

A Theoretical Study of Dirhodium-Catalyzed Intramolecular Aliphatic C–H Bond Amination of Aryl Azides†

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1. Rh₂(OCHO)₄ catalyzed C–H bond amination with aryl azide **1**

The aryl azide **1** may coordinate with the catalyst Rh₂(OCHO)₄ (**II**) to form intermediate **A** or **A^{iso}** (Figure S1). **A^{iso}** and **A** are two coordination complexes between the catalyst and substrate. Figure S1 suggests an isomerization between **A^{iso}** and **A**. The energy of separate Rh₂(OCHO)₄ and **1** is 12.4 kcal/mol lower than **A**. And **A^{iso}** is 5.9 kcal/mol lower than **A**. These three structures can be exchanged with each other easily. The γ -coordination complex **A^{iso}** is more stable than the α -coordination complex **A**. However, **A** would be the reactant for elimination of nitrogen gas to form metal nitrene intermediate **B**, but **A^{iso}** might not.

The α -coordination complex **A** cleavages the N–N bond via the transition state **A-TS** and its activation barrier is 20.0 kcal/mol. The extrusion of N₂ produces the metal nitrene intermediate **^sB**.

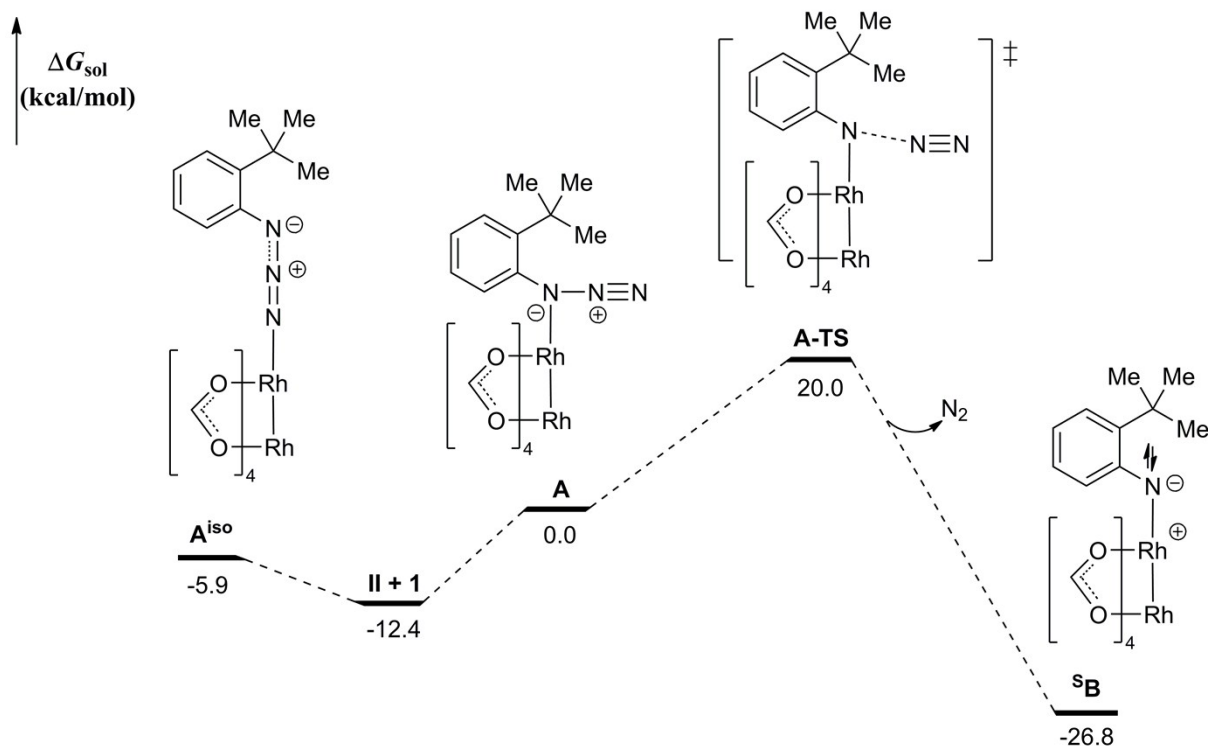


Figure S1. Reaction profiles of metal nitrene formation from Rh₂(OCHO)₄ (**II**) and **1**.

Following the extrusion of nitrogen gas, the dirhodium nitrene mediated amination would take place in an intramolecular mechanism (see Figure S2).

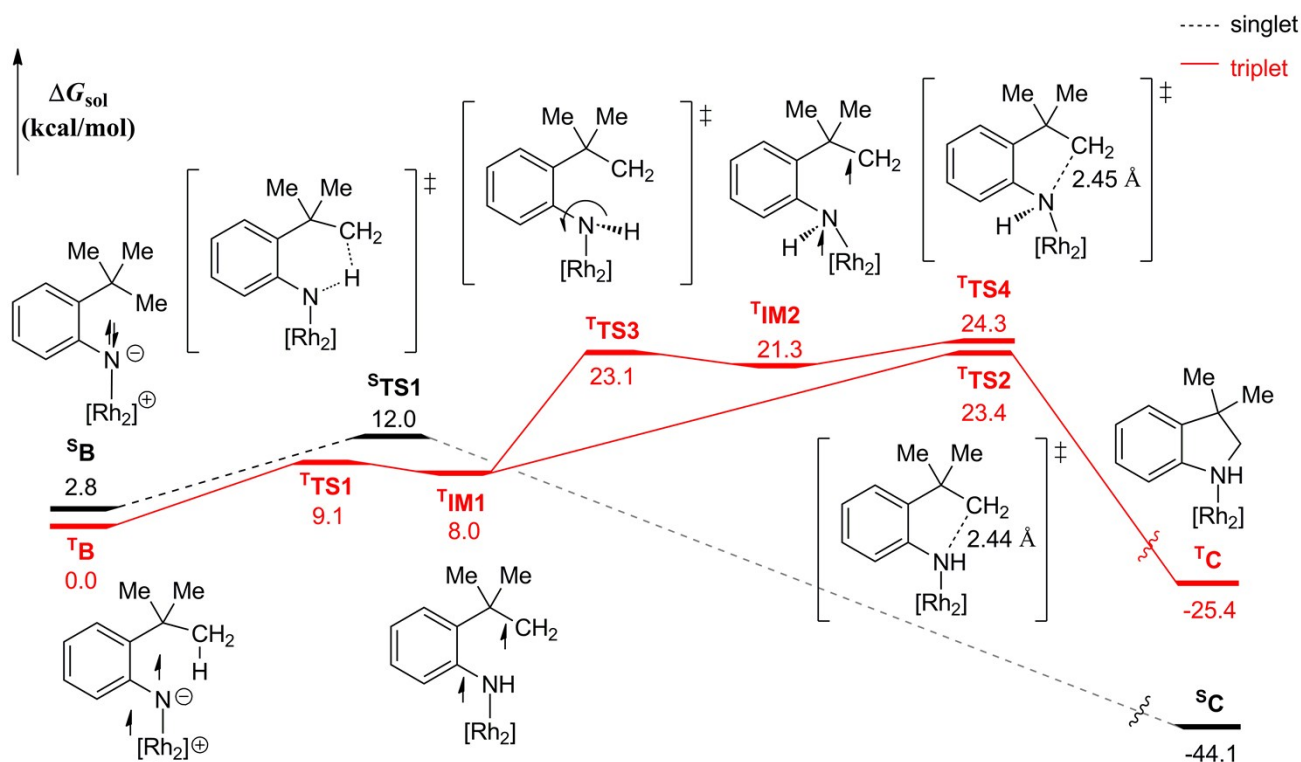


Figure S2. Reaction profiles of amination mediated by **B** from $\text{Rh}_2(\text{OCHO})_4$ and **1**.

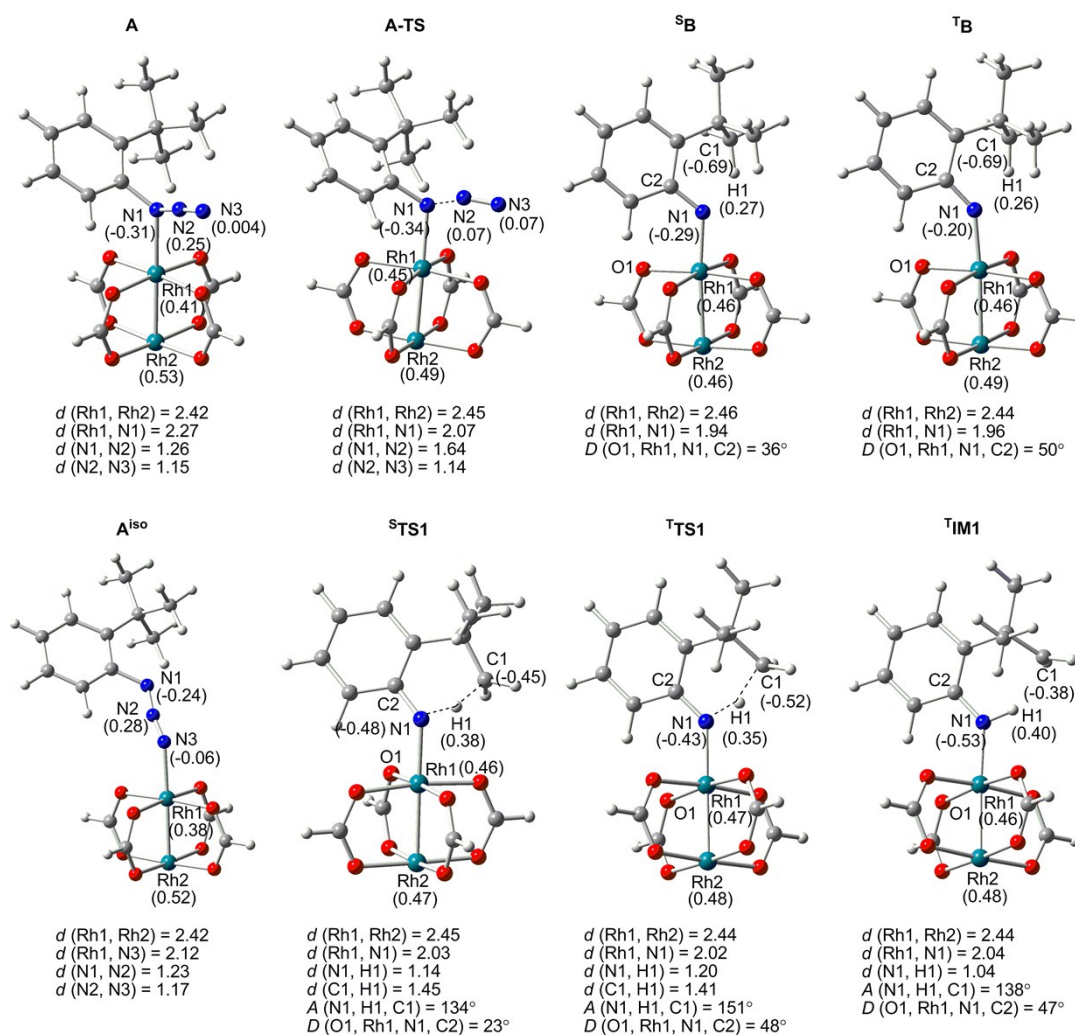


Figure S3. Shown are optimized structures in the reaction of $\text{Rh}_2(\text{OCHO})_4$ and **1**. Selected NBO charges are in parentheses. Bond distances are in angstrom.

2. Comparison of metal nitrenoid species in the reaction of $\text{Rh}_2(\text{OCHO})_4$ and **1**

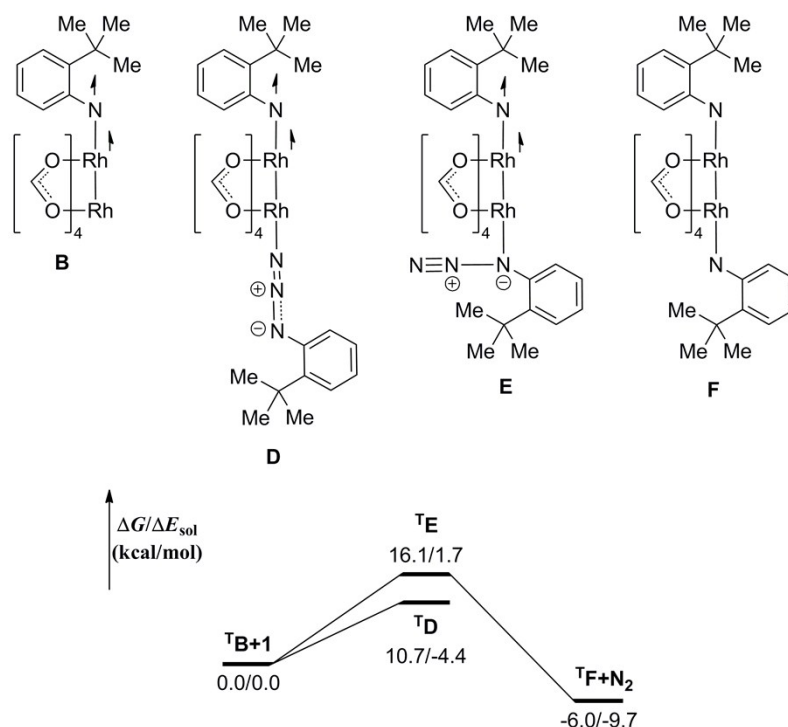


Figure S4. The relative energies of metal nitrenoid species as compared to T_{B} .

As previous reports (A. I. Olivos Suarez, H. Jiang, X. P. Zhang and B. de Bruin, *Dalton Trans.*, 2011, **40**, 5697-5705.) about metal nitrene suggest that bis-nitrene species and nitrene-azide species might be involved in the reactions, we also constructed and optimized some relative analogues derived from T_{B} (see Figure S1). One should mention that the two rhodium metal centers in the dirhodium catalyst could both react with the aryl azide substrate, which leads to **D** and **E** with sub.:cat.=2:1. With weaker electron-donating ability of rhodium centers, the energies of T_{D} and T_{E} are higher than the corresponding transition state in the amination reaction mediated by T_{B} . Thus T_{D} and T_{E} are not expected to form and subsequently produce bis-nitrene **F**. According to our calculations, T_{B} should mainly be the active intermediate for subsequent amination reactions.

3. Rh₂(esp)₂ catalyzed C–H bond amination with aryl azide 1

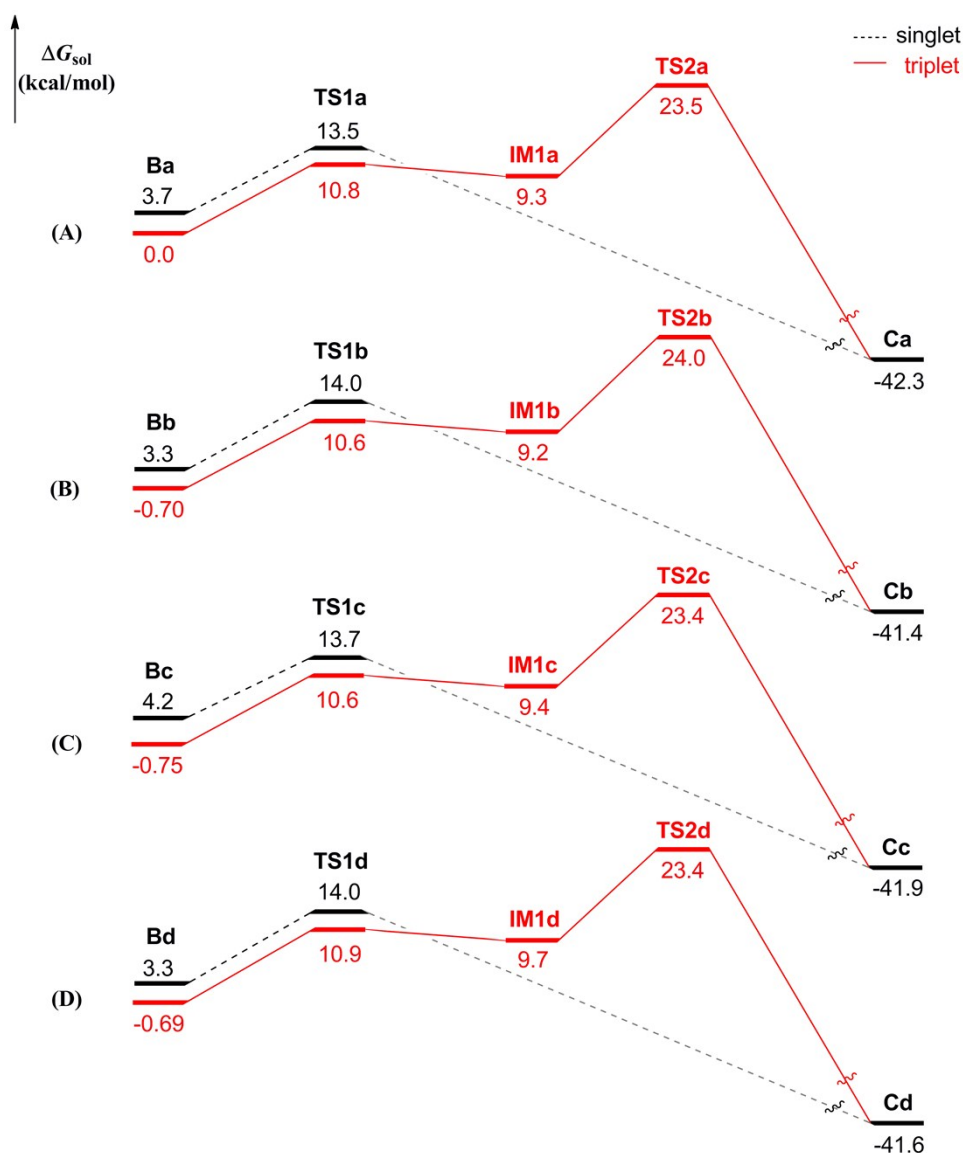


Figure S5. Reaction profiles of amination mediated by **Ba~d**.

Figure S5 depicts the reaction profiles of metal nitrene mediated amination from **Ba~d** with the free energy of the triplet **^TBa** as zero point energy. The free energy differences between the singlet and triplet metal nitrenes are about 3.5~5.0 kcal/mol ($\Delta G_{\text{ST}} = 3.7, 4.0, 5.0$ and 4.0 kcal/mol for **Ba**, **Bb**, **Bc** and **Bd**, respectively). It is noticeable that the enthalpy differences ΔH_{ST} are about 2.6 kcal/mol. Moreover, the triplet transition states **^TTS1a~d** are all lower in energy than the corresponding singlet transition states **^STS1a~d** by more than 2.5 kcal/mol. Therefore, the C-H bond amination from metal nitrene intermediates would be favored through the triplet transition states **^TTS1a~d**.

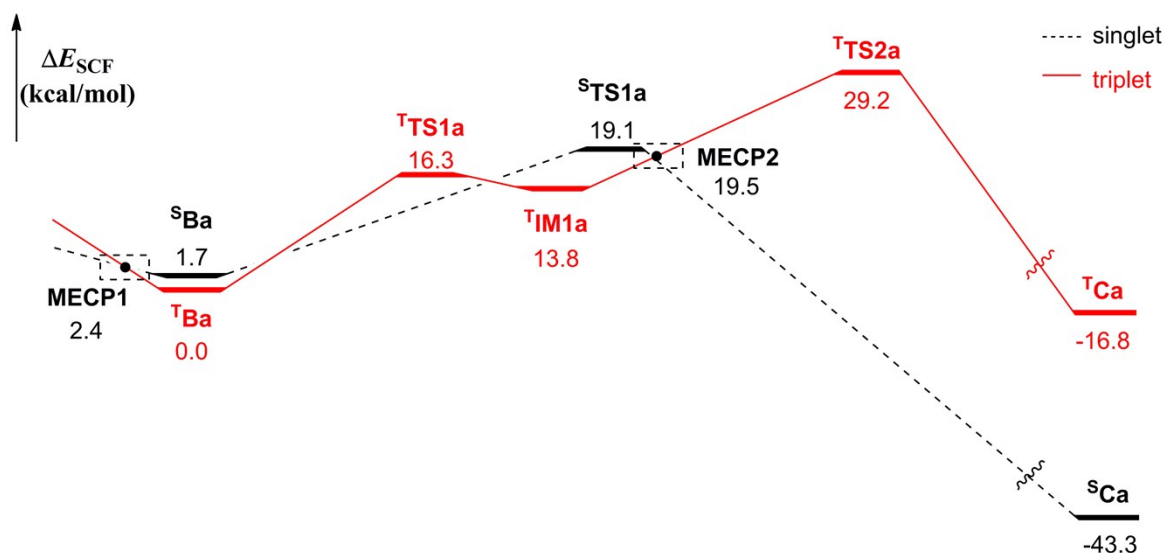


Figure S6. Reaction profiles of amination mediated by **Ba** from $\text{Rh}_2(\text{esp})_2$ (**I**) and **1** (relative energies in gas phase, sum of electronic energies/ E_{SCF}).

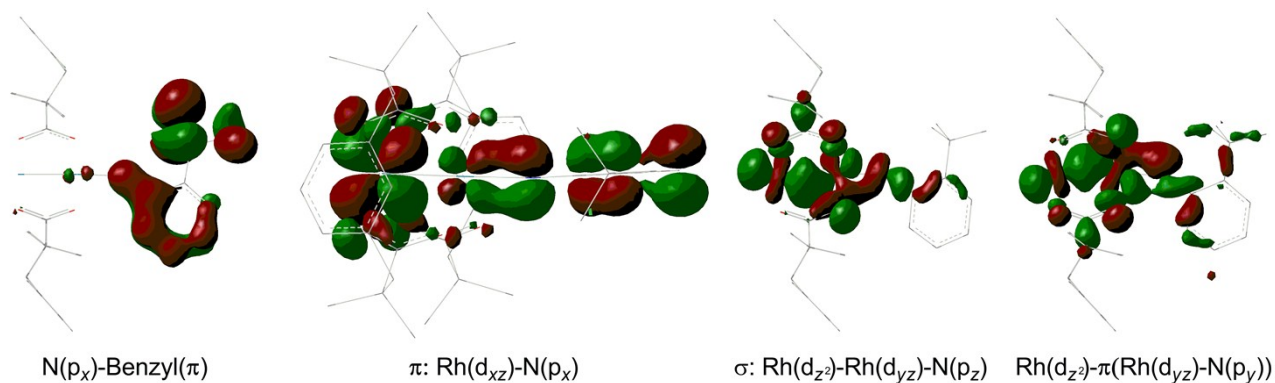


Figure S7. Kohn-Sham frontier orbitals of metal nitrene $t\text{Ba}$.

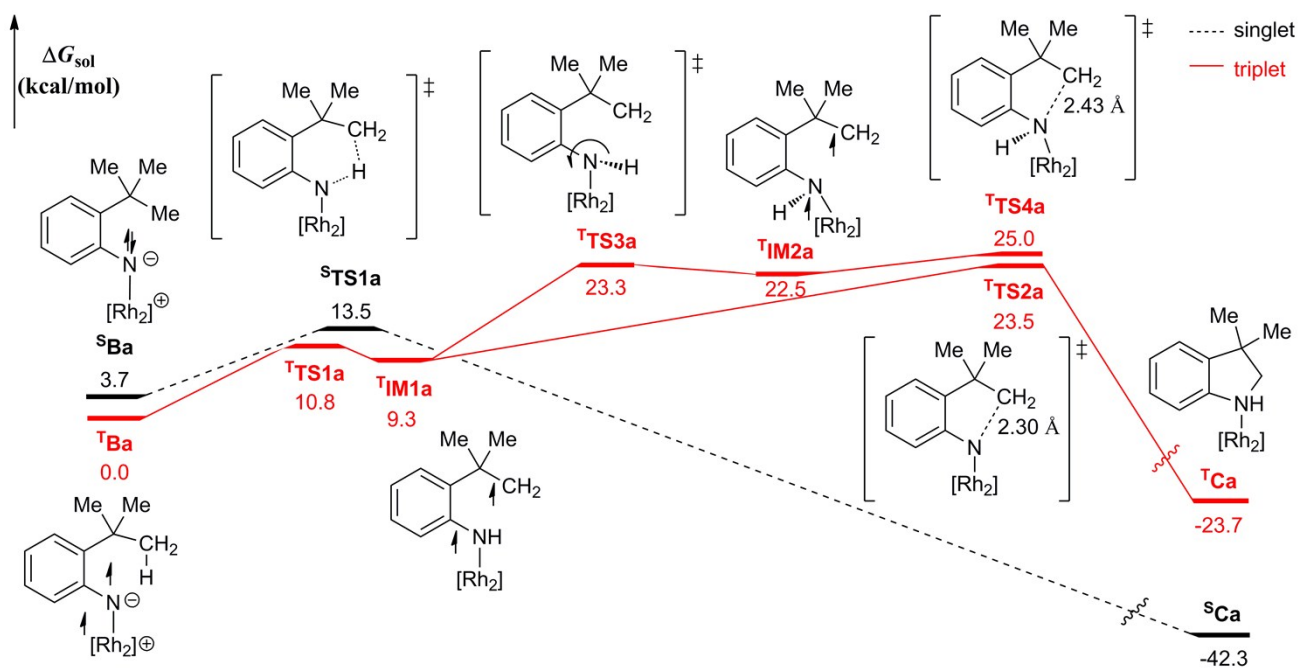


Figure S8. Reaction profiles of amination mediated by **Ba**.

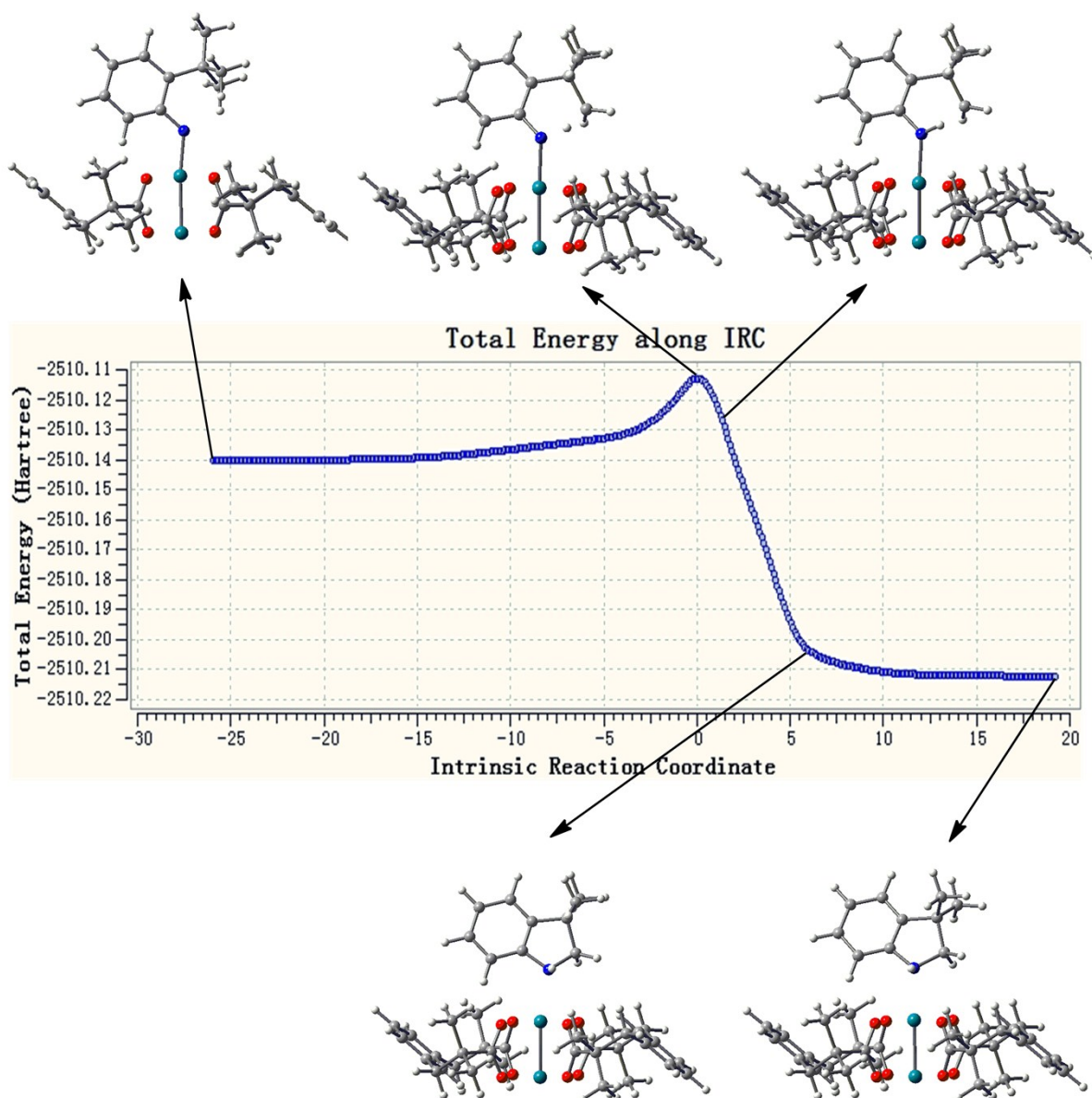


Figure S9. Shown is IRC calculation for $^8\text{TS1a}$.

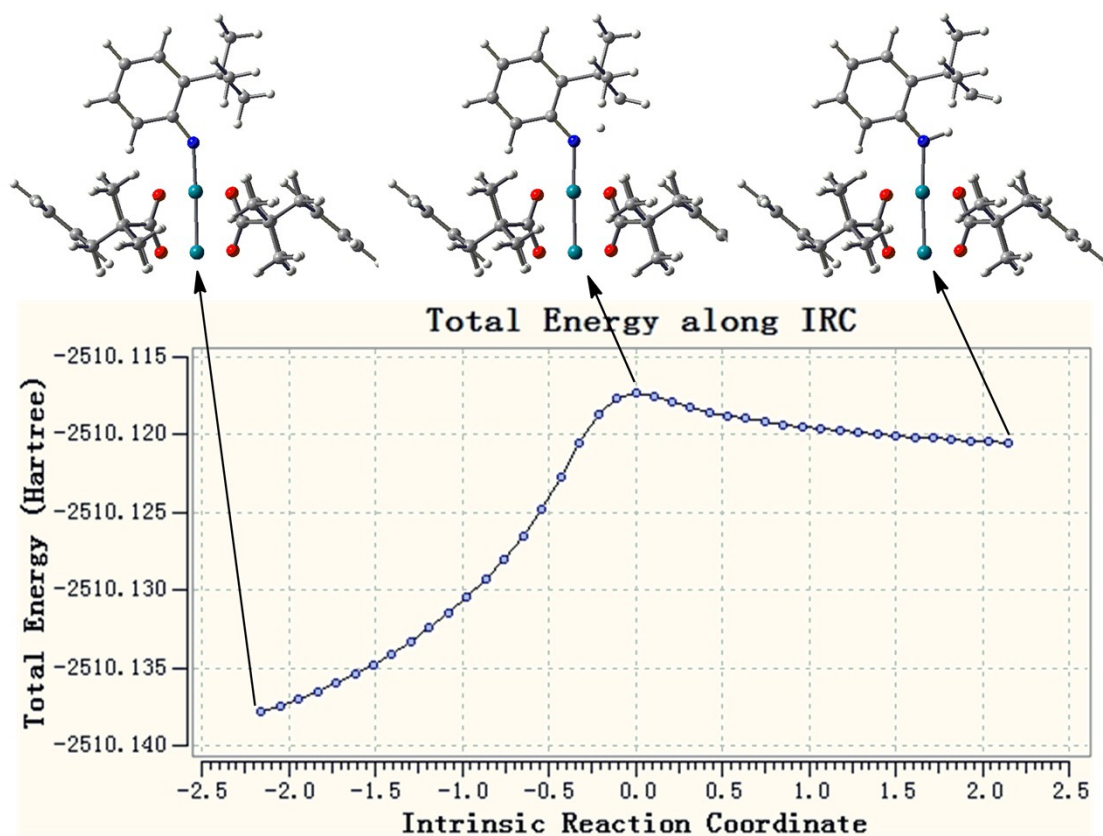


Figure S10. Shown is IRC calculation for $^1\text{TS1a}$.

4. Relative energies of important species calculated by BPW91 and M06L

Table S1. Relative energies of important species calculated by BPW91 and M06L (kcal/mol).

species	BPW91		M06L	
	ΔH_{sol}	ΔG_{sol}	ΔH_{sol}	ΔG_{sol}
A	0.0	0.0	0.0	0.0
A-TS	18.5	20.0	21.7	22.2
^sB	-13.8	-26.8	-6.5	-19.6
^sTS1	-5.5	-17.7	6.5	-6.0
^sC	-62.9	-73.7	-55.8	-67.9
^tB	-15.3	-29.7	-10.1	-24.9
^tTS1	-7.1	-20.5	4.4	-9.1
^tIM1	-7.0	-21.7	0.7	-14.6
^tTS2	8.0	-6.2	15.1	0.4
Aa	0.0	0.0	0.0	0.0
Aa-TS	17.8	19.2	19.3	19.8
^sBa	-15.4	-26.8	-5.4	-17.5
^sTS1a	-5.4	-17.0	7.4	-6.0
^sCa	-61.8	-72.8	-53.0	-64.1
^tBa	-18.0	-30.5	-9.0	-22.4
^tTS1a	-8.2	-19.7	4.9	-7.4
^tIM1a	-8.1	-21.2	3.3	-9.6
^tTS2a	5.6	-7.0	18.1	3.3

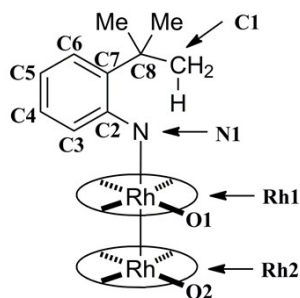
5. Relative energies of important species optimized at BPW91/BS3

Table S2. Relative energies of important species optimized at BPW91/BS3 (kcal/mol).

species	ΔH_{sol}	ΔG_{sol}
Aa	0.0	0.0
Aa-TS	17.9	18.7
^sBa	-15.4	-26.9
^sTS1a	-5.5	-17.4
^sCa	-61.7	-73.0
^tBa	-17.9	-30.7
^tTS1a	-8.0	-19.5
^tIM1a	-7.9	-21.3
^tTS2a	5.4	-9.3

6. Mulliken atomic spin densities

Table S3. Mulliken atomic spin densities for selected atoms in the optimized structures (O1 and O2 refer to the oxygen atoms coordinated to Rh1 and Rh2 centers, respectively).



species	S ²	Rh1	Rh2	N1	C1	C2~C7	C8	O1	O2
^T Ba	2.0	0.35144	0.17714	1.01652	0.01862	0.43445	-0.01374	0.01380	-0.00078
^T TS1a	2.0	0.27220	0.15576	0.66819	0.62105	0.35248	-0.03573	0.01276	0.00091
^T IM1a	2.0	0.23965	0.12388	0.41706	0.97665	0.32604	-0.06174	0.00861	0.00030
^T TS2a	2.0	0.56689	0.53185	0.08558	0.68271	0.12989	-0.03728	0.04503	0.02267
MECP2	2.0	0.25164	0.13980	0.42711	0.98734	0.28963	-0.06124	0.00960	0.00096
^T Ca	2.0	1.20929	0.54673	0.00237	0.00314	0.00196	0.00284	0.20148	0.01516
^T B	2.0	0.31082	0.16225	1.05954	0.01987	0.44538	-0.01378	0.01235	-0.00147
^T TS1	2.0	0.24234	0.13674	0.69869	0.61583	0.37561	-0.03568	0.01055	-0.00034
^T IM1	2.0	0.21313	0.09606	0.44523	0.97536	0.35662	-0.06223	0.00662	-0.00090
^T TS2	2.0	0.69457	0.27422	0.19871	0.73393	0.06490	-0.04286	0.10513	-0.00175
^T C	2.0	1.21631	0.55266	0.00022	0.00333	0.00208	0.00273	0.19763	0.00814

7. Coordinates of optimized structures (BPW91/BS1)

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I = Rh₂(esp)₂ (E = -2066.60898668)

Rh	-0.03812100	-0.00000200	1.18733800
O	1.40088400	-1.47471600	1.17818600
O	1.40088300	1.47471200	1.17818600
O	1.48227400	-1.44976100	-1.10520400
O	1.48227200	1.44975700	-1.10520300
C	1.85880600	-1.88214200	0.04488600
C	2.92870000	-2.99434700	0.07985500
C	2.30056000	-4.23629600	0.76257900
H	1.94299000	-3.99698300	1.77546200
H	3.05189200	-5.04045800	0.83603300
H	1.45100500	-4.62144600	0.17505500
C	3.38508500	-3.35818300	-1.34549200
H	2.53945600	-3.71475800	-1.95300300
H	4.13701100	-4.16405500	-1.29502200
H	3.83163200	-2.49656600	-1.86217400
C	4.14551100	-2.52089300	0.95537700
H	3.79074100	-2.40962200	1.99335400
H	4.87851800	-3.34723200	0.94952700
C	4.80607500	-1.23160900	0.50689800
C	5.90408000	-1.21718800	-0.37551000
H	6.33602600	-2.16180400	-0.72095700
C	6.45459400	0.00000300	-0.80314500
H	7.31776800	0.00000300	-1.47547600
C	5.90407800	1.21719400	-0.37551200
H	6.33602300	2.16181100	-0.72096100
C	4.80607400	1.23161500	0.50689600
C	4.29769200	0.00000300	0.95868600
H	3.47153700	0.00000400	1.67380500
C	4.14550800	2.52090000	0.95537300
H	4.87851300	3.34724100	0.94952000
H	3.79074100	2.40963000	1.99335200
C	2.92869300	2.99434800	0.07985300
C	3.38507300	3.35818700	-1.34549500
H	3.83162400	2.49657300	-1.86217700
H	4.13699500	4.16406300	-1.29502500
H	2.53944200	3.71475800	-1.95300400
C	2.30054800	4.23629400	0.76258000
H	1.45099000	4.62144000	0.17505800
H	3.05187600	5.04045900	0.83603300
H	1.94298100	3.99697800	1.77546300
C	1.85880500	1.88213800	0.04488600
Rh	0.03812500	-0.00000300	-1.18732900
O	-1.40087700	1.47471200	-1.17817700
O	-1.40087700	-1.47471800	-1.17817800
O	-1.48227200	1.44975400	1.10521300
O	-1.48227200	-1.44975900	1.10521100
C	-1.85880600	1.88213200	-0.04487700
C	-2.92869400	2.99434300	-0.07984700
C	-2.30054100	4.23629300	-0.76255800
H	-1.94296700	3.99698500	-1.77544100
H	-3.05186600	5.04046100	-0.83600900
H	-1.45098600	4.62143100	-0.17502600
C	-3.38508700	3.35817200	1.34550000
H	-2.53946200	3.71473900	1.95301900
H	-4.13700900	4.16404900	1.29502900
H	-3.83164300	2.49655500	1.86217300
C	-4.14550100	2.52090200	-0.95538200
H	-3.79072200	2.40963700	-1.99335700
H	-4.87850400	3.34724400	-0.94953200
C	-4.80607300	1.23161600	-0.50691700
C	-5.90409300	1.21719400	0.37547200
H	-6.33604300	2.16181000	0.72091400

C	-6.45461500	0.00000300	0.80309500
H	-7.31780000	0.00000200	1.47541100
C	-5.90409300	-1.21718800	0.37546900
H	-6.33604400	-2.16180400	0.72090900
C	-4.80607300	-1.23160800	-0.50692000
C	-4.29768300	0.00000500	-0.95869900
H	-3.47151700	0.00000500	-1.67380600
C	-4.14550200	-2.52089300	-0.95538600
H	-4.87850800	-3.34723300	-0.94954200
H	-3.79071900	-2.40962600	-1.99336000
C	-2.92870100	-2.99434200	-0.07984700
C	-3.38510100	-3.35816300	1.34549900
H	-3.83165200	-2.49653900	1.86216700
H	-4.13702900	-4.16403300	1.29502900
H	-2.53948100	-3.71473300	1.95302200
C	-2.30055700	-4.23630000	-0.76255300
H	-1.45100800	-4.62144500	-0.17501600
H	-3.05188900	-5.04046100	-0.83600400
H	-1.94297700	-3.99699800	-1.77543500
C	-1.85880200	-1.88214200	-0.04487800

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II = Rh₂(OCHO)₄ (E = -978.06555768)

Rh	-0.00099500	0.00143100	1.19586100
O	1.44982200	-1.45053200	1.15410000
O	-1.45302000	-1.44921600	1.15203100
O	1.45404000	-1.45100000	-1.14893800
O	-1.44861400	-1.45462500	-1.15100100
C	1.84690600	-1.84555000	0.00338000
C	-1.84578400	-1.84671200	0.00067700
Rh	0.00095500	-0.00148300	-1.19585700
O	-1.45212600	1.44819300	-1.15410100
O	1.45059200	1.45153900	-1.15203200
O	-1.45165000	1.45341500	1.14893500
O	1.45095100	1.45223400	1.15101000
C	-1.84656300	1.84588600	-0.00339600
C	1.84572300	1.84669300	-0.00068800
H	2.62745700	-2.62647900	0.00495100
H	-2.62664300	-2.62733400	0.00104000
H	-2.62715000	2.62678000	-0.00498100
H	2.62651000	2.62738800	-0.00105600

44

A^{iso} (E = -1531.10410652)

N	-2.96593800	-0.47846800	-0.59386300
Rh	3.40263200	0.03436600	0.60110300
O	3.05298500	-1.79612100	1.45874400
O	2.50942600	0.95599800	2.20730000
O	0.98504200	-1.93029400	0.45281100
O	0.44108200	0.83592800	1.20287500
C	1.93690600	-2.35721400	1.19453300
C	1.24926400	1.14397300	2.14737000
Rh	1.23522100	-0.09253700	-0.46518600
O	1.62342800	1.75268200	-1.31021300
O	2.15880800	-1.01448000	-2.06556100
O	3.68643200	1.86259600	-0.29104300
O	4.21774400	-0.88711800	-1.04055100
C	2.74651700	2.30182100	-1.03520700
C	3.42223600	-1.19884400	-1.99019000
H	1.76610700	-3.34164600	1.66655400
H	0.78997400	1.63727800	3.02315700
H	2.92183800	3.28601700	-1.50620900
H	3.88346900	-1.69323900	-2.86416400
C	-3.45830600	1.91790600	-0.33112100

C	-3.87871600	0.57241900	-0.28363000
C	-5.21002500	0.21267400	0.07704500
C	-6.07023000	1.28743800	0.38162300
C	-5.66317400	2.62860200	0.33714300
C	-4.34806900	2.94813300	-0.02242200
H	-2.42558900	2.14841700	-0.60797000
H	-7.10134300	1.07487200	0.66522100
H	-6.37703400	3.41876700	0.58480700
H	-4.01228600	3.98767700	-0.06142000
C	-5.70333500	-1.25283800	0.13635600
C	-4.88294200	-2.05293400	1.18512000
C	-7.19060900	-1.34143100	0.55265200
C	-5.57716800	-1.91702600	-1.26213800
H	-3.81314700	-2.08665300	0.93454800
H	-4.98891900	-1.60705400	2.18813800
H	-5.25368400	-3.09108300	1.23356600
H	-7.85560600	-0.82993000	-0.16316900
H	-7.49188400	-2.40119100	0.58076000
H	-7.36935300	-0.92318400	1.55734200
H	-5.96193000	-2.95027300	-1.21959300
H	-6.16739200	-1.36520700	-2.01260800
H	-4.53412600	-1.95900000	-1.60676000
N	-1.80596700	-0.22565400	-0.93244300
N	-0.70611200	-0.19251700	-1.32314900

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A (E = -1531.09447504)

N	1.58685800	0.03864400	0.96930500
Rh	-2.86838000	-0.04235500	-0.51406400
O	-2.95910700	1.98678300	-0.20909700
O	-3.46090300	-0.35672000	1.42811500
O	-0.77426100	2.03650200	0.51869000
O	-1.27985000	-0.31466400	2.16326300
C	-1.90875400	2.55955600	0.23384800
C	-2.54758200	-0.41959900	2.31652400
Rh	-0.57066900	-0.00363100	0.25206000
O	-0.52404900	-2.04765500	-0.03859500
O	0.00132600	0.31285500	-1.70597200
O	-2.70372200	-2.06824100	-0.78320800
O	-2.18793600	0.27374900	-2.42517300
C	-1.58525700	-2.60709900	-0.48526000
C	-0.92511200	0.37940700	-2.58602300
H	-1.98359000	3.65065300	0.39353600
H	-2.88874100	-0.58667100	3.35397900
H	-1.52223800	-3.70080900	-0.63058700
H	-0.58411300	0.55233500	-3.62298400
C	2.54932800	2.18031000	0.34240500
C	2.68684700	0.78221900	0.33745100
C	3.79443500	0.12361900	-0.26086500
C	4.75546300	0.98421100	-0.83887600
C	4.63870900	2.38067500	-0.83449000
C	3.52767000	2.98995200	-0.24253400
H	1.65352800	2.61461000	0.79083900
H	5.63725600	0.54951100	-1.30981700
H	5.42198300	2.98678400	-1.29828200
H	3.41656200	4.07734500	-0.23440500
C	3.98120300	-1.41301400	-0.31310500
C	2.85443200	-2.04470800	-1.17083400
C	5.33365400	-1.80395900	-0.95677600
C	3.96701500	-2.03199300	1.11133600
H	1.85818300	-1.86173600	-0.74702700
H	2.87057800	-1.64080100	-2.19638800
H	3.00186900	-3.13719200	-1.23044900
H	6.19593700	-1.41247400	-0.39101700
H	5.41787700	-2.90280700	-0.96764800
H	5.41568600	-1.46215900	-2.00170900
H	4.24563900	-3.09767100	1.05086900
H	4.69303400	-1.53233700	1.77420500

H	2.97420600	-1.98879600	1.57950200
N	1.54952800	-0.06782400	3.37113200
N	1.62207400	0.03249900	2.22764900

44

A-TS (E = -1531.06390285)

N	1.48061600	-0.29089200	0.86051800
Rh	-2.76912200	0.04324200	-0.59977000
O	-2.99603000	1.88307100	0.28634700
O	-3.42590800	-0.86764600	1.11996700
O	-0.87714100	1.78879700	1.17925900
O	-1.28860900	-0.95700500	1.96542600
C	-2.02099500	2.33116100	0.97085100
C	-2.55452300	-1.16464000	2.00052200
Rh	-0.49949500	-0.04526300	0.30627400
O	-0.36573700	-1.91854400	-0.58897800
O	0.10622900	0.88867900	-1.44061600
O	-2.49701300	-1.79480400	-1.45411900
O	-2.03730600	0.95320400	-2.28357400
C	-1.37073300	-2.35774800	-1.24766400
C	-0.78042500	1.16909300	-2.32004000
H	-2.17130300	3.31381800	1.45339700
H	-2.92489000	-1.66209800	2.91433000
H	-1.24062900	-3.35986500	-1.69526500
H	-0.39966000	1.66577400	-3.23084400
C	2.22577100	2.03526700	0.73877100
C	2.45654200	0.66330300	0.46887600
C	3.64810900	0.24954200	-0.22516900
C	4.51020500	1.28630000	-0.64141600
C	4.27229300	2.63965900	-0.36591100
C	3.12642500	3.02213500	0.34427800
H	1.31407100	2.29909300	1.27596000
H	5.41765900	1.03458100	-1.19033400
H	4.99170700	3.39134000	-0.70402100
H	2.93402400	4.07285400	0.57803100
C	4.00480000	-1.22256200	-0.53998400
C	2.94023800	-1.83884100	-1.48381600
C	5.37625700	-1.34749800	-1.24926800
C	4.08971200	-2.05360200	0.76717800
H	1.94782600	-1.86079700	-1.01433100
H	2.86815200	-1.26537500	-2.42325900
H	3.22494500	-2.87500400	-1.73829200
H	6.20489700	-0.95338900	-0.63695800
H	5.58369600	-2.41388600	-1.43542500
H	5.38970600	-0.83820900	-2.22726200
H	4.43898800	-3.07374400	0.53313400
H	4.80373800	-1.60710100	1.47941200
H	3.11082700	-2.14044200	1.25607700
N	1.12899800	-1.19469300	3.28846600
N	1.54810500	-0.50185300	2.48530700

42

^sB (E = -1421.59681961)

N	-1.52260100	-0.30608800	-0.32638500
Rh	2.83720200	-0.00751100	0.15944200
O	3.01027100	-1.36261800	-1.36855900
O	2.69978200	-1.54842500	1.49723100
O	0.72551900	-1.42463000	-1.67719500
O	0.41373500	-1.64248300	1.23027600
C	1.93461800	-1.75828900	-1.92982800
C	1.53466800	-2.01775600	1.71968900
Rh	0.39188800	-0.06614400	-0.13533100
O	0.26338000	1.28090300	1.42456100
O	0.62738400	1.49450900	-1.47098300
O	2.55167000	1.34119300	1.69127100
O	2.91269100	1.53077500	-1.19795000
C	1.35606400	1.66957200	1.97522000
C	1.81410300	1.92929400	-1.69878700

H	2.05737300	-2.49081200	-2.74871200
H	1.47798000	-2.86236800	2.43034500
H	1.22833600	2.38630800	2.80693800
H	1.87535000	2.75789200	-2.42729200
C	-2.19808200	2.04344700	-0.16681000
C	-2.48044100	0.62708000	-0.16177100
C	-3.87330000	0.18259500	-0.00784700
C	-4.84263100	1.18264400	0.15145400
C	-4.53035000	2.55383700	0.13393800
C	-3.20432600	2.98903700	-0.03823700
H	-1.16408500	2.34927300	-0.31471200
H	-5.88795300	0.90207200	0.28627400
H	-5.33538400	3.28558100	0.25108400
H	-2.96968200	4.05677900	-0.06428400
C	-4.26099300	-1.30638500	0.00135300
C	-5.77941800	-1.50946200	0.21724600
C	-3.88601000	-1.95286200	-1.36309500
C	-3.52130200	-2.04434900	1.15307700
H	-6.12181400	-1.10939900	1.18675400
H	-6.38335500	-1.05144400	-0.58441700
H	-5.99782800	-2.58962300	0.21325700
H	-2.80315600	-1.89690000	-1.53835800
H	-4.19301500	-3.01285500	-1.36152300
H	-4.40871300	-1.44951900	-2.19406300
H	-2.43250300	-2.00381700	1.00915700
H	-3.76580900	-1.59686500	2.13165700
H	-3.83766300	-3.10142400	1.17476300

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¹B (E = -1421.59858456)

N	1.52891000	-0.05627600	-0.30831100
Rh	-2.84346900	0.01909900	0.16448000
O	-2.73433400	-1.72738700	1.22780500
O	-3.05420400	-1.04351000	-1.57798900
O	-0.45022400	-1.82717500	0.96199900
O	-0.77197800	-1.15252100	-1.87105400
C	-1.58169400	-2.24869900	1.38843900
C	-1.98935700	-1.38575400	-2.19168700
Rh	-0.42452400	-0.07346100	-0.13955100
O	-0.62149900	1.67775800	-1.23355100
O	-0.27111900	1.01111000	1.61870100
O	-2.90024000	1.76657200	-0.91071600
O	-2.55666600	1.07596500	1.90145800
C	-1.78912000	2.18866700	-1.36867200
C	-1.35122000	1.32778200	2.23009500
H	-1.54651200	-3.18742500	1.96998600
H	-2.12818900	-1.96011600	-3.12537000
H	-1.82725300	3.11909200	-1.96375600
H	-1.20932600	1.89557500	3.16749000
C	2.45046900	2.14839100	-0.13915200
C	2.60678300	0.71290600	-0.15299200
C	3.94477900	0.13655800	-0.01546500
C	5.00668400	1.03776500	0.11711500
C	4.83439100	2.43535300	0.12811700
C	3.54750600	2.98675300	0.00083800
H	1.44130500	2.54378300	-0.25221000
H	6.02077600	0.64841400	0.22125300
H	5.70653400	3.08568600	0.23632800
H	3.40472600	4.07124700	0.00873700
C	4.15717700	-1.38777600	-0.00816800
C	5.65046700	-1.76169200	0.13817900
C	3.39132300	-2.01564400	1.18812300
C	3.64249200	-2.00158000	-1.33798200
H	6.25953800	-1.37470700	-0.69599600
H	6.08022200	-1.39369200	1.08505300
H	5.74920600	-2.85948900	0.13721600
H	2.30871800	-1.83204400	1.11848400
H	3.55217500	-3.10755300	1.20178000

H	3.75212900	-1.60468100	2.14607300
H	2.56679400	-1.81373300	-1.47779200
H	4.18294800	-1.58126700	-2.20270400
H	3.80157300	-3.09355400	-1.33218000

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N₂ (E = -109.51428868)

N	0.00000000	0.00000000	0.55811100
N	0.00000000	0.00000000	-0.55811100

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¹D (E = -1974.62622682)

N	4.79758700	-0.55117300	0.02415600
C	5.39159500	1.61966600	-0.97026400
C	5.71446400	0.52732900	-0.13888600
C	6.95238400	0.46148300	0.56527900
C	7.82402900	1.55244600	0.37274900
C	7.51388100	2.64239600	-0.45345400
C	6.28899300	2.67746400	-1.13046400
H	4.42838200	1.63390600	-1.48868800
H	8.78633400	1.55699700	0.88552000
H	8.23168800	3.45969700	-0.56358500
H	6.02794000	3.51898100	-1.77768100
C	7.33612600	-0.72212700	1.48538900
C	7.37270900	-2.04492600	0.67205700
C	8.73756500	-0.53348500	2.11262100
C	6.32016200	-0.84113900	2.65426800
H	6.39072400	-2.29371100	0.24574100
H	8.10153300	-1.97694000	-0.15274500
H	7.67871400	-2.87740000	1.32860800
H	8.79558100	0.36896800	2.74390400
H	8.96039100	-1.39921300	2.75755400
H	9.53237100	-0.47902500	1.34988100
H	6.60960300	-1.67563200	3.31586600
H	6.30691100	0.08211500	3.25726900
H	5.29900200	-1.03178400	2.29468300
N	3.74183400	-0.58779900	-0.61765800
N	2.73196000	-0.81206200	-1.15156200
N	-3.77413900	0.19455600	0.13141200
Rh	0.53326900	-0.47199700	-0.76311100
O	0.43912900	1.03972200	-2.16767200
O	-0.03785200	-1.83749300	-2.19052500
O	-1.78176900	1.43805500	-1.71337800
O	-2.26254500	-1.44222700	-1.74960300
C	-0.67554500	1.63961700	-2.32151300
C	-1.28963700	-2.00642000	-2.35894500
Rh	-1.83856000	-0.04398500	-0.27669500
O	-1.71624300	-1.56087800	1.12784800
O	-1.21861200	1.32074300	1.14355500
O	0.50684500	-1.94938200	0.67534000
O	1.00174700	0.92031000	0.69044200
C	-0.59409500	-2.15272500	1.28480000
C	0.03879500	1.48925700	1.30313100
H	-0.69323900	2.44270300	-3.08126400
H	-1.57973100	-2.73819200	-3.13544300
H	-0.58256200	-2.94738400	2.05361100
H	0.32320200	2.22757800	2.07535600
C	-5.01992500	-1.84859200	0.19783800
C	-4.92974400	-0.41796400	0.37709700
C	-6.11195300	0.32344200	0.81958400
C	-7.27450900	-0.42058200	1.04608500
C	-7.34155400	-1.81641500	0.86818100
C	-6.20562800	-2.52734100	0.44200300
H	-4.12279000	-2.36795700	-0.13909900
H	-8.17760700	0.09592400	1.37667600
H	-8.28112200	-2.34053400	1.06289600
H	-6.25050800	-3.61118900	0.30051300
C	-6.05823800	1.84817100	1.02369100

C	-5.67186700	2.54533700	-0.30924800
C	-7.42176600	2.41828600	1.47650300
C	-5.01101000	2.19390200	2.11712600
H	-4.68361200	2.21606500	-0.66521600
H	-6.41330100	2.32822100	-1.09657100
H	-5.63727100	3.63891200	-0.16360500
H	-7.74726700	1.99842100	2.44319200
H	-7.33261900	3.50947100	1.60446800
H	-8.21486000	2.23641200	0.73185000
H	-4.98026600	3.28620300	2.27353000
H	-5.27319200	1.71844200	3.07735600
H	-4.00203700	1.86119700	1.83046300

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^TE (E = -1974.61763550)

N	3.47443600	-0.62037200	-0.65805700
C	4.28403300	-1.61026600	1.41517800
C	4.41035700	-0.58069000	0.46703100
C	5.35494800	0.47091600	0.60966300
C	6.15805200	0.40316100	1.77073600
C	6.04841900	-0.62105000	2.72108000
C	5.10651000	-1.63997200	2.54543700
H	3.51294900	-2.36853800	1.26431500
H	6.90691100	1.17728700	1.94101100
H	6.70265100	-0.61505900	3.59744400
H	5.00261200	-2.44517100	3.27765600
C	5.54289700	1.61561200	-0.41576900
C	6.67049100	2.58653100	0.00885100
C	5.93761800	1.03999200	-1.80318800
C	4.23975500	2.44574200	-0.54028000
H	6.45782800	3.07480400	0.97439300
H	7.65156800	2.08707500	0.07775400
H	6.75964600	3.38332500	-0.74756900
H	5.12797100	0.45203600	-2.25745100
H	6.16754500	1.86719100	-2.49622100
H	6.83418900	0.40206700	-1.72942800
H	4.39285800	3.26912400	-1.25994500
H	3.39267700	1.84216800	-0.89140600
H	3.96426100	2.88768300	0.43113400
N	-3.32200200	0.17055800	0.23472000
C	-4.48660300	-1.91693500	0.09412800
C	-4.48516100	-0.47637200	0.20140500
C	-5.76196700	0.23550900	0.27724200
C	-6.92241800	-0.54410800	0.23023800
C	-6.90259300	-1.94821500	0.11855200
C	-5.67559600	-2.63160700	0.05246600
H	-3.51885100	-2.41587500	0.04594900
H	-7.89444700	-0.05020900	0.28159200
H	-7.84578000	-2.50022700	0.08550200
H	-5.65173000	-3.72212300	-0.03144900
C	-5.80556300	1.76905000	0.40282700
C	-7.25510600	2.30283900	0.47046400
C	-5.07645000	2.20897300	1.70141000
C	-5.11774000	2.41896700	-0.82839400
H	-7.83100000	2.05979800	-0.43842300
H	-7.80159100	1.91163400	1.34515000
H	-7.23124600	3.40120900	0.56089500
H	-4.01878400	1.90447000	1.69107400
H	-5.11661100	3.30756500	1.80039500
H	-5.55572500	1.76695500	2.59113000
H	-5.15369600	3.51856700	-0.73880200
H	-4.06270600	2.11690300	-0.90869700
H	-5.63180100	2.13461600	-1.76200400
Rh	-1.35603000	0.00308500	-0.00904400
O	-0.86615600	1.31402800	1.50895000
O	-1.27402300	-1.58071900	1.32769100
O	1.38766700	0.98484900	1.18056700
O	0.97766600	-1.90534400	0.97943400

C	0.37485100	1.50217200	1.75553800
C	-0.15221400	-2.16396000	1.51188700
Rh	1.05008700	-0.34011000	-0.36096500
O	0.60614300	-1.64713500	-1.88451900
O	1.00561700	1.22444200	-1.70142900
O	-1.65129500	-1.33692000	-1.56608300
O	-1.24697100	1.55471200	-1.36702900
C	-0.62798100	-1.84391300	-2.13945300
C	-0.11140000	1.80703200	-1.89806500
N	3.72180000	-2.34445900	-2.31026100
N	3.66069300	-1.55164700	-1.47623800
H	-0.16969500	-3.00456400	2.23020000
H	0.59072800	2.20882600	2.57784800
H	-0.84632700	-2.54592100	-2.96508500
H	-0.10347200	2.64223300	-2.62226200

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^TF (E = -1865.11424975)

N	-3.20183100	0.25004200	-0.36537900
C	-3.90964200	-2.07506800	-0.17206700
C	-4.16765500	-0.65389600	-0.17278900
C	-5.55385900	-0.19031800	-0.00195000
C	-6.53801300	-1.17475000	0.13908000
C	-6.25526300	-2.55392300	0.13969500
C	-4.93128500	-3.00012400	-0.01612100
H	-2.87911200	-2.39530100	-0.31216000
H	-7.57814300	-0.86910600	0.26412800
H	-7.07090900	-3.27195100	0.26174000
H	-4.70383300	-4.07026700	-0.02094300
C	-5.90329200	1.30943100	0.01494400
C	-7.41831100	1.54953700	0.21404900
C	-5.15823600	2.01113200	1.18365700
C	-5.49639200	1.96424800	-1.33352100
H	-8.02097100	1.11479400	-0.60126400
H	-7.78208600	1.14328100	1.17296500
H	-7.61105000	2.63484600	0.22230200
H	-4.06807800	1.91880700	1.07434600
H	-5.41683400	3.08415200	1.19816100
H	-5.45128600	1.57617200	2.15430600
H	-5.76398500	3.03514900	-1.32443400
H	-4.41276500	1.87620700	-1.50257000
H	-6.02204400	1.48763200	-2.17820200
N	3.20183100	-0.25001000	0.36540900
C	3.90959000	2.07509400	0.17184700
C	4.16763900	0.65392900	0.17274300
C	5.55385600	0.19036500	0.00197100
C	6.53798700	1.17480500	-0.13916900
C	6.25520200	2.55397100	-0.13994600
C	4.93121300	3.00015800	0.01580400
H	2.87905100	2.39531900	0.31188400
H	7.57812500	0.86917300	-0.26417400
H	7.07083200	3.27200500	-0.26206900
H	4.70373300	4.07029500	0.02049700
C	5.90332900	-1.30937800	-0.01475500
C	7.41833500	-1.54947000	-0.21397200
C	5.49657900	-1.96403000	1.33383500
C	5.15818300	-2.01125800	-1.18330300
H	7.78200200	-1.14335500	-1.17298800
H	8.02106200	-1.11458100	0.60121300
H	7.61110600	-2.63477500	-0.22207300
H	4.41296400	-1.87601000	1.50297300
H	5.76421400	-3.03492000	1.32486900
H	6.02228900	-1.48727800	2.17840300
H	5.41681300	-3.08427200	-1.19768900
H	4.06803300	-1.91895300	-1.07389900
H	5.45112600	-1.57641700	-2.15403700
Rh	1.22424900	-0.17022800	0.21837800
O	1.16713300	-1.79587600	-1.06176100

O	0.76619300	-1.38482400	1.81347900
O	-1.07378200	-1.46609000	-1.48293700
O	-1.48285200	-1.06851300	1.43081000
C	0.05051700	-2.05859400	-1.61805900
C	-0.47758700	-1.54637900	2.05505400
Rh	-1.22424700	0.17019100	-0.21839600
O	-1.16713400	1.79584000	1.06174600
O	-0.76619600	1.38478300	-1.81350100
O	1.07378000	1.46604900	1.48292400
O	1.48285000	1.06846600	-1.43083600
C	-0.05051900	2.05855500	1.61804600
C	0.47758400	1.54633200	-2.05508100
H	-0.05210200	2.91890300	2.31257500
H	0.71693800	2.18902400	-2.92188900
H	-0.71694200	-2.18908100	2.92185600
H	0.05209900	-2.91894800	-2.31257900

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^sTS1 (E = -1421.57229463)

N	-1.55842400	-0.20963700	-0.71046600
Rh	2.80385200	0.02655800	0.25754200
O	3.11830100	-1.07749000	-1.44895300
O	2.61118700	-1.70355100	1.34223700
O	0.85675900	-1.20844900	-1.88561100
O	0.35322300	-1.80830500	0.91510500
C	2.09410700	-1.44158200	-2.11712300
C	1.45408900	-2.22665400	1.42567900
Rh	0.40306200	-0.07804400	-0.20080200
O	0.10497800	1.01892100	1.52418600
O	0.68277900	1.66446600	-1.29743400
O	2.37016400	1.12384700	1.94726100
O	2.93775000	1.75033500	-0.84020900
C	1.14256000	1.36202500	2.19427300
C	1.85718900	2.17111900	-1.36802400
H	2.29850000	-2.04153700	-3.02332400
H	1.37697000	-3.16024300	2.01194600
H	0.93574800	1.94381500	3.11142900
H	1.93574100	3.09561300	-1.96858200
C	-2.34250300	2.04962700	-0.30963600
C	-2.57188400	0.64659800	-0.30226800
C	-3.88054900	0.15979900	0.02833100
C	-4.90218100	1.07774400	0.28088900
C	-4.67382800	2.46580900	0.23797800
C	-3.39000600	2.94069800	-0.06068600
H	-1.34779100	2.41278300	-0.56539000
H	-5.89947100	0.71214700	0.54205400
H	-5.48788800	3.16045400	0.46038600
H	-3.19259800	4.01619900	-0.08882900
C	-4.10431600	-1.36447600	0.01820300
C	-5.07347800	-1.81975100	1.14646800
C	-4.67870300	-1.78226200	-1.36384300
C	-2.76599900	-2.03155800	0.25333000
H	-4.73332100	-1.46442000	2.13163500
H	-6.09211200	-1.43502900	0.96937700
H	-5.13838700	-2.92017400	1.17356700
H	-3.99248700	-1.50605100	-2.18058800
H	-4.84879900	-2.87181500	-1.40587500
H	-5.64059900	-1.27828500	-1.54953800
H	-1.94719200	-1.27952600	-0.67902100
H	-2.30327400	-1.89764800	1.23638000
H	-2.59333700	-3.02293900	-0.18978300

42

^sC (E = -1421.67401138)

N	-1.76536400	-0.40422300	-0.68056700
Rh	2.78505000	0.13231800	0.23028200
O	3.11369000	-1.29373600	-1.22025800
O	2.67097800	-1.34382300	1.65394700

O	0.85583200	-1.54967300	-1.60366800
O	0.40989100	-1.60401600	1.29091300
C	2.09817100	-1.80050900	-1.79936700
C	1.52763100	-1.86923700	1.85929300
Rh	0.39655400	-0.13453300	-0.16512100
O	0.07586500	1.28444900	1.30130400
O	0.54014200	1.34212200	-1.60928200
O	2.33905100	1.53906300	1.65843300
O	2.79645900	1.59405600	-1.21725800
C	1.10558700	1.78627100	1.87273200
C	1.69757400	1.86108000	-1.80272200
H	2.31133500	-2.55957500	-2.57478500
H	1.49065400	-2.66129600	2.62997200
H	0.89331000	2.53660600	2.65664000
H	1.74105200	2.64414700	-2.58221700
C	-2.51488700	2.02037900	-0.46628400
C	-2.72120700	0.64309100	-0.34689000
C	-3.93313500	0.10281600	0.11094100
C	-4.97230500	0.96301400	0.48643500
C	-4.78054300	2.35193500	0.38859600
C	-3.56669700	2.87237700	-0.09155100
H	-1.56167800	2.41059900	-0.82538700
H	-5.92541500	0.56350800	0.84579100
H	-5.58314800	3.03239100	0.68636800
H	-3.43094000	3.95501300	-0.16429100
C	-3.90906500	-1.42125400	0.01815300
C	-4.45881300	-2.12638800	1.27237400
C	-4.69152900	-1.87824500	-1.23927100
C	-2.37734900	-1.67063800	-0.14445100
H	-3.93963700	-1.78319400	2.18172600
H	-5.53608800	-1.92818800	1.39953000
H	-4.33185200	-3.21968500	1.19388000
H	-4.28774800	-1.41687400	-2.15639300
H	-4.64024000	-2.97458200	-1.35450500
H	-5.75349100	-1.59207300	-1.16549000
H	-1.65381600	-0.46361700	-1.70144500
H	-1.91243000	-1.86116400	0.83342600
H	-2.13034000	-2.50842700	-0.81206200

42

^tTS1 (E = -1421.57500231)

N	1.57397900	-0.18170500	-0.34887400
Rh	-2.84747200	0.01253000	0.17752700
O	-2.71794500	-1.75584500	1.20684300
O	-3.06931700	-1.02225700	-1.58197100
O	-0.43584900	-1.84650000	0.90502400
O	-0.78860600	-1.12042300	-1.89560100
C	-1.56198800	-2.27852400	1.33552700
C	-2.00836400	-1.35385500	-2.20757400
Rh	-0.43032100	-0.06280100	-0.15292600
O	-0.62396000	1.70794200	-1.20703200
O	-0.25276900	0.99228300	1.61788000
O	-2.90146800	1.78047900	-0.86777400
O	-2.53550400	1.04283600	1.92724600
C	-1.79468000	2.21742300	-1.32250600
C	-1.32742300	1.29629500	2.24515700
H	-1.51944800	-3.23228600	1.89267800
H	-2.15451500	-1.91778500	-3.14693000
H	-1.84146100	3.16156100	-1.89543100
H	-1.17897900	1.85271500	3.18866500
C	2.40936200	2.07870300	-0.09942400
C	2.62174500	0.66350600	-0.17697500
C	3.97618500	0.14484200	-0.08620400
C	5.02358500	1.06240300	0.03074300
C	4.79786900	2.45079000	0.08433500
C	3.48440800	2.95125800	0.02763600
H	1.38669700	2.44698200	-0.17460000
H	6.05188400	0.69789700	0.09226900

H	5.64624500	3.13451100	0.17399900
H	3.30410800	4.02909100	0.07157400
C	4.19031900	-1.37797400	-0.00597700
C	5.60671700	-1.80069400	-0.48073300
C	4.00112100	-1.80883200	1.47663000
C	3.15815900	-2.08450000	-0.87455800
H	5.81640100	-1.43449900	-1.49848700
H	6.39246100	-1.42330100	0.19553600
H	5.68139300	-2.90009500	-0.48694200
H	2.98738000	-1.56694400	1.83309800
H	4.15326500	-2.89708000	1.57998400
H	4.72581100	-1.29448000	2.12805700
H	2.04403300	-1.25777500	-0.60434700
H	3.27013700	-1.96314500	-1.96099100
H	2.85867900	-3.09440300	-0.56644900

42

^tIM1 (E = -1421.57929760)

N	1.57479800	-0.19553200	-0.35429100
Rh	-2.86680100	-0.02429800	0.17778200
O	-2.69980900	-1.82079500	1.15425600
O	-3.06835900	-1.01239000	-1.61054400
O	-0.41667600	-1.85377900	0.84878600
O	-0.78559300	-1.05791000	-1.92152200
C	-1.53356700	-2.32336900	1.26546400
C	-1.99999700	-1.30629300	-2.24241800
Rh	-0.45106700	-0.03916100	-0.15110900
O	-0.67240200	1.75781400	-1.15150900
O	-0.28782700	0.97141100	1.64412400
O	-2.95124100	1.77084000	-0.81459200
O	-2.57093700	0.96416600	1.95352300
C	-1.85319000	2.24646500	-1.25246800
C	-1.36845900	1.23636000	2.27848400
H	-1.47044400	-3.29359300	1.79138900
H	-2.13398300	-1.84722300	-3.19705200
H	-1.92006800	3.20775600	-1.79395000
H	-1.23277000	1.77200700	3.23581500
C	2.38494300	2.05447900	-0.09893100
C	2.62976400	0.64607000	-0.18055300
C	3.99680100	0.15915500	-0.08697800
C	5.01531200	1.11188600	0.03024500
C	4.75597400	2.49427400	0.08396600
C	3.43097000	2.96033000	0.02860400
H	1.35239600	2.39472000	-0.17450100
H	6.05376100	0.78081600	0.09205700
H	5.58830100	3.19742900	0.17421500
H	3.21978600	4.03232300	0.07445000
C	4.28940200	-1.35416600	-0.01577200
C	5.80341900	-1.67189700	-0.21473700
C	3.87613500	-1.87309400	1.39387700
C	3.54507200	-2.11032700	-1.09017500
H	6.18021800	-1.27523700	-1.17086400
H	6.41437900	-1.25835700	0.60620000
H	5.94924100	-2.76367400	-0.21543200
H	2.80819000	-1.69709300	1.59381700
H	4.06810600	-2.95685900	1.47299100
H	4.45923900	-1.36175400	2.17638100
H	1.88143100	-1.17250500	-0.54409900
H	3.55331800	-1.74425800	-2.12102900
H	3.29668100	-3.16423800	-0.93246600

42

^tTS2 (E = -1421.55226091)

N	-1.54918800	-0.13407400	-0.71000400
Rh	2.76857200	0.08153200	0.20059100
O	3.03626500	-1.29775500	-1.30692600
O	2.73736800	-1.43207900	1.57645400
O	0.76908700	-1.50655200	-1.66411600

O	0.48508100	-1.71142700	1.29401100
C	2.00154100	-1.76598200	-1.88882200
C	1.61514200	-1.99290400	1.81227900
Rh	0.36359600	-0.13487500	-0.13952600
O	0.10253600	1.24031700	1.41139500
O	0.68547400	1.56748100	-1.56451000
O	2.38186000	1.44671400	1.69028900
O	2.93941300	1.58834900	-1.15162700
C	1.15963800	1.70534600	1.95804900
C	1.86743200	1.99482600	-1.72766100
H	2.19477600	-2.49665900	-2.69617300
H	1.62768300	-2.81572200	2.55039500
H	0.99307800	2.43162700	2.77518900
H	2.01223700	2.81965000	-2.45182100
C	-2.45063000	2.10128600	-0.31672100
C	-2.62387600	0.70028400	-0.35606300
C	-3.88384900	0.12631300	-0.01422200
C	-4.94547900	0.98453300	0.30639800
C	-4.77586100	2.37915300	0.31878700
C	-3.52445700	2.93435900	0.01507300
H	-1.47489200	2.50962900	-0.58261900
H	-5.91933500	0.56791700	0.57609300
H	-5.61842000	3.02532100	0.58033600
H	-3.38368500	4.01881400	0.03009200
C	-3.99078900	-1.41229500	-0.00209900
C	-5.06527100	-1.90604100	1.01363100
C	-4.37714400	-1.92498600	-1.41677400
C	-2.66561400	-1.97215000	0.43691400
H	-4.86690400	-1.51714600	2.02461100
H	-6.07716500	-1.58844700	0.70941000
H	-5.06443400	-3.00698900	1.05738900
H	-3.64389900	-1.62187100	-2.18255600
H	-4.44094600	-3.02643100	-1.42647200
H	-5.35550400	-1.51955800	-1.71969500
H	-1.74549600	-0.77385400	-1.48777400
H	-2.25262300	-1.69246800	1.40772800
H	-2.22904000	-2.84570300	-0.05442900

42

^tC (E = -1421.63131254)

N	-1.78466600	-0.33033500	-0.70659100
Rh	2.73249800	0.10239500	0.22028000
O	3.06361200	-0.81993500	-1.59226700
O	2.86500500	-1.69286400	1.16499200
O	0.80921100	-1.04120300	-1.99769500
O	0.63971300	-2.16072700	0.94171000
C	2.04749400	-1.17727400	-2.28011200
C	1.81170700	-2.41805500	1.32492900
Rh	0.36153600	-0.11711000	-0.17059400
O	0.03971200	0.81006600	1.67251500
O	0.62861800	1.98920700	-1.21056600
O	2.30868200	1.01451100	2.01403900
O	2.85162100	1.91951900	-0.68332800
C	1.07606400	1.15702300	2.33002600
C	1.79687500	2.46070400	-1.18838600
H	2.27454400	-1.66744800	-3.24509500
H	1.99749500	-3.36935400	1.86137900
H	0.89097100	1.64749200	3.30373800
H	1.97817800	3.45179000	-1.64959200
C	-2.57783800	2.06250500	-0.34942700
C	-2.76275700	0.67807300	-0.31452600
C	-3.96457400	0.08420900	0.10185900
C	-5.02548600	0.90029000	0.51196600
C	-4.86114800	2.29632800	0.49320100
C	-3.65267300	2.86898700	0.06130400
H	-1.62599800	2.49103900	-0.67020400
H	-5.97272400	0.46205200	0.84007100
H	-5.68161900	2.94190100	0.81859400

H	-3.53903600	3.95643800	0.05455000
C	-3.89880700	-1.43336300	-0.05900300
C	-4.44437200	-2.20830200	1.15528000
C	-4.64637000	-1.85916900	-1.34784800
C	-2.35849700	-1.63282300	-0.20596000
H	-3.94863100	-1.89014600	2.08651900
H	-5.52878000	-2.04759500	1.27384000
H	-4.28300600	-3.29270200	1.03129100
H	-4.24091000	-1.35018900	-2.23865300
H	-4.56225100	-2.94804700	-1.50566700
H	-5.71688200	-1.60547200	-1.28121700
H	-1.69330900	-0.35362800	-1.73201100
H	-1.90319500	-1.82961500	0.77548000
H	-2.07078400	-2.44539900	-0.88775600

42

^tTS3 (E = -1421.55434608)

N	1.48003500	0.15639400	-1.05482000
Rh	-2.72507200	-0.03052000	0.40577200
O	-2.59920000	-2.06265900	0.59660200
O	-3.25957700	-0.25872400	-1.57070200
O	-0.41446900	-2.04934000	-0.11804900
O	-1.06143400	-0.19939500	-2.26247300
C	-1.49102700	-2.61196900	0.28877100
C	-2.32886700	-0.28570000	-2.44070300
Rh	-0.39438200	0.00369100	-0.31329600
O	-0.62067900	2.06497800	-0.45860900
O	0.14078300	0.22205300	1.66900100
O	-2.82439000	1.99993600	0.20013300
O	-2.06628800	0.20141100	2.34083100
C	-1.75717100	2.58479900	-0.17986300
C	-0.80637400	0.27409900	2.52985000
H	-1.44471700	-3.71160100	0.38110100
H	-2.64912300	-0.39940800	-3.49230000
H	-1.81291500	3.68332500	-0.28455800
H	-0.48035300	0.39980900	3.57825200
C	2.65038600	2.20453600	-0.52029400
C	2.62811500	0.78902800	-0.51137900
C	3.74464300	0.05550000	0.00248700
C	4.82110900	0.81300300	0.50859500
C	4.82436600	2.21443900	0.52452000
C	3.73301500	2.91779900	0.00128700
H	1.77934900	2.72839800	-0.91909200
H	5.69679200	0.29327400	0.90027200
H	5.68519100	2.74919100	0.93606000
H	3.71975900	4.01147300	-0.00315000
C	3.81812500	-1.49721400	-0.04423300
C	5.25054100	-2.01583800	0.26021900
C	2.86177000	-2.09556900	1.01849000
C	3.45580800	-1.98242500	-1.42632500
H	5.99719700	-1.59862600	-0.43583900
H	5.56651200	-1.78526100	1.29181500
H	5.26206100	-3.11170400	0.14912700
H	1.81987800	-1.81158400	0.82714800
H	2.92696000	-3.19726100	1.00161700
H	3.13769500	-1.74620800	2.02704900
H	1.40682900	0.28408600	-2.07397300
H	4.16389800	-1.85354900	-2.24973500
H	2.45554900	-2.35483400	-1.65392000

42

^tIM2 (E = -1421.55782444)

N	1.50473100	0.62013500	-1.06929200
Rh	-2.68466700	-0.05819200	0.44458900
O	-2.47706600	-2.08960800	0.58080700
O	-3.27780100	-0.25446400	-1.51469500
O	-0.31621900	-1.96892600	-0.19843200
O	-1.10954200	-0.08317500	-2.27714700

C	-1.35721800	-2.58332700	0.22488000
C	-2.37594700	-0.21619300	-2.41631700
Rh	-0.38056200	0.09015700	-0.34914000
O	-0.69999900	2.14868900	-0.46034300
O	0.18865500	0.27954100	1.63131600
O	-2.86830700	1.97476700	0.28829500
O	-1.99217700	0.14775700	2.36818200
C	-1.84631900	2.61253000	-0.12738400
C	-0.73143600	0.26941200	2.52209900
H	-1.26638000	-3.68270300	0.28723800
H	-2.72903500	-0.31129100	-3.45923400
H	-1.95762500	3.70878200	-0.21313800
H	-0.37929400	0.38185000	3.56369600
C	3.11172800	2.30194400	-0.48952200
C	2.72898600	0.91968700	-0.50729800
C	3.65171700	-0.06256100	0.01427300
C	4.83089300	0.42462100	0.60751500
C	5.15274500	1.78765600	0.67710900
C	4.29063100	2.73680600	0.10114200
H	2.41509800	3.02777300	-0.92127700
H	5.54642600	-0.28919200	1.01878400
H	6.08396500	2.10171400	1.15656900
H	4.53661900	3.80200400	0.12028800
C	3.43701000	-1.59196800	-0.12196700
C	4.80520500	-2.33769600	-0.24612700
C	2.72065800	-2.12212300	1.14809700
C	2.66820700	-1.92585300	-1.37146800
H	5.40955500	-1.93784200	-1.07656500
H	5.40309800	-2.28384900	0.67938600
H	4.61104400	-3.40321400	-0.44614800
H	1.75337900	-1.62657900	1.29773200
H	2.54873100	-3.20838200	1.05697100
H	3.34212200	-1.94459500	2.04155500
H	1.22312900	1.40538400	-1.67338200
H	3.06455400	-1.62125400	-2.34344700
H	1.69529200	-2.41224800	-1.33322000

42

^tTS4 (E = -1421.55458404)

N	1.50671400	0.38828100	-1.18710200
Rh	-2.62944500	0.06840300	0.45605700
O	-2.66695800	-1.96684700	0.66240100
O	-3.24897900	-0.12250900	-1.50209100
O	-0.53045200	-2.14050400	-0.14388900
O	-1.08396700	-0.18883300	-2.29469100
C	-1.62490500	-2.61328500	0.31479800
C	-2.35955200	-0.19596600	-2.41346400
Rh	-0.32276000	-0.04697000	-0.36713000
O	-0.52533900	2.11771800	-0.48673300
O	0.28737500	0.13647600	1.61095100
O	-2.68693900	2.09915000	0.28162400
O	-1.88961400	0.25999300	2.36485600
C	-1.62438500	2.66449400	-0.14870100
C	-0.62095200	0.25273600	2.50523100
H	-1.67353900	-3.71227500	0.42172600
H	-2.73724100	-0.27982000	-3.44917800
H	-1.67257400	3.76637600	-0.23574800
H	-0.25142600	0.36225000	3.54142500
C	2.94447500	2.26045700	-0.58722400
C	2.65784100	0.86560400	-0.57478900
C	3.58003000	-0.03595300	0.04155700
C	4.70072600	0.50674600	0.69220100
C	4.94599800	1.88713200	0.72062500
C	4.07089800	2.76598300	0.05775900
H	2.23595900	2.93164200	-1.08009100
H	5.41670600	-0.16264600	1.17635500
H	5.82711100	2.27237900	1.24105300
H	4.26506900	3.84221600	0.05377300

C	3.38138600	-1.56476500	-0.08340100
C	4.74310100	-2.24813700	-0.44002400
C	2.86687800	-2.14612300	1.25868500
C	2.44288300	-1.87919600	-1.20991100
H	5.17460100	-1.82363200	-1.36068600
H	5.48018300	-2.13286900	0.37160500
H	4.58860800	-3.32827300	-0.59432500
H	1.90347500	-1.69773400	1.53665000
H	2.74043600	-3.23931300	1.17685900
H	3.58703400	-1.94370500	2.06841300
H	1.24231500	0.95550500	-2.00367000
H	2.75527300	-1.67989200	-2.23790500
H	1.55266200	-2.48818700	-1.05771100

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Aa (E = -2619.63377716)

Rh	-0.06752800	0.10436400	-0.26541300
O	-1.45163200	1.09586200	0.92525000
O	-1.57016900	-0.55814500	-1.52731000
O	-1.81367000	-0.77741400	2.18526500
O	-1.94531300	-2.39174500	-0.21845500
C	-2.02937700	0.44970200	1.87850300
C	-3.05052300	1.23345400	2.73406700
C	-2.29265900	2.38746200	3.43857800
H	-1.80037400	3.04668700	2.70837600
H	-2.99958300	2.98903900	4.03463500
H	-1.52403000	1.99342900	4.12372900
C	-3.69488500	0.31636700	3.79086800
H	-2.93494200	-0.10368600	4.46692200
H	-4.41039200	0.89963300	4.39565700
H	-4.23378100	-0.52312500	3.32854700
C	-4.14424000	1.86576400	1.80004400
H	-3.64636300	2.60343400	1.14969700
H	-4.83508400	2.42470000	2.45623600
C	-4.92041300	0.88243200	0.94519600
C	-6.15274700	0.33957000	1.35878300
H	-6.59677300	0.65992600	2.30667600
C	-6.81959700	-0.59807800	0.55662600
H	-7.78395800	-1.00192900	0.87936100
C	-6.25700700	-1.02272700	-0.65610300
H	-6.78198700	-1.76045200	-1.27137700
C	-5.02599900	-0.49576400	-1.09431600
C	-4.39523900	0.47521400	-0.29486200
H	-3.45796900	0.91738400	-0.64021800
C	-4.35904100	-0.95793900	-2.37589100
H	-5.11866700	-1.33079400	-3.08580800
H	-3.85715500	-1.10328000	-2.85866300
C	-3.29970200	-2.10639100	-2.20847300
C	-3.96976000	-3.39824800	-1.70267700
H	-4.44832300	-3.25134500	-0.72379700
H	-4.74109100	-3.71777000	-2.42419200
H	-3.23628500	-4.21222800	-1.60035900
C	-2.64405900	-2.36380700	-3.58928500
H	-1.89951800	-3.17455000	-3.52601700
H	-3.41482600	-2.67076600	-4.31626300
H	-2.14295000	-1.46139400	-3.97006500
C	-2.19029900	-1.65095100	-1.23492300
Rh	-0.46321900	-1.84213600	1.08291500
O	0.88876200	-2.86297000	-0.09508200
O	1.02671100	-1.21154200	2.35564600
O	1.29173300	-1.00331400	-1.35899400
O	1.40927600	0.64116000	1.07066000
C	1.47832700	-2.23870700	-1.04966100
C	2.47785300	-3.05718200	-1.89734800
C	1.70035300	-4.23374300	-2.54063500
H	1.20828900	-4.85158500	-1.77469300
H	2.39469700	-4.87059800	-3.11443900
H	0.92944800	-3.86323700	-3.23631900

C	3.11316900	-2.19306900	-3.00217600
H	2.34515400	-1.76657200	-3.66501600
H	3.78729700	-2.81671100	-3.61382500
H	3.70068500	-1.36280000	-2.58380800
C	3.58222700	-3.65990700	-0.95450600
H	3.09196000	-4.38729600	-0.28696700
H	4.27503300	-4.22719800	-1.60124800
C	4.35164900	-2.65387300	-0.11996600
C	5.56868900	-2.09102300	-0.55266300
H	6.00809100	-2.41063900	-1.50308000
C	6.23061800	-1.13975000	0.23817200
H	7.18647100	-0.72492400	-0.09636800
C	5.67863800	-0.72172600	1.45829300
H	6.20206600	0.02263700	2.06681200
C	4.46274900	-1.26793700	1.91516700
C	3.83691100	-2.25090100	1.12618200
H	2.91379600	-2.70981800	1.48810000
C	3.80941400	-0.82211900	3.20949500
H	4.57609400	-0.45796400	3.91640000
H	3.31432400	-1.68538500	3.68382800
C	2.74399400	0.32536900	3.07165600
C	3.40806500	1.63649200	2.61256000
H	3.88866100	1.52802400	1.63020400
H	4.17489500	1.93639700	3.34740000
H	2.67002100	2.44890300	2.53512700
C	2.07938800	0.53322000	4.45639900
H	1.33269000	1.34341400	4.41610400
H	2.84406500	0.81623800	5.19952000
H	1.57730300	-0.38374800	4.80013400
C	1.64286800	-0.11599300	2.08125300
N	0.38014000	1.89524100	-1.65557000
C	2.80297300	2.06465000	-1.66585400
C	1.57794200	2.74625400	-1.59085000
C	1.49478300	4.15512300	-1.43095600
C	2.73905200	4.82375900	-1.37466400
C	3.97045300	4.16042500	-1.46207500
C	4.00927700	2.76951100	-1.60538700
H	2.78582000	0.97647500	-1.75244200
H	2.75075400	5.90797700	-1.26165200
H	4.89730900	4.73908800	-1.41338800
H	4.95945600	2.23265100	-1.66362100
C	0.16886500	4.94585100	-1.31169500
C	-0.59858900	4.48582500	-0.04530200
C	0.41849500	6.46786100	-1.17835500
C	-0.72050100	4.74539600	-2.56890100
H	-0.83600200	3.41321400	-0.06689800
H	-0.00405500	4.68474500	0.86191100
H	-1.54627100	5.04601800	0.03889100
H	0.92815600	6.88699800	-2.06225900
H	-0.55214000	6.98134600	-1.08315200
H	1.00973800	6.71786100	-0.28206700
H	-1.58269700	5.43227100	-2.52440000
H	-0.16301800	4.96496800	-3.49458900
H	-1.12744500	3.72758200	-2.63921700
N	-0.36955100	1.20405500	-3.83238100
N	0.05066000	1.55987000	-2.82168200

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Aa-TS (E = -2619.60440801)

Rh	-0.04473300	0.09265100	-0.36362500
O	-1.46876800	1.16155700	0.74069200
O	-1.55025600	-0.80837500	-1.44849100
O	-1.71295000	-0.52396700	2.26294100
O	-1.83381800	-2.44131900	0.11483800
C	-1.99876000	0.63191700	1.78839900
C	-3.04588900	1.47551700	2.55188200
C	-2.31788300	2.71289900	3.13692700
H	-1.84782800	3.31431200	2.34501500

H	-3.04028800	3.34768200	3.67733000
H	-1.53730900	2.40729400	3.85309400
C	-3.66881000	0.65543400	3.69817800
H	-2.89921400	0.32149400	4.41001600
H	-4.39462800	1.28255700	4.24359900
H	-4.19172100	-0.23582100	3.32279600
C	-4.15335200	1.97807900	1.55832300
H	-3.67245400	2.64069500	0.82051100
H	-4.84810900	2.60132100	2.14886500
C	-4.92025200	0.88474200	0.83861600
C	-6.14733900	0.38885600	1.32137100
H	-6.59664900	0.82900700	2.21738700
C	-6.80224900	-0.65727600	0.65475600
H	-7.76266000	-1.02388700	1.02947000
C	-6.23101700	-1.23901200	-0.48655600
H	-6.74529900	-2.06138100	-0.99422600
C	-5.00543600	-0.76210600	-0.99159400
C	-4.38836500	0.31798200	-0.33429000
H	-3.45822600	0.72057200	-0.74046000
C	-4.32727600	-1.39159700	-2.19308200
H	-5.07819800	-1.88062400	-2.83895000
H	-3.84199500	-0.60787000	-2.79716700
C	-3.24743300	-2.48307200	-1.85905400
C	-3.88699700	-3.68683200	-1.14140100
H	-4.34681400	-3.39369600	-0.18668700
H	-4.66902500	-4.12172900	-1.78671500
H	-3.13974700	-4.46707200	-0.93184900
C	-2.60563400	-2.94841300	-3.19189900
H	-1.84250400	-3.72384600	-3.01356200
H	-3.38200300	-3.38334700	-3.84363200
H	-2.13402300	-2.10868100	-3.72339500
C	-2.13227700	-1.86528700	-0.98834300
Rh	-0.34414500	-1.66417100	1.28080700
O	1.02152700	-2.79856100	0.23645500
O	1.14528100	-0.82033000	2.41270900
O	1.30085900	-1.14930000	-1.31339000
O	1.46053600	0.82643500	0.85921900
C	1.55251300	-2.31374500	-0.82416800
C	2.55495700	-3.21032300	-1.58418400
C	1.78819700	-4.47098400	-2.06038400
H	1.32914800	-5.00191300	-1.21278900
H	2.48295900	-5.15870200	-2.57119800
H	0.99337500	-4.20288200	-2.77565200
C	3.15155800	-2.47649700	-2.79921000
H	2.36344100	-2.14976000	-3.49427500
H	3.82849600	-3.15719000	-3.34280100
H	3.72779600	-1.59060100	-2.49525300
C	3.68844300	-3.66950300	-0.59662800
H	3.22685800	-4.31364600	0.16978000
H	4.37804200	-4.30415600	-1.18109400
C	4.45534700	-2.54946500	0.08101100
C	5.65612200	-2.03421500	-0.44636100
H	6.08667300	-2.47539700	-1.35114900
C	6.31303700	-0.97141100	0.19189400
H	7.25535700	-0.59216000	-0.21510200
C	5.77187700	-0.39490500	1.35051800
H	6.29093000	0.43623400	1.83839000
C	4.57317400	-0.89066800	1.90016300
C	3.95223800	-1.98343200	1.26739700
H	3.04223100	-2.39843500	1.70657500
C	3.93178400	-0.27595700	3.12931200
H	4.70343500	0.19238600	3.76603400
H	3.45581800	-1.06976400	3.72835300
C	2.85007100	0.82926600	2.84881600
C	3.48521600	2.06354900	2.18392500
H	3.94434800	1.81639600	1.21658800
H	4.26419100	2.47639000	2.84763000
H	2.73448300	2.84755300	2.00470600

C	2.21352900	1.23211500	4.20372900
H	1.45774500	2.02269000	4.06526200
H	2.99247300	1.62465400	4.87901900
H	1.72998300	0.37081000	4.68867300
C	1.73240800	0.23082100	1.96485200
N	0.09949100	1.72417100	-1.63645100
C	2.52497800	1.75401700	-1.92757800
C	1.31060000	2.46250900	-1.76228400
C	1.31159900	3.90075400	-1.71437700
C	2.57267100	4.52344300	-1.82463100
C	3.76654200	3.81062400	-2.00458900
C	3.74722700	2.41148100	-2.06286300
H	2.47213300	0.66513800	-1.95693800
H	2.63515100	5.61118800	-1.78441100
H	4.70951700	4.35741100	-2.09995000
H	4.66907400	1.84050400	-2.20217300
C	0.04138200	4.76355800	-1.52402700
C	-0.60409700	4.44136200	-0.15187000
C	0.35784300	6.27922300	-1.54241600
C	-0.98622600	4.50118500	-2.65618900
H	-0.89550600	3.38403600	-0.08407600
H	0.09597400	4.66180000	0.67187400
H	-1.50476100	5.06434800	-0.00843300
H	0.79577400	6.60437000	-2.50120800
H	-0.58080600	6.84008500	-1.40294000
H	1.03924200	6.57623800	-0.72777500
H	-1.82847300	5.20789800	-2.56033400
H	-0.53268300	4.64981800	-3.65045600
H	-1.39635200	3.48496300	-2.60391400
N	-1.29320900	0.81399100	-3.63633300
N	-0.36932300	1.25100600	-3.12405900

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⁵Ba (E = -2510.14051693)

N	0.02268200	2.23463100	-0.42307400
C	-2.39234300	2.65499100	-0.46346500
C	-1.01769300	3.09213200	-0.47121900
C	-0.73377900	4.53079400	-0.56306300
C	-1.83629900	5.39346900	-0.63126300
C	-3.16433300	4.92966100	-0.63181800
C	-3.44575200	3.55454900	-0.55300400
H	-2.57816800	1.58425900	-0.40529400
H	-1.67433900	6.47047500	-0.69320400
H	-3.98222200	5.65386100	-0.69623900
H	-4.47938700	3.19757000	-0.55776600
C	0.70456000	5.08175000	-0.57295100
C	0.73775900	6.62714200	-0.64588300
C	1.44405200	4.65890900	0.72756300
C	1.46965200	4.53602600	-1.81200600
H	0.27296900	7.01442000	-1.56846100
H	0.24365000	7.09892800	0.22045200
H	1.78849000	6.96023700	-0.64484200
H	1.51000500	3.56412500	0.79755200
H	2.46426200	5.08051500	0.72537600
H	0.92102700	5.04071400	1.62117700
H	1.53569600	3.44028100	-1.77458000
H	0.96474200	4.83098300	-2.74772600
H	2.48979300	4.95757400	-1.82960600
Rh	-0.00600300	0.32534000	-0.09661100
O	1.46690400	0.09569600	-1.56721900
O	1.44982600	0.58319200	1.38239300
O	1.67133000	-2.14195200	-1.14805700
O	1.67316600	-1.66495400	1.70825000
C	1.98175000	-1.06637300	-1.77164800
C	3.05348000	-1.16074900	-2.88216000
C	2.39755400	-0.72856100	-4.21808900
H	1.97950000	0.28683500	-4.14708900
H	3.15002300	-0.74414800	-5.02465200

H	1.58674700	-1.41997000	-4.50154600
C	3.58364000	-2.60205500	-3.00400500
H	2.77135200	-3.30450200	-3.24498800
H	4.33197800	-2.64936000	-3.81366400
H	4.05621300	-2.94225100	-2.07143700
C	4.22124100	-0.15920300	-2.56508200
H	3.81366900	0.86329300	-2.62511800
H	4.95784000	-0.26448000	-3.38158000
C	4.89759000	-0.35392500	-1.22206800
C	6.05002200	-1.14973700	-1.07111100
H	6.50647400	-1.61659900	-1.94976100
C	6.62336100	-1.33522800	0.19548900
H	7.52733000	-1.94286400	0.29977800
C	6.04428300	-0.74642700	1.32923000
H	6.49658500	-0.90011000	2.31422000
C	4.89121000	0.05358000	1.20664600
C	4.35441100	0.25867400	-0.07770200
H	3.48044500	0.90500800	-0.18953800
C	4.21024900	0.67759500	2.40921200
H	4.94502800	0.84706700	3.21659000
H	3.80386600	1.66328900	2.12915700
C	3.04026800	-0.16326200	3.03637200
C	3.56890800	-1.48217900	3.63179200
H	4.04707100	-2.11125200	2.86752900
H	4.31200600	-1.25693600	4.41574400
H	2.75506400	-2.06652200	4.08740400
C	2.37921600	0.68729200	4.15032900
H	1.56086400	0.13233200	4.63820900
H	3.12665200	0.93344000	4.92326400
H	1.96971200	1.62496800	3.74587200
C	1.97387000	-0.44434400	1.95377600
Rh	0.24422500	-2.06911600	0.30964500
O	-1.19281100	-1.90046800	1.78195400
O	-1.18797200	-2.40612100	-1.13234000
O	-1.44447000	0.33529600	1.38321600
O	-1.43956800	-0.16803000	-1.49810700
C	-1.72508600	-0.75646400	2.00597100
C	-2.78466100	-0.67885200	3.12958100
C	-2.11439000	-1.14536200	4.44685300
H	-1.69187500	-2.15586800	4.34257700
H	-2.85995300	-1.15667300	5.25983900
H	-1.30445700	-0.45829000	4.74236100
C	-3.31616500	0.75660200	3.29889900
H	-2.50099100	1.45629100	3.53778100
H	-4.04553100	0.78119400	4.12663100
H	-3.81289000	1.11932100	2.38785100
C	-3.95559700	-1.67381400	2.79965700
H	-3.55088200	-2.69797800	2.85135500
H	-4.69346300	-1.57425500	3.61556000
C	-4.62814600	-1.46890400	1.45624200
C	-5.77161300	-0.66044400	1.30136300
H	-6.22586400	-0.18813000	2.17819400
C	-6.34200400	-0.47403000	0.03307900
H	-7.24232800	0.13886800	-0.07332800
C	-5.76941400	-1.07377300	-1.09873300
H	-6.22214300	-0.92180600	-2.08376200
C	-4.62594000	-1.88745000	-0.97230900
C	-4.09307500	-2.09235800	0.31381300
H	-3.22821100	-2.75028400	0.42847800
C	-3.95202400	-2.53052700	-2.16866200
H	-4.68944200	-2.70895700	-2.97152600
H	-3.54858800	-3.51348300	-1.87470500
C	-2.77871700	-1.70499600	-2.81140700
C	-3.30648800	-0.40802800	-3.45249800
H	-3.80998900	0.23608400	-2.71760400
H	-4.02986100	-0.66082000	-4.24635300
H	-2.48879500	0.17344500	-3.90456800
C	-2.10704400	-2.58709900	-3.89435600

H	-1.29079100	-2.04274300	-4.39708200
H	-2.84998500	-2.86434800	-4.66103100
H	-1.69226000	-3.50740000	-3.45675700
C	-1.72095400	-1.40387400	-1.72550700
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¹³⁵ Ba (E = -2510.14323240)			
N	-0.26199500	2.22817000	-0.33792800
C	-2.57713700	2.84256300	-0.46651200
C	-1.17731800	3.19326000	-0.42763900
C	-0.79482300	4.60455900	-0.49333800
C	-1.83287600	5.53732700	-0.59270000
C	-3.19336500	5.17469400	-0.62867900
C	-3.55950000	3.81902700	-0.56432800
H	-2.82946800	1.78365500	-0.41718100
H	-1.58697100	6.59966000	-0.64392700
H	-3.95778000	5.95263300	-0.70622400
H	-4.61339700	3.52667700	-0.59102200
C	0.68466400	5.02962100	-0.44665300
C	0.85114800	6.56370600	-0.53867800
C	1.32009100	4.56482100	0.89178300
C	1.45512400	4.39799600	-1.63735600
H	0.45086300	6.96939400	-1.48308200
H	0.36168400	7.08602800	0.30061400
H	1.92425100	6.81389800	-0.50079600
H	1.27384000	3.47071300	0.99919700
H	2.37987900	4.87228400	0.93064700
H	0.80032300	5.02019000	1.75176200
H	1.41235300	3.29876500	-1.60346800
H	1.03300500	4.73170200	-2.60028400
H	2.51517000	4.70476100	-1.60325700
Rh	0.00892500	0.30993700	-0.07883600
O	1.45808500	0.15231500	-1.55968100
O	1.46290500	0.57909500	1.38179700
O	1.68519200	-2.09058900	-1.19758100
O	1.69356800	-1.67173700	1.67435500
C	1.98248600	-1.00022900	-1.80084400
C	3.04295200	-1.05679800	-2.92252100
C	2.37551400	-0.58149300	-4.23822300
H	1.95654600	0.43023200	-4.13077200
H	3.12208800	-0.56913000	-5.05015000
H	1.56346200	-1.26407300	-4.53859800
C	3.57331800	-2.49277000	-3.09487300
H	2.76004300	-3.18842000	-3.35164500
H	4.31458000	-2.51232800	-3.91200200
H	4.05466000	-2.86171800	-2.17785100
C	4.21326000	-0.06488500	-2.58261700
H	3.80738700	0.95954200	-2.61544600
H	4.94621100	-0.15013600	-3.40454500
C	4.89423600	-0.29453400	-1.24746300
C	6.04242600	-1.10036100	-1.11869100
H	6.49342900	-1.54976800	-2.00911100
C	6.61944200	-1.31666500	0.14136200
H	7.52035700	-1.93138900	0.22858300
C	6.04858700	-0.74959300	1.29033300
H	6.50443200	-0.92742100	2.26954500
C	4.89988800	0.05978500	1.19025200
C	4.35994500	0.29571600	-0.08742700
H	3.48996000	0.95012200	-0.18112900
C	4.22631300	0.66190900	2.40815800
H	4.96496900	0.81415500	3.21524900
H	3.82142300	1.65402000	2.14932600
C	3.05723200	-0.18856500	3.02510300
C	3.58807800	-1.51594900	3.60005500
H	4.06617900	-2.13324000	2.82612100
H	4.33176700	-1.30165500	4.38636200
H	2.77555900	-2.10787400	4.04819800
C	2.39664600	0.64460400	4.15229000

H	1.58074200	0.08070800	4.63379800
H	3.14547700	0.88089000	4.92681400
H	1.98398300	1.58718800	3.76291400
C	1.99156300	-0.45514800	1.93998100
Rh	0.26382500	-2.06912100	0.26993400
O	-1.16195200	-1.98350600	1.75037400
O	-1.16600900	-2.41545300	-1.16804800
O	-1.42130400	0.26213100	1.41736400
O	-1.42641500	-0.17032500	-1.49465600
C	-1.69776900	-0.84561800	2.00804800
C	-2.75672900	-0.80502500	3.13329700
C	-2.08223400	-1.30145200	4.43755700
H	-1.65576500	-2.30743200	4.30783100
H	-2.82659600	-1.33628300	5.25089100
H	-1.27490600	-0.61851800	4.74937500
C	-3.29681000	0.62257900	3.33748500
H	-2.48680800	1.32089300	3.59683200
H	-4.02913500	0.62134500	4.16291900
H	-3.79171000	1.00553900	2.43385500
C	-3.92137800	-1.79924500	2.77824800
H	-3.51046800	-2.82194400	2.80434300
H	-4.65853900	-1.72422200	3.59736600
C	-4.59751000	-1.56520100	1.44131200
C	-5.74365700	-0.75676600	1.30795700
H	-6.19710600	-0.30590200	2.19634100
C	-6.31714800	-0.54204000	0.04573700
H	-7.21839800	0.07193700	-0.04438200
C	-5.74502200	-1.11244100	-1.10121900
H	-6.19952400	-0.93710700	-2.08149400
C	-4.59862500	-1.92487200	-0.99658700
C	-4.06294000	-2.15939200	0.28327600
H	-3.19600900	-2.81739800	0.38022800
C	-3.92378600	-2.53482700	-2.20972700
H	-4.66194300	-2.69772800	-3.01520000
H	-3.51470800	-3.52268500	-1.94084900
C	-2.75696600	-1.68688700	-2.83534600
C	-3.29414300	-0.37892200	-3.44612100
H	-3.79480600	0.24826500	-2.69501600
H	-4.02105400	-0.61844200	-4.24082500
H	-2.48176600	0.21545900	-3.89087400
C	-2.08024200	-2.53938400	-3.93839200
H	-1.26772700	-1.97814900	-4.42852100
H	-2.82181500	-2.80254600	-4.71128500
H	-1.66000600	-3.46754700	-3.52305800
C	-1.70135800	-1.40092400	-1.74337100

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Ab (E = -2619.63347807)

Rh	0.11305800	0.13534200	-0.29183300
O	1.59397800	-0.53851000	-1.57264300
O	1.47421000	1.37829000	0.68031000
O	2.21650300	-2.17096600	-0.10120100
O	2.07358600	-0.29691900	2.11152600
C	2.32815100	-1.53457600	-1.20844300
C	3.41344000	-1.99928700	-2.20507800
C	2.70771800	-2.42090300	-3.51915300
H	2.11315300	-1.59410400	-3.93577000
H	3.46147500	-2.72157200	-4.26636200
H	2.03890900	-3.28079700	-3.34993900
C	4.20234700	-3.19164600	-1.63154700
H	3.53651500	-4.04267000	-1.42243000
H	4.95891200	-3.51828100	-2.36540500
H	4.71506200	-2.92758600	-0.69553300
C	4.37410700	-0.79992300	-2.53542400
H	3.78735800	-0.03413100	-3.06862400
H	5.12585600	-1.18596000	-3.24669800
C	5.06362400	-0.16562000	-1.34322800
C	6.34445400	-0.56514400	-0.91394500

H	6.89003100	-1.33210000	-1.47285600
C	6.93051600	0.02500400	0.21554900
H	7.93246800	-0.28119700	0.53097000
C	6.24000200	1.00542100	0.94338900
H	6.70395500	1.45595900	1.82657800
C	4.95767300	1.42308300	0.53659300
C	4.40548100	0.84675600	-0.62168300
H	3.42685800	1.18768800	-0.96615900
C	4.15519800	2.44627700	1.31727900
H	4.83353900	3.11934600	1.87140300
H	3.58144100	3.07470200	0.61581900
C	3.15188600	1.85172200	2.36896800
C	3.91088600	1.10958900	3.48657000
H	4.49757600	0.26835000	3.09079100
H	4.59877200	1.81065800	3.98949200
H	3.21582500	0.70900100	4.23981400
C	2.34183600	3.01931900	2.98584800
H	1.62411100	2.64890500	3.73616900
H	3.02584200	3.72202100	3.49109000
H	1.78139000	3.57219600	2.21730800
C	2.16012800	0.89876900	1.66236400
Rh	0.76762100	-1.60348700	1.23218100
O	-0.70042100	-0.95935500	2.52447400
O	-0.53904900	-2.87316400	0.28395500
O	-1.34024600	0.68141100	1.06634500
O	-1.18006300	-1.22365000	-1.16247000
C	-1.44478700	0.02684500	2.16655400
C	-2.54278600	0.46042800	3.16431600
C	-1.84336800	0.89786400	4.47656700
H	-1.21938300	0.08824000	4.88428200
H	-2.60113700	1.17124300	5.23029300
H	-1.20288200	1.77916900	4.30706500
C	-3.37187100	1.62951200	2.60169700
H	-2.73468000	2.49871200	2.38137700
H	-4.12849900	1.93414700	3.34510100
H	-3.88957100	1.34923000	1.67339300
C	-3.46332900	-0.77068300	3.49302200
H	-2.84956100	-1.51789600	4.02245800
H	-4.22560900	-0.41200800	4.20751900
C	-4.13417900	-1.42680000	2.30136800
C	-5.42421800	-1.06124800	1.86884700
H	-5.98973400	-0.30639800	2.42448800
C	-5.99436400	-1.67170700	0.74184900
H	-7.00439200	-1.39397100	0.42539700
C	-5.27889800	-2.63842300	0.01954900
H	-5.73156200	-3.10673400	-0.86037300
C	-3.98696000	-3.02249800	0.42950100
C	-3.45038200	-2.42683900	1.58600900
H	-2.46393800	-2.74273800	1.93294100
C	-3.15977500	-4.03288300	-0.34193300
H	-3.82099100	-4.73037800	-0.88658700
H	-2.56550500	-4.63494900	0.36496500
C	-2.17244700	-3.42662400	-1.40361100
C	-2.94866800	-2.75239900	-2.54963500
H	-3.58513000	-1.93445300	-2.18367500
H	-3.59152800	-3.49922600	-3.04644000
H	-2.26267600	-2.33508400	-3.30244400
C	-1.30514200	-4.57959600	-1.96968700
H	-0.60919700	-4.20803900	-2.73994800
H	-1.95335600	-5.33867000	-2.43944600
H	-0.71704500	-5.06323300	-1.17539900
C	-1.22718600	-2.42293700	-0.70463200
N	-0.51514100	1.85293800	-1.69980300
C	-0.43450300	3.84452300	-0.31611400
C	-1.15573300	3.10384000	-1.26636100
C	-2.43225400	3.50988200	-1.74016600
C	-2.91416000	4.72135200	-1.19345800
C	-2.20159400	5.47783800	-0.25354800

C	-0.95075200	5.04004800	0.19353000
H	0.52109000	3.44603600	0.02951900
H	-3.88682300	5.09561800	-1.51416800
H	-2.63315700	6.40785100	0.12736100
H	-0.38267700	5.61346000	0.93097300
C	-3.26751700	2.73100800	-2.78442100
C	-3.55049400	1.29276500	-2.28290400
C	-4.63622000	3.40546200	-3.04416700
C	-2.52401200	2.68467700	-4.14691000
H	-2.63187300	0.71656300	-2.11036700
H	-4.11823200	1.31073800	-1.33875800
H	-4.15523800	0.75395000	-3.03276900
H	-4.53381900	4.41728100	-3.47121200
H	-5.19894300	2.79849900	-3.77195800
H	-5.24745300	3.47146600	-2.12882700
H	-3.17575100	2.22426900	-4.90888600
H	-2.26369400	3.69870000	-4.49359000
H	-1.60358000	2.08570800	-4.10886200
N	1.15551700	1.95541200	-3.42424500
N	0.35360600	1.98428300	-2.59752900

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Ab-TS (E = -2619.60429476)

Rh	-0.12298900	0.20149900	0.31099400
O	-1.57947200	-0.62318000	1.51199200
O	-1.52312500	1.46568300	-0.55638700
O	-2.16249300	-2.14229100	-0.08389000
O	-2.07776100	-0.08785500	-2.13178500
C	-2.28973100	-1.60899100	1.07233200
C	-3.35484100	-2.18844800	2.02687600
C	-2.63263600	-2.70724900	3.29658600
H	-2.06273000	-1.90545100	3.78884200
H	-3.37624700	-3.09908800	4.01078000
H	-1.93936100	-3.52767400	3.04816700
C	-4.11120300	-3.34604200	1.34672700
H	-3.42235600	-4.15229800	1.05259400
H	-4.84963800	-3.76348200	2.05226200
H	-4.64192200	-3.01028800	0.44424200
C	-4.34942900	-1.05148800	2.46117500
H	-3.78453400	-0.32102900	3.06228400
H	-5.08914900	-1.52247800	3.13281100
C	-5.05664400	-0.33526600	1.32688900
C	-6.32275400	-0.73584800	0.85704800
H	-6.84460100	-1.56613600	1.34326300
C	-6.92453800	-0.06722700	-0.21920800
H	-7.91553800	-0.37544400	-0.56560400
C	-6.26306700	0.99395100	-0.85500900
H	-6.73883900	1.50614200	-1.69742100
C	-4.99559400	1.41425400	-0.40621600
C	-4.42915800	0.75720900	0.70089300
H	-3.46519700	1.09990900	1.08258400
C	-4.22228900	2.52450900	-1.09136900
H	-4.91910200	3.22684400	-1.58256200
H	-3.65987800	3.10046300	-0.33791200
C	-3.20804600	2.05334300	-2.19503400
C	-3.95058100	1.40089100	-3.37729900
H	-4.51856400	0.51480900	-3.05994300
H	-4.65397600	2.12995300	-3.81451200
H	-3.24690200	1.08713100	-4.16291600
C	-2.42417900	3.29266100	-2.69627700
H	-1.69826700	3.01207100	-3.47700300
H	-3.12410300	4.02411200	-3.13388100
H	-1.87848300	3.78362600	-1.87647900
C	-2.19648700	1.05987800	-1.58174300
Rh	-0.73745500	-1.43113200	-1.36745000
O	0.70327000	-0.66412200	-2.61156200
O	0.58983500	-2.75903200	-0.55845100
O	1.30088900	0.87994700	-1.03454900

O	1.20211000	-1.24154900	1.03759800
C	1.41993600	0.31255500	-2.18114700
C	2.50389600	0.85742200	-3.13852500
C	1.78812200	1.40588900	-4.39958000
H	1.17285800	0.62968300	-4.87941400
H	2.53755200	1.75990800	-5.12753300
H	1.13730300	2.25846300	-4.14423600
C	3.31802900	1.98173200	-2.47196200
H	2.66954700	2.81416100	-2.16170500
H	4.06163500	2.37020200	-3.18897200
H	3.84971600	1.62317400	-1.57911900
C	3.44078200	-0.32269300	-3.58553800
H	2.83457800	-1.02714600	-4.17819400
H	4.19166800	0.11434100	-4.26785200
C	4.13180200	-1.07457400	-2.46374400
C	5.41946500	-0.72835600	-2.00908900
H	5.96742200	0.08410600	-2.49683000
C	6.00954200	-1.43046600	-0.94782000
H	7.01777200	-1.16625300	-0.61475700
C	5.31578100	-2.47074800	-0.31147400
H	5.78432800	-3.01053100	0.51773000
C	4.02627500	-2.83719800	-0.74485300
C	3.47099200	-2.14833400	-1.83911600
H	2.48862700	-2.44912900	-2.20983000
C	3.22255700	-3.92889100	-0.06401500
H	3.90053600	-4.66174300	0.40862100
H	2.63141400	-4.47249800	-0.81909000
C	2.23435700	-3.44444600	1.05965600
C	3.01070100	-2.88288800	2.26338700
H	3.65175900	-2.03900500	1.97335000
H	3.65000400	-3.67544200	2.68871500
H	2.32637400	-2.53315700	3.05092000
C	1.38230800	-4.65935600	1.50871000
H	0.68927500	-4.37652100	2.31821700
H	2.04197100	-5.45527700	1.89351900
H	0.79301800	-5.06482900	0.67254000
C	1.27100100	-2.39061800	0.46749100
N	0.58003800	1.47673800	1.78922900
C	0.53365400	3.59799500	0.57515300
C	1.17908300	2.73320400	1.49176800
C	2.41516000	3.12978200	2.11245400
C	2.91775300	4.39498600	1.74259800
C	2.25996400	5.24969100	0.84724000
C	1.05319800	4.85264300	0.25718100
H	-0.40160500	3.25220100	0.13308100
H	3.85437700	4.74193200	2.17905400
H	2.69564500	6.22662600	0.61722800
H	0.52552000	5.51131400	-0.43851700
C	3.21033200	2.24617300	3.10218000
C	3.65518400	0.94738400	2.38382400
C	4.48778100	2.95343600	3.61845000
C	2.35640500	1.88666400	4.34648600
H	2.79068700	0.36574300	2.03514300
H	4.29237800	1.17389200	1.51301100
H	4.24029400	0.31993800	3.07897600
H	4.26133100	3.88002700	4.17299700
H	5.01190300	2.27547900	4.31179000
H	5.19235000	3.19508200	2.80527800
H	2.98564700	1.36060900	5.08506900
H	1.95282000	2.79116300	4.83199900
H	1.52270100	1.22218800	4.08760800
N	-1.27791400	1.12168100	3.57794500
N	-0.61860300	1.73150700	2.87023900

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⁵Bb (E = -2510.13862803)

Rh	-0.03265300	0.33458400	-0.08400300
O	1.43484700	-0.06364700	-1.52782800

O	1.40512800	0.45095300	1.40279200
O	1.38907200	-2.30997400	-1.11716900
O	1.39864200	-1.80969900	1.72947600
C	1.82681700	-1.27246200	-1.72904100
C	2.90438700	-1.47659200	-2.81796700
C	2.29616600	-1.03407400	-4.17341800
H	1.95805400	0.01245300	-4.13589300
H	3.05207800	-1.13139600	-4.97092100
H	1.43599000	-1.66782100	-4.44530000
C	3.32710300	-2.95599800	-2.89319300
H	2.46664900	-3.60371800	-3.11865000
H	4.07441400	-3.08306300	-3.69503900
H	3.76942700	-3.30095400	-1.94743200
C	4.13939500	-0.55582100	-2.51135000
H	3.80727200	0.49229200	-2.59114400
H	4.87034800	-0.72743400	-3.32146500
C	4.79615500	-0.77675300	-1.16199100
C	5.90508100	-1.63017900	-0.99908800
H	6.34253800	-2.12492000	-1.87214500
C	6.46030900	-1.83798300	0.27216300
H	7.33149400	-2.49025300	0.38515700
C	5.90447200	-1.21581500	1.39973400
H	6.34158900	-1.38907100	2.38838500
C	4.79548800	-0.35736100	1.26558300
C	4.27980300	-0.13036800	-0.02360900
H	3.44402200	0.56242600	-0.14480100
C	4.13995600	0.30614000	2.46159500
H	4.87205900	0.41762100	3.28119400
H	3.80862300	1.32035400	2.18362000
C	2.90463900	-0.45522000	3.06521100
C	3.32621400	-1.82502900	3.63006200
H	3.75696200	-2.46983700	2.85085100
H	4.08250800	-1.67874000	4.42003200
H	2.46778100	-2.35526700	4.06942100
C	2.30998500	0.41726800	4.19995000
H	1.43638500	-0.07294900	4.66076300
H	3.06611600	0.56735300	4.98891100
H	1.99999800	1.40415700	3.82443200
C	1.82062900	-0.62912200	1.97775400
Rh	-0.05178900	-2.07754500	0.30452400
O	-1.50414700	-1.76755400	1.73421100
O	-1.47399700	-2.26170500	-1.16038600
O	-1.49286000	0.48493200	1.36424100
O	-1.50338000	-0.00540400	-1.52028300
C	-1.92092800	-0.57705000	1.95551400
C	-3.01158900	-0.39928900	3.03623500
C	-2.39974600	-0.83773400	4.39191700
H	-2.03494200	-1.87512000	4.34728600
H	-3.16302500	-0.76753500	5.18514900
H	-1.55773500	-0.18495500	4.67634100
C	-3.47926900	1.06553500	3.12368000
H	-2.64510900	1.73725600	3.37561500
H	-4.24433600	1.15894100	3.91320200
H	-3.91479300	1.41100200	2.17508000
C	-4.21963500	-1.35123700	2.71510000
H	-3.85847100	-2.39039700	2.78557900
H	-4.95668000	-1.20792000	3.52529400
C	-4.87726700	-1.13447300	1.36567000
C	-5.99677500	-0.29498500	1.20239200
H	-6.44512000	0.18948200	2.07571900
C	-6.54857200	-0.08878200	-0.07064400
H	-7.42809000	0.55202700	-0.18470900
C	-5.97891200	-0.69776800	-1.19865200
H	-6.41317900	-0.52490400	-2.18853800
C	-4.85962300	-1.54266100	-1.06388000
C	-4.34835200	-1.76960700	0.22718100
H	-3.50463900	-2.45246000	0.34826600
C	-4.18661400	-2.19088200	-2.25825300

H	-4.91274600	-2.31697000	-3.08101200
H	-3.83502200	-3.19786000	-1.97920300
C	-2.96428500	-1.40346000	-2.85552000
C	-3.41508800	-0.05256400	-3.44161400
H	-3.87566500	0.58913900	-2.67680900
H	-4.15419300	-0.22818300	-4.24193100
H	-2.56464600	0.49616000	-3.87321700
C	-2.32926400	-2.27359000	-3.97019100
H	-1.47364200	-1.75664300	-4.43503400
H	-3.07459200	-2.46906400	-4.75961900
H	-1.97844200	-3.23769000	-3.57200700
C	-1.89854000	-1.20401500	-1.75375000
N	0.02245700	2.20058900	-0.60596400
C	0.00310600	3.22280400	1.62598300
C	0.08066300	3.29177800	0.18681100
C	0.21511600	4.60977000	-0.44830400
C	0.26544000	5.72427500	0.40144000
C	0.18327300	5.61757800	1.80102200
C	0.04793900	4.36170300	2.41809800
H	-0.10606700	2.23726900	2.07419400
H	0.36827100	6.72276800	-0.02561900
H	0.22376300	6.52622000	2.40941900
H	-0.02025700	4.28481400	3.50714600
C	0.29684700	4.77897000	-1.97686500
C	-1.00254100	4.23633100	-2.63637900
C	0.44807300	6.26183800	-2.39128300
C	1.52808500	4.00902900	-2.53248700
H	-1.12461200	3.16451000	-2.42946000
H	-1.88934300	4.77474900	-2.26058700
H	-0.95188800	4.38763300	-3.72869500
H	1.37040800	6.71752900	-1.99238100
H	0.50342700	6.32018000	-3.49052600
H	-0.41200900	6.87588200	-2.07436000
H	1.59692700	4.16261700	-3.62355900
H	2.46317100	4.37998800	-2.07863200
H	1.43632600	2.93332100	-2.32818500

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^TBb (E = -2510.14171654)

Rh	-0.03135800	0.30790200	-0.09790700
O	1.42251700	-0.03883900	-1.54432000
O	1.42101600	0.46887400	1.38297400
O	1.44450100	-2.27794800	-1.10225500
O	1.45549700	-1.78599500	1.74750300
C	1.84916900	-1.23989300	-1.73451600
C	2.92018300	-1.42955700	-2.83075600
C	2.29931900	-0.99220800	-4.18219100
H	1.95246700	0.05131800	-4.14335000
H	3.05172600	-1.08269200	-4.98363700
H	1.44356400	-1.63374200	-4.44982200
C	3.35807200	-2.90451400	-2.91066700
H	2.50324700	-3.56114000	-3.13227200
H	4.10124900	-3.02198400	-3.71762100
H	3.81024300	-3.24640100	-1.96853100
C	4.14762800	-0.49617200	-2.53018600
H	3.80594600	0.54888100	-2.61090000
H	4.87657300	-0.66273900	-3.34309900
C	4.81004200	-0.70878600	-1.18254000
C	5.92090800	-1.55945900	-1.01889000
H	6.35702700	-2.05752800	-1.89069700
C	6.47992900	-1.75972100	0.25190800
H	7.35271700	-2.40963300	0.36587200
C	5.92590800	-1.13278900	1.37773600
H	6.36616800	-1.29991400	2.36597700
C	4.81490100	-0.27708600	1.24250700
C	4.29535300	-0.05746600	-0.04641300
H	3.45860200	0.63427200	-0.16827000
C	4.15975300	0.39067100	2.43606300

H	4.89555200	0.52107400	3.24948100
H	3.81274700	1.39698600	2.14913300
C	2.93925300	-0.38111400	3.05586800
C	3.38505100	-1.73342600	3.64436200
H	3.82637600	-2.38504900	2.87674500
H	4.13914200	-1.55920100	4.43067700
H	2.53663100	-2.27035300	4.09499000
C	2.33064300	0.50108600	4.17573700
H	1.46651900	0.00384600	4.64669100
H	3.08537400	0.67802400	4.96040200
H	2.00277100	1.47527600	3.78306400
C	1.85681600	-0.59147300	1.97358600
Rh	0.00715300	-2.07218200	0.33183800
O	-1.43741700	-1.80678100	1.77314600
O	-1.42099500	-2.30602000	-1.12417700
O	-1.49027300	0.44059300	1.36438400
O	-1.49501800	-0.05818100	-1.51430900
C	-1.88219300	-0.62008300	1.97687800
C	-2.96523200	-0.45068600	3.06683700
C	-2.33920700	-0.87850300	4.41921600
H	-1.96443700	-1.91236300	4.37619600
H	-3.09776000	-0.81259200	5.21730900
H	-1.50223700	-0.21589900	4.69520600
C	-3.44447400	1.01070500	3.15233700
H	-2.61269100	1.69056200	3.38957800
H	-4.20046600	1.10149600	3.95084700
H	-3.89390400	1.34822500	2.20743700
C	-4.16708800	-1.41457100	2.75819600
H	-3.79798800	-2.45062500	2.83458700
H	-4.90169100	-1.27085700	3.57047000
C	-4.83121300	-1.21251700	1.41003200
C	-5.95482900	-0.37935900	1.24324200
H	-6.40177800	0.11123600	2.11375500
C	-6.51197700	-0.18660600	-0.02955800
H	-7.39438100	0.44969100	-0.14612100
C	-5.94368100	-0.80298300	-1.15418600
H	-6.38223900	-0.64091500	-2.14397700
C	-4.81999500	-1.64139900	-1.01564900
C	-4.30314400	-1.85492500	0.27531000
H	-3.45582700	-2.53295000	0.39984000
C	-4.14710500	-2.29631300	-2.20621500
H	-4.87643500	-2.44261200	-3.02275900
H	-3.78056200	-3.29500300	-1.91677600
C	-2.93966100	-1.50061900	-2.82218500
C	-3.41344400	-0.16612300	-3.42781500
H	-3.87732200	0.48243400	-2.67094000
H	-4.15592900	-0.36664600	-4.21889800
H	-2.57470200	0.38664300	-3.87692500
C	-2.29681500	-2.37902500	-3.92618100
H	-1.45079300	-1.85769800	-4.40357700
H	-3.04322700	-2.59679000	-4.70853900
H	-1.93101300	-3.33203900	-3.51502800
C	-1.87208700	-1.26752200	-1.73054200
N	-0.03334600	2.24327600	-0.37288400
C	-0.00258200	3.47983300	1.68310000
C	0.00910600	3.42632000	0.24057200
C	0.06472500	4.67715900	-0.51728600
C	0.10912700	5.86369700	0.22267600
C	0.09959300	5.89435100	1.63072400
C	0.04188800	4.69263700	2.35794200
H	-0.05019500	2.53027200	2.21574400
H	0.15307000	6.81648500	-0.30816900
H	0.13600200	6.85551800	2.15059100
H	0.03105900	4.70734900	3.45201400
C	0.07142800	4.67165500	-2.05707300
C	-1.22425400	3.99781100	-2.58435900
C	0.13121600	6.10108800	-2.64335000
C	1.31262500	3.89635500	-2.57610000

H	-1.30865900	2.95869900	-2.23232600
H	-2.11836700	4.55044100	-2.24972100
H	-1.22036800	3.99014700	-3.68832800
H	1.04786100	6.63604500	-2.34269400
H	0.13168400	6.03867000	-3.74400000
H	-0.74049500	6.70882800	-2.34771200
H	1.32243700	3.90101000	-3.68012700
H	2.24608700	4.36753300	-2.22432400
H	1.30271500	2.84966600	-2.23671600

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Ac (E = -2619.63230573)

Rh	-0.12048100	0.12276400	-0.27914900
O	1.23625100	-1.01365500	-1.37676100
O	1.36712200	0.73261300	1.03833900
O	0.96365300	-2.80545200	0.01509100
O	1.05312800	-1.10538800	2.36260000
C	1.49459200	-2.21703000	-0.99200100
C	2.51762300	-3.01786500	-1.82945300
C	1.97183800	-3.13031400	-3.27542700
H	1.79126500	-2.13780900	-3.71547700
H	2.69795300	-3.66751800	-3.90861700
H	1.02494100	-3.69449600	-3.29606100
C	2.71745600	-4.42765400	-1.24061800
H	1.76967800	-4.98641700	-1.21943900
H	3.43463600	-4.98747000	-1.86511100
H	3.10633000	-4.38718400	-0.21310800
C	3.88167100	-2.24003300	-1.87879100
H	3.71361200	-1.29902100	-2.42808100
H	4.57156400	-2.85051600	-2.48849000
C	4.51010400	-1.93105900	-0.53331600
C	5.47758500	-2.77124100	0.05173800
H	5.82447200	-3.65877900	-0.48711000
C	6.00917900	-2.46846900	1.31398100
H	6.77164100	-3.11883700	1.75318600
C	5.56947300	-1.33684300	2.01651800
H	5.98720000	-1.11141700	3.00300600
C	4.60277500	-0.47975000	1.45458000
C	4.11072400	-0.78077800	0.17139800
H	3.38766700	-0.10308800	-0.28805400
C	4.07019400	0.73268300	2.19408500
H	4.82475400	1.09969300	2.91273800
H	3.88243900	1.54750800	1.47577100
C	2.74861500	0.49773400	3.01025000
C	2.98144300	-0.50604700	4.15547500
H	3.30702700	-1.48629200	3.77886200
H	3.75983600	-0.11571000	4.83345600
H	2.06178400	-0.65871400	4.74018500
C	2.29689600	1.85876500	3.59746400
H	1.38023100	1.74361900	4.19911900
H	3.08481600	2.26119200	4.25643000
H	2.09851400	2.59064500	2.80062600
C	1.63763500	-0.00380800	2.05995200
Rh	-0.42309100	-1.79710600	1.13213700
O	-1.79766400	-0.71887700	2.22002000
O	-1.88291400	-2.44915900	-0.16392200
O	-1.52489800	1.10632500	0.87105300
O	-1.62224000	-0.60700000	-1.48761600
C	-2.06544600	0.48548900	1.85848100
C	-3.10986400	1.24828200	2.70521600
C	-2.55015900	1.36774800	4.14606000
H	-2.33307700	0.37667200	4.57227100
H	-3.28683800	1.87500200	4.79175400
H	-1.62222100	1.96303400	4.16086400
C	-3.36908300	2.65372700	2.13132600
H	-2.44540600	3.25076500	2.11283100
H	-4.10545200	3.17809700	2.76426700
H	-3.76191900	2.60896400	1.10521700

C	-4.44261500	0.41808000	2.76785000
H	-4.23030700	-0.51956200	3.30728500
H	-5.14666400	0.99916700	3.38992800
C	-5.07434100	0.09667500	1.42720100
C	-6.05986500	0.91784400	0.84473700
H	-6.42421100	1.79683500	1.38600600
C	-6.58757500	0.60635700	-0.41706700
H	-7.36472900	1.24112300	-0.85339200
C	-6.12526700	-0.51405700	-1.12322100
H	-6.53918400	-0.74551000	-2.10988800
C	-5.14119500	-1.35267200	-0.56357400
C	-4.65560600	-1.04540900	0.72068100
H	-3.91827000	-1.70763800	1.17995500
C	-4.57933700	-2.54909700	-1.30681300
H	-5.32588400	-2.93858200	-2.02181500
H	-4.36380500	-3.35841300	-0.58998900
C	-3.26877600	-2.27588100	-2.13067100
C	-3.54363700	-1.30194700	-3.29080600
H	-3.91059200	-0.33033600	-2.93060600
H	-4.30553100	-1.73567600	-3.96092700
H	-2.63298700	-1.11955700	-3.88038300
C	-2.76620600	-3.62999100	-2.69477800
H	-1.85858600	-3.49015000	-3.30497700
H	-3.54169100	-4.07461200	-3.34110200
H	-2.53493700	-4.33882200	-1.88539900
C	-2.17678000	-1.72776800	-1.18563800
N	0.15986000	1.96886800	-1.64951300
C	2.38586800	1.86936700	-2.61467100
C	1.42130600	2.65513700	-1.96217400
C	1.65602600	4.01150200	-1.60991000
C	2.92954400	4.51024000	-1.96791500
C	3.90014400	3.74050700	-2.62300400
C	3.63179500	2.40786600	-2.95176900
H	2.14318000	0.82728800	-2.83177300
H	3.17470900	5.54569200	-1.73114800
H	4.86525900	4.18996200	-2.87301700
H	4.37757800	1.79118600	-3.46012200
C	0.62965800	4.92181600	-0.89135300
C	0.29205700	4.33531600	0.50273900
C	1.18549600	6.35011900	-0.67246000
C	-0.66857900	5.06852100	-1.73071200
H	-0.13592900	3.32578000	0.43846100
H	1.19609700	4.28509100	1.13142300
H	-0.43959200	4.98703900	1.01138700
H	1.40677000	6.86441700	-1.62292700
H	0.42729200	6.94983400	-0.14320800
H	2.09664700	6.35421600	-0.05169800
H	-1.32028900	5.83081600	-1.27100600
H	-0.44576500	5.39331800	-2.76066500
H	-1.25041100	4.13798900	-1.77512200
N	-1.45031000	1.78446600	-3.42504700
N	-0.63449200	1.89822500	-2.62154500

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Ac-TS (E = -2619.60220082)

Rh	-0.09195500	0.13649300	-0.40677900
O	1.24234300	-1.17056700	-1.32598800
O	1.43490900	0.91079700	0.79748900
O	1.01231400	-2.72534300	0.32712900
O	1.14438900	-0.70148100	2.38967100
C	1.50763300	-2.30677100	-0.77490200
C	2.48853800	-3.23674800	-1.52344100
C	1.91241700	-3.51299800	-2.93487200
H	1.75731600	-2.57871000	-3.49526400
H	2.60951600	-4.15109200	-3.50353200
H	0.94741900	-4.04187800	-2.87136400
C	2.65846900	-4.56469000	-0.76066900
H	1.69512200	-5.08510700	-0.64924700

H	3.34318400	-5.22359300	-1.32137000
H	3.07290600	-4.40463000	0.24488400
C	3.87416700	-2.51520000	-1.69218200
H	3.72962100	-1.65853500	-2.37143200
H	4.53899800	-3.22809400	-2.21181200
C	4.52204100	-2.03373300	-0.40822900
C	5.46689500	-2.80733200	0.29383400
H	5.78261200	-3.77593800	-0.10677000
C	6.01684400	-2.33520700	1.49507700
H	6.76199600	-2.93626200	2.02478800
C	5.61831700	-1.09721500	2.02056100
H	6.05283700	-0.73932600	2.95939800
C	4.67369400	-0.30469600	1.33940400
C	4.16309600	-0.77950700	0.11786000
H	3.46103700	-0.15229700	-0.43608700
C	4.18169700	1.02174500	1.88465500
H	4.95681100	1.48072700	2.52394700
H	3.99798000	1.71498600	1.04747100
C	2.87229300	0.95186800	2.74920900
C	3.10662800	0.12937500	4.03118800
H	3.39342300	-0.90707700	3.80321000
H	3.91519800	0.59518500	4.62017600
H	2.20056000	0.09853500	4.65507700
C	2.46692600	2.39818700	3.12681400
H	1.54805700	2.40601100	3.73582600
H	3.27005400	2.86668400	3.72032400
H	2.29322100	3.00944600	2.22934900
C	1.72851200	0.33377100	1.91125900
Rh	-0.34985100	-1.56048400	1.30725600
O	-1.71923400	-0.36651200	2.25668700
O	-1.81902800	-2.41310000	0.15871000
O	-1.53316400	1.23013700	0.63413800
O	-1.61988800	-0.79167100	-1.42905800
C	-2.03702900	0.75444700	1.71575200
C	-3.09558300	1.60734300	2.45496000
C	-2.48466900	2.01960600	3.81969900
H	-2.20209700	1.13673200	4.41306900
H	-3.22012700	2.60828200	4.39370300
H	-1.58849300	2.64588600	3.67770100
C	-3.46140600	2.86586900	1.64725100
H	-2.57991300	3.50154200	1.48229000
H	-4.20999600	3.45380700	2.20550700
H	-3.88269900	2.61093200	0.66418400
C	-4.37305900	0.73701900	2.73585600
H	-4.07952400	-0.08927200	3.40382200
H	-5.07218300	1.37915400	3.30072000
C	-5.05871200	0.17743000	1.50433300
C	-6.12936500	0.84023400	0.87229900
H	-6.52288300	1.76787600	1.30008800
C	-6.70072400	0.31228300	-0.29504600
H	-7.54220500	0.82635300	-0.76917500
C	-6.19591000	-0.86756800	-0.86140800
H	-6.64179900	-1.26498100	-1.77881000
C	-5.12705300	-1.55081100	-0.24912100
C	-4.60049500	-1.03008800	0.94709900
H	-3.80056600	-1.57416400	1.45349200
C	-4.51601100	-2.80059100	-0.85171200
H	-5.26197500	-3.32795500	-1.47250000
H	-4.21719900	-3.49106700	-0.04612100
C	-3.26297200	-2.55875300	-1.76873900
C	-3.64536400	-1.74116900	-3.01494400
H	-4.03189800	-0.74730200	-2.74976500
H	-4.42574600	-2.28071400	-3.57830600
H	-2.77999200	-1.59867400	-3.67866900
C	-2.71049100	-3.94200700	-2.20245400
H	-1.83772500	-3.82693400	-2.86611600
H	-3.48710100	-4.49214500	-2.75994300
H	-2.41072600	-4.54418400	-1.33140300

C	-2.15631800	-1.86029600	-0.94812400
N	0.04580400	1.77769800	-1.66014800
C	2.29801100	1.50728500	-2.57946400
C	1.30361900	2.34265200	-2.01520200
C	1.56608900	3.74253200	-1.81376400
C	2.86270300	4.18609600	-2.15171900
C	3.83979800	3.34829400	-2.70651400
C	3.55280300	1.99745900	-2.94096300
H	2.04616400	0.45719500	-2.73379400
H	3.12177200	5.23446200	-2.00144300
H	4.81975200	3.76060100	-2.96451000
H	4.29781700	1.33561300	-3.39121400
C	0.52386300	4.75030600	-1.27322200
C	0.07440700	4.34733400	0.15249500
C	1.09323900	6.18778900	-1.18810900
C	-0.71016100	4.80272800	-2.21293800
H	-0.38280900	3.34859300	0.16315800
H	0.93009000	4.34585700	0.84729800
H	-0.66538400	5.07622900	0.52797200
H	1.39891800	6.57860900	-2.17327900
H	0.30947800	6.85752900	-0.79800400
H	1.95369600	6.25806800	-0.50165600
H	-1.39825800	5.59708300	-1.87572200
H	-0.41303400	5.03143900	-3.25018000
H	-1.26435700	3.85549800	-2.20491200
N	-1.85362900	1.22307900	-3.35697000
N	-0.79088700	1.49706600	-3.04115300

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^sBc (E = -2510.13562538)

Rh	-0.03612500	0.33624300	-0.21565500
O	1.45122300	-0.18766200	-1.57888000
O	1.40688600	0.80552600	1.20773100
O	1.55201100	-2.33069600	-0.80163400
O	1.48654400	-1.35773100	1.94451400
C	1.92452300	-1.39031900	-1.58175900
C	3.01276600	-1.71381600	-2.63058500
C	2.44988500	-1.37859000	-4.03454400
H	2.14106400	-0.32465600	-4.10156100
H	3.22066500	-1.56926700	-4.80017500
H	1.57749100	-2.00983300	-4.27029300
C	3.39367000	-3.20553000	-2.56258100
H	2.51879600	-3.84747000	-2.74614100
H	4.15028600	-3.42460600	-3.33525900
H	3.80762100	-3.47525500	-1.58050700
C	4.27576300	-0.81177300	-2.38208500
H	3.99659300	0.23035000	-2.61175000
H	5.02877800	-1.11353000	-3.13169600
C	4.86969700	-0.87481400	-0.98774400
C	5.91075100	-1.75843100	-0.64154900
H	6.34535900	-2.41346900	-1.40319600
C	6.40455500	-1.79070900	0.67158700
H	7.22315900	-2.47050800	0.92616200
C	5.86075600	-0.95611200	1.66013600
H	6.25608800	-0.99052600	2.68023200
C	4.81982700	-0.06270300	1.34103700
C	4.36335400	-0.02710100	0.01225800
H	3.57772400	0.68433100	-0.24616400
C	4.16968400	0.84697500	2.36558900
H	4.88329200	1.08295400	3.17496600
H	3.90172900	1.80196200	1.88349100
C	2.87811500	0.27940400	3.05826800
C	3.23038000	-0.92579400	3.95156200
H	3.68384400	-1.74286300	3.37240900
H	3.94551900	-0.60731900	4.72926000
H	2.33476800	-1.32553100	4.45082100
C	2.25842000	1.40851600	3.91918900
H	1.36228500	1.05097200	4.45250300

H	2.98841100	1.74482100	4.67470900
H	1.97042800	2.27098600	3.29973600
C	1.84534000	-0.13082800	1.98218600
Rh	0.09154500	-1.96939000	0.57615100
O	-1.37079900	-1.57100700	1.95107700
O	-1.31235900	-2.49226600	-0.83365500
O	-1.52318700	0.59055100	1.23380100
O	-1.47477000	-0.33065600	-1.56067200
C	-1.87279300	-0.38923300	1.98548500
C	-2.96981700	-0.12888700	3.04370900
C	-2.32710600	-0.33288700	4.43996600
H	-1.90250400	-1.34325200	4.53997000
H	-3.08984400	-0.19264200	5.22445500
H	-1.52402200	0.40177500	4.61586500
C	-3.52416000	1.30270100	2.93033600
H	-2.72842100	2.04867600	3.07412700
H	-4.28998600	1.46180400	3.70873400
H	-3.98318400	1.48399700	1.94804200
C	-4.11771800	-1.18867600	2.87545900
H	-3.69499100	-2.18216400	3.09834900
H	-4.86460800	-0.96990200	3.65942400
C	-4.78362300	-1.21745300	1.51322500
C	-5.94874400	-0.47778400	1.23018300
H	-6.42610400	0.10867800	2.02177000
C	-6.50816500	-0.50039100	-0.05601200
H	-7.42259600	0.06438800	-0.26121000
C	-5.90170500	-1.24134200	-1.08119200
H	-6.34209800	-1.24689000	-2.08337500
C	-4.73629000	-1.99026700	-0.82527700
C	-4.21645700	-1.98834600	0.48206000
H	-3.33478900	-2.59495000	0.70029500
C	-4.02110100	-2.77077100	-1.91121300
H	-4.73605500	-3.06897000	-2.69877400
H	-3.60491700	-3.69756300	-1.48301800
C	-2.85257500	-2.00759300	-2.63256500
C	-3.38873600	-0.79436100	-3.41528400
H	-3.88231200	-0.06920000	-2.75257800
H	-4.12071400	-1.13700000	-4.16668300
H	-2.57577100	-0.27039600	-3.94008400
C	-2.16124500	-2.99612100	-3.60643600
H	-1.34177600	-2.50191200	-4.15404300
H	-2.89158600	-3.35937700	-4.34910700
H	-1.74776400	-3.86250600	-3.06822200
C	-1.80011500	-1.57220500	-1.58632000
N	-0.38626200	2.15558200	-0.79781700
C	1.89767500	2.93195300	-1.17648600
C	0.48915400	3.16492500	-0.98401500
C	-0.01255700	4.54292200	-1.05705700
C	0.93439100	5.55188400	-1.28305900
C	2.30194300	5.28471000	-1.47625800
C	2.78623100	3.96561400	-1.43794500
H	2.22821500	1.89493300	-1.16511000
H	0.60968900	6.59240300	-1.32790700
H	2.98777000	6.11603300	-1.66536600
H	3.84728100	3.75831000	-1.60410400
C	-1.50332000	4.88027000	-0.87715700
C	-1.77065200	6.40201700	-0.95414600
C	-2.33354700	4.19599600	-2.00024600
C	-1.99479300	4.38562500	0.51110900
H	-1.24230700	6.96133700	-0.16323700
H	-1.49018800	6.82879100	-1.93213800
H	-2.84952400	6.58137100	-0.81744100
H	-2.22620300	3.10390900	-1.95314400
H	-3.39939200	4.45594000	-1.87863000
H	-2.01041200	4.54517000	-2.99579700
H	-3.05400700	4.66373800	0.64949000
H	-1.90283600	3.29317900	0.58988500
H	-1.41236800	4.85072600	1.32521300

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Tb (E = -2510.14031216)

Rh	0.04364600	0.31908500	-0.07984500
O	-1.33349800	0.52109800	1.46574100
O	-1.49670400	0.03431500	-1.46970800
O	-1.44466800	-1.73977100	1.77966400
O	-1.59680600	-2.21088100	-1.07524800
C	-1.77650000	-0.53431300	2.05788400
C	-2.78053300	-0.30942000	3.21021500
C	-2.09284700	0.57503000	4.28070300
H	-1.76261900	1.53387500	3.85408300
H	-2.79860600	0.77953000	5.10328300
H	-1.21470200	0.06456000	4.70948300
C	-3.19949500	-1.65435600	3.83353200
H	-2.32742900	-2.19896900	4.22625700
H	-3.89461900	-1.46860400	4.67001600
H	-3.69969300	-2.30406700	3.10113900
C	-4.03384900	0.46781300	2.66520500
H	-3.70227000	1.47608200	2.36659900
H	-4.72305700	0.59251300	3.51923200
C	-4.75451000	-0.18985100	1.50429300
C	-5.85064400	-1.05487400	1.69142000
H	-6.23193400	-1.23876800	2.70088100
C	-6.46558800	-1.66957500	0.59073200
H	-7.32582800	-2.32754700	0.74611400
C	-5.98554100	-1.44526800	-0.70802900
H	-6.47117200	-1.93185200	-1.55986800
C	-4.89131500	-0.58469600	-0.92369600
C	-4.31265900	0.05034400	0.19039400
H	-3.48664900	0.74772100	0.03253600
C	-4.31441600	-0.34136400	-2.30536100
H	-5.09452000	-0.48283800	-3.07437700
H	-3.97789000	0.70591300	-2.38057300
C	-3.11264900	-1.26775500	-2.71251600
C	-3.57424200	-2.73281100	-2.83663700
H	-3.98091500	-3.11328300	-1.88873100
H	-4.36006800	-2.80300100	-3.60800000
H	-2.74147500	-3.38809300	-3.13328800
C	-2.56158600	-0.77621700	-4.07509300
H	-1.73459000	-1.41786500	-4.42093300
H	-3.35982500	-0.81672500	-4.83511800
H	-2.19218400	0.25830700	-4.01045500
C	-1.98396800	-1.14364000	-1.66488500
Rh	-0.08710200	-2.06807300	0.28489700
O	1.26925900	-2.32913500	-1.24153000
O	1.42568300	-1.90042000	1.66130900
O	1.42099500	-0.07379000	-1.57172600
O	1.57040000	0.34976000	1.31326300
C	1.73306600	-1.29094600	-1.83879200
C	2.73694800	-1.52767600	-2.98909000
C	2.01651500	-2.36276800	-4.07814500
H	1.64459300	-3.31446100	-3.66957800
H	2.71675300	-2.58232500	-4.90157000
H	1.16298800	-1.80739000	-4.50058400
C	3.21613600	-0.19190100	-3.58801900
H	2.37056400	0.39570800	-3.97637200
H	3.90863500	-0.39272100	-4.42322500
H	3.73838600	0.42445000	-2.84236100
C	3.95202400	-2.36912600	-2.45342100
H	3.57512200	-3.36760300	-2.17647500
H	4.63941900	-2.50694700	-3.30699800
C	4.69448200	-1.76706800	-1.27620900
C	5.82922500	-0.94863400	-1.44114300
H	6.22557200	-0.76461100	-2.44479500
C	6.46215100	-0.38042100	-0.32567100
H	7.35250000	0.24040700	-0.46357800
C	5.96047800	-0.60242500	0.96532700

H	6.45896300	-0.15037700	1.82870000
C	4.82694000	-1.41629900	1.15873000
C	4.23259400	-2.01025600	0.03037300
H	3.37663100	-2.67399100	0.17277700
C	4.22061000	-1.64802800	2.52937200
H	4.99652200	-1.55796300	3.31029400
H	3.82164000	-2.67423400	2.58501200
C	3.06614300	-0.66056100	2.93202800
C	3.59722400	0.77877700	3.06531200
H	4.01988200	1.14641700	2.11947700
H	4.38697300	0.80645700	3.83547400
H	2.79741800	1.47046400	3.36896700
C	2.48154200	-1.13045000	4.28891800
H	1.68134000	-0.45315200	4.63000000
H	3.27493500	-1.12727700	5.05520300
H	2.06876400	-2.14787500	4.21520600
C	1.93641500	-0.74314100	1.88219300
N	0.10064900	2.26098000	-0.36859000
C	-1.66143100	3.23209100	-1.66944000
C	-0.47853100	3.36068100	-0.85163800
C	0.05591800	4.69684800	-0.58201000
C	-0.63415900	5.77839500	-1.14091700
C	-1.79007200	5.63112700	-1.93164400
C	-2.29965000	4.34791100	-2.19431600
H	-2.02306800	2.22170400	-1.85959200
H	-0.26705000	6.79027700	-0.96036000
H	-2.28359100	6.51797900	-2.33832400
H	-3.19557100	4.22262000	-2.80995400
C	1.31764000	4.89065200	0.27861700
C	1.69950600	6.38198500	0.42022000
C	1.06982700	4.32687500	1.70384000
C	2.51783500	4.15384600	-0.37487100
H	1.92365900	6.84729800	-0.55437200
H	0.90667900	6.96952200	0.91317800
H	2.60604300	6.46497900	1.04201700
H	0.84039400	3.25153400	1.67310000
H	1.97120300	4.46982000	2.32465900
H	0.23057100	4.84957300	2.19332300
H	3.42459500	4.29656000	0.23804400
H	2.32775100	3.07355900	-0.45987000
H	2.72027100	4.55165900	-1.38364400

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Ad (E = -2619.63425321)

Rh	0.13560700	0.20441900	-0.20301800
O	-1.31667900	0.53587700	1.24642400
O	-1.22431600	-0.80043300	-1.41249000
O	-0.88802500	-1.47785700	2.23886900
O	-0.81159300	-2.78073400	-0.34844500
C	-1.52048200	-0.36618700	2.14276300
C	-2.61075300	-0.07174400	3.19765200
C	-2.20717800	1.21678200	3.95765000
H	-2.09194500	2.06655600	3.26849900
H	-2.98184100	1.46914900	4.70144900
H	-1.25635600	1.07370900	4.49743500
C	-2.73959900	-1.24306100	4.19013500
H	-1.78985400	-1.42363400	4.71609600
H	-3.51023400	-1.00275000	4.94262400
H	-3.02590700	-2.17571800	3.68331200
C	-3.97848800	0.19781700	2.47332900
H	-3.86844400	1.12018700	1.87963700
H	-4.71986900	0.40741900	3.26497100
C	-4.47528000	-0.92083700	1.57755500
C	-5.36700900	-1.91091000	2.03451800
H	-5.75137100	-1.86548400	3.05850000
C	-5.77575700	-2.94618700	1.18060300
H	-6.47939100	-3.70255600	1.54126400
C	-5.28933100	-3.01727600	-0.13331700

H	-5.61296100	-3.83031800	-0.79108600
C	-4.39829900	-2.03933900	-0.61669100
C	-4.02703500	-0.99156200	0.24610700
H	-3.35798000	-0.21264200	-0.12618400
C	-3.82582500	-2.08762100	-2.02031500
H	-4.51052800	-2.63780600	-2.69022500
H	-3.74295600	-1.06193700	-2.41534100
C	-2.41819100	-2.77072500	-2.15787600
C	-2.50732300	-4.27170300	-1.82141000
H	-2.85520100	-4.43774200	-0.79167600
H	-3.21446600	-4.76079800	-2.51310200
H	-1.52774100	-4.76208300	-1.92772400
C	-1.93498400	-2.58973800	-3.61889400
H	-0.95617100	-3.07292300	-3.77339800
H	-2.65508200	-3.05783100	-4.31121200
H	-1.84003400	-1.52479500	-3.87848000
C	-1.40735300	-2.06257400	-1.22807300
Rh	0.56769400	-1.90129400	0.87206900
O	2.00343000	-2.27136900	-0.56098500
O	1.94098000	-0.94022100	2.07439100
O	1.61761000	-0.25378500	-1.55728700
O	1.53890100	1.06042600	1.04913200
C	2.22963500	-1.38035400	-1.45818700
C	3.31368500	-1.70797600	-2.50915600
C	2.85985300	-2.97725100	-3.27458000
H	2.70125700	-3.82179400	-2.58722800
H	3.62902300	-3.26298000	-4.01185100
H	1.92043300	-2.79311100	-3.82148800
C	3.50005100	-0.54270900	-3.49853400
H	2.56296700	-0.32050300	-4.03128300
H	4.26370500	-0.81660400	-4.24646200
H	3.82508400	0.37608700	-2.99025800
C	4.66396200	-2.03878500	-1.77609000
H	4.51308100	-2.96121300	-1.19134400
H	5.40251300	-2.27071700	-2.56404900
C	5.19635700	-0.94869700	-0.86592400
C	6.12039100	0.01722200	-1.31039800
H	6.50695900	-0.03043600	-2.33338000
C	6.55849500	1.03086300	-0.44527300
H	7.28844100	1.76683600	-0.79557600
C	6.06545400	1.10772100	0.86570800
H	6.40992000	1.90591100	1.53110600
C	5.14035400	0.15497700	1.33591400
C	4.74590400	-0.87744700	0.46503200
H	4.05628700	-1.64190100	0.83034700
C	4.54632600	0.22213700	2.72957200
H	5.24711900	0.72675800	3.41846000
H	4.39433800	-0.80010800	3.11350500
C	3.17729400	0.98566400	2.84170100
C	3.35639400	2.47575100	2.49809700
H	3.70111200	2.61718300	1.46364900
H	4.10119000	2.92326800	3.17807300
H	2.41211800	3.02800600	2.62150100
C	2.66445100	0.84157600	4.29748400
H	1.70765200	1.37224700	4.43387400
H	3.39640900	1.27975300	4.99686400
H	2.51477000	-0.21573000	4.56282800
C	2.14109300	0.31723100	1.90962200
N	-0.19771400	2.26751900	-1.18958800
C	-0.54739200	3.79821800	0.66365900
C	-0.97506600	3.36907700	-0.60332400
C	-2.09920500	3.93659500	-1.26157400
C	-2.75180700	4.96779600	-0.54775700
C	-2.33259600	5.41259900	0.71325300
C	-1.22086800	4.82770200	1.32871100
H	0.31221200	3.29859400	1.11486500
H	-3.62035000	5.45238900	-0.99475300
H	-2.88105200	6.21875200	1.20871000

H	-0.87939700	5.16187300	2.31203300
C	-2.60594100	3.50290900	-2.65892400
C	-3.02312500	2.01085100	-2.63152700
C	-3.84230400	4.32141100	-3.10170700
C	-1.50920500	3.72364000	-3.73619500
H	-2.19510100	1.34906600	-2.34332100
H	-3.85239300	1.85214200	-1.92247100
H	-3.37160900	1.70590500	-3.63387600
H	-3.62009200	5.39715900	-3.20196900
H	-4.17438200	3.96082500	-4.08892300
H	-4.69108900	4.20192900	-2.40824200
H	-1.93000000	3.52563000	-4.73677400
H	-1.14047700	4.76275400	-3.72480100
H	-0.65212900	3.04820100	-3.61045900
N	1.88549400	2.83491400	-2.24795900
N	0.88692700	2.62968700	-1.71486200

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Ad-TS (E = -2619.60391917)

Rh	0.14638700	0.28386800	-0.20722300
O	-1.30275300	0.66377800	1.24588000
O	-1.21979900	-0.80128000	-1.36730600
O	-0.90420200	-1.32185800	2.30459900
O	-0.82330400	-2.73668000	-0.21913700
C	-1.51886500	-0.20599000	2.17181100
C	-2.60573700	0.14451700	3.21343600
C	-2.19446800	1.46336300	3.91472400
H	-2.08185100	2.28252300	3.18913800
H	-2.96503400	1.74901900	4.65062800
H	-1.24153200	1.34157900	4.45608200
C	-2.73942600	-0.98046400	4.25742000
H	-1.79055700	-1.14041500	4.79164600
H	-3.50914900	-0.70210300	4.99747900
H	-3.02942100	-1.93396100	3.79359100
C	-3.97172500	0.38983000	2.47682000
H	-3.85534900	1.28396900	1.84263000
H	-4.71158200	0.63935900	3.25825500
C	-4.47396800	-0.76593500	1.63285000
C	-5.36579400	-1.73274800	2.13691800
H	-5.74791100	-1.63972300	3.15846700
C	-5.77731100	-2.80571400	1.33257600
H	-6.48113200	-3.54375600	1.72901800
C	-5.29349700	-2.93770800	0.02249900
H	-5.61975700	-3.78004400	-0.59597100
C	-4.40301800	-1.98385500	-0.50795800
C	-4.02911400	-0.89746200	0.30468100
H	-3.36414200	-0.13393600	-0.10547600
C	-3.83622900	-2.09823100	-1.91017300
H	-4.52559100	-2.67666100	-2.55076700
H	-3.75253000	-1.09263100	-2.35275700
C	-2.43239200	-2.79369200	-2.02299500
C	-2.52793400	-4.27715800	-1.61677100
H	-2.87297700	-4.39331400	-0.57931800
H	-3.24067400	-4.79267400	-2.28292100
H	-1.55175200	-4.77788700	-1.70452100
C	-1.95355600	-2.68279100	-3.49224800
H	-0.97846300	-3.17891700	-3.62784300
H	-2.67936700	-3.17837800	-4.15884600
H	-1.85359000	-1.63191900	-3.80186700
C	-1.41384800	-2.05245200	-1.12792700
Rh	0.54824400	-1.80289500	0.95581100
O	1.97762400	-2.24518000	-0.45353900
O	1.92770900	-0.81300700	2.12468600
O	1.63283900	-0.26473200	-1.53143800
O	1.56165800	1.14502400	1.01302100
C	2.22210700	-1.40014400	-1.38710700
C	3.29742100	-1.80364100	-2.42074000
C	2.81513800	-3.10416900	-3.11354100

H	2.63586500	-3.90439000	-2.37995200
H	3.57962900	-3.44832000	-3.83034800
H	1.88193600	-2.93001800	-3.67407400
C	3.51054100	-0.70269100	-3.47436800
H	2.57679200	-0.48138800	-4.01270900
H	4.25985500	-1.04273800	-4.20958000
H	3.86556400	0.23332600	-3.02184800
C	4.63991900	-2.12469400	-1.66727800
H	4.47044100	-3.01652200	-1.04165200
H	5.37524500	-2.40604700	-2.44198800
C	5.18975000	-1.00396600	-0.80614900
C	6.12543400	-0.07034200	-1.29335100
H	6.51038700	-0.16776900	-2.31330300
C	6.57663800	0.97502700	-0.47409100
H	7.31544800	1.68553600	-0.85677000
C	6.08523000	1.11651100	0.83201200
H	6.43958300	1.93997700	1.46037200
C	5.14901300	0.19705300	1.34469000
C	4.74213500	-0.86872500	0.52104300
H	4.04508600	-1.60929100	0.92015000
C	4.55385800	0.33819800	2.73243400
H	5.26106600	0.86382900	3.39851700
H	4.38305700	-0.66155700	3.16436000
C	3.19835700	1.13061800	2.80333400
C	3.40135700	2.59715900	2.37944800
H	3.75171500	2.67520900	1.34038600
H	4.15122600	3.06876100	3.03700500
H	2.46580100	3.17020800	2.46696400
C	2.68046200	1.07308000	4.26350100
H	1.73355600	1.62793600	4.36900100
H	3.41956300	1.53594300	4.93890200
H	2.51205600	0.03458800	4.58640400
C	2.15251300	0.43008900	1.90779100
N	-0.28326100	1.99257800	-1.30287100
C	-0.67205600	3.55267200	0.53868800
C	-1.02762100	3.06956000	-0.74347000
C	-2.11555200	3.66878800	-1.46915600
C	-2.79621200	4.71553000	-0.81167800
C	-2.42603400	5.19515100	0.45253000
C	-1.34658800	4.61808000	1.13424100
H	0.16954400	3.07165900	1.03926400
H	-3.63802100	5.19838700	-1.30877400
H	-2.98207700	6.02654000	0.89591900
H	-1.03724700	4.99201400	2.11433100
C	-2.56848200	3.21765900	-2.87848100
C	-3.06537800	1.75109800	-2.82193900
C	-3.73518700	4.08053100	-3.41912800
C	-1.40704400	3.33045300	-3.90082500
H	-2.27174000	1.07018000	-2.48363800
H	-3.92371400	1.65463200	-2.13567400
H	-3.39632100	1.43015700	-3.82561200
H	-3.45760600	5.14290800	-3.52444400
H	-4.01487900	3.71294400	-4.42007400
H	-4.63516900	4.01411700	-2.78545400
H	-1.78757800	3.11624000	-4.91452500
H	-0.97758500	4.34620500	-3.90961500
H	-0.60720500	2.61032400	-3.68625400
N	1.98434200	2.33875600	-2.54808700
N	1.13670600	2.60004000	-1.83003700

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^sBd (E = -2510.13862670)

Rh	0.03260200	0.33455100	-0.08418600
O	-1.40520200	0.45149100	1.40256300
O	-1.43478800	-0.06423300	-1.52779900
O	-1.39857000	-1.80900800	1.73029400
O	-1.38914900	-2.31037700	-1.11616600
C	-1.82066800	-0.62832500	1.97799100

C	-2.90467100	-0.45399300	3.06539000
C	-2.31005900	0.41896400	4.19978500
H	-2.00010700	1.40572100	3.82389300
H	-3.06619500	0.56932800	4.98868800
H	-1.43644200	-0.07104200	4.66079500
C	-3.32624200	-1.82357500	3.63077400
H	-2.46777500	-2.35370100	4.07020600
H	-4.08241700	-1.67697700	4.42080100
H	-3.75712200	-2.46863700	2.85184600
C	-4.13995600	0.30710900	2.46139900
H	-3.80859000	1.32119700	2.18299900
H	-4.87210800	0.41897700	3.28090400
C	-4.79545000	-0.35689200	1.26564000
C	-5.90436400	-1.21538800	1.40011800
H	-6.34147900	-1.38830000	2.38883100
C	-6.46014100	-1.83803900	0.27278600
H	-7.33126600	-2.49034500	0.38603100
C	-5.90490300	-1.63070500	-0.99854200
H	-6.34231400	-2.12581600	-1.87141100
C	-4.79603600	-0.77726400	-1.16176800
C	-4.27976100	-0.13037900	-0.02363000
H	-3.44401000	0.56240300	-0.14507800
C	-4.13927400	-0.55682100	-2.51121500
H	-4.87023400	-0.72875100	-3.32125900
H	-3.80718300	0.49127100	-2.59140800
C	-2.90423200	-1.47767600	-2.81750200
C	-3.32692100	-2.95711600	-2.89222100
H	-3.76942200	-3.30170300	-1.94640800
H	-4.07407200	-3.08451000	-3.69416300
H	-2.46641400	-3.60491700	-3.11724400
C	-2.29598700	-1.03562900	-4.17308300
H	-1.43582700	-1.66949000	-4.44475200
H	-3.05189400	-1.13319800	-4.97056000
H	-1.95784700	0.01090200	-4.13591300
C	-1.82676700	-1.27314200	-1.72854900
Rh	0.05178200	-2.07741000	0.30542200
O	1.47388400	-2.26204600	-1.15960200
O	1.50418800	-1.76692000	1.73481800
O	1.50327300	-0.00588900	-1.52040300
O	1.49305700	0.48540100	1.36382500
C	1.89839600	-1.20462600	-1.75339000
C	2.96401000	-1.40454700	-2.85520800
C	2.32889700	-2.27517700	-3.96943000
H	1.97800300	-3.23904700	-3.57075500
H	3.07419200	-2.47109700	-4.75877600
H	1.47330600	-1.75838800	-4.43450600
C	3.41478900	-0.05393300	-3.44196300
H	2.56430600	0.49464700	-3.87367400
H	4.15374500	-0.22995200	-4.24233000
H	3.87550900	0.58809100	-2.67751400
C	4.18636000	-2.19173600	-2.25765800
H	3.83475300	-3.19859300	-1.97818200
H	4.91247500	-2.31820900	-3.08037600
C	4.85943800	-1.54308800	-1.06354500
C	5.97875500	-0.69828500	-1.19865700
H	6.41298900	-0.52579000	-2.18862200
C	6.54849900	-0.08893400	-0.07088800
H	7.42803000	0.55180800	-0.18521800
C	5.99675700	-0.29467200	1.20224700
H	6.44516800	0.19007100	2.07538600
C	4.87723500	-1.13407400	1.36587100
C	4.34822800	-1.76957300	0.22762400
H	3.50445500	-2.45230300	0.34899100
C	4.21963700	-1.35033200	2.71540600
H	4.95671500	-1.20681100	3.52553300
H	3.85838500	-2.38943900	2.78623900
C	3.01167900	-0.39818500	3.03625000
C	3.47947100	1.06665000	3.12305500

H	3.91523300	1.41160200	2.17437600
H	4.24436000	1.16040200	3.91270600
H	2.64530800	1.73857100	3.37446100
C	2.39988000	-0.83602600	4.39214900
H	1.55793200	-0.18307100	4.67635700
H	3.16321900	-0.76553900	5.18529500
H	2.03500600	-1.87340400	4.34797000
C	1.92104600	-0.57631100	1.95559000
N	-0.02210800	2.20045600	-0.60670400
C	-0.00257100	3.22324700	1.62499400
C	-0.08048500	3.29181600	0.18579900
C	-0.21512400	4.60965900	-0.44962900
C	-0.26533600	5.72438700	0.39982600
C	-0.18271300	5.61809800	1.79940700
C	-0.04713200	4.36238500	2.41677000
H	0.10685500	2.23785400	2.07344300
H	-0.36830100	6.72275500	-0.02749800
H	-0.22294800	6.52690700	2.40756600
H	0.02143000	4.28580900	3.50581800
C	-0.29716400	4.77842000	-1.97821800
C	-0.44844200	6.26120000	-2.39296100
C	1.00205800	4.23561600	-2.63795400
C	-1.52855000	4.00836300	-2.53341300
H	-1.37071100	6.71700800	-1.99402700
H	0.41170100	6.87530700	-2.07631600
H	-0.50394100	6.31929100	-3.49220500
H	1.12424300	3.16385500	-2.43083900
H	0.95107900	4.38663000	-3.73029700
H	1.88894800	4.77416000	-2.26256600
H	-1.59790300	4.16208700	-3.62442300
H	-1.43647400	2.93262200	-2.32934300
H	-2.46350700	4.37902100	-2.07906100

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¹Bd (E = -2510.14171494)

Rh	0.03142800	0.30793900	-0.09785300
O	-1.42104500	0.46804000	1.38303100
O	-1.42226700	-0.03935000	-1.54432500
O	-1.45468700	-1.78689400	1.74733300
O	-1.44360400	-2.27849800	-1.10239900
C	-1.85647400	-0.59253400	1.97350600
C	-2.93899800	-0.38267400	3.05580600
C	-2.33060600	0.49934100	4.17593400
H	-2.00291400	1.47371000	3.78355400
H	-3.08540400	0.67591600	4.96061600
H	-1.46640200	0.00214500	4.64678900
C	-3.38454400	-1.73523100	3.64392200
H	-2.53603700	-2.27206700	4.09449600
H	-4.13875100	-1.56138200	4.43020800
H	-3.82564000	-2.38676200	2.87609500
C	-4.15960700	0.38906200	2.43614200
H	-3.81271100	1.39546700	2.14940100
H	-4.89543600	0.51923100	3.24957100
C	-4.81465900	-0.27856600	1.24246100
C	-5.92560400	-1.13437700	1.37752000
H	-6.36591200	-1.30166000	2.36571200
C	-6.47951700	-1.76120100	0.25157900
H	-7.35226400	-2.41119000	0.36541100
C	-5.92043300	-1.56074200	-1.01916100
H	-6.35646400	-2.05873800	-1.89105500
C	-4.80962700	-0.70995800	-1.18264100
C	-4.29506100	-0.05873400	-0.04640100
H	-3.45836800	0.63309600	-0.16812300
C	-4.14714100	-0.49714800	-2.53021900
H	-4.87603000	-0.66370800	-3.34318400
H	-3.80554200	0.54794000	-2.61082500
C	-2.91957800	-1.43039300	-2.83081000
C	-3.35728200	-2.90540700	-2.91060900

H	-3.80939200	-3.24727400	-1.96843700
H	-4.10045900	-3.02303400	-3.71754000
H	-2.50237500	-3.56194100	-3.13217800
C	-2.29886100	-0.99302200	-4.18229200
H	-1.44299900	-1.63441400	-4.44992400
H	-3.05129300	-1.08369600	-4.98369100
H	-1.95219700	0.05057200	-4.14354200
C	-1.84854300	-1.24051700	-1.73462500
Rh	-0.00623700	-2.07221800	0.33161200
O	1.42194800	-2.30520100	-1.12448300
O	1.43831600	-1.80626800	1.77286100
O	1.49530200	-0.05728300	-1.51424000
O	1.49026200	0.44118000	1.36444700
C	1.87273100	-1.26648100	-1.73067700
C	2.94044200	-1.49909300	-2.82229100
C	2.29785200	-2.37729500	-3.92659000
H	1.93215200	-3.33048300	-3.51575000
H	3.04438100	-2.59472700	-4.70892900
H	1.45180200	-1.85596600	-4.40393500
C	3.41407000	-0.16435100	-3.42749100
H	2.57527100	0.38842200	-3.87649000
H	4.15663500	-0.36452100	-4.21858600
H	3.87779900	0.48404600	-2.67038800
C	4.14794800	-2.29477300	-2.20640000
H	3.78147000	-3.29353200	-1.91711900
H	4.87732000	-2.44089700	-3.02293800
C	4.82075100	-1.63996300	-1.01572700
C	5.94440600	-0.80148200	-1.15412000
H	6.38301300	-0.63929500	-2.14387000
C	6.51261500	-0.18519200	-0.02940100
H	7.39500200	0.45114900	-0.14585600
C	5.95540200	-0.37808200	1.24335000
H	6.40228600	0.11244700	2.11393300
C	4.83181400	-1.21130700	1.41000100
C	4.30384000	-1.85363600	0.27518600
H	3.45655300	-2.53171500	0.39960600
C	4.16762700	-1.41350800	2.75811300
H	4.90216900	-1.26974000	3.57043400
H	3.79864900	-2.44961000	2.83444400
C	2.96561900	-0.44979400	3.06672700
C	3.44460900	1.01168400	3.15214900
H	3.89399600	1.34921300	2.20723200
H	4.20057100	1.10266300	3.95066300
H	2.61269600	1.69140500	3.38932600
C	2.33967100	-0.87766300	4.41912000
H	1.50256600	-0.21521300	4.69507400
H	3.09820500	-0.81156700	5.21721400
H	1.96510000	-1.91159900	4.37615100
C	1.88260900	-0.61943700	1.97678300
N	0.03265900	2.24333500	-0.37261600
C	0.00029000	3.47973200	1.68344100
C	-0.01101800	3.42629000	0.24091900
C	-0.06746300	4.67714200	-0.51688700
C	-0.11307100	5.86359700	0.22313400
C	-0.10392500	5.89417000	1.63118900
C	-0.04535800	4.69246200	2.35834100
H	0.04860800	2.53018700	2.21605000
H	-0.15763600	6.81638100	-0.30766400
H	-0.14126400	6.85526900	2.15111400
H	-0.03476500	4.70712000	3.45241700
C	-0.07353300	4.67173500	-2.05667800
C	-0.13423600	6.10116200	-2.64288100
C	1.22292400	3.99901100	-2.58350100
C	-1.31388000	3.89543100	-2.57622200
H	-1.05140700	6.63536800	-2.34249800
H	0.73690000	6.70954800	-2.34687700
H	-0.13425700	6.03885200	-3.74353600
H	1.30817300	2.96000300	-2.23135700

H	1.21935100	3.99126400	-3.68746900
H	2.11642100	4.55249900	-2.24864100
H	-1.32336100	3.90022900	-3.68025500
H	-1.30316400	2.84869800	-2.23700600
H	-2.24786600	4.36574500	-2.22467400

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^sTS1a (E = -2510.11283559)

N	0.09456200	1.97611900	-1.32684300
C	2.47107300	2.44572300	-1.33537300
C	1.12583600	2.90332400	-1.33985300
C	0.87139500	4.31143600	-1.45558400
C	1.95015200	5.18379300	-1.61793400
C	3.27803400	4.71757600	-1.64656500
C	3.52712500	3.34570700	-1.50522700
H	2.65323300	1.37586400	-1.24146600
H	1.76373200	6.25854700	-1.70131700
H	4.10326500	5.42656900	-1.75352900
H	4.55334900	2.96743800	-1.51301100
C	-0.59705400	4.77783300	-1.46351700
C	-0.78332800	6.14509800	-0.74605800
C	-1.08633400	4.89354800	-2.93408600
C	-1.41579000	3.74103000	-0.72379300
H	-0.37420700	6.11713300	0.27604200
H	-0.28194600	6.95683000	-1.30025800
H	-1.85452600	6.40105900	-0.68759200
H	-0.99776200	3.92891500	-3.45963800
H	-2.14167400	5.21446200	-2.97261600
H	-0.48261400	5.63223500	-3.48512500
H	-0.88786900	2.51658400	-1.39431400
H	-1.21991700	3.61323100	0.34538800
H	-2.47048500	3.61601600	-1.00729800
Rh	-0.01705600	0.24983700	-0.26294200
O	-1.45376800	0.97840300	1.02777200
O	-1.49657000	-0.36711900	-1.59473500
O	-1.68361200	-1.04607800	2.05141200
O	-1.71200400	-2.37892400	-0.52778500
C	-1.98216800	0.18790200	1.90203200
C	-3.03812400	0.79880000	2.84875300
C	-2.35999600	1.93491100	3.65547000
H	-1.94940000	2.70983800	2.99069400
H	-3.09624400	2.40534100	4.32880300
H	-1.53798200	1.54191600	4.27585000
C	-3.57863700	-0.27192400	3.81611200
H	-2.76856800	-0.70180800	4.42427200
H	-4.31465300	0.18861400	4.49697400
H	-4.06813400	-1.09589700	3.27745400
C	-4.20581600	1.42540300	2.00461300
H	-3.79413600	2.27681400	1.43756800
H	-4.93015700	1.84134900	2.72758800
C	-4.90649100	0.47616100	1.05134500
C	-6.07232400	-0.22715600	1.41285300
H	-6.52203200	-0.06498700	2.39760400
C	-6.66617700	-1.12456100	0.51302700
H	-7.57932800	-1.65548000	0.79839600
C	-6.09707500	-1.34616600	-0.74990100
H	-6.56618600	-2.05216000	-1.44248700
C	-4.93192400	-0.65590500	-1.13753700
C	-4.37396900	0.26636300	-0.23365200
H	-3.48529000	0.82457200	-0.53610100
C	-4.25704400	-0.89179100	-2.47519800
H	-4.99770700	-1.23722800	-3.21831600
H	-3.84228300	0.05906200	-2.84892900
C	-3.09737100	-1.95172500	-2.46891200
C	-3.64281700	-3.35618700	-2.14777300
H	-4.12143200	-3.39125700	-1.15851600
H	-4.38948800	-3.64223300	-2.90842500
H	-2.83703800	-4.10552800	-2.15730100

C	-2.43967900	-1.95362000	-3.87224400
H	-1.63390500	-2.70400800	-3.92789800
H	-3.19176700	-2.21000400	-4.63755600
H	-2.01275200	-0.96854100	-4.11373500
C	-2.01965800	-1.53500000	-1.44076500
Rh	-0.26753500	-1.89368300	0.84492100
O	1.14217700	-2.69430200	-0.40919900
O	1.18289300	-1.30295800	2.18607400
O	1.41480900	-0.67926600	-1.44791300
C	1.42814100	0.71775000	1.14099600
C	1.68069200	-1.92552800	-1.28493800
C	2.72613400	-2.56365900	-2.22736800
C	2.03282400	-3.72162800	-2.98909700
H	1.60993500	-4.46065000	-2.29227100
H	2.76384700	-4.22915600	-3.64087400
H	1.21857300	-3.34138300	-3.62775900
C	3.27001700	-1.53368800	-3.23490000
H	2.45783800	-1.10215400	-3.83916300
H	3.98194400	-2.02945600	-3.91672300
H	3.79141600	-0.70581500	-2.73336600
C	3.89073400	-3.17363100	-1.36510400
H	3.47395100	-4.01186300	-0.78277000
H	4.61908000	-3.60325500	-2.07602700
C	4.58474200	-2.20609000	-0.42584100
C	5.74140000	-1.49313800	-0.79879500
H	6.19042400	-1.66197100	-1.78278900
C	6.32947000	-0.58094400	0.09027700
H	7.23817700	-0.04594500	-0.20220300
C	5.76262000	-0.35321600	1.35318600
H	6.22799500	0.36286600	2.03793800
C	4.60665300	-1.05305100	1.75207900
C	4.05535400	-1.99144700	0.86023500
H	3.17890200	-2.56359300	1.17315400
C	3.93661100	-0.81422800	3.09164300
H	4.68141300	-0.47954900	3.83565100
H	3.51232400	-1.76257600	3.46043300
C	2.78748300	0.25840100	3.09314600
C	3.34789900	1.66280000	2.80140300
H	3.83268200	1.71336100	1.81635300
H	4.09145000	1.92820100	3.57256000
H	2.54938000	2.41980500	2.81850500
C	2.11885400	0.24291500	4.49125600
H	1.31999100	1.00026900	4.55423000
H	2.86783200	0.47886800	5.26609300
H	1.68190100	-0.74241100	4.71278800
C	1.71584100	-0.14221100	2.05273800

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^sCa (E = -2510.21224223)

N	0.18327500	2.14575400	-1.45217300
C	2.68870800	2.53040200	-1.25260900
C	1.37030900	2.98035700	-1.35981900
C	1.04385800	4.34532300	-1.41223700
C	2.06432400	5.30102000	-1.33791700
C	3.39748200	4.87031400	-1.22146100
C	3.70434900	3.49913800	-1.18793500
H	2.90755800	1.46311400	-1.20308700
H	1.83261900	6.36981100	-1.37762000
H	4.20173500	5.60870000	-1.15757900
H	4.74531600	3.17729600	-1.09655200
C	-0.45535500	4.52620100	-1.64379000
C	-1.09836700	5.59476200	-0.73992700
C	-0.71883600	4.85840300	-3.13424100
C	-0.96711000	3.09727400	-1.28304500
H	-0.88217700	5.40015100	0.32296300
H	-0.72279800	6.60221800	-0.98482400
H	-2.19392700	5.61074500	-0.87217000
H	-0.30840300	4.07974000	-3.79924200

H	-1.80182400	4.94238800	-3.32996500
H	-0.24632800	5.81446600	-3.41309400
H	0.14561200	1.69541500	-2.37602700
H	-1.26341600	3.04932900	-0.22509700
H	-1.81584900	2.76010600	-1.89481600
Rh	-0.02339400	0.25038700	-0.25072200
O	-1.43800300	1.02961900	1.06089600
O	-1.50678500	-0.30131300	-1.59496600
O	-1.72208500	-1.00160100	2.07099300
O	-1.78987800	-2.30447600	-0.53056600
C	-1.97972200	0.24424700	1.92896300
C	-3.01772700	0.87285000	2.88683500
C	-2.31133800	1.99157100	3.69302300
H	-1.88066700	2.75398000	3.02642900
H	-3.03404300	2.48154800	4.36739200
H	-1.49902200	1.57711000	4.31233900
C	-3.57903400	-0.18740200	3.85363400
H	-2.77527500	-0.64270300	4.45159800
H	-4.29635300	0.28841200	4.54426200
H	-4.09499400	-0.99524200	3.31512300
C	-4.17560800	1.52881200	2.05164800
H	-3.74800600	2.37449000	1.48765600
H	-4.88913100	1.95574800	2.77918100
C	-4.90053800	0.60187200	1.09444400
C	-6.08231300	-0.07552100	1.45360000
H	-6.52446500	0.08977400	2.44124500
C	-6.70172300	-0.95011500	0.54848600
H	-7.62678300	-1.46063000	0.83282600
C	-6.14367200	-1.17400900	-0.71895700
H	-6.63334000	-1.86083500	-1.41664800
C	-4.96263300	-0.51000000	-1.10422000
C	-4.37738300	0.38846600	-0.19389200
H	-3.47439000	0.92543300	-0.49173800
C	-4.30225000	-0.74787600	-2.44895500
H	-5.05641900	-1.06692900	-3.19050100
H	-3.86947200	0.19804100	-2.81565300
C	-3.16648200	-1.83372900	-2.46566500
C	-3.74179900	-3.22810900	-2.15258700
H	-4.20926400	-3.26075800	-1.15808400
H	-4.50351200	-3.48952700	-2.90722000
H	-2.95384100	-3.99590000	-2.17783800
C	-2.52796300	-1.83908400	-3.87748400
H	-1.73296700	-2.59963700	-3.94767600
H	-3.29314500	-2.08078700	-4.63458200
H	-2.09159800	-0.85872900	-4.12265900
C	-2.07021400	-1.45354600	-1.44346600
Rh	-0.33041600	-1.87760100	0.85173000
O	1.06947800	-2.66969100	-0.44177500
O	1.13666200	-1.34286000	2.19073900
O	1.36905600	-0.65596000	-1.48089400
O	1.44101500	0.67021200	1.14655500
C	1.61285900	-1.90967400	-1.32044100
C	2.63926900	-2.56856700	-2.27074900
C	1.91510100	-3.70013900	-3.04308500
H	1.47066500	-4.43133700	-2.35148000
H	2.63114200	-4.22415100	-3.69860900
H	1.11153100	-3.29243400	-3.67860700
C	3.21337500	-1.54666900	-3.26956900
H	2.41483500	-1.09213800	-3.87580700
H	3.91513100	-2.05481600	-3.95295400
H	3.75438900	-0.73612200	-2.76020800
C	3.78767400	-3.21955200	-1.41736400
H	3.34715000	-4.05126800	-0.84346900
H	4.50355000	-3.66233600	-2.13314000
C	4.50992500	-2.28344400	-0.46728100
C	5.68602500	-1.59910300	-0.83334000
H	6.12795100	-1.76747000	-1.82072200
C	6.30363900	-0.71844600	0.06757300

H	7.22752300	-0.20689000	-0.21957500
C	5.74790300	-0.49418000	1.33619300
H	6.23701100	0.19577000	2.03126900
C	4.57286800	-1.16554700	1.72830500
C	3.99049000	-2.07222800	0.82345400
H	3.09747500	-2.62149400	1.13013900
C	3.91531300	-0.93092500	3.07478800
H	4.67167200	-0.62403700	3.81926000
H	3.47247800	-1.87535200	3.43179000
C	2.78827800	0.16497700	3.09854400
C	3.37645900	1.56123800	2.82447500
H	3.86141400	1.61402900	1.83960600
H	4.12583000	1.80302800	3.59788200
H	2.59255000	2.33314500	2.85108100
C	2.12904700	0.14247900	4.50079500
H	1.34635100	0.91500300	4.58000400
H	2.88715200	0.35038400	5.27495300
H	1.67201800	-0.83649600	4.70927700
C	1.70340600	-0.19658800	2.05744200

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^tTS1a (E = -2510.11727780)

N	-0.14076900	2.28279800	-0.43106400
C	-2.50760200	2.79713200	-0.46478100
C	-1.13515900	3.20481200	-0.50242600
C	-0.82202000	4.61759300	-0.63069400
C	-1.88403900	5.51869600	-0.74920700
C	-3.22698400	5.09840600	-0.72921400
C	-3.53035900	3.73319800	-0.57814100
H	-2.72044500	1.73365400	-0.36385100
H	-1.67211400	6.58567400	-0.85428000
H	-4.02787400	5.83626000	-0.82741600
H	-4.57176600	3.39943800	-0.55882300
C	0.64493400	5.07435900	-0.52160400
C	0.89389400	6.43629100	-1.22482200
C	0.99380200	5.21271300	0.98747500
C	1.55260400	4.02986800	-1.15594900
H	0.57618100	6.40837400	-2.27955900
H	0.36043600	7.26054900	-0.72130300
H	1.96909800	6.67648100	-1.19524300
H	0.86982400	4.25122300	1.51066500
H	2.04077400	5.54067200	1.11029200
H	0.33942100	5.95440900	1.47314200
H	0.86668400	2.85472000	-0.71459300
H	1.48686500	3.92751600	-2.24794500
H	2.57467200	3.95924400	-0.76206000
Rh	0.00811200	0.30027400	-0.09703700
O	1.46895000	0.12176600	-1.56407400
O	1.46727100	0.60376700	1.35605600
O	1.69484200	-2.11552100	-1.16256100
O	1.70022000	-1.64110200	1.69980300
C	1.99474900	-1.03516000	-1.78117100
C	3.06085500	-1.11540200	-2.89744800
C	2.39667500	-0.67585900	-4.22695200
H	1.97295000	0.33649800	-4.14624700
H	3.14538100	-0.68094500	-5.03714200
H	1.58795600	-1.36884500	-4.51195300
C	3.59654000	-2.55348400	-3.03331200
H	2.78595900	-3.25745600	-3.27524700
H	4.34083400	-2.59138600	-3.84715800
H	4.07528200	-2.89867700	-2.10572300
C	4.22828500	-0.11330900	-2.58027900
H	3.81948400	0.90908200	-2.63618000
H	4.96208000	-0.21427200	-3.39978900
C	4.91019900	-0.31006700	-1.24030600
C	6.06586100	-1.10195700	-1.09357200
H	6.52172000	-1.56624900	-1.97383200
C	6.64286600	-1.28698000	0.17155600

H	7.54906400	-1.89177700	0.27255300
C	6.06539400	-0.70169800	1.30810600
H	6.52111100	-0.85549800	2.29144500
C	4.90916700	0.09431200	1.18997000
C	4.36913900	0.29796000	-0.09293200
H	3.49039700	0.93800900	-0.20023000
C	4.22728900	0.71565700	2.39343900
H	4.96198100	0.88668600	3.20052400
H	3.81902700	1.70105500	2.11425400
C	3.05865500	-0.12734500	3.02010800
C	3.59297600	-1.44090100	3.62237700
H	4.07593500	-2.07074600	2.86171700
H	4.33305900	-1.20881900	4.40720700
H	2.78098800	-2.02756000	4.07810100
C	2.39175000	0.72452900	4.12947500
H	1.57591000	0.16720500	4.61861400
H	3.13655500	0.97905800	4.90226500
H	1.97641500	1.65763600	3.72021000
C	1.99535300	-0.41783000	1.93684500
Rh	0.27014100	-2.07083900	0.30346300
O	-1.16060600	-1.94181100	1.77840200
O	-1.16211700	-2.43454000	-1.12994500
O	-1.42615200	0.29536600	1.39319800
O	-1.43047900	-0.19668700	-1.49774600
C	-1.69923500	-0.79931100	2.00926600
C	-2.75673300	-0.73757400	3.13581100
C	-2.07694600	-1.19506300	4.45133200
H	-1.64183800	-2.20020900	4.34618600
H	-2.81975200	-1.21578300	5.26670000
H	-1.27500900	-0.49753300	4.74436100
C	-3.30642500	0.69093200	3.30507200
H	-2.50064900	1.40074800	3.54585900
H	-4.03805500	0.70605800	4.13109700
H	-3.80476100	1.04780800	2.39268000
C	-3.91580100	-1.74778300	2.81021200
H	-3.49743200	-2.76663400	2.85883500
H	-4.65093400	-1.65870400	3.62986600
C	-4.59791100	-1.55017000	1.47057700
C	-5.75324600	-0.75747800	1.32300500
H	-6.20939600	-0.29283400	2.20294000
C	-6.33184600	-0.57569600	0.05789200
H	-7.24014300	0.02619300	-0.04305700
C	-5.75584400	-1.16402200	-1.07804400
H	-6.21415800	-1.01455900	-2.06085700
C	-4.60037800	-1.96147000	-0.95896300
C	-4.05933400	-2.16297600	0.32418600
H	-3.18419500	-2.80808400	0.43277600
C	-3.92155100	-2.58974800	-2.16037600
H	-4.65948300	-2.77528900	-2.96126100
H	-3.50329500	-3.56823000	-1.87209700
C	-2.76271200	-1.74466600	-2.80366600
C	-3.31119100	-0.45102400	-3.43398700
H	-3.81079800	0.18580200	-2.69029200
H	-4.04145500	-0.70829200	-4.22017600
H	-2.50452400	0.14002700	-3.89332300
C	-2.08506600	-2.61166900	-3.89487100
H	-1.27890200	-2.05342100	-4.39882900
H	-2.82786900	-2.89502700	-4.65951700
H	-1.65554400	-3.52867200	-3.46442600
C	-1.70344900	-1.43259600	-1.72176500

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^TIM1a (E = -2510.12118357)

N	-0.04770300	2.29839400	-0.41901200
C	-2.38601000	2.85568000	-0.48808200
C	-1.01228000	3.25568500	-0.50406700
C	-0.69122800	4.66900600	-0.61555600
C	-1.75674000	5.56771200	-0.74794900

C	-3.10099700	5.15226800	-0.75411700
C	-3.40963400	3.78817200	-0.61321400
H	-2.60081800	1.79165600	-0.39388800
H	-1.54842800	6.63525300	-0.84411900
H	-3.89670100	5.89436000	-0.86235000
H	-4.45102400	3.45418800	-0.60963500
C	0.76780100	5.15664700	-0.49171900
C	0.93206300	6.64639200	-0.92308300
C	1.20714700	5.04399400	0.99838100
C	1.69312400	4.35068500	-1.37102100
H	0.57810500	6.81263200	-1.95296300
H	0.38457700	7.32548600	-0.24679400
H	1.99699900	6.92492400	-0.87812900
H	1.12319800	4.00972600	1.36550400
H	2.25523600	5.37024800	1.11487900
H	0.57418100	5.68425300	1.63356500
H	0.90192300	2.68911600	-0.58369300
H	1.40765000	4.12742500	-2.40306800
H	2.75654500	4.29068600	-1.11938400
Rh	-0.00270300	0.28310000	-0.09258200
O	1.45763800	0.09278200	-1.56054400
O	1.46540600	0.56558200	1.35511500
O	1.65321000	-2.14941600	-1.16844500
O	1.66720000	-1.68302500	1.69487900
C	1.96700800	-1.07042200	-1.78276700
C	3.03004600	-1.16159600	-2.90134900
C	2.36840600	-0.71019300	-4.22819800
H	1.95807300	0.30739900	-4.14375400
H	3.11479200	-0.72307500	-5.04046300
H	1.54982300	-1.39170500	-4.51270700
C	3.54718400	-2.60596500	-3.04229500
H	2.72682800	-3.29907300	-3.28249100
H	4.28788800	-2.65164600	-3.85901100
H	4.02499000	-2.95926100	-2.11724600
C	4.21084800	-0.17529400	-2.58467100
H	3.81481700	0.85236900	-2.63714300
H	4.94151900	-0.28314400	-3.40609300
C	4.89329900	-0.38405200	-1.24679600
C	6.03950400	-1.19037700	-1.10444400
H	6.48814500	-1.65757700	-1.98686300
C	6.61624200	-1.38626400	0.15919000
H	7.51507200	-2.00250000	0.25682900
C	6.04773600	-0.79775100	1.29861600
H	6.50291700	-0.96066300	2.28073000
C	4.90110500	0.01271000	1.18496900
C	4.36190400	0.22681000	-0.09649700
H	3.49058500	0.87741600	-0.20047700
C	4.22822500	0.63811000	2.39141600
H	4.96563300	0.79646400	3.19856100
H	3.83295000	1.63003700	2.11657600
C	3.04930100	-0.19229200	3.01558400
C	3.56789100	-1.51524600	3.61128200
H	4.04222400	-2.14756900	2.84722300
H	4.31156500	-1.29633400	4.39650800
H	2.74912700	-2.09393400	4.06504100
C	2.39490600	0.66252300	4.13019400
H	1.57214800	0.11345500	4.61706300
H	3.14363900	0.90298800	4.90373400
H	1.99142800	1.60335900	3.72677600
C	1.98032000	-0.46458100	1.93319500
Rh	0.22978500	-2.08974400	0.29865600
O	-1.19924200	-1.93917100	1.77368700
O	-1.20773100	-2.42313500	-1.13538500
O	-1.43659500	0.30188300	1.39338100
O	-1.44850400	-0.18097800	-1.49380500
C	-1.72380800	-0.79029900	2.00729200
C	-2.78012500	-0.71725200	3.13399700
C	-2.10666600	-1.18682500	4.44852500

H	-1.68605900	-2.19794500	4.34147200
H	-2.84947100	-1.19834800	5.26409000
H	-1.29462400	-0.50151100	4.74263700
C	-3.31007700	0.71844800	3.30616300
H	-2.49421800	1.41682900	3.54640600
H	-4.04007600	0.74242500	4.13342600
H	-3.80490600	1.08320700	2.39494400
C	-3.95298300	-1.71050100	2.80615500
H	-3.54869600	-2.73518200	2.85168700
H	-4.68677100	-1.61387300	3.62617700
C	-4.63206800	-1.49909500	1.46712100
C	-5.77444600	-0.68746900	1.32147700
H	-6.22346400	-0.21813200	2.20258800
C	-6.34923600	-0.49236800	0.05665300
H	-7.24736700	0.12481300	-0.04295400
C	-5.78230000	-1.08658300	-1.08076100
H	-6.23758500	-0.92660000	-2.06333800
C	-4.63992500	-1.90295900	-0.96355500
C	-4.10266100	-2.11679400	0.31913700
H	-3.23752500	-2.77553800	0.42617300
C	-3.97017100	-2.53777500	-2.16657100
H	-4.71036700	-2.71055000	-2.96820800
H	-3.56591400	-3.52291700	-1.88099200
C	-2.79935100	-1.70703300	-2.80670600
C	-3.33002300	-0.40408000	-3.43332800
H	-3.82418600	0.23554900	-2.68837900
H	-4.06097000	-0.64903100	-4.22281200
H	-2.51490200	0.17914300	-3.88775200
C	-2.13303500	-2.57965300	-3.90039600
H	-1.31834300	-2.03120000	-4.40142000
H	-2.87894900	-2.84941200	-4.66695900
H	-1.71719300	-3.50438400	-3.47304700
C	-1.73694400	-1.41216700	-1.72350000

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^tTS2a (E = -2510.09670425)

Rh	0.01686200	0.31201700	-0.10740900
O	-1.46849500	0.55848500	1.40632600
O	-1.45087000	0.14837700	-1.56499200
O	-1.67179100	-1.69048200	1.69876400
O	-1.68341500	-2.09247500	-1.17468000
C	-1.98457500	-0.47277200	1.96529800
C	-3.05463300	-0.23269700	3.05394500
C	-2.40242100	0.59642600	4.18867900
H	-1.99750300	1.54540200	3.80629900
H	-3.15262500	0.82027300	4.96574300
H	-1.58109600	0.03587600	4.66471600
C	-3.57406000	-1.56933100	3.61738900
H	-2.75602100	-2.15775600	4.06004400
H	-4.32000900	-1.37024600	4.40582400
H	-4.04616000	-2.18435200	2.83785200
C	-4.23119700	0.61265700	2.44558400
H	-3.83274300	1.60873700	2.19159500
H	-4.96944800	0.75606600	3.25470100
C	-4.90566000	0.01472900	1.22590900
C	-6.05795300	-0.78969000	1.32401000
H	-6.51306300	-0.96931000	2.30322500
C	-6.63263300	-1.35024500	0.17372800
H	-7.53562600	-1.96203100	0.26005400
C	-6.05739500	-1.13073500	-1.08657400
H	-6.51173000	-1.57461000	-1.97807400
C	-4.90569000	-0.32975100	-1.21383300
C	-4.36609900	0.25128500	-0.05185900
H	-3.48932300	0.89689500	-0.14222700
C	-4.22910500	-0.09514000	-2.55067500
H	-4.96477900	-0.18315200	-3.36993800
H	-3.83047600	0.93247800	-2.58458700
C	-3.05380900	-1.07856900	-2.89633900

C	-3.57649800	-2.51899000	-3.05553700
H	-4.04619900	-2.88563600	-2.13171300
H	-4.32533900	-2.54897100	-3.86550000
H	-2.76079900	-3.21056100	-3.31543300
C	-2.40547200	-0.60799400	-4.22297300
H	-1.58798600	-1.28335100	-4.52479500
H	-3.15946200	-0.61166700	-5.02814500
H	-1.99673900	0.40955700	-4.13048700
C	-1.98086000	-1.00760100	-1.78565400
Rh	-0.24929100	-2.07614600	0.29661400
O	1.17645500	-2.42720300	-1.14338400
O	1.19258500	-1.93050400	1.76384300
O	1.44526000	-0.20112200	-1.52166400
O	1.45594100	0.31011900	1.37452300
C	1.72194000	-1.43391400	-1.74798800
C	2.77484100	-1.75348900	-2.83114000
C	2.09413200	-2.63060200	-3.91240300
H	1.67072400	-3.54672500	-3.47399500
H	2.83405800	-2.91599500	-4.67893800
H	1.28304600	-2.07920000	-4.41605500
C	3.31594500	-0.46192200	-3.47221400
H	2.50532600	0.12348100	-3.93204900
H	4.04337600	-0.72152000	-4.26012200
H	3.81650600	0.18087800	-2.73435300
C	3.93919500	-2.58950100	-2.18578100
H	3.52651400	-3.56836600	-1.89064900
H	4.67513500	-2.77620600	-2.98818200
C	4.61816100	-1.95016100	-0.99024400
C	5.76440100	-1.14103700	-1.11878500
H	6.21589000	-0.99014800	-2.10451800
C	6.34010800	-0.54246600	0.01183200
H	7.24090500	0.06925400	-0.09633600
C	5.77057000	-0.72609800	1.28070300
H	6.22665300	-0.25345300	2.15633400
C	4.62425400	-1.52996500	1.43762600
C	4.08581700	-2.15236000	0.29635400
H	3.21783900	-2.80588700	0.41249000
C	3.95085700	-1.72874600	2.78144300
H	4.69039700	-1.63638100	3.59672000
H	3.53640100	-2.74903500	2.83329300
C	2.79036400	-0.72199800	3.11285800
C	3.33621000	0.70806100	3.28147400
H	3.82880500	1.06820500	2.36734100
H	4.07105100	0.72442400	4.10464900
H	2.52899600	1.41493000	3.52585200
C	2.11697300	-1.18306100	4.43034500
H	1.31381900	-0.48838800	4.72672900
H	2.86285400	-1.20172800	5.24294600
H	1.68507500	-2.18970600	4.32610300
C	1.72920400	-0.78398900	1.98941200
N	-0.03082400	2.37990600	-0.43244700
C	2.38614400	2.85781600	-0.41166900
C	1.04229300	3.29423900	-0.47460300
C	0.76652300	4.69847900	-0.50781100
C	1.83458100	5.60490200	-0.52019600
C	3.16640600	5.16000100	-0.48389300
C	3.43469000	3.78395500	-0.42235200
H	2.58967400	1.78815900	-0.37139000
H	1.63254200	6.67958600	-0.54080300
H	3.98459100	5.88560300	-0.49036600
H	4.46763200	3.42580300	-0.38548000
C	-0.71462900	5.11123200	-0.52569300
C	-0.94787800	6.47875800	0.17953000
C	-1.20953300	5.21686100	-1.99435600
C	-1.47192000	4.04686800	0.22102900
H	-0.56223300	6.46379400	1.21119000
H	-0.45399200	7.30318700	-0.36329900
H	-2.02589500	6.70555700	0.21475100

H	-1.06761300	4.26985300	-2.54201400
H	-2.28299900	5.47191100	-2.02691000
H	-0.65251200	5.99783000	-2.53608000
H	-0.66538400	2.48422000	-1.23540900
H	-1.24857800	3.87682000	1.27601900
H	-2.45127400	3.70983500	-0.13109300

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^TCa (E = -2510.17002503)

Rh	-0.02668700	0.39607500	-0.30354700
O	-1.64864600	1.14373900	1.21013800
O	-1.50918500	-0.11912400	-1.69582500
O	-1.83232700	-0.97782200	1.98518600
O	-1.82182400	-2.13114200	-0.66047700
C	-2.17657400	0.26826300	1.96087200
C	-3.30605800	0.69308200	2.93044400
C	-2.71327700	1.73547900	3.91156600
H	-2.29264200	2.59641500	3.36962100
H	-3.49951500	2.09958200	4.59446700
H	-1.91391300	1.28762800	4.52464100
C	-3.85800400	-0.50906300	3.71814100
H	-3.06466500	-0.99101200	4.30954900
H	-4.64597700	-0.16846400	4.41233400
H	-4.28867000	-1.26907200	3.05029200
C	-4.44286900	1.39299000	2.10455800
H	-4.01108300	2.29716200	1.64357200
H	-5.20423100	1.73099800	2.83006100
C	-5.09853300	0.54305300	1.03142500
C	-6.31094600	-0.13644000	1.26128800
H	-6.81400000	-0.03552600	2.22839900
C	-6.88415600	-0.92911600	0.25622500
H	-7.83327800	-1.44090300	0.44202600
C	-6.24889600	-1.06722000	-0.98633500
H	-6.70388600	-1.68785800	-1.76500000
C	-5.03447900	-0.40095100	-1.24444000
C	-4.49269700	0.41363900	-0.23299900
H	-3.56552300	0.95704600	-0.43029700
C	-4.30833300	-0.54760200	-2.56892300
H	-5.02792800	-0.81961200	-3.36171300
H	-3.86469200	0.42083800	-2.85521700
C	-3.16703100	-1.62688800	-2.60963500
C	-3.73483200	-3.03374200	-2.34410100
H	-4.21235800	-3.09899000	-1.35619100
H	-4.48778200	-3.27768400	-3.11321800
H	-2.94133200	-3.79522100	-2.38563900
C	-2.51411600	-1.58357700	-4.01443500
H	-1.70169100	-2.32437800	-4.09539900
H	-3.26667200	-1.82193100	-4.78496800
H	-2.09575700	-0.58868300	-4.23047900
C	-2.08277400	-1.26416900	-1.56981600
Rh	-0.39412500	-1.72061300	0.76319000
O	0.99216700	-2.68482900	-0.38783600
O	1.03093200	-1.22058400	2.16128300
O	1.52976000	-0.82124200	-1.56133400
O	1.42465800	0.78877600	1.14409100
C	1.66549100	-2.05115300	-1.29725700
C	2.68255900	-2.90718100	-2.09366900
C	1.91441700	-4.06473200	-2.77803100
H	1.37607200	-4.67594000	-2.03842800
H	2.61968200	-4.71342300	-3.32533300
H	1.18088600	-3.67686200	-3.50448200
C	3.38640700	-2.04957700	-3.16172600
H	2.65665800	-1.60667200	-3.85688800
H	4.08037900	-2.67863800	-3.74539000
H	3.96130300	-1.22812800	-2.70968600
C	3.73052500	-3.53319900	-1.10403300
H	3.20616200	-4.28309500	-0.48891400
H	4.46568500	-4.07892800	-1.72263200

C	4.44265500	-2.55392200	-0.19010900
C	5.66674200	-1.94880300	-0.53807700
H	6.15328900	-2.21071800	-1.48318300
C	6.27553700	-1.03000900	0.33025100
H	7.23574800	-0.58017300	0.05932100
C	5.66682300	-0.69198400	1.54825300
H	6.15293100	0.02209800	2.22064100
C	4.44335300	-1.28245800	1.92184500
C	3.86632900	-2.22504400	1.05086300
H	2.93187600	-2.70952600	1.34271900
C	3.73674700	-0.93398000	3.21860600
H	4.47531300	-0.64282800	3.98704000
H	3.21335000	-1.82784400	3.59557400
C	2.69048100	0.23518200	3.13693700
C	3.38812500	1.57580100	2.84109400
H	3.91273900	1.55732400	1.87526500
H	4.12244700	1.79148200	3.63626500
H	2.66132900	2.40145200	2.81027500
C	1.95580700	0.31838100	4.49951100
H	1.22379300	1.14283300	4.50152300
H	2.68327100	0.51008100	5.30651400
H	1.42338100	-0.61880100	4.72207100
C	1.63654200	-0.08677500	2.05350000
N	0.31849800	2.25091800	-1.50721200
C	2.85754700	2.31332200	-1.53228600
C	1.60462500	2.92931300	-1.47983300
C	1.44801500	4.32179900	-1.40452200
C	2.58500600	5.13809500	-1.36608300
C	3.85715700	4.54114400	-1.41049800
C	3.98958900	3.14470000	-1.50043300
H	2.93998200	1.22575000	-1.57745400
H	2.48968100	6.22666200	-1.30868600
H	4.75119200	5.17001900	-1.37483600
H	4.98503800	2.69355600	-1.53019800
C	-0.03022200	4.70085500	-1.46776100
C	-0.44465500	5.74844600	-0.41677100
C	-0.38273000	5.20324400	-2.89082700
C	-0.69349100	3.31786700	-1.17454700
H	-0.17012000	5.42316600	0.59964700
H	0.04449600	6.71791500	-0.60853600
H	-1.53480100	5.91794800	-0.44229500
H	-0.13428300	4.45056400	-3.65810300
H	-1.45964500	5.43198200	-2.96881200
H	0.17880600	6.12032200	-3.13329100
H	0.13936700	1.86279700	-2.44303200
H	-0.92643900	3.22090900	-0.10380300
H	-1.61600200	3.13758600	-1.74439000

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^TTS3a (E = -2510.09518127)

Rh	0.06920100	0.18939900	-0.39199800
O	1.51492500	-0.69606300	-1.58978700
O	1.51723500	1.28251100	0.61620300
O	1.89581100	-2.32008200	-0.02738200
O	1.85651700	-0.38837300	2.12552200
C	2.11934400	-1.74895900	-1.15113300
C	3.18680000	-2.37099500	-2.07983600
C	2.48726600	-2.79503400	-3.39654700
H	2.00168300	-1.93707100	-3.88573600
H	3.23008500	-3.21963600	-4.09256800
H	1.72268000	-3.56647100	-3.20796300
C	3.83420000	-3.60032800	-1.41498000
H	3.08076000	-4.36823100	-1.18311600
H	4.57588400	-4.04061900	-2.10307500
H	4.34313300	-3.33416200	-0.47752500
C	4.27199700	-1.28993000	-2.43147900
H	3.78098200	-0.49502300	-3.01731400
H	5.00100100	-1.78126900	-3.10027800

C	4.98657300	-0.67434300	-1.24402300
C	6.21056400	-1.17701600	-0.76037900
H	6.69628900	-2.01313300	-1.27360300
C	6.81743700	-0.60290000	0.36638600
H	7.77607600	-0.99026800	0.72421900
C	6.20158800	0.46298300	1.03865400
H	6.67969200	0.89857700	1.92177700
C	4.97681800	0.98438400	0.57745200
C	4.40718900	0.42200200	-0.57968200
H	3.47707100	0.84264200	-0.96836600
C	4.25073700	2.10073000	1.30362200
H	4.97281600	2.72845900	1.85528200
H	3.74883400	2.75387700	0.57117100
C	3.17546200	1.63137400	2.34835300
C	3.83187000	0.83865700	3.49522600
H	4.33990900	-0.06405100	3.12690600
H	4.57573000	1.47754200	4.00086000
H	3.08402300	0.52647400	4.23955000
C	2.47240200	2.88865800	2.92091200
H	1.71246400	2.60847200	3.66877800
H	3.21542200	3.53264200	3.42067100
H	1.98161000	3.47092300	2.12727800
C	2.10701800	0.77032300	1.64194600
Rh	0.45878100	-1.56002500	1.23163400
O	-0.98841900	-0.69627900	2.41720600
O	-0.92731500	-2.74306200	0.30406000
O	-1.37952700	0.94554600	0.87142900
O	-1.33144400	-1.10584000	-1.23101800
C	-1.60276700	0.34803100	1.98764400
C	-2.69055700	0.94495900	2.90984300
C	-1.99563500	1.41147800	4.21512500
H	-1.46494600	0.58004500	4.70347900
H	-2.74966700	1.80670500	4.91661400
H	-1.27082000	2.21650400	4.01051900
C	-3.39294500	2.13839400	2.23687600
H	-2.67512800	2.93749700	2.00029800
H	-4.15387100	2.54934100	2.92232500
H	-3.88779500	1.84447500	1.30038200
C	-3.72663000	-0.17538900	3.28517300
H	-3.19684100	-0.94148000	3.87478800
H	-4.46927100	0.29480700	3.95432900
C	-4.42568600	-0.83484700	2.11220800
C	-5.65779300	-0.36881400	1.61253700
H	-6.16124000	0.47011900	2.10331100
C	-6.24955000	-0.98199900	0.49861500
H	-7.21474400	-0.62286100	0.12907200
C	-5.61051900	-2.05172000	-0.14580500
H	-6.07816100	-2.51958800	-1.01817900
C	-4.37755000	-2.53741300	0.33239900
C	-3.82306400	-1.93613200	1.47741100
H	-2.88697200	-2.32855600	1.88092100
C	-3.62571500	-3.65741000	-0.36096700
H	-4.33172800	-4.31803300	-0.89503600
H	-3.10921000	-4.27574400	0.39140000
C	-2.55696700	-3.19550800	-1.41734300
C	-3.23354400	-2.48892300	-2.60570400
H	-3.79087400	-1.59849800	-2.28143000
H	-3.94007800	-3.18280000	-3.09192300
H	-2.49144700	-2.17704100	-3.35657600
C	-1.79762300	-4.45088800	-1.91836400
H	-1.04395500	-4.18043800	-2.67627500
H	-2.50802700	-5.15313800	-2.38608700
H	-1.28847300	-4.96657600	-1.09024100
C	-1.52960400	-2.27065300	-0.72669400
N	-0.25277600	1.50872900	-1.90916400
C	-2.52257700	1.56699700	-2.75555000
C	-1.40806500	2.26741900	-2.23431700
C	-1.46815400	3.69126700	-2.09178100

C	-2.67593000	4.32036900	-2.45835500
C	-3.78519100	3.61384000	-2.94270800
C	-3.70637000	2.22507300	-3.09957600
H	-2.44272800	0.48270300	-2.84943100
H	-2.75658600	5.40514700	-2.37325900
H	-4.69907100	4.15403000	-3.20671300
H	-4.55688500	1.65477900	-3.48433200
C	-0.24550500	4.53293200	-1.62985700
C	-0.47645600	6.05498000	-1.83440600
C	0.01197200	4.29258700	-0.12225600
C	0.96231000	4.15075700	-2.44919200
H	-0.68934600	6.30375400	-2.88740800
H	-1.30323500	6.43592700	-1.21103400
H	0.43706000	6.59561100	-1.53941000
H	0.23041300	3.23742600	0.08385200
H	0.87326600	4.89870000	0.20951400
H	-0.86856700	4.59036900	0.47080600
H	0.15053900	1.06829900	-2.74794700
H	1.03106000	4.47022300	-3.49293600
H	1.69623300	3.43490700	-2.07633000

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¹IM2a (E = -2510.09725199)

Rh	0.05430800	0.17803000	-0.41632900
O	1.50156800	-0.76722300	-1.56814900
O	1.50240500	1.31364000	0.55790800
O	1.86321900	-2.33174200	0.05526300
O	1.84181500	-0.31301500	2.11751900
C	2.09529300	-1.80657700	-1.08972200
C	3.15934200	-2.47401000	-1.98958000
C	2.45401700	-2.96289000	-3.28056800
H	1.97347500	-2.12847100	-3.81377700
H	3.19253600	-3.42918400	-3.95421500
H	1.68525600	-3.71843200	-3.04921400
C	3.80879300	-3.66894000	-1.26653100
H	3.05609000	-4.42476200	-0.99592900
H	4.54942200	-4.14222500	-1.93350700
H	4.31935300	-3.35582000	-0.34462800
C	4.24166800	-1.41074200	-2.39908900
H	3.74383200	-0.64065700	-3.01137700
H	4.96304600	-1.93065800	-3.05441200
C	4.96863200	-0.74840500	-1.24479100
C	6.19643300	-1.23359600	-0.75327400
H	6.67642900	-2.08954800	-1.23845500
C	6.81381700	-0.61789000	0.34549100
H	7.77525800	-0.99239200	0.70951000
C	6.20422300	0.47302200	0.98229300
H	6.69003300	0.94120700	1.84435700
C	4.97587900	0.97798800	0.51216800
C	4.39568300	0.37325400	-0.61783300
H	3.46386700	0.78025400	-1.01646100
C	4.25791200	2.12162400	1.20275000
H	4.98604900	2.76247000	1.73111900
H	3.75882600	2.75475200	0.45081400
C	3.18469800	1.69360300	2.26707700
C	3.84248800	0.92414400	3.42905500
H	4.33165700	0.00299100	3.08173400
H	4.60278500	1.56570800	3.90620700
H	3.09890000	0.64655800	4.19113400
C	2.50627300	2.97508200	2.81375400
H	1.74632100	2.72624600	3.57258700
H	3.26303900	3.61918000	3.29238800
H	2.02012900	3.54531000	2.00903600
C	2.09740000	0.82702700	1.59393700
Rh	0.43339400	-1.51110300	1.27284000
O	-1.00774600	-0.61541900	2.43624500
O	-0.96121700	-2.72281200	0.38286400
O	-1.40029300	0.96556700	0.83142000

O	-1.34137600	-1.14733600	-1.22188400
C	-1.62499200	0.41036600	1.96855500
C	-2.71559900	1.03479100	2.86942300
C	-2.02179000	1.55129500	4.15646600
H	-1.49361900	0.73896500	4.67857000
H	-2.77602800	1.97635800	4.84007700
H	-1.29456600	2.34568900	3.92093800
C	-3.42613700	2.19995200	2.15686900
H	-2.71492400	2.99555700	1.89185600
H	-4.18875600	2.62889400	2.82928600
H	-3.92167500	1.86988200	1.23279800
C	-3.74628500	-0.07634800	3.28473000
H	-3.21066200	-0.82303300	3.89345800
H	-4.48630100	0.41161600	3.94403900
C	-4.44951500	-0.77099200	2.13479500
C	-5.68440400	-0.32133100	1.62714000
H	-6.18793700	0.52940500	2.09708300
C	-6.27817300	-0.96524800	0.53172300
H	-7.24531700	-0.61828800	0.15565200
C	-5.63855700	-2.05029100	-0.08598200
H	-6.10770800	-2.54223500	-0.94419800
C	-4.40335200	-2.52082700	0.40161400
C	-3.84660600	-1.88784800	1.52810300
H	-2.90850900	-2.26763700	1.93874700
C	-3.65273300	-3.65974900	-0.26128300
H	-4.36030800	-4.33420700	-0.77573100
H	-3.13614800	-4.25718400	0.50778600
C	-2.58463300	-3.22982100	-1.33144200
C	-3.26127900	-2.55310400	-2.53752800
H	-3.80046000	-1.64211200	-2.24049200
H	-3.98212100	-3.25215400	-2.99462200
H	-2.52003600	-2.27937700	-3.30405500
C	-1.83147900	-4.50206300	-1.79824100
H	-1.07849600	-4.25687100	-2.56533800
H	-2.54541600	-5.21556800	-2.24303200
H	-1.32217000	-4.99483900	-0.95631600
C	-1.55223800	-2.28878000	-0.67051900
N	-0.46105000	1.31075400	-2.10134600
C	-2.52357300	1.78231900	-3.23744600
C	-1.42062400	2.24460900	-2.44863800
C	-1.34628400	3.64869000	-2.12274700
C	-2.42274400	4.45834100	-2.53114200
C	-3.52429100	3.97144900	-3.24964500
C	-3.56506000	2.61781300	-3.62247500
H	-2.54842900	0.72024800	-3.49967500
H	-2.39825600	5.52464500	-2.29983300
H	-4.33127700	4.65236600	-3.53438100
H	-4.40226100	2.22127700	-4.20379600
C	-0.12057300	4.29465300	-1.42407300
C	0.03672900	5.79126800	-1.83511100
C	-0.32711800	4.23967300	0.11065900
C	1.15765100	3.60648600	-1.82301900
H	0.08435200	5.90866200	-2.93021800
H	-0.78089000	6.42445700	-1.45140300
H	0.97574000	6.17946800	-1.40943800
H	-0.40134000	3.20293800	0.46409200
H	0.52045900	4.72868300	0.62078100
H	-1.25025600	4.77249500	0.39383400
H	-0.52529600	0.52705500	-2.76595900
H	1.48389700	3.64656800	-2.86603100
H	1.67885200	2.93746600	-1.13999800

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^tTS4a (E = -2510.09333115)

Rh	0.08821800	0.24368200	-0.47015200
O	1.55110100	-0.73821700	-1.59067600
O	1.56297200	1.39451600	0.52906900
O	1.88513600	-2.25710200	0.08428700

O	1.88035100	-0.19854100	2.11379600
C	2.13204200	-1.76509100	-1.07236400
C	3.20684000	-2.46504800	-1.93527700
C	2.52239800	-2.97804900	-3.22790800
H	2.05990200	-2.15236700	-3.78991900
H	3.26900200	-3.46748800	-3.87584600
H	1.74147600	-3.72006200	-2.99362800
C	3.83139500	-3.64841600	-1.17243900
H	3.06631600	-4.39020900	-0.89782400
H	4.57945800	-4.14504400	-1.81380500
H	4.32757200	-3.31829200	-0.24868000
C	4.30695500	-1.42154200	-2.34798700
H	3.82677700	-0.65849000	-2.98283500
H	5.03261900	-1.96113300	-2.98231200
C	5.02506900	-0.74374800	-1.19677400
C	6.24233200	-1.23093600	-0.68160600
H	6.71849300	-2.10169400	-1.14357200
C	6.85418600	-0.59943500	0.41120100
H	7.80732600	-0.97669200	0.79370200
C	6.25054300	0.51177500	1.01777600
H	6.73330500	0.99372500	1.87399100
C	5.03293000	1.01983700	0.52367600
C	4.45724300	0.39618400	-0.59843200
H	3.53173900	0.80203100	-1.01304600
C	4.32461900	2.19064900	1.17789500
H	5.05707900	2.83497600	1.69605400
H	3.84362700	2.81065300	0.40310400
C	3.23204200	1.80994000	2.24064000
C	3.86475800	1.07602800	3.43822000
H	4.35341400	0.14090700	3.12935900
H	4.62098900	1.72749500	3.90855200
H	3.10579700	0.82720100	4.19521300
C	2.55556900	3.11659100	2.72761500
H	1.78599500	2.90350000	3.48750000
H	3.31025100	3.77704000	3.18697000
H	2.07999300	3.65535200	1.89467500
C	2.14865200	0.93251900	1.57684300
Rh	0.45994600	-1.39478400	1.28316600
O	-0.97871900	-0.44085400	2.41076800
O	-0.92189600	-2.68017300	0.50992300
O	-1.37072400	1.08293900	0.74949700
O	-1.34580000	-1.23277200	-1.19459700
C	-1.59604600	0.56634800	1.90345800
C	-2.68541700	1.22424200	2.78273900
C	-1.97887000	1.82869100	4.02397500
H	-1.43448500	1.05648400	4.58872900
H	-2.72709400	2.29001600	4.69048300
H	-1.26340000	2.61335200	3.72707700
C	-3.42553500	2.33492500	2.01433200
H	-2.73296100	3.12560600	1.69115300
H	-4.18482400	2.79055200	2.67293800
H	-3.92928200	1.94484500	1.11846500
C	-3.69167000	0.12654400	3.28251500
H	-3.13566800	-0.57034300	3.93058900
H	-4.43004500	0.64459700	3.92035500
C	-4.40166000	-0.65588700	2.19410700
C	-5.65743500	-0.26730100	1.68741400
H	-6.16759600	0.60414500	2.10979800
C	-6.26361500	-0.99929000	0.65587300
H	-7.24692900	-0.69914600	0.28129300
C	-5.61703900	-2.11391800	0.10129400
H	-6.09732200	-2.67624200	-0.70609600
C	-4.36078600	-2.52482800	0.58931700
C	-3.79009400	-1.80149000	1.65245800
H	-2.83421600	-2.13269200	2.06363900
C	-3.60682000	-3.69966900	-0.00375400
H	-4.31642600	-4.41893200	-0.45070900
H	-3.06749700	-4.23125800	0.79750300

C	-2.56590200	-3.34034000	-1.12518000
C	-3.27676500	-2.77648800	-2.36827300
H	-3.83592900	-1.85946600	-2.13221100
H	-3.98610200	-3.52551500	-2.75988600
H	-2.55376700	-2.54254800	-3.16490300
C	-1.79882300	-4.63397300	-1.50111200
H	-1.06987400	-4.44207800	-2.30580800
H	-2.50845600	-5.39688200	-1.86360100
H	-1.25867700	-5.04163300	-0.63340800
C	-1.53753400	-2.32884700	-0.56545600
N	-0.49833700	1.18653400	-2.20366100
C	-2.78873800	1.40629000	-3.01658500
C	-1.60772100	1.98173400	-2.47049900
C	-1.55591300	3.39106200	-2.24494000
C	-2.71150700	4.14844200	-2.50117200
C	-3.88691000	3.56365100	-2.99433100
C	-3.91604000	2.18574500	-3.27070500
H	-2.80377200	0.32869800	-3.19738900
H	-2.69498900	5.22840800	-2.33198800
H	-4.76823400	4.18425200	-3.17892600
H	-4.82006500	1.72119700	-3.67502100
C	-0.23083400	4.05367900	-1.80256000
C	-0.00393000	5.38145800	-2.59432700
C	-0.28833900	4.37666500	-0.28797300
C	0.92910100	3.15485200	-2.11858000
H	-0.01615400	5.20389600	-3.68175700
H	-0.77448500	6.13440900	-2.35926200
H	0.97308700	5.81348600	-2.32375600
H	-0.41010800	3.45738300	0.30184400
H	0.64025600	4.88155700	0.03023600
H	-1.13447600	5.04826300	-0.06753900
H	-0.40850900	0.42009900	-2.88349400
H	1.19516000	2.96897100	-3.16202300
H	1.63693900	2.84923700	-1.34922100

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^sTS1b (E = -2510.11357331)

Rh	0.05555900	0.30040900	-0.21409100
O	1.49215500	-0.19449200	-1.63557800
O	1.51593200	1.08793800	1.05538600
O	1.93735400	-2.18366400	-0.59699300
O	1.94283100	-0.93738400	2.01824200
C	2.12375800	-1.31145300	-1.51670200
C	3.18558400	-1.61768300	-2.59836500
C	2.46042200	-1.70073900	-3.96553300
H	1.92973300	-0.76350600	-4.19227200
H	3.19343500	-1.89197100	-4.76736300
H	1.72921200	-2.52593300	-3.97413200
C	3.89505000	-2.95237900	-2.30327300
H	3.17685500	-3.78577600	-2.27663200
H	4.63442000	-3.15868100	-3.09612800
H	4.41790700	-2.92810900	-1.33647800
C	4.22026400	-0.43653100	-2.66656900
H	3.67858000	0.46696600	-2.99183500
H	4.93841400	-0.69131700	-3.46640100
C	4.96109900	-0.14412000	-1.37571400
C	6.22353400	-0.70211000	-1.09436400
H	6.71649300	-1.33474700	-1.83946000
C	6.85777700	-0.44138500	0.12934300
H	7.84533800	-0.86677700	0.33190100
C	6.23229800	0.35973000	1.09597300
H	6.73156700	0.55106500	2.05128100
C	4.97019600	0.93104900	0.84027800
C	4.37038600	0.69139700	-0.40988400
H	3.40959700	1.15971200	-0.63474800
C	4.23956300	1.76707400	1.87400800
H	4.96442000	2.23909000	2.56132600
H	3.69302300	2.58085500	1.36958100

C	3.21492400	0.98503900	2.77077200
C	3.93086900	-0.07023000	3.63529000
H	4.45188400	-0.81602900	3.01811600
H	4.67283100	0.42927700	4.28146800
H	3.21691400	-0.60494300	4.27965000
C	2.49945900	2.00842000	3.68948600
H	1.76475300	1.50817700	4.34169600
H	3.23984900	2.50823600	4.33679600
H	1.97787800	2.77898400	3.10179800
C	2.14515500	0.31870200	1.87611600
Rh	0.52592700	-1.82525800	0.85114800
O	-0.90683000	-1.36197400	2.25877400
O	-0.89023000	-2.67600500	-0.36766300
O	-1.37379600	0.63342200	1.24160500
O	-1.34627500	-0.67563900	-1.36364600
C	-1.55362800	-0.25801200	2.15115600
C	-2.62622500	0.02873500	3.22731300
C	-1.89957200	0.13692700	4.59251800
H	-1.33626600	-0.78139000	4.81769900
H	-2.63632100	0.30434700	5.39624700
H	-1.19655500	0.98626600	4.59793900
C	-3.37623200	1.34017400	2.92964600
H	-2.68515400	2.19470000	2.88686900
H	-4.11404700	1.53025500	3.72807400
H	-3.90838100	1.29303300	1.96865600
C	-3.62654100	-1.18140700	3.30221400
H	-3.06020600	-2.06681900	3.63452600
H	-4.35309500	-0.94151100	4.09896100
C	-4.35574500	-1.50330400	2.01172200
C	-5.62666200	-0.97304500	1.71440900
H	-6.13701600	-0.34122100	2.44827800
C	-6.24779600	-1.26150100	0.49002700
H	-7.24267600	-0.85892200	0.27679300
C	-5.60092800	-2.06252300	-0.46286000
H	-6.09129800	-2.27779800	-1.41779800
C	-4.33006800	-2.60664300	-0.19115500
C	-3.74424100	-2.34014100	1.06023800
H	-2.77665400	-2.78741300	1.29735000
C	-3.57420200	-3.44115700	-1.20773700
H	-4.28233000	-3.93916400	-1.89407600
H	-3.01224700	-4.23455700	-0.68836900
C	-2.55964800	-2.64873100	-2.10829300
C	-3.29840900	-1.64316900	-3.00913400
H	-3.87109000	-0.91373700	-2.41811400
H	-4.00131300	-2.18514700	-3.66470600
H	-2.59292300	-1.09104100	-3.64798100
C	-1.79395600	-3.67169100	-2.98710200
H	-1.08892600	-3.16108700	-3.66369700
H	-2.50861300	-4.23784500	-3.60806900
H	-1.22776300	-4.38307900	-2.36719200
C	-1.52277600	-1.94232400	-1.20696000
N	-0.19287000	2.06609500	-1.18732700
C	-0.46971600	3.64405600	0.62937900
C	-0.77337500	3.22652700	-0.69438700
C	-1.59491900	4.06942400	-1.51446300
C	-2.02552800	5.29848600	-1.00799700
C	-1.69184300	5.71841800	0.29285600
C	-0.91172100	4.88264800	1.10336100
H	0.15075600	2.99311100	1.24447500
H	-2.65696200	5.94337400	-1.62642000
H	-2.06043100	6.67611400	0.66957200
H	-0.65175600	5.18966800	2.12081800
C	-1.90056500	3.59842300	-2.94915700
C	-1.78010100	2.09009800	-2.97675400
C	-3.34244300	3.97462300	-3.39502300
C	-0.87226200	4.23691400	-3.92329900
H	-0.48669500	1.93308000	-2.26438500
H	-2.51145500	1.51353800	-2.40271300

H	-1.46659500	1.61198200	-3.91559800
H	-3.45913700	5.06835000	-3.48115100
H	-3.55897100	3.54215400	-4.38613000
H	-4.09067900	3.60003700	-2.67914400
H	-1.06315600	3.91595900	-4.96199700
H	-0.93671100	5.33607600	-3.88679900
H	0.15828000	3.95250900	-3.65563300

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^sCb (E = -2510.21157981)

Rh	0.05170900	0.28397900	-0.22075500
O	1.52750800	-0.23886700	-1.58482700
O	1.48267500	1.13337800	1.03235800
O	1.88792800	-2.22229200	-0.50783400
O	1.84406800	-0.87297800	2.06776600
C	2.12885200	-1.37117700	-1.43173500
C	3.21540600	-1.73063200	-2.47201000
C	2.53272200	-1.82336800	-3.86023000
H	2.03933900	-0.87629800	-4.12726000
H	3.28400500	-2.05744200	-4.63345400
H	1.77532200	-2.62428200	-3.87277400
C	3.87190200	-3.08097600	-2.12721900
H	3.12582000	-3.88950100	-2.10649000
H	4.62858400	-3.32806100	-2.89165600
H	4.36400100	-3.05365900	-1.14441200
C	4.29297100	-0.58901600	-2.53292100
H	3.79822700	0.32298900	-2.90696700
H	5.03199200	-0.89123600	-3.29640000
C	4.99409300	-0.28095400	-1.22359800
C	6.22748900	-0.86598200	-0.87649700
H	6.72764300	-1.53730300	-1.58177500
C	6.82291400	-0.58405200	0.36209200
H	7.78808800	-1.03258000	0.61593600
C	6.18822100	0.26811400	1.27789900
H	6.65746800	0.47740100	2.24447900
C	4.95411900	0.86664400	0.95677200
C	4.39447500	0.60029400	-0.30590600
H	3.45091300	1.07933100	-0.57537300
C	4.21059500	1.75991100	1.93134900
H	4.92338900	2.23287900	2.63070200
H	3.71379600	2.57380000	1.37721500
C	3.12348400	1.04456800	2.81039400
C	3.77338600	0.00577800	3.74417900
H	4.29307700	-0.78006200	3.17760900
H	4.50581400	0.50872700	4.39883600
H	3.01926300	-0.48115400	4.38066900
C	2.40516700	2.12529300	3.65742400
H	1.62449100	1.67517000	4.29226100
H	3.13182900	2.62631300	4.31930100
H	1.93617300	2.88844800	3.01783700
C	2.07063000	0.37460300	1.89597500
Rh	0.44703300	-1.81882500	0.90132700
O	-1.00970600	-1.31119300	2.26169600
O	-0.95272400	-2.68544400	-0.33526000
O	-1.40022800	0.67604600	1.19789200
O	-1.35279200	-0.69432800	-1.38471100
C	-1.62563300	-0.19217500	2.11740000
C	-2.71512800	0.13978600	3.16402100
C	-2.01659600	0.26713200	4.54206200
H	-1.47972500	-0.65752600	4.80315200
H	-2.76596200	0.47277600	5.32521500
H	-1.29352400	1.09967300	4.54119000
C	-3.43185800	1.45826600	2.81929700
H	-2.72328900	2.29848500	2.77854300
H	-4.18714700	1.67951200	3.59310600
H	-3.93791900	1.40121400	1.84487300
C	-3.74262400	-1.04624600	3.24672000
H	-3.20222200	-1.93500500	3.61170200

H	-4.48061600	-0.77265700	4.02200800
C	-4.45087400	-1.38423100	1.94872100
C	-5.70533400	-0.83824000	1.61261700
H	-6.21872500	-0.18027700	2.32110200
C	-6.30605000	-1.14360900	0.38212900
H	-7.28846600	-0.72773300	0.13844300
C	-5.65446600	-1.97851100	-0.53784700
H	-6.12810400	-2.20725500	-1.49809500
C	-4.39952200	-2.53840800	-0.22706400
C	-3.83463400	-2.25315200	1.02963000
H	-2.87885800	-2.70954600	1.29540600
C	-3.63843800	-3.40995100	-1.20781900
H	-4.34253200	-3.91154900	-1.89598900
H	-3.10240700	-4.20031700	-0.65719300
C	-2.59001300	-2.65876700	-2.10447600
C	-3.29084700	-1.65760400	-3.04051400
H	-3.84228400	-0.89233300	-2.47516300
H	-4.00656800	-2.19574700	-3.68566800
H	-2.56355300	-1.14702000	-3.69005700
C	-1.83248900	-3.71824400	-2.94555300
H	-1.09932700	-3.23937200	-3.61555400
H	-2.54639900	-4.28008200	-3.57153300
H	-1.29810500	-4.42978200	-2.29806100
C	-1.55394800	-1.95133400	-1.19973900
N	-0.14713800	2.21622700	-1.36480900
C	-0.60098400	3.82407100	0.55341700
C	-0.74483500	3.40191600	-0.77033700
C	-1.50235900	4.12075400	-1.70985900
C	-2.15432200	5.29511000	-1.31543600
C	-2.02940200	5.73340500	0.01459600
C	-1.25423800	5.00806800	0.93558000
H	-0.01472200	3.23341000	1.25867500
H	-2.74992800	5.87086200	-2.03044800
H	-2.53987500	6.64613700	0.33448300
H	-1.16693500	5.36099900	1.96701900
C	-1.38769200	3.47492000	-3.08932600
C	-0.84099100	2.07013800	-2.69005800
C	-2.72904200	3.36033300	-3.83693300
C	-0.36058800	4.25446700	-3.94907900
H	0.85939700	2.37254900	-1.50685000
H	-1.66918300	1.36365300	-2.53585800
H	-0.14662800	1.63278600	-3.42133200
H	-3.12679100	4.35520900	-4.09815900
H	-2.60372700	2.79827300	-4.77830900
H	-3.48343400	2.84130900	-3.22400700
H	-0.22376900	3.76700500	-4.92979700
H	-0.69945800	5.28836600	-4.12591500
H	0.62321100	4.30874300	-3.45261100

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^tTS1b (E = -2510.11612559)

Rh	-0.03283200	0.29873200	-0.09279000
O	1.42296700	-0.07285700	-1.53329400
O	1.40507300	0.43393300	1.39938700
O	1.39514700	-2.31506200	-1.10036700
O	1.38759400	-1.82434200	1.75057700
C	1.82760100	-1.28153900	-1.72151400
C	2.91185900	-1.48883300	-2.80268400
C	2.31225700	-1.05613700	-4.16510300
H	1.97790800	-0.00795300	-4.13876900
H	3.07201500	-1.16216400	-4.95779900
H	1.45133700	-1.68902500	-4.43661800
C	3.33847800	-2.96766300	-2.86761200
H	2.48113400	-3.61849500	-3.09613200
H	4.09207400	-3.09723200	-3.66311800
H	3.77444700	-3.30650300	-1.91680900
C	4.14370800	-0.56434400	-2.49450400
H	3.80939100	0.48300000	-2.57779000

H	4.87723500	-0.73559500	-3.30243500
C	4.79784400	-0.77999100	-1.14299000
C	5.91188200	-1.62600800	-0.97675500
H	6.35462900	-2.11905100	-1.84813900
C	6.46518500	-1.82851500	0.29618300
H	7.34027000	-2.47501000	0.41224900
C	5.90270600	-1.20809200	1.42143300
H	6.33867700	-1.37691400	2.41134100
C	4.78839900	-0.35708500	1.28389400
C	4.27408300	-0.13577700	-0.00693100
H	3.43311900	0.55043200	-0.12984300
C	4.12653100	0.30485900	2.47723300
H	4.85607300	0.42047200	3.29852400
H	3.79152400	1.31713400	2.19694400
C	2.89262300	-0.46107800	3.07735100
C	3.31871300	-1.82719600	3.64768000
H	3.75604300	-2.47228400	2.87223200
H	4.07085600	-1.67514700	4.44058600
H	2.46102900	-2.36038500	4.08485900
C	2.28877000	0.41168800	4.20716700
H	1.41682700	-0.08280600	4.66643800
H	3.04124100	0.56969100	4.99814900
H	1.97289800	1.39473700	3.82666400
C	1.81303000	-0.63974800	1.98608200
Rh	-0.05421900	-2.08517600	0.32053200
O	-1.50691700	-1.77946500	1.74638000
O	-1.47630300	-2.26814900	-1.15283500
O	-1.49598900	0.47129300	1.35580900
O	-1.48436500	-0.01573000	-1.53351000
C	-1.92325100	-0.58338400	1.95480100
C	-3.01545700	-0.39841400	3.03295900
C	-2.40893300	-0.83335800	4.39201800
H	-2.04800000	-1.87234200	4.35290000
H	-3.17363600	-0.75654800	5.18332500
H	-1.56506700	-0.18250200	4.67502400
C	-3.47620800	1.06907900	3.11245500
H	-2.63766800	1.73834900	3.35575000
H	-4.23834700	1.17144300	3.90378800
H	-3.91286000	1.41030200	2.16283700
C	-4.22694000	-1.34636700	2.71359800
H	-3.87066400	-2.38692100	2.78919300
H	-4.96557500	-1.19660300	3.52116300
C	-4.88079700	-1.13290400	1.36179500
C	-6.00055700	-0.29484400	1.19321000
H	-6.45103400	0.19206600	2.06404300
C	-6.54986100	-0.09299100	-0.08162600
H	-7.42986700	0.54650200	-0.19942000
C	-5.97744100	-0.70510400	-1.20655300
H	-6.41050800	-0.53667800	-2.19780600
C	-4.85739100	-1.54820200	-1.06657300
C	-4.34845900	-1.77042900	0.22618900
H	-3.50387200	-2.45140400	0.35139900
C	-4.18220600	-2.20054600	-2.25762100
H	-4.90718900	-2.33025200	-3.08088200
H	-3.83052800	-3.20627500	-1.97437700
C	-2.95919800	-1.41544800	-2.85622400
C	-3.41039800	-0.06609900	-3.44560800
H	-3.86863700	0.57785200	-2.68118800
H	-4.15209100	-0.24341800	-4.24307600
H	-2.56087200	0.47988000	-3.88274900
C	-2.32550200	-2.28864400	-3.96952300
H	-1.46932700	-1.77412100	-4.43627000
H	-3.07122500	-2.48586800	-4.75812800
H	-1.97537500	-3.25199900	-3.56891300
C	-1.89247000	-1.21398700	-1.75655700
N	-0.00613300	2.27073500	-0.50509400
C	0.01485300	3.41870700	1.62778200
C	0.04998300	3.43220300	0.19559300

C	0.13625300	4.70781700	-0.49440100
C	0.14364000	5.87367700	0.27696400
C	0.08843400	5.84221000	1.68268400
C	0.03239400	4.60626700	2.35189900
H	-0.04679200	2.45086600	2.12426900
H	0.20100600	6.84444700	-0.22178500
H	0.09372900	6.77833300	2.24745300
H	-0.00752700	4.57483500	3.44472700
C	0.32633000	4.72521400	-2.02342300
C	-0.42885800	3.55931300	-2.64597600
C	-0.18596200	6.04318000	-2.66525200
C	1.84535300	4.57363600	-2.31901000
H	-0.17974900	2.57615400	-1.64856800
H	-1.52546800	3.62173200	-2.62268000
H	-0.02613000	3.15262000	-3.58263600
H	0.41483800	6.91340300	-2.35014400
H	-0.11114500	5.97389800	-3.76260900
H	-1.23912400	6.23388200	-2.40317800
H	2.02681100	4.58565600	-3.40780700
H	2.41720700	5.39834300	-1.86401900
H	2.23241900	3.62461600	-1.91530000

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¹IM1b (E = -2510.12038603)

Rh	-0.03129600	0.28751200	-0.07418100
O	1.42039100	-0.02372100	-1.53290400
O	1.40681000	0.39780000	1.41566200
O	1.41916100	-2.27752400	-1.16260900
O	1.40307300	-1.86905200	1.70332100
C	1.83640900	-1.22242800	-1.75745100
C	2.91688500	-1.38697200	-2.84969700
C	2.31180600	-0.90761600	-4.19390000
H	1.97311600	0.13756800	-4.12911200
H	3.06990300	-0.98169300	-4.99181300
H	1.45273500	-1.53380100	-4.48607200
C	3.34883000	-2.86078800	-2.96998200
H	2.49294300	-3.50644600	-3.21786600
H	4.09904000	-2.95824400	-3.77327800
H	3.79075600	-3.23199800	-2.03414600
C	4.14657000	-0.47003600	-2.51208200
H	3.80954800	0.57860800	-2.56088300
H	4.88025700	-0.61269700	-3.32542500
C	4.80132400	-0.72837900	-1.16844200
C	5.91319100	-1.58208400	-1.02905100
H	6.35455900	-2.04867300	-1.91557000
C	6.46602900	-1.82582800	0.23680900
H	7.33936600	-2.47802700	0.33236900
C	5.90552900	-1.23918200	1.38100500
H	6.34145800	-1.43988500	2.36495000
C	4.79340900	-0.38140200	1.27047800
C	4.27927800	-0.11876000	-0.01272100
H	3.43991800	0.57315200	-0.11355000
C	4.13422200	0.24566800	2.48396100
H	4.86598200	0.33843900	3.30618400
H	3.79795100	1.26523100	2.23314200
C	2.90214600	-0.53723500	3.06651200
C	3.33086100	-1.91731900	3.60006900
H	3.76446300	-2.54269500	2.80658100
H	4.08651500	-1.78571700	4.39332100
H	2.47492300	-2.46146200	4.02711600
C	2.30015200	0.30548800	4.21963500
H	1.43117200	-0.20275200	4.66944100
H	3.05502900	0.44571600	5.01167000
H	1.98011400	1.29671700	3.86472300
C	1.82172700	-0.68897000	1.97247400
Rh	-0.03285600	-2.10504800	0.26354800
O	-1.48857500	-1.85240800	1.69643800
O	-1.45233600	-2.25762200	-1.21602900

O	-1.49707000	0.40860600	1.37267500
O	-1.47366500	0.00529000	-1.53115300
C	-1.91656900	-0.66675400	1.93949400
C	-3.01261000	-0.52469500	3.01988700
C	-2.40761400	-1.00214100	4.36532400
H	-2.04079700	-2.03723400	4.29226800
H	-3.17507600	-0.95602900	5.15635300
H	-1.56806700	-0.35669600	4.67257300
C	-3.48191800	0.93659100	3.14796000
H	-2.64814300	1.60183600	3.41711900
H	-4.24741300	1.00702200	3.93961100
H	-3.91721000	1.30776200	2.20901100
C	-4.21799700	-1.46775400	2.66525300
H	-3.85641500	-2.50830900	2.70808800
H	-4.96022300	-1.34821300	3.47457000
C	-4.86825200	-1.21352000	1.31873400
C	-5.98823100	-0.37149700	1.17238700
H	-6.44210900	0.08777300	2.05635700
C	-6.53339700	-0.13059200	-0.09741400
H	-7.41358700	0.51157100	-0.19822700
C	-5.95684200	-0.70719300	-1.23889300
H	-6.38693500	-0.50849900	-2.22584300
C	-4.83646200	-1.55321700	-1.12134000
C	-4.33156800	-1.81493000	0.16568800
H	-3.48686700	-2.49898300	0.27239700
C	-4.15660800	-2.16767700	-2.32977100
H	-4.87900200	-2.27349800	-3.15870900
H	-3.80406000	-3.18098000	-2.07608600
C	-2.93295800	-1.36290500	-2.90105900
C	-3.38561600	0.00141200	-3.45399200
H	-3.84573900	0.62374100	-2.67296800
H	-4.12584200	-0.15474600	-4.25727300
H	-2.53616300	0.56053300	-3.87461500
C	-2.29352900	-2.20288100	-4.03602300
H	-1.43799100	-1.67269700	-4.48612200
H	-3.03652100	-2.38097500	-4.83172600
H	-1.94095200	-3.17561800	-3.66112300
C	-1.87206900	-1.18868500	-1.79110600
N	-0.02023800	2.28847400	-0.48469200
C	-0.03193800	3.33285900	1.68183000
C	0.01081400	3.43209000	0.25447400
C	0.08263700	4.74990300	-0.35509200
C	0.06539300	5.86105000	0.49750500
C	0.00147000	5.74237000	1.89764500
C	-0.03851800	4.46670600	2.48620300
H	-0.08029400	2.33429700	2.11434100
H	0.10840600	6.86484400	0.07001400
H	-0.01163700	6.64244600	2.51822400
H	-0.08326300	4.36198900	3.57418000
C	0.26857400	4.90646200	-1.87913500
C	-0.68485600	4.02134800	-2.64454500
C	0.00042800	6.36637600	-2.35855600
C	1.74064100	4.55031000	-2.24141500
H	-0.12116000	2.48401900	-1.50123100
H	-1.73930300	3.97689700	-2.35764900
H	-0.42557900	3.70350600	-3.65917700
H	0.74246800	7.07139200	-1.94559400
H	0.07937300	6.41156800	-3.45645800
H	-1.00733200	6.70803400	-2.07342400
H	1.89882500	4.63850200	-3.33015700
H	2.43804700	5.23644700	-1.73472700
H	1.99237700	3.52266900	-1.93765300

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^tTS2b (E = -2510.09582177)

Rh	-0.01687100	0.31510300	-0.08765300
O	1.43277000	0.06203800	-1.55460500
O	1.44307200	0.51904100	1.38333300

O	1.54988400	-2.18478500	-1.14947600
O	1.56090600	-1.72837100	1.71784700
C	1.90273000	-1.12071000	-1.76776200
C	2.97042400	-1.25594500	-2.87738500
C	2.33456500	-0.79652900	-4.21396600
H	1.96670900	0.23855800	-4.14761900
H	3.08418000	-0.85086300	-5.02136800
H	1.48993900	-1.44726500	-4.49419100
C	3.44133300	-2.71766400	-3.00239700
H	2.60009900	-3.38646800	-3.23894500
H	4.18321100	-2.79519800	-3.81550500
H	3.90456300	-3.07677400	-2.07223700
C	4.18021900	-0.30614100	-2.55802600
H	3.81845600	0.73403000	-2.61479600
H	4.91062600	-0.43893800	-3.37592300
C	4.85023100	-0.53402300	-1.21672800
C	5.97188700	-1.37372900	-1.07131600
H	6.41010700	-1.85263400	-1.95269200
C	6.53839500	-1.58760600	0.19393600
H	7.41888500	-2.22935100	0.29393200
C	5.98286300	-0.98428400	1.33188700
H	6.42998000	-1.16114500	2.31527800
C	4.86095500	-0.14021400	1.21523600
C	4.33257600	0.09155200	-0.06786200
H	3.48425000	0.77181200	-0.17379100
C	4.20395500	0.50336900	2.42086200
H	4.94407700	0.64041200	3.22922800
H	3.83587100	1.50575300	2.14633100
C	3.00261700	-0.29576600	3.04403900
C	3.47945100	-1.63980800	3.62727000
H	3.93068300	-2.28074800	2.85636200
H	4.23272100	-1.45235900	4.41133000
H	2.64393000	-2.19517500	4.07984100
C	2.37983400	0.57113900	4.16764300
H	1.53097300	0.05287800	4.64344000
H	3.13494000	0.76635900	4.94756100
H	2.02503700	1.53654200	3.77678700
C	1.92378600	-0.52488500	1.96418300
Rh	0.11656100	-2.08700300	0.31760000
O	-1.32388200	-1.85586800	1.77804300
O	-1.31176000	-2.39459300	-1.11482200
O	-1.46748900	0.39346500	1.37777600
O	-1.49367500	-0.16049500	-1.51933200
C	-1.81036900	-0.68417700	1.98783600
C	-2.88820900	-0.56233000	3.09052300
C	-2.23452500	-0.97180800	4.43521400
H	-1.81933700	-1.98972000	4.38338300
H	-2.98799800	-0.93986900	5.24032200
H	-1.42238200	-0.27742500	4.70722500
C	-3.41964100	0.88024700	3.18754500
H	-2.61114400	1.58841400	3.42228700
H	-4.17342400	0.93938700	3.99133600
H	-3.88616700	1.20652200	2.24699500
C	-4.05735300	-1.56809100	2.79145000
H	-3.65155800	-2.59031200	2.86743300
H	-4.79187000	-1.44842200	3.60782100
C	-4.73651600	-1.39445200	1.44706300
C	-5.88148900	-0.59069100	1.28099900
H	-6.33288900	-0.10177100	2.15013800
C	-6.45392700	-0.42526600	0.01113800
H	-7.35253300	0.18824700	-0.10441900
C	-5.88105100	-1.04099900	-1.11157500
H	-6.33258200	-0.90185800	-2.09907000
C	-4.73604900	-1.85011400	-0.97364000
C	-4.20242200	-2.03580200	0.31467700
H	-3.33628400	-2.68982400	0.43874200
C	-4.05775700	-2.50354800	-2.16179000
H	-4.79232900	-2.68755300	-2.96619200

H	-3.65601200	-3.48475900	-1.85958600
C	-2.88317700	-1.68200900	-2.80586800
C	-3.40791300	-0.37950400	-3.43801500
H	-3.88543800	0.27040500	-2.69094000
H	-4.15039400	-0.62298500	-4.21712900
H	-2.59138400	0.18973000	-3.90727800
C	-2.22010800	-2.56375100	-3.89441400
H	-1.39767400	-2.02491100	-4.39345300
H	-2.96498900	-2.82849900	-4.66374500
H	-1.81535900	-3.49170700	-3.46313800
C	-1.81740500	-1.38000200	-1.72754600
N	-0.09800400	2.33783900	-0.67623100
C	-0.11885200	3.40091200	1.54957100
C	-0.12891700	3.49003300	0.13812100
C	-0.25419000	4.77727600	-0.47476500
C	-0.30666400	5.91979200	0.33369500
C	-0.25990300	5.82231200	1.73424300
C	-0.17693800	4.55721600	2.33548000
H	-0.04840000	2.41693000	2.01171700
H	-0.40581700	6.90582700	-0.12898300
H	-0.30606900	6.72683000	2.34703300
H	-0.15553800	4.46858100	3.42586600
C	-0.33774200	4.79924300	-2.01026500
C	-1.20358400	5.98363900	-2.52860600
C	1.08773000	4.92335600	-2.61452800
C	-0.98953200	3.50566700	-2.42210200
H	-2.21023500	5.96421100	-2.08194200
H	-0.73919100	6.95709000	-2.29360000
H	-1.30847400	5.92356500	-3.62413900
H	1.74796600	4.10527300	-2.28060600
H	1.04658200	4.89944400	-3.71725600
H	1.55681800	5.87144300	-2.30698600
H	0.65342300	2.38469000	-1.37739500
H	-2.01283900	3.30217600	-2.10032700
H	-0.64025600	2.96311500	-3.30560900

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^sTS1c (E = -2510.11135369)

Rh	-0.06916100	0.27415600	-0.28068000
O	1.42160200	-0.48727800	-1.54385900
O	1.36482400	0.91462400	1.07982200
O	1.46214600	-2.50271800	-0.47392200
O	1.41295600	-1.13596100	2.09305800
C	1.86179400	-1.68666500	-1.37562100
C	2.95032900	-2.18099500	-2.35517700
C	2.40193700	-2.04947800	-3.79806300
H	2.10897100	-1.01286300	-4.02227200
H	3.17442200	-2.36145700	-4.52111900
H	1.52204700	-2.69719200	-3.94503200
C	3.30769700	-3.65149000	-2.06401400
H	2.42485800	-4.30137500	-2.16201700
H	4.06882100	-3.99256100	-2.78659300
H	3.70749900	-3.77873700	-1.04782700
C	4.22415500	-1.26932400	-2.23062700
H	3.96089600	-0.26862000	-2.61208300
H	4.97860800	-1.68686400	-2.92094500
C	4.80646700	-1.13655900	-0.83645900
C	5.82773200	-1.98079400	-0.35786000
H	6.25386400	-2.74661000	-1.01380500
C	6.31358300	-1.83393500	0.95020500
H	7.11700000	-2.48551700	1.30679800
C	5.78043600	-0.85579000	1.80337300
H	6.16839700	-0.75091800	2.82154700
C	4.75994100	0.00249600	1.34956500
C	4.31107900	-0.14232400	0.02515700
H	3.54388200	0.54283000	-0.34027700
C	4.12302100	1.06081100	2.22924800
H	4.83840200	1.39886700	3.00011500

H	3.87092100	1.93935800	1.61228600
C	2.82042400	0.61769900	2.98949400
C	3.14887000	-0.45785200	4.04280500
H	3.58687500	-1.35591200	3.58425800
H	3.86942800	-0.04829500	4.77154900
H	2.24525600	-0.76746000	4.58993400
C	2.22136700	1.86641600	3.68283300
H	1.31621300	1.60357500	4.25509000
H	2.95493400	2.29014800	4.38943000
H	1.95464800	2.63985300	2.94721600
C	1.78494400	0.08309500	1.97227800
Rh	0.00582900	-1.89269300	0.80670900
O	-1.45372400	-1.23376100	2.09368100
O	-1.41069100	-2.55450000	-0.53653900
O	-1.54057900	0.79660600	1.06087100
O	-1.52401300	-0.50372400	-1.54151100
C	-1.92120500	-0.04869900	1.95559700
C	-3.00706100	0.39654100	2.96037200
C	-2.38574400	0.33915900	4.37950200
H	-2.00956900	-0.66919000	4.60831300
H	-3.14672000	0.61027600	5.13065800
H	-1.54933500	1.05122700	4.47445000
C	-3.49388900	1.82676700	2.66587800
H	-2.66480100	2.54829100	2.72352200
H	-4.25103500	2.11784800	3.41379500
H	-3.94748000	1.90400200	1.66737300
C	-4.20518600	-0.61968800	2.91071700
H	-3.83454600	-1.59317800	3.27123800
H	-4.95128000	-0.26364900	3.64336500
C	-4.85148500	-0.79964300	1.55058100
C	-5.96778800	-0.04335500	1.14162500
H	-6.42299200	0.67297200	1.83322100
C	-6.51061300	-0.21714900	-0.14030000
H	-7.38921500	0.36141000	-0.44161800
C	-5.93629400	-1.13013700	-1.03736100
H	-6.36572000	-1.25546700	-2.03643700
C	-4.81958900	-1.89904700	-0.65427500
C	-4.31614900	-1.73817500	0.64971300
H	-3.47337000	-2.35546400	0.96908300
C	-4.13851000	-2.86872400	-1.60035200
H	-4.86087700	-3.24283100	-2.34756900
H	-3.77866800	-3.74194300	-1.03165800
C	-2.92030800	-2.28441200	-2.40326600
C	-3.38344000	-1.18901000	-3.38206000
H	-3.86611600	-0.35236900	-2.85645300
H	-4.10668500	-1.61647900	-4.09766600
H	-2.53406300	-0.78248200	-3.95139600
C	-2.26244500	-3.44542900	-3.19133400
H	-1.41230400	-3.08165000	-3.79172600
H	-2.99727200	-3.89148400	-3.88283200
H	-1.89672000	-4.23055800	-2.51258700
C	-1.87018800	-1.73308700	-1.41083700
N	-0.25150000	2.01227300	-1.32460700
C	2.03782200	2.69572000	-1.69984500
C	0.68027300	3.03197400	-1.44918500
C	0.30378600	4.41622200	-1.43939700
C	1.27303800	5.38579500	-1.71180200
C	2.61126900	5.04073200	-1.97571500
C	2.98206600	3.68932200	-1.97265800
H	2.30352300	1.63962200	-1.73160100
H	0.99185000	6.44316500	-1.69974900
H	3.35151500	5.82303600	-2.16249400
H	4.01797500	3.40133700	-2.17461200
C	-1.18071100	4.75854800	-1.20971300
C	-1.35591900	6.04366500	-0.35080100
C	-1.87141900	4.95406200	-2.58772100
C	-1.81814000	3.60575300	-0.46537300
H	-0.80913200	5.96199100	0.60173100

H	-0.98726400	6.93402600	-0.88788500
H	-2.42280100	6.21227200	-0.12822700
H	-1.79539800	4.04240100	-3.20211700
H	-2.93987800	5.19999800	-2.46083800
H	-1.39379000	5.77549800	-3.14524800
H	-2.87950800	3.39019500	-0.65206100
H	-1.28223600	2.46790800	-1.22550800
H	-1.50750500	3.44283600	0.57066000

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^sCc (E = -2510.21052819)

Rh	-0.07313900	0.27672800	-0.22060900
O	1.39975700	-0.46147000	-1.50655600
O	1.35370700	0.78087000	1.19985400
O	1.32231700	-2.52152600	-0.52128800
O	1.26235700	-1.31380200	2.11803100
C	1.78036400	-1.68708700	-1.37663100
C	2.87035600	-2.18933400	-2.35256800
C	2.33234500	-2.03347600	-3.79731200
H	2.06344200	-0.98827800	-4.01328100
H	3.10095900	-2.35400400	-4.52092000
H	1.43942000	-2.66059100	-3.95453800
C	3.20407100	-3.66837700	-2.07925700
H	2.31224000	-4.30312400	-2.19269100
H	3.96641400	-4.01191000	-2.79959200
H	3.59360500	-3.81480200	-1.06160100
C	4.15758500	-1.30003600	-2.21369800
H	3.90808700	-0.28602800	-2.56854500
H	4.90265600	-1.70976900	-2.91886600
C	4.75259400	-1.21300700	-0.82132100
C	5.80076000	-2.05399300	-0.39905600
H	6.23297800	-2.77732200	-1.09804400
C	6.30385800	-1.95865700	0.90703100
H	7.12833700	-2.60633400	1.22013300
C	5.75881900	-1.03687700	1.81325100
H	6.15777300	-0.97163100	2.83054200
C	4.71017200	-0.18382700	1.41702400
C	4.24418300	-0.27294100	0.09300300
H	3.45376700	0.40822400	-0.22892000
C	4.06669000	0.80894500	2.36595800
H	4.78467000	1.10029200	3.15348600
H	3.80323200	1.72465500	1.81127100
C	2.77272000	0.30452600	3.09987000
C	3.10297000	-0.86809600	4.04264300
H	3.51216900	-1.72792500	3.49312400
H	3.84886500	-0.54168100	4.78762800
H	2.20568200	-1.21014900	4.58029300
C	2.19357700	1.48683400	3.91744500
H	1.28648100	1.18039400	4.46424100
H	2.93504700	1.82898500	4.65934100
H	1.93554600	2.33377800	3.26370000
C	1.71385600	-0.11546300	2.05318100
Rh	-0.14871400	-1.92629200	0.76823100
O	-1.61270600	-1.25451400	2.05116200
O	-1.56649900	-2.43118900	-0.65476700
O	-1.56716800	0.82451300	1.10574200
O	-1.49204700	-0.34392800	-1.58243900
C	-2.01240700	-0.04003900	1.94719500
C	-3.11192200	0.41135300	2.93691200
C	-2.54763100	0.25910700	4.37249200
H	-2.23057100	-0.77656100	4.56649100
H	-3.31986600	0.53541000	5.11045300
H	-1.68012700	0.92175700	4.52740500
C	-3.51749600	1.87625600	2.69234200
H	-2.65702400	2.55116800	2.81792700
H	-4.29155900	2.17072800	3.42171300
H	-3.92174400	2.02249400	1.68018100
C	-4.35549700	-0.53991100	2.80135400

H	-4.04270500	-1.54642700	3.12413500
H	-5.10792000	-0.18404500	3.52765900
C	-4.96764100	-0.62449500	1.41652200
C	-6.04391000	0.19293800	1.01827400
H	-6.49129500	0.88976700	1.73449000
C	-6.55805800	0.10474700	-0.28408000
H	-7.40699700	0.73010600	-0.57696700
C	-5.99356400	-0.78341500	-1.21180100
H	-6.40108400	-0.84373800	-2.22611100
C	-4.91644800	-1.61216700	-0.84018800
C	-4.44248900	-1.53602700	0.48246400
H	-3.63148900	-2.19972600	0.79049400
C	-4.24934100	-2.56010400	-1.81827800
H	-4.96604400	-2.86429100	-2.60204500
H	-3.93989800	-3.47529400	-1.28759100
C	-2.98625600	-1.98919400	-2.55803500
C	-3.37531900	-0.81779600	-3.47899800
H	-3.81777200	0.01409000	-2.91175500
H	-4.11408900	-1.16212400	-4.22280300
H	-2.49864200	-0.43223300	-4.02178100
C	-2.36620500	-3.13287700	-3.40081700
H	-1.48511900	-2.77756700	-3.96047500
H	-3.10438400	-3.50283600	-4.13255800
H	-2.05453200	-3.97274100	-2.76165500
C	-1.93489000	-1.55063600	-1.51202200
N	-0.19954400	2.30485800	-1.24917800
C	2.21868200	2.65303000	-1.96048700
C	0.97477900	3.11709600	-1.52432000
C	0.71943000	4.48271900	-1.31457900
C	1.74183000	5.41640300	-1.52067900
C	3.00549800	4.96749500	-1.94258300
C	3.23600300	3.59987000	-2.16829600
H	2.38259100	1.58537700	-2.11385300
H	1.56156800	6.48421900	-1.36319800
H	3.81304700	5.68815800	-2.09900000
H	4.22292900	3.26313100	-2.49765400
C	-0.75002600	4.70028300	-0.96346000
C	-0.97005200	5.67207600	0.21138600
C	-1.52014600	5.19467200	-2.21430700
C	-1.16191300	3.24705600	-0.57885900
H	-0.39992700	5.35793900	1.10062600
H	-0.65254500	6.69460200	-0.05296000
H	-2.03809300	5.71861700	0.48499500
H	-1.41269900	4.49309800	-3.05881900
H	-2.59584200	5.30158000	-1.99157500
H	-1.14150900	6.17480700	-2.54815900
H	-2.19175900	2.98315200	-0.85661300
H	-0.59867600	1.95064100	-2.12846800
H	-1.05475800	3.09329300	0.50378200

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^tTS1c (E = -2510.11423303)

Rh	0.05296600	0.27674400	-0.23286900
O	-1.37910900	0.79626200	1.18615900
O	-1.44233500	-0.37788300	-1.53531500
O	-1.37854400	-1.30868700	2.07570800
O	-1.48286000	-2.45749300	-0.59021500
C	-1.77846800	-0.09265200	2.03012400
C	-2.81384800	0.35952500	3.08589800
C	-2.19210500	1.52188400	3.90055100
H	-1.91030800	2.36091300	3.24674600
H	-2.91886300	1.88603700	4.64630500
H	-1.29265000	1.18631700	4.44271500
C	-3.16889500	-0.80701500	4.02769800
H	-2.27686900	-1.17840600	4.55448600
H	-3.89574900	-0.46020700	4.78197200
H	-3.61051000	-1.65163000	3.47968900
C	-4.10020400	0.90241600	2.36562800

H	-3.82088500	1.82278300	1.82660500
H	-4.80805200	1.19441600	3.16184900
C	-4.76555500	-0.06014900	1.40105400
C	-5.81887100	-0.91324200	1.78406600
H	-6.21005600	-0.87064300	2.80549900
C	-6.37949400	-1.80576800	0.85797200
H	-7.20793900	-2.45326800	1.16061500
C	-5.88778500	-1.87250500	-0.45435800
H	-6.33319600	-2.57307300	-1.16792600
C	-4.83481800	-1.03092600	-0.86346900
C	-4.31212900	-0.12022800	0.07144800
H	-3.51976300	0.56377500	-0.23882200
C	-4.24597000	-1.08460600	-2.25989800
H	-5.00323800	-1.44564400	-2.97835600
H	-3.96370000	-0.06678700	-2.57702700
C	-2.98709400	-2.00858100	-2.43491800
C	-3.36671400	-3.48696800	-2.22442000
H	-3.76236200	-3.66560100	-1.21432700
H	-4.13738600	-3.77476400	-2.95993900
H	-2.49489700	-4.14383800	-2.36528800
C	-2.43917000	-1.80712900	-3.87026800
H	-1.56665900	-2.45555500	-4.05322100
H	-3.21635600	-2.07276000	-4.60673500
H	-2.13611800	-0.76316200	-4.04064400
C	-1.88722400	-1.58445300	-1.43451100
Rh	0.00398400	-1.94793400	0.71471900
O	1.39130900	-2.52458000	-0.69159100
O	1.49117400	-1.37695800	2.01589400
O	1.46836500	-0.41654700	-1.56769000
O	1.57041300	0.71798500	1.10980800
C	1.82835400	-1.64877200	-1.52368300
C	2.85741000	-2.12497800	-2.57395600
C	2.17058600	-3.20396500	-3.44960700
H	1.80066200	-4.03936200	-2.83614300
H	2.88995700	-3.60046000	-4.18603200
H	1.31974300	-2.77702200	-4.00569300
C	3.32334600	-0.95432600	-3.45993200
H	2.47372700	-0.49163600	-3.98428900
H	4.03516700	-1.32658600	-4.21657000
H	3.82140700	-0.17200200	-2.86925400
C	4.07617100	-2.79313100	-1.84134200
H	3.70736000	-3.69801300	-1.33096700
H	4.77455200	-3.12585600	-2.62978500
C	4.79676400	-1.90773200	-0.84296500
C	5.92548300	-1.14184400	-1.19519800
H	6.33526700	-1.21154100	-2.20789600
C	6.53529700	-0.30185900	-0.25160800
H	7.42210400	0.27542500	-0.53030700
C	6.01503600	-0.19708200	1.04695600
H	6.49546500	0.46513100	1.77439700
C	4.88723900	-0.95187100	1.42579200
C	4.31717300	-1.81995100	0.47689200
H	3.46474100	-2.43671100	0.77029900
C	4.26477800	-0.84035600	2.80422700
H	5.02862900	-0.53623000	3.54201200
H	3.88664200	-1.82757700	3.11654000
C	3.08316700	0.18816300	2.93321600
C	3.58183900	1.62550400	2.69728600
H	4.01648300	1.74339500	1.69432900
H	4.35620300	1.87253000	3.44359100
H	2.76172100	2.35163200	2.79975500
C	2.49502200	0.06646700	4.36253900
H	1.66876200	0.78101000	4.51192400
H	3.27629200	0.29339600	5.10756000
H	2.11407700	-0.94853300	4.55140300
C	1.96426400	-0.18650900	1.93426400
N	0.17967000	2.17382000	-0.91892900
C	-2.01009400	2.84800100	-1.69653500

C	-0.66732900	3.16027000	-1.31229500
C	-0.22270800	4.54154500	-1.36577900
C	-1.12932400	5.50740800	-1.81287100
C	-2.44429900	5.18052700	-2.19317600
C	-2.87966100	3.84466800	-2.12768400
H	-2.30840500	1.80004600	-1.67144300
H	-0.81613400	6.55332400	-1.86347300
H	-3.12121800	5.96708800	-2.53741700
H	-3.89953600	3.58353700	-2.42491000
C	1.17544400	4.89957400	-0.82815800
C	1.73211200	6.20571000	-1.45604600
C	1.06430800	5.08438400	0.71163900
C	2.14209000	3.76302600	-1.13322400
H	1.74745500	6.14865900	-2.55638700
H	1.13798600	7.08755300	-1.16105000
H	2.76329500	6.37372000	-1.10523100
H	0.71483400	4.15828600	1.19448300
H	2.04863400	5.34622600	1.13705500
H	0.35478000	5.89070400	0.95848300
H	2.98528500	3.63077900	-0.44397200
H	1.27377500	2.66653600	-0.89528200
H	2.40334500	3.61884700	-2.19081500

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TM1c (E = -2510.11878607)

Rh	0.04692300	0.25725400	-0.22972100
O	-1.37527900	0.79351100	1.18697200
O	-1.45328800	-0.38400500	-1.52962800
O	-1.38791900	-1.30807700	2.08253800
O	-1.50487400	-2.46033200	-0.57845000
C	-1.78051400	-0.08953500	2.03389800
C	-2.81207000	0.37386400	3.08796000
C	-2.17551400	1.52495100	3.90731000
H	-1.87953800	2.36131800	3.25632900
H	-2.89906500	1.89803000	4.65178500
H	-1.28270600	1.17489500	4.45133300
C	-3.18604600	-0.78987900	4.02570000
H	-2.30057100	-1.17511800	4.55355600
H	-3.90988200	-0.43517600	4.77922400
H	-3.63804100	-1.62666100	3.47414400
C	-4.08785000	0.93822000	2.36513300
H	-3.79168900	1.85328100	1.82618300
H	-4.79204300	1.24247000	3.16002000
C	-4.76722000	-0.01430200	1.40043500
C	-5.83319400	-0.85085400	1.78515200
H	-6.22432800	-0.79943900	2.80621100
C	-6.40604400	-1.73824200	0.86174600
H	-7.24414200	-2.37257200	1.16573600
C	-5.91330600	-1.81695000	-0.44944100
H	-6.36713400	-2.51417800	-1.16098100
C	-4.84803300	-0.99183600	-0.86028700
C	-4.31353100	-0.08419000	0.07117800
H	-3.51188900	0.58796800	-0.24180600
C	-4.25739900	-1.06287500	-2.25511200
H	-5.01830700	-1.41816100	-2.97259900
H	-3.95950900	-0.05151900	-2.57830400
C	-3.01159500	-2.00622100	-2.42043100
C	-3.41117600	-3.47735900	-2.19655000
H	-3.80957000	-3.64154800	-1.18509300
H	-4.18543600	-3.76165600	-2.92965800
H	-2.54816200	-4.14704600	-2.33097800
C	-2.45992600	-1.82615000	-3.85731100
H	-1.59564400	-2.48751000	-4.03298300
H	-3.23987200	-2.08912500	-4.59181200
H	-2.14338700	-0.78792200	-4.03803100
C	-1.90640200	-1.58700000	-1.42420000
Rh	-0.01073800	-1.96231000	0.72287100
O	1.36850600	-2.55206100	-0.68464800

O	1.48552500	-1.39226100	2.01743300
O	1.45500500	-0.44713000	-1.56704800
O	1.57431800	0.69692400	1.09934000
C	1.80785900	-1.68103100	-1.52102800
C	2.82975900	-2.16711500	-2.57374200
C	2.13328100	-3.24565800	-3.44224900
H	1.76136500	-4.07650600	-2.82383800
H	2.84725700	-3.64905700	-4.18019000
H	1.28239400	-2.81620900	-3.99631800
C	3.29814000	-1.00241900	-3.46630400
H	2.44850200	-0.53587200	-3.98716600
H	4.00315700	-1.38181400	-4.22577900
H	3.80467500	-0.22137200	-2.88111000
C	4.04824600	-2.83925800	-1.84444200
H	3.67695100	-3.74030000	-1.32908400
H	4.74125600	-3.17867200	-2.63476000
C	4.77818700	-1.95434600	-0.85251900
C	5.91072000	-1.19735900	-1.21176000
H	6.31648600	-1.27383100	-2.22559600
C	6.52951600	-0.35773900	-0.27366900
H	7.41918600	0.21245600	-0.55783000
C	6.01469800	-0.24445500	1.02635700
H	6.50209000	0.41736300	1.74952400
C	4.88326000	-0.99025700	1.41207000
C	4.30384700	-1.85804300	0.46862000
H	3.44804500	-2.46744500	0.76752200
C	4.26617600	-0.86923500	2.79207100
H	5.03421500	-0.56678400	3.52619800
H	3.88285600	-1.85273600	3.10972600
C	3.09145700	0.16711300	2.92007200
C	3.59869400	1.60003900	2.67532600
H	4.02742100	1.71201600	1.66910600
H	4.37983300	1.84412700	3.41551000
H	2.78472100	2.33246900	2.78189000
C	2.50831500	0.05660400	4.35239800
H	1.68724200	0.77715100	4.50158600
H	3.29410600	0.28215800	5.09307100
H	2.12161100	-0.95495100	4.54785800
C	1.96617100	-0.20587600	1.92758400
N	0.25250000	2.18460400	-0.89398600
C	-1.89715300	2.83198700	-1.74861300
C	-0.57664200	3.17759900	-1.32118400
C	-0.16562600	4.57089800	-1.36722500
C	-1.08776900	5.50335600	-1.85858700
C	-2.37886400	5.14091700	-2.28424600
C	-2.78109500	3.79566800	-2.22090200
H	-2.16837500	1.77623800	-1.72348800
H	-0.80675900	6.55722900	-1.91074000
H	-3.06127700	5.90830600	-2.65962500
H	-3.78226400	3.50273700	-2.55004500
C	1.20119700	5.00761500	-0.79973600
C	1.57181600	6.46687700	-1.20730000
C	1.13564600	4.95460000	0.75528600
C	2.31301800	4.12185000	-1.30806600
H	1.57662500	6.59508800	-2.30142800
H	0.87320000	7.20002300	-0.76811000
H	2.57893900	6.70532500	-0.82996700
H	0.88640200	3.94470200	1.11423800
H	2.10786400	5.24647100	1.18863800
H	0.36824300	5.65101000	1.13003300
H	3.22821700	4.01203100	-0.71892800
H	1.22427900	2.52502900	-0.75003000
H	2.36247800	3.86218700	-2.36939200

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^TTS2c (E = -2510.09502620)

Rh	-0.04170900	0.33317800	-0.13127300
O	1.45137100	0.02544000	-1.57372500

O	1.39093100	0.59651000	1.35136400
O	1.55877700	-2.19926500	-1.11098900
O	1.52232900	-1.65605800	1.73620200
C	1.93125100	-1.15574000	-1.75393100
C	3.02039300	-1.32909700	-2.83439400
C	2.44241300	-0.83416700	-4.18419800
H	2.10960300	0.21255400	-4.11664600
H	3.21382600	-0.90795100	-4.96905600
H	1.58418800	-1.45189900	-4.49631200
C	3.43329700	-2.80904400	-2.95265000
H	2.57088900	-3.44379800	-3.20680100
H	4.18689300	-2.91560100	-3.75153200
H	3.86393700	-3.18661200	-2.01410600
C	4.26229000	-0.43583100	-2.47634700
H	3.95400100	0.61974400	-2.55983700
H	5.01472100	-0.61409900	-3.26500200
C	4.87236200	-0.67292900	-1.10751000
C	5.94920400	-1.55666800	-0.89825600
H	6.39766500	-2.08019900	-1.74858500
C	6.46091200	-1.75582400	0.39306300
H	7.30698700	-2.43324600	0.54272700
C	5.89892800	-1.09091500	1.49357200
H	6.30852600	-1.25377900	2.49553500
C	4.82119700	-0.20193900	1.31302600
C	4.34555800	0.00421500	0.00627600
H	3.52987200	0.71292000	-0.14576100
C	4.15580600	0.52600300	2.46547100
H	4.87338100	0.66458700	3.29364900
H	3.84913800	1.53130400	2.13190200
C	2.89372400	-0.18204800	3.07826800
C	3.29298600	-1.50355400	3.76251100
H	3.76317000	-2.20190500	3.05538300
H	4.00853600	-1.29228300	4.57556500
H	2.41640500	-2.00623600	4.19881100
C	2.25882800	0.77698600	4.11631800
H	1.37954800	0.31406400	4.59400000
H	2.99104200	1.00627200	4.90882600
H	1.94100000	1.71961600	3.64637400
C	1.85417800	-0.43840100	1.96275000
Rh	0.10963700	-2.06035700	0.31221500
O	-1.33768400	-1.90024000	1.74959600
O	-1.31239500	-2.34205200	-1.16373100
O	-1.54675700	0.33652500	1.37451400
O	-1.48514400	-0.09467000	-1.54180000
C	-1.85942500	-0.74398900	1.97989800
C	-2.93468300	-0.67758600	3.08962600
C	-2.28615400	-1.15724300	4.41280400
H	-1.87307400	-2.17183500	4.30943900
H	-3.04150900	-1.16445100	5.21686800
H	-1.47230300	-0.48066100	4.72182900
C	-3.45960600	0.76003200	3.25931100
H	-2.64423800	1.45007500	3.52399200
H	-4.20881400	0.78467300	4.06919800
H	-3.92986900	1.13156900	2.33773600
C	-4.10731000	-1.66146300	2.73582700
H	-3.70949600	-2.68880100	2.77801300
H	-4.85294800	-1.56835800	3.54553600
C	-4.76450900	-1.43279300	1.38866100
C	-5.90140400	-0.61535500	1.23365800
H	-6.36396500	-0.15532000	2.11269800
C	-6.45375600	-0.40243100	-0.03822100
H	-7.34765800	0.21951300	-0.14560400
C	-5.86920400	-0.98435100	-1.17303900
H	-6.30753100	-0.81093100	-2.16109000
C	-4.73124300	-1.80557100	-1.04650500
C	-4.21712300	-2.03744800	0.24236300
H	-3.35647500	-2.70073600	0.35620200
C	-4.04338100	-2.42850600	-2.24576000

H	-4.77151500	-2.59078400	-3.06056700
H	-3.64643100	-3.41783700	-1.96479400
C	-2.86092700	-1.59493500	-2.85969100
C	-3.37872500	-0.28081800	-3.47410200
H	-3.87047100	0.35325200	-2.72226700
H	-4.10993900	-0.51044700	-4.26777600
H	-2.55759000	0.29857200	-3.92317100
C	-2.18656000	-2.45543400	-3.95847400
H	-1.35958100	-1.90676200	-4.43881000
H	-2.92378300	-2.70608400	-4.73971600
H	-1.78594600	-3.39090700	-3.53993000
C	-1.80572700	-1.32037600	-1.76389100
N	-0.45724500	2.36143100	-0.45349600
C	1.83047100	3.23101500	-0.69553700
C	0.43597500	3.44183400	-0.59545700
C	-0.06055000	4.78411700	-0.56498400
C	0.84409900	5.84988200	-0.66010700
C	2.22631400	5.62606400	-0.77455700
C	2.71437700	4.31075200	-0.78857800
H	2.19579000	2.20570400	-0.72888200
H	0.47369300	6.87837500	-0.62817400
H	2.91340800	6.47406300	-0.84239100
H	3.78862500	4.12261700	-0.87569000
C	-1.58234800	4.95412900	-0.42725200
C	-1.95745600	6.26528100	0.32225600
C	-2.23278000	4.98223900	-1.83762800
C	-2.08144500	3.78087500	0.37106400
H	-1.47109700	6.31124800	1.30949300
H	-1.65925200	7.15860500	-0.25328000
H	-3.04835200	6.31641500	0.46974200
H	-2.00133400	4.06987100	-2.41254700
H	-3.33053300	5.06463600	-1.75795000
H	-1.86243200	5.84210700	-2.41836400
H	-1.19297800	2.35559600	-1.17187300
H	-1.72968500	3.64561500	1.39548500
H	-3.01501100	3.27764700	0.10422000

106

^sTS1d (E = -2510.11264920)

Rh	0.07882900	0.30502800	-0.20220600
O	-1.37104900	0.63536000	1.24965600
O	-1.32187200	-0.56882200	-1.44523200
O	-1.03477000	-1.43450200	2.16401900
O	-1.02251600	-2.61256900	-0.47869200
C	-1.62238500	-0.29804000	2.10360400
C	-2.71313600	0.00575800	3.15676800
C	-2.21992600	1.19760600	4.01682800
H	-2.03273700	2.08628500	3.39545300
H	-2.98197100	1.45150400	4.77293400
H	-1.28971300	0.93998400	4.54982900
C	-2.95629100	-1.22005000	4.05770600
H	-2.03596500	-1.51514300	4.58383600
H	-3.72188400	-0.97285500	4.81297000
H	-3.30550600	-2.08745200	3.47918100
C	-4.03903600	0.44152100	2.43657800
H	-3.83989400	1.38699000	1.90582400
H	-4.77248000	0.66405700	3.23204700
C	-4.61801100	-0.57024900	1.46615000
C	-5.61208100	-1.49289300	1.84694100
H	-6.01610700	-1.46677200	2.86397000
C	-6.09635500	-2.43493900	0.92721800
H	-6.87956100	-3.13685000	1.22897300
C	-5.58168000	-2.48380100	-0.37680900
H	-5.96194900	-3.22639600	-1.08563400
C	-4.58700900	-1.57333900	-0.78392000
C	-4.14464000	-0.61084100	0.14196900
H	-3.39751300	0.12201900	-0.17070200
C	-3.97196700	-1.61651200	-2.16957900

H	-4.67870200	-2.07377300	-2.88476800
H	-3.78223100	-0.58796700	-2.51971500
C	-2.62827200	-2.42186500	-2.28728300
C	-2.85745400	-3.91473100	-1.98522600
H	-3.23792300	-4.06887800	-0.96530000
H	-3.59283000	-4.32421100	-2.69865100
H	-1.92309900	-4.48708600	-2.08695100
C	-2.09172100	-2.25723100	-3.73219200
H	-1.15127700	-2.81536400	-3.86967900
H	-2.82812000	-2.65359700	-4.45139700
H	-1.90489300	-1.19934600	-3.97070900
C	-1.57944300	-1.82831100	-1.32120000
Rh	0.41018900	-1.88579800	0.78266000
O	1.82942000	-2.25111600	-0.67258200
O	1.83346200	-1.10183000	2.03407500
O	1.53508200	-0.17789000	-1.59448500
O	1.54387900	0.96799100	1.11554800
C	2.09357600	-1.33383000	-1.53216300
C	3.16393200	-1.66423900	-2.59909200
C	2.62518000	-2.83924100	-3.45524200
H	2.40369300	-3.71833700	-2.83110200
H	3.37596200	-3.12502100	-4.21131000
H	1.70440400	-2.54899600	-3.98787600
C	3.44015800	-0.44752300	-3.50241500
H	2.52767600	-0.12894500	-4.02888000
H	4.19766400	-0.71637100	-4.25845600
H	3.81301000	0.41101800	-2.92557500
C	4.48057000	-2.14263300	-1.88852900
H	4.25636300	-3.08621600	-1.36444000
H	5.20394100	-2.37949900	-2.68923800
C	5.08983000	-1.15515400	-0.91183900
C	6.09341000	-0.24343000	-1.29405500
H	6.48551700	-0.26391000	-2.31593900
C	6.60263400	0.67993300	-0.36891700
H	7.39386400	1.37267100	-0.67111100
C	6.10279600	0.72157100	0.94110400
H	6.50237100	1.45021800	1.65376400
C	5.09919000	-0.17862600	1.34968100
C	4.63350300	-1.12498800	0.41871100
H	3.88322700	-1.85287400	0.73507500
C	4.49732000	-0.14207100	2.74112300
H	5.22477900	0.27695600	3.45901900
H	4.27143300	-1.16961700	3.07075800
C	3.18356300	0.70802300	2.88598500
C	3.46071600	2.19596700	2.60411600
H	3.81779200	2.35663300	1.57674200
H	4.23035300	2.56462000	3.30365700
H	2.55423500	2.80384300	2.74475400
C	2.65797700	0.53524600	4.33448600
H	1.73934000	1.12365700	4.49422300
H	3.41615300	0.89209600	5.05186300
H	2.43651600	-0.52019300	4.55364000
C	2.10530300	0.14803300	1.93026200
N	-0.05505800	2.12978900	-1.08128400
C	-0.36775000	3.59836700	0.82091100
C	-0.60955100	3.28223500	-0.54383100
C	-1.34186800	4.21661400	-1.35048900
C	-1.75261800	5.42646000	-0.78456600
C	-1.48382300	5.74211900	0.56030000
C	-0.78685800	4.82091000	1.35353700
H	0.19370700	2.88539400	1.42334900
H	-2.31691900	6.13999100	-1.39233100
H	-1.83568700	6.68777700	0.98086500
H	-0.57289800	5.04837100	2.40213700
C	-1.57080900	3.86158100	-2.83238400
C	-2.95594500	4.34904700	-3.34458300
C	-0.44420900	4.50892300	-3.68473600
C	-1.52246000	2.35403700	-2.96309500

H	-3.77102000	3.97496000	-2.70533100
H	-3.00661100	5.45096200	-3.36519600
H	-3.12771600	3.99363300	-4.37429600
H	0.54908500	4.15389800	-3.36584700
H	-0.57255900	4.26898800	-4.75436000
H	-0.46014400	5.60499300	-3.57463100
H	-1.17313800	1.92630900	-3.91355400
H	-0.28793200	2.08280000	-2.18015900
H	-2.32178700	1.78171200	-2.48261000

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^sCd (E = -2510.21271258)

Rh	0.08236400	0.28221300	-0.20228700
O	-1.38893200	0.69609300	1.20798600
O	-1.32385500	-0.59978800	-1.45673200
O	-1.14083500	-1.36003300	2.17974100
O	-1.08383900	-2.62220400	-0.41864300
C	-1.69286800	-0.20753000	2.07476900
C	-2.80429700	0.14996400	3.08979100
C	-2.29575900	1.33653100	3.94820800
H	-2.06354400	2.21002700	3.32039400
H	-3.06874000	1.62677000	4.67991100
H	-1.38880000	1.05675300	4.50937500
C	-3.11876800	-1.05119600	4.00134800
H	-2.22702200	-1.36691600	4.56345300
H	-3.90162700	-0.76711000	4.72547000
H	-3.47603200	-1.91620300	3.42430900
C	-4.09096800	0.62222900	2.32321700
H	-3.83681500	1.54363900	1.77394500
H	-4.83540300	0.89612300	3.09221900
C	-4.68695100	-0.39020100	1.36376100
C	-5.73596100	-1.25195400	1.73980400
H	-6.17040900	-1.17332400	2.74152500
C	-6.23434500	-2.20057700	0.83466800
H	-7.05971800	-2.85473400	1.13159000
C	-5.67938000	-2.31739500	-0.44827700
H	-6.07038300	-3.06603900	-1.14492900
C	-4.62959600	-1.46856000	-0.85048800
C	-4.17339000	-0.49605000	0.05823500
H	-3.38282200	0.19020400	-0.25295600
C	-3.97183200	-1.59010300	-2.21181400
H	-4.67473200	-2.04588200	-2.93193800
H	-3.72624500	-0.58491600	-2.59275100
C	-2.65970900	-2.45173400	-2.25169300
C	-2.95626100	-3.91722500	-1.88086200
H	-3.36457500	-4.00230500	-0.86361600
H	-3.69265700	-4.33457400	-2.58898000
H	-2.04403300	-4.53043400	-1.93052000
C	-2.08159900	-2.38471800	-3.68839000
H	-1.15973100	-2.98377700	-3.76979300
H	-2.81333000	-2.79176600	-4.40662600
H	-1.84796200	-1.34859900	-3.97775600
C	-1.60943700	-1.84651400	-1.29119400
Rh	0.33131100	-1.87509500	0.85713100
O	1.78696400	-2.30732500	-0.54793800
O	1.73544500	-1.01506100	2.10609000
O	1.57338400	-0.25350300	-1.52750400
O	1.51557100	1.02030800	1.09060500
C	2.10345800	-1.42177800	-1.42026900
C	3.19970300	-1.81089000	-2.43980500
C	2.66939700	-3.01306100	-3.26283400
H	2.40885200	-3.85785200	-2.60749700
H	3.43994200	-3.34716100	-3.97824600
H	1.77272400	-2.73143800	-3.83940100
C	3.52403700	-0.63891700	-3.38442000
H	2.63204800	-0.32685100	-3.94898700
H	4.29545300	-0.95200600	-4.10865900
H	3.90210100	0.23467600	-2.83351400

C	4.48651300	-2.27857800	-1.66971100
H	4.22896500	-3.19414100	-1.11242500
H	5.23031700	-2.56158300	-2.43591700
C	5.08215700	-1.25981500	-0.71693100
C	6.11738800	-0.38586500	-1.10358700
H	6.54430200	-0.46063900	-2.10891800
C	6.61536600	0.56672800	-0.20214400
H	7.43269400	1.22796100	-0.50578800
C	6.07303100	0.67559900	1.08703600
H	6.46631200	1.42479800	1.78179600
C	5.03658400	-0.18500400	1.49964500
C	4.58183800	-1.16169400	0.59453000
H	3.80556800	-1.85937300	0.91629400
C	4.39108600	-0.07530500	2.86758400
H	5.10424500	0.36071500	3.58979400
H	4.13311600	-1.08253500	3.23363800
C	3.08969900	0.80244700	2.92913400
C	3.40747500	2.27215100	2.59696600
H	3.81892300	2.37970200	1.58276900
H	4.14990500	2.66022700	3.31517300
H	2.50644300	2.90019200	2.66697500
C	2.51077300	0.70344500	4.36391400
H	1.60081100	1.31790000	4.46496200
H	3.25067000	1.07307600	5.09391400
H	2.25563900	-0.33650400	4.61780100
C	2.03379900	0.22308100	1.95872300
N	0.07245300	2.27521200	-1.25461600
C	-0.52348700	3.78883800	0.69707400
C	-0.56792900	3.43123600	-0.65340600
C	-1.25150700	4.19849600	-1.61023600
C	-1.93544200	5.35219100	-1.20749100
C	-1.91393400	5.72294700	0.14833000
C	-1.20626100	4.95286400	1.08742500
H	0.01308700	3.16668700	1.41447500
H	-2.47326100	5.96582500	-1.93663700
H	-2.44882100	6.61955700	0.47381900
H	-1.19442600	5.25575500	2.13825400
C	-1.01851600	3.63453200	-3.01041900
C	-2.29936700	3.53740900	-3.86056300
C	0.04544700	4.48905600	-3.74523300
C	-0.46356400	2.21846300	-2.65815200
H	-3.08338700	2.96745000	-3.33640500
H	-2.70197800	4.53802800	-4.09046500
H	-2.09235100	3.03677100	-4.82196800
H	0.98856100	4.53754100	-3.17510300
H	0.26700400	4.06541500	-4.74007300
H	-0.31005800	5.52300200	-3.88591100
H	0.32633400	1.86919200	-3.33798300
H	1.09314700	2.40005100	-1.25966200
H	-1.27182400	1.47266600	-2.66039900

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^TTS1d (E = -2510.11639721)

Rh	0.02591900	0.29540500	-0.09342400
O	-1.42938900	0.52734100	1.37096800
O	-1.41435600	0.01788100	-1.56817700
O	-1.55951100	-1.72422500	1.73043100
O	-1.54058400	-2.21923900	-1.12433200
C	-1.91185800	-0.51473500	1.95734000
C	-2.99453200	-0.26433500	3.03112800
C	-2.37175200	0.61229200	4.14699400
H	-2.01224100	1.57193800	3.74633200
H	-3.12787100	0.81943200	4.92297700
H	-1.52620800	0.09598000	4.63100700
C	-3.48214900	-1.59768300	3.62979700
H	-2.65192100	-2.15253000	4.09257000
H	-4.23735200	-1.39493900	4.40828800
H	-3.93418300	-2.24564200	2.86537200

C	-4.18858800	0.53413000	2.39398900
H	-3.81265800	1.52979800	2.10624800
H	-4.93046900	0.68745400	3.19798700
C	-4.84650000	-0.12167900	1.19548000
C	-5.97512000	-0.95539300	1.32164400
H	-6.42585600	-1.11420600	2.30650900
C	-6.53230600	-1.57158400	0.19146800
H	-7.41788400	-2.20520200	0.29858300
C	-5.96051700	-1.38084600	-1.07507600
H	-6.39960000	-1.86970800	-1.95058900
C	-4.83204500	-0.55200300	-1.22975300
C	-4.31231200	0.08734500	-0.08922100
H	-3.45824400	0.75924300	-0.20341500
C	-4.15711100	-0.35008900	-2.57264600
H	-4.88638700	-0.49106800	-3.39028900
H	-3.78676800	0.68595200	-2.64437600
C	-2.95303300	-1.31341800	-2.87302500
C	-3.43183200	-2.77443800	-2.97345200
H	-3.89900400	-3.11503800	-2.03829500
H	-4.17227300	-2.86218200	-3.78685500
H	-2.59363200	-3.45171000	-3.19668700
C	-2.31127000	-0.88042500	-4.21545700
H	-1.47251100	-1.54359900	-4.48417800
H	-3.06017800	-0.94048600	-5.02319300
H	-1.93415300	0.15194500	-4.16333000
C	-1.88804400	-1.16514400	-1.76310700
Rh	-0.11154900	-2.08234100	0.33012200
O	1.32422200	-2.37157300	-1.11335000
O	1.32705100	-1.86132300	1.78816900
O	1.48167000	-0.12672400	-1.50223000
O	1.46647300	0.38434800	1.38519000
C	1.81421400	-1.34894800	-1.71643600
C	2.88246100	-1.62027200	-2.79993100
C	2.22893200	-2.49592600	-3.89917000
H	1.83475400	-3.43339900	-3.47882500
H	2.97655800	-2.74306700	-4.67170100
H	1.40042300	-1.96013600	-4.39126200
C	3.39207100	-0.30407600	-3.41657600
H	2.56905100	0.26255500	-3.87783700
H	4.13551000	-0.53011700	-4.19999500
H	3.86477400	0.34174900	-2.66282200
C	4.06713000	-2.43651600	-2.16719800
H	3.67617600	-3.42523500	-1.87559800
H	4.80208200	-2.60351200	-2.97488500
C	4.74099000	-1.78991700	-0.97276500
C	5.87940100	-0.97028800	-1.10334400
H	6.32840800	-0.81685800	-2.08987700
C	6.44914400	-0.36228400	0.02516800
H	7.34277200	0.25944200	-0.08503700
C	5.87998100	-0.54604400	1.29399200
H	6.32901800	-0.06332800	2.16784500
C	4.74162800	-1.36060800	1.45281900
C	4.21062000	-1.99363300	0.31426200
H	3.34969300	-2.65564100	0.43231800
C	4.06583600	-1.55411700	2.79622700
H	4.79961100	-1.43390400	3.61318200
H	3.67105300	-2.58127600	2.86327800
C	2.88550400	-0.56409800	3.10506900
C	3.40179900	0.88303000	3.21416600
H	3.86550000	1.22202800	2.27670900
H	4.15449100	0.94362900	4.01882600
H	2.58586300	1.58055500	3.45557400
C	2.23731800	-0.99249400	4.44636000
H	1.41728000	-0.31008700	4.72505100
H	2.99073500	-0.95952500	5.25149100
H	1.83309500	-2.01422700	4.38534100
C	1.81054300	-0.69100200	2.00074500
N	0.08801900	2.26590300	-0.51367900

C	0.11151200	3.41944900	1.61638000
C	0.11363100	3.43044500	0.18362600
C	0.13478900	4.70703200	-0.50996200
C	0.10628300	5.87404100	0.25921500
C	0.07942600	5.84399600	1.66573100
C	0.09322400	4.60847600	2.33798900
H	0.10967700	2.45129800	2.11592200
H	0.11252700	6.84505800	-0.24227700
H	0.05504000	6.78093300	2.22865000
H	0.08156900	4.57812300	3.43151800
C	0.30226800	4.72959900	-2.04152100
C	-0.27485700	6.02305500	-2.67842100
C	1.82241400	4.64260300	-2.35656800
C	-0.40972000	3.53140300	-2.65334700
H	-1.33204400	6.16874000	-2.40369200
H	0.29158300	6.91903700	-2.37191300
H	-0.21018100	5.95497900	-3.77652500
H	2.25539700	3.71177700	-1.95710800
H	1.98866200	4.66126500	-3.44765700
H	2.36353400	5.49210300	-1.90969900
H	0.00100100	3.13803300	-3.59212900
H	-0.10919300	2.56263500	-1.65500900
H	-1.50787000	3.55044500	-2.62120900

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TM1d (E = -2510.12055174)

Rh	0.02693800	0.28488400	-0.07496300
O	-1.42940800	0.46333100	1.38992400
O	-1.40604900	0.03860100	-1.56273800
O	-1.53242500	-1.79851000	1.68630800
O	-1.51747800	-2.21146600	-1.18269400
C	-1.90003200	-0.60009200	1.94687500
C	-2.98640300	-0.39462600	3.02570400
C	-2.37338000	0.45040200	4.17089000
H	-2.01935400	1.42478700	3.80214400
H	-3.13322300	0.62739700	4.95070500
H	-1.52561600	-0.07525700	4.64074700
C	-3.46345100	-1.75131000	3.57881400
H	-2.62963100	-2.31295200	4.02673100
H	-4.22388300	-1.58212500	4.36024900
H	-3.90601000	-2.37846700	2.79174900
C	-4.18661100	0.41400000	2.41272000
H	-3.81892300	1.42148200	2.15718200
H	-4.93025200	0.53553500	3.22046800
C	-4.83903400	-0.20850500	1.19351900
C	-5.96377100	-1.05109500	1.29240000
H	-6.41503600	-1.24230100	2.27125600
C	-6.51652200	-1.63505700	0.14308300
H	-7.39916400	-2.27590600	0.22948100
C	-5.94423300	-1.40273800	-1.11624800
H	-6.38001300	-1.86643700	-2.00698600
C	-4.81969900	-0.56397200	-1.24387900
C	-4.30430100	0.04234800	-0.08353600
H	-3.45338500	0.72161200	-0.17569200
C	-4.14439700	-0.31750000	-2.57917900
H	-4.87200700	-0.43835900	-3.40153100
H	-3.78039200	0.72246400	-2.61939700
C	-2.93396500	-1.26353500	-2.90692900
C	-3.40364500	-2.72347500	-3.05294800
H	-3.87081200	-3.09451700	-2.12943500
H	-4.14213800	-2.79057300	-3.87013100
H	-2.56117300	-3.38894600	-3.29470300
C	-2.29341600	-0.78477700	-4.23447600
H	-1.44913100	-1.43279700	-4.52223800
H	-3.04062300	-0.82533300	-5.04502300
H	-1.92421900	0.24842000	-4.14950100
C	-1.87099900	-1.14167300	-1.79171100
Rh	-0.08560100	-2.10347300	0.27263600

O	1.34896600	-2.33286600	-1.18077100
O	1.35418700	-1.90724200	1.73268500
O	1.48009600	-0.07572400	-1.50423700
O	1.47005200	0.35059500	1.39901300
C	1.82462500	-1.28744600	-1.75604100
C	2.88979500	-1.51528200	-2.85201700
C	2.23870400	-2.35895100	-3.97719200
H	1.85368700	-3.31307200	-3.58691700
H	2.98491600	-2.57419500	-4.76057200
H	1.40390600	-1.81357600	-4.44764800
C	3.38761100	-0.17569400	-3.42687400
H	2.55907900	0.39874600	-3.86847600
H	4.13111900	-0.36954000	-4.21880100
H	3.85695600	0.44933900	-2.65364400
C	4.08333100	-2.34301200	-2.25096800
H	3.70113000	-3.34371300	-1.99016100
H	4.81603600	-2.47819500	-3.06656300
C	4.75790200	-1.73060900	-1.03889400
C	5.89270200	-0.90288400	-1.14760500
H	6.33832100	-0.71764300	-2.13023300
C	6.46319600	-0.32717600	-0.00263400
H	7.35409200	0.30115500	-0.09632300
C	5.89845400	-0.55169200	1.26158900
H	6.34825500	-0.09404800	2.14844000
C	4.76382900	-1.37540800	1.39884200
C	4.23206200	-1.97545000	0.24293200
H	3.37427900	-2.64437700	0.34316400
C	4.09297900	-1.61270100	2.73789300
H	4.82887900	-1.51330900	3.55571400
H	3.70358000	-2.64338900	2.77531600
C	2.90882200	-0.63860600	3.08048900
C	3.41771500	0.80753200	3.22858600
H	3.87513700	1.17529100	2.29889900
H	4.17412100	0.84892500	4.03102000
H	2.59938100	1.49351200	3.49351500
C	2.26936100	-1.10936900	4.41194300
H	1.44576700	-0.44097500	4.71324000
H	3.02597800	-1.09417800	5.21459900
H	1.87178400	-2.13171900	4.32327300
C	1.82853300	-0.73967800	1.97915500
N	0.06537200	2.28505100	-0.49217900
C	0.08802900	3.33373300	1.67246700
C	0.07360800	3.43068400	0.24435600
C	0.06527600	4.74899700	-0.36871700
C	0.02033000	5.86034200	0.48257700
C	0.00784500	5.74258700	1.88421000
C	0.05430100	4.46823800	2.47522000
H	0.11249500	2.33549500	2.10760400
H	0.00026600	6.86381400	0.05258800
H	-0.02948400	6.64262800	2.50386200
H	0.05724600	4.36472400	3.56423000
C	0.20295700	4.90991900	-1.89742300
C	-0.13555000	6.35679800	-2.37102800
C	1.67827600	4.61264700	-2.29828800
C	-0.73400400	3.98601800	-2.63661500
H	-1.14907700	6.65853600	-2.06204900
H	0.58764000	7.09121100	-1.97636800
H	-0.08471800	6.40310100	-3.47050000
H	1.98411100	3.59915500	-1.99636700
H	1.80236700	4.70044000	-3.39146600
H	2.35926800	5.33146100	-1.81516100
H	-0.48626400	3.67131800	-3.65506300
H	-0.06791000	2.47498300	-1.50580500
H	-1.77963200	3.90616800	-2.32579700

106

^tTS2d (E = -2510.09629912)

Rh	0.04826300	0.31785400	-0.08078700
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O	-1.40164000	0.43413800	1.39577600
O	-1.43723200	-0.10204300	-1.55616000
O	-1.38187400	-1.83045000	1.72911300
O	-1.38218800	-2.33616800	-1.11692700
C	-1.80837700	-0.64544500	1.97021700
C	-2.89237400	-0.47841600	3.05954700
C	-2.29578300	0.39322000	4.19417900
H	-1.98229300	1.37852700	3.81782900
H	-3.05159000	0.54509100	4.98318200
H	-1.42358200	-0.09957700	4.65497700
C	-3.31415400	-1.84858900	3.62301300
H	-2.45587600	-2.37901500	4.06247500
H	-4.07068200	-1.70319300	4.41300800
H	-3.74487700	-2.49322400	2.84352600
C	-4.12733400	0.28474300	2.45805900
H	-3.79268900	1.29600500	2.17391800
H	-4.85580500	0.40269600	3.27995800
C	-4.79121400	-0.38248800	1.26873200
C	-5.90825200	-1.22886200	1.41300400
H	-6.34352600	-1.38966300	2.40456600
C	-6.47431600	-1.85475200	0.29268000
H	-7.35137800	-2.49761100	0.41396800
C	-5.92192100	-1.66205200	-0.98211400
H	-6.36740000	-2.15902200	-1.84990300
C	-4.80531700	-0.82084300	-1.15524200
C	-4.27725400	-0.17112500	-0.02400100
H	-3.43402300	0.51141000	-0.15249200
C	-4.15486000	-0.61618400	-2.51034900
H	-4.89037100	-0.79642300	-3.31452100
H	-3.82223400	0.43076700	-2.60410600
C	-2.92175100	-1.54035700	-2.81293700
C	-3.34164200	-3.02171600	-2.85509900
H	-3.76940600	-3.34953700	-1.89670800
H	-4.10030600	-3.16640500	-3.64323600
H	-2.48268300	-3.67141200	-3.08103500
C	-2.33051100	-1.12351700	-4.18388100
H	-1.46775600	-1.75593100	-4.45077000
H	-3.09316600	-1.24349700	-4.97177500
H	-2.00150900	-0.07336200	-4.17233500
C	-1.83285200	-1.30683000	-1.74148200
Rh	0.06072900	-2.09143100	0.29365200
O	1.48810600	-2.22368700	-1.19293300
O	1.50978200	-1.80488300	1.72276100
O	1.50420500	0.03920300	-1.51994600
O	1.51632500	0.44355300	1.37708100
C	1.90774700	-1.15666300	-1.77043000
C	2.97517700	-1.33675700	-2.87330500
C	2.34335000	-2.18764400	-4.00467000
H	1.99243500	-3.15843500	-3.62339200
H	3.09060300	-2.36964800	-4.79542000
H	1.48801400	-1.66413300	-4.46280600
C	3.42795000	0.02345700	-3.43626200
H	2.58014300	0.57575200	-3.86952400
H	4.17336600	-0.13848800	-4.23340600
H	3.88328700	0.65426300	-2.65906300
C	4.19759200	-2.13393800	-2.28888600
H	3.84566400	-3.14579000	-2.02892500
H	4.92455000	-2.24509400	-3.11304300
C	4.86970700	-1.50832300	-1.08184800
C	5.98619000	-0.65723300	-1.20058200
H	6.41892900	-0.46253300	-2.18713700
C	6.55622800	-0.07118600	-0.06064500
H	7.43362800	0.57456200	-0.16233500
C	6.00830300	-0.30758500	1.20880400
H	6.45719800	0.15884100	2.09153100
C	4.89230300	-1.15463300	1.35640500
C	4.36211900	-1.76524800	0.20511200
H	3.52147000	-2.45418300	0.31295600

C	4.23941800	-1.40427400	2.70249200
H	4.97786200	-1.27486800	3.51362300
H	3.88405700	-2.44678300	2.75139100
C	3.02756100	-0.46550200	3.04661700
C	3.48683600	0.99969300	3.16689900
H	3.92696000	1.36644400	2.22840400
H	4.24603200	1.08116900	3.96334600
H	2.64678200	1.66139900	3.42520600
C	2.41753200	-0.93773100	4.39170800
H	1.57217300	-0.29569000	4.68964700
H	3.18045300	-0.88075000	5.18627500
H	2.05807500	-1.97577300	4.32438600
C	1.93959300	-0.61849000	1.96199500
N	-0.00618200	2.33443900	-0.65184000
C	-0.01365600	3.38269700	1.57897400
C	-0.06588500	3.48040800	0.16875500
C	-0.25936300	4.76529200	-0.43137500
C	-0.34693900	5.89780500	0.38860600
C	-0.26580700	5.79244300	1.78690800
C	-0.10655000	4.52895400	2.37587200
H	0.12248700	2.40060300	2.03637700
H	-0.49943100	6.88196000	-0.06330200
H	-0.34037000	6.68952900	2.40778000
H	-0.05004700	4.43405600	3.46446500
C	-0.36308500	4.80151600	-1.96556500
C	-1.28337200	5.95567700	-2.45858300
C	1.04957800	4.99263800	-2.58184100
C	-0.96384600	3.48839600	-2.39006700
H	-2.28315500	5.88967900	-2.00091600
H	-0.85629500	6.94432200	-2.21651300
H	-1.39843500	5.90480100	-3.55352900
H	1.74511900	4.19680900	-2.26671500
H	0.99752400	4.98337700	-3.68433200
H	1.48294800	5.95450700	-2.26483200
H	0.74029600	2.39707000	-1.35663000
H	-1.97471200	3.23817500	-2.06207100
H	-0.59628900	2.96750800	-3.27896600

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MECP1 ($E_{\text{singlet}} = -2510.13939842$, $E_{\text{triplet}} = -2510.13938675$)

N	-0.06641800	2.23591600	-0.41050300
C	-2.45740800	2.67437500	-0.46219500
C	-1.08231700	3.11227200	-0.46423000
C	-0.79782500	4.54929700	-0.55007400
C	-1.89983800	5.41051000	-0.61901100
C	-3.23038300	4.95251200	-0.61968400
C	-3.50907300	3.57683800	-0.54506900
H	-2.63858000	1.60269400	-0.40685100
H	-1.73118800	6.48637700	-0.67950500
H	-4.04719500	5.67829400	-0.67962100
H	-4.54181900	3.21704700	-0.54837200
C	0.64294800	5.09448100	-0.55880500
C	0.68311100	6.63984800	-0.62881900
C	1.38280300	4.66339700	0.73718200
C	1.40655900	4.54494600	-1.79544800
H	0.21857400	7.03066800	-1.55013500
H	0.18992400	7.11092200	0.23848000
H	1.73517600	6.96977100	-0.62720200
H	1.44070700	3.56763200	0.80784100
H	2.40804500	5.07296100	0.73117700
H	0.86748400	5.04798600	1.63366100
H	1.46575700	3.44782400	-1.76103000
H	0.90736100	4.84303500	-2.73287300
H	2.43141400	4.95525000	-1.80982800
Rh	0.01116700	0.31756800	-0.09430200
O	1.47471600	0.10627600	-1.56690900
O	1.46092700	0.58698500	1.38014700

O	1.68850500	-2.13090700	-1.15573300
O	1.68979900	-1.66032100	1.70407600
C	1.99479500	-1.05270500	-1.77780500
C	3.06374400	-1.13592700	-2.89011900
C	2.39949500	-0.70314400	-4.22200600
H	1.97262800	0.30799200	-4.14329000
H	3.14914300	-0.70744800	-5.03126200
H	1.59382400	-1.40020900	-4.50610200
C	3.60638000	-2.57201200	-3.01967400
H	2.80032800	-3.28091000	-3.26314700
H	4.35317700	-2.60853800	-3.83121000
H	4.08448500	-2.91332800	-2.09025500
C	4.22146700	-0.12290100	-2.57061900
H	3.80187000	0.89481300	-2.62840600
H	4.95878800	-0.21805800	-3.38766600
C	4.90038800	-0.31327300	-1.22804500
C	6.05891900	-1.10062300	-1.08033000
H	6.51759100	-1.56172400	-1.96081000
C	6.63572400	-1.28454600	0.18489600
H	7.54484900	-1.88471900	0.28632000
C	6.05322400	-0.70365800	1.32093300
H	6.50759300	-0.85659000	2.30504200
C	4.89412900	0.08793800	1.20222000
C	4.35481600	0.29342800	-0.08134500
H	3.47736000	0.93529400	-0.19046000
C	4.21035900	0.70093900	2.40909600
H	4.94564300	0.87530000	3.21496000
H	3.79242300	1.68313700	2.13397200
C	3.04989700	-0.15357100	3.03628500
C	3.59026900	-1.46850000	3.63029800
H	4.07431800	-2.09353800	2.86633500
H	4.33125600	-1.23721000	4.41440700
H	2.78197600	-2.06028700	4.08636400
C	2.37937600	0.68953900	4.15042300
H	1.56576700	0.12628300	4.63665800
H	3.12323800	0.94283100	4.92442700
H	1.96126000	1.62296600	3.74501300
C	1.98723100	-0.43929600	1.95248900
Rh	0.26210400	-2.07096300	0.30375900
O	-1.17291700	-1.92670200	1.77634200
O	-1.16771500	-2.42033900	-1.13568500
O	-1.42680100	0.31104500	1.38945200
O	-1.42480800	-0.18126900	-1.49757600
C	-1.70729700	-0.78356400	2.00562700
C	-2.76893500	-0.71303600	3.12747900
C	-2.09828400	-1.17504200	4.44622200
H	-1.66895100	-2.18301900	4.34424200
H	-2.84657900	-1.19024600	5.25660300
H	-1.29391200	-0.48230800	4.74374100
C	-3.30786900	0.71974700	3.29415700
H	-2.49700100	1.42370800	3.53457500
H	-4.03995800	0.74143000	4.11941300
H	-3.80331100	1.07873600	2.38103900
C	-3.93581400	-1.71294400	2.79766800
H	-3.52732300	-2.73586600	2.84669800
H	-4.67204200	-1.61668400	3.61547800
C	-4.61277100	-1.50852500	1.45632600
C	-5.76352900	-0.70952600	1.30535200
H	-6.22054000	-0.24302000	2.18384600
C	-6.33746500	-0.52493500	0.03839000
H	-7.24355900	0.08009100	-0.06499200
C	-5.76090500	-1.11570200	-1.09612900
H	-6.21603200	-0.96405700	-2.08009700
C	-4.60995600	-1.91952000	-0.97353100
C	-4.07439700	-2.12401000	0.31136500
H	-3.20480800	-2.77614800	0.42309900
C	-3.93081900	-2.55380800	-2.17163800
H	-4.66632400	-2.73263300	-2.97623100

H	-3.52244100	-3.53578600	-1.88091900
C	-2.76216900	-1.71895400	-2.81105500
C	-3.29860100	-0.42130300	-3.44317700
H	-3.80220400	0.21605300	-2.70263700
H	-4.02397500	-0.67352400	-4.23528000
H	-2.48580200	0.16678000	-3.89525500
C	-2.08903800	-2.59170100	-3.90066200
H	-1.27806700	-2.04020400	-4.40419100
H	-2.83416400	-2.86848500	-4.66536700
H	-1.66755400	-3.51228600	-3.46992700
C	-1.70336600	-1.41664900	-1.72617400

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MECP2 ($E_{\text{singlet}} = -2510.11211330$, $E_{\text{triplet}} = -2510.11213859$)

N	0.10864100	2.05821200	-1.17776100
C	2.47005900	2.54996900	-1.23630000
C	1.11724200	2.99215200	-1.26725800
C	0.84796800	4.40204500	-1.40393700
C	1.93009600	5.27681900	-1.54874700
C	3.26238600	4.82214300	-1.54020600
C	3.52389700	3.45323000	-1.38007400
H	2.65679900	1.48182700	-1.13037900
H	1.74348700	6.34924800	-1.64870000
H	4.08374700	5.53719400	-1.64016200
H	4.55370400	3.08534000	-1.36761500
C	-0.61618500	4.88247800	-1.40650500
C	-0.74653300	6.36868400	-0.94477400
C	-1.20084600	4.76943400	-2.84445500
C	-1.41159900	4.04953000	-0.43608500
H	-0.26946600	6.52450200	0.03546700
H	-0.28807100	7.05978500	-1.67390000
H	-1.81116100	6.64048300	-0.86009700
H	-1.14310500	3.73893600	-3.23142300
H	-2.25892300	5.08299200	-2.86127500
H	-0.63958100	5.41577300	-3.53833500
H	-0.81728100	2.42037500	-1.45895400
H	-1.02746500	3.87951700	0.57179500
H	-2.49088400	3.93480000	-0.58116500
Rh	-0.00661200	0.22943400	-0.26272000
O	-1.45294500	0.94244200	1.04244800
O	-1.48760800	-0.35545900	-1.60278100
O	-1.68328200	-1.09824100	2.03801700
O	-1.71260800	-2.37944900	-0.56346500
C	-1.97781100	0.14041100	1.90459900
C	-3.03011900	0.73791500	2.86491200
C	-2.34455200	1.85952100	3.68520600
H	-1.93717200	2.64227800	3.02796500
H	-3.07426400	2.32099400	4.37186500
H	-1.51914800	1.45420300	4.29325200
C	-3.57038600	-0.34551400	3.81801400
H	-2.75959700	-0.78711100	4.41685000
H	-4.30162600	0.10711100	4.50917600
H	-4.06547500	-1.15944900	3.26919600
C	-4.19864500	1.38079500	2.03383100
H	-3.78582600	2.23947500	1.47907900
H	-4.92140400	1.78613400	2.76423700
C	-4.90204500	0.44745100	1.06693100
C	-6.06458400	-0.26540800	1.42059100
H	-6.51124600	-0.12132300	2.40954000
C	-6.65902700	-1.14974800	0.50817000
H	-7.56847600	-1.68970300	0.78820700
C	-6.09353600	-1.34830500	-0.76021200
H	-6.56230000	-2.04492600	-1.46246000
C	-4.93178500	-0.64781700	-1.14021400
C	-4.37345600	0.26129900	-0.22340900
H	-3.48806900	0.82914300	-0.51798600
C	-4.25973400	-0.86258100	-2.48294100

H	-5.00160600	-1.19771600	-3.22956200
H	-3.84649200	0.09394200	-2.84375600
C	-3.10084500	-1.92351800	-2.49420500
C	-3.64765400	-3.33053700	-2.18511100
H	-4.11601000	-3.37579900	-1.19152100
H	-4.40339700	-3.60521600	-2.94088900
H	-2.84438400	-4.08207200	-2.21191200
C	-2.44952400	-1.91260400	-3.90043500
H	-1.64004300	-2.65832300	-3.96495800
H	-3.20388400	-2.16840200	-4.66379700
H	-2.02940400	-0.92363400	-4.13831600
C	-2.01843000	-1.52279200	-1.46511700
Rh	-0.26861500	-1.92099300	0.81481900
O	1.14089100	-2.69398300	-0.46013900
O	1.18081200	-1.36285500	2.16759100
O	1.41874700	-0.66504400	-1.46973100
O	1.43870300	0.66533200	1.14425700
C	1.68062700	-1.91500400	-1.32651100
C	2.72167300	-2.54391500	-2.27938200
C	2.02773800	-3.69339300	-3.05322400
H	1.60018900	-4.43765300	-2.36480000
H	2.76012600	-4.19703900	-3.70650600
H	1.21726300	-3.30532500	-3.69203300
C	3.26405100	-1.50337700	-3.27677900
H	2.45017400	-1.06456900	-3.87356300
H	3.97202000	-1.99309700	-3.96691000
H	3.78853700	-0.68172700	-2.76837700
C	3.88770400	-3.16540400	-1.42742400
H	3.47215200	-4.01196200	-0.85642500
H	4.61464200	-3.58518300	-2.14554700
C	4.58277800	-2.21173100	-0.47523400
C	5.73716900	-1.49139000	-0.84019500
H	6.18268200	-1.64372900	-1.82859100
C	6.32763700	-0.59378700	0.06190500
H	7.23540200	-0.05403300	-0.22457900
C	5.76454000	-0.38732400	1.33035700
H	6.23148000	0.31802300	2.02524800
C	4.61094500	-1.09541800	1.72157200
C	4.05760100	-2.01917100	0.81596900
H	3.18303300	-2.59783900	1.12263700
C	3.94584700	-0.88200100	3.06798900
H	4.69239800	-0.55632700	3.81410000
H	3.52742000	-1.83795800	3.42359700
C	2.79194600	0.18487900	3.09222600
C	3.34434500	1.59634300	2.81973600
H	3.83271700	1.66124800	1.83733700
H	4.08308300	1.85750800	3.59671500
H	2.54126500	2.34822100	2.84172600
C	2.12808200	0.14494600	4.49177200
H	1.33124200	0.90292000	4.57069200
H	2.88032700	0.36614100	5.26780300
H	1.68950700	-0.84315600	4.69700400
C	1.72053600	-0.20332200	2.04849800