6.26947935	14.04436305	21.73246195

H	5.33883246	14.24185335	21.20558676
C	4.38009072	9.58718063	11.92999785
C	4.86995717	9.95977601	21.40450753
C	3.41569040	12.03545525	20.94932921
H	3.18172308	12.12023732	22.00540012
C	9.02645327	13.61280505	18.61613332
C	4.18485070	9.86643085	22.76867503
H	4.70106760	9.14550131	23.40872047
H	3.13516168	9.56779681	22.67610901
H	4.23292700	10.83089129	23.28181100
C	4.96550008	6.21125216	20.57159080
H	4.88654335	5.25107313	21.07279450
C	3.11283941	15.54000170	14.56490091
H	2.77520820	16.45613377	14.09146769
C	3.19202308	8.95714383	14.00917906
C	4.38395849	18.07732920	15.31471187
H	4.06839588	18.11072860	14.26832472
H	5.04392885	18.93555556	15.47025311
H	3.50072302	18.19065371	15.95234337
C	5.92030016	11.59622013	10.70153681
H	6.50218483	12.37972652	10.22372004
C	5.89658726	5.88552654	16.25921053
C	2.93479381	12.99205339	20.06278703
H	2.31924831	13.80881647	20.43064174
C	6.36572034	16.69529285	14.67655952
H	6.91649554	15.76237166	14.83242881
H	7.03675350	17.53607283	14.88610423
H	6.05563897	16.73524413	13.62780586
C	5.39604237	14.75437473	11.74857142
H	4.49558575	14.23461371	12.06964625
C	4.46236460	9.68538236	10.54182223
H	3.93434245	8.97119176	9.91889667
C	7.79996288	14.94700532	11.70922688
H	8.78427316	14.57345845	11.97832118
C	2.48980364	9.87435118	16.55790082
H	2.19892049	10.22677267	17.54488378
C	6.29251650	14.07337361	23.12084097
H	5.38340287	14.30875130	23.66785960
C	2.82700592	13.17828178	14.96315789
H	2.25379334	12.26873328	14.80120765
C	11.19521161	11.67046558	13.26896789
H	12.25474934	11.43275565	13.31015117
C	5.22198506	10.67890043	9.92817967
H	5.26889432	10.73314256	8.84468765
C	6.34771256	10.37346612	21.62809515
H	6.39329268	11.32163222	22.17286053
H	6.86943008	10.50312423	20.67393641
H	6.86554508	9.60133772	22.20873707
C	9.26207341	12.77266790	14.19793049
H	8.81591865	13.39012345	14.97687374
C	9.04527025	11.45880354	12.18645070
H	8.43652385	11.05309721	11.38318278
C	2.10479711	8.40197856	14.68820420
H	1.52524493	7.60660244	14.23116592
C	7.68725287	16.12287266	10.96810138
H	8.58590465	16.65474538	10.66742576
C	10.62202258	12.48099801	14.24583591
H	11.22603595	12.87513941	15.05812865
C	4.73114660	5.16069113	15.97592712
H	3.76158151	5.64838625	16.06529102
C	10.40325124	11.15511780	12.24459712
H	10.84403357	10.51372807	11.48611574
C	3.67374071	8.44820499	12.65403265
C	7.47166992	13.78927981	23.80973476
H	7.48751879	13.80337541	24.89586797
C	2.40714914	14.36036912	14.35863826
H	1.52256363	14.36395855	13.72725430
B	4.34731131	11.74939903	16.59264587
C	8.61106776	13.47242652	21.70159941
H	9.52378253	13.24419762	21.15829833
C	6.43490676	16.60957237	10.60707868
H	6.35006769	17.52392608	10.02660958
C	1.76059915	8.85156801	15.95752801
H	0.91540703	8.40716837	16.47624594
C	9.68568255	12.37792323	18.56375537
H	9.14665451	11.46771982	18.82150709
C	9.71713099	14.76673348	18.23391457
H	9.21569107	15.73029729	18.25153651
C	5.28816242	15.91770858	10.99802621
H	4.30483379	16.29231717	10.72642907
C	8.62712556	13.48844670	23.09574947
H	9.55209419	13.27065591	23.62280820
C	4.80332443	3.82876137	15.58445164
H	3.89063190	3.27719416	15.37619430
C	11.02390726	12.30587094	18.19087369
H	11.52824185	11.34407599	18.17438777
C	4.71377974	7.32514752	12.89029687
H	4.25270672	6.48975630	13.42785042
H	5.55153314	7.68885692	13.49252998
H	5.10330678	6.96395933	11.93153081
C	11.70971267	13.46223550	17.82692060
H	12.75308002	13.40680589	17.52802093
C	7.13585042	5.25623515	16.11663835
H	8.04995040	5.80423315	16.32784295
C	11.04918495	14.68846716	17.83486844
H	11.57544096	15.59199262	17.53887753
C	6.04384038	3.20853480	15.44410153
H	6.10213039	2.17113296	15.12672795
C	7.20720221	3.92642172	15.70620894
H	8.17742177	3.44939850	15.59655009
C	8.26721127	8.28194985	17.81556765
H	7.91516075	7.90825110	18.77379266
C	7.41238526	8.26926543	16.70830679
C	7.88362888	8.76428237	15.48449205
H	7.22025077	8.79192855	14.62246700
C	9.18772741	9.23116443	15.36074144
H	9.53690232	9.61193983	14.40544246
C	10.03452233	9.22747615	16.46588173
H	11.05092566	9.59886951	16.36951450
C	9.56983653	8.75971534	17.69296054
H	10.22489982	8.76154953	18.56068428
C	2.52175768	7.87719580	11.81866016
H	2.89087151	7.47880269	10.86986510
H	1.76335092	8.63924265	11.61090011
H	2.04531929	7.04234908	12.33799120
N	5.96405695	11.54440069	16.46473117
H	6.30418302	11.88915244	15.56204693
H	6.44412352	12.06250825	17.20589857
H	6.23443141	10.56611667	16.55049936

CageNH3_ipr

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P	16.43627014	5.42161141	5.98950499
P	12.81417574	9.24053023	7.06746579
P	13.93437116	4.80215152	10.75390113
O	13.62428060	8.96845560	9.89453625
O	16.72205158	5.52009678	10.17526911
O	17.10467499	8.24423221	6.49318831
N	15.34962221	7.32739164	8.58581181
H	15.80098970	6.70866171	7.89766918
H	14.65022134	7.88477919	8.08013535
H	14.84808854	6.72072342	9.24300993
C	17.92702845	6.13089456	9.84678064
C	14.48982843	9.09834720	10.98398632
C	16.96301093	9.52987464	7.02063542
C	17.82881892	7.48340685	9.47260756
C	15.82508483	8.73681418	10.77075381
C	16.61506613	9.61146629	8.37627167
C	17.78718830	3.35182899	10.30351495
C	15.35945411	3.63820019	10.56512221
C	16.83126585	8.06737041	5.15908454
C	12.59052149	9.86650361	9.79273883
C	16.43127350	6.78538402	4.74822377
C	17.19352179	10.63244187	6.19612963
C	13.98286838	9.58572941	12.19047451
C	16.64992190	4.16338637	10.33708254
C	12.11863157	10.16678417	8.50576654
C	19.04290005	8.13593448	9.24203031
H	19.02115908	9.18543990	8.95751402
C	13.91336674	5.02095740	12.63332491
H	13.04575274	5.67426630	12.80398271
C	17.60295474	1.97240073	10.42560590
H	18.46802388	1.31624166	10.40766929
C	14.87946329	9.76006761	13.24503471
H	14.53354238	10.14964100	14.19685425
C	16.98688537	9.13086095	4.26235400
C	19.12913778	5.42554371	9.91158282
C	15.18380723	4.20575908	5.32276154
H	15.38750363	3.95959168	4.27230747
C	16.49217509	10.91127597	8.88074553
H	16.22617117	11.04007776	9.92705510
C	15.23250567	2.25347051	10.67788346
H	14.25588507	1.81242838	10.84790157
C	16.67243264	8.91455702	11.87173553
H	17.72315053	8.65464824	11.76262918
C	19.18870149	3.94025785	10.23769057
C	18.10193661	4.61327205	5.65046071
H	18.12234081	3.76902364	6.35576221
C	16.34161216	1.41910239	10.59011945
H	16.22372602	0.34324561	10.67825602
C	16.07823382	6.62169325	3.40468007

H	15.75041932	5.65000940	3.04793162
C	12.58932187	10.41547240	5.63028196
H	11.54369820	10.74345266	5.56183142
C	17.04861239	11.90239511	6.75646483
H	17.21110058	12.78774312	6.15066062
C	12.03682983	10.41952110	10.95265245
C	11.11531753	11.13648027	8.40433535
H	10.73445797	11.41593464	7.42667917
C	20.30726767	6.14105749	9.67512569
H	21.26582845	5.63434036	9.74237079
C	20.27106696	7.48978093	9.35820799
H	21.19594440	8.03293714	9.18443030
C	15.16428817	5.78068634	13.07687051
H	16.06383278	5.16885481	12.93884878
H	15.09092277	6.02987310	14.14229718
H	15.29777574	6.70924405	12.51636661
C	12.43980846	3.70517832	10.46775057
H	12.50187764	2.80580137	11.09335653
C	16.60484871	8.92594826	2.93831527
H	16.68574227	9.73510142	2.21998923
C	16.22048759	9.42702871	13.08422200
H	16.91246519	9.56139201	13.91130628
C	12.48517471	9.83916554	12.28668789
C	17.67178616	10.38942780	4.77223902
C	16.13262646	7.68692220	2.51369705
H	15.83622796	7.54531448	1.47853476
C	10.60445667	11.76270484	9.53529399
H	9.83835473	12.52570349	9.43339544
C	16.69628419	12.04111076	8.09252945
H	16.58462021	13.03286601	8.52246947
C	11.05110061	11.39184148	10.80154629
H	10.61383533	11.86159981	11.67650933
B	16.41689972	8.28980991	9.32259564
C	11.45620564	7.95401620	6.79530012
H	11.83536527	7.34957950	5.95793353
C	13.79164173	4.83608287	5.43100070
H	13.56856191	5.09831959	6.47255780
H	13.02496193	4.13004648	5.08961150
H	13.71061436	5.74788010	4.82982193
C	13.73933345	3.73626834	13.44050758
H	12.79891976	3.22118597	13.22130134
H	13.74425530	3.97287666	14.51190971
H	14.56435162	3.04072695	13.24976322
C	18.30448878	4.08243103	4.23319803
H	17.54797333	3.34292314	3.95155855
H	19.28703230	3.60035990	4.15425626
H	18.27544385	4.89892431	3.50305174
C	20.02033416	3.20995158	9.16194911
H	20.10077510	2.14143501	9.38081129
H	21.03683754	3.60978533	9.11819152
H	19.56060112	3.33046653	8.17629043
C	15.27301251	2.92036944	6.15317706
H	16.22068883	2.39463978	5.99838066
H	14.46070519	2.23714044	5.87786686
H	15.18003840	3.13944833	7.22460240
C	19.85970498	3.74822001	11.61812667
H	19.28535231	4.26071767	12.39668745
H	20.87461597	4.15900687	11.60947971
H	19.91825261	2.68430538	11.87289106
C	11.78063372	8.46845231	12.46588029
H	12.02964957	7.78893037	11.64399837
H	10.69300175	8.60140129	12.49212003
H	12.10772033	8.00760214	13.40489405
C	11.17835304	4.47778641	10.87213987
H	11.15840134	4.70808517	11.94191207
H	10.28720960	3.88188524	10.64165059
H	11.10262708	5.42197034	10.32096596
C	19.21292937	5.59103915	6.04444905
H	19.24145979	6.44329653	5.35463356
H	20.18804626	5.09128566	5.99698398
H	19.07592097	5.97946596	7.05869021
C	13.48826603	11.63740895	5.82594186
H	13.23852737	12.19027445	6.73738757
H	13.38586335	12.32063931	4.97373847
H	14.53937270	11.33662350	5.89641570
C	12.11403126	10.73527321	13.46766416
H	12.42071189	10.27083418	14.40893027
H	11.02978440	10.86953888	13.52093833
H	12.58729760	11.72014184	13.39301662
C	12.95846138	9.67081037	4.34152210
H	13.98542271	9.28787583	4.39477660
H	12.90106474	10.35351752	3.48517723
H	12.28973988	8.82678057	4.14238035
C	11.37918458	7.05474766	8.03165364
H	12.35783650	6.64804949	8.31035058
H	10.70018596	6.21346555	7.84699110
H	10.99386049	7.61313091	8.89382416
C	19.19509288	10.10110519	4.82559205
H	19.72463055	10.97887053	5.21228763
H	19.57173393	9.86872094	3.82291285
H	19.40792667	9.25269661	5.48390013
C	17.43196400	11.59180237	3.85799719
H	16.36683052	11.83824899	3.78694854
H	17.81559140	11.39184749	2.85355041
H	17.96961955	12.46799473	4.22923724
C	12.36841305	3.28117364	8.99882566
H	12.27518142	4.15646273	8.34681433
H	11.49101285	2.64429507	8.83270554
H	13.25665457	2.72297366	8.68788386
C	10.07431228	8.49259369	6.43194865
H	9.67241832	9.11469551	7.23933461
H	9.37937565	7.65697030	6.27977031
H	10.08443089	9.08580540	5.51243839

CageTbunc

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P	6.41506294	13.20587207	12.83864831
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P	6.15241593	7.55787358	16.72931035
O	5.74067459	14.32422777	17.05765056
O	5.31302749	9.78218343	18.64023652
O	4.93444645	10.76036924	13.91003555
C	4.61677493	14.38063945	16.22761469
C	6.02850039	15.44672123	17.80184337
C	5.13030123	16.81013359	15.90824705
C	4.21232984	15.61549454	15.71011779
C	5.26488318	8.54428997	19.24258192
C	5.67123110	16.71773872	17.32321607
C	4.44764540	10.76233041	19.13569232
C	3.99759826	11.73246891	18.23299903
C	6.68746161	15.28688218	19.02835547
C	3.94997667	13.17670262	15.97375939
C	4.06603873	10.71666980	20.48049064
C	4.91243239	8.43534862	20.59761706
C	3.89068274	10.10276627	14.56847321
C	4.84856848	10.85213255	12.53827140
C	5.58545723	7.41485504	18.47788810
C	5.44520746	11.94837807	11.90125486
C	6.81572794	13.81459613	21.41920381
C	6.92304832	16.42793147	19.80518252
H	7.41957749	16.31501551	20.76527479
C	5.90750842	17.82213116	18.13523566
H	5.61945972	18.81121128	17.79531107
C	3.59721410	10.51487927	15.87340555
C	5.90589261	14.72378308	11.91492355
C	8.12131794	12.91266562	12.20282010
C	5.48012462	6.15642359	19.08275421
H	5.71369488	5.27156686	18.49674554
C	6.52313303	17.68317112	19.37690212
H	6.70050777	18.55534042	19.99894591
C	3.06908529	12.64970719	18.74107057
H	2.67901269	13.41746096	18.07812808
C	4.80055351	7.16511022	21.15324291
H	4.50875637	7.05600321	22.19246783
C	5.45154742	13.91497294	21.71755995
H	4.72334258	13.93662638	20.91062718
C	4.18428394	9.85345243	11.80833228
C	4.76810228	9.72199612	21.38957700
C	3.09910972	11.62041511	20.91662983
H	2.75582770	11.59544608	21.94523364
C	9.07383459	13.82353570	19.63711747
C	4.04120699	9.52320732	22.71883992
H	4.59165957	8.82528368	23.35607900
H	3.02422439	9.14237142	22.57542763
H	3.98842235	10.47106862	23.26239141
C	5.07284530	6.02527052	20.40053865
H	4.98163557	5.04052784	20.84896259
C	3.01714295	15.66377269	14.99488027
H	2.65783660	16.60824471	14.60076084
C	3.19372858	9.09150946	13.89874289
C	4.43398539	18.14169338	15.62728356
H	4.08230488	18.17130159	14.59199154
H	5.13472631	18.97325700	15.74423282
H	3.58030555	18.30262632	16.29434121
C	5.30330169	12.06208253	10.51278364
H	5.75055696	12.91392494	10.00751097
C	5.30852873	6.07451990	16.02059335
C	2.59601849	12.58015354	20.04732324
H	1.84870595	13.28898092	20.39406263
C	6.32917946	16.67481217	14.93407393
H	6.84096003	15.71589314	15.06801797

H	7.04655516	17.48400289	15.11288881
H	5.97611312	16.72990175	13.89922748
C	4.55992999	15.09178146	12.03287999
H	3.87671925	14.46226688	12.59725952
C	4.04898122	10.01591380	10.43354072
H	3.52096835	9.26701072	9.85278996
C	6.77036868	15.55299402	11.19731093
H	7.81532175	15.28378404	11.07649060
C	2.49337818	9.89478388	16.47225133
H	2.21640088	10.18761732	17.48149493
C	5.01602799	13.97131581	23.03499445
H	3.95235209	14.04869041	23.24466373
C	2.78387489	13.27779477	15.20472228
H	2.22383524	12.37197321	14.98825576
C	10.80823690	12.46734987	11.51378078
H	11.84711172	12.29366744	11.24775710
C	4.59622319	11.11970788	9.78370158
H	4.48294480	11.23234437	8.70965209
C	6.19409421	10.25168144	21.69235851
H	6.13225742	11.19539699	22.24376715
H	6.75249130	10.43275668	20.76799833
H	6.74141496	9.51763327	22.29482806
C	9.13195832	13.77650828	12.65169495
H	8.87630306	14.62356307	13.28617767
C	8.48291454	11.81606883	11.41393856
H	7.72191253	11.12382242	11.06645429
C	2.07313960	8.54679599	14.52273385
H	1.49101785	7.78056128	14.02188204
C	6.29919797	16.73226242	10.62099757
H	6.98466913	17.36609597	10.06474207
C	10.45971975	13.56434555	12.30006843
H	11.22547930	14.25084291	12.65080475
C	3.90941949	6.12175757	15.99461442
H	3.39152860	6.97535359	16.42458320
C	9.81674156	11.59441960	11.07721562
H	10.07861933	10.73390285	10.46746422
C	3.73860267	8.61457456	12.56303080
C	5.93663163	13.91609660	24.08097294
H	5.59701778	13.95174027	25.11232954
C	2.29934778	14.49966396	14.75026912
H	1.37204648	14.54217293	14.18502468
B	4.35803066	11.74184963	16.63948504
C	7.73443569	13.77408997	22.47003608
H	8.79909847	13.71218720	22.26611795
C	4.96127544	17.09293946	10.74610702
H	4.59749180	18.01219711	10.29564206
C	1.71795537	8.95354969	15.80295297
H	0.84765805	8.52057772	16.28897696
C	9.82807993	12.75313171	20.14163251
H	9.32170727	11.89122186	20.57286182
C	9.75059745	14.90262535	19.05992860
H	9.18993237	15.73607461	18.64730216
C	4.09043092	16.26141498	11.44968222
H	3.04224692	16.52920122	11.55469359
C	7.29439341	13.82032567	23.79245931
H	8.02187877	13.78797262	24.59914040
C	3.17553230	5.09756425	15.41097289
H	2.09008936	5.15383778	15.40178994
C	11.21691888	12.77517899	20.09616082
H	11.78174420	11.94007651	20.50144039
C	4.99689153	7.74607734	12.82569756
H	4.71830040	6.83987964	13.37363102
H	5.73434497	8.29236369	13.42293915
H	5.45680939	7.46233300	11.87214442
C	11.88061599	13.85683569	19.51952221
H	12.96590164	13.87043580	19.47285174
C	5.95627186	4.97714243	15.44953515
H	7.03961664	4.90676644	15.46997164
C	11.14264606	14.91507831	18.99866900
H	11.65034407	15.76060367	18.54244122
C	3.82790787	4.01061878	14.82982315
H	3.25578486	3.21233000	14.36536127
C	5.21789371	3.95483761	14.85400411
H	5.73692639	3.10735139	14.41423895
C	8.57179311	6.78329104	18.06503090
H	8.03386203	6.87200498	19.00419410
C	7.90266405	6.99126500	16.85483147
C	8.63194172	6.88788906	15.66043089
H	8.13625144	7.06676926	14.70775819
C	9.98264184	6.56131954	15.67531819
H	10.52615508	6.47743699	14.73819910
C	10.63935857	6.35687922	16.88781132
H	11.69776202	6.11243110	16.90185069
C	9.93018257	6.47308006	18.07921832
H	10.43381816	6.32038657	19.02995068
C	2.73181593	7.77326318	11.77975584
H	3.17546829	7.41663598	10.84569694
H	1.82255425	8.33707190	11.54472215
H	2.45563873	6.88494395	12.35532715
C	8.47946876	11.24936762	16.19674655
C	5.91498039	11.54113259	16.47076634
N	7.05164058	11.40278639	16.33843772
C	8.98574022	10.50479300	17.43479293
H	8.57415304	9.49354065	17.47271348
H	10.07690301	10.43981588	17.38386534
H	8.70573100	11.04324191	18.34357432
C	9.08150783	12.65409817	16.10206369
H	10.15975763	12.56430760	15.93835515
H	8.64085856	13.20038455	15.26461776
H	8.91142706	13.21218854	17.02568818
C	8.73513589	10.44621926	14.91916336
H	9.81096276	10.26986757	14.82486413
H	8.22273254	9.48213896	14.96542837
H	8.39119258	10.99462046	14.03921000

H2O

Energy: -76.47985644

O	5.96158259	11.54754347	16.41310444
H	6.24743477	10.63775328	16.54611580
H	6.27686023	11.76046599	15.52856939

MeNH

Energy: -95.94252194

N	10.02386468	3.94538165	5.74571813
C	8.78616681	3.48633962	5.09300117
H	8.69993958	3.95505867	4.10681144
H	7.86011804	3.70094951	5.65115598
H	8.83913311	2.40391295	4.93404745
H	10.09302989	3.52513258	6.66680037
H	9.96624789	4.94542501	5.90846546

NH3

Energy: -56.60686768

N	5.94246392	11.54719867	16.46745443
H	6.31244117	11.88063693	15.58321761
H	6.44876126	12.05326093	17.18680687
H	6.24312854	10.58108151	16.54569712

OpenCage

Energy: -4403.964741

P	-5.64757722	1.40157518	-0.28831858
P	3.62944903	1.59689244	0.38951000
P	2.78181250	-2.76955406	-1.18404387
O	1.02852978	2.62759079	-0.78661778
O	1.24063617	-1.59068480	1.14448227
O	-3.54577234	-0.80657742	-0.21443605
C	-0.31982219	2.96356023	-0.69601888
C	1.91479897	3.65664958	-0.54763973
C	0.27993930	5.16716625	-1.68610773
C	-0.74410372	4.24406336	-1.05924500
C	1.92639417	-2.72282702	1.53539818
C	1.56436349	4.97122858	-0.89598453
C	0.56822068	-0.83260642	2.07383918
C	-0.16865286	0.27425825	1.57575768
C	3.13852819	3.35168334	0.05154018
C	-1.18387708	1.97572926	-0.23523155
C	0.65615568	-1.10515411	3.43944307
C	1.93028588	-3.16792588	2.86136444
C	-2.42720625	-1.35738894	-0.84934329
C	-4.78978932	-1.27590823	-0.59917908
C	2.60874803	-3.43284252	0.52955662
C	-5.88198048	-0.39437914	-0.58680255
C	4.04431601	1.78321165	2.18151334
C	3.99552926	4.41052538	0.37061604
H	4.94634964	4.19280838	0.84968531
C	2.44034312	5.99562236	-0.55274696
H	2.18822557	7.02343206	-0.79140339
C	-1.21067911	-0.66643780	-0.79248269
C	-6.99130778	1.74474371	0.89866532
C	-6.24491845	2.12787360	-1.86521732
C	3.17776998	-4.66615041	0.85698193
H	3.65450839	-5.24798953	0.07314916
C	3.64703045	5.72191734	0.08963985
H	4.31729879	6.53368897	0.35595905
C	-0.67555344	1.17314639	2.53544440
H	-1.20673800	2.05399174	2.19044405
C	2.54586288	-4.38746410	3.14564202
H	2.55539131	-4.74872665	4.16978798

C	2.95085292	1.69219791	3.05398891
H	1.95857915	1.50289635	2.65297963
C	-4.94342022	-2.60314390	-1.03131872
C	1.34478760	-2.34152191	3.99017352
C	0.07529215	-0.20203081	4.33432978
H	0.14526663	-0.39781986	5.40048208
C	5.28572696	1.54652336	-0.41316865
C	0.31144815	-3.17731217	4.77712734
H	0.77841600	-4.05986461	5.22410798
H	-0.49671017	-3.50727989	4.11647349
H	-0.12456829	-2.58757970	5.58878404
C	3.14182724	-5.15367105	2.15463463
H	3.58975441	-6.11290031	2.39540582
C	-2.08298036	4.57372288	-0.86311434
H	-2.44215378	5.56672060	-1.11142225
C	-2.55008813	-2.58878756	-1.50335278
C	-0.17631554	6.62549366	-1.71185648
H	-1.08846159	6.72583001	-2.30677310
H	0.58180145	7.25450832	-2.18723214
H	-0.37049316	7.00874858	-0.70442018
C	-7.15116493	-0.89744026	-0.88936515
H	-8.00408592	-0.22485258	-0.85602502
C	2.42950486	-4.33067613	-2.11854086
C	-0.55992094	0.94720579	3.89927226
H	-0.97375297	1.65403376	4.61187027
C	0.53117922	4.70604105	-3.14525908
H	0.86015504	3.66356791	-3.18147681
H	1.30406444	5.33154047	-3.60537330
H	-0.39320554	4.79732700	-3.72572981
C	-6.67819568	1.56913381	2.25381600
H	-5.67334959	1.25982389	2.53538230
C	-6.21852409	-3.05387290	-1.36114510
H	-6.35524312	-4.07738360	-1.69314329
C	-8.28208237	2.16434371	0.55684091
H	-8.54457270	2.31400166	-0.48701312
C	-0.20401804	-1.10404328	-1.66477330
H	0.74995330	-0.58390612	-1.67611821
C	3.11334086	1.85256830	4.42547684
H	2.24691503	1.77787757	5.07690977
C	-2.52119973	2.34325304	-0.08309406
H	-3.22727876	1.61184769	0.28504804
C	-6.89201606	3.40524168	-4.28102416
H	-7.14656349	3.89791880	-5.21509258
C	-7.32723122	-2.21862021	-1.26531453
H	-8.31731820	-2.59403327	-1.50578254
C	2.49827539	-1.91490086	4.92812229
H	2.11869753	-1.33238985	5.77343409
H	3.22277698	-1.29951599	4.38540562
H	3.01440271	-2.79329486	5.32824543
C	-6.53922744	3.49978644	-1.89538715
H	-6.51634868	4.07936895	-0.97477056
C	-6.25545283	1.41411082	-3.06829419
H	-6.01548641	0.35480632	-3.07274273
C	-1.53215940	-2.97448495	-2.37113908
H	-1.61338025	-3.89936169	-2.93207770
C	-9.23454218	2.39833979	1.54505678
H	-10.23163146	2.72605802	1.26330813
C	-6.87278239	4.12802829	-3.08884673
H	-7.11210867	5.18794232	-3.08929883
C	1.24325984	-5.01817597	-1.82250619
H	0.61017052	-4.67543985	-1.00785850
C	-6.57585827	2.05061651	-4.26555394
H	-6.58011339	1.47942469	-5.18993216
C	-3.71009755	-3.48203894	-1.09455339
C	4.37823257	2.08740402	4.95779695
H	4.51016875	2.20234365	6.03014153
C	-2.96672640	3.62771984	-0.35916739
H	-4.01178925	3.87863850	-0.20237653
B	-0.79074197	0.51363226	0.16475602
C	5.30735493	2.02869165	2.72777832
H	6.17417097	2.11171988	2.07798078
C	-8.91670980	2.20631689	2.88709964
H	-9.66210002	2.38800150	3.65628658
C	-0.38679377	-2.19767552	-2.50010548
H	0.39789302	-2.49368346	-3.18825700
C	6.21275864	0.58342059	0.00984452
H	5.96257310	-0.09062630	0.82587919
C	5.61484547	2.35682401	-1.50558811
H	4.90589841	3.09583780	-1.86715728
C	-7.63554829	1.78644825	3.23857183
H	-7.37663082	1.64056962	4.28363866
C	5.47321226	2.17397375	4.10283945
H	6.46526851	2.36334794	4.50414083
C	0.86824318	-6.13694648	-2.55587578
H	-0.05183372	-6.65852071	-2.30488931
C	7.46065690	0.48917374	-0.59340993
H	8.17238776	-0.24866069	-0.23613289
C	-3.88552696	-4.67782526	-2.03068300
H	-2.97136130	-5.27829499	-2.05015849
H	-4.11897523	-4.36222554	-3.05308444
H	-4.68404890	-5.33444156	-1.67479132
C	7.78992049	1.31853004	-1.66293547
H	8.76381233	1.23848094	-2.13796488
C	3.22244850	-4.79062713	-3.17350861
H	4.15040490	-4.28336876	-3.42115214
C	6.85537995	2.23832182	-2.12764227
H	7.09344883	2.87980613	-2.97192255
C	1.66579430	-6.58934747	-3.60620745
H	1.37287486	-7.46451870	-4.17928983
C	2.84237625	-5.91191347	-3.90946722
H	3.47758150	-6.25888374	-4.72010083
C	5.59975498	-3.11829162	-0.56390005
H	5.32952460	-3.57387415	0.38334893
C	4.60907340	-2.63061727	-1.42046196
C	5.00182714	-1.99777293	-2.60910952
H	4.24520901	-1.56935721	-3.26396422
C	6.34300766	-1.92538146	-2.96861651
H	6.62655890	-1.44080021	-3.89869738
C	7.31808861	-2.45441754	-2.12827250
H	8.36752631	-2.39261381	-2.40305873
C	6.94370061	-3.03122331	-0.91857548
H	7.70148069	-3.41978887	-0.24309128
C	-3.41195287	-4.01371008	0.33182473
H	-4.23379650	-4.65471650	0.67007219
H	-3.29922098	-3.18973176	1.04293762
H	-2.48306524	-4.59517261	0.32719537

Tbunc

Energy: -250.8898552

C	8.46772060	11.25179992	16.19810578
C	5.88374023	11.53174719	16.46702379
N	7.03830549	11.40281847	16.33748774
C	8.98746187	10.50334316	17.43101850
H	8.52586390	9.51456163	17.50584492
H	10.07097555	10.37965495	17.34287195
H	8.77095175	11.06524019	18.34411939
C	9.08574634	12.65197723	16.10710767
H	10.17030535	12.55670529	15.99927160
H	8.69254084	13.19227440	15.24119017
H	8.87170426	13.22888982	17.01139026
C	8.73840978	10.45179152	14.91863596
H	9.81864496	10.32911511	14.79636448
H	8.27645795	9.46197720	14.97583291
H	8.34336299	10.97660711	14.04402220

Cage_ipr

Energy: -3724.869859

P	16.28908538	5.51304780	6.19935964
P	12.98344040	9.25050189	6.91969051
P	13.95161220	4.90745963	10.76430239
O	13.83147032	8.97595794	9.79002824
O	16.78566296	5.63563429	10.14298427
O	17.10281901	8.30739238	6.59893310
C	17.99779387	6.20203114	9.80378943
C	14.58872585	9.03556993	10.94707599
C	16.95665603	9.58402574	7.10003183
C	17.96411280	7.56199930	9.42913460
C	15.93834627	8.67003104	10.83841635
C	16.63331059	9.69661475	8.46350632
C	17.78727834	3.42659940	10.17048081
C	15.36977708	3.75665536	10.46141318
C	16.79566199	8.10792376	5.26735954
C	12.77401057	9.86035286	9.67429244
C	16.34890359	6.82917770	4.90330258
C	17.11309377	10.68229241	6.25253147
C	14.00243135	9.43247929	12.15074308
C	16.67003538	4.26437266	10.24734320
C	12.33337844	10.18581010	8.38049204
C	19.18955817	8.16377849	9.10250238
H	19.19430355	9.20856090	8.80208059
C	14.01336503	4.97940170	12.66288954
H	13.22750216	5.70505846	12.91629380
C	17.57374757	2.04643676	10.21159655
H	18.42273954	1.37281765	10.15752900
C	14.81634841	9.49468673	13.28328751
H	14.39747439	9.81795797	14.23039987
C	16.95639833	9.14978877	4.34993058
C	19.18149894	5.46085622	9.81972006
C	15.08770325	4.26224328	5.49652398
H	15.35370780	3.98996524	4.46729986

C	16.38169915	10.99710174	8.93493419
H	16.12023222	11.13228771	9.98144664
C	15.21561277	2.36912705	10.49800580
H	14.23206897	1.94140604	10.65783709
C	16.69971593	8.69922196	12.01928798
H	17.74828400	8.41435126	11.97202000
C	19.20264497	3.98395121	10.17721621
C	17.96777822	4.68770828	5.90459981
H	18.02172153	3.93460274	6.70494029
C	16.30090597	1.51438556	10.34919579
H	16.15728979	0.43824633	10.37621363
C	15.99541206	6.63772277	3.56313215
H	15.63543621	5.66812976	3.23332590
C	12.59547123	10.38177450	5.47653654
H	11.53653773	10.66795489	5.48443620
C	16.86686581	11.94992381	6.77986073
H	16.96530327	12.82664908	6.14799582
C	12.16469863	10.36865240	10.82809569
C	11.33449455	11.16111670	8.27806451
H	10.97049444	11.45606187	7.29933514
C	20.37549854	6.13221312	9.53940770
H	21.31469310	5.59028792	9.58960572
C	20.39121530	7.47327827	9.18898009
H	21.33078853	7.97124533	8.96854721
C	15.35220638	5.56209560	13.11483346
H	16.16821959	4.85173639	12.93426747
H	15.32410438	5.77284407	14.19078686
H	15.58920084	6.49099690	12.59174350
C	12.44320440	3.81778304	10.49973066
H	12.52132988	2.91190851	11.11316653
C	16.57623890	8.91749248	3.02913916
H	16.66817038	9.70709662	2.29059835
C	16.15721234	9.13043199	13.22294418
H	16.77181248	9.17161142	14.11751900
C	12.51188875	9.72369168	12.16267448
C	17.62028249	10.42752442	4.84060766
C	16.08710887	7.67372667	2.63968826
H	15.79419571	7.50659672	1.60714403
C	10.79220782	11.76513392	9.40578131
H	10.03174318	12.53314161	9.29824845
C	16.48789954	12.10901979	8.10937299
H	16.29244830	13.10254879	8.50228881
C	11.18736600	11.34964025	10.67344027
H	10.71239529	11.78433731	11.54639331
B	16.74081780	8.53584711	9.50702295
C	11.61918543	7.94268255	6.77149127
H	11.96007612	7.30984069	5.93977696
C	13.67856487	4.85955592	5.50764869
H	13.39638361	5.16125266	6.52278002
H	12.94809927	4.11923952	5.15898490
H	13.60485290	5.74158547	4.86265502
C	13.73053176	3.66603445	13.39045909
H	12.72095983	3.28760959	13.20757820
H	13.83410732	3.82066283	14.47198723
H	14.44840305	2.89123837	13.09681152
C	18.14143228	3.99766086	4.55337919
H	17.42100370	3.19038860	4.39363685
H	19.14716117	3.56256149	4.49053602
H	18.04044322	4.71656123	3.73194763
C	20.09912416	3.21055743	9.18914395
H	20.15765308	2.15290934	9.45704925
H	21.12130514	3.59575440	9.20392174
H	19.71230016	3.29146883	8.16843772
C	15.15856831	3.00362011	6.36989067
H	16.12201741	2.49119257	6.28061919
H	14.37303076	2.29709957	6.07589766
H	15.00810337	3.25448141	7.42711130
C	19.77132055	3.82527544	11.60757554
H	19.14980349	4.36519425	12.32996054
H	20.79057578	4.22415233	11.65659901
H	19.79508402	2.76691549	11.88972167
C	11.76244065	8.36845864	12.23454529
H	12.05791396	7.71052419	11.41062242
H	10.68059890	8.53408412	12.17751095
H	11.99583745	7.86496481	13.17958313
C	11.20539317	4.59757972	10.96308294
H	11.24889467	4.85510826	12.02630492
H	10.30540226	3.99239235	10.80132803
H	11.09250618	5.52747096	10.39449977
C	19.08519492	5.70848698	6.13165997
H	19.10442474	6.44283020	5.31750899
H	20.05768062	5.20150974	6.14921736
H	18.96415193	6.24865293	7.07398831
C	13.45415183	11.64496746	5.54899323
H	13.27980436	12.21162096	6.46981692
H	13.23248882	12.30021154	4.69764294
H	14.51801100	11.38865480	5.51189915
C	12.08928545	10.58035558	13.35664933
H	12.31958678	10.06846135	14.29472488
H	11.00806529	10.74222817	13.34585929
H	12.59136641	11.55380010	13.35418918
C	12.88095411	9.61037709	4.18203583
H	13.92239592	9.26635148	4.15579442
H	12.72105575	10.26320992	3.31531280
H	12.23134823	8.73647647	4.06667529
C	11.60226030	7.08847801	8.03931540
H	12.59784339	6.71500779	8.30279595
H	10.93736812	6.22806724	7.89896847
H	11.22401870	7.66515953	8.89249640
C	19.14709788	10.16570838	4.92594344
H	19.65604141	11.05927582	5.30416566
H	19.54010930	9.92550305	3.93183324
H	19.36664606	9.33028977	5.59854887
C	17.38178387	11.61055277	3.90212292
H	16.31542708	11.83719204	3.79631710
H	17.79483325	11.39791592	2.91230357
H	17.89584753	12.50129988	4.27328800
C	12.29878153	3.40573641	9.03399835
H	12.22192118	4.28467815	8.38688868
H	11.38609257	2.81137181	8.90295663
H	13.14429868	2.80565292	8.68734003
C	10.21595960	8.45756569	6.45703763
H	9.85952801	9.13239481	7.24353403
H	9.51941771	7.61110521	6.40488525
H	10.16556010	8.98635440	5.50071694

OpenCage_ipr

Energy: -3724.849915

P	-4.59985256	0.60082963	1.10083657
P	3.28471913	1.62396076	0.84973450
P	2.49181130	-2.98542076	-1.14745726
O	1.22513365	2.65325114	-1.05447698
O	0.42200637	-1.68450519	0.62934163
O	-3.01659489	-1.33235215	-0.48965363
C	0.05865770	2.88559313	-1.75672784
C	1.72957542	3.68486407	-0.28621362
C	0.73605116	5.29524910	-1.93357228
C	-0.23719838	4.16543736	-2.22782644
C	1.40014095	-2.32985393	1.37625941
C	1.38989033	5.00860313	-0.58767470
C	-0.15838129	-0.57104546	1.21975425
C	-0.54347606	0.49436966	0.38440379
C	2.59811878	3.34257471	0.76286716
C	-0.77365753	1.77381897	-1.97606204
C	-0.29137218	-0.53130714	2.61020171
C	1.28437000	-2.35995068	2.77280417
C	-2.27319530	-1.68791873	-1.60314304
C	-4.33611514	-1.74840689	-0.43250524
C	2.47378512	-2.93069967	0.69892808
C	-5.22065279	-0.95965296	0.32124578
C	2.98752554	4.37579451	1.62230803
H	3.64340147	4.16320043	2.46024129
C	1.79237935	6.00049583	0.30495556
H	1.52659744	7.03608784	0.12238991
C	-1.21048346	-0.84025067	-1.95177702
C	3.48112284	-3.50207793	1.48777517
H	4.32771965	-3.97426308	1.00485542
C	2.55692911	5.68234745	1.42331162
H	2.85711259	6.46371374	2.11541409
C	-0.91165777	1.68197651	1.04601559
H	-1.17675873	2.54691394	0.44737075
C	2.32032880	-2.92307224	3.51279431
H	2.26659011	-2.93835208	4.59627911
C	-4.74271602	-2.90665013	-1.10157726
C	0.00627465	-1.80682519	3.37941434
C	-0.69623560	0.66316739	3.20466693
H	-0.78024542	0.72820177	4.28453256
C	-1.14096948	-2.81761519	3.12125626
H	-0.92485227	-3.76301133	3.63094219
H	-1.26290890	-3.01873728	2.05278067
H	-2.08349684	-2.41274122	3.50654610
C	3.42360361	-3.48068119	2.87420637
H	4.22811023	-3.91771265	3.45877439
C	-1.38493796	4.32117802	-3.00815813
H	-1.64526173	5.30128952	-3.39432187
C	-2.63139932	-2.81561111	-2.35015782
C	0.06261475	6.66872344	-1.97285380
H	-0.35473147	6.86389580	-2.96375470
H	0.79445923	7.45853257	-1.78362894
H	-0.74002967	6.74620038	-1.23164303
C	-6.54908119	-1.38969951	0.40143317

H	-7.26744595	-0.81857703	0.97998835
C	-0.97224561	1.78087249	2.42682015
H	-1.26372310	2.71602921	2.89627521
C	1.84800973	5.25553524	-3.01350138
H	2.32928949	4.27306426	-3.04165633
H	2.61000747	6.01252863	-2.79722647
H	1.41376329	5.45673554	-3.99915117
C	-6.08500486	-3.27597114	-1.01877134
H	-6.43382616	-4.16584648	-1.53135754
C	-0.55515509	-1.12545532	-3.16133865
H	0.25046036	-0.47048987	-3.48529960
C	-1.87974826	1.97701633	-2.82094706
H	-2.53280491	1.13513971	-3.03690916
C	-6.98250770	-2.52958626	-0.26472357
H	-8.02261690	-2.83527235	-0.19741986
C	0.11620983	-1.57947032	4.88575943
H	-0.82772605	-1.18964705	5.27771240
H	0.91720573	-0.87569537	5.13633084
H	0.30861960	-2.52601955	5.39886569
C	-1.94286499	-3.05136929	-3.53988342
H	-2.20289705	-3.90615986	-4.15521106
C	-3.68529123	-3.75688978	-1.78488233
C	-2.18944057	3.23255807	-3.32685637
H	-3.06524335	3.37018640	-3.95429359
B	-0.75956723	0.43825041	-1.15947777
C	-0.91154760	-2.21130218	-3.94907180
H	-0.38730231	-2.40900534	-4.87957422
C	-4.27506673	-4.68091646	-2.85233422
H	-3.48910860	-5.29755218	-3.29641936
H	-4.77189977	-4.11529872	-3.64774588
H	-4.99679243	-5.37022896	-2.40683692
C	-3.02122941	-4.63294255	-0.69221259
H	-3.77810010	-5.26705800	-0.21702531
H	-2.55176361	-4.01204362	0.07777352
H	-2.25301348	-5.26955711	-1.14068798
C	-5.91432095	0.93684834	2.39720149
H	-6.92057213	0.89761495	1.96090412
C	-4.99026958	1.77106048	-0.34299148
H	-4.52999631	1.24501382	-1.19378417
C	-6.47695328	1.96097901	-0.63898155
H	-6.59969425	2.53967448	-1.56312304
H	-6.99667366	1.00661890	-0.76857293
H	-6.97328908	2.51677899	0.16442975
C	-4.27721874	3.11896193	-0.19628219
H	-3.20041555	2.99049333	-0.06109579
H	-4.43182240	3.71732316	-1.10232071
H	-4.66251250	3.69437738	0.65099088
C	-5.79030744	-0.12929990	3.49291732
H	-6.54638524	0.04044551	4.26901220
H	-5.92343832	-1.14412569	3.10530533
H	-4.80242012	-0.07608964	3.96713828
C	-5.71045397	2.33147080	3.00121486
H	-5.94452992	3.12925766	2.29169230
H	-6.36923728	2.45556929	3.86923738
H	-4.67658028	2.46809046	3.34249022
C	4.30468350	-2.88218507	-1.67841245
H	4.16917619	-2.63931299	-2.74401174
C	4.94154309	-1.65713472	-1.01853669
H	5.18344766	-1.85205529	0.03189856
H	5.86905932	-1.38289208	-1.53554796
H	4.26466234	-0.79685522	-1.04796817
C	5.23319072	-4.09773666	-1.63016835
H	4.81041622	-4.95912904	-2.15466337
H	6.17572239	-3.83860577	-2.12992643
H	5.48422271	-4.40145447	-0.60984198
C	1.98137537	-4.78153133	-1.44189556
H	2.31203404	-4.97699755	-2.47374247
C	0.45260564	-4.84013559	-1.39346372
H	-0.00989908	-4.14421355	-2.09830137
H	0.10244354	-5.85406189	-1.62482431
H	0.09120646	-4.58868243	-0.38788453
C	2.55710128	-5.85371630	-0.51455564
H	2.23671936	-6.84333866	-0.86491351
H	3.64739679	-5.85107947	-0.46895485
H	2.17635615	-5.72313927	0.50405095
C	4.86594252	1.89464250	-0.16216554
H	5.37985917	0.92648243	-0.08896301
C	3.95149899	1.51352313	2.59849317
H	4.58132924	2.38123820	2.83071023
C	4.50279290	2.13070004	-1.63039281
H	4.03392104	3.11316392	-1.75773849
H	5.40843386	2.11187749	-2.24829262
H	3.80959398	1.37339221	-2.01219271
C	5.80942249	2.98441729	0.34197313
H	5.32707811	3.96775950	0.31274168
H	6.15256784	2.80117607	1.36482680
H	6.69669142	3.02882100	-0.30243382
C	2.78880473	1.45556403	3.59119352
H	2.17834331	0.56327478	3.41312762
H	3.17206175	1.40516922	4.61773725
H	2.13187354	2.32836510	3.51382101
C	4.81229889	0.24955052	2.70962172
H	5.12747928	0.10540159	3.75015084
H	4.24478095	-0.63904290	2.40536495
H	5.71421380	0.30662503	2.09182870

F_CO

Energy: -4526.23970241 Eh

P	6.97035600	12.83005200	13.35887200
P	7.02255400	13.59673900	19.50937000
P	5.80341400	7.75614400	16.53889300
O	5.63789200	14.22413100	16.94420900
O	5.25358600	9.92677100	18.47513300
O	4.97035600	10.82163100	14.18898000
C	4.55068900	14.25816700	16.08595900
C	5.91825800	15.38653000	17.63655600
C	5.08925300	16.66756200	15.65416500
C	4.19029000	15.45539400	15.46063200
C	5.26238900	8.71033100	19.12580200
C	5.58783100	16.63112700	17.08870200
C	4.47539200	10.93097100	19.02464600
C	3.95190200	11.88429300	18.14111600
C	6.56178200	15.26484600	18.87492500
C	3.83213800	13.06735400	15.91296500
C	4.23606700	10.96098600	20.39926400
C	5.03097900	8.64000500	20.50319200
C	3.92485700	10.12895800	14.75176600
C	5.36485600	10.54841500	12.90674700
C	5.53889300	7.57400800	18.35346900
C	6.35419800	11.39243700	12.37651300
C	7.26643300	13.98871800	21.29786800
C	6.82972000	16.43694000	19.58910000
H	7.32969700	16.36928600	20.55035100
C	5.84028400	17.77088700	17.84884800
H	5.57649500	18.74849000	17.45995200
C	3.54268500	10.57308100	16.02828300
C	6.54288600	14.15675600	12.14524900
C	8.79721300	12.68969100	13.21873100
C	5.54931100	6.33383200	18.99901500
H	5.76327900	5.43776200	18.42506900
C	6.45125300	17.67752200	19.09509500
H	6.65059400	18.57576100	19.67188100
C	3.14777700	12.88279800	18.68331600
H	2.71993500	13.63190700	18.02403600
C	5.01526600	7.38040800	21.09979600
H	4.82285600	7.28859900	22.16341100
C	6.10435600	14.15382300	22.06487100
H	5.13065600	14.07693700	21.58509000
C	4.80395500	9.50916200	12.15806800
C	4.94502700	9.94275100	21.28123700
C	3.41252600	11.97114900	20.89654300
H	3.19806000	12.02269000	21.95847800
C	8.75662500	13.44082100	18.90519300
C	4.25997600	9.77326500	22.63851000
H	4.80696100	9.05748400	23.25774200
H	3.22577400	9.42902200	22.53091300
H	4.26136900	10.72014100	23.18514800
C	5.26950700	6.23333400	20.35530000
H	5.26511700	5.26046600	20.83781300
C	3.04473900	15.46222200	14.66559400
H	2.72980100	16.37688100	14.17559400
C	3.29694000	9.06993400	14.10380500
C	4.38023900	17.97872700	15.31095300
H	4.06951400	17.97753600	14.26266100
H	5.06167500	18.82502200	15.43240900
H	3.49907300	18.14143500	15.94067600
C	6.78037600	11.17943300	11.06556400
H	7.52230800	11.84730000	10.63523400
C	5.63142400	5.99703100	16.00878500
C	2.87404500	12.92783200	20.04607400
H	2.23885400	13.71348600	20.44470000
C	6.32753100	16.52862400	14.73376300
H	6.84788300	15.58298700	14.91604800
H	7.02260800	17.35403400	14.92518900
H	6.02187000	16.55197800	13.68291200
C	5.17710600	14.44356600	12.02016100
H	4.45046900	13.88063500	12.60319500
C	5.28483100	9.31567200	10.86210700
H	4.87414500	8.50945300	10.26100400
C	7.46129500	14.90648300	11.40861000
H	8.52420800	14.69583400	11.48329000

C	2.50940500	9.89933100	16.66459300
H	2.19243000	10.22552400	17.65057800
C	6.18362600	14.40714200	23.42871900
H	5.27237800	14.53877300	24.00609900
C	2.70343700	13.11908600	15.09637100
H	2.11696500	12.21663300	14.95534500
C	11.59814000	12.52795600	13.35439800
H	12.68152200	12.46521200	13.40463000
C	6.26320600	10.13501100	10.31180500
H	6.60657400	9.96889800	9.29528000
C	6.39832700	10.42236100	21.52076400
H	6.39885300	11.37758200	22.05598500
H	6.91931600	10.56230000	20.56878000
H	6.94131700	9.67685700	22.11286200
C	9.55760800	13.76899900	13.69442200
H	9.05854100	14.67450100	14.03469700
C	9.46285000	11.52084100	12.83916200
H	8.89664700	10.65972300	12.49780900
C	2.26878900	8.41540800	14.78827100
H	1.76646800	7.57415500	14.31881200
C	7.02143800	15.92989000	10.56958800
H	7.74762200	16.50667700	10.00289300
C	10.94374400	13.69476100	13.74589000
H	11.51479300	14.54589400	14.10627600
C	4.32458500	5.49710400	15.92439400
H	3.48772600	6.14278400	16.18513600
C	10.85201800	11.44207000	12.90899200
H	11.35160400	10.52343700	12.61279400
C	3.69963100	8.61895100	12.70735100
C	7.42702800	14.47870400	24.05630400
H	7.49048800	14.66526400	25.12470300
C	2.30515400	14.30156500	14.48332200
H	1.41605000	14.31537200	13.85969300
C	8.50776800	14.07236800	21.93229600
H	9.42174200	13.95753000	21.35703700
C	5.66334400	16.20811400	10.44895800
H	5.32454300	17.00614400	9.79423500
C	1.88039300	8.81518300	16.05704700
H	1.08021800	8.29239000	16.57252500
C	9.47767400	12.29894100	19.28484500
H	9.02260500	11.56762600	19.94978200
C	9.35320000	14.35007400	18.02731900
H	8.81181800	15.23864600	17.71458600
C	4.74038500	15.45406600	11.17332000
H	3.67697700	15.66258400	11.08973300
C	8.58516600	14.30967400	23.30425000
H	9.55890200	14.37053400	23.78296700
C	4.08936300	4.19343100	15.50631900
H	3.07036200	3.81939100	15.45343600
C	10.77053300	12.08967100	18.82195000
H	11.31617300	11.20298500	19.13285600
C	4.20073400	7.15978700	12.75391100
H	3.42895300	6.49659100	13.15639300
H	5.08312900	7.07569500	13.39510600
H	4.46169300	6.80877500	11.75023400
C	11.35548500	13.00019500	17.94379400
H	12.35944800	12.82787300	17.56603200
C	6.69474500	5.16689900	15.64603000
H	7.71546100	5.53346500	15.70743100
C	10.64147000	14.12604100	17.54695100
H	11.08754100	14.83866500	16.85890900
C	5.15595100	3.37303300	15.13980800
H	4.97272400	2.35708900	14.80119000
C	6.45574300	3.86509000	15.20772600
H	7.29314600	3.23163200	14.92753500
C	8.47314600	8.09612700	17.52620300
H	8.07197900	7.97554700	18.52910400
C	7.62105500	8.01393600	16.42160500
C	8.15749700	8.18018100	15.13675700
H	7.50005000	8.14603700	14.26883600
C	9.52053800	8.38255100	14.96158000
H	9.92370100	8.50019100	13.95985800
C	10.36421600	8.46207300	16.06838000
H	11.42697900	8.64152800	15.93145100
C	9.83588700	8.32591300	17.34823500
H	10.48630100	8.39353000	18.21619700
C	2.46843800	8.70926000	11.77713900
H	2.71902700	8.37600100	10.76546800
H	2.10374400	9.74010600	11.72398100
H	1.65869900	8.07357000	12.14730100
C	4.22562100	11.78776100	16.64580400
O	8.98842400	11.44040800	16.07911400
C	7.93468400	11.37283800	16.48683200
H	5.30958100	11.65690300	16.52260000

R_acn

Energy: -4531.77380382 Eh

P	6.17948000	13.20195200	13.14312900
P	6.82307600	13.48387800	19.48863700
P	5.90423200	7.89097100	16.62432700
O	5.29890400	14.19359000	17.04395400
O	4.92372700	9.98041000	18.48304000
O	4.61494200	10.88080100	14.10915200
C	4.40825200	14.29408400	15.98372500
C	5.98575300	15.29633100	17.48496500
C	5.16735800	16.70378500	15.52365800
C	4.36130900	15.45543300	15.20008000
C	5.38055800	8.91004700	19.20899100
C	5.93322300	16.52543100	16.82033900
C	4.30578100	11.05035800	19.11519400
C	3.69057200	12.00599900	18.28575600
C	6.76235000	15.12982700	18.65171000
C	3.59413200	13.17399700	15.73238300
C	4.33329500	11.16607800	20.51195000
C	5.36344600	8.89147900	20.60686400
C	3.77147400	9.99312200	14.76190800
C	4.98582400	10.66220500	12.80674700
C	5.88039800	7.81618500	18.46989800
C	5.74271600	11.68115100	12.18936900
C	7.15820300	14.00800800	21.22457300
C	7.45118300	16.23478900	19.15449100
H	8.01877500	16.12978000	20.07421700
C	6.65597000	17.59500300	17.35277000
H	6.63574800	18.55316700	16.84188700
C	3.28479400	10.39253300	16.02047100
C	6.31916500	14.42568900	11.77135000
C	7.95997200	12.92144000	13.55893000
C	6.32550700	6.69162500	19.16649700
H	6.67581500	5.82821700	18.60892300
C	7.40304500	17.46553500	18.51383400
H	7.94802800	18.31503600	18.91447200
C	3.21953400	13.15743700	18.93134200
H	2.76735200	13.94037000	18.32448800
C	5.83627100	7.74962400	21.25722300
H	5.84069800	7.72277400	22.34296700
C	6.21810000	14.83440800	21.85894800
H	5.38922900	15.24130300	21.28486100
C	4.64491700	9.49496900	12.11682800
C	4.90279300	10.08636600	21.41925700
C	3.82310800	12.32752400	21.08734300
H	3.86605900	12.45469500	22.16528700
C	8.48314100	12.84100500	18.98225200
C	3.81011800	9.64561500	22.41883600
H	4.18313300	8.87483500	23.09988400
H	2.94374400	9.24516700	21.88231700
H	3.47792200	10.49108000	23.02791900
C	6.30557900	6.65027800	20.55415300
H	6.65850300	5.76972000	21.08257900
C	3.54822200	15.45460300	14.06919500
H	3.52307800	16.32998100	13.42642500
C	3.45919900	8.75323400	14.18728200
C	4.20575800	17.90671800	15.64785900
H	3.65742400	18.06199700	14.71463500
H	4.75305600	18.82864800	15.86497500
H	3.48107300	17.73564800	16.45064900
C	6.11741300	11.51505700	10.85528400
H	6.66750600	12.30810100	10.35769200
C	5.78148200	6.09543200	16.21918100
C	3.29592900	13.34140100	20.30256800
H	2.92847900	14.25607200	20.75997000
C	6.18413500	16.97236500	14.39163700
H	6.88810200	16.13882200	14.30931400
H	6.75177000	17.88801100	14.59005800
H	5.67759500	17.08170800	13.42743300
C	5.18450100	14.66410800	10.98080000
H	4.29994800	14.04562100	11.11327000
C	5.05726100	9.36979200	10.78848500
H	4.81002900	8.46486000	10.24102000
C	7.43801200	15.24495300	11.59009700
H	8.32677600	15.09115900	12.19520200
C	2.56660700	9.42021500	16.72972000
H	2.19858500	9.67218800	17.72303500
C	6.33571500	15.14433100	23.20788100
H	5.60143800	15.79466600	23.67612800
C	2.81975600	13.23558600	14.56580100
H	2.20052300	12.37674500	14.31153600
C	10.64792000	12.74823300	14.32657200
H	11.69146800	12.68257100	14.62355000
C	5.77899700	10.36755300	10.15074000

H	6.08027500	10.25065100	9.11402500
C	6.11815900	10.64514200	22.19111200
H	5.84289300	11.52981000	22.77386000
H	6.90827800	10.93430100	21.49150000
H	6.52061500	9.89168100	22.87669500
C	8.34849500	13.22997700	14.86566500
H	7.59732800	13.54350400	15.58808400
C	8.93399200	12.50492100	12.64334100
H	8.65140800	12.25378600	11.62461400
C	2.71949600	7.84521200	14.94109700
H	2.49502100	6.86556900	14.52889200
C	7.42724900	16.26565400	10.64086000
H	8.30856100	16.88943500	10.51657900
C	9.68526300	13.14307800	15.24889900
H	9.96731100	13.38164800	16.26937000
C	4.64722900	5.39396400	16.65515200
H	3.93471000	5.88406300	17.31433900
C	10.26987700	12.42599800	13.02263200
H	11.01806500	12.10858000	12.30074900
C	3.90056400	8.35639900	12.78690900
C	7.38770900	14.62130600	23.96023300
H	7.47792400	14.86001600	25.01625100
C	2.80102700	14.33833600	13.72709200
H	2.19486800	14.33801200	12.82519700
B	3.26282300	11.88879900	16.70266200
C	8.20765800	13.48826400	21.98890000
H	8.94477400	12.83745300	21.52752100
C	6.30057700	16.48535000	9.85528600
H	6.29443900	17.27908200	9.11351600
C	2.29830500	8.15821800	16.22421200
H	1.74789500	7.43089200	16.81497900
C	8.54234800	11.49718800	18.60283500
H	7.62609600	10.91207700	18.55290400
C	9.66915400	13.58406200	19.02716000
H	9.64326400	14.63235100	19.31141400
C	5.17783800	15.67555100	10.02867100
H	4.29121500	15.83564600	9.42075200
C	8.31985700	13.79247200	23.34462000
H	9.14441900	13.37835800	23.91897700
C	4.42545100	4.08049600	16.26081100
H	3.54521800	3.55307800	16.61911800
C	9.76186300	10.89979300	18.29066500
H	9.78632600	9.85708000	17.99097300
C	4.84774600	7.13842400	12.86438000
H	4.37243600	6.30111100	13.38482400
H	5.75889100	7.40027300	13.41107600
H	5.13095600	6.80499700	11.86026000
C	10.93617000	11.64123500	18.35704400
H	11.88820900	11.17574100	18.11536800
C	6.67468200	5.44530800	15.36146300
H	7.55563700	5.96737000	14.99952100
C	10.88802500	12.98654300	18.72370500
H	11.80242100	13.57262200	18.76875800
C	5.32403300	3.44167200	15.40593600
H	5.14856000	2.41597100	15.09377600
C	6.44643500	4.13067300	14.95852100
H	7.15446500	3.64507100	14.29206900
C	8.75735300	7.53012600	16.84576100
H	8.56969700	6.80521300	17.63301000
C	7.68823300	8.21448400	16.25495500
C	7.95662700	9.15149600	15.25306600
H	7.13427700	9.69851700	14.79572700
C	9.26422700	9.38742000	14.83303700
H	9.45406600	10.12280800	14.05773400
C	10.31701000	8.68660900	15.41087400
H	11.33704700	8.86768700	15.08199000
C	10.06203900	7.75912400	16.42160100
H	10.88277900	7.21567800	16.88280000
C	2.65250700	7.98861900	11.95300400
H	2.93041700	7.69043800	10.93777100
H	1.97174000	8.84380100	11.89041300
H	2.11567900	7.15150900	12.40807600
C	0.57991000	12.20742500	16.95587900
C	-0.84197700	12.37360300	17.09030000
H	-1.34297000	11.42437600	16.87760600
H	-1.07908000	12.68918600	18.11080100
H	-1.18947800	13.13416300	16.38455300
N	1.71464000	12.07510200	16.84680200

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Energy: -4492.03491718 Eh

P	6.17577300	13.21751600	13.13824000
P	6.80635700	13.48438400	19.50880800
P	5.87843100	7.87233500	16.62306700
O	5.30390800	14.19639500	17.05769700
O	4.92411100	9.96502300	18.48290600
O	4.62370100	10.88818100	14.09941100
C	4.41607400	14.29486800	15.98393300
C	5.99800600	15.28967500	17.49064300
C	5.19464400	16.70186500	15.52651200
C	4.38828400	15.45496400	15.19707600
C	5.39656200	8.90783500	19.20604000
C	5.96210200	16.51868000	16.82105000
C	4.31066100	11.04683000	19.11803900
C	3.68792200	11.99548600	18.28800800
C	6.77422900	15.12448400	18.66010600
C	3.59596000	13.17923800	15.73873500
C	4.35601000	11.16248900	20.51461400
C	5.39879700	8.89239400	20.60577300
C	3.78064500	9.99060700	14.75777500
C	5.00849400	10.66571100	12.80852500
C	5.89882800	7.81152300	18.46851600
C	5.76792500	11.68511200	12.19042300
C	7.15421600	14.01826500	21.23967300
C	7.47743200	16.22289400	19.15637500
H	8.04324000	16.11541900	20.07707800
C	6.69703400	17.58199700	17.34846900
H	6.68503300	18.53809600	16.83294100
C	3.28453300	10.39428500	16.01003600
C	6.31565300	14.43023500	11.75628200
C	7.95854100	12.95860000	13.56847800
C	6.36925000	6.69703700	19.16397400
H	6.72138200	5.83494000	18.60529500
C	7.44417500	17.45126700	18.50980700
H	7.99827800	18.29700100	18.90640600
C	3.22087300	13.14493900	18.94237900
H	2.73664200	13.91108300	18.33995600
C	5.89314100	7.75920100	21.25458300
H	5.90719300	7.73736800	22.34059100
C	6.21919600	14.85445900	21.86955100
H	5.38874000	15.25602000	21.29411600
C	4.68464900	9.49241200	12.11684600
C	4.92612300	10.08088600	21.41974100
C	3.85229000	12.32391900	21.09519400
H	3.90036500	12.45076200	22.17325200
C	8.45815300	12.81359300	19.00470000
C	3.82809000	9.62635300	22.40795300
H	4.19845200	8.84885600	23.08385700
H	2.96694000	9.23069100	21.85984400
H	3.48834400	10.46634500	23.02059800
C	6.36912400	6.66186600	20.55211200
H	6.73908100	5.78804700	21.08046100
C	3.58447700	15.45873300	14.05990400
H	3.56691000	16.33381900	13.41595300
C	3.48618900	8.74761200	14.18002900
C	4.23190400	17.90344300	15.66026900
H	3.68390500	18.06365700	14.72759400
H	4.77738900	18.82472900	15.88755800
H	3.50578500	17.72167000	16.45922000
C	6.16157500	11.51366500	10.86275800
H	6.71153500	12.30829300	10.36734400
C	5.76649500	6.07175900	16.23740900
C	3.31463600	13.33343100	20.31121600
H	2.93754100	14.24378900	20.77021100
C	6.20941700	16.98097400	14.39507500
H	6.91427000	16.14864100	14.30591500
H	6.77676300	17.89653600	14.59691000
H	5.70085500	17.09470300	13.43254800
C	5.18350700	14.64818000	10.95561000
H	4.30438700	14.02289100	11.09151200
C	5.11490600	9.36298000	10.79504400
H	4.87724200	8.45394400	10.24971400
C	7.42482900	15.26285300	11.57440900
H	8.31039500	15.12750100	12.18853500
C	2.56635900	9.41381500	16.71013300
H	2.16563500	9.67713700	17.68705200
C	6.34057500	15.17514200	23.21542200
H	5.60805000	15.83069900	23.67926100
C	2.82778400	13.25015800	14.56728400
H	2.18017700	12.40783300	14.33175800
C	10.63704800	12.79151400	14.37432400
H	11.67620100	12.72672300	14.68701400
C	5.83984000	10.36039200	10.15961700
H	6.15396200	10.23993800	9.12693400
C	6.13172300	10.64042900	22.20648100
H	5.84634400	11.52033700	22.79135100
H	6.92600700	10.93891500	21.51531300
H	6.53368200	9.88616800	22.89202500
C	8.32500700	13.24253900	14.88703200
H	7.55949700	13.53257400	15.60420800
C	8.95118500	12.57113900	12.65986900

H	8.68593100	12.33805600	11.63219600
C	2.74978000	7.83258200	14.92824100
H	2.53166200	6.85200400	14.51405900
C	7.40839900	16.27425700	10.61516900
H	8.28240300	16.90888500	10.49258100
C	9.65653600	13.15865700	15.28931200
H	9.91973100	13.37636700	16.31943900
C	4.64346000	5.36887600	16.70077500
H	3.93790100	5.86506900	17.36287700
C	10.28197600	12.49530300	13.05771500
H	11.04375800	12.19881300	12.34090900
C	3.93267100	8.35528500	12.77981700
C	7.39132700	14.65375100	23.97113200
H	7.48338300	14.89991000	25.02543700
C	2.82819700	14.34693800	13.72161900
H	2.21604100	14.35166300	12.82337500
B	3.23079600	11.89132700	16.70483800
C	8.20151000	13.49944500	22.00791500
H	8.93342300	12.83938400	21.55138400
C	6.28486100	16.47234800	9.81939600
H	6.27332400	17.25975100	9.07075600
C	2.31597400	8.14791800	16.20694500
H	1.75528100	7.42285800	16.79141900
C	8.48903400	11.47467000	18.60509600
H	7.55960100	10.91170600	18.54545300
C	9.66016900	13.52985000	19.06082200
H	9.65560100	14.57449600	19.35970500
C	5.17094800	15.65030100	9.99401300
H	4.28496900	15.79497600	9.38118900
C	8.31771100	13.81443500	23.36099800
H	9.14009200	13.39896800	23.93785600
C	4.42140400	4.05023300	16.32509000
H	3.54833200	3.52429000	16.70275400
C	9.69557700	10.85600200	18.28348700
H	9.69773400	9.81783300	17.96718000
C	4.87268400	7.13143900	12.85389600
H	4.38903800	6.29424000	13.36653500
H	5.78118200	7.38516500	13.40908700
H	5.16152600	6.80145500	11.84982200
C	10.88560600	11.57099100	18.36062400
H	11.82724100	11.08892900	18.11014400
C	6.64640000	5.41580800	15.37011800
H	7.51667000	5.93897800	14.98464800
C	10.86633200	12.91119200	18.74837300
H	11.79309400	13.47719600	18.80129500
C	5.30791800	3.40540800	15.46170200
H	5.13118500	2.37572100	15.16315900
C	6.41806900	4.09537800	14.98602900
H	7.11567600	3.60675900	14.31053800
C	8.74338800	7.52394000	16.75793000
H	8.58232600	6.77126100	17.52500400
C	7.65234900	8.21345200	16.21456900
C	7.88741400	9.18625200	15.23891200
H	7.04784300	9.73767700	14.81984200
C	9.18224500	9.45436100	14.79913300
H	9.34492200	10.21859700	14.04596100
C	10.25655900	8.74906900	15.32987000
H	11.26686800	8.95646800	14.98627300
C	10.03554100	7.78386700	16.31309800
H	10.87320500	7.23649800	16.73831500
C	2.68657600	7.99816300	11.93757800
H	2.96656000	7.70655300	10.92034200
H	2.00961300	8.85664200	11.88114800
H	2.14464000	7.16136900	12.38723900
C	1.61940800	12.08540200	16.85422300
N	0.46988600	12.22325300	16.96125800

R_CO

Energy: -4512.39126994 Eh

P	6.18834100	13.20269800	13.12821800
P	6.82188400	13.49948200	19.50171000
P	5.89511700	7.86860900	16.63632100
O	5.32170300	14.20546800	17.05100900
O	4.94387300	9.96236700	18.49261600
O	4.64027900	10.87627000	14.09113000
C	4.43683900	14.30610900	15.99333600
C	6.00790100	15.31186600	17.49226100
C	5.17864700	16.71657000	15.53246500
C	4.37144700	15.46762200	15.21494200
C	5.40282900	8.89190400	19.22247400
C	5.95314900	16.53816200	16.82493600
C	4.32782900	11.02736700	19.12287600
C	3.73535700	11.99407100	18.28725800
C	6.77922300	15.14410400	18.66065000
C	3.64353400	13.17270700	15.72792500
C	4.33477200	11.14347800	20.51783500
C	5.38767200	8.87991800	20.61937200
C	3.79914500	9.99063800	14.73804700
C	5.01013900	10.65840000	12.78538700
C	5.89791500	7.79827700	18.48243100
C	5.76360400	11.68004900	12.17125500
C	7.15504200	14.02338100	21.23718600
C	7.47050200	16.24815400	19.16170300
H	8.03619700	16.14441400	20.08277900
C	6.67883300	17.60701900	17.35519200
H	6.65961800	18.56496900	16.84399600
C	3.33375800	10.38168400	16.00874600
C	6.31765400	14.43100700	11.76053900
C	7.96808000	12.93298900	13.55094700
C	6.35172100	6.67798600	19.18001500
H	6.70025600	5.81295400	18.62381100
C	7.42627400	17.47667900	18.51609200
H	7.97359000	18.32570500	18.91443100
C	3.23227500	13.13788700	18.92370300
H	2.78872400	13.92229400	18.31089200
C	5.87006900	7.74263600	21.27099700
H	5.87860400	7.71809300	22.35669400
C	6.21111400	14.84818900	21.86793400
H	5.38205200	15.25229900	21.29179900
C	4.66773700	9.49127600	12.09798900
C	4.91301200	10.07209700	21.42914400
C	3.80257000	12.30024100	21.08531800
H	3.82580700	12.42507800	22.16398500
C	8.47198700	12.83514700	18.99463200
C	3.82318200	9.62166900	22.42707300
H	4.20477800	8.85662000	23.10952400
H	2.96195100	9.21052400	21.89064600
H	3.48103000	10.46374800	23.03522500
C	6.34194100	6.64407400	20.56814000
H	6.70261500	5.76758700	21.09800700
C	3.54393600	15.46267000	14.09313900
H	3.50185300	16.34185400	13.45679100
C	3.46837800	8.75793400	14.16335100
C	4.21766300	17.91898000	15.66273600
H	3.66304500	18.07473400	14.73336100
H	4.76763100	18.84024300	15.87500100
H	3.49870000	17.74923600	16.47074800
C	6.14008500	11.51457000	10.83766400
H	6.68783700	12.30896600	10.33961800
C	5.76740500	6.07344900	16.23584500
C	3.27534500	13.31134800	20.29760700
H	2.88284000	14.21585300	20.75289300
C	6.18673700	16.98171600	14.39208700
H	6.88983200	16.14781900	14.30580000
H	6.75572700	17.89754300	14.58486000
H	5.67244300	17.08991500	13.43179000
C	5.17830100	14.66512800	10.97555000
H	4.29717000	14.04195100	11.10985100
C	5.08327700	9.36595700	10.77054400
H	4.83749000	8.46136200	10.22203100
C	7.43175300	15.25615100	11.57754800
H	8.32348900	15.10554100	12.17905200
C	2.59015600	9.42639800	16.71632400
H	2.23201600	9.67932600	17.71394000
C	6.32537000	15.16040600	23.21663100
H	5.58856400	15.80933800	23.68268400
C	2.84582900	13.23135700	14.57623400
H	2.23679900	12.36478800	14.32001400
C	10.65199900	12.76158800	14.33231600
H	11.69401900	12.69645600	14.63458800
C	5.80546000	10.36482600	10.13474300
H	6.10884000	10.24746400	9.09874600
C	6.11993700	10.64933800	22.20042200
H	5.83158300	11.53267000	22.77891200
H	6.90834000	10.94538000	21.50170900
H	6.52975100	9.90384100	22.89017900
C	8.34818600	13.23163400	14.86246700
H	7.59228600	13.53632600	15.58365100
C	8.94867000	12.52850300	12.63688600
H	8.67289100	12.28571600	11.61431000
C	2.71195700	7.86172900	14.91685600
H	2.46948700	6.88804700	14.50119700
C	7.41185100	16.27890200	10.63069900
H	8.28930600	16.90760600	10.50430300
C	9.68299300	13.14580200	15.25254200
H	9.95838700	13.37622500	16.27673000
C	4.63332200	5.37782900	16.68169800
H	3.92615700	5.87250800	17.34353700
C	10.28255100	12.45016600	13.02330800
H	11.03584900	12.14172200	12.30295200
C	3.91597800	8.35556700	12.76675800

C	7.37719900	14.64074900	23.97146600
H	7.46454200	14.88095700	25.02734700
C	2.80042900	14.34399900	13.75197000
H	2.17692700	14.34774000	12.86275700
B	3.39183100	11.87098700	16.69010700
C	8.20419000	13.50668600	22.00369700
H	8.94362400	12.85690200	21.54455900
C	6.28090400	16.49434600	9.85014100
H	6.26777700	17.28979300	9.11035600
C	2.29221100	8.17568300	16.19991500
H	1.72106300	7.45924400	16.78306700
C	8.51223900	11.49226100	18.60918200
H	7.58805800	10.91995400	18.55834300
C	9.66754900	13.56264100	19.04050300
H	9.65606600	14.60979400	19.32995300
C	5.16281200	15.67874300	10.02582200
H	4.27305900	15.83601300	9.42187400
C	8.31262400	13.81313200	23.35922700
H	9.13674800	13.40177600	23.93611500
C	4.40492500	4.06366900	16.29354000
H	3.52523800	3.54033200	16.65888800
C	9.72293700	10.88025400	18.29146700
H	9.73356600	9.83848600	17.98748800
C	4.85946500	7.13573400	12.85763600
H	4.37584400	6.30102700	13.37473900
H	5.76578100	7.39628200	13.41301400
H	5.15161600	6.79959600	11.85711000
C	10.90688000	11.60627200	18.35801300
H	11.85209700	11.12944300	18.11184300
C	6.65304800	5.41829900	15.37436700
H	7.53306700	5.93657700	15.00476400
C	10.87756500	12.95031600	18.73109500
H	11.79979100	13.52387000	18.77671200
C	5.29625100	3.41929400	15.43529900
H	5.11549000	2.39312000	15.12788300
C	6.41785200	4.10293100	14.97780900
H	7.11973500	3.61250700	14.30845000
C	8.75205200	7.51686500	16.80401200
H	8.58079500	6.77289500	17.57716100
C	7.67010600	8.20558000	16.24207700
C	7.91790800	9.16597700	15.25721900
H	7.08537900	9.71612300	14.82281500
C	9.21784500	9.42230200	14.82606900
H	9.39172000	10.17562700	14.06443100
C	10.28355000	8.71828800	15.37557100
H	11.29779500	8.91540500	15.03817000
C	10.04920200	7.76631600	16.36835200
H	10.88017300	7.21968300	16.80680600
C	2.67228800	7.98851900	11.92673500
H	2.95696700	7.68493500	10.91520600
H	1.99429500	8.84504500	11.85539600
H	2.13001200	7.15445400	12.38067300
C	1.79507700	12.06129600	16.83611300
O	0.67106200	12.19402400	16.93824300

R_h2o_2

Energy: -4475.49421046 Eh

P	6.19568500	13.20797900	13.14876500
P	6.84640300	13.49390100	19.47002300
P	5.90646900	7.87646700	16.62846900
O	5.32433200	14.19104500	17.02098300
O	4.94026700	9.96515500	18.48374000
O	4.64870600	10.87678400	14.11268800
C	4.41257100	14.28853700	15.98079000
C	5.99324300	15.30296800	17.46926900
C	5.13594800	16.70739900	15.52229700
C	4.33551300	15.45333000	15.20657300
C	5.38201000	8.88937600	19.21271600
C	5.91577600	16.53432200	16.81219500
C	4.33243100	11.03914700	19.11121700
C	3.74184800	12.00224500	18.27200700
C	6.77606700	15.13973000	18.63192600
C	3.61246300	13.15525200	15.73862600
C	4.34764300	11.15575700	20.50707200
C	5.35601700	8.87189400	20.60977300
C	3.79022000	9.99689700	14.75716300
C	5.00568100	10.66921700	12.80395100
C	5.87383900	7.79283400	18.47392300
C	5.75474300	11.69395300	12.18748700
C	7.17727000	14.01663700	21.20698900
C	7.45578100	16.25082600	19.13385400
H	8.03027900	16.14967700	20.04970500
C	6.62897300	17.61040100	17.34445100
H	6.59243400	18.57123300	16.83963800
C	3.29867700	10.40102900	16.01350600
C	6.33710800	14.44068400	11.78546700
C	7.97476300	12.91884900	13.56227400
C	6.30265700	6.66271700	19.17151100
H	6.64746300	5.79624800	18.61515500
C	7.38828500	17.48323900	18.49798200
H	7.92681800	18.33722600	18.89773000
C	3.29155200	13.16659000	18.91352800
H	2.90768700	13.98758600	18.30426800
C	5.81309800	7.72446800	21.26173200
H	5.81160700	7.69597600	22.34743200
C	6.24293600	14.85084000	21.83955500
H	5.42139900	15.26906900	21.26313600
C	4.65929300	9.50663300	12.10931400
C	4.90424200	10.07318200	21.41860900
C	3.84185200	12.32263500	21.07729500
H	3.87326400	12.44889800	22.15556100
C	8.50737700	12.85296000	18.96741400
C	3.80660600	9.64615300	22.41815100
H	4.17268200	8.87524600	23.10253400
H	2.93752300	9.25067200	21.88252300
H	3.48084000	10.49616900	23.02430300
C	6.27413200	6.62107500	20.55924400
H	6.61443800	5.73625900	21.08879200
C	3.50329400	15.44631500	14.08873200
H	3.45492900	16.32464700	13.45161500
C	3.46866400	8.76339800	14.17564200
C	4.16827400	17.90432500	15.65343000
H	3.61147100	18.05638900	14.72478600
H	4.71210200	18.82942800	15.86464600
H	3.45138600	17.73052700	16.46257000
C	6.12030000	11.53726300	10.84969200
H	6.66530300	12.33459500	10.35328100
C	5.77927100	6.08360400	16.21441500
C	3.34151100	13.34515100	20.28817600
H	2.98763100	14.26746000	20.74003200
C	6.14107000	16.97912000	14.38062500
H	6.85191300	16.15169700	14.29668000
H	6.70185000	17.90050900	14.57154200
H	5.62606200	17.07969900	13.41978200
C	5.19836100	14.69565000	11.00623500
H	4.30899400	14.08445100	11.14111800
C	5.06359600	9.38998000	10.77763900
H	4.81475100	8.48796800	10.22621900
C	7.46251400	15.25007300	11.60139500
H	8.35470900	15.08267800	12.19785200
C	2.56175100	9.43511100	16.71454700
H	2.18580200	9.69045600	17.70254100
C	6.35769300	15.15556300	23.18995200
H	5.62827100	15.81226700	23.65683600
C	2.82831700	13.20853700	14.57620400
H	2.25485900	12.32395500	14.29149900
C	10.66399500	12.72880100	14.32001000
H	11.70813200	12.65630100	14.61325000
C	5.77974800	10.39276100	10.14130300
H	6.07470700	10.28215500	9.10210200
C	6.12411800	10.62629900	22.18800300
H	5.85543800	11.51467000	22.76835700
H	6.91599300	10.90768800	21.48702000
H	6.52093600	9.87149800	22.87526100
C	8.37160400	13.23801900	14.86389800
H	7.62655000	13.56555300	15.58632800
C	8.94050300	12.48317000	12.64696400
H	8.65057900	12.22280000	11.63260800
C	2.71432000	7.86201300	14.92307600
H	2.48322100	6.88522500	14.50769400
C	7.45376600	16.27807000	10.65998400
H	8.33998900	16.89423700	10.53288900
C	9.70924000	13.14291700	15.24207300
H	9.99824600	13.38971000	16.25861900
C	4.63326900	5.38967700	16.63133800
H	3.91377000	5.88350100	17.28018900
C	10.27720900	12.39573800	13.02138900
H	11.01913100	12.06311400	12.29992000
C	3.91862900	8.36489700	12.77843300
C	7.40094600	14.61962900	23.94525100
H	7.48899200	14.85448100	25.00228700
C	2.77217100	14.31940600	13.74801800
H	2.16007500	14.31091000	12.85049100
B	3.31885600	11.87395000	16.70367700
C	8.21809400	13.48392300	21.97435700
H	8.95061900	12.82712700	21.51413000
C	6.32295100	16.51428300	9.88526600
H	6.31849100	17.31355700	9.14949100
C	2.28430300	8.17756500	16.20240100
H	1.71901800	7.45583100	16.78571100
C	8.56954900	11.50743600	18.59450300

H	7.65441200	10.92042100	18.54527800
C	9.69184300	13.59827500	19.01321800
H	9.66346600	14.64750000	19.29386800
C	5.19385500	15.71399700	10.06146500
H	4.30415900	15.88702400	9.46168000
C	8.32740400	13.78319000	23.33132700
H	9.14528200	13.35928300	23.90803600
C	4.40834900	4.07871200	16.23058400
H	3.51888100	3.55686700	16.57382100
C	9.79090700	10.91049000	18.28897500
H	9.81781700	9.86630900	17.99454300
C	4.87209000	7.15235600	12.86381900
H	4.39722400	6.31379100	13.38288200
H	5.77869600	7.41930600	13.41566900
H	5.16302500	6.81915900	11.86174800
C	10.96374700	11.65430600	18.35554200
H	11.91735000	11.18925700	18.11935400
C	6.68074500	5.42974500	15.36850700
H	7.57060700	5.94652400	15.02103700
C	10.91246300	13.00120700	18.71600200
H	11.82591300	13.58866500	18.76162500
C	5.31531600	3.43576300	15.38773400
H	5.13719300	2.41218200	15.07019400
C	6.44909200	4.11775500	14.95875000
H	7.16338600	3.62870000	14.30160000
C	8.75667900	7.51451000	16.87455500
H	8.56123700	6.79430300	17.66428800
C	7.69348600	8.19727400	16.27145600
C	7.97141400	9.12878500	15.26684800
H	7.15386400	9.67561600	14.80079100
C	9.28262700	9.35927600	14.85510100
H	9.48004400	10.08987900	14.07707800
C	10.32948800	8.65906200	15.44443300
H	11.35231400	8.83568600	15.12188000
C	10.06502000	7.73836400	16.45888100
H	10.88110800	7.19577300	16.92921200
C	2.67722900	7.98746100	11.93917800
H	2.96174600	7.68650700	10.92675200
H	1.99189000	8.83839400	11.86957200
H	2.14240800	7.14897000	12.39368700
O	1.69541200	12.03778700	16.92771900
H	1.23099200	12.25011800	16.09962100
H	1.49594300	12.75474800	17.55521700

R_menh3

Energy: -4494.88175558 Eh

P	6.21594800	13.18460300	13.14186800
P	6.84303700	13.49727700	19.46599700
P	5.95903700	7.89577400	16.60308400
O	5.30811600	14.20014300	17.02554500
O	4.96496200	9.98216700	18.46050800
O	4.65900900	10.85963000	14.10449400
C	4.41491400	14.28992200	15.96647800
C	5.97492900	15.31095400	17.47535100
C	5.14089600	16.71107700	15.51614500
C	4.35452400	15.45173900	15.18599800
C	5.39015000	8.89808200	19.18577700
C	5.90087300	16.54286400	16.81813100
C	4.33705200	11.04900700	19.08642900
C	3.74216500	12.01109800	18.24518800
C	6.75493400	15.14851700	18.64062100
C	3.62854500	13.14821700	15.70662600
C	4.34539500	11.15805500	20.48361200
C	5.34502300	8.86998000	20.58269300
C	3.80264300	9.98380200	14.75444900
C	5.00618900	10.65448100	12.79364500
C	5.88801700	7.80331300	18.44698800
C	5.76331000	11.67430800	12.17814000
C	7.17186600	14.00888000	21.20680700
C	7.42506500	16.26197000	19.15021800
H	7.99637600	16.16062800	20.06805700
C	6.60366600	17.62153600	17.35872100
H	6.56731700	18.58281200	16.85463900
C	3.33186700	10.38862200	16.01856500
C	6.37715400	14.41839700	11.78105500
C	7.99213000	12.88650700	13.55971300
C	6.29980400	6.66597600	19.14362800
H	6.64997100	5.80212900	18.58660900
C	7.35336000	17.49644300	18.51879800
H	7.88335300	18.35256100	18.92538600
C	3.29725700	13.17474800	18.89313000
H	2.90538500	13.99216400	18.28869800
C	5.78496300	7.71524000	21.23330100
H	5.76922800	7.67994800	22.31868200
C	6.23535600	14.83478300	21.84699600
H	5.41230000	15.25520700	21.27452900
C	4.64325400	9.49819800	12.09713800
C	4.89840500	10.07172100	21.39317800
C	3.84084100	12.32325400	21.05676300
H	3.86952800	12.44636900	22.13554200
C	8.51213500	12.87947100	18.95888800
C	3.80014500	9.64861300	22.39370000
H	4.16342200	8.87789900	23.07975700
H	2.92971300	9.25469100	21.85889300
H	3.47671800	10.50025300	22.99866300
C	6.24917700	6.61369100	20.53019200
H	6.57654700	5.72308600	21.05819600
C	3.55658300	15.43582500	14.04373800
H	3.51692600	16.31345900	13.40477000
C	3.47340400	8.75085500	14.17538600
C	4.16360300	17.90175000	15.63029600
H	3.62183600	18.04977300	14.69206000
H	4.69706600	18.83076600	15.85131400
H	3.43362800	17.72262100	16.42651800
C	6.12112400	11.51725700	10.83826300
H	6.67456000	12.30914200	10.34247400
C	5.83582900	6.10569100	16.17259100
C	3.34932700	13.35028500	20.26712800
H	2.99908600	14.27366500	20.72007900
C	6.16463900	16.98913300	14.39215500
H	6.88159600	16.16556700	14.32155300
H	6.71692200	17.91397200	14.59151100
H	5.66660300	17.08531800	13.42205200
C	5.25367600	14.67605000	10.98073600
H	4.36269200	14.06345900	11.09491000
C	5.03671800	9.38314100	10.76209500
H	4.77364700	8.48673700	10.20802800
C	7.50552300	15.22918900	11.62119000
H	8.38656500	15.05956700	12.23338500
C	2.63792200	9.40616600	16.73957000
H	2.30634600	9.63650200	17.75140000
C	6.35003500	15.12871300	23.19983900
H	5.61879900	15.77929000	23.67246900
C	2.90457700	13.18476000	14.50638900
H	2.36595700	12.29169800	14.20372500
C	10.68247400	12.71296300	14.31589800
H	11.72737200	12.64758500	14.60814700
C	5.76178600	10.38022900	10.12664700
H	6.04989800	10.27067100	9.08540300
C	6.12164000	10.61678500	22.16307600
H	5.85703700	11.50448400	22.74637900
H	6.91371200	10.89756100	21.46206100
H	6.51607300	9.85758800	22.84701600
C	8.39099300	13.23158400	14.85410300
H	7.64672200	13.57375400	15.57072900
C	8.95577600	12.43212700	12.65159100
H	8.66332200	12.15277800	11.64291600
C	2.73754800	7.84421900	14.93494500
H	2.49796200	6.86902600	14.52083100
C	7.51425000	16.26110800	10.68418300
H	8.40257000	16.87797300	10.57645700
C	9.72948900	13.14537300	15.23137400
H	10.02049300	13.41383600	16.24183600
C	4.69445900	5.39844900	16.57913800
H	3.97293800	5.87744000	17.23641300
C	10.29314400	12.35258500	13.02530400
H	11.03406700	12.00591400	12.30934500
C	3.90187300	8.35829600	12.76968900
C	7.39563600	14.59032400	23.95008900
H	7.48381400	14.81700900	25.00890600
C	2.86167200	14.29476100	13.67653500
H	2.28659000	14.27417500	12.75473300
B	3.32619600	11.87542400	16.67177700
C	8.21516300	13.47369900	21.96930100
H	8.94970200	12.82325900	21.50328000
C	6.39813100	16.50047300	9.88933000
H	6.40714100	17.30289800	9.15701800
C	2.34892700	8.15008800	16.23018300
H	1.81038800	7.42092900	16.82940200
C	8.59152600	11.53630400	18.58067500
H	7.68346800	10.93870200	18.52606100
C	9.68757700	13.63860700	19.00992300
H	9.64587200	14.68647200	19.29401300
C	5.26661200	15.69864500	10.04056800
H	4.38835900	15.87348300	9.42461600
C	8.32456400	13.76221200	23.32854200
H	9.14454300	13.33663500	23.90105200
C	4.47735500	4.09211400	16.15910300
H	3.59136100	3.55982500	16.49530400
C	9.82090300	10.95496500	18.27673500
H	9.86101000	9.91236900	17.97811500

C	4.84975700	7.13989500	12.83659300
H	4.37966100	6.30185700	13.36092800
H	5.76612400	7.40100400	13.37485800
H	5.12297800	6.80855600	11.82901000
C	10.98478200	11.71203800	18.35038100
H	11.94461900	11.25910200	18.11583700
C	6.74181800	5.46883900	15.31821800
H	7.62912600	5.99547400	14.97904800
C	10.91617100	13.05718100	18.71459500
H	11.82237000	13.65540300	18.76497200
C	5.38803200	3.46688200	15.30712800
H	5.21621400	2.44692100	14.97480600
C	6.51812800	4.16177000	14.88914700
H	7.23600300	3.68650200	14.22582400
C	8.80037100	7.52883200	16.92311300
H	8.58379000	6.83444600	17.73020400
C	7.75497600	8.20166300	16.27956400
C	8.05942200	9.09899500	15.25177600
H	7.25552800	9.63745200	14.75300200
C	9.38006800	9.30387800	14.85671000
H	9.59814600	10.00658600	14.05884600
C	10.40964800	8.61440600	15.48768000
H	11.43973900	8.77159900	15.17855900
C	10.11824000	7.72911800	16.52589700
H	10.92059900	7.19501700	17.02844500
C	2.64662100	7.99327100	11.94609200
H	2.91537600	7.69606100	10.92825000
H	1.96603000	8.84910600	11.89040300
H	2.11272800	7.15577700	12.40386300
N	1.54811300	12.08157900	16.93817600
H	1.41668200	13.05839300	17.19260800
C	0.50786900	11.71171400	15.93829200
H	-0.46509300	11.61076800	16.43022700
H	0.43990900	12.48794800	15.17606600
H	0.77809600	10.76134500	15.47250000
H	1.37134300	11.56158100	17.79529900

R_menh3_ipr

Energy: -3816.26393554 Eh

P	1.97870300	31.26044200	14.52643100
P	4.49239200	36.60923100	17.11199900
P	6.42898200	32.78466500	12.70320100
O	1.24495300	34.05740100	14.97355900
O	3.68365400	33.12437100	11.42702200
O	4.98468500	36.68994400	14.06660800
C	2.29604000	33.26461200	11.39283600
C	1.17348900	35.42740800	15.08090900
C	4.91494100	36.73365600	12.67649200
C	1.95931800	36.16136400	14.17071900
C	3.80750500	36.12463000	12.05393300
C	1.70304800	34.30409300	12.12426700
C	1.55170300	32.36159900	10.61418600
C	5.75371000	37.61840400	14.73690900
C	0.30181300	34.21600200	12.22757600
H	-0.22135800	34.94557900	12.84429500
C	0.29976600	33.26212800	15.56604600
C	3.86203700	36.07660700	10.64985800
H	3.08258900	35.52991600	10.12801500
C	5.41839900	31.51260400	11.81519300
C	6.75510400	38.33594900	14.06356400
C	4.19455300	31.85722500	11.21388100
C	3.50969400	30.96119500	10.37975600
C	0.35365700	36.02991900	16.04290900
C	5.87550500	37.35852700	10.55797000
H	6.65478600	37.83746300	9.97608400
C	-0.71512800	33.79035000	16.36534100
C	2.07662900	37.53064200	14.45182400
H	2.73184800	38.13982100	13.83012300
C	5.94936800	37.34812900	11.94874300
C	4.84533200	36.70033400	9.90164600
H	4.82770900	36.65307100	8.81603500
C	0.43072400	31.87764000	15.33368900
C	2.31514700	31.50341700	9.62363700
C	5.55647700	37.76758100	16.12310400
C	-0.45757900	33.24137100	11.60146100
H	-1.53427700	33.20852900	11.74276700
C	0.16876600	32.34039500	10.74715200
H	-0.42356600	31.62223900	10.19022700
C	-1.69665600	32.91282300	16.83398000
H	-2.50087800	33.29374100	17.45673300
C	5.87020900	30.19875500	11.63819700
H	6.79812900	29.88735700	12.10523300
C	7.45211900	39.32118800	14.75894600
H	8.21019500	39.90708900	14.25140400
C	-0.70167200	35.24384000	16.81142000
C	1.36532600	38.15312100	15.46747000
H	1.47391500	39.22028800	15.63667000
C	7.17059100	37.87694800	12.67898100
C	3.99299100	29.66353400	10.24171800
H	3.45971000	28.95093300	9.62128000
C	0.47266400	37.40805900	16.22629000
H	-0.13720000	37.90424800	16.97668500
C	7.64586800	33.20962300	11.30749800
H	8.27389900	33.99454000	11.75066100
C	-0.58095700	31.04678100	15.81429600
H	-0.52865500	29.97693800	15.64318800
C	1.57565700	29.45997300	14.18364100
H	1.09600300	28.98668900	15.05015500
C	6.32892600	38.72717200	16.78711400
H	6.22507100	38.84078200	17.86173200
C	2.83855200	32.41881700	8.48446100
H	3.43818500	31.83188900	7.77953900
H	3.46233200	33.22699200	8.87828700
H	1.99285000	32.86333500	7.94756300
C	3.97858200	37.67875800	18.59703400
H	4.85546700	37.79561600	19.25171000
C	-1.65510000	31.55916800	16.53576200
H	-2.43459100	30.89543800	16.89812100
C	3.06468100	31.12074400	16.07033800
H	3.95973200	30.60773500	15.69395300
C	0.63390700	29.38532000	12.97825600
H	-0.28612900	29.95924100	13.13225100
H	0.36013100	28.34332500	12.77074300
H	1.13115900	29.79284900	12.09099900
C	5.16138800	29.27330800	10.88481500
H	5.53045500	28.25701000	10.78125500
C	7.51650000	31.74321000	13.82648000
H	8.01723500	30.95199400	13.25496900
C	7.23176500	39.53478500	16.11359100
H	7.79592700	40.29358200	16.64788600
C	5.95994100	35.68804800	17.89230400
H	6.65376800	36.45487200	18.26885200
C	2.87887900	28.70890900	13.88713300
H	3.46123500	29.22114900	13.11153600
H	2.65281600	27.69955900	13.52162600
H	3.50933300	28.60730400	14.77611200
C	1.45813300	30.40885800	8.99050400
H	0.61635600	30.85436900	8.45223700
H	1.06408100	29.70872700	9.73452600
H	2.04210700	29.84511800	8.25696600
C	8.54997300	32.08405600	10.80934000
H	9.19246500	31.67522200	11.59511900
H	9.20390300	32.46624400	10.01484500
H	7.96002400	31.26454400	10.38444900
B	2.38159400	35.67086500	12.67898300
C	-0.39557900	35.27664400	18.32517800
H	-0.38015600	36.30755100	18.69442500
H	0.57874400	34.82051100	18.52737800
H	-1.15972500	34.72461400	18.88262600
C	6.86578500	33.82665100	10.14738900
H	6.26807700	33.06322000	9.63405100
H	7.55347800	34.26380600	9.41273100
H	6.18755300	34.61206500	10.48828300
C	8.59817400	32.64919300	14.42545900
H	8.15013800	33.49761200	14.95358400
H	9.27328600	33.04662400	13.66057200
H	9.20343300	32.08564400	15.14595700
C	8.15138300	36.69000200	12.86739600
H	8.48129200	36.32786600	11.88708400
H	7.66586400	35.86215400	13.39590500
H	9.02671200	37.01014200	13.44444800
C	2.48295300	30.30907900	17.22558100
H	1.57749800	30.78320800	17.62039900
H	3.21312200	30.24771500	18.04307600
H	2.22862500	29.28548100	16.93207000
C	-2.08199800	35.88879200	16.55733500
H	-2.86904700	35.35971800	17.10230200
H	-2.32437300	35.86660800	15.48978200
H	-2.09152000	36.92940000	16.89341200
C	3.49543000	32.51054800	16.54216000
H	3.87532800	33.12592500	15.71952000
H	4.28641500	32.41443800	17.29558700
H	2.66144200	33.05212700	17.00391400
C	3.43719700	39.06173400	18.22722100
H	4.14737100	39.67098600	17.66416500
H	3.17167200	39.60534400	19.14275300
H	2.53019500	38.95939400	17.62612200
C	2.87945600	36.92527600	19.36039100
H	1.97420000	36.87949400	18.74682900
H	2.63561000	37.45469500	20.29014400
H	3.15359500	35.89934600	19.61733700

C	6.67079700	34.87395300	16.81126900
H	5.99358800	34.14070000	16.35962400
H	7.51840100	34.32946200	17.24592200
H	7.05573900	35.51137000	16.00812500
C	7.89202500	38.97830200	11.89446600
H	8.79139700	39.30101500	12.42452000
H	7.24542700	39.84752000	11.73417600
H	8.22910600	38.60650300	10.92443000
C	6.67086700	31.09582000	14.92322700
H	7.30685100	30.51630300	15.60379900
H	5.91771500	30.42083300	14.50326300
H	6.14921700	31.85742500	15.51343400
C	5.54128300	34.79488500	19.06150900
H	5.22336100	35.37789800	19.93026100
H	6.39056500	34.17414300	19.37332800
H	4.72285800	34.12273000	18.78006900
N	1.28738200	36.89648400	11.82480300
H	1.74529100	37.79506300	11.96265200
H	0.46321400	36.92891300	12.42092600
C	0.84414600	36.80258600	10.40677900
H	0.59802600	35.76443500	10.17153100
H	-0.04144900	37.42717200	10.24837600
H	1.64148200	37.14795700	9.74847600

R_nh3

Energy: -4455.62500396 Eh

P	6.18748700	13.19896700	13.14252600
P	6.83909000	13.49021800	19.48190900
P	5.92649800	7.89189800	16.62348800
O	5.31666000	14.19406700	17.03439400
O	4.95169500	9.98240600	18.48382200
O	4.63323300	10.87473700	14.11020600
C	4.41641400	14.29159100	15.98218900
C	5.98904200	15.30276300	17.48315800
C	5.15476500	16.70824500	15.52749900
C	4.35351700	15.45629000	15.20562100
C	5.38869000	8.90292100	19.20873300
C	5.92204600	16.53412000	16.82428400
C	4.32667900	11.04963400	19.11329500
C	3.72366700	12.00783500	18.27551000
C	6.76649000	15.13844300	18.64959200
C	3.61547500	13.15964300	15.73277200
C	4.34079200	11.15956000	20.51023700
C	5.35714300	8.87879600	20.60616700
C	3.78535100	9.99239400	14.76377000
C	4.98730800	10.66395100	12.80173300
C	5.88371200	7.80767600	18.46864100
C	5.74088100	11.68451600	12.18339400
C	7.17292800	14.00864500	21.21973000
C	7.44515000	16.24804400	19.15615700
H	8.01454500	16.14507500	20.07499900
C	6.63440300	17.60857300	17.36088600
H	6.60456900	18.56882100	16.85448900
C	3.31559600	10.39422000	16.02968800
C	6.33652700	14.42877500	11.77723900
C	7.96550500	12.90615900	13.55817800
C	6.31026100	6.67541600	19.16449200
H	6.65759900	5.81098300	18.60660500
C	7.38434700	17.48081500	18.52037900
H	7.92175700	18.33375600	18.92388700
C	3.26195900	13.16383400	18.92303100
H	2.85024000	13.97127200	18.31827300
C	5.81202200	7.72926300	21.25582500
H	5.80700700	7.69741600	22.34141500
C	6.23451300	14.83423600	21.85757500
H	5.40744300	15.24681900	21.28502300
C	4.63377600	9.50253600	12.10887100
C	4.90445300	10.07735400	21.41816800
C	3.82959200	12.32150400	21.08441100
H	3.86271600	12.44604300	22.16293100
C	8.50201300	12.85745500	18.97303200
C	3.81155600	9.64528500	22.42093200
H	4.18172100	8.87518400	23.10405900
H	2.94207400	9.24716000	21.88770700
H	3.48459200	10.49378100	23.02846300
C	6.27643900	6.62839500	20.55177300
H	6.61542500	5.74195400	21.07946000
C	3.53526000	15.45174400	14.07801600
H	3.49708800	16.32957400	13.43939400
C	3.45909800	8.75855900	14.18494500
C	4.18988100	17.90854600	15.64887300
H	3.64082800	18.06063300	14.71563100
H	4.73456700	18.83254900	15.86307200
H	3.46591600	17.73811500	16.45245700
C	6.10296200	11.52439700	10.84510400
H	6.65235400	12.31780700	10.34726400
C	5.79999700	6.09950100	16.20503700
C	3.32015500	13.34152200	20.29671800
H	2.95903400	14.25978800	20.75166900
C	6.17092900	16.97652000	14.39459400
H	6.87793300	16.14525500	14.31519500
H	6.73513300	17.89477200	14.59079100
H	5.66416000	17.08072500	13.42982700
C	5.20291900	14.68367800	10.99040800
H	4.31236000	14.07326400	11.12025400
C	5.03283000	9.38345300	10.77582400
H	4.77690800	8.48284100	10.22527100
C	7.46335300	15.23776800	11.59949800
H	8.35164200	15.07074900	12.20182500
C	2.60771100	9.41539900	16.74330400
H	2.28014700	9.64292300	17.75716500
C	6.35190600	15.13695800	23.20818000
H	5.61911100	15.78698000	23.67914700
C	2.84535400	13.21712100	14.56144500
H	2.26152500	12.34194300	14.27807500
C	10.65467800	12.72318700	14.31760300
H	11.69890200	12.65380300	14.61132900
C	5.75323700	10.38196400	10.13756400
H	6.04490000	10.26949000	9.09762800
C	6.12501500	10.63097500	22.18591800
H	5.85561100	11.51773100	22.76839800
H	6.91463900	10.91553900	21.48375200
H	6.52517000	9.87555100	22.87071800
C	8.36142000	13.23119400	14.85868100
H	7.61560400	13.56104700	15.57934800
C	8.93200300	12.46756700	12.64512600
H	8.64265100	12.20332600	11.63154700
C	2.71945800	7.85194900	14.94109400
H	2.48359800	6.87607300	14.52653400
C	7.46112800	16.26483600	10.65706000
H	8.34841100	16.88054900	10.53518700
C	9.69907500	13.13966900	15.23771800
H	9.98742500	13.39155800	16.25322800
C	4.66158100	5.39684400	16.62783300
H	3.94622900	5.88233000	17.28725600
C	10.26871200	12.38372900	13.02036100
H	11.01146800	12.04930700	12.30053400
C	3.89277200	8.36307100	12.78171700
C	7.40196800	14.60738100	23.95857600
H	7.49206300	14.84058700	25.01581700
C	2.80519600	14.32629400	13.73076500
H	2.20149300	14.31952500	12.82737800
B	3.31289500	11.88206400	16.70136600
C	8.22056900	13.48232000	21.98213900
H	8.95645800	12.83215700	21.51787200
C	6.33542700	16.50082700	9.87485900
H	6.33598500	17.29940500	9.13830500
C	2.31938400	8.15948100	16.23175500
H	1.77631900	7.43099500	16.82766500
C	8.56950200	11.51377900	18.59443100
H	7.65687100	10.92289400	18.54473600
C	9.68324100	13.60801600	19.01757900
H	9.65067000	14.65624000	19.30146900
C	5.20492500	15.70117400	10.04471600
H	4.31904200	15.87406300	9.43925500
C	8.33250600	13.77935000	23.33943600
H	9.15567400	13.36040000	23.91225400
C	4.43955900	4.08725900	16.22084700
H	3.55611000	3.55862300	16.56927100
C	9.79280100	10.92379300	18.28293100
H	9.82375800	9.88105200	17.98389000
C	4.84158600	7.14587300	12.85511300
H	4.36898000	6.30774100	13.37689800
H	5.75450600	7.40812300	13.39870400
H	5.12121400	6.81385600	11.84952500
C	10.96247300	11.67255600	18.34928200
H	11.91750000	11.21282400	18.10841600
C	6.69746200	5.45483500	15.34764900
H	7.58206000	5.97790400	14.99615800
C	10.90585100	13.01787500	18.71475200
H	11.81659000	13.60960000	18.75973000
C	5.34211100	3.45398700	15.36607300
H	5.16645900	2.43139200	15.04401300
C	6.46885500	4.14428500	14.93182800
H	7.18018500	3.66276900	14.26595500
C	8.77404200	7.52667200	16.88920800
H	8.57284900	6.81892800	17.68864100
C	7.71595800	8.20492200	16.27236600
C	8.00109600	9.11982300	15.25467900
H	7.18736200	9.66226300	14.77676300
C	9.31474300	9.33835400	14.84405200

H	9.51781400	10.05563900	14.05522500
C	10.35671500	8.64354100	15.44823500
H	11.38140500	8.81119800	15.12685900
C	10.08483200	7.73943600	16.47552600
H	10.89701300	7.20096400	16.95720800
C	2.64122000	7.99429400	11.95390500
H	2.91470000	7.69491200	10.93795200
H	1.95986000	8.84912600	11.89291700
H	2.10636500	7.15736000	12.41148500
N	1.58445700	12.08527700	16.87071100
H	1.34152500	13.05945800	17.03539800
H	1.09315300	11.78176400	16.03309600
H	1.22563100	11.54195200	17.65252800

R_nh3_ipr

Energy: -3777.00682298 Eh

P	1.95739300	31.29279700	14.50236800
P	4.49422200	36.60039100	17.11242100
P	6.41574700	32.81195200	12.70169200
O	1.22311800	34.08913900	14.96837800
O	3.67035300	33.15725000	11.43008600
O	4.98767600	36.68462900	14.06511000
C	2.28315800	33.30088100	11.38490500
C	1.14911800	35.45949800	15.08258800
C	4.91321300	36.74460500	12.67573000
C	1.92866900	36.19913600	14.17348200
C	3.79368500	36.16430900	12.05097200
C	1.68644000	34.34052200	12.11294100
C	1.54265300	32.40289900	10.59683500
C	5.76118800	37.60709300	14.74018800
C	0.28200600	34.26496800	12.19199600
H	-0.24302500	34.99174700	12.81081800
C	0.28376800	33.28925200	15.56402100
C	3.82247000	36.17046800	10.64319800
H	3.01846300	35.66859800	10.10657200
C	5.40159500	31.54106800	11.81760100
C	6.76766000	38.32072500	14.07011200
C	4.18014200	31.88980100	11.21398500
C	3.49856800	30.99759000	10.37308200
C	0.32669900	36.05684600	16.04586900
C	5.86370800	37.40814000	10.56297000
H	6.64487000	37.88912200	9.98553100
C	-0.72877100	33.81165200	16.37054300
C	2.02664600	37.57136300	14.44262700
H	2.66660000	38.18432600	13.80855600
C	5.95083800	37.36027900	11.95141900
C	4.80981400	36.79402700	9.90084300
H	4.77344200	36.78583300	8.81490000
C	0.41659100	31.90541200	15.32681400
C	2.31090800	31.54454100	9.61034400
C	5.56352200	37.75501600	16.12601700
C	-0.47503400	33.29427400	11.55586800
H	-1.55356300	33.26679200	11.68362600
C	0.15800800	32.38871200	10.71218300
H	-0.43060400	31.67340500	10.14776500
C	-1.70371300	32.92948500	16.84413400
H	-2.50535000	33.30635500	17.47262900
C	5.85194800	30.22702100	11.63880200
H	6.77865900	29.91329800	12.10659500
C	7.46713500	39.30320100	14.76659800
H	8.22748200	39.88709200	14.26014700
C	-0.72206300	35.26491300	16.81706000
C	1.31238600	38.18974300	15.45894000
H	1.40567600	39.25939600	15.62266500
C	7.18130500	37.85936400	12.68617800
C	3.98029800	29.69958800	10.23274600
H	3.44895300	28.99030900	9.60693300
C	0.43354000	37.43643200	16.22594800
H	-0.17814000	37.92841400	16.97761900
C	7.61377100	33.24422200	11.29227700
H	8.25990200	34.01270200	11.73749400
C	-0.58900400	31.07010200	15.81251700
H	-0.53475700	30.00095800	15.63792400
C	1.55140300	29.49365100	14.15585900
H	1.07789200	29.01732200	15.02405800
C	6.33901800	38.71073500	16.79227500
H	6.23414700	38.82312200	17.86695000
C	2.84497400	32.46150000	8.47731200
H	3.45116000	31.87558800	7.77715300
H	3.46497800	33.26907100	8.87838000
H	2.00433600	32.90670700	7.93309000
C	3.97329000	37.67454500	18.59024900
H	4.84465300	37.79387100	19.25184600
C	-1.65945800	31.57666200	16.54328000
H	-2.43391700	30.90934500	16.90981600
C	3.05971100	31.14495500	16.03356300
H	3.94970500	30.63189000	15.64526600
C	0.60066100	29.42346800	12.95727100
H	-0.31909600	29.99515900	13.12130300
H	0.32662600	28.38209400	12.74699900
H	1.08997100	29.83605700	12.06797200
C	5.14468400	29.30486900	10.88012700
H	5.51253700	28.28830400	10.77494800
C	7.51991300	31.77028800	13.80853300
H	8.01693700	30.98269200	13.22875400
C	7.24537400	39.51625800	16.12116900
H	7.81106400	40.27275900	16.65709600
C	5.95667800	35.67814600	17.90042200
H	6.64738700	36.44466300	18.28326800
C	2.85236200	28.74324200	13.84823900
H	3.43231100	29.26010700	13.07406900
H	2.62363400	27.73669600	13.47666300
H	3.48628800	28.63471700	14.73390400
C	1.45603300	30.45372500	8.96798400
H	0.61951500	30.90241400	8.42426300
H	1.05465800	29.75261100	9.70719000
H	2.04417300	29.89045600	8.23744700
C	8.49557600	32.11552900	10.76279200
H	9.14416300	31.68688600	11.53301100
H	9.14282500	32.50198000	9.96490500
H	7.88948500	31.30965500	10.33457300
B	2.35784900	35.71722700	12.67948200
C	-0.41326700	35.29965900	18.33021800
H	-0.39763500	36.33113000	18.69793200
H	0.56153400	34.84411800	18.53109500
H	-1.17605400	34.74792500	18.88985200
C	6.82346100	33.89093900	10.15539800
H	6.20487000	33.14550900	9.64035100
H	7.50551800	34.32821700	9.41554600
H	6.16395600	34.68178100	10.51974800
C	8.60559300	32.67715900	14.39904900
H	8.16153300	33.52336100	14.93414000
H	9.27238500	33.07780100	13.62852300
H	9.21921700	32.11266800	15.11165700
C	8.13566900	36.65140200	12.87419000
H	8.46679700	36.29096900	11.89382400
H	7.62902400	35.82955900	13.39193300
H	9.01236600	36.94940600	13.46092700
C	2.48900700	30.32986300	17.19183000
H	1.59193900	30.80717000	17.60171700
H	3.22984200	30.25946500	17.99893900
H	2.22416400	29.30954900	16.89615300
C	-2.10676400	35.90179400	16.56607100
H	-2.88986300	35.36594800	17.11004800
H	-2.34986200	35.88124800	15.49866700
H	-2.12304300	36.94129700	16.90528500
C	3.49844700	32.53183800	16.50601000
H	3.87821600	33.14632800	15.68258600
H	4.29202400	32.43072400	17.25605000
H	2.66903400	33.07669500	16.97194700
C	3.43620700	39.05463500	18.20463700
H	4.16332500	39.67054700	17.67136100
H	3.13094400	39.59364300	19.11046900
H	2.55464200	38.94638300	17.56747000
C	2.86666600	36.92533300	19.34652600
H	1.96595300	36.88156000	18.72616700
H	2.61740300	37.45669600	20.27371400
H	3.13625700	35.89881000	19.60665700
C	6.67555000	34.86693800	16.82240600
H	6.00096600	34.13712800	16.36146400
H	7.51847400	34.31896600	17.26178000
H	7.06836200	35.50743200	16.02552700
C	7.93025600	38.94703500	11.90937900
H	8.83309800	39.24844300	12.44621100
H	7.30406300	39.83081900	11.74751500
H	8.26502600	38.57025200	10.94034300
C	6.68873000	31.11590400	14.91238400
H	7.33506600	30.53943700	15.58570700
H	5.93575700	30.43663400	14.49906700
H	6.16790800	31.87308100	15.50901400
C	5.52938700	34.78381200	19.06554600
H	5.20337300	35.36646300	19.93160000
H	6.37677000	34.16410900	19.38446400
H	4.71397100	34.11079500	18.77746100
N	1.34470100	36.86484700	11.79113000
H	1.77537800	37.78646700	11.77305400
H	1.19993000	36.57048500	10.82817000
H	0.43092700	36.96122700	12.22757700

R_tbu

Energy: -4649.58887552 Eh

P	6.22140400	13.16401900	13.10283300
P	6.82518000	13.50691000	19.47501800
P	5.94992600	7.85178000	16.64425500
O	5.32722500	14.18404600	17.01039600
O	4.97216000	9.95585500	18.48062300
O	4.68468300	10.83116700	14.07949500
C	4.44535400	14.26935400	15.94259400
C	6.00675800	15.29453400	17.44367100
C	5.18730400	16.68016000	15.46670600
C	4.38805600	15.42507800	15.15246100
C	5.43975800	8.89825500	19.21878000
C	5.95320500	16.51601100	16.76560900
C	4.34675600	11.02732900	19.10139300
C	3.73887900	11.97560000	18.25773400
C	6.77571300	15.14250000	18.61712000
C	3.65084400	13.13517500	15.69073500
C	4.35976800	11.15343100	20.49694300
C	5.42523500	8.89625200	20.61662600
C	3.84395900	9.94203700	14.73267400
C	5.06611700	10.60505100	12.78123300
C	5.94743600	7.80083200	18.49082100
C	5.81626500	11.62687000	12.16066100
C	7.15137600	14.05194700	21.20580400
C	7.46167800	16.25345300	19.11011300
H	8.02480400	16.15982500	20.03383900
C	6.67284400	17.59226600	17.28893900
H	6.65313400	18.54491700	16.76779900
C	3.35650800	10.34589400	15.98973400
C	6.35417600	14.37562400	11.72006700
C	8.00093000	12.91311900	13.54050800
C	6.41124600	6.69133300	19.19893700
H	6.76915500	5.82519000	18.65045300
C	7.41597700	17.47629700	18.45402700
H	7.95908800	18.33073100	18.84663600
C	3.23982500	13.12252600	18.89144700
H	2.78424700	13.89540900	18.27336100
C	5.91681000	7.76916000	21.27882500
H	5.92467600	7.75528000	22.36478700
C	6.20303900	14.88083100	21.82466200
H	5.37442500	15.27523100	21.24127300
C	4.74114700	9.42837900	12.09983300
C	4.94283700	10.09135900	21.41638500
C	3.82662400	12.31154100	21.05920200
H	3.85567800	12.44616200	22.13666700
C	8.48296100	12.84968500	18.98153600
C	3.85468900	9.64146200	22.41679100
H	4.23895700	8.88257100	23.10485900
H	2.99627700	9.22237000	21.88177200
H	3.50737000	10.48627000	23.01828700
C	6.39967300	6.66831100	20.58721400
H	6.76780300	5.79982600	21.12515700
C	3.57394900	15.41035300	14.02175400
H	3.53947600	16.28261100	13.37526800
C	3.53605800	8.69910000	14.16383400
C	4.22009900	17.87946300	15.58143300
H	3.67250400	18.02679900	14.64648200
H	4.76339500	18.80487900	15.79363700
H	3.49496900	17.71052900	16.38426100
C	6.20517500	11.45162400	10.83194100
H	6.75027200	12.24583700	10.33071100
C	5.84177600	6.05066900	16.26361700
C	3.29273300	13.31279800	20.26284800
H	2.90257200	14.22253600	20.71095000
C	6.20284200	16.94387100	14.33250000
H	6.91188300	16.11379500	14.25879300
H	6.76499400	17.86466400	14.52244900
H	5.69610700	17.04094700	13.36709800
C	5.22066000	14.59067700	10.92107000
H	4.34352900	13.96196300	11.05534100
C	5.16808200	9.29425000	10.77694300
H	4.93503500	8.38190300	10.23558800
C	7.46271900	15.20833500	11.53670600
H	8.34978600	15.07340600	12.14873300
C	2.62457300	9.38132300	16.69667000
H	2.24879600	9.64198200	17.68543500
C	6.31160100	15.20843900	23.17013300
H	5.57106000	15.86024600	23.62627500
C	2.87089000	13.18496600	14.52657900
H	2.26094400	12.31727100	14.27772000
C	10.68021400	12.77194900	14.34488200
H	11.72025500	12.71847900	14.65620700
C	5.88640700	10.29286300	10.13655900
H	6.19931900	10.16837300	9.10418600
C	6.14547700	10.67925500	22.18652100
H	5.85170600	11.56470900	22.75886400
H	6.93301700	10.97542100	21.48691300
H	6.55916100	9.94073300	22.88167400
C	8.36754000	13.22246300	14.85336000
H	7.60256500	13.52354700	15.56649700
C	8.99315200	12.51324200	12.63697500
H	8.72816500	12.26221700	11.61353600
C	2.78738100	7.79709200	14.91700800
H	2.56413300	6.81558500	14.50869500
C	7.44360600	16.21866800	10.57654400
H	8.31702200	16.85315700	10.45076800
C	9.69988300	13.15171100	15.25488600
H	9.96438600	13.39058400	16.27999100
C	4.71341500	5.34865700	16.71424300
H	3.99975900	5.84430300	17.36828400
C	10.32452900	12.44991300	13.03462100
H	11.08666800	12.14473400	12.32214700
C	3.99672000	8.29107100	12.77291000
C	7.36235000	14.70070700	23.93467200
H	7.44536200	14.95306300	24.98810100
C	2.83638700	14.28576600	13.68586400
H	2.22566100	14.27697400	12.78718800
B	3.35209600	11.84518100	16.66533700
C	8.19925000	13.54736700	21.98227400
H	8.94227800	12.89457200	21.53334400
C	6.31864100	16.41466300	9.78236500
H	6.30606100	17.20040300	9.03222600
C	2.35344700	8.11894400	16.19371000
H	1.79144300	7.39826200	16.78152600
C	8.53266000	11.50565200	18.60133600
H	7.61151900	10.92880100	18.54642000
C	9.67474600	13.58311200	19.03228600
H	9.65616500	14.63132500	19.31759300
C	5.20580200	15.59182900	9.95826700
H	4.32048400	15.73380900	9.34399600
C	8.30219000	13.86914600	23.33471200
H	9.12554800	13.46645100	23.91883100
C	4.49841700	4.02825500	16.34002700
H	3.62275800	3.50066500	16.70907500
C	9.74844700	10.89851300	18.29362300
H	9.76603400	9.85575700	17.99338400
C	4.95139500	7.08090600	12.87645100
H	4.47400500	6.24522300	13.39763300
H	5.85232900	7.35461600	13.43424300
H	5.25231600	6.74027300	11.87992100
C	10.92836800	11.63055300	18.36516100
H	11.87752400	11.15754700	18.12677000
C	6.73538700	5.39408700	15.41137900
H	7.61119000	5.91663100	15.03782600
C	10.88987000	12.97581700	18.73314800
H	11.80889700	13.55425800	18.78240500
C	5.39782300	3.38272900	15.49098200
H	5.22763900	2.35151800	15.19447100
C	6.51381300	4.07222500	15.02863800
H	7.22198500	3.58143100	14.36615200
C	8.81034100	7.52311100	16.82138800
H	8.64308200	6.78219900	17.59837800
C	7.72411600	8.19973000	16.25297500
C	7.96695100	9.15708000	15.26390500
H	7.13107200	9.69865000	14.82509900
C	9.26594700	9.42162800	14.83475100
H	9.43562700	10.17266700	14.06993500
C	10.33589400	8.72894300	15.39032600
H	11.34939300	8.93254800	15.05443600
C	10.10661500	7.78044100	16.38764300
H	10.94084300	7.24297100	16.83129800
C	2.76251100	7.90518800	11.92701400
H	3.05616900	7.59785900	10.91899900
H	2.07653000	8.75458000	11.84567600
H	2.22553700	7.06907800	12.38363500
C	1.74767400	12.02913900	16.80017900
N	0.60168700	12.16029800	16.89923600
C	-0.82911900	12.32588300	16.97930600
C	-1.25820100	13.20456400	15.79919100
H	-0.76774300	14.18124100	15.84469800
H	-1.00758700	12.72535700	14.84841600
H	-2.34125000	13.35090400	15.84532500
C	-1.46124400	10.93246900	16.89524800
H	-1.19550700	10.44301600	15.95382100
H	-1.12938700	10.30538300	17.72778200
H	-2.54894500	11.03670200	16.94450500
C	-1.14257900	13.00115600	18.31895500
H	-0.79425900	12.38639600	19.15390900
H	-0.66505400	13.98344700	18.37721000
H	-2.22542100	13.13008400	18.40378400