

Retro-metal-Ene versus retro-Aldol: Mechanistic insight into Rh-catalysed formal [3+2] cycloaddition

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1. Complete reference for Gaussian 09

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; and Fox, D. J. Gaussian 09, revision D.01; Gaussian, Inc.: Wallingford, CT, **2013**.

2. Isomerization from intermediate CP6 to intermediate CP8.

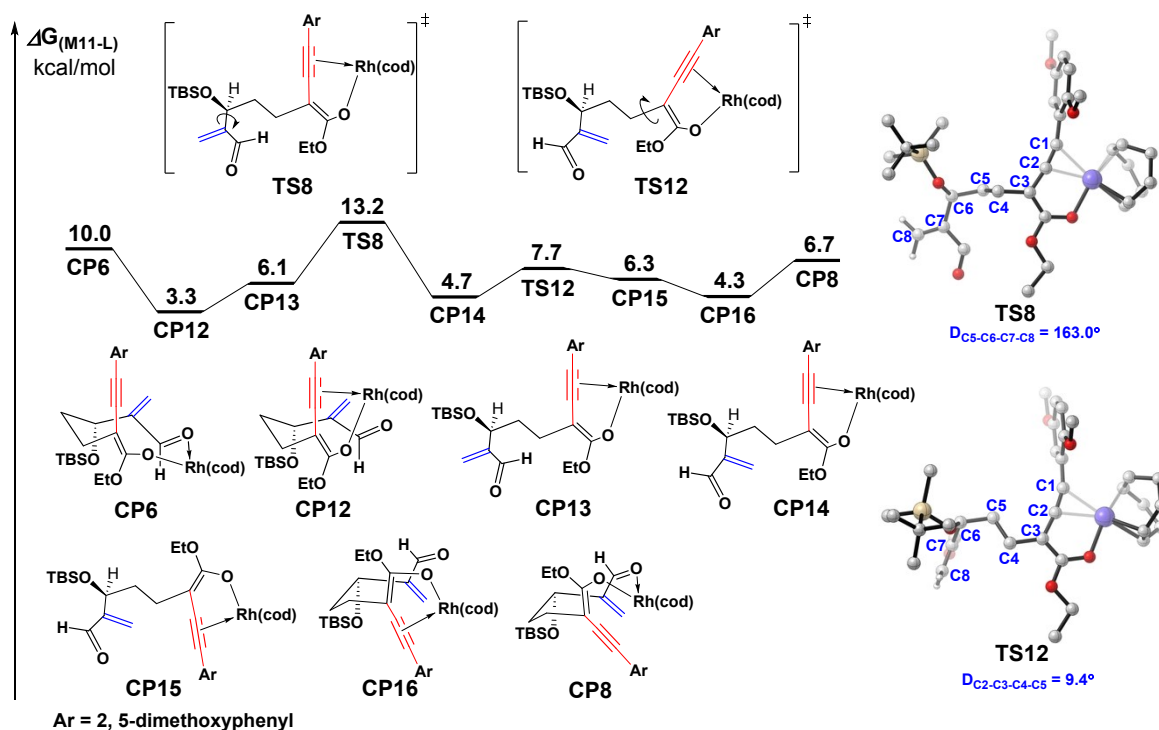


Figure S1. Gibbs free energy profiles for the isomerization from intermediate CP6 to intermediate CP8. The bond lengths are given in angstrom.

The Gibbs free energy profiles for the isomerization from intermediate CP6 to intermediate CP8 are shown in Figure S1. As shown in Figure S1, the enolate-Rh intermediate CP6 can isomerize to the open-ring intermediate CP12 with 6.7 kcal/mol exothermic. With the ring opened, intermediate CP12 can isomerize to CP13 further (2.7 kcal/mol endothermic). The subsequent rotation of vinyl aldehyde in CP13 can occur through transition state TS8, generates intermediate CP14. The activation free energy of this rotation is only 9.9 kcal/mol. The enolate-rhodium and acetylene in CP14 can also rotate via transition state TS12, with a barrier of only 3.0 kcal/mol, to get intermediate CP15. Intermediate CP15 can also isomerize to CP16 with 1.5 kcal/mol exothermic. With closing the ring in CP16, the ten-membered-ring alleno-rhodium intermediate CP8 is generated. The calculated results indicated that the overall barrier for the isomerization from intermediate CP6 to intermediate CP8 is only 9.9 kcal/mol. Meanwhile, this isomerization is exergonic by 3.3 kcal/mol.

3. The coordination capabilities of terminal alkyne and aryl alkyne.

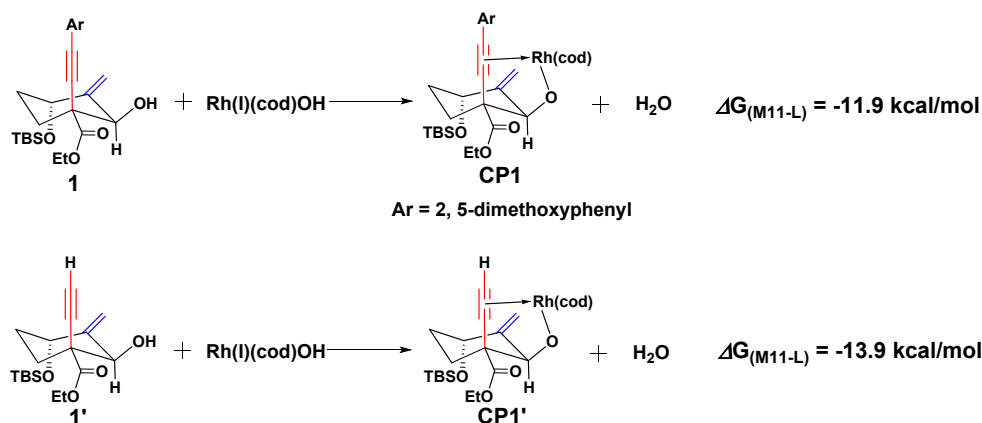


Figure S2. The reaction Gibbs energies of ligand exchange for Rh(I)LnOH with aryl alkyne **1** and terminal alkyne **1'**.

The reaction Gibbs energies of ligand exchange for Rh(I)LnOH with **1** and **1'** are shown in Figure S2. The reaction Gibbs energies of ligand exchange between Rh(I)LnOH and **1**, with aryl alkyne, is -11.9 kcal/mol . While the reaction Gibbs energies of ligand exchange between Rh(I)LnOH and **1'**, with terminal alkyne, is -13.9 kcal/mol . The calculated results indicated that the coordination capability of terminal alkyne in **1'** is stronger than aryl alkyne in **1**. The lower coordination capability of aryl alkyne in **1a** also makes contribution to conduct the retro-Aldol type reaction to cleave the C-C bond.

4. The intramolecular Michael-type addition of acetylene to enal moiety in allene-Rhodium intermediate **CP17**.

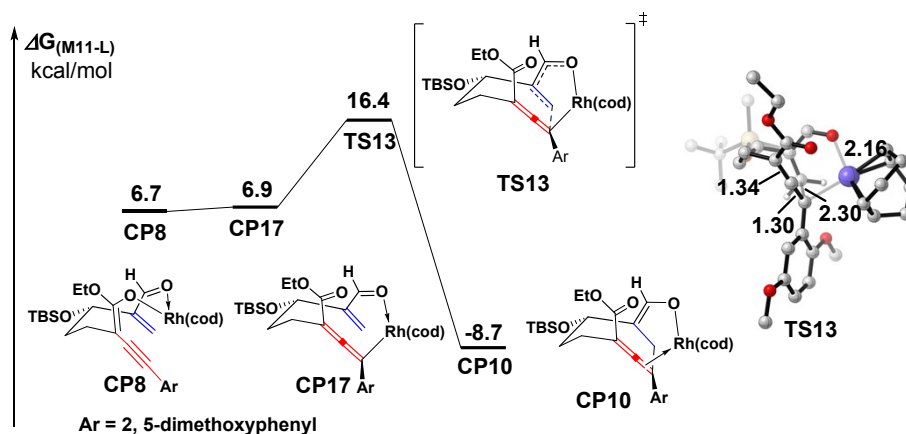


Figure S3. The Gibbs energies profile for intramolecular Michael-type addition of acetylene to enal moiety in allene-Rh intermediate **CP17**.

As shown in Figure S3, the intermediate **CP8** isomerize to allene-Rhodium intermediate **CP17** with 0.2 kcal/mol endothermic. The intramolecular Michael-type addition of acetylene to enal moiety in enolate-Rhodium intermediate **CP17** then occurs via transition state **TS13**. The activation energy of

TS13 is 4.7 kcal/mol higher than that of **TS9**, which indicates that this intramolecular Michael-type addition of allene-Rhodium intermediate **CP17** is unfavorable.

5. The pathway of the 3,3-sigmatropic migration of the isomer of **CP1**.

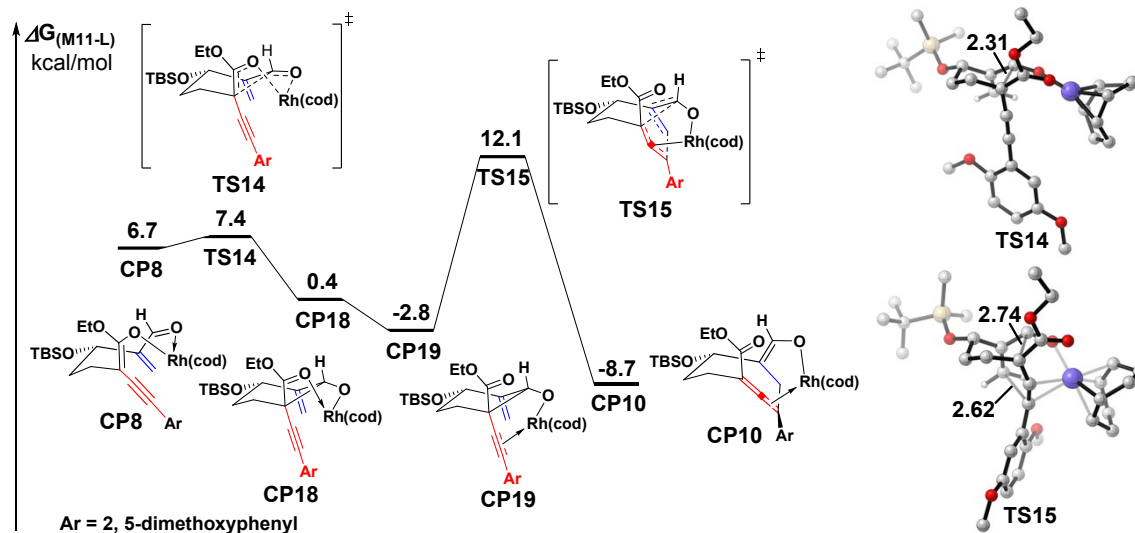


Figure S4. The Gibbs energies profile for 3,3-sigmatropic migration of the isomer of **CP1**.

As shown in Figure S4, the Aldol reaction of intermediate **CP8** occurs via transition state **TS14**, with an energy barrier of 0.7 kcal/mol, to give the allyloxy-rhodium intermediate **CP18**. The coordination of the alkyne group in intermediate **CP18** generates intermediate **CP19**, which is isomer of **CP1**. Then, the intramolecular 3,3-sigmatropic migration from **CP19** to **CP10** occurs via concerted transition state **TS15** with an energy barrier of 14.9 kcal/mol. The activation energy of **TS15** is 0.4 kcal/mol higher than that of **TS9**, which indicates that this 3,3-sigmatropic migration of **CP19** is also unfavorable, but could not be ruled out.

6. Computational Methods.

All DFT calculations were carried out with the GAUSSIAN 09 series of programs. Density functional B3-LYP¹ with a standard 6-31G(d) basis set (LANL08² basis set for Rhodium) was used for geometry optimizations. Harmonic frequency calculations were performed for all stationary points to confirm them as local minima or transition structures and to derive the thermochemical corrections for the enthalpies and Gibbs energies. All minima have zero imaginary frequency and all transition states have only one imaginary frequency. The solvent effects were considered by single point calculations on the gas-phase stationary points with a continuum solvation model SMD.³ The DFT method M11-L⁴

functional with the 6-311+G(d) (LANL08 basis set for Rhodium) basis set was used to calculate the single point energies with trimethylbenzene as solvent and provide highly accurate energy information.⁵ The energies given in this report are the M11-L calculated Gibbs energies in trimethylbenzene solvent. The optimized structures were displayed using CYLview.⁶ In addition, the concentration correction of 1.89 kcal/mol for the G(sol) values was applied to account for the condition change from 1 atm to 1 M concentration when going from gas phase to solution.⁷

7. B3LYP and M06 absolute calculation energies, enthalpies, and free energies.

Geometry	E _(elec-B3LYP) ¹	H _(corr-B3LYP) ²	G _(corr-B3LYP) ³	E _(solv-M06) ⁴	IF ⁵
CP1	-2175.450247	0.820973	0.688771	-2175.660015	-
TS1	-2175.421755	0.818024	0.688200	-2175.637604	-188.3
CP2	-2175.454283	0.821228	0.693355	-2175.672448	-
TS2	-2175.423989	0.818972	0.690701	-2175.644506	-355.5
CP3	-2175.487689	0.821459	0.692184	-2175.69954	-
1	-1754.440215	0.639501	0.525583	-1754.470171	-
TS3	-3929.891238	1.457291	1.236382	-3930.137654	-1452.7
2	-1754.498803	0.640011	0.529058	-1754.534383	-
TS4	-2175.424134	0.818676	0.685361	-2175.633410	-272.9
CP4	-2175.433341	0.819740	0.683947	-2175.641123	-
TS5	-2175.416555	0.818544	0.685796	-2175.629691	-245.2
CP5	-2175.453137	0.821185	0.688089	-2175.656859	-
TS6	-2175.437223	0.818714	0.685662	-2175.638246	-105.4
CP6	-2175.437386	0.819463	0.684557	-2175.639857	-
TS7	-2175.426407	0.818383	0.686984	-2175.637670	-200.8
CP7	-2175.457426	0.821156	0.690095	-2175.670977	-
TS8	-2175.429053	0.819320	0.683938	-2175.634087	-362.0
CP8	-2175.435679	0.819664	0.685041	-2175.645574	-
TS9	-2175.431405	0.818482	0.687474	-2175.64002	-207.2
CP9	-2175.459561	0.821235	0.690916	-2175.669506	-

CP10	-2175.462371	0.821398	0.693038	-2175.678142	-
TS10	-2175.430179	0.819207	0.690342	-2175.649350	-370.2
CP11	-2175.488277	0.821423	0.690131	-2175.701174	-
TS11	-3929.891592	1.457002	1.236843	-3930.141935	-1335.8
2a	-1754.498803	0.640011	0.529058	-1754.532432	-
CP12	-2175.438112	0.819723	0.681946	-2175.647883	-
CP13	-2175.435651	0.819879	0.679889	-2175.641459	-
CP14	-2175.436786	0.819676	0.680151	-2175.643839	-
TS12	-2175.433656	0.818688	0.682988	-2175.642019	-12.1
CP15	-2175.436776	0.819826	0.681340	-2175.642566	-
CP16	-2175.435710	0.819758	0.682853	-2175.646491	-
1'	-1294.338961	0.481895	0.393615	-1294.365776	-
Rh(I)(cod)OH	-497.399936	0.207254	0.16139	-497.5871125	-
CP1'	-1715.352663	0.663521	0.555159	-1715.55711	-
H₂O	-76.407024	0.024919	0.003474	-76.42160269	-
CP17	-2175.434655	0.819563	0.684344	-2175.644661	-
TS13	-2175.419891	0.818720	0.686951	-2175.632022	-224.3
TS14	-2175.436624	0.818467	0.684674	-2175.644046	-93.8
CP18	-2175.449898	0.820868	0.684497	-2175.655022	-
CP19	-2175.450647	0.820720	0.686767	-2175.662457	-
TS15	-2175.424441	0.817902	0.68733	-2175.639219	-96.4

¹The electronic energy calculated by B3LYP in gas phase. ²The thermal correction to enthalpy calculated by B3LYP in gas phase. ³The thermal correction to Gibbs free energy calculated by B3LYP in gas phase. ⁴The electronic energy calculated by M11-L in trimethylbenzene solvent. ⁵The B3LYP calculated imaginary frequencies for the transition states.

8. B3LYP geometries for all the optimized compounds and transition states.

CP1				H	-2.48121800	0.26285300	2.20785900
C	-1.34118600	-0.61905900	-0.29389200	H	-0.97542600	0.87670400	2.90003000
C	-0.72671700	-0.38688000	1.13759300	H	-2.31356900	2.68109300	1.76890200
C	-1.50389600	0.68477200	1.95855900	H	-0.73489400	2.47372800	0.99568300
C	-1.70121900	1.98843200	1.17931800	H	-2.43288000	2.68597600	-0.72945800
C	-2.38783600	1.74037300	-0.17101900	O	-0.51660900	-1.48255100	-0.99391300
H	-2.32221200	-1.09489600	-0.13644800	C	-1.59956700	0.72347000	-0.97560000

C	-1.15241300	0.99230600	-2.20546800
H	-0.57643100	0.25696500	-2.75737000
H	-1.35108800	1.94809200	-2.68679900
C	0.67137400	0.02288600	0.88530400
C	1.72015500	0.65693400	0.78465400
O	-3.72145900	1.28890700	0.10541700
Si	-5.00433800	1.15836600	-0.97708000
C	-6.55968500	1.20691100	0.14147700
C	-4.91121700	-0.46142600	-1.94641900
H	-5.73886100	-0.55017400	-2.66127900
H	-3.97368000	-0.51401400	-2.51097500
H	-4.94538700	-1.33439700	-1.28458100
C	-4.97730400	2.60938900	-2.19458600
H	-5.85924100	2.58831900	-2.84664500
H	-4.96666300	3.57870900	-1.68259900
H	-4.09455800	2.56416700	-2.84325900
C	-6.62253300	2.55176900	0.89621700
H	-7.49674000	2.57757600	1.56366100
H	-5.72871800	2.70925700	1.51027100
H	-6.71249000	3.40246000	0.20911500
C	-6.49384600	0.05900200	1.17201200
H	-7.37183200	0.08764200	1.83464100
H	-6.48280700	-0.92570900	0.68862800
H	-5.59839000	0.13318200	1.79898800
C	-7.83558600	1.04683200	-0.71321400
H	-7.85392700	0.09101900	-1.25113600
H	-8.73074600	1.07782700	-0.07478100
H	-7.93898300	1.85006900	-1.45382500
Rh	1.51720200	-1.24535200	-0.84616300
C	-0.72953400	-1.72240700	1.90077700
O	0.24293700	-2.28710300	2.35210100
O	-1.98839600	-2.18819000	2.03944300
C	-2.12514300	-3.44588200	2.73656100
H	-1.53121900	-4.20223500	2.21387000
H	-1.71099600	-3.33710100	3.74439700
C	-3.60178700	-3.79475900	2.75956900
H	-4.17935200	-3.02075600	3.27540000
H	-3.99407700	-3.89646300	1.74265100
H	-3.75141200	-4.74489400	3.28435200
C	2.84299400	1.54061900	0.88118100
C	3.83632600	1.34110800	1.87639300
C	2.94805500	2.63879500	0.01900200
C	4.88997200	2.24849400	1.97603200
C	4.00853500	3.54624100	0.12670000
H	2.19415800	2.79809900	-0.74458900
C	4.97980400	3.34607200	1.11042800
H	5.65852900	2.11735600	2.72880100
H	5.81465200	4.02851800	1.22065800
O	3.67288900	0.24884100	2.67329700
O	3.99844200	4.58053900	-0.76763400
C	4.61606300	0.01935600	3.70754900
H	5.62514100	-0.14136800	3.30488500
H	4.64011000	0.85370000	4.42114400
H	4.28106400	-0.88504300	4.21737500
C	5.05063300	5.52713600	-0.70164500
H	6.02878400	5.05886300	-0.87781100
H	4.85207600	6.25264200	-1.49267900
H	5.06983800	6.04495000	0.26717300
C	1.59057600	-2.47511200	-2.62792000
C	1.56136500	-3.28440100	-1.47482900
C	2.73300500	-4.01117400	-0.84559000
C	3.99445800	-3.12836200	-0.72851100
C	3.65102500	-1.65966700	-0.49303900

C	3.50660800	-0.71205500	-1.52005200
C	3.61428100	-0.98063100	-3.01302100
C	2.83775400	-2.23513400	-3.47153600
H	0.63427700	-2.29634500	-3.11344500
H	0.58158100	-3.64791400	-1.17234900
H	2.95736700	-4.93721600	-1.39972500
H	2.41952200	-4.31959500	0.15805000
H	4.61149400	-3.49106100	0.10188600
H	4.61431800	-3.22389300	-1.62733000
H	3.86956500	-1.28650300	0.50448900
H	3.67507300	0.33012000	-1.25715900
H	4.67118900	-1.04529800	-3.31976900
H	3.20233600	-0.10469300	-3.52837800
H	2.54507100	-2.11435400	-4.52096900
H	3.48479300	-3.11947700	-3.44073700

TS1

C	-1.26505600	-0.28589200	-1.24017000
C	-0.65592000	-0.28895000	1.44398900
C	-1.54086200	0.78602000	2.05537600
C	-1.62017700	2.08705400	1.23988200
C	-2.11077400	1.91475100	-0.21551000
H	-2.24691800	-0.73543800	-1.04746400
H	-2.54617700	0.37331800	2.16664800
H	-1.19460600	1.04091500	3.06768900
H	-2.30310700	2.77914000	1.75073200
H	-0.63651300	2.57083500	1.21254800
H	-2.19158900	2.92712700	-0.64093600
O	-0.33154500	-1.03848200	-1.66935300
C	-1.11761900	1.12221500	-1.05771500
C	0.09180500	1.66899600	-1.40319100
H	0.74607500	1.13883800	-2.08218100
H	0.31390200	2.71815100	-1.22537400
C	0.61325500	-0.02143800	0.97823000
C	1.46987500	0.70198500	0.33696200
O	-3.39983200	1.30149200	-0.19058100
Si	-4.70442200	1.68183500	-1.17868800
C	-6.13695400	0.62594800	-0.47628400
C	-4.33155900	1.24410500	-2.98109300
H	-4.19911800	0.16522300	-3.12156100
H	-5.13714200	1.57364300	-3.64892300
H	-3.40623600	1.72959400	-3.31395600
C	-5.07358700	3.53641200	-1.06885700
H	-5.97611800	3.79453600	-1.63668200
H	-5.22635100	3.85836200	-0.03261300
H	-4.25194700	4.13314700	-1.48374200
C	-6.48883300	1.09446500	0.95249700
H	-7.28812900	0.46710600	1.37424800
H	-5.62493300	1.02718100	1.62342300
H	-6.84772200	2.13112000	0.96812800
C	-5.70671900	-0.85639500	-0.42084100
H	-6.52169500	-1.47495200	-0.01560700
H	-5.46370900	-1.25161900	-1.41530500
H	-4.82794600	-0.99333400	0.21921800
C	-7.38577900	0.75881500	-1.37460900
H	-7.19914500	0.40013000	-2.39437800
H	-8.21529300	0.16280200	-0.96670800
H	-7.73662100	1.79650200	-1.44331700
Rh	1.42512400	-1.54250800	-0.40948100
C	-1.05741000	-1.68307600	1.42969700
O	-0.40520900	-2.59324300	0.89239900
O	-2.23806300	-1.94275500	2.04119100
C	-2.69192900	-3.30986100	2.00401200

H	-2.80565500	-3.62112500	0.96016500	C	0.55652800	-0.09178300	0.81394600
H	-1.92991300	-3.95170300	2.45841900	C	1.22295100	0.90707200	0.13758500
C	-4.00729700	-3.37253800	2.75979800	O	-3.33483000	1.33723700	-0.06122500
H	-3.87725200	-3.04791700	3.79744200	Si	-4.66255300	1.78410900	-0.98435500
H	-4.75979900	-2.73104900	2.28992600	C	-6.08989100	0.73074100	-0.26299700
H	-4.38507900	-4.40114000	2.76449300	C	-4.38568300	1.41470100	-2.81846100
C	2.59248700	1.59803400	0.48345300	H	-5.17832900	1.85021000	-3.43959500
C	2.82195400	2.28787700	1.71002900	H	-3.42813000	1.83155500	-3.15152700
C	3.44501400	1.86582600	-0.59523800	H	-4.35313400	0.33790400	-3.01944400
C	3.88283500	3.18670200	1.80717000	C	-4.99189800	3.64023700	-0.78926300
C	4.51473100	2.76089800	-0.49007700	H	-5.91927900	3.93167200	-1.29814600
H	3.27388400	1.36200400	-1.54031400	H	-5.08271600	3.93089800	0.26349900
C	4.73283600	3.42530800	0.71826500	H	-4.18327600	4.23649400	-1.22946300
H	4.07118700	3.71598800	2.73414300	C	-6.36549500	1.14476000	1.19856800
H	5.54919800	4.12848100	0.83590000	H	-7.15946900	0.51808800	1.63172800
O	1.95331900	2.01576100	2.72842100	H	-5.47240100	1.02993800	1.82342600
O	5.27560100	2.91301900	-1.61948900	H	-6.69752700	2.18771900	1.27407500
C	2.14336000	2.67416500	3.96825000	C	-5.69398900	-0.76203600	-0.28910200
H	3.11941200	2.43163800	4.41006300	H	-6.50325000	-1.37888300	0.13041900
H	2.05724500	3.76444000	3.86475200	H	-5.50828100	-1.12054600	-1.30936700
H	1.35046800	2.31024000	4.62412100	H	-4.78779700	-0.94504700	0.29902300
C	6.35837700	3.82392400	-1.57246100	C	-7.37408600	0.92949200	-1.09644000
H	7.10433400	3.53066700	-0.82062000	H	-7.23928400	0.62075000	-2.14034500
H	6.81801800	3.79748700	-2.56248000	H	-8.19684600	0.32797700	-0.68249200
H	6.01946500	4.84722700	-1.35906400	H	-7.70717800	1.97536000	-1.09729300
C	2.59989700	-2.06386500	-2.17316300	Rh	1.27553600	-1.36913200	-0.72103400
C	1.71572700	-3.11268900	-1.83715400	C	-1.02569600	-1.77910900	1.38406800
C	2.08945300	-4.40673600	-1.13278600	O	-0.49008800	-2.63257500	0.67552000
C	2.96213400	-4.17365100	0.12087800	O	-2.10892200	-2.06109400	2.13449900
C	2.67071100	-2.82921700	0.78448200	C	-2.62709000	-3.40584400	2.03814400
C	3.38219600	-1.64831800	0.50175800	H	-2.85562900	-3.62182500	0.98993700
C	4.48498800	-1.52248200	-0.53615000	H	-1.84989000	-4.10697700	2.36009100
C	4.10366600	-2.11814700	-1.91005000	C	-3.86148800	-3.48057300	2.91802600
H	2.27687400	-1.38453500	-2.96003200	H	-3.61534800	-3.24823300	3.95932400
H	0.77623900	-3.14971500	-2.38560000	H	-4.62595000	-2.77477500	2.57773900
H	2.58692100	-5.10698400	-1.82297700	H	-4.28334900	-4.49102400	2.88019500
H	1.15387200	-4.88729100	-0.82653600	C	2.50080400	1.54265500	0.53567700
H	2.78258900	-4.97602500	0.84528700	C	3.03485800	1.44919900	1.85094700
H	4.02674900	-4.22849200	-0.13500400	C	3.18924600	2.33945100	-0.38811400
H	2.15037500	-2.88038000	1.73862300	C	4.20588800	2.13234600	2.17883500
H	3.42003500	-0.89607500	1.28689000	C	4.36622600	3.02108100	-0.06046800
H	5.41413200	-1.97807900	-0.15606500	H	2.81776200	2.43954900	-1.40130600
H	4.69827000	-0.45634800	-0.65682500	C	4.87659700	2.91782500	1.23430900
H	4.62935400	-1.56792500	-2.69888300	H	4.61456500	2.06778700	3.18050000
H	4.44830800	-3.15633900	-1.98841700	H	5.78265800	3.43470200	1.52875800
CP2				O	2.34420000	0.67126400	2.73717900
C	-1.26147600	0.00285000	-1.50030700	O	4.92804200	3.75339300	-1.07100900
C	-0.57581500	-0.37636300	1.47555900	C	2.81273300	0.57572800	4.07162400
C	-1.45173300	0.66747600	2.15792600	H	3.81599900	0.13146700	4.11749700
C	-1.55319200	2.01510500	1.41695600	H	2.82999600	1.55769600	4.56299200
C	-2.04474000	1.94862500	-0.05619500	H	2.10582800	-0.07581100	4.58815700
H	-2.26057300	-0.44158500	-1.52994100	C	6.12329200	4.46054800	-0.79342400
H	-2.45493500	0.24613500	2.25778400	H	6.93634400	3.78285000	-0.49829500
H	-1.09621400	0.86044900	3.18011800	H	6.39654300	4.96622500	-1.72154800
H	-2.25190400	2.65365100	1.97356600	H	5.97750900	5.21013000	-0.00332200
H	-0.58523100	2.52986000	1.43679800	C	2.46695400	-1.72426600	-2.55585000
H	-2.14017100	3.00001400	-0.38222300	C	1.59104300	-2.79768000	-2.33324700
O	-0.27719300	-0.74109300	-1.98466700	C	1.95327300	-4.14844100	-1.74301100
C	-1.05829800	1.22736100	-0.95204600	C	2.84910700	-4.05019500	-0.48739000
C	0.36563800	1.68969300	-0.91850400	C	2.58816500	-2.79340400	0.34033100
H	0.82534700	1.57694900	-1.90540400	C	3.27889700	-1.59002100	0.18569500
H	0.43410000	2.75135600	-0.64533600	C	4.33272700	-1.28565000	-0.86413200
				C	3.96587100	-1.78023400	-2.28161800

H	2.12729300	-0.95309300	-3.24337200
H	0.64334200	-2.76715300	-2.86500600
H	2.42982100	-4.79364500	-2.49850800
H	1.01422500	-4.64150600	-1.46806900
H	2.67952500	-4.92974400	0.14427100
H	3.90786300	-4.08220700	-0.76906000
H	2.07814600	-2.95165300	1.28743100
H	3.30478000	-0.93732300	1.05195400
H	5.30866600	-1.69438700	-0.55399800
H	4.45336900	-0.19744300	-0.89115200
H	4.49051100	-1.16275800	-3.02000300
H	4.32751100	-2.80348900	-2.43574500

TS2

C	-1.27583100	-0.00108300	-1.45869300
C	-0.67283400	-0.13804600	1.13955600
C	-1.39097300	0.76127200	2.16016600
C	-1.82331400	2.11077500	1.54816900
C	-2.23711500	1.87908700	0.08246200
H	-2.28705700	-0.40415800	-1.62741100
H	-2.27492500	0.23753200	2.52515400
H	-0.73232300	0.93192800	3.01776400
H	-2.64485500	2.56166000	2.11658700
H	-0.98948300	2.82127500	1.56820700
H	-2.32807600	2.85760500	-0.41822800
O	-0.27900100	-0.58140900	-1.96277600
C	-1.11563800	1.08809400	-0.55147900
C	0.23351400	1.76901800	-0.61602700
H	0.61184800	1.69983200	-1.64273900
H	0.15886600	2.83641600	-0.36810500
C	0.73593400	-0.05733100	0.92207900
C	1.25237200	1.06019600	0.31490500
O	-3.47837300	1.18175500	0.01742400
Si	-4.87795500	1.79755600	-0.68705300
C	-6.19194200	0.43523500	-0.41443100
C	-4.57802900	2.12957500	-2.52605900
H	-5.45970900	2.57650500	-3.00132300
H	-3.74385300	2.82737700	-2.67082600
H	-4.33251900	1.21019500	-3.06973400
C	-5.36948400	3.42144700	0.15381600
H	-6.29774300	3.82314800	-0.27086500
H	-5.52310800	3.29104100	1.23105100
H	-4.59617000	4.18807100	0.02069300
C	-6.42834100	0.23809400	1.09832300
H	-7.15929900	-0.56606300	1.27052500
H	-5.50126400	-0.03326100	1.61600500
H	-6.82534500	1.14387500	1.57280700
C	-5.69399900	-0.89416100	-1.02082600
H	-6.43448000	-1.69122900	-0.85719100
H	-5.53404500	-0.81711800	-2.10333600
H	-4.74987700	-1.20962300	-0.56345000
C	-7.52095300	0.83695200	-1.08995500
H	-7.40923500	0.96465500	-2.17374400
H	-8.28089900	0.05816000	-0.93092500
H	-7.92594900	1.77196200	-0.68235100
Rh	1.49245600	-1.51668400	-0.37864800
C	-1.24301100	-1.51295400	0.95664300
O	-0.65570000	-2.40125300	0.34262800
O	-2.44504900	-1.72973600	1.51514600
C	-2.98582400	-3.06528700	1.37543700
H	-3.24676400	-3.22571500	0.32416900
H	-2.20815600	-3.78730000	1.63998400
C	-4.19531500	-3.16975300	2.28542100

H	-3.91367800	-2.99751900	3.32938100
H	-4.96298300	-2.44094700	2.00880800
H	-4.62852300	-4.17313900	2.20698900
C	2.58141600	1.67564400	0.45756600
C	3.33793300	1.58248900	1.66388400
C	3.09884600	2.48678500	-0.56248500
C	4.54787600	2.26575700	1.78316800
C	4.31542600	3.16692100	-0.44221800
H	2.55961300	2.59751000	-1.49627500
C	5.04649600	3.05646600	0.73995900
H	5.12489800	2.19831700	2.69790400
H	5.99149700	3.57015600	0.87352900
O	2.80963500	0.81886600	2.66784200
O	4.69024000	3.90879100	-1.53264300
C	3.50480600	0.74277800	3.89792800
H	4.49790800	0.28837300	3.77689400
H	3.61853300	1.73157600	4.36401700
H	2.89662500	0.10688500	4.54423000
C	5.91719700	4.61030300	-1.46465900
H	6.76732900	3.92938900	-1.31805400
H	6.02760900	5.12032300	-2.42387900
H	5.91530400	5.35653900	-0.65766100
C	2.35053300	-2.15617900	-2.31978200
C	1.54532400	-3.17227800	-1.79256100
C	2.03476700	-4.41416100	-1.06707100
C	3.09220200	-4.10288700	0.01919700
C	2.90727600	-2.71296400	0.63539100
C	3.54025500	-1.53399700	0.14488500
C	4.44664900	-1.44542300	-1.07131800
C	3.87426700	-2.18496500	-2.30011200
H	1.88446800	-1.47746900	-3.03050600
H	0.51783800	-3.21747700	-2.14968400
H	2.42086000	-5.16298300	-1.77747600
H	1.16078600	-4.86885100	-0.58702900
H	3.02661800	-4.85949500	0.80992800
H	4.10479500	-4.18991800	-0.39323800
H	2.64336200	-2.70985700	1.69263300
H	3.72055900	-0.75519000	0.88018300
H	5.46022500	-1.81073300	-0.83454600
H	4.55453300	-0.38141900	-1.31282300
H	4.25658500	-1.72075900	-3.21690800
H	4.22355200	-3.22374500	-2.31987800

CP3

C	-1.89545500	0.50828700	-1.49603600
C	-0.50169100	-0.64763100	0.35902900
C	-0.95590800	-1.02737900	1.80809700
C	-2.47918300	-0.84847800	1.80814200
C	-2.74732800	0.38898800	0.92413800
H	-2.63294500	1.29108500	-1.76225400
H	-0.63961300	-2.03334200	2.10366100
H	-0.47525700	-0.32371200	2.49725700
H	-2.96174300	-1.70654500	1.33150200
H	-2.89558600	-0.74173600	2.81631200
H	-2.78247700	1.29356300	1.54562300
O	-1.40606700	-0.19291500	-2.35722800
C	-1.50690000	0.48910600	-0.03079100
C	-0.65262700	1.78415700	0.18399000
H	-0.85319800	2.54262100	-0.58827000
H	-0.90011600	2.26193900	1.13965700
C	0.90964500	-0.04155500	0.27280400
C	0.79363000	1.30118200	0.15181600
O	-3.96311000	0.27871200	0.18826600

Si	-5.49040800	0.78240700	0.68967100	H	2.56184600	-4.07347000	2.25135200
C	-6.60674500	0.51498700	-0.83923000	H	3.75199800	-2.52304900	3.52686400
C	-5.42537200	2.60126800	1.21086200	H	5.09100100	-2.41218200	2.40929000
H	-6.42405000	2.96909500	1.47644800	H	2.75005900	-0.63467300	2.56412700
H	-4.78697900	2.74467200	2.09125900	H	3.73548000	0.62943700	0.80935100
H	-5.03541600	3.24231300	0.41222500	H	6.12918000	-0.48271700	0.61650900
C	-6.08199400	-0.24751700	2.16354100	H	5.22685800	-0.17696500	-0.85879900
H	-7.09383300	0.04318600	2.47186000	H	5.97029500	-2.38055700	-1.21322200
H	-6.09780900	-1.31812100	1.93044800	H	5.82144000	-2.84484300	0.46618600
H	-5.42682900	-0.10935800	3.03214100				
C	-6.56159300	-0.96821200	-1.26803700	1			
H	-7.19498600	-1.12818800	-2.15284300	C	-0.61654800	0.81412200	1.02796800
H	-5.54327300	-1.28131600	-1.52432100	C	0.12880600	1.25815100	-0.28944300
H	-6.93046900	-1.63524300	-0.47895600	C	-0.62615100	0.69233300	-1.53176900
C	-6.11848500	1.38829300	-2.01557000	C	-0.76471100	-0.83198400	-1.45912600
H	-6.75407400	1.22873300	-2.89880600	C	-1.50129500	-1.26518500	-0.18445500
H	-6.15651400	2.45860700	-1.77767400	H	-1.59343800	1.30578100	1.01609500
H	-5.08965100	1.14272100	-2.30132100	H	-1.61713000	1.15311400	-1.56925700
C	-8.06463000	0.89756800	-0.49991000	H	-0.08576100	0.98465700	-2.43893700
H	-8.15970000	1.95180400	-0.21054500	H	-1.32263100	-1.19634900	-2.32959200
H	-8.71130000	0.74268500	-1.37563500	H	0.22680200	-1.30041300	-1.47063900
H	-8.47294800	0.28768400	0.31539900	H	-1.49635800	-2.36170600	-0.11636900
Rh	2.29903100	-1.51586200	0.08580000	O	0.05134900	1.31930300	2.16637900
C	-0.51549000	-1.89092700	-0.51199100	H	0.98318100	1.04406300	2.09143900
O	0.52861600	-2.41393000	-0.92678100	C	-0.81870500	-0.69070700	1.04462600
O	-1.69906400	-2.45775100	-0.70964600	C	-0.41106600	-1.45805200	2.05775000
C	-1.74476100	-3.60142600	-1.60313200	H	0.06983800	-1.03290900	2.93287500
H	-1.34747000	-3.28454000	-2.57139300	H	-0.55304200	-2.53613900	2.04395300
H	-1.09406300	-4.38459400	-1.20330100	C	1.50600100	0.75520900	-0.25137300
C	-3.19171100	-4.04533300	-1.69434500	C	2.61590600	0.26903400	-0.20650000
H	-3.57336200	-4.34975100	-0.71424100	O	-2.85207700	-0.79695200	-0.28883900
H	-3.82255700	-3.23702300	-2.07673700	Si	-4.19684300	-1.32052300	0.58199400
H	-3.27230900	-4.89961900	-2.37540800	C	-5.68031200	-0.89793900	-0.55307300
C	1.88000200	2.27908100	-0.09614800	C	-4.31960100	-0.41166200	2.23464300
C	2.02208100	3.46267100	0.67161800	H	-5.20156200	-0.73165700	2.80321500
C	2.77552700	2.07033600	-1.14599700	H	-3.43529200	-0.60972200	2.85060900
C	3.03446500	4.37342400	0.37682200	H	-4.38750600	0.67358500	2.09642300
C	3.80576200	2.97573400	-1.43600300	C	-4.07802900	-3.18237600	0.90809300
H	2.67600000	1.17710300	-1.75359200	H	-4.99351300	-3.54929100	1.38818000
C	3.93179800	4.13675100	-0.67534700	H	-3.93517800	-3.75754500	-0.01401600
H	3.15270800	5.27744700	0.96336900	H	-3.24546300	-3.41749300	1.58165900
H	4.70895100	4.86508100	-0.87694000	C	-5.55768000	-1.66875000	-1.88532800
O	1.12949600	3.62059600	1.70697400	H	-6.38968200	-1.40904800	-2.55635300
O	4.62360100	2.62655700	-2.48160300	H	-4.62310700	-1.42739400	-2.40410000
C	1.23578400	4.78049300	2.50867400	H	-5.58853900	-2.75541100	-1.73605000
H	2.20873600	4.83583400	3.01655600	C	-5.69277600	0.61660000	-0.85425100
H	1.08865400	5.69779700	1.92123100	H	-6.52847100	0.86608200	-1.52481000
H	0.44489300	4.70417900	3.25816700	H	-5.81712800	1.21476300	0.05685900
C	5.65614500	3.52402800	-2.84058600	H	-4.76586900	0.93766900	-1.34252700
H	6.37244100	3.67145200	-2.01980700	C	-7.00692900	-1.28664400	0.13506600
H	6.17215200	3.06888000	-3.68863600	H	-7.15811200	-0.74360900	1.07613700
H	5.25700200	4.50235100	-3.14360600	H	-7.85959900	-1.04900500	-0.51757900
C	3.97097400	-2.90173800	-0.63303700	H	-7.05848900	-2.36033400	0.35572300
C	3.18563100	-3.57264800	0.28933500	C	0.15406800	2.79962800	-0.34008500
C	3.49110100	-3.75323100	1.76482400	C	3.93302400	-0.27829400	-0.17800300
C	3.99719300	-2.46513800	2.45961500	C	5.02959500	0.53436800	0.12717600
C	3.39528800	-1.18264300	1.87932700	C	4.14599900	-1.65318100	-0.46375100
C	3.97122100	-0.43076900	0.82831500	C	6.32963900	0.01546500	0.15672800
C	5.22879700	-0.78359600	0.05495500	H	4.87662700	1.58640700	0.34156400
C	5.32633900	-2.28003800	-0.33129000	C	5.44217500	-2.16242300	-0.43292800
H	3.73142600	-3.03922300	-1.68704600	C	6.53232900	-1.33692800	-0.12421800
H	2.39721400	-4.21606600	-0.09978500	H	5.62915000	-3.20807200	-0.64818100
H	4.21266800	-4.57208900	1.91934800	H	7.52605600	-1.76948300	-0.10980700

O	3.02963500	-2.38412800	-0.75542900
O	7.31775100	0.90911200	0.46873500
C	3.19078100	-3.76251100	-1.04022000
H	3.81895800	-3.92214400	-1.92713700
H	3.62681900	-4.30298700	-0.18906200
H	2.18821900	-4.14742100	-1.23557700
C	8.65241400	0.43773800	0.50610600
H	9.26908500	1.30014500	0.76648200
H	8.78571400	-0.34436900	1.26648500
H	8.97216600	0.04635200	-0.46963600
O	-1.10009900	3.29844700	-0.32811700
C	-1.20469600	4.74091400	-0.35122900
H	-0.65630600	5.14419600	0.50562600
H	-0.72062600	5.11278700	-1.25999000
C	-2.67989200	5.09248900	-0.30388000
H	-3.21193300	4.66928200	-1.16211400
H	-3.14354900	4.71163000	0.61175500
H	-2.80207900	6.18104400	-0.32507300
O	1.14837400	3.48569000	-0.39739700

TS3

Rh	0.08665100	-2.01227400	0.03529700
C	1.67624300	-3.43404000	0.52903600
C	1.28123700	-3.60211300	-0.80624300
C	0.37757300	-4.70078800	-1.33543800
C	-0.88195200	-4.91034700	-0.46416200
C	-1.35267700	-3.61381200	0.19465300
C	-0.97084200	-3.18212300	1.47956900
C	0.01283700	-3.88363400	2.39898200
C	1.28944000	-4.36492200	1.67137300
H	2.54342200	-2.80319100	0.71422900
H	1.89060300	-3.11316400	-1.56747100
H	0.93376200	-5.64558300	-1.44372500
H	0.06740400	-4.41207400	-2.34676600
H	-1.68906000	-5.30970300	-1.08916500
H	-0.69525000	-5.66991600	0.30304000
H	-2.29856100	-3.22766700	-0.18193000
H	-1.66045800	-2.51535500	1.99145600
H	-0.47404000	-4.72506900	2.91877000
H	0.29647900	-3.16651600	3.17790100
H	2.11666400	-4.41250400	2.38901100
H	1.15814500	-5.38556600	1.29552700
C	2.57577600	-0.13801000	-0.72417400
C	2.93959500	1.04813500	-1.69214100
C	4.50128400	1.15090800	-1.77322000
C	5.11816800	1.38095300	-0.39110400
C	4.72579500	0.26204600	0.58204500
H	3.04752200	-1.02221400	-1.16876100
H	4.88559900	0.22104500	-2.20337400
H	4.76349200	1.96971100	-2.45202600
H	6.21117900	1.41420400	-0.47178000
H	4.78190100	2.34301200	0.01204800
H	5.07699300	0.52203600	1.58955100
O	1.18084200	-0.38176700	-0.76698700
H	0.23232000	0.08485900	-0.24362100
C	3.21697400	0.07407200	0.63242800
C	2.55515300	0.08730400	1.78898000
H	1.48280400	-0.05129500	1.84495100
H	3.07244400	0.25027000	2.73148700
C	2.39684700	2.31863300	-1.20600700
C	2.06927500	3.37353600	-0.70555200
O	5.34209800	-0.96397800	0.14157300
Si	6.38392800	-1.90865600	1.06520400

C	6.99566500	-3.27335600	-0.12833100
C	5.47123400	-2.64285300	2.55226000
H	6.14406700	-3.24316200	3.17684600
H	5.05304500	-1.85256300	3.18724100
H	4.63841100	-3.28361200	2.24108800
C	7.81407100	-0.84755100	1.70939000
H	8.51552900	-1.44506600	2.30462800
H	8.37995100	-0.38194600	0.89450900
H	7.45001800	-0.04156500	2.35837300
C	7.78969100	-2.63983800	-1.29134500
H	8.12011400	-3.41687100	-1.99626700
H	7.18028500	-1.92087900	-1.85052600
H	8.68751700	-2.11762800	-0.93891200
C	5.79081200	-4.04336600	-0.71151100
H	6.13595900	-4.81949500	-1.41063200
H	5.20501000	-4.54546100	0.06844000
H	5.11592300	-3.37649900	-1.25940600
C	7.90946600	-4.26117000	0.62952200
H	7.38027400	-4.76850300	1.44571400
H	8.27797300	-5.04078900	-0.05293200
H	8.78923500	-3.76450400	1.05774600
C	2.41420900	0.74168700	-3.10635400
C	1.68217400	4.61477800	-0.11340300
C	0.31858000	4.89151000	0.11263800
C	2.65606700	5.55576400	0.27443000
C	-0.06299000	6.09034100	0.71828700
H	-0.40811300	4.15361200	-0.20101100
C	2.26020100	6.75063200	0.87924300
C	0.91497200	7.02061500	1.10538600
H	3.02643100	7.45862100	1.18147400
H	0.59803300	7.94360500	1.58096000
O	4.00265200	5.29548100	0.10012000
O	-1.35603900	6.44029900	0.97554900
C	4.49700500	5.62758600	-1.19640300
H	3.99288600	5.04464100	-1.97720300
H	4.36833800	6.69842300	-1.40666200
H	5.56310400	5.38567000	-1.19338700
C	-2.37564000	5.50079500	0.65218900
H	-3.31680800	5.97139600	0.94202100
H	-2.39448900	5.27163300	-0.41973600
H	-2.24662600	4.56341900	1.20709300
O	2.75847000	-0.50245300	-3.50053300
C	2.34820100	-0.87909300	-4.83458000
H	1.25839300	-0.80190800	-4.89934600
H	2.77636100	-0.16739400	-5.54778000
C	2.83581700	-2.29471400	-5.08039800
H	3.92573000	-2.35467300	-4.99586900
H	2.39497600	-2.99147500	-4.35965900
H	2.55000300	-2.61610900	-6.08807800
O	1.82289900	1.52279600	-3.81897100
C	-4.34557400	1.53102000	-1.40717700
C	-2.10307200	0.18997900	-1.25663700
C	-2.23790000	-0.97779100	-2.28209900
C	-3.72247300	-1.39181300	-2.28517900
C	-4.27725500	-0.91016000	-0.93779200
H	-4.42422900	1.39417400	-2.50782400
H	-1.90250500	-0.68231900	-3.27678800
H	-1.59783800	-1.80492000	-1.95883800
H	-4.27456900	-0.88383800	-3.08506400
H	-3.86886900	-2.46837500	-2.43148100
H	-3.97436300	-1.60093200	-0.13758700
O	-4.86383200	2.49088700	-0.87860100
C	-3.56544300	0.44969200	-0.67189100

C	-3.35916900	0.77649600	0.80882300
H	-3.42594800	1.85753800	0.98006400
H	-4.11400100	0.31039700	1.45286300
C	-1.25457100	-0.11944900	0.01582600
C	-1.96082800	0.27325100	1.11163900
O	-5.68460500	-0.74241100	-0.93719100
Si	-6.88939700	-1.76014400	-0.35725600
C	-8.45482900	-0.66440100	-0.34949000
C	-6.44090300	-2.37228700	1.37790300
H	-7.24338300	-2.99378200	1.79400100
H	-5.53010700	-2.98370000	1.36131300
H	-6.26699400	-1.53757600	2.06603500
C	-7.07962200	-3.26397400	-1.49207200
H	-7.88736600	-3.92405100	-1.15208000
H	-7.30088100	-2.96879300	-2.52405100
H	-6.15889500	-3.86050200	-1.50987500
C	-8.75319700	-0.17458300	-1.78331200
H	-9.64037900	0.47526100	-1.78687300
H	-7.91669800	0.40201700	-2.19265300
H	-8.95673900	-1.00821700	-2.46691600
C	-8.22450100	0.56326500	0.55965300
H	-9.11296700	1.21170400	0.55415700
H	-8.04337500	0.27278000	1.60233000
H	-7.37164200	1.16302700	0.22431200
C	-9.66442000	-1.46849800	0.17420300
H	-9.51069400	-1.82209600	1.20156600
H	-10.56636700	-0.83969000	0.17930700
H	-9.88261200	-2.34255100	-0.45250700
C	-1.59965500	1.51755200	-1.84169000
O	-1.43483400	2.50843600	-1.15345700
O	-1.44241200	1.52143100	-3.17385400
C	-1.05580500	2.79236600	-3.76584200
H	-1.79454000	3.54413800	-3.47043700
H	-0.08301400	3.07383700	-3.36035100
C	-1.00323300	2.59366100	-5.26772700
H	-0.23797100	1.85664700	-5.52536600
H	-1.97098700	2.26160300	-5.65947900
H	-0.74297700	3.54124600	-5.75274700
C	-1.47638500	0.38315100	2.51320200
C	-2.09828800	-0.30012700	3.58794900
C	-0.45724400	1.28783700	2.80802000
C	-1.66447500	-0.08986800	4.89422300
C	-0.01851100	1.50401900	4.12442100
H	0.00074700	1.86049300	2.00876200
C	-0.62592800	0.81150900	5.16977900
H	-2.12474000	-0.61711500	5.72182800
H	-0.31618100	0.95594400	6.19845500
O	-3.11045800	-1.16975700	3.24818500
O	0.99854800	2.40717200	4.26659700
C	-3.77703200	-1.85903600	4.29269300
H	-3.09289900	-2.52050800	4.84144100
H	-4.24551800	-1.16170300	4.99998100
H	-4.55100000	-2.45822600	3.81044100
C	1.43266900	2.71941000	5.57722300
H	1.84773400	1.83977100	6.08952800
H	2.21565000	3.47154000	5.46356800
H	0.61713900	3.13430900	6.18566300

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C	-0.96208300	-0.19276800	1.65732300
C	0.00454600	1.29320400	-0.28429100
C	-0.69370700	1.27686800	-1.67783600
C	-0.72002000	-0.20692200	-2.06472100

C	-1.10046600	-0.90069500	-0.75173300
H	-1.81115800	0.51096800	1.74346600
H	-1.71393400	1.65478200	-1.59258300
H	-0.15775800	1.90094900	-2.40074300
H	-1.43219600	-0.43717700	-2.86335000
H	0.27434300	-0.54185700	-2.38468200
H	-0.86415900	-1.97236900	-0.75122400
O	-0.69277100	-0.94426200	2.56928300
C	-0.22478200	-0.16922200	0.32137800
C	1.18448900	-0.80353700	0.43480600
H	1.37520800	-1.09892000	1.47284400
H	1.25484000	-1.72441700	-0.16084400
C	1.50826400	1.36881100	-0.41466600
C	2.16112300	0.24786400	-0.05900800
O	-2.48651900	-0.69678800	-0.48401600
Si	-3.67265100	-1.89692500	-0.44749300
C	-5.29284900	-0.94303600	-0.09916900
C	-3.26547800	-3.15121900	0.90750000
H	-4.06786300	-3.89049800	1.02060400
H	-2.34881800	-3.70521100	0.67002800
H	-3.10673800	-2.66853400	1.87789400
C	-3.73096600	-2.79551100	-2.11265300
H	-4.48217900	-3.59493300	-2.10595100
H	-3.97194000	-2.11711800	-2.93886200
H	-2.76524600	-3.26363800	-2.34068400
C	-5.57603400	0.05064100	-1.24665900
H	-6.49508500	0.61884600	-1.04074800
H	-4.75872700	0.77061800	-1.36707200
H	-5.71873400	-0.46033300	-2.20675400
C	-5.16635800	-0.15460900	1.22232200
H	-6.09943500	0.38848400	1.43353900
H	-4.97107700	-0.81195400	2.07838600
H	-4.35603900	0.58177800	1.17237600
C	-6.47114800	-1.93539600	0.01336100
H	-6.33470200	-2.64557700	0.83812800
H	-7.40873200	-1.39322400	0.20323400
H	-6.61290200	-2.51399300	-0.90825200
C	-0.47104700	2.40946400	0.65588900
O	0.18286100	2.82490500	1.59006900
O	-1.70669400	2.87254200	0.36397900
C	-2.21474400	3.90610400	1.24021100
H	-2.23701800	3.51922700	2.26398200
H	-1.52034100	4.75205200	1.22336400
C	-3.59609000	4.28853600	0.74221900
H	-3.55190200	4.66590000	-0.28464800
H	-4.27345300	3.42863000	0.76452300
H	-4.01559000	5.07413500	1.38034200
C	3.60706000	-0.04024500	-0.09471800
C	4.59374900	0.86207400	-0.58817900
C	4.05738800	-1.27835900	0.38094600
C	5.93889900	0.49904800	-0.58005800
C	5.40888300	-1.64276200	0.38835000
H	3.35324600	-2.00212500	0.77318000
C	6.35829300	-0.74643000	-0.09567400
H	6.69073200	1.18383200	-0.95383000
H	7.41496900	-0.98743100	-0.10734400
O	4.15522000	2.06966100	-1.06150200
O	5.68229500	-2.88908800	0.88689400
C	5.10984700	3.00401900	-1.53209500
H	5.82030400	3.28773100	-0.74437400
H	5.66591400	2.61551900	-2.39604800
H	4.54104200	3.88455100	-1.83740600
C	7.03566900	-3.30136800	0.92925800

H	7.64202600	-2.63981500	1.56350500
H	7.03236100	-4.30545400	1.35817900
H	7.48060700	-3.33918200	-0.07501500
H	1.97748900	2.26963100	-0.78251900

TS4

C	-1.41664100	-0.63542700	-0.30635300
C	-0.72871700	0.17360300	1.61644500
C	-1.68065300	1.34542000	1.88561200
C	-1.78940300	2.35636600	0.74346000
C	-2.37699200	1.74292800	-0.53613000
H	-2.37526300	-0.95490700	0.11977000
H	-2.67194100	0.93822000	2.09170300
H	-1.36662400	1.87039700	2.79897900
H	-2.43487700	3.18671100	1.05534200
H	-0.80494900	2.77706000	0.50255800
H	-2.43405700	2.53395800	-1.29758600
O	-0.57027000	-1.55906700	-0.55846700
C	-1.48303000	0.63722000	-1.07118300
C	-0.77764500	0.80093800	-2.20193100
H	-0.12724600	0.02128300	-2.58617600
H	-0.83921900	1.72326900	-2.77542500
C	0.56692100	0.41673300	1.18314000
C	1.67382200	0.58275000	0.61514000
O	-3.68975300	1.25937300	-0.24039600
Si	-4.98048200	1.09424900	-1.31050200
C	-6.46246000	0.67214300	-0.17749200
C	-4.65332000	-0.28574000	-2.56185500
H	-5.48719600	-0.38874500	-3.26724300
H	-3.74867400	-0.07853900	-3.14475400
H	-4.50860400	-1.25450700	-2.07013200
C	-5.24173100	2.71777800	-2.24986600
H	-6.12079700	2.65490400	-2.90305600
H	-5.39062900	3.56466000	-1.57035300
H	-4.38323000	2.95329300	-2.89076800
C	-6.71160700	1.82509500	0.81890200
H	-7.54790600	1.57673100	1.48873200
H	-5.83067200	2.01665100	1.44151300
H	-6.97187700	2.75996800	0.30701200
C	-6.15772300	-0.61739200	0.61674400
H	-6.99591800	-0.85894800	1.28695900
H	-6.01137300	-1.48075400	-0.04424800
H	-5.25752800	-0.50922000	1.23235000
C	-7.73407300	0.45429400	-1.02661700
H	-7.62152700	-0.37710100	-1.73352800
H	-8.58920800	0.21544400	-0.37773700
H	-8.00472900	1.34909300	-1.60137000
Rh	1.47432800	-1.23701900	-0.89431200
C	-0.87773400	-1.05917800	2.43416700
O	-0.03949100	-1.93162200	2.56795600
O	-2.12261800	-1.15497400	2.98640100
C	-2.37321000	-2.35189500	3.74635400
H	-2.23309200	-3.22366900	3.09836600
H	-1.63589100	-2.42373700	4.55310900
C	-3.79158700	-2.26385100	4.28150900
H	-3.91286100	-1.38615400	4.92501500
H	-4.51502000	-2.19094100	3.46256800
H	-4.02583800	-3.15812700	4.86999600
C	2.91602700	1.32873900	0.79622600
C	3.84537700	0.98206900	1.81054600
C	3.19387700	2.42714900	-0.01960200
C	5.00072500	1.74391200	1.97552800
C	4.35366600	3.19586900	0.15325900

H	2.49453900	2.70595400	-0.80137700
C	5.26073000	2.85069100	1.15463300
H	5.71705400	1.49223700	2.74942900
H	6.16936400	3.41982800	1.31338900
O	3.52235800	-0.11077100	2.56471300
O	4.49611400	4.25142000	-0.70906400
C	4.37784700	-0.46933000	3.63408300
H	5.38183300	-0.74123400	3.27875700
H	4.46678700	0.34237500	4.36924700
H	3.91439400	-1.33697700	4.10647400
C	5.65114100	5.05937900	-0.58110500
H	6.57147100	4.48196600	-0.74663100
H	5.56784800	5.82970500	-1.35053000
H	5.70414800	5.53930000	0.40609100
C	1.41186300	-2.54893600	-2.61050800
C	1.49368400	-3.30496700	-1.42069600
C	2.73390900	-3.98219600	-0.87251400
C	3.97795400	-3.06918100	-0.91398000
C	3.61402800	-1.59908100	-0.72038000
C	3.36315000	-0.70246100	-1.77242200
C	3.36353000	-1.04823600	-3.25269500
C	2.57628300	-2.33763000	-3.57487300
H	0.41689500	-2.43097700	-3.03821200
H	0.55564600	-3.68465900	-1.01908100
H	2.92749000	-4.92785800	-1.40431000
H	2.52208400	-4.25141000	0.16823900
H	4.67433100	-3.37153700	-0.12354500
H	4.52015200	-3.19629300	-1.85767300
H	3.90196100	-1.17818700	0.23853100
H	3.51620300	0.35390300	-1.56287200
H	4.39576500	-1.11744000	-3.63254100
H	2.90209500	-0.20776800	-3.78488000
H	2.19095800	-2.28113000	-4.59945600
H	3.23893700	-3.21005900	-3.55203700

CP4

C	-1.41454200	1.08821300	-0.75647900
C	-0.59918900	-1.88699700	-0.44278000
C	-1.88000100	-1.98950400	0.38655300
C	-1.97046100	-1.11959000	1.64994800
C	-2.45948800	0.33368600	1.45989700
H	-2.36043300	0.85022900	-1.26100400
H	-2.75232000	-1.79273800	-0.24780700
H	-1.99239600	-3.03798600	0.69279500
H	-2.68423500	-1.59166200	2.33680800
H	-1.00261800	-1.09170200	2.16590600
H	-2.56905800	0.76410700	2.46645600
O	-0.41463100	1.27514400	-1.45778900
C	-1.46646100	1.20530100	0.70928900
C	-0.67192800	2.09211000	1.32948600
H	0.04961100	2.69150800	0.78075000
H	-0.72057200	2.23924700	2.40591900
C	0.48286700	-1.18644700	-0.09884500
C	1.52634000	-0.46967400	0.18003600
O	-3.71215700	0.34745700	0.77265300
Si	-5.18089300	0.86964500	1.41984400
C	-6.43890800	0.66896400	-0.00517100
C	-5.02511300	2.67099800	1.97870500
H	-5.97444900	3.04627200	2.38009900
H	-4.27570600	2.77641800	2.77290200
H	-4.72596600	3.32886200	1.15514700
C	-5.63069100	-0.19534600	2.91736100
H	-6.57854900	0.12616700	3.36605300

H	-5.72865900	-1.25340700	2.64951600
H	-4.86425700	-0.12350600	3.69929100
C	-6.48904000	-0.80490400	-0.46323000
H	-7.20576000	-0.92270000	-1.28898600
H	-5.51211900	-1.15128800	-0.81821500
H	-6.80987200	-1.47489200	0.34369300
C	-6.02964800	1.55077200	-1.20505100
H	-6.74957700	1.43240700	-2.02785600
H	-6.00532300	2.61624400	-0.94533300
H	-5.04129600	1.27555100	-1.59066200
C	-7.84219600	1.09745100	0.47904900
H	-7.86469700	2.14511700	0.80413000
H	-8.57332100	0.99449400	-0.33548800
H	-8.19745000	0.47968600	1.31311400
Rh	1.69881000	1.34421300	-0.96016400
C	-0.50507700	-2.70169400	-1.68181800
O	0.42616900	-2.73820800	-2.46480600
O	-1.64042900	-3.44089000	-1.87341200
C	-1.65393500	-4.25828500	-3.05601600
H	-1.50916200	-3.62124300	-3.93543600
H	-0.81044100	-4.95646700	-3.02015200
C	-2.98750500	-4.98421500	-3.09543400
H	-3.11507300	-5.61589600	-2.20998900
H	-3.81912800	-4.27248800	-3.13076100
H	-3.04157700	-5.62208200	-3.98492300
C	2.55203500	-0.99059600	1.13041000
C	3.50278700	-1.96629900	0.73945600
C	2.58363900	-0.52964800	2.44630000
C	4.42785700	-2.44682500	1.66537000
C	3.51101300	-1.01475600	3.38028500
H	1.86812400	0.22071800	2.76898300
C	4.43731600	-1.97935600	2.98764600
H	5.15593700	-3.19630800	1.37499100
H	5.16985400	-2.37702700	3.68062600
O	3.43976500	-2.36949200	-0.56714500
O	3.41779700	-0.47923900	4.64119900
C	4.25251600	-3.44960500	-0.98151700
H	5.32294400	-3.20224800	-0.92923600
H	4.06583400	-4.34861400	-0.37780700
H	3.97601500	-3.64691300	-2.01860300
C	4.32213100	-0.94662000	5.62309800
H	5.36596700	-0.73845200	5.34849500
H	4.07911000	-0.40695800	6.54110300
H	4.21029100	-2.02591200	5.79864500
C	1.90172200	3.43600300	-1.73646500
C	1.91938700	2.52583400	-2.79524400
C	3.14680100	2.01903600	-3.52833600
C	4.30619700	1.63222300	-2.58291700
C	3.81081000	1.06352300	-1.25388900
C	3.58762200	1.83335000	-0.09339600
C	3.75020100	3.34016500	0.01938400
C	3.13657700	4.12171600	-1.16576400
H	0.94885600	3.91714000	-1.51732800
H	0.97892800	2.36101900	-3.32023700
H	3.48847700	2.75678800	-4.27246600
H	2.84137100	1.13140800	-4.09391200
H	4.93371500	0.88265000	-3.07840200
H	4.95695500	2.49482000	-2.39916700
H	3.99167200	0.00073200	-1.11821300
H	3.65704900	1.31383800	0.85951500
H	4.81380300	3.60314800	0.14224000
H	3.25479000	3.65381700	0.94659500
H	2.86627600	5.12987600	-0.82984000

H	3.88056700	4.26153700	-1.95751000
TS5			
C	-1.50207100	-0.39153900	-1.15969700
C	-0.55984700	-0.58884000	1.69651800
C	-1.69872400	0.29804200	2.20401300
C	-1.78903500	1.69030000	1.56698400
C	-2.23798100	1.70695100	0.08782200
H	-2.52679400	-0.77431700	-1.10165800
H	-2.64297100	-0.22888700	2.04293700
H	-1.60777000	0.42178800	3.29336300
H	-2.51204000	2.28983300	2.13501000
H	-0.82341400	2.20629900	1.63950100
H	-2.25905100	2.76488000	-0.21743300
O	-0.61514600	-1.21940600	-1.54033900
C	-1.27227600	0.96079900	-0.82422900
C	-0.03009800	1.50443300	-1.11996500
H	0.54374000	1.11143400	-1.95381400
H	0.19507300	2.53295700	-0.85058800
C	0.57368200	-0.06114800	1.20366600
C	1.37923500	0.64722900	0.48380400
O	-3.55501300	1.15843900	0.00712500
Si	-4.82449800	1.80475200	-0.88968000
C	-6.33011900	0.71168500	-0.44234000
C	-4.42763700	1.73440600	-2.73855700
H	-5.18316100	2.26238200	-3.33315500
H	-3.45784300	2.20378800	-2.94302900
H	-4.37234500	0.70277800	-3.10490700
C	-5.10296400	3.61130100	-0.39227200
H	-5.97004500	4.03518900	-0.91371600
H	-5.27899400	3.71099300	0.68483400
H	-4.23867400	4.23709200	-0.64623100
C	-6.66091200	0.86359400	1.05787600
H	-7.51073200	0.22039700	1.33004800
H	-5.81158800	0.57775100	1.68857100
H	-6.93762200	1.89396400	1.31260200
C	-6.00744800	-0.76946100	-0.73533800
H	-6.86726800	-1.40637100	-0.48001900
H	-5.78196500	-0.93897000	-1.79574200
H	-5.14940900	-1.11677400	-0.14910000
C	-7.55628600	1.13815400	-1.27889800
H	-7.37939100	1.02415100	-2.35557800
H	-8.42693700	0.51644100	-1.02428600
H	-7.83984900	2.18210800	-1.09409900
Rh	1.48912200	-1.10947900	-1.13676800
C	-0.62644900	-2.05168500	1.86840800
O	0.24967900	-2.85294200	1.57696200
O	-1.81540800	-2.44861400	2.40316700
C	-1.97579800	-3.86632600	2.58679200
H	-1.87696800	-4.36669600	1.61732900
H	-1.17034300	-4.23821900	3.22934100
C	-3.34450300	-4.09421200	3.20407100
H	-3.42620300	-3.58738700	4.17129900
H	-4.13617300	-3.71423700	2.54993800
H	-3.51094300	-5.16595100	3.36068500
C	2.51622300	1.50629300	0.83543500
C	3.13849800	1.44615500	2.11516500
C	3.00877400	2.43811700	-0.08439300
C	4.19598300	2.30370000	2.41521000
C	4.06765400	3.30316100	0.21999300
H	2.56755500	2.50434300	-1.07277900
C	4.66381600	3.23503600	1.47832700
H	4.67536600	2.26360000	3.38663100

H	5.48597300	3.88662300	1.75098400
O	2.64329400	0.51736200	2.98403200
O	4.43450100	4.16494400	-0.78063300
C	3.23040300	0.40788400	4.26778300
H	4.29337000	0.13735200	4.20537900
H	3.13049800	1.34091900	4.83920200
H	2.68508700	-0.38847700	4.77732700
C	5.50125900	5.05964100	-0.52457800
H	6.43623200	4.52517200	-0.30587500
H	5.62857700	5.64687600	-1.43624900
H	5.27266000	5.73540000	0.31130000
C	1.81857100	-2.34969400	-2.87513100
C	1.44585100	-3.14698300	-1.77226000
C	2.35677200	-3.98548600	-0.89898200
C	3.64039000	-3.23528200	-0.48451600
C	3.39732700	-1.73689800	-0.32691500
C	3.60235300	-0.79482400	-1.35018700
C	4.03514000	-1.10193000	-2.77490800
C	3.24369300	-2.26277700	-3.41575500
H	1.02636900	-2.09336400	-3.57762500
H	0.39145100	-3.40705200	-1.69847800
H	2.60571000	-4.93669000	-1.39694500
H	1.78608600	-4.23331400	0.00059300
H	4.00310200	-3.64035000	0.46675500
H	4.44233100	-3.40373700	-1.21283300
H	3.39976900	-1.36723200	0.69654900
H	3.80303800	0.22763700	-1.04089500
H	5.11855600	-1.30037500	-2.81317500
H	3.87411600	-0.19283500	-3.36699700
H	3.21059000	-2.12187400	-4.50223300
H	3.75959200	-3.21607400	-3.25282700

CP5

C	0.92152700	-0.05156600	-0.28579700
C	0.12749100	-0.67663900	0.95298000
C	0.94996800	-1.85399900	1.57248300
C	1.27661000	-2.93373000	0.53977600
C	2.05911700	-2.35288300	-0.64206400
H	1.86548000	0.31347100	0.16699400
H	1.88428700	-1.44541000	1.97494500
H	0.39057900	-2.28254400	2.40699900
H	1.87097000	-3.72538400	1.01165700
H	0.34852200	-3.38339000	0.16671300
H	2.18921400	-3.12808900	-1.40985600
O	0.24682800	0.93712700	-0.95995700
C	1.29377700	-1.19013800	-1.23735200
C	0.92876700	-1.17259900	-2.52137200
H	0.35315600	-0.34460000	-2.91812200
H	1.18855100	-1.98732100	-3.19435400
C	-1.20463000	-1.14087500	0.55554300
C	-2.29024200	-1.58446300	0.24655400
O	3.35040700	-1.95978400	-0.14881500
Si	4.67812300	-1.46407200	-1.05668000
C	6.17808100	-1.82780300	0.07976100
C	4.56359100	0.37777400	-1.46782200
H	5.40015000	0.70225800	-2.09931400
H	3.63325600	0.58593300	-2.00819400
H	4.56598800	0.99796600	-0.56395100
C	4.78055600	-2.45104700	-2.66925100
H	5.69758100	-2.20433500	-3.21837500
H	4.77988100	-3.53307000	-2.49351400
H	3.93515000	-2.21772500	-3.32679800
C	6.27080000	-3.34339100	0.35733900

H	7.11205000	-3.55980200	1.03266800
H	5.35737700	-3.72068000	0.83091500
H	6.43535500	-3.91950300	-0.56183500
C	6.00869400	-1.08669200	1.42401900
H	6.85383000	-1.30834000	2.09285400
H	5.97598800	0.00202400	1.29197500
H	5.08867500	-1.39052700	1.93572000
C	7.48430800	-1.35525300	-0.59438000
H	7.47617400	-0.27685700	-0.79579300
H	8.34714400	-1.55820600	0.05704600
H	7.66916800	-1.87183000	-1.54489500
Rh	-0.21405300	2.66831400	-0.03661800
C	-0.08091800	0.40002900	2.03132500
O	-0.05337200	1.62261500	1.86821600
O	-0.30905300	-0.10652200	3.23770500
C	-0.57405800	0.82484400	4.32121800
H	0.29612700	1.47783000	4.43635600
H	-1.42952300	1.44570000	4.03959500
C	-0.84444600	0.00047100	5.56477200
H	-1.71199900	-0.65090000	5.42090500
H	0.01946600	-0.62208100	5.81787900
H	-1.04860800	0.66735700	6.40939700
C	-3.55767000	-2.12012100	-0.12543500
C	-3.76321300	-3.52628100	-0.13852600
C	-4.61399100	-1.27520700	-0.48058400
C	-5.00908300	-4.03094200	-0.50266200
C	-5.86474500	-1.78932800	-0.84335000
H	-4.46686600	-0.20064900	-0.48049900
C	-6.05981800	-3.17123400	-0.85342700
H	-5.18670600	-5.10001600	-0.52079400
H	-7.01516300	-3.60150300	-1.13109300
O	-2.68834500	-4.29050900	0.21709000
O	-6.81658800	-0.85951700	-1.16766000
C	-2.83982500	-5.69856000	0.21210100
H	-3.61587200	-6.02525400	0.91791600
H	-3.08444800	-6.07622500	-0.79012300
H	-1.87579000	-6.10461800	0.52407900
C	-8.09387500	-1.32766200	-1.55883500
H	-8.58175400	-1.89734800	-0.75551700
H	-8.68714500	-0.43779400	-1.77851700
H	-8.03780200	-1.95587100	-2.45870400
C	-0.93206000	3.49775600	-1.86245300
C	0.45701100	3.72185000	-1.75099200
C	1.12277100	5.02379000	-1.33963200
C	0.45357700	5.68082800	-0.10991500
C	-0.11991700	4.64176200	0.85234700
C	-1.45300400	4.19101900	0.82745900
C	-2.51184500	4.59982200	-0.18532000
C	-1.99642200	4.57278300	-1.64514200
H	-1.23769800	2.63942700	-2.45908500
H	1.10451900	3.01898100	-2.27302300
H	1.15648100	5.72971000	-2.18549100
H	2.16610900	4.79087500	-1.09530900
H	1.19302300	6.29515900	0.41743600
H	-0.33634300	6.37127700	-0.42586700
H	0.41946600	4.52859800	1.79298700
H	-1.85311700	3.78347500	1.75759100
H	-2.92825900	5.59165000	0.05475400
H	-3.34266800	3.89020100	-0.09156700
H	-2.83921400	4.38647300	-2.32071900
H	-1.59641100	5.55319900	-1.92755600

TS6

C	1.07401900	-0.11559200	-0.59483800
C	0.40254500	-0.57681900	1.52266400
C	1.43820300	-1.56120300	2.06923500
C	1.71343900	-2.75499900	1.14894700
C	2.29291900	-2.35762800	-0.21952300
H	1.93489700	0.40931400	-0.16744100
H	2.37489300	-1.02804500	2.24019300
H	1.11104300	-1.94156100	3.04822000
H	2.42586000	-3.43010500	1.63959500
H	0.79086800	-3.32187000	0.97310500
H	2.47819000	-3.28335800	-0.78269900
O	0.14015100	0.54384600	-1.16175100
C	1.30676100	-1.51965400	-1.01313300
C	0.60366400	-2.03852500	-2.03160700
H	-0.13976500	-1.44453700	-2.55119000
H	0.75313700	-3.06396400	-2.36059600
C	-0.89653300	-1.06560300	1.23704400
C	-1.98310800	-1.53514300	0.94173300
O	3.53017000	-1.67096200	-0.00690000
Si	4.81459800	-1.54637600	-1.08881000
C	6.27623300	-0.95580200	-0.00290300
C	4.41706200	-0.30255100	-2.45747400
H	3.51092700	-0.60281000	-2.99608900
H	4.24198300	0.70222100	-2.05557800
H	5.23212000	-0.23357400	-3.18846800
C	5.15954100	-3.23302200	-1.87718500
H	4.32754300	-3.55437800	-2.51552000
H	6.05330200	-3.19163300	-2.51178800
H	5.32180900	-4.01332200	-1.12483100
C	6.57396700	-2.00818500	1.08637500
H	7.39556600	-1.66885500	1.73446300
H	5.69930000	-2.18632500	1.72165300
H	6.87731900	-2.96988900	0.65424900
C	5.91113600	0.38063700	0.68001800
H	6.73658100	0.71891100	1.32379300
H	5.72253200	1.17582800	-0.05202400
H	5.01681400	0.28027800	1.30580300
C	7.53658400	-0.75218900	-0.87144200
H	7.38231600	0.00281800	-1.65230000
H	8.37788100	-0.41065900	-0.25093300
H	7.85347500	-1.68122000	-1.36198800
Rh	-0.91427600	2.20577900	-0.43889400
C	0.50823600	0.80839600	1.88950100
O	-0.29354000	1.73126200	1.57943100
O	1.62391300	1.12705000	2.58207200
C	1.85906100	2.52224300	2.86455200
H	1.89694500	3.07937800	1.92254200
H	1.02052200	2.91346900	3.44923000
C	3.16952300	2.61088000	3.62609200
H	3.11685100	2.04392600	4.56111200
H	3.99694600	2.21413300	3.02886700
H	3.38830300	3.65686400	3.86807300
C	-3.25162900	-2.10099400	0.63300500
C	-4.45022500	-1.35228200	0.76276300
C	-3.34323700	-3.42493700	0.17264400
C	-5.66868100	-1.92926700	0.42590900
C	-4.57527200	-3.99885400	-0.15680100
H	-2.44365800	-4.01952700	0.05644600
C	-5.74934300	-3.24641100	-0.03783700
H	-6.56710700	-1.32722300	0.52572500
H	-6.71621800	-3.66364500	-0.29409800
O	-4.43221200	-0.03473300	1.17547600
O	-4.52317000	-5.29588200	-0.59231100

C	-4.24487800	0.14830700	2.58018300
H	-5.05680800	-0.32830700	3.14674400
H	-3.28084700	-0.25359900	2.90939600
H	-4.26548900	1.22667100	2.75528800
C	-5.73993000	-5.93025000	-0.94136600
H	-6.24220000	-5.41712500	-1.77306100
H	-5.47336300	-6.94226700	-1.25291900
H	-6.42904100	-5.98518600	-0.08735300
C	-1.99940100	2.35044500	-2.26328500
C	-0.81468300	3.11854800	-2.34177300
C	-0.72524200	4.62991300	-2.20813300
C	-1.53173900	5.16887000	-1.00368300
C	-1.57582700	4.16543600	0.14757000
C	-2.60916400	3.22780900	0.33830200
C	-3.79828700	3.00261500	-0.58030000
C	-3.39791700	2.93441000	-2.07383900
H	-1.96071100	1.35103600	-2.69476300
H	0.02954000	2.65794400	-2.85602700
H	-1.04139700	5.12569900	-3.13988200
H	0.33273000	4.88405100	-2.07167400
H	-1.07982500	6.10380300	-0.65257100
H	-2.55220600	5.42411600	-1.30934400
H	-0.97930200	4.42212100	1.02246900
H	-2.73571200	2.83661600	1.34772900
H	-4.56490700	3.77838500	-0.42257600
H	-4.24994900	2.05052100	-0.28458400
H	-4.12177600	2.31135700	-2.61090200
H	-3.45114200	3.92647600	-2.53656100

CP6

C	1.05529600	-0.16887400	-0.71294500
C	0.36659800	-0.64425700	1.63325700
C	1.41048000	-1.65052500	2.10631000
C	1.65297300	-2.81874800	1.14060400
C	2.21595700	-2.41384700	-0.23576800
H	1.89582900	0.33428600	-0.22751700
H	2.35397900	-1.12843900	2.27371300
H	1.11010700	-2.07240400	3.07744800
H	2.36342500	-3.51766700	1.60069300
H	0.71899400	-3.36870300	0.97049600
H	2.40546700	-3.34407400	-0.79086500
O	0.10810900	0.49627100	-1.21356000
C	1.21854100	-1.59597800	-1.04006000
C	0.43838300	-2.15496500	-1.98054800
H	-0.31307800	-1.56895800	-2.49798300
H	0.52913800	-3.20555000	-2.24460100
C	-0.92771900	-1.09970800	1.30979500
C	-2.01826300	-1.54675500	0.98709100
O	3.44129500	-1.70305200	-0.04540100
Si	4.80101100	-1.76393200	-1.03703300
C	6.14425300	-0.85124100	-0.02700100
C	4.46288400	-0.90619500	-2.68993800
H	3.60781900	-1.36605100	-3.19965600
H	4.23101400	0.15717800	-2.55894600
H	5.32690300	-0.98011300	-3.36185700
C	5.27350300	-3.56551100	-1.37738300
H	4.50382600	-4.07960000	-1.96581800
H	6.20541900	-3.62122000	-1.95340600
H	5.41865200	-4.13436800	-0.45211900
C	6.40342100	-1.60143000	1.29735000
H	7.15881000	-1.07117000	1.89574600
H	5.49244000	-1.67802600	1.90119400
H	6.77963600	-2.61750500	1.12546500

C	5.66487700	0.58091800	0.29675300	C	-1.91164200	2.19136700	1.56787800
H	6.41801000	1.10803700	0.90122400	C	-2.32487200	1.97398000	0.09444300
H	5.50449000	1.17509800	-0.61172300	H	-2.46290800	-0.62231800	-0.66416900
H	4.72652100	0.57092000	0.86302100	H	-2.61839700	0.31657100	2.37860200
C	7.45909700	-0.77591500	-0.83319800	H	-1.50431200	1.17943800	3.42631200
H	7.33388100	-0.23185900	-1.77759700	H	-2.69313800	2.79408100	2.04812600
H	8.23214600	-0.24941100	-0.25492700	H	-0.99308900	2.79053100	1.57716200
H	7.85498300	-1.77172000	-1.06950900	H	-2.40560000	2.97650700	-0.35455800
Rh	-0.84514500	2.21984500	-0.43461100	O	-0.63148600	-0.99957200	-1.44680800
C	0.54394300	0.74309800	1.87345200	C	-1.29240200	1.18124400	-0.70679900
O	-0.25891200	1.67695500	1.56132000	C	-0.08799600	1.76320200	-1.05328700
O	1.71967200	1.07949500	2.46890700	H	0.59041000	1.23716400	-1.71339600
C	1.98064200	2.47839000	2.68342700	H	0.04572200	2.83776100	-0.96878400
H	2.02272400	2.99532200	1.71788300	C	0.59595500	0.62965900	1.40364000
H	1.15655500	2.91470100	3.25674700	C	1.39755200	1.34590600	0.75845800
C	3.29942500	2.58098300	3.43007100	O	-3.60698100	1.33980200	0.07909800
H	3.24490000	2.05687400	4.38974000	Si	-4.88488000	1.72005300	-0.94468700
H	4.11630100	2.14481800	2.84608600	C	-6.33566600	0.65254900	-0.29855300
H	3.53670600	3.63314600	3.62356800	C	-4.45312100	1.30191500	-2.73878200
C	-3.29672600	-2.06750200	0.64882400	H	-3.52854600	1.80831700	-3.04129900
C	-4.46575800	-1.26401300	0.71504200	H	-4.29427100	0.22702300	-2.88235300
C	-3.43338000	-3.39832700	0.21810300	H	-5.24550200	1.62011000	-3.42759800
C	-5.69539400	-1.79385100	0.34451500	C	-5.26955500	3.57125100	-0.83209900
C	-4.67701300	-3.92420100	-0.14535600	H	-4.44021500	4.17612500	-1.21880300
H	-2.55877000	-4.03630900	0.15115700	H	-6.15677000	3.82776000	-1.42424100
C	-5.81935700	-3.11740400	-0.09137800	H	-5.45401600	3.88539700	0.20131100
H	-6.56850800	-1.14985800	0.39619000	C	-6.72410900	1.09652600	1.12848400
H	-6.79388600	-3.49662700	-0.37587800	H	-7.53810800	0.46639500	1.51658100
O	-4.40366200	0.06041200	1.10208500	H	-5.87900900	1.01220600	1.82105800
O	-4.66776700	-5.23329900	-0.54848900	H	-7.07727700	2.13490700	1.15327300
C	-4.26335900	0.26216800	2.50987300	C	-5.91458400	-0.83277700	-0.25978800
H	-5.12110900	-0.16095300	3.05092700	H	-6.74376600	-1.45529200	0.10819500
H	-3.33531000	-0.18117800	2.88556300	H	-5.64185200	-1.20932800	-1.25369400
H	-4.23527700	1.34344900	2.66472300	H	-5.05777600	-0.98833600	0.40538800
C	-5.89783900	-5.82053700	-0.93066200	C	-7.55990900	0.80589700	-1.22748900
H	-6.34436000	-5.30563100	-1.79259400	H	-7.34732400	0.46429000	-2.24809600
H	-5.66630300	-6.85074900	-1.20907900	H	-8.40165400	0.20568100	-0.85218800
H	-6.62116700	-5.82427700	-0.10354800	H	-7.90562000	1.84575400	-1.28718100
C	-1.96248300	2.45814300	-2.23343900	Rh	1.12132200	-1.95292000	-0.68088700
C	-0.74458100	3.17113300	-2.31981900	C	-0.66604100	-1.38654900	1.78528400
C	-0.58126200	4.67338600	-2.15394700	O	0.12804300	-2.18409900	1.21775000
C	-1.33187400	5.22050700	-0.91727900	O	-1.72477500	-1.89610500	2.45021300
C	-1.40105100	4.19131300	0.20967200	C	-1.94025800	-3.31883600	2.36361400
C	-2.47361300	3.29849000	0.40104200	H	-1.99435400	-3.61085100	1.30989700
C	-3.69064000	3.14800900	-0.49489800	H	-1.08495900	-3.83738500	2.80943500
C	-3.32611300	3.10474600	-1.99804500	C	-3.23140000	-3.62268500	3.10266600
H	-1.98377300	1.46971600	-2.69088300	H	-3.16387400	-3.31303300	4.15061000
H	0.06503000	2.68689200	-2.86760900	H	-4.07653400	-3.10005500	2.64290000
H	-0.89608400	5.20570500	-3.06570700	H	-3.43279300	-4.69925200	3.07221400
H	0.49039100	4.87494600	-2.03816700	C	2.68713900	1.98485800	0.70124800
H	-0.82462100	6.12151100	-0.55356300	C	3.67179200	1.70633500	1.69619800
H	-2.34479300	5.53495700	-1.19123400	C	3.01668100	2.88482200	-0.31732000
H	-0.77537200	4.39556500	1.07778100	C	4.91310700	2.33502900	1.63355500
H	-2.59212600	2.88584700	1.40255100	C	4.26494300	3.51787000	-0.37269800
H	-4.42000300	3.95019400	-0.29767800	H	2.29595000	3.11300000	-1.09302700
H	-4.17473000	2.20669100	-0.21621000	C	5.21686700	3.24141700	0.60714800
H	-4.09114300	2.53394200	-2.53604300	H	5.66865600	2.13369300	2.38426400
H	-3.33926100	4.11138600	-2.43127600	H	6.19330200	3.71174600	0.59564200
TS7				O	3.31314300	0.81507100	2.66642300
C	-1.47683900	-0.21000200	-0.91441700	O	4.44415900	4.38018400	-1.42304200
C	-0.56703300	0.04044200	1.82297800	C	4.23382700	0.55171100	3.70963100
C	-1.69652100	0.90337200	2.37920900	H	5.16048300	0.09903300	3.33036600
				H	4.48359200	1.46427900	4.26797600

H	3.73543400	-0.15442700	4.37638800
C	5.68540300	5.05293100	-1.52153600
H	6.52129400	4.34919500	-1.63972000
H	5.61823700	5.68246000	-2.41118600
H	5.87456800	5.68692200	-0.64404100
C	2.30144800	-1.51820400	-2.40778000
C	1.51752000	-2.67284400	-2.62677000
C	2.00984800	-4.10953400	-2.55831600
C	2.87717300	-4.38536500	-1.30791200
C	2.44785300	-3.52355900	-0.12117300
C	3.02147600	-2.26819800	0.18778700
C	4.10899700	-1.57217700	-0.61417600
C	3.80380200	-1.54112500	-2.13014800
H	1.91301100	-0.58572100	-2.81486700
H	0.59070800	-2.53610700	-3.18416000
H	2.55310800	-4.38093900	-3.47773600
H	1.12357000	-4.75404500	-2.52470400
H	2.79468500	-5.44404000	-1.03639600
H	3.93665400	-4.21289000	-1.52856100
H	1.95234100	-4.05042700	0.69328500
H	2.92988500	-1.92105900	1.21710600
H	5.09013700	-2.03726900	-0.42522100
H	4.18068200	-0.54437800	-0.24416100
H	4.26536200	-0.65207900	-2.57415700
H	4.25927600	-2.40127900	-2.63437200

CP7

C	-1.36087400	-0.16749900	-1.14626300
C	-0.50670500	0.14748800	1.97017500
C	-1.67115100	1.02074300	2.44175900
C	-1.87113400	2.23942500	1.52200900
C	-2.19355900	1.91724200	0.03388200
H	-2.37476700	-0.57769500	-1.08152000
H	-2.57803200	0.40983100	2.43497600
H	-1.52921800	1.35918600	3.47663400
H	-2.70318200	2.84012800	1.91019100
H	-0.98031700	2.87805800	1.55676600
H	-2.25675800	2.90534300	-0.45945800
O	-0.45872400	-0.94886700	-1.71728000
C	-1.13796300	1.09308500	-0.68879800
C	0.24936100	1.66880700	-0.77853500
H	0.75981300	1.23719200	-1.64613500
H	0.20578700	2.75910500	-0.92302200
C	0.54662100	0.69740600	1.38994200
C	1.14276600	1.44048200	0.48437300
O	-3.47963600	1.28995900	0.00146800
Si	-4.73326700	1.72487500	-1.02905600
C	-6.17137800	0.55535100	-0.54768200
C	-4.23027200	1.51608400	-2.84029200
H	-3.29705300	2.05429600	-3.04394900
H	-4.05558100	0.46634200	-3.09990600
H	-4.99780900	1.91172600	-3.51707900
C	-5.20119500	3.54058700	-0.74582300
H	-4.36736900	4.20913400	-0.99313100
H	-6.04722000	3.83403300	-1.37987400
H	-5.48117600	3.73304500	0.29622000
C	-6.59747600	0.81705600	0.91267700
H	-7.40596200	0.13056200	1.20566300
H	-5.76353700	0.66637000	1.60760200
H	-6.97143500	1.83860700	1.05351800
C	-5.71604200	-0.91420000	-0.67817300
H	-6.53370100	-1.59506600	-0.39751400
H	-5.42302800	-1.16382400	-1.70535700

H	-4.86159100	-1.12745600	-0.02640700
C	-7.37904600	0.79538900	-1.47923300
H	-7.13287000	0.59704400	-2.52971600
H	-8.21058900	0.12850900	-1.20776900
H	-7.75417300	1.82456600	-1.41144400
Rh	1.06195200	-1.95381900	-0.72923800
C	-0.63798100	-1.31812700	1.94269700
O	-0.00554900	-2.09679500	1.21783300
O	-1.55314400	-1.78356400	2.80032000
C	-1.81518700	-3.20831400	2.78241300
H	-2.08117400	-3.50228400	1.76273400
H	-0.89496100	-3.73486800	3.05473700
C	-2.93780300	-3.47205900	3.76814600
H	-2.65473800	-3.15943800	4.77836800
H	-3.84524300	-2.93214800	3.47998700
H	-3.16553000	-4.54333700	3.78920700
C	2.47792800	2.05409900	0.56719700
C	3.29171900	1.89677400	1.72249000
C	2.98997400	2.79761600	-0.49929700
C	4.55754000	2.47489600	1.76833200
C	4.26250200	3.38218500	-0.45160400
H	2.40852500	2.93808500	-1.40258100
C	5.04924600	3.22048400	0.68787200
H	5.18284300	2.35847800	2.64593600
H	6.03742500	3.65959600	0.75976100
O	2.75095300	1.16079600	2.73785500
O	4.63070900	4.08270600	-1.56899100
C	3.50667600	0.97255600	3.92166100
H	4.44508100	0.43869300	3.72082700
H	3.73312600	1.92986000	4.40984300
H	2.88136600	0.36888300	4.58196600
C	5.90978500	4.68951800	-1.58032400
H	6.71263800	3.94629300	-1.47722900
H	6.00056000	5.18366100	-2.54963400
H	6.01119000	5.43832800	-0.78245500
C	2.31230200	-1.64205100	-2.42077500
C	1.50788500	-2.78956000	-2.61382800
C	1.96006500	-4.23187400	-2.46160500
C	2.77893000	-4.47153700	-1.17132300
C	2.33484800	-3.55036000	-0.03606400
C	2.92760300	-2.30041400	0.23866200
C	4.05365500	-1.65737300	-0.55644000
C	3.80216400	-1.68690400	-2.08291900
H	1.95953600	-0.72565200	-2.89052500
H	0.60396300	-2.65174100	-3.20531400
H	2.52751800	-4.55863900	-3.34827200
H	1.05725700	-4.85348800	-2.43085900
H	2.66343000	-5.51597700	-0.85852400
H	3.84880700	-4.33394000	-1.36557500
H	1.79968900	-4.03239500	0.78102700
H	2.81724500	-1.91355500	1.25264800
H	5.02280000	-2.12426500	-0.31576100
H	4.12737200	-0.61388800	-0.23036500
H	4.30240500	-0.82938000	-2.54730400
H	4.25685400	-2.57822400	-2.53092400

TS8

C	-3.74386200	-3.44995500	-0.94715400
C	-0.27567200	-1.25047200	0.23320500
C	-1.75955500	-0.94874100	0.22633800
C	-2.34406400	-0.78481700	-1.19750400
C	-3.88328300	-0.82312200	-1.29981800
H	-2.70241900	-3.30570600	-0.62302700

H	-2.27654800	-1.74910600	0.76521400
H	-1.96087800	-0.03385100	0.79347100
H	-1.99813100	0.17591700	-1.59881800
H	-1.92589200	-1.55167800	-1.86282600
H	-4.15793200	-0.34815300	-2.25399400
O	-4.21088300	-4.57826100	-0.97835600
C	-4.50790700	-2.22497300	-1.34132100
C	-5.76907000	-2.39812100	-1.76287100
H	-6.20206200	-3.39408300	-1.78605300
H	-6.39108800	-1.56613200	-2.08168400
C	0.69150300	-0.23391700	0.13038900
C	1.39239100	0.79479000	0.06588800
O	-4.47226000	-0.08920700	-0.22030400
Si	-5.11734900	1.46024300	-0.27513000
C	-5.75877400	1.76514300	1.50034900
C	-6.51820300	1.53797100	-1.54943000
H	-6.94412400	2.54711700	-1.60860900
H	-6.15784400	1.28329900	-2.55408700
H	-7.33214000	0.84658900	-1.30318900
C	-3.79609300	2.72202400	-0.77302600
H	-4.20279000	3.74099700	-0.78536300
H	-2.94136500	2.71052300	-0.08743700
H	-3.41238800	2.51559400	-1.77998100
C	-4.58604700	1.68632400	2.50168100
H	-4.94931800	1.84712400	3.52748600
H	-4.09642800	0.70690400	2.47099000
H	-3.82368300	2.44998800	2.30294200
C	-6.80244700	0.68820800	1.86887100
H	-7.15946600	0.83899600	2.89835600
H	-7.68072600	0.72663800	1.21217300
H	-6.37916100	-0.31993700	1.80487700
C	-6.41421300	3.16029400	1.59578100
H	-7.27316800	3.26001400	0.92020500
H	-6.78270900	3.33912800	2.61643800
H	-5.70736800	3.96619400	1.36112300
Rh	2.81955600	-1.12887900	0.03068500
C	0.25956300	-2.52189000	0.31848600
O	1.53008200	-2.75993600	0.27203100
O	-0.58524000	-3.57399800	0.46043400
C	-0.03183000	-4.90232200	0.44928300
H	0.40302800	-5.10186500	-0.53778900
H	0.77336100	-4.96745900	1.18753000
C	-1.16388900	-5.86543800	0.76631400
H	-1.55775100	-5.68001400	1.77127200
H	-1.98933800	-5.76388200	0.05394800
H	-0.79385000	-6.89640700	0.72729000
C	1.79237000	2.17444600	0.02723300
C	2.15542400	2.86759900	1.21558200
C	1.77854000	2.87905500	-1.18258400
C	2.47777600	4.22210100	1.14885700
C	2.10249400	4.24075100	-1.24413000
H	1.49252900	2.36815400	-2.09592000
C	2.45313000	4.91096100	-0.07153500
H	2.74975800	4.76753800	2.04515500
H	2.70855200	5.96438500	-0.08119600
O	2.15822400	2.12929700	2.36290300
O	2.04111700	4.80961300	-2.48738600
C	2.44675600	2.78659700	3.58492700
H	3.46374800	3.20252600	3.59263500
H	1.72795900	3.59156000	3.78896900
H	2.36394000	2.02315800	4.36027800
C	2.35112400	6.18678900	-2.60305000
H	3.38272300	6.39826300	-2.28922800

H	2.24014800	6.43279000	-3.66086400
H	1.66307600	6.80823200	-2.01337500
C	4.25475200	-2.63581400	-0.57064300
C	4.28395400	-2.47883000	0.82906000
C	5.33046600	-1.72038600	1.62065700
C	5.68510900	-0.36100700	0.98275400
C	4.48735900	0.27804800	0.28188400
C	4.19078700	0.13177000	-1.08359200
C	4.95003000	-0.72432700	-2.08158900
C	5.32050700	-2.11598300	-1.52774100
H	3.62875800	-3.43971900	-0.95084500
H	3.69730300	-3.18925900	1.40850200
H	6.23500500	-2.33457100	1.75804200
H	4.92183100	-1.54839100	2.62306800
H	6.04453100	0.32089900	1.76196700
H	6.51437600	-0.47062600	0.27548700
H	4.08549300	1.15404500	0.77995200
H	3.60556500	0.92491800	-1.54348300
H	5.84734300	-0.19139500	-2.43582400
H	4.30534300	-0.85180900	-2.95897300
H	5.42985800	-2.82000300	-2.36043700
H	6.29410900	-2.08789800	-1.02726800

CP8

C	0.81628100	-1.21867500	-0.42096200
C	0.23946300	-0.65523700	1.99264500
C	1.58751100	-0.53843500	2.69636300
C	2.65561400	0.25429300	1.92669900
C	3.01338100	-0.35252300	0.55438900
H	1.07792000	-2.20425600	-0.01165700
H	3.20819800	-1.42888200	0.70019900
O	-0.25761100	-1.06971400	-1.06098400
C	1.86226300	-0.19180300	-0.42684900
C	1.72760500	0.89117900	-1.21239000
H	0.86523800	0.99580700	-1.86090300
H	2.47878000	1.67277500	-1.22009100
C	-0.44631900	0.52563000	1.65547500
C	-0.94950400	1.59067000	1.33173500
O	4.18777000	0.29996800	0.07631400
Si	5.47710700	-0.46872400	-0.68299900
C	6.64538400	0.95381000	-1.20525100
C	4.87235200	-1.46976400	-2.17144700
H	5.70951400	-1.93568600	-2.70571100
H	4.20090200	-2.27876500	-1.85755800
H	4.32059400	-0.84603100	-2.88288400
C	6.31771000	-1.64956800	0.53600200
H	7.14892900	-2.18799800	0.06442300
H	6.71383900	-1.11797700	1.40866100
H	5.61185800	-2.40483000	0.90359300
C	7.03831600	1.78851800	0.03295800
H	7.70324200	2.61507700	-0.25801800
H	6.15860900	2.22113800	0.52175200
H	7.57397500	1.18744300	0.77806800
C	5.93476900	1.87114300	-2.22289200
H	6.59568200	2.69904500	-2.51951500
H	5.65765500	1.33192500	-3.13699100
H	5.02286300	2.30932500	-1.80188600
C	7.92319800	0.37577000	-1.85218300
H	7.70250200	-0.21153700	-2.75258500
H	8.59928800	1.18900800	-2.15392500
H	8.48010900	-0.26818400	-1.16019300
Rh	-2.23579600	-1.68457300	-0.54753300
C	-0.47213700	-1.87910900	1.98139600

O	-1.60581900	-2.10356300	1.45090600	C	1.02742700	0.53564400	-0.55434100
O	0.16122200	-2.92432900	2.58221400	H	0.21904400	0.67168600	-1.26272800
C	-0.48124100	-4.20990800	2.53057000	H	1.66426800	1.38957800	-0.35837200
H	-1.46704900	-4.14068800	3.00206600	C	-0.35401400	0.14958400	1.76567700
H	-0.63387200	-4.50273600	1.48583100	C	-0.35317000	1.25812300	1.19243100
C	0.41946900	-5.19139700	3.26073200	O	3.84507400	-0.24049700	0.14173000
H	1.40102800	-5.25543200	2.77943100	Si	4.83115700	-0.61336400	-1.16522200
H	0.56669400	-4.88485000	4.30133800	C	6.44334800	0.36287200	-0.81884000
H	-0.03341900	-6.18912100	3.25484400	C	4.05190700	-0.07735100	-2.80466100
C	-1.58593200	2.81002500	0.98688700	H	3.09619900	-0.58936500	-2.96249500
C	-0.83800100	4.01623700	0.87644100	H	3.85235700	1.00019000	-2.82773900
C	-2.96474800	2.85345200	0.73758200	H	4.70421400	-0.31626600	-3.65409200
C	-1.48494700	5.19806600	0.52800100	C	5.15212500	-2.47949200	-1.23602700
C	-3.60649300	4.04362000	0.37816600	H	5.89732300	-2.71641900	-2.00549000
H	-3.55154600	1.94609100	0.82967500	H	5.52323800	-2.87211700	-0.28234300
C	-2.86579600	5.22157100	0.27582200	H	4.24006300	-3.03253300	-1.49124700
H	-0.92820100	6.12433600	0.44236600	C	7.08854700	-0.14625000	0.48755900
H	-3.33299300	6.16105400	0.00414500	H	7.99897900	0.42743200	0.71707800
O	0.50186600	3.90739800	1.12841200	H	6.40571900	-0.04372900	1.33835300
O	-4.95670600	3.94152100	0.15086800	H	7.37961000	-1.20164300	0.41547800
C	1.29171400	5.07820900	1.04302300	C	6.11419100	1.86310600	-0.66077100
H	1.26890300	5.51121900	0.03310000	H	7.02635800	2.43574400	-0.43556800
H	0.96671900	5.84037900	1.76500100	H	5.68166500	2.28597500	-1.57615800
H	2.31222000	4.77051800	1.27931700	H	5.40201000	2.03002400	0.15531700
C	-5.65748400	5.11962900	-0.19914700	C	7.44299200	0.18332400	-1.98152200
H	-5.28661000	5.54970000	-1.14021900	H	7.03865300	0.55033100	-2.93291600
H	-6.70126500	4.82470500	-0.32685900	H	8.36786000	0.74451000	-1.78273000
H	-5.59215600	5.88160400	0.59014300	H	7.72693800	-0.86750500	-2.12189600
C	-2.80024300	-2.03425700	-2.58025300	Rh	-2.37505900	-1.34119700	-0.67168900
C	-2.92876900	-0.66308800	-2.26872400	C	-0.93498500	-2.17456300	1.97443300
C	-4.22596100	0.06575500	-1.96294800	O	-2.00606100	-2.12883900	1.30854200
C	-5.11604300	-0.69411200	-0.95137000	O	-0.61230700	-3.32681900	2.60352600
C	-4.28908700	-1.52154200	0.03185700	C	-1.47050700	-4.46424900	2.38947000
C	-3.94669400	-2.87631600	-0.16332200	H	-2.48086700	-4.21945300	2.73302700
C	-4.28930100	-3.71745700	-1.38168000	H	-1.52584100	-4.67848100	1.31694100
C	-3.98466000	-2.99150400	-2.71217000	C	-0.87811900	-5.62574300	3.16793800
H	-1.89045800	-2.33507400	-3.09915800	H	0.13157500	-5.85900100	2.81451500
H	-2.10452500	-0.01471400	-2.56509800	H	-0.82323700	-5.39193200	4.23605100
H	-4.78389800	0.27206400	-2.89021800	H	-1.50304200	-6.51659600	3.04044900
H	-3.96100300	1.04146000	-1.54180200	C	-0.73304500	2.63150500	1.04017700
H	-5.72230200	0.02781300	-0.39307800	C	0.23914300	3.66861600	1.03660200
H	-5.82667800	-1.34418300	-1.47410400	C	-2.07829100	2.97886400	0.86640500
H	-4.27059000	-1.15848600	1.05869000	C	-0.16173200	4.98990100	0.86074800
H	-3.70256300	-3.44843600	0.73149500	C	-2.47603900	4.30859600	0.68546100
H	-5.34118100	-4.04336000	-1.34792800	H	-2.83460400	2.20320100	0.88196100
H	-3.68523400	-4.63094200	-1.32825200	C	-1.51421500	5.31909000	0.68218000
H	-3.76614300	-3.73317500	-3.48886900	H	0.56997300	5.78974000	0.86096800
H	-4.86653900	-2.44223400	-3.06054700	H	-1.78672500	6.35900700	0.54482300
H	2.32941800	1.28920000	1.76863500	O	1.53610700	3.26870400	1.21796300
H	3.57461300	0.28625600	2.52487100	O	-3.82406800	4.50265700	0.52091400
H	1.45099900	-0.05547500	3.67529200	C	2.55062800	4.25827000	1.22488300
H	1.96347700	-1.54454600	2.90333600	H	2.58548700	4.80840000	0.27469500
TS9				H	2.41095700	4.97171500	2.04830400
C	0.73048600	-1.88405100	-0.65015100	H	3.49021500	3.72104100	1.36508200
C	-0.00275900	-1.11060000	2.16493100	C	-4.28496100	5.83024200	0.34848200
C	1.36734200	-1.32436200	2.80278100	H	-3.86381100	6.29234800	-0.55525800
C	2.49493300	-0.56478600	2.07779100	H	-5.36978800	5.76260600	0.24463700
C	2.70310400	-0.97406800	0.60360000	H	-4.04374900	6.45904000	1.21663900
H	1.22063500	-2.86053800	-0.48602100	C	-3.02490200	-1.45734500	-2.69859300
H	2.93526100	-2.05133400	0.58556100	C	-2.57119300	-0.15050300	-2.41420500
O	-0.40011500	-1.92293700	-1.22871500	C	-3.45225700	1.05670100	-2.14435800
C	1.47760600	-0.74407700	-0.26833300	C	-4.57798700	0.76125200	-1.12592500
				C	-4.17002800	-0.31562900	-0.11959900

C	-4.42583200	-1.69520200	-0.28500800
C	-5.08405800	-2.34196700	-1.49254000
C	-4.49980200	-1.83460600	-2.83066100
H	-2.31842600	-2.12523200	-3.19005200
H	-1.55772900	0.08947200	-2.73599500
H	-3.87144600	1.45125300	-3.08378200
H	-2.81047700	1.84616400	-1.73896700
H	-4.82520300	1.68455100	-0.59015200
H	-5.49605800	0.45500300	-1.64062900
H	-4.01623100	0.02773800	0.90294600
H	-4.45133400	-2.29783500	0.62258500
H	-6.17617100	-2.19929100	-1.46603300
H	-4.91528900	-3.42268600	-1.41632600
H	-4.60722300	-2.61343700	-3.59406600
H	-5.06957800	-0.97264600	-3.19511200
H	1.58445000	-2.39746600	2.81063500
H	1.36313200	-1.00826100	3.85590100
H	2.30665700	0.51408600	2.11025300
H	3.44111400	-0.73934600	2.60534300

CP9

C	0.73342800	-1.79404000	-0.74173600
C	-0.13431700	-0.86632700	2.26017100
C	1.20769300	-1.11143300	2.95446200
C	2.38832700	-0.49395300	2.17739600
C	2.57674300	-1.00005200	0.72220200
H	1.14125900	-2.80522500	-0.57206800
H	2.73278000	-2.09001600	0.76676900
O	-0.35719900	-1.74221900	-1.47539800
C	1.42060500	-0.74106600	-0.21538300
C	0.92862900	0.66673400	-0.41709300
H	0.36688600	0.73672600	-1.35499900
H	1.76617200	1.36959100	-0.46872900
C	-0.33085900	0.25421600	1.58637300
C	0.00605700	1.18464100	0.73035800
O	3.80421700	-0.37692100	0.28427700
Si	4.67958000	-0.75256900	-1.09737200
C	6.42989600	-0.06085000	-0.72528100
C	3.95461800	0.07174100	-2.63851600
H	4.55386900	-0.14752800	-3.53131400
H	2.93698400	-0.29142400	-2.81896500
H	3.90381300	1.16141700	-2.52909500
C	4.71943300	-2.62682600	-1.36793400
H	5.36819500	-2.89174600	-2.21200300
H	5.08673400	-3.16295000	-0.48491400
H	3.71644600	-3.00571400	-1.59648600
C	7.03418700	-0.78975900	0.49376700
H	8.02493600	-0.37761600	0.73784500
H	6.39914600	-0.68147000	1.38025700
H	7.16605500	-1.86223800	0.30348400
C	6.33400100	1.44676900	-0.40367200
H	7.32937800	1.85464600	-0.17087000
H	5.93723400	2.02118000	-1.25042400
H	5.68500900	1.62928800	0.46050200
C	7.35884200	-0.25788100	-1.94235000
H	6.99004400	0.26900900	-2.83102100
H	8.36417300	0.13324900	-1.72592700
H	7.47364400	-1.31709600	-2.20570600
Rh	-2.28851900	-1.31659400	-0.83331100
C	-1.12716800	-1.94806200	2.13571300
O	-1.98656000	-2.04976200	1.25190500
O	-1.01655900	-2.88018600	3.08749900
C	-1.90108500	-4.02567100	3.00402200

H	-2.93461000	-3.67123700	3.06736600
H	-1.76699200	-4.49955300	2.02691300
C	-1.54435000	-4.95468300	4.14882800
H	-0.50629900	-5.29280900	4.06989800
H	-1.67340600	-4.45461800	5.11391000
H	-2.19629600	-5.83460000	4.12581300
C	-0.45600500	2.59550300	0.77092800
C	0.45787700	3.67726400	0.80132300
C	-1.82190900	2.87146500	0.76981500
C	-0.02393100	4.98490300	0.80485100
C	-2.30700300	4.18724200	0.77301800
H	-2.53186000	2.05240100	0.74944200
C	-1.40174100	5.24684000	0.78590000
H	0.66243200	5.82338700	0.83076400
H	-1.73860300	6.27711300	0.78331400
O	1.78435400	3.34286600	0.85827600
O	-3.67160500	4.31287800	0.75309000
C	2.74683200	4.38276900	0.87648200
H	2.68155900	5.00979000	-0.02302600
H	2.63711200	5.01741300	1.76633000
H	3.71895000	3.88742300	0.90198100
C	-4.21591000	5.62040100	0.75319300
H	-3.90574000	6.18896800	-0.13451100
H	-5.30048900	5.49618700	0.73930600
H	-3.92764000	6.17935100	1.65418700
C	-2.89484600	-1.43633300	-2.87083600
C	-2.47000300	-0.12283700	-2.57021900
C	-3.37795600	1.06717900	-2.31483200
C	-4.52372000	0.75360900	-1.32279800
C	-4.13267700	-0.32402300	-0.31049600
C	-4.35692600	-1.70501300	-0.48943400
C	-4.96656000	-2.36151700	-1.71781400
C	-4.35953400	-1.83587500	-3.03849400
H	-2.16156300	-2.08837400	-3.34210700
H	-1.45112500	0.13051200	-2.85829300
H	-3.78221300	1.45657000	-3.26320900
H	-2.75799000	1.86764200	-1.89631200
H	-4.79104400	1.67132100	-0.78648200
H	-5.42718300	0.44434900	-1.86132600
H	-4.02489600	0.01916600	0.71847500
H	-4.40698700	-2.31172500	0.41496800
H	-6.06259500	-2.24709300	-1.72302000
H	-4.77267800	-3.43836300	-1.64197200
H	-4.43763000	-2.61118000	-3.80925300
H	-4.93560800	-0.98069600	-3.40964700
H	1.20285500	-0.71946600	3.97989000
H	1.34561900	-2.19436800	3.04752200
H	2.29965000	0.59769600	2.15580500
H	3.31453300	-0.71830400	2.72050000

CP10

C	0.92195300	-1.48047300	-1.40615400
C	-0.34370800	-1.68252200	1.40221500
C	0.89458000	-1.72075300	2.29250800
C	2.05220600	-0.79660000	1.86105900
C	2.56598100	-0.95941100	0.40666000
H	1.35134800	-2.48663400	-1.51979400
H	2.83245500	-2.01637400	0.24697000
O	-0.21943200	-1.27432500	-2.03600800
C	1.53949900	-0.56185600	-0.61851700
C	0.87186200	0.77276000	-0.48145300
H	0.63913200	1.19612300	-1.46412900
H	1.53851900	1.47885500	0.02845300

C	-0.79013900	-0.57410700	0.79441900	H	-2.37344600	-1.77392700	-3.33725700
C	-0.43688700	0.69129700	0.36701300	H	-1.53213400	0.43947900	-3.42413200
O	3.76860400	-0.16331500	0.35266800	H	-3.84818300	1.85476900	-3.56525900
Si	4.89142700	-0.14524000	-0.89517400	H	-2.55939800	2.37928300	-2.49334200
C	6.46357700	0.60169700	-0.08972800	H	-4.39181700	2.47324100	-1.04573600
C	4.30808000	0.91994700	-2.34651300	H	-5.20307100	1.09384600	-1.75066100
H	5.05573000	0.95449700	-3.14901400	H	-3.34724300	1.12471100	0.55914500
H	3.38296000	0.50855500	-2.76500200	H	-3.78620600	-1.18355000	0.83423300
H	4.10253900	1.95119200	-2.03622900	H	-5.78493300	-1.58948000	-0.88758500
C	5.20902600	-1.90455900	-1.52293900	H	-4.41706500	-2.69724700	-0.89114500
H	6.00808300	-1.91650200	-2.27458600	H	-4.69330500	-2.27115900	-3.18662800
H	5.50319600	-2.58423300	-0.71453600	H	-5.10902100	-0.58651400	-2.97132100
H	4.31135900	-2.31890900	-1.99715900	H	1.77782500	0.25438800	2.01272800
C	6.94540400	-0.30648000	1.06172300	H	2.90128600	-0.98293500	2.53006100
H	7.83340300	0.12580500	1.54708600	H	0.62877500	-1.47524900	3.33058000
H	6.17150700	-0.42705600	1.82802000	H	1.24981800	-2.75611500	2.31686100
H	7.22388200	-1.30610600	0.70515800				
C	6.13948700	1.99846900	0.48276000	TS10			
H	7.02746900	2.43068500	0.96846600	C	1.29711200	-1.27768100	-0.70738100
H	5.82383200	2.69863500	-0.30078000	C	0.26039000	-0.94843100	1.68655200
H	5.33945300	1.94901800	1.22969700	C	1.04391300	-0.39425300	2.90239000
C	7.59179800	0.73283600	-1.13496600	C	2.35040600	0.31856000	2.47500400
H	7.30984000	1.39410400	-1.96357300	C	2.76484700	-0.17492400	1.08123900
H	8.49569800	1.15708900	-0.67315600	H	2.00554600	-2.12842800	-0.70429500
H	7.87246700	-0.23807400	-1.56288100	H	3.17626000	-1.19219900	1.15946800
Rh	-1.90687400	-0.61479100	-0.99088900	O	0.27068200	-1.34600100	-1.43502800
C	-1.04985400	-2.93274100	1.05271600	C	1.50732800	-0.23022700	0.23739800
O	-1.91383800	-3.02850700	0.18290800	C	0.73498300	1.04691800	-0.02962900
O	-0.65022200	-4.00156000	1.77483000	H	0.67863800	1.23893900	-1.10280700
C	-1.27186300	-5.26328500	1.44930900	H	1.23295100	1.91284200	0.42706100
H	-2.35523000	-5.16669000	1.57519600	C	-0.90629500	-0.27140800	1.20730400
H	-1.08088300	-5.48989600	0.39539100	C	-0.70844000	0.89564300	0.51442700
C	-0.68275400	-6.31279900	2.37403300	O	3.76633500	0.70971900	0.57605500
H	0.40025700	-6.39317500	2.23537600	Si	4.86108500	0.43676100	-0.67085800
H	-0.87833800	-6.06522800	3.42247000	C	6.24184500	1.72819100	-0.36819400
H	-1.13087100	-7.28950000	2.16060700	C	4.04888900	0.69716800	-2.35982600
C	-0.95079100	1.96899900	0.91603800	H	4.77305200	0.56600500	-3.17364600
C	-1.66109700	2.05080100	2.14611500	H	3.23427300	-0.01715800	-2.52627000
C	-0.68518500	3.16529900	0.23894000	H	3.62380100	1.70345800	-2.44906100
C	-2.06518600	3.29236000	2.63715800	C	5.53216500	-1.33284400	-0.57863700
C	-1.09700700	4.40961100	0.72750700	H	5.96308600	-1.55888300	0.40359200
H	-0.14706000	3.15068500	-0.70147600	H	4.74715400	-2.07298800	-0.77607200
C	-1.78902000	4.47276100	1.93812200	H	6.31640900	-1.48955300	-1.32942100
H	-2.60094100	3.36100000	3.57666600	C	6.89041000	1.48640100	1.01202000
H	-2.11796000	5.41838100	2.35320900	H	7.66492000	2.24216500	1.20938700
O	-1.91265700	0.87030100	2.78508900	H	6.15089900	1.54738800	1.81812900
O	-0.77244500	5.48844300	-0.04879700	H	7.37341800	0.50293100	1.07211300
C	-2.59050100	0.89652900	4.02960500	C	5.63620500	3.14866900	-0.39130400
H	-2.02952000	1.46737300	4.78146300	H	6.41444500	3.89998400	-0.19093300
H	-3.59878800	1.32095300	3.93218500	H	5.19474800	3.38971700	-1.36628200
H	-2.66634600	-0.14466900	4.34786500	H	4.85535200	3.26447900	0.36837900
C	-1.13923900	6.77547000	0.41544800	C	7.32500300	1.62086400	-1.46310200
H	-0.67000700	7.00645200	1.38165700	H	6.92000100	1.81118800	-2.46471200
H	-0.77943800	7.48045000	-0.33635100	H	8.11974000	2.36090600	-1.28869200
H	-2.22910200	6.87677200	0.51303500	H	7.80168900	0.63250200	-1.47722400
C	-2.98851800	-1.00386200	-2.87723700	Rh	-1.87123400	-1.26694900	-0.40697700
C	-2.48658600	0.30169800	-2.92052700	C	0.21905600	-2.44462800	1.56345200
C	-3.27738200	1.57000200	-2.66651800	O	-0.62742400	-3.05130000	0.91660200
C	-4.21970700	1.46766300	-1.44635600	O	1.22543400	-3.07698100	2.20204300
C	-3.66230400	0.58902300	-0.32839500	C	1.25435400	-4.52351400	2.12215100
C	-3.91894600	-0.77430600	-0.16525600	H	1.79559200	-4.82774900	3.02139300
C	-4.70774200	-1.66409600	-1.10921400	H	0.22897100	-4.89717900	2.17193000
C	-4.44257600	-1.37544600	-2.60689600	C	1.95599100	-5.00537700	0.86097100

H	1.39900900	-4.70429100	-0.03055300	Si	-5.33605400	-0.23154900	-0.78158200
H	2.97263400	-4.60257600	0.80050700	C	-6.11482000	1.47742700	-0.43456000
H	2.02210100	-6.09958900	0.87199000	C	-6.01188500	-1.56462300	0.38034600
C	-1.66158100	2.02190600	0.41183400	H	-7.08553300	-1.72267800	0.21975300
C	-1.80909300	2.84362500	-0.73932000	H	-5.51671800	-2.52948200	0.21469100
C	-2.43144800	2.33801600	1.53749800	H	-5.86666600	-1.29516000	1.43257500
C	-2.68158800	3.92999000	-0.71277700	C	-5.62341000	-0.78689800	-2.56899200
C	-3.31855500	3.42244000	1.56076800	H	-6.69321100	-0.90679400	-2.78108900
H	-2.32584500	1.73189700	2.43063200	H	-5.21895600	-0.06708000	-3.28951300
C	-3.43620100	4.22941100	0.43035800	H	-5.14554900	-1.75506000	-2.76410100
H	-2.80076700	4.55941400	-1.58705800	C	-5.52537900	2.52560200	-1.40375900
H	-4.09863000	5.08715000	0.41204200	H	-5.94264700	3.52035800	-1.18974500
O	-1.09642000	2.48053100	-1.85317800	H	-4.43604400	2.59375600	-1.30958600
O	-3.99930100	3.60828400	2.73523500	H	-5.75898500	2.29378100	-2.45037900
C	-1.14949000	3.31841000	-2.99384400	C	-5.81000700	1.91019800	1.01632200
H	-2.16253900	3.36636100	-3.41594400	H	-6.24423800	2.90068700	1.21663300
H	-0.80843700	4.33696600	-2.76361400	H	-6.23571500	1.21438700	1.74995900
H	-0.47745800	2.86821500	-3.72685500	H	-4.73230000	1.97475100	1.20145300
C	-4.90521100	4.69297500	2.80995400	C	-7.64530100	1.40878100	-0.63138100
H	-5.70894700	4.60341800	2.06576300	H	-8.11827800	0.69602600	0.05580100
H	-5.33828800	4.65659600	3.81166100	H	-8.09801200	2.39237500	-0.44010900
H	-4.39709800	5.65769100	2.67146300	H	-7.91765400	1.12019800	-1.65440900
C	-2.60453500	-2.66612000	-1.93247300	Rh	2.67724000	-1.05701400	-0.36439000
C	-2.46399400	-1.39152700	-2.50096800	C	0.37192500	-2.69620700	0.32988700
C	-3.58509100	-0.40284200	-2.76415900	O	1.59956300	-2.84216200	0.39104600
C	-4.55428600	-0.26338900	-1.56950100	O	-0.45825500	-3.67271600	0.67994100
C	-3.84296700	-0.45593700	-0.22918200	C	0.12758000	-4.89404000	1.21482500
C	-3.74505600	-1.69200700	0.45869200	H	0.71968500	-5.36298400	0.42320700
C	-4.26140200	-3.03263900	-0.03631900	H	0.80237400	-4.62068400	2.03004100
C	-3.93369000	-3.29461700	-1.52545400	C	-1.01399600	-5.77482300	1.68315900
H	-1.77452000	-3.35695700	-2.07292400	H	-1.59166800	-5.27723000	2.46816700
H	-1.54197900	-1.19490700	-3.04394000	H	-1.68706400	-6.02180200	0.85581600
H	-4.13587600	-0.66644000	-3.68227700	H	-0.61194800	-6.70907400	2.08974100
H	-3.11634600	0.56970500	-2.95152800	C	0.79640300	2.11491000	0.69313800
H	-5.01006400	0.73327600	-1.58978700	C	1.08766500	2.56931500	2.00364100
H	-5.38283700	-0.97543900	-1.65792400	C	1.02619600	2.98290300	-0.37182700
H	-3.77169000	0.43864300	0.38383800	C	1.60554800	3.84821400	2.19986600
H	-3.62243900	-1.63329800	1.54022100	C	1.54782800	4.27224000	-0.17958000
H	-5.34491700	-3.12319600	0.14593000	H	0.79419200	2.66529000	-1.38342300
H	-3.78189400	-3.80848100	0.57218200	C	1.83734200	4.70467700	1.11258200
H	-3.89015500	-4.37614200	-1.69949700	H	1.84029900	4.20241700	3.19731400
H	-4.73857800	-2.92044900	-2.16788500	H	2.23853100	5.69400200	1.30106000
H	3.15777100	0.16204000	3.19850800	O	0.84159700	1.67411400	3.01126200
H	2.19460900	1.40076300	2.40873700	O	1.72659700	5.01564500	-1.31855300
H	0.39360500	0.30013900	3.44107000	C	1.08964300	2.07705900	4.34396400
H	1.27068200	-1.21578600	3.58569500	H	2.15104300	2.31233100	4.50570700
CP11				H	0.48404900	2.95049500	4.62440100
C	-2.08387400	-1.71755500	1.66539500	H	0.80926500	1.22814500	4.97029600
C	-0.25822900	-1.43742200	-0.21223500	C	2.24632200	6.32349400	-1.17739900
C	-0.65111500	-1.70053100	-1.71586600	H	3.24943400	6.31668100	-0.72795000
C	-1.85070300	-0.78363000	-1.95564900	H	2.30871200	6.73555500	-2.18688000
C	-2.65805300	-0.95770500	-0.66762200	H	1.58852200	6.95937300	-0.56812700
H	-2.79392300	-2.53465000	1.40773400	C	4.44097700	-2.20542400	-1.20374100
H	-3.08042500	-1.97812000	-0.66671400	C	4.68121500	-1.91008200	0.13150200
O	-1.76153400	-1.53731200	2.81954800	C	5.52341400	-0.76407400	0.65973800
C	-1.60472000	-0.89259800	0.47587600	C	5.27280300	0.57333900	-0.07737200
C	-1.24013100	0.55151000	0.90199200	C	3.82045000	0.74267100	-0.52485800
H	-1.31900100	0.65645600	1.98950100	C	3.32409000	0.37209900	-1.79470100
H	-1.93208000	1.27460200	0.45454200	C	4.11618400	-0.31343600	-2.89511200
C	0.78481500	-0.30788300	-0.08927800	C	5.03500700	-1.45195100	-2.38657500
C	0.19717500	0.77357600	0.45998800	H	4.01987700	-3.18478100	-1.42835000
O	-3.69201100	-0.00649100	-0.49714300	H	4.45444900	-2.68797300	0.86154400
				H	6.59585400	-1.01706400	0.63015900

H	5.27069400	-0.63519800	1.71899800
H	5.53553300	1.39989500	0.59320200
H	5.94290800	0.66469600	-0.93984200
H	3.27073400	1.51784900	0.00113400
H	2.45303800	0.91651300	-2.15535800
H	4.70848800	0.42337200	-3.46299400
H	3.39365400	-0.73259800	-3.60644500
H	5.21472700	-2.15761000	-3.20669700
H	6.01831200	-1.05358800	-2.11578900
H	0.20176500	-1.49745600	-2.36863700
H	-0.95007600	-2.74789300	-1.85882300
H	-1.53143500	0.26073400	-2.04571000
H	-2.42245000	-1.04586100	-2.85212800

TS11

C	-3.59823900	-2.95936500	-0.53048900
C	-1.69927700	-1.22471100	-0.96366800
C	-1.86670400	0.12897800	-1.77530700
C	-3.23151300	0.69832800	-1.37019000
C	-4.09369000	-0.54207800	-1.13786300
H	-4.50434400	-3.11925400	-1.15799600
H	-4.33360700	-0.99673400	-2.10973500
O	-3.05034700	-3.91058500	-0.01190800
C	-3.15750100	-1.51260900	-0.37609700
C	-3.02158800	-1.16605800	1.13042600
H	-3.39188300	-1.97070100	1.77133900
H	-3.61099400	-0.27533100	1.38243600
C	-0.76720600	-1.04589000	0.25415100
C	-1.53779100	-0.93941800	1.36821000
O	-5.29080900	-0.24818500	-0.43254700
Si	-6.88915300	-0.59741400	-0.82256900
C	-7.88321600	0.99771500	-0.45376100
C	-7.47790200	-2.03130700	0.26064000
H	-8.52972000	-2.27891200	0.07196200
H	-6.88765000	-2.93477700	0.06459200
H	-7.37493500	-1.79850900	1.32671200
C	-7.03824200	-1.09620800	-2.64390600
H	-8.09296200	-1.22684900	-2.91582900
H	-6.61524700	-0.34363000	-3.31904100
H	-6.53312300	-2.04782800	-2.84856300
C	-7.40338100	2.13660000	-1.37898700
H	-7.94920000	3.06562200	-1.15872900
H	-6.33504800	2.34204100	-1.24613400
H	-7.57292200	1.90314000	-2.43756200
C	-7.65939400	1.41892900	1.01462000
H	-8.19856100	2.35251400	1.23252600
H	-8.02279800	0.66046000	1.71907300
H	-6.59774900	1.59069300	1.22386300
C	-9.39018000	0.75643600	-0.68763100
H	-9.78848900	-0.02830200	-0.03276500
H	-9.96071900	1.67342600	-0.48053600
H	-9.60610500	0.46936100	-1.72452200
Rh	1.24523600	-2.26517600	0.27521900
C	-1.22780100	-2.25494400	-1.97952100
O	-0.09227800	-2.66053800	-2.12779200
O	-2.23724800	-2.63652800	-2.80485000
C	-1.89822500	-3.58426500	-3.84217700
H	-1.10712300	-3.15458500	-4.46497400
H	-1.50047600	-4.48939800	-3.37305200
C	-3.15950800	-3.86336600	-4.63875400
H	-3.93723000	-4.29811000	-4.00246000
H	-3.55147000	-2.94466900	-5.08743700
H	-2.93995300	-4.57277100	-5.44428800

C	-1.10563500	-0.55440600	2.74084900
C	-1.41456000	-1.34831700	3.86824600
C	-0.44286300	0.66802700	2.94774000
C	-1.04670600	-0.92458600	5.14975200
C	-0.07745200	1.09405400	4.23237800
H	-0.20793000	1.26924000	2.07775200
C	-0.38747200	0.28836000	5.33122700
H	-1.27079200	-1.53405200	6.01765300
H	-0.10637600	0.62608700	6.32378500
O	-2.04695000	-2.54258300	3.61961900
O	0.58141700	2.25853400	4.51793800
C	-2.35419700	-3.39047600	4.71194400
H	-1.44768000	-3.70766100	5.24488200
H	-3.03745000	-2.90544900	5.42244200
H	-2.84284700	-4.26569000	4.28022300
C	0.75079000	3.21715100	3.48229200
H	-0.21441400	3.55616500	3.08598200
H	1.26591600	4.06270500	3.94338400
H	1.35832100	2.82607600	2.65823700
C	3.27437800	-2.87475000	0.75305700
C	2.91415600	-3.31575000	-0.53532000
C	2.49773400	-4.72563400	-0.91517300
C	1.46323900	-5.32669100	0.06486100
C	0.55497400	-4.25763100	0.67000700
C	0.81238800	-3.59178000	1.88698500
C	2.03252400	-3.78642400	2.77071900
C	3.35587700	-3.78352600	1.97506300
H	3.84093900	-1.94776200	0.82007900
H	3.24354000	-2.70355400	-1.37660400
H	3.37695900	-5.38423400	-1.00345200
H	2.04817600	-4.66938400	-1.91242600
H	0.84726100	-6.05991600	-0.46812200
H	1.96804700	-5.88282500	0.86351100
H	-0.48455700	-4.28598900	0.34838100
H	-0.05509700	-3.19456000	2.40749800
H	1.93842800	-4.71144500	3.36351400
H	2.04834800	-2.96149400	3.49268900
H	4.17166500	-3.44331800	2.62368700
H	3.62101200	-4.80048000	1.66515800
C	2.59708600	0.62564200	-0.62705200
C	2.17024500	1.86382700	-1.49803700
C	3.39531100	2.82497400	-1.64805900
C	3.92518900	3.27068100	-0.28288500
C	4.32717600	2.06492100	0.57627500
H	3.41944300	0.16090900	-1.18497400
H	4.18129000	2.29558900	-2.19428500
H	3.09401700	3.69347800	-2.24343400
H	4.79703100	3.92191800	-0.41397200
H	3.15553900	3.84674100	0.24476500
H	4.60155300	2.41198500	1.58197300
O	1.55124900	-0.31461000	-0.60917200
H	0.50578600	-0.29396000	-0.08863400
C	3.18039300	1.07123700	0.70171400
C	2.78584100	0.61070500	1.89068600
H	1.99092900	-0.12030800	1.99175800
H	3.26410800	0.94502300	2.80942500
C	1.03977100	2.60064000	-0.92041400
C	0.12377900	3.29745800	-0.53472900
O	5.45048300	1.42633500	-0.05213900
Si	6.89006700	0.97775200	0.69609500
C	8.01038000	0.39199400	-0.73983800
C	6.59493800	-0.40292800	1.95498500
H	7.52445700	-0.67721600	2.46859300

H	5.87641700	-0.08922100	2.72155400
H	6.19223500	-1.30496700	1.48053600
C	7.63022200	2.46776700	1.60198300
H	8.58945300	2.20900800	2.06722600
H	7.80424600	3.31291200	0.92631400
H	6.96972200	2.81746200	2.40508000
C	8.27777800	1.56034200	-1.71293300
H	8.90492500	1.22358900	-2.55140400
H	7.34594900	1.95624800	-2.13229800
H	8.80495000	2.38870400	-1.22400200
C	7.31848000	-0.75216800	-1.51261700
H	7.95815500	-1.09565500	-2.33910500
H	7.12102000	-1.62085400	-0.87222400
H	6.36404300	-0.42806800	-1.94209800
C	9.35661900	-0.11830200	-0.17998400
H	9.22539500	-0.97606400	0.49128800
H	10.01102300	-0.44618200	-1.00071800
H	9.89676200	0.66101900	0.37248300
C	1.76533200	1.36092300	-2.90266600
C	-0.94379500	4.17324000	-0.16630200
C	-1.91070800	3.78676400	0.78768800
C	-1.03068400	5.45170300	-0.75628300
C	-2.93257200	4.66433300	1.15813000
H	-1.83825300	2.79807000	1.22256900
C	-2.05681000	6.32026300	-0.37226300
C	-2.99625800	5.94099700	0.57767000
H	-2.09613000	7.30425300	-0.82966400
H	-3.79346500	6.61150900	0.88249300
O	-0.09901300	5.88358000	-1.67079200
O	-3.90572400	4.38198900	2.07207900
C	-0.28245300	5.38569500	-3.00140000
H	-0.17802000	4.29605300	-3.04499900
H	-1.26604100	5.67800100	-3.39373400
H	0.49909800	5.85056000	-3.60760400
C	-3.92184300	3.09248600	2.66578800
H	-4.77252200	3.08982400	3.34975200
H	-4.06031300	2.30505200	1.91291100
H	-3.00249400	2.89067400	3.23048400
O	2.72396700	0.57609500	-3.42965900
C	2.44174100	0.01568800	-4.73274500
H	1.51533600	-0.56265700	-4.66620000
H	2.27802900	0.83534800	-5.43973700
C	3.62631400	-0.84882000	-5.12146100
H	4.54705700	-0.25783900	-5.16402900
H	3.76879900	-1.66044300	-4.40067500
H	3.45461900	-1.29098300	-6.10913300
O	0.74599200	1.65449400	-3.48973900
H	-3.65496800	1.36814100	-2.12613200
H	-3.16150800	1.26614200	-0.43551100
H	-1.85270000	-0.06671700	-2.85287100
H	-1.04217800	0.81109500	-1.56887400

2a

C	-1.00726900	1.75593500	-1.46407300
C	0.30958800	1.98335000	0.80129800
C	-0.47216700	1.91369900	2.16125800
C	-1.24335900	0.59451500	2.09138000
C	-1.74281100	0.58334500	0.64449700
H	-1.96067200	2.31168000	-1.34025800
H	0.21710000	1.97217000	3.00956600
H	-1.16973000	2.75513000	2.23714000
H	-2.51688600	1.36398000	0.54812100
O	-0.44619500	1.73978100	-2.53725400

C	-0.51812500	1.03828000	-0.20664900
C	0.45049900	-0.12008400	-0.56667600
H	0.64465700	-0.12511000	-1.64567600
H	0.01534500	-1.08732900	-0.30953500
C	1.64673900	1.29433600	0.89647400
C	1.72811700	0.15661300	0.19642700
O	-2.25725500	-0.66762400	0.23038000
Si	-3.87106200	-1.03494900	-0.08560800
C	-3.88946900	-2.93224700	-0.31882200
C	-4.44455700	-0.12336100	-1.64073500
H	-5.47269600	-0.39649600	-1.90890000
H	-4.42939500	0.96348300	-1.49147200
H	-3.80287300	-0.34598300	-2.50055900
C	-4.94957300	-0.48676500	1.37073500
H	-6.00952000	-0.69536200	1.18161800
H	-4.66906200	-0.99275300	2.30137200
H	-4.86029300	0.59329000	1.54263600
C	-3.32990000	-3.61953900	0.94537500
H	-3.31886300	-4.71153800	0.81339000
H	-2.30490100	-3.29513400	1.15727600
H	-3.93888700	-3.40622500	1.83270200
C	-3.01338900	-3.32109700	-1.52990000
H	-3.00391700	-4.41360000	-1.65752400
H	-3.39054200	-2.88857200	-2.46463900
H	-1.97631100	-2.99103400	-1.40285900
C	-5.33453000	-3.41896600	-0.56409900
H	-5.77386700	-2.97097600	-1.46428800
H	-5.35028400	-4.50941200	-0.70456700
H	-5.99552700	-3.19174600	0.28157400
C	0.49705100	3.44172600	0.38020600
O	1.56188900	4.01520100	0.31265300
O	-0.68775100	4.05124300	0.12895900
C	-0.61287700	5.44392300	-0.26125200
H	-0.10039700	6.00080400	0.52941200
H	-0.00587600	5.52021000	-1.16848200
C	-2.03168200	5.93573900	-0.47898000
H	-2.52522600	5.37162500	-1.27704200
H	-2.62617300	5.83566200	0.43515700
H	-2.01697700	6.99299400	-0.76550600
C	2.94432300	-0.68151100	0.09318700
C	2.90461300	-2.09282100	0.22264900
C	4.17829000	-0.07214500	-0.13795900
C	4.07922500	-2.83357900	0.10695600
C	5.36196000	-0.81529600	-0.24772400
H	4.22995200	1.00451800	-0.26218600
C	5.30880400	-2.20333800	-0.12943700
H	4.06216100	-3.91275000	0.20617600
H	6.20129100	-2.81219000	-0.21837300
O	1.67673800	-2.64415800	0.48932000
O	6.49902300	-0.08836800	-0.48000200
C	1.58253500	-4.05200400	0.60314700
H	1.89483500	-4.55547700	-0.32200400
H	2.18613100	-4.43199200	1.43889500
H	0.52912100	-4.26793300	0.79268100
C	7.71767100	-0.79330700	-0.62352300
H	7.68694100	-1.48831200	-1.47432000
H	8.48433400	-0.03736900	-0.80514700
H	7.97261600	-1.35459900	0.28640000
H	2.44019200	1.71544300	1.50510100
H	-2.06142100	0.53214100	2.81683500
H	-0.57937900	-0.26297400	2.25077700

CP12

C	1.71636100	-0.30211100	1.40738300
C	0.59784000	-0.44214000	-1.32729600
C	1.62184100	0.44083700	-2.00949400
C	1.88371700	1.79371700	-1.32710100
C	2.57427900	1.75249700	0.05287500
H	2.46730100	-0.87544600	0.83966300
H	2.56076300	-0.11566200	-2.07833000
H	1.31303500	0.65564000	-3.04481300
H	2.52138000	2.39513300	-1.98918000
H	0.94153100	2.34540200	-1.21131100
H	2.78070500	2.80007900	0.32109500
O	0.98667000	-0.85538200	2.21800800
C	1.71739200	1.17419400	1.16917700
C	0.98343800	1.95380500	1.97625500
H	0.37663000	1.50579900	2.75729300
H	0.97245000	3.03740500	1.88383500
C	-0.67976100	0.04265200	-0.98066300
C	-1.74497700	0.65538000	-0.78256000
O	3.80024200	1.01975600	-0.03559700
Si	5.34752400	1.65159300	0.15291700
C	6.49471200	0.12150000	0.13611100
C	5.46515300	2.60819200	1.78249900
H	6.48324100	2.98074800	1.95066300
H	4.79940800	3.47993100	1.77996800
H	5.18833300	1.98591600	2.64064600
C	5.73394600	2.83772200	-1.27124800
H	6.72703700	3.29043100	-1.16203300
H	5.69999100	2.33049100	-2.24215900
H	5.00522000	3.65737900	-1.30256800
C	6.24242700	-0.70367900	-1.14425000
H	6.89353400	-1.59044500	-1.16188100
H	5.20383200	-1.04739100	-1.20349500
H	6.45624900	-0.12669600	-2.05273400
C	6.20527700	-0.76238900	1.36837900
H	6.84174200	-1.65949200	1.35420800
H	6.40816000	-0.23469000	2.30834000
H	5.16187700	-1.09674200	1.39101000
C	7.97239700	0.56912900	0.17013300
H	8.20630900	1.15323900	1.06939300
H	8.63696700	-0.30702600	0.17112900
H	8.23843200	1.17724200	-0.70322900
Rh	-1.87720200	-1.56240600	0.14880600
C	0.73618400	-1.81358200	-1.14669200
O	-0.17480900	-2.54395600	-0.60567200
O	1.88642800	-2.40963500	-1.54032200
C	2.03657800	-3.81169300	-1.25401500
H	1.94706000	-3.97388100	-0.17446000
H	1.23139900	-4.37074500	-1.74256300
C	3.40063900	-4.23250100	-1.77251900
H	3.47701900	-4.06144100	-2.85132200
H	4.19809700	-3.66821400	-1.27808500
H	3.56040600	-5.29919800	-1.57899600
C	-2.75030300	1.67796700	-0.72779400
C	-3.86091600	1.67283300	-1.61716000
C	-2.62092300	2.73720400	0.17939600
C	-4.78273200	2.71710200	-1.56865800
C	-3.54788100	3.78655800	0.21970600
H	-1.77507900	2.75554600	0.85823800
C	-4.63278100	3.77186400	-0.65759600
H	-5.63164700	2.73253500	-2.24218900
H	-5.37071200	4.56592900	-0.65305000
O	-3.93772600	0.61524700	-2.47572200
O	-3.29789900	4.76371600	1.14548600

C	-5.00605600	0.58108100	-3.40591800
H	-5.98145700	0.54008600	-2.90174000
H	-4.98512600	1.45027000	-4.07723600
H	-4.86328300	-0.32967000	-3.98994300
C	-4.20545900	5.84766400	1.22673200
H	-5.21694000	5.51123500	1.49346400
H	-3.82531100	6.50084700	2.01461000
H	-4.25249700	6.40910100	0.28329900
C	-1.95936300	-3.23079600	1.52569800
C	-2.66375000	-3.55100300	0.34908000
C	-4.17072900	-3.54086600	0.18345400
C	-4.82621600	-2.29401900	0.81337300
C	-3.92908900	-1.06009000	0.72290100
C	-3.03517900	-0.63871900	1.72361000
C	-2.72696600	-1.34923700	3.02810000
C	-2.59487200	-2.87731700	2.86377700
H	-0.91913600	-3.54340100	1.56956200
H	-2.12356100	-4.12737900	-0.40031700
H	-4.61474100	-4.46313900	0.59173800
H	-4.38160400	-3.54962200	-0.89235700
H	-5.76987400	-2.08279000	0.29696100
H	-5.09451400	-2.48490100	1.85797500
H	-4.27732800	-0.30016900	0.03136800
H	-2.77959000	0.41895500	1.73281700
H	-3.48500900	-1.09916100	3.78834900
H	-1.77293100	-0.95275100	3.39206500
H	-1.96888800	-3.27330000	3.67109800
H	-3.56872600	-3.36850400	2.96460600

CP13

C	4.34542000	3.22851400	1.06148100
C	-0.14327700	1.79346400	0.18585900
C	1.35630500	1.95333400	0.30916200
C	2.09129500	1.78649000	-1.03443600
C	3.63137300	1.75769500	-0.96046400
H	3.96944000	2.38902200	1.67374900
H	1.56028400	2.94700700	0.72468500
H	1.74778700	1.21784900	1.02204200
H	1.77283300	0.84442000	-1.49897200
H	1.79287800	2.59560100	-1.71386600
H	3.99514600	1.62945600	-1.99139100
O	4.81077400	4.22248900	1.58917500
C	4.25001900	3.03814800	-0.42084000
C	4.71917100	4.00624800	-1.21920800
H	5.13531300	4.91210300	-0.78794300
H	4.69729800	3.92455900	-2.30328000
C	-0.73766100	0.51826400	0.15681500
C	-1.06387900	-0.68422400	0.19984300
O	4.04825600	0.65513100	-0.14836600
Si	4.99194700	-0.64491900	-0.65222600
C	5.04175800	-1.81012700	0.86256900
C	6.71894300	-0.04138300	-1.13716400
H	7.35536600	-0.87225700	-1.46608100
H	6.66756800	0.67630300	-1.96523500
H	7.22311800	0.45785000	-0.30214300
C	4.19248600	-1.47842300	-2.15262500
H	4.79948300	-2.31984800	-2.50914900
H	3.19255200	-1.86175600	-1.91983500
H	4.09103200	-0.77846000	-2.99147500
C	3.60668000	-2.22802800	1.25004000
H	3.62675600	-2.88810900	2.12978600
H	2.98639200	-1.35990900	1.49771000
H	3.10512600	-2.77593000	0.44306700

C	5.69385200	-1.08471500	2.05948400	C	2.16915300	1.75727400	-0.86476400
H	5.71575000	-1.74339800	2.94015100	C	3.71051200	1.71978300	-0.75903600
H	6.72909800	-0.79111900	1.84638800	H	3.76628500	4.02656600	-2.09009800
H	5.13913700	-0.18088900	2.33498000	H	1.65695100	2.85738900	0.93451800
C	5.86488500	-3.07410500	0.52890400	H	1.81073600	1.12046100	1.16639500
H	6.90190400	-2.83456400	0.26175800	H	1.85192800	0.83342900	-1.36422300
H	5.90133200	-3.74481700	1.39970100	H	1.87155700	2.58522300	-1.52285600
H	5.42759700	-3.64367800	-0.30070700	H	4.10036800	1.60822200	-1.78667400
Rh	-3.01592200	0.66835100	-0.12026400	O	4.58371300	5.32729900	-0.78328600
C	-1.04857300	2.83123500	0.08378800	C	4.28699200	3.01089800	-0.20294800
O	-2.32389300	2.64197000	-0.03747700	C	4.86592600	3.12428000	0.99932700
O	-0.59142200	4.10615300	0.11403500	H	5.25055300	4.08676100	1.32369200
C	-1.56115100	5.16441800	0.07589000	H	4.96504900	2.27151400	1.66107600
H	-2.15219200	5.08810700	-0.84362000	C	-0.68374400	0.49582400	0.23242700
H	-2.25003700	5.06116500	0.92211000	C	-1.03187700	-0.70088500	0.19597100
C	-0.79626500	6.47532500	0.13962000	O	4.11152500	0.61327500	0.03882500
H	-0.20768400	6.53791600	1.06059900	Si	4.82008900	-0.80500400	-0.52839400
H	-0.11272400	6.56900100	-0.71055300	C	4.96859400	-1.91911600	1.01824700
H	-1.49566600	7.31860300	0.11654100	C	6.50924200	-0.41230200	-1.28642000
C	-0.97416400	-2.11785900	0.24365400	H	7.01757600	-1.32282000	-1.62693000
C	-1.20801500	-2.83598100	1.44853700	H	6.40669800	0.24437400	-2.15933800
C	-0.58701800	-2.83153000	-0.89794100	H	7.16766800	0.09393000	-0.57195200
C	-1.04080200	-4.21983100	1.46711200	C	3.73543000	-1.59930900	-1.86065400
C	-0.41850600	-4.22202700	-0.87373500	H	4.20492600	-2.50619300	-2.26152600
H	-0.39594700	-2.29739100	-1.82274700	H	2.74658000	-1.87613200	-1.47793800
C	-0.64814900	-4.91522400	0.31558800	H	3.58295000	-0.91683700	-2.70623000
H	-1.20807700	-4.78200900	2.37857300	C	3.57043900	-2.16159800	1.62821800
H	-0.52773100	-5.99102300	0.37097800	H	3.65060400	-2.80425900	2.51751800
O	-1.58729600	-2.09063900	2.52721500	H	3.09601500	-1.22358300	1.93667700
O	-0.02943300	-4.79354200	-2.05504500	H	2.89371700	-2.66128700	0.92462200
C	-1.75308700	-2.74612300	3.77305600	C	5.86457500	-1.24249600	2.07815600
H	-2.56050400	-3.49044900	3.73660800	H	5.94427500	-1.87798000	2.97246200
H	-0.82553100	-3.23734900	4.09589400	H	6.88328300	-1.07143400	1.70865500
H	-2.01572400	-1.96456100	4.48793900	H	5.45447500	-0.27669500	2.39418000
C	0.16412800	-6.19638400	-2.08168600	C	5.59041100	-3.27824100	0.62647400
H	-0.76182100	-6.73850100	-1.84469300	H	6.59891200	-3.16786300	0.20822100
H	0.47100400	-6.43874200	-3.10096400	H	5.67555500	-3.92579600	1.51128600
H	0.95156900	-6.51045800	-1.38267300	H	4.97872000	-3.81447000	-0.10966800
C	-4.79305300	1.55289400	-0.98411300	Rh	-2.95332700	0.69724600	-0.08727800
C	-4.88466100	1.57333100	0.42152600	C	-0.95855400	2.81307100	0.28425600
C	-5.70649700	0.63009000	1.27733600	O	-2.23436000	2.65065100	0.13075400
C	-5.56758100	-0.84219300	0.83737700	O	-0.48399000	4.07704300	0.39403800
C	-4.17940900	-1.15131300	0.27920300	C	-1.43507300	5.15268300	0.36769100
C	-3.84006500	-1.09684900	-1.08287600	H	-1.98675300	5.13133800	-0.57900300
C	-4.75194100	-0.66423200	-2.21734400	H	-2.16175800	5.01963500	1.17721100
C	-5.56753300	0.60474000	-1.89217300	C	-0.65410700	6.44557400	0.52858500
H	-4.41994100	2.45980300	-1.45453500	H	-0.10825400	6.45469000	1.47757000
H	-4.59320400	2.49998500	0.91210600	H	0.07008900	6.56790700	-0.28328400
H	-6.76517800	0.93576800	1.28694200	H	-1.33895700	7.30091600	0.51413900
H	-5.35006200	0.73001700	2.30908900	C	-0.97031500	-2.13657600	0.18335000
H	-5.75738700	-1.49582900	1.69650100	C	-1.24070100	-2.89687300	1.35453500
H	-6.33150200	-1.09584700	0.09419100	C	-0.57933300	-2.81309900	-0.97949700
H	-3.56178400	-1.77420900	0.91747600	C	-1.10519500	-4.28390500	1.31992700
H	-3.00483500	-1.71403000	-1.40459600	C	-0.44225700	-4.20728600	-1.00843000
H	-5.41729500	-1.49300300	-2.50903200	H	-0.36231100	-2.24758600	-1.87961700
H	-4.11630100	-0.46402200	-3.08773600	C	-0.70853800	-4.94197200	0.14783000
H	-5.81604600	1.12397800	-2.82473500	H	-1.30122300	-4.87778500	2.20520400
H	-6.52539800	0.34235700	-1.43031500	H	-0.61395700	-6.02169400	0.16172700
CP14				O	-1.62116700	-2.18659900	2.45592300
C	4.20339700	4.21128900	-1.08302000	O	-0.04601500	-4.73990100	-2.20520500
C	-0.07008500	1.75720900	0.34132600	C	-1.82652700	-2.88772900	3.67047300
C	1.43084000	1.88682300	0.48080800	H	-2.65141900	-3.60903600	3.58925300
				H	-0.91774100	-3.41539700	3.98936100

H	-2.08310300	-2.12941500	4.41210900
C	0.11652500	-6.14458500	-2.28557400
H	-0.82569000	-6.67438700	-2.08810600
H	0.43752900	-6.35254400	-3.30808500
H	0.88311100	-6.50482500	-1.58562000
C	-4.69405800	1.66328500	-0.93888900
C	-4.82367000	1.59493200	0.46220500
C	-5.68273500	0.61247700	1.23284300
C	-5.54940900	-0.83155600	0.70541600
C	-4.15162000	-1.12496200	0.16266300
C	-3.77504300	-0.98888300	-1.18387200
C	-4.64747200	-0.46900700	-2.31236000
C	-5.45587000	0.78770900	-1.92691100
H	-4.29444900	2.59194400	-1.33975000
H	-4.53326600	2.48385000	1.01882900
H	-6.73728800	0.93224400	1.23024500
H	-5.35698700	0.64282000	2.27901200
H	-5.76799300	-1.53431200	1.51764300
H	-6.29788100	-1.02951500	-0.06961600
H	-3.56121000	-1.80066600	0.77233500
H	-2.94005900	-1.59818800	-1.52124400
H	-5.31451100	-1.26685700	-2.67737200
H	-3.98404300	-0.22138200	-3.14923500
H	-5.67199600	1.36994600	-2.82986300
H	-6.42953100	0.50922900	-1.50921300

TS12

C	3.44742200	0.71915600	3.75116100
C	0.17595500	-1.38000800	0.41201900
C	1.65796100	-1.15080200	0.66314100
C	2.01863400	0.32101000	0.89204200
C	3.51370100	0.56787000	1.19435500
H	2.85246700	1.63722900	3.54420900
H	1.97048100	-1.74402900	1.53254300
H	2.25084700	-1.52563800	-0.18169900
H	1.76013100	0.90931200	0.00320400
H	1.42189600	0.73098400	1.71835900
H	3.64567100	1.66282200	1.24940400
O	3.66742600	0.38577500	4.90015300
C	3.93374500	-0.00239900	2.54025800
C	4.70359300	-1.08733600	2.69642000
H	4.95176800	-1.43278800	3.69578800
H	5.09277800	-1.63339900	1.84446100
C	-0.74575400	-0.34010700	0.20167800
C	-1.41396000	0.69807200	0.02140600
O	4.30182000	0.03388100	0.14043900
Si	5.50747800	0.84588700	-0.70817100
C	6.13085200	-0.43142400	-1.98702700
C	6.87717900	1.40329400	0.47260200
H	7.66936800	1.94294500	-0.06070700
H	6.48158500	2.08238600	1.23806700
H	7.33743900	0.55796600	0.99577600
C	4.77468400	2.37840300	-1.54456700
H	5.53519700	2.92159400	-2.11911900
H	3.95989900	2.11607900	-2.22855600
H	4.36948500	3.07954100	-0.80417200
C	4.97138100	-0.85021900	-2.91731700
H	5.31771500	-1.59852200	-3.64534900
H	4.14241100	-1.29268300	-2.35372300
H	4.57421600	-0.00159900	-3.48772900
C	6.66679900	-1.68678200	-1.26516300
H	7.02163700	-2.42585000	-1.99846100
H	7.51084500	-1.45234000	-0.60479100

H	5.88781700	-2.16722600	-0.66242800
C	7.26438400	0.18727500	-2.83463600
H	8.12755500	0.47634600	-2.22221100
H	7.62324800	-0.53818700	-3.57907100
H	6.93027300	1.07627800	-3.38423900
Rh	-2.88827100	-1.16957100	-0.05573100
C	-0.38747600	-2.63881400	0.33402200
O	-1.65088500	-2.84232700	0.13584000
O	0.42093100	-3.71635600	0.47591700
C	-0.18971700	-5.01546100	0.45113500
H	-0.93883100	-5.08408200	1.24830000
H	-0.70795500	-5.15936700	-0.50351700
C	0.91935500	-6.03598300	0.64108200
H	1.66143500	-5.95692300	-0.16013200
H	1.42959400	-5.88230500	1.59752000
H	0.50262000	-7.04939100	0.62902600
C	-1.74253000	2.08886200	-0.13978200
C	-1.84271600	2.68141000	-1.42933600
C	-1.91452600	2.90379400	0.98619900
C	-2.09847800	4.04728100	-1.53980100
C	-2.16976600	4.27658300	0.87001900
H	-1.83230600	2.46984100	1.97720200
C	-2.26190100	4.84662700	-0.40012800
H	-2.17111000	4.51658600	-2.51417400
H	-2.45799700	5.90497100	-0.52852500
O	-1.67422800	1.84098900	-2.49193800
O	-2.30786500	4.95658400	2.04956100
C	-1.71404600	2.39166800	-3.79685100
H	-2.69275400	2.83875500	-4.01945700
H	-0.93252400	3.15038500	-3.93856500
H	-1.53555400	1.55770900	-4.47778900
C	-2.55833700	6.34912800	1.98777000
H	-3.50180000	6.56919600	1.46920100
H	-2.63006600	6.68843300	3.02290700
H	-1.74100500	6.88658100	1.48723800
C	-4.47671900	-2.56922300	0.39763700
C	-4.21727400	-2.57340400	-0.98724400
C	-5.05028400	-1.89166700	-2.05428700
C	-5.46883100	-0.46176800	-1.65392400
C	-4.41166200	0.23130700	-0.79570800
C	-4.40509100	0.23835100	0.60880600
C	-5.38648700	-0.48311900	1.51491300
C	-5.69093200	-1.92413600	1.05502800
H	-3.97435200	-3.33602100	0.98280800
H	-3.55665600	-3.35652400	-1.35408100
H	-5.93354700	-2.50007100	-2.30764700
H	-4.44072700	-1.84385800	-2.96412500
H	-5.63514700	0.13299900	-2.55953700
H	-6.42789100	-0.47401000	-1.12460700
H	-3.87825100	1.03354700	-1.29420200
H	-3.89261700	1.06724800	1.09106900
H	-6.31555400	0.10176200	1.61272700
H	-4.94173600	-0.51654900	2.51625700
H	-5.99121000	-2.52447000	1.92135000
H	-6.54383300	-1.94038600	0.36820900

CP15

C	-2.48133100	3.66482300	1.53064800
C	-0.43573100	-0.61667300	-0.29258100
C	-1.67752900	0.24267900	-0.40275900
C	-2.33583500	0.52012600	0.96189200
C	-3.57941400	1.43630000	0.90975900
H	-2.29083300	3.14430400	2.49624600

H	-1.41908800	1.19196100	-0.88673300
H	-2.40802700	-0.25201300	-1.05113900
H	-2.63726800	-0.43449200	1.40944000
H	-1.59521000	0.96483800	1.64082000
H	-3.99287100	1.47431500	1.93353600
O	-2.09871700	4.80910000	1.37418600
C	-3.23085500	2.86398500	0.52139000
C	-3.56764800	3.43393200	-0.64286800
H	-3.27772900	4.46084200	-0.84508800
H	-4.13316500	2.89218700	-1.39217400
C	0.84673200	-0.04364000	-0.20892100
C	1.87856800	0.65199900	-0.13559300
O	-4.54295700	0.89985500	0.01274800
Si	-6.01281900	0.20480900	0.44803700
C	-6.81200400	-0.31126300	-1.21025400
C	-7.07286300	1.47085400	1.37393400
H	-8.02386900	1.03149400	1.69904900
H	-6.56132400	1.83423600	2.27390400
H	-7.30007600	2.34336500	0.75127700
C	-5.71722700	-1.28532900	1.57737700
H	-6.65790700	-1.78982700	1.83116600
H	-5.05565300	-2.02011800	1.10491600
H	-5.24950100	-0.97986900	2.52167100
C	-5.93272400	-1.36801300	-1.91401900
H	-6.37113500	-1.64375700	-2.88445700
H	-4.92025100	-0.99268200	-2.09987000
H	-5.84508600	-2.28794400	-1.32302100
C	-6.95149700	0.91667000	-2.13577600
H	-7.42125100	0.62560900	-3.08692900
H	-7.57700500	1.70016600	-1.69031800
H	-5.97602900	1.35730300	-2.36962600
C	-8.21335000	-0.90858000	-0.95250800
H	-8.89080400	-0.18408500	-0.48351800
H	-8.67536900	-1.21781500	-1.90132100
H	-8.17269200	-1.79574500	-0.30801000
Rh	2.47144800	-1.66478800	-0.03570700
C	-0.43463000	-1.99377400	-0.19736200
O	0.64905200	-2.69360400	-0.08542500
O	-1.62135100	-2.65175400	-0.22350900
C	-1.58444200	-4.08676200	-0.20586200
H	-1.00893000	-4.44987000	-1.06509700
H	-1.07622800	-4.43103700	0.70166600
C	-3.02239800	-4.57427700	-0.25610000
H	-3.58588400	-4.21380400	0.61121800
H	-3.52224800	-4.21822400	-1.16289300
H	-3.04827200	-5.66979000	-0.25290100
C	2.75794900	1.78905600	-0.14927500
C	3.20823100	2.38856000	1.05873700
C	3.13905100	2.36573300	-1.36739400
C	4.00396500	3.53179400	1.00283900
C	3.93957200	3.51395200	-1.41839100
H	2.79186600	1.92852900	-2.29762200
C	4.37155900	4.09603600	-0.22586500
H	4.34782100	4.00814100	1.91358100
H	4.98903000	4.98681800	-0.22678700
O	2.81146600	1.78117500	2.21567900
O	4.23303200	3.97774100	-2.67190900
C	3.17301100	2.38254300	3.44718900
H	4.26338700	2.41473800	3.57884000
H	2.77010700	3.40055100	3.53198200
H	2.73534600	1.75452000	4.22512800
C	5.01238400	5.15554000	-2.77892000
H	6.01100200	5.02332900	-2.33962900

H	5.11429300	5.35288600	-3.84781000
H	4.52024200	6.01219200	-2.29833600
C	3.33390100	-3.60293200	-0.47492800
C	3.17366100	-3.45398400	0.91677400
C	4.26779100	-3.13130600	1.91491000
C	5.20073400	-2.00293400	1.42923200
C	4.46593400	-0.97236300	0.57441800
C	4.38676500	-1.01326600	-0.82740700
C	4.94908200	-2.09936900	-1.72735600
C	4.66746700	-3.52545800	-1.20916700
H	2.53471800	-4.12333700	-0.99772100
H	2.27520800	-3.88938000	1.34993600
H	4.84650000	-4.03536000	2.16445300
H	3.77922900	-2.81503500	2.84379600
H	5.63734600	-1.49652600	2.29773300
H	6.04610200	-2.41578200	0.86797900
H	4.32457000	-0.00638000	1.04758900
H	4.22595500	-0.06537300	-1.33519800
H	6.02939700	-1.94481300	-1.88149700
H	4.48159300	-1.98054700	-2.71180600
H	4.65178400	-4.22128500	-2.05574100
H	5.47703900	-3.86734900	-0.55533300

CP16

C	0.93817500	2.56528000	1.64854500
C	0.08169200	1.43225500	-1.29671400
C	1.49904400	1.42376100	-1.84069700
C	2.49481300	2.31509200	-1.07092900
C	2.97310700	1.77108900	0.29171500
H	1.17214400	3.55146700	1.19108000
H	1.87421600	0.39493100	-1.85138000
H	1.49421800	1.76256900	-2.88629700
H	3.39652900	2.46009200	-1.68049400
H	2.05217000	3.30743200	-0.93236400
H	3.58557900	2.57242000	0.74366800
O	-0.00434200	2.46852800	2.41696500
C	1.85456200	1.45539200	1.27416700
C	1.67553400	0.25308800	1.83805300
H	0.85884800	0.10250300	2.53442800
H	2.31385300	-0.58741700	1.59535900
C	-0.53450900	0.26476000	-0.81333000
C	-0.86638900	-0.85802100	-0.37944800
O	3.77933800	0.61492500	0.07829400
Si	5.42453600	0.49617000	0.40123400
C	5.90250800	-1.26888200	-0.16186800
C	5.74167000	0.76076600	2.24917400
H	6.81464200	0.74907500	2.47620200
H	5.35134400	1.73220900	2.57735200
H	5.25841500	-0.00797400	2.86251700
C	6.37950100	1.81688700	-0.56413200
H	7.45743200	1.74928000	-0.37112800
H	6.22640500	1.72233700	-1.64515000
H	6.06219500	2.82607300	-0.27345200
C	5.66886100	-1.41700800	-1.68088000
H	5.91543900	-2.43793500	-2.00794800
H	4.62391900	-1.22495400	-1.94872900
H	6.29640600	-0.72949100	-2.26113200
C	5.03755300	-2.31122700	0.57912100
H	5.30897800	-3.32876100	0.26093100
H	5.17735300	-2.26238300	1.66643800
H	3.97167800	-2.17035600	0.36852100
C	7.39152200	-1.53247400	0.15100400
H	7.60324900	-1.46920900	1.22564500

H	7.67852300	-2.54179100	-0.17810700
H	8.05304700	-0.82422200	-0.36365400
Rh	-2.65202700	0.71295900	-0.01724700
C	-0.74636900	2.54502500	-1.27729300
O	-1.93754400	2.52948100	-0.78646200
O	-0.28143700	3.70945100	-1.79545000
C	-1.15417700	4.85132300	-1.74569400
H	-2.08206800	4.62357900	-2.28139300
H	-1.41667500	5.06575200	-0.70393400
C	-0.41270800	6.01197100	-2.38602300
H	0.51117200	6.23393100	-1.84158600
H	-0.15239300	5.78232800	-3.42444500
H	-1.04247200	6.90860200	-2.37683500
C	-0.93737000	-2.29603200	-0.32847800
C	-0.72361400	-3.02397200	0.87320100
C	-1.17310600	-3.01380400	-1.50926900
C	-0.74750000	-4.41779100	0.84765100
C	-1.19514900	-4.41365900	-1.53066700
H	-1.33390600	-2.47464600	-2.43669700
C	-0.98081400	-5.11608800	-0.34385900
H	-0.58201900	-4.98646200	1.75516500
H	-0.99056100	-6.19974800	-0.32129600
O	-0.50125900	-2.28429000	2.00147600
O	-1.43115300	-4.98578400	-2.75129100
C	-0.24427500	-2.96907500	3.21610700
H	-1.09665200	-3.59264900	3.51831500
H	0.65304500	-3.59770700	3.14169500
H	-0.08122700	-2.19341300	3.96623100
C	-1.44895900	-6.39965700	-2.82920000
H	-2.24400100	-6.83102500	-2.20515600
H	-1.64373800	-6.64125700	-3.87588100
H	-0.48477100	-6.83429200	-2.53132700
C	-4.56492500	1.73437300	-0.01418300
C	-3.88336100	1.97878900	1.19451100
C	-4.15628000	1.32181200	2.53212800
C	-4.37389500	-0.20054800	2.41105600
C	-3.52371700	-0.81514000	1.30149600
C	-3.95912100	-1.01764400	-0.01894700
C	-5.31090500	-0.62077800	-0.58721700
C	-5.75591200	0.79483400	-0.16464900
H	-4.45476800	2.48775500	-0.79076000
H	-3.31146200	2.90278700	1.25353200
H	-5.01399600	1.80022300	3.03209500
H	-3.28325100	1.50979800	3.16653300
H	-4.11290900	-0.67826300	3.36250100
H	-5.43142200	-0.42929000	2.24054100
H	-2.69089300	-1.41576400	1.64972000
H	-3.45878400	-1.79756800	-0.58850500
H	-6.07364100	-1.36891900	-0.31625800
H	-5.22631100	-0.65435000	-1.67978800
H	-6.43948200	1.19936200	-0.91996500
H	-6.32745400	0.75913100	0.76904800

1'

C	1.47628600	-0.74619000	0.82461600
C	2.35218800	-0.48567800	-0.46130000
C	1.42331100	-0.25303600	-1.69207800
C	0.44624100	-1.41513500	-1.89775800
C	-0.41415700	-1.65118200	-0.64854100
H	0.93692000	0.18334000	1.02612800
H	0.86440300	0.67104000	-1.52303600
H	2.04302700	-0.11072100	-2.58438400
H	-0.21296100	-1.19967400	-2.74638400

H	0.99737000	-2.33514300	-2.12645800
H	-1.03215700	-2.54703200	-0.79618600
O	2.30191800	-0.96175900	1.95054000
H	2.92074100	-1.67715300	1.71690000
C	0.46995600	-1.85396300	0.56970200
C	0.37680700	-2.93296600	1.34977600
H	1.01047200	-3.05671000	2.22228200
H	-0.34437400	-3.72054600	1.14434800
C	3.22723500	-1.64567100	-0.67420700
C	3.89919300	-2.64079500	-0.80576000
O	-1.25558700	-0.50401300	-0.48508800
Si	-2.68716700	-0.38786700	0.39923300
C	-3.62572300	1.06486200	-0.42162300
C	-2.32011300	-0.02807100	2.21793000
H	-3.24322300	0.02820300	2.80806900
H	-1.69658000	-0.81959400	2.64855600
H	-1.78469200	0.91979900	2.34601500
C	-3.65769000	-2.00891000	0.27292500
H	-4.64126700	-1.90671600	0.74763700
H	-3.82314200	-2.31328700	-0.76705500
H	-3.13849200	-2.82903200	0.78309600
C	-3.95082300	0.71785200	-1.89022300
H	-4.47011200	1.55667700	-2.37661100
H	-3.04109300	0.51152600	-2.46548000
H	-4.60535500	-0.15914700	-1.96933700
C	-2.75046400	2.33681500	-0.39166400
H	-3.27897400	3.17523400	-0.86888800
H	-2.50979500	2.64537100	0.63319600
H	-1.80643600	2.18852800	-0.92765600
C	-4.94292100	1.34203100	0.33606900
H	-4.76610600	1.62289200	1.38162400
H	-5.48641400	2.17332700	-0.13605100
H	-5.61367800	0.47348700	0.33108000
C	3.22655400	0.76260200	-0.21706100
O	2.45558400	1.83688000	0.04791600
C	3.16270100	3.07059500	0.31777900
H	3.82674200	2.91050700	1.17278000
H	3.78720600	3.31267100	-0.54795400
C	2.12315700	4.14092600	0.59206100
H	1.46485800	4.27923100	-0.27175100
H	1.50692200	3.87527000	1.45696400
H	2.62026300	5.09420200	0.80267700
O	4.43403700	0.79593400	-0.26815400
H	4.51824100	-3.49727000	-0.94895100

Rh(I)(cod)OH

Rh	-0.86685300	-0.15313000	-0.33169600
C	1.00509500	0.14809700	-1.41756400
C	0.91759500	-1.18061600	-0.96474300
C	1.62234100	-1.74589300	0.26081800
C	1.44972700	-0.86093900	1.51896300
C	0.13190700	-0.08412600	1.50510300
C	-0.01254000	1.23497800	0.96516900
C	1.08355100	2.03992800	0.28995900
C	1.87256000	1.21777100	-0.75668700
H	0.74071800	0.33370900	-2.45960700
H	0.61366200	-1.93281800	-1.69695700
H	2.69128600	-1.91762100	0.05824400
H	1.18787000	-2.73204800	0.46136900
H	1.48437900	-1.49311700	2.41306400
H	2.28561200	-0.15820800	1.61459100
H	-0.57436000	-0.36383000	2.28776000
H	-0.81291400	1.84506300	1.38733600

H	1.76450400	2.47109000	1.04173300
H	0.60179800	2.88960500	-0.20760300
H	2.26543000	1.89350400	-1.52480300
H	2.74953800	0.75076300	-0.29429600
O	-2.69527400	0.04660400	0.27996000
H	-2.84838100	0.31671400	1.19971300

CP1'

C	0.26700000	0.08370200	-0.10692900
C	0.00498400	1.02980400	1.12794400
C	1.20147400	1.07475100	2.12439000
C	1.67181700	-0.32354900	2.53493000
C	2.03020400	-1.17396600	1.30855400
H	1.04557000	0.57586400	-0.71063100
H	2.02159400	1.59821800	1.62626600
H	0.92064900	1.66239000	3.00659200
H	2.55263500	-0.24018800	3.18231600
H	0.88872800	-0.84053900	3.10333100
H	2.29306600	-2.18911900	1.63748800
O	-0.89954300	-0.00708500	-0.84881800
C	0.84209800	-1.25026600	0.36626400
C	0.32496100	-2.42055800	-0.01778400
H	-0.53667300	-2.45704300	-0.67533500
H	0.74629200	-3.36591600	0.31827100
C	-1.21687600	0.49969400	1.75669100
C	-2.16461300	0.00424600	2.35935500
O	3.17211500	-0.56639400	0.69036000
Si	4.15043600	-1.21563800	-0.51797100
C	5.83490300	-0.33258200	-0.28381400
C	3.42125700	-0.85883000	-2.22472500
H	4.05331600	-1.26264200	-3.02543300
H	2.43047200	-1.31764900	-2.31778600
H	3.30559600	0.21697000	-2.39995500
C	4.31068800	-3.08917200	-0.29467300
H	5.02624400	-3.50680100	-1.01362700
H	4.65352300	-3.36175000	0.71021900
H	3.34964000	-3.58735300	-0.46774100
C	6.41368100	-0.67173400	1.10611500
H	7.36830200	-0.14827700	1.26443100
H	5.73125400	-0.37059700	1.90894700
H	6.61005500	-1.74546200	1.21667000
C	5.64295400	1.19606900	-0.38599500
H	6.60372900	1.71347900	-0.24581900
H	5.25283600	1.49395800	-1.36696100
H	4.94931600	1.56650600	0.37706300
C	6.83004200	-0.78959000	-1.37253100
H	6.47537200	-0.54884000	-2.38234200
H	7.79920700	-0.28677600	-1.23996400
H	7.01846500	-1.86996100	-1.33244900
Rh	-2.67999500	-0.29338800	0.13629600
C	-0.29429000	2.45156500	0.61652600
O	-1.30428400	3.08370800	0.83533400
O	0.74717400	2.93010800	-0.09118100
C	0.58896200	4.26332000	-0.62880700
H	-0.30911700	4.28330600	-1.25376200
H	0.43232900	4.95990200	0.20127700
C	1.84347800	4.58648200	-1.41852200
H	2.73095200	4.54658400	-0.77865000
H	1.97930000	3.87753200	-2.24148900
H	1.76688300	5.59478200	-1.84020700
C	-3.36166400	-1.17093700	-1.73206100
C	-3.54128000	0.22323500	-1.75844900
C	-4.84562400	0.97009300	-1.56578000

C	-5.66976700	0.44637000	-0.36850000
C	-4.78585700	-0.07268800	0.76311900
C	-4.38057300	-1.41170000	0.89931300
C	-4.69328600	-2.54957200	-0.05816100
C	-4.49319000	-2.17474600	-1.54310700
H	-2.45008900	-1.54763700	-2.18906700
H	-2.74478100	0.80132100	-2.22223600
H	-5.44625400	0.94372400	-2.48921200
H	-4.59528500	2.02257400	-1.39220200
H	-6.30122100	1.25608600	0.01427700
H	-6.35772500	-0.34362400	-0.69061700
H	-4.78593600	0.54104400	1.66163300
H	-4.13345000	-1.75710100	1.90254100
H	-5.71419500	-2.92815900	0.11323800
H	-4.01698600	-3.37583500	0.19082000
H	-4.26926600	-3.08209300	-2.11557300
H	-5.42105800	-1.77458900	-1.96655300
H	-2.84219000	-0.28422900	3.13477700

H2O

O	0.00000000	0.00000000	0.11942600
H	0.00000000	0.76261700	-0.47770500
H	0.00000000	-0.76261700	-0.47770500

CP17

C	-1.05748200	0.32457100	-2.12405100
C	0.13705600	2.48955900	-0.16289200
C	-1.33084900	2.80628400	0.12060400
C	-2.21183800	1.67979900	0.68820500
C	-2.84094900	0.71464800	-0.34451800
H	-1.58613900	1.04855100	-2.76733900
H	-3.29526800	1.32655300	-1.14296100
O	0.08852000	0.00656700	-2.45893600
C	-1.80295500	-0.19732300	-0.97585000
C	-1.56081500	-1.44272500	-0.53486400
H	-0.79465200	-2.06519000	-0.98716400
H	-2.13392100	-1.85623700	0.28714700
C	0.75330200	1.34218600	0.12227800
C	1.39607500	0.23670300	0.33296500
O	-3.83356700	-0.06309200	0.31407800
Si	-5.48684100	-0.02994300	-0.01039900
C	-6.23171100	-1.32136100	1.18620100
C	-5.79203800	-0.48040600	-1.82319300
H	-6.86421100	-0.50715800	-2.05328300
H	-5.33799800	0.25554100	-2.49846300
H	-5.37084300	-1.46076000	-2.07247300
C	-6.17218500	1.70435700	0.31181000
H	-7.24145500	1.76094400	0.07419500
H	-6.04571500	2.00365100	1.35843200
H	-5.66427400	2.45382000	-0.30799900
C	-5.84637000	-0.96978200	2.63970900
H	-6.25688400	-1.71703700	3.33454200
H	-4.75949100	-0.94698900	2.77407700
H	-6.24172700	0.00741700	2.94306600
C	-5.69151800	-2.72847300	0.85147400
H	-6.10450300	-3.47147100	1.54932600
H	-5.96784700	-3.04514700	-0.16178800
H	-4.59921300	-2.77194200	0.93029100
C	-7.77101800	-1.32922000	1.05765000
H	-8.10025400	-1.58967500	0.04379700
H	-8.20633900	-2.07269200	1.74078400
H	-8.21008600	-0.35729100	1.31419100
Rh	1.68091000	-1.01173700	-1.38706700

C	0.99640900	3.57586300	-0.69951900
O	2.19326900	3.51545500	-0.91905500
O	0.27273400	4.70990800	-0.93939800
C	1.02155000	5.82591300	-1.45350600
H	1.83212200	6.06490400	-0.75691500
H	1.48472300	5.53976600	-2.40414200
C	0.05633900	6.98653000	-1.62020900
H	-0.74736500	6.73052600	-2.31882400
H	-0.39690400	7.25878200	-0.66118700
H	0.58680700	7.86191900	-2.01152700
C	2.03446800	0.01023300	1.65960800
C	1.59770200	-1.02080600	2.52868400
C	3.09224700	0.82147100	2.07319400
C	2.23256000	-1.21313400	3.75390600
C	3.73404000	0.62615600	3.30611300
H	3.42319100	1.63121900	1.43013500
C	3.30316400	-0.39685200	4.14859000
H	1.90488700	-1.99496300	4.42980900
H	3.77342700	-0.57724900	5.10839600
O	0.53482900	-1.77545600	2.08878800
O	4.76061500	1.49097100	3.58395500
C	0.07548800	-2.81947500	2.92394000
H	0.85743300	-3.56969600	3.10911800
H	-0.28712900	-2.43968400	3.88948000
H	-0.75328300	-3.29162700	2.39167300
C	5.42776800	1.34746900	4.82252900
H	5.91057900	0.36409900	4.91387300
H	6.19338000	2.12589600	4.84604400
H	4.74426700	1.48766900	5.67192500
C	2.41180400	-1.74521000	-3.36310300
C	1.57171500	-2.70481300	-2.79593900
C	2.01647700	-3.95922500	-2.06591700
C	3.15340600	-3.70272700	-1.04931900
C	3.08707600	-2.31104500	-0.41654900
C	3.75412200	-1.17353800	-0.92068100
C	4.57664800	-1.09707800	-2.19337300
C	3.93134200	-1.83450800	-3.38849100
H	1.96422800	-1.04980800	-4.07112600
H	0.53783400	-2.72247700	-3.14407200
H	2.31290100	-4.74385900	-2.78075500
H	1.14461600	-4.35368400	-1.52996900
H	3.09554200	-4.45652900	-0.25546600
H	4.13006900	-3.84802200	-1.52472100
H	2.85986600	-2.30404300	0.64572200
H	3.99132400	-0.39117700	-0.20238700
H	5.59658300	-1.47496800	-2.01379300
H	4.68433900	-0.03565000	-2.44546300
H	4.30075600	-1.39594500	-4.32275500
H	4.24262500	-2.88458500	-3.40497600
H	-1.35439400	3.63933900	0.83553900
H	-1.79814400	3.21837000	-0.78565400
H	-1.65983100	1.08462000	1.42465200
H	-3.05616300	2.14026900	1.21422400

TS13

C	1.04364300	-1.88421700	-1.00231300
C	-0.26721700	-1.52131900	1.82835700
C	1.09589200	-1.53087000	2.52578200
C	2.13951500	-0.53007000	2.01042800
C	2.68585500	-0.83379000	0.59908300
H	1.61535300	-2.82378000	-0.93331900
H	3.05794000	-1.87128500	0.59917600
O	-0.09823500	-1.97156100	-1.54422900

C	1.62436300	-0.71095000	-0.47435300
C	1.04246000	0.51161000	-0.77837000
H	0.48755000	0.64506600	-1.69844200
H	1.44191800	1.42473500	-0.35059000
C	-0.74660800	-0.42839400	1.21894100
C	-0.89037100	0.62096600	0.47284500
O	3.78458100	0.06194100	0.39317000
Si	5.01837500	-0.08037500	-0.73854400
C	6.42784200	1.01033100	-0.03723300
C	4.46555200	0.54093800	-2.43838200
H	5.27054600	0.45599200	-3.17900200
H	3.61254800	-0.04277100	-2.80199200
H	4.15280900	1.59090800	-2.40187700
C	5.55398000	-1.89046000	-0.90040400
H	6.42799000	-1.97841200	-1.55740100
H	5.82109000	-2.33042500	0.06744800
H	4.75974500	-2.50694900	-1.33870200
C	6.88167800	0.46529100	1.33401700
H	7.67237700	1.10208100	1.75761600
H	6.05260600	0.44199300	2.05000400
H	7.28903300	-0.55062800	1.25739900
C	5.92101500	2.45752700	0.14678300
H	6.71573300	3.09084500	0.56837900
H	5.61665800	2.90940500	-0.80564300
H	5.06387200	2.49932900	0.82790500
C	7.63237300	1.01497000	-1.00348300
H	7.36894000	1.41492400	-1.99046400
H	8.44112800	1.64401600	-0.60360400
H	8.04782500	0.00975600	-1.14977800
Rh	-1.74963700	-0.59996300	-1.31342100
C	-1.16285600	-2.69135500	1.93709400
O	-2.29449500	-2.77492400	1.48472800
O	-0.57969800	-3.71658200	2.61785800
C	-1.38269800	-4.90209500	2.76982600
H	-2.31924700	-4.63699700	3.27173200
H	-1.64147100	-5.28805800	1.77794300
C	-0.57162700	-5.90304300	3.57352800
H	0.36058500	-6.15596700	3.05761500
H	-0.31978300	-5.49997600	4.55997800
H	-1.14824800	-6.82414200	3.71413700
C	-1.36361200	1.95850500	0.88538700
C	-1.20905700	3.11028700	0.06833200
C	-1.96927300	2.12613400	2.13734100
C	-1.64543100	4.35331400	0.52750800
C	-2.41011400	3.37252900	2.59660500
H	-2.10384300	1.26399000	2.78241600
C	-2.24534100	4.49472300	1.78448700
H	-1.52615100	5.23727400	-0.08782800
H	-2.57292000	5.47777100	2.10238300
O	-0.62348700	2.92672500	-1.15916100
O	-2.98056300	3.38002500	3.84126600
C	-0.42983700	4.05799100	-1.98909900
H	-1.38301400	4.53509100	-2.25490800
H	0.22285400	4.80278600	-1.51372000
H	0.05044400	3.68568300	-2.89611400
C	-3.43891000	4.61804500	4.35254300
H	-4.22770200	5.05104900	3.72167700
H	-3.84845400	4.40303200	5.34154400
H	-2.62071300	5.34506900	4.45080700
C	-2.84157200	-2.06311700	-2.48233200
C	-2.25917200	-1.10117600	-3.33128000
C	-2.99167100	0.05347700	-3.99095000
C	-3.92455500	0.80004100	-3.01119100

C	-3.38707800	0.79391200	-1.58000600
C	-3.72451000	-0.16211100	-0.60410700
C	-4.60246900	-1.38496700	-0.79458400
C	-4.31844600	-2.12940900	-2.11801600
H	-2.27267700	-2.97627700	-2.31974700
H	-1.31706800	-1.37786100	-3.80563300
H	-3.55246400	-0.29100200	-4.87465800
H	-2.23428500	0.75280600	-4.36471800
H	-4.04092300	1.83814300	-3.34372200
H	-4.92962100	0.36535800	-3.03119000
H	-3.04192200	1.75738900	-1.21653100
H	-3.61320200	0.13932600	0.43603600
H	-5.66699200	-1.10777100	-0.72434400
H	-4.39189000	-2.05667900	0.04307500
H	-4.61351400	-3.17922500	-2.00969600
H	-4.92790600	-1.72515900	-2.93358800
H	0.94892700	-1.35015200	3.60066100
H	1.50119400	-2.54634900	2.45944300
H	2.99487500	-0.53625400	2.69681200
H	1.74057000	0.49139400	2.02086700

TS14

C	0.72106300	-1.60650400	-0.42508900
C	0.14035200	-1.09127600	1.75106500
C	1.46255400	-1.14260800	2.51544200
C	2.57852300	-0.29700900	1.88947400
C	2.96207200	-0.75682400	0.47065800
H	1.02216800	-2.60621300	-0.07346500
H	3.22681200	-1.82705800	0.52096400
O	-0.31446800	-1.50052300	-1.15927800
C	1.79088500	-0.58928300	-0.48393600
C	1.66549500	0.47121100	-1.29638000
H	0.79421700	0.57210200	-1.93302800
H	2.43076800	1.23731400	-1.33852400
C	-0.43346100	0.18024900	1.52400000
C	-0.81955100	1.31664800	1.30310500
O	4.09123800	0.00597600	0.05838800
Si	5.42653300	-0.54884500	-0.79783100
C	6.60826100	0.95672300	-0.82359400
C	4.94156400	-1.09117100	-2.54406700
H	5.80403500	-1.48934300	-3.09315400
H	4.18014000	-1.87962200	-2.50960200
H	4.52248200	-0.26287500	-3.12595100
C	6.19909600	-2.02688700	0.10102500
H	7.11720800	-2.35761200	-0.40022900
H	6.45368700	-1.78341500	1.13873800
H	5.51758600	-2.88630600	0.12029500
C	7.00590600	1.33058300	0.62059100
H	7.65819600	2.21638600	0.62209500
H	6.12646500	1.56062300	1.23235600
H	7.55618400	0.52051700	1.11483700
C	5.90020700	2.16447700	-1.47474900
H	6.56836100	3.03839800	-1.48916200
H	5.61006700	1.95944500	-2.51276600
H	4.99592700	2.44400000	-0.92247500
C	7.88184300	0.62312800	-1.63077300
H	7.65537100	0.37525700	-2.67521700
H	8.56372900	1.48597500	-1.64203600
H	8.43507400	-0.22026200	-1.19869000
Rh	-2.38269800	-1.49814900	-0.66443300
C	-0.75290400	-2.21057000	1.82172200
O	-1.87676400	-2.31142000	1.25943600
O	-0.28852000	-3.27038400	2.51835800

C	-1.07753400	-4.47853700	2.49729500
H	-2.06120300	-4.26873600	2.92907300
H	-1.22888800	-4.79133300	1.45900100
C	-0.32093100	-5.52188700	3.29988200
H	0.65974800	-5.72243700	2.85616600
H	-0.17044000	-5.18711600	4.33125200
H	-0.88863000	-6.45870700	3.32004300
C	-1.28516100	2.63936400	1.08114400
C	-0.36177000	3.70752200	0.89985500
C	-2.65646900	2.92228700	1.02713600
C	-0.83736200	4.99602700	0.67340800
C	-3.12704700	4.21884400	0.78999300
H	-3.37405200	2.12325300	1.17696300
C	-2.21450900	5.25986900	0.61515600
H	-0.14650700	5.81978600	0.53448300
H	-2.54560200	6.27593700	0.43454000
O	0.95956300	3.36570600	0.96325900
O	-4.49189900	4.35392900	0.75088500
C	1.92431700	4.38398400	0.77271700
H	1.82886000	4.85273500	-0.21650200
H	1.85089300	5.16191100	1.54542400
H	2.89620400	3.89233200	0.84632500
C	-5.02151400	5.64640200	0.52346600
H	-4.70713400	6.04937100	-0.44953400
H	-6.10770700	5.53397000	0.53106500
H	-4.72628400	6.35140900	1.31308400
C	-2.96544100	-1.59774500	-2.71838100
C	-2.75020200	-0.25433200	-2.34518500
C	-3.82635200	0.76757400	-2.02023300
C	-4.90363500	0.21712400	-1.05782800
C	-4.32990300	-0.83274500	-0.10681600
C	-4.34477100	-2.22368500	-0.35941400
C	-4.86457100	-2.89389400	-1.62066700
C	-4.34958200	-2.21658000	-2.91154800
H	-2.14516300	-2.10170500	-3.22851300
H	-1.78006400	0.17166700	-2.59844000
H	-4.28856200	1.15424700	-2.94265400
H	-3.33061100	1.61973000	-1.54314800
H	-5.32025700	1.04601700	-0.47468300
H	-5.74329100	-0.21047400	-1.61798600
H	-4.25372500	-0.52979800	0.93731600
H	-4.28950800	-2.87836300	0.51038200
H	-5.96553200	-2.93664100	-1.61691400
H	-4.51834200	-3.93405800	-1.60232600
H	-4.30418300	-2.95806700	-3.71734000
H	-5.05313200	-1.44752300	-3.24995800
H	1.30934200	-0.80635000	3.55134600
H	1.78909700	-2.18573100	2.58172800
H	2.28179200	0.75699300	1.83511400
H	3.47433000	-0.35827800	2.51957300

CP18

C	0.22520900	-1.29442600	0.24288400
C	-0.07525100	-0.25644100	1.42079200
C	1.11932300	-0.24597100	2.42991300
C	2.45771500	0.04710500	1.75030200
C	2.74557300	-0.97342100	0.64115100
H	0.32445500	-2.26700900	0.77640000
H	2.78517000	-1.97191800	1.11365100
O	-0.73339200	-1.33297000	-0.73726300
C	1.59919700	-0.96597400	-0.35129100
C	1.74599200	-0.67136500	-1.64218200
H	0.88235700	-0.66633100	-2.29619200

H	2.71893600	-0.42795900	-2.05441200
C	-0.30902200	1.09184200	0.89878300
C	-0.44917900	2.22797700	0.49890900
O	4.00056100	-0.67115500	0.04643900
Si	5.24969700	-1.75860900	-0.23240300
C	6.67780900	-0.66662300	-0.88964700
C	4.73206800	-3.08010500	-1.48299500
H	5.52065100	-3.83037800	-1.62044000
H	3.83226900	-3.60592100	-1.14122700
H	4.49976600	-2.64833300	-2.46251900
C	5.72730000	-2.62463600	1.38493500
H	6.55598000	-3.32600900	1.22727000
H	6.03571300	-1.91046200	2.15699800
H	4.88841500	-3.20545900	1.78809000
C	7.05934200	0.38466100	0.17444400
H	7.86313200	1.03599000	-0.20018100
H	6.20536500	1.02079100	0.43251100
H	7.42264700	-0.08136300	1.09886900
C	6.22891600	0.06383500	-2.17380600
H	7.03731700	0.70853000	-2.54989000
H	5.97427700	-0.63915000	-2.97659300
H	5.35329000	0.69650900	-1.99109000
C	7.91094300	-1.53931000	-1.20862100
H	7.69415500	-2.29117100	-1.97762100
H	8.73380500	-0.91550100	-1.58750100
H	8.28524500	-2.06536400	-0.32131400
Rh	-2.60863300	-1.93420200	-0.30494000
C	-1.34457400	-0.67628900	2.18055900
O	-2.21977500	-1.45081500	1.78541900
O	-1.44031800	-0.11681900	3.38158100
C	-2.63092700	-0.40010100	4.16555300
H	-3.50760900	-0.13363500	3.56833000
H	-2.66782400	-1.47598600	4.36118200
C	-2.53235400	0.41433400	5.44072200
H	-1.64144100	0.13982000	6.01431800
H	-2.48570800	1.48469100	5.21777600
H	-3.41425000	0.22839600	6.06315400
C	-0.59039400	3.56417000	0.02308700
C	0.52617700	4.44351500	0.02540500
C	-1.82131700	4.02890500	-0.45097600
C	0.37054700	5.74494000	-0.44564600
C	-1.97088800	5.33925700	-0.92064000
H	-2.67962200	3.36589000	-0.46194200
C	-0.87007200	6.19702000	-0.91717500
H	1.20934300	6.43139200	-0.45431900
H	-0.95139200	7.21670900	-1.27570500
O	1.69408300	3.92423600	0.50366800
O	-3.22584200	5.67389900	-1.35654000
C	2.85192800	4.73954300	0.47010100
H	3.09646500	5.05046000	-0.55454400
H	2.73691700	5.63296700	1.09935100
H	3.66292600	4.12374700	0.86278200
C	-3.42691700	6.98487800	-1.85100500
H	-2.79579000	7.19006200	-2.72688000
H	-4.47709100	7.03885400	-2.14493000
H	-3.22778800	7.74434700	-1.08196300
C	-2.79287300	-2.92549000	-2.18969800
C	-3.11446100	-1.55883900	-2.32517100
C	-4.51501200	-0.97693300	-2.41198700
C	-5.48214900	-1.55900500	-1.35170700
C	-4.76360500	-1.93933400	-0.05762800
C	-4.23953300	-3.21880700	0.20922400
C	-4.26576300	-4.41240600	-0.73244300

C	-3.82362800	-4.05281200	-2.17056900
H	-1.77660400	-3.21132500	-2.45540500
H	-2.32201700	-0.90661700	-2.68990900
H	-4.92968900	-1.10814100	-3.42466100
H	-4.42661000	0.10478900	-2.25739900
H	-6.25887100	-0.81762400	-1.13053500
H	-6.00983200	-2.43135200	-1.75428400
H	-4.98545000	-1.30973000	0.80420900
H	-4.10536600	-3.48194000	1.26028200
H	-5.25976400	-4.88861500	-0.74300000
H	-3.57333400	-5.16031600	-0.32750000
H	-3.39507700	-4.94071700	-2.64974500
H	-4.69093500	-3.77314100	-2.77915000
H	0.92175400	0.48928200	3.21291600
H	1.15992200	-1.23091800	2.91750800
H	2.44853600	1.05014400	1.30859600
H	3.26269400	0.01544300	2.49472900

CP19

C	0.80871600	-1.92154000	-0.01509900
C	0.12965200	-1.51440400	1.35090800
C	1.15762700	-1.04372400	2.42143300
C	2.14061900	-0.00010800	1.88151600
C	2.86164200	-0.52052700	0.62766500
H	1.36411500	-2.85587900	0.18471200
H	3.38870800	-1.44943600	0.91371500
O	-0.18590500	-2.17079500	-0.94131600
C	1.83785800	-0.86919200	-0.43539100
C	1.82295500	-0.31749200	-1.64852100
H	1.05644900	-0.59744500	-2.36195000
H	2.56595800	0.41556100	-1.94291300
C	-0.81494300	-0.43701100	0.99176800
C	-1.37758600	0.64986200	0.86384200
O	3.79916400	0.45463000	0.18758300
Si	5.44136700	0.19386000	-0.04965900
C	6.10796500	1.88609500	-0.64780300
C	5.71479200	-1.17260200	-1.32935000
H	6.78158300	-1.39015100	-1.46303100
H	5.22942900	-2.10375000	-1.01183100
H	5.29624200	-0.90835600	-2.30641600
C	6.25684100	-0.34191000	1.57488700
H	7.33440300	-0.50229000	1.44547400
H	6.12182300	0.40351100	2.36674900
H	5.83215500	-1.28750400	1.93441400
C	5.88514300	2.95357800	0.44540700
H	6.24492100	3.93467400	0.10120100
H	4.82362500	3.05581700	0.69727200
H	6.42772300	2.71455800	1.36829300
C	5.36080200	2.32039000	-1.92684700
H	5.73087600	3.29646000	-2.27479600
H	5.50288100	1.60762200	-2.74857900
H	4.28389900	2.41515600	-1.74764600
C	7.61774200	1.78148000	-0.95387600
H	7.82731700	1.05480300	-1.74860700
H	8.00827500	2.75304500	-1.29031800
H	8.19781100	1.48820300	-0.06980000
Rh	-1.83899500	-0.94673600	-0.97863300
C	-0.66697800	-2.71507600	1.88635900
O	-1.86113100	-2.74087500	2.09171600
O	0.14977500	-3.76117300	2.13292200
C	-0.48982700	-4.96122100	2.62225800
H	-1.01398600	-4.72644900	3.55436100
H	-1.23914400	-5.28027600	1.89114200

C	0.59322200	-6.00509900	2.82228600	O	3.85012200	0.30866600	0.23129700
H	1.10761600	-6.21906200	1.87993300	Si	5.10535600	-0.11918100	-0.80102500
H	1.33566700	-5.66516400	3.55185500	C	6.48777000	1.14517500	-0.40523100
H	0.14839600	-6.93564200	3.19187900	C	4.57908100	-0.00770200	-2.61504700
C	-1.94819600	1.95767100	0.96882000	H	5.39155000	-0.30976600	-3.28765300
C	-1.33807800	3.05379500	0.30086200	H	3.72250900	-0.66268300	-2.80944100
C	-3.08920300	2.17737400	1.74813100	H	4.27689500	1.01016100	-2.88681800
C	-1.89791800	4.32363600	0.42780400	C	5.66064700	-1.89571300	-0.44496200
C	-3.64571900	3.45689100	1.87018500	H	6.54788700	-2.15264100	-1.03676500
H	-3.55106500	1.35135200	2.27776500	H	5.91091400	-2.04485500	0.61164700
C	-3.04647900	4.52841400	1.20490600	H	4.87996900	-2.62033400	-0.70695300
H	-1.44938800	5.17404800	-0.07251000	C	6.93990500	0.98865300	1.06267800
H	-3.45260300	5.53063700	1.27954500	H	7.71163900	1.73343000	1.30789100
O	-0.22288400	2.75913800	-0.41900800	H	6.10444800	1.13292300	1.75682200
O	-4.75956400	3.54482800	2.65869400	H	7.37103800	-0.00154500	1.25636900
C	0.45400500	3.81189200	-1.08576900	C	5.95422900	2.57975100	-0.61030600
H	-0.18440500	4.28382200	-1.84474000	H	6.73595000	3.31638100	-0.37171100
H	0.80166200	4.57679900	-0.37857900	H	5.64559700	2.75795000	-1.64804700
H	1.31369900	3.34722300	-1.57024500	H	5.09350000	2.78319900	0.03604900
C	-5.36270400	4.81651600	2.81921300	C	7.69812300	0.91748300	-1.33620100
H	-5.71035100	5.22439100	1.86005000	H	7.43437800	1.04829100	-2.39295300
H	-6.22105300	4.66130400	3.47551300	H	8.49700400	1.63839900	-1.10858500
H	-4.67549300	5.53512000	3.28672000	H	8.12582900	-0.08651600	-1.21978700
C	-2.69585900	-2.44808400	-2.26917500	Rh	-2.06744000	-1.04267200	-0.62347000
C	-1.94410400	-1.54396200	-3.04278300	C	-0.52508100	-2.61516200	1.57867200
C	-2.50654700	-0.41547200	-3.88527900	O	-1.45189500	-2.99545700	0.84354300
C	-3.62113800	0.37207800	-3.16210300	O	0.15755400	-3.50316300	2.34796000
C	-3.39177700	0.45150800	-1.65301900	C	-0.24001600	-4.88217800	2.23794300
C	-3.92735500	-0.44739300	-0.71393000	H	-1.30023600	-4.97216700	2.49716700
C	-4.76687800	-1.67490300	-1.02080500	H	-0.12750900	-5.20780000	1.19810100
C	-4.21781800	-2.49989500	-2.20638300	C	0.64059300	-5.68439000	3.17985700
H	-2.17544100	-3.34864400	-1.95076400	H	1.69664200	-5.58661700	2.90725500
H	-0.92723300	-1.84529800	-3.28349600	H	0.51972500	-5.34276700	4.21309300
H	-2.86726400	-0.79679100	-4.85461700	H	0.36913100	-6.74490600	3.13265700
H	-1.67909000	0.26635500	-4.11494700	C	-1.47611900	2.16519600	0.52934600
H	-3.66477700	1.38916800	-3.56943900	C	-1.60413400	3.05792900	-0.57227400
H	-4.60113000	-0.07240800	-3.36803600	C	-1.73736300	2.66462100	1.81615300
H	-3.12351300	1.43882100	-1.28633800	C	-1.97286400	4.38323000	-0.34682900
H	-4.04475900	-0.08162000	0.30521200	C	-2.09976000	3.99750900	2.03797400
H	-5.81766400	-1.39368000	-1.19872600	H	-1.65045800	2.00121900	2.66982400
H	-4.76359100	-2.30186100	-0.12179600	C	-2.21934800	4.86027900	0.94727900
H	-4.53535300	-3.54339500	-2.09785700	H	-2.07208400	5.07323200	-1.17655000
H	-4.64600900	-2.15169400	-3.15242000	H	-2.50117700	5.89877600	1.07742300
H	0.62087400	-0.64936700	3.29227400	O	-1.34626000	2.54754500	-1.81446400
H	1.70863800	-1.92895900	2.75956400	O	-2.31578400	4.34656000	3.34374400
H	2.88303900	0.24142500	2.65173400	C	-1.29977600	3.44451900	-2.91234400
H	1.62266600	0.92893200	1.61730100	H	-2.28109600	3.89598100	-3.11150600
TS15				H	-0.56356500	4.24234900	-2.74773100
C	0.94253400	-1.65118300	-0.84341000	H	-0.99977400	2.84608200	-3.77447100
C	-0.06410400	-1.24696100	1.67876500	C	-2.69319700	5.68330200	3.61955600
C	1.10967400	-0.85726800	2.56732500	H	-3.64286100	5.94569000	3.13288700
C	2.16314500	0.05067600	1.90427600	H	-2.81614300	5.74434500	4.70263300
C	2.70646400	-0.48470900	0.56360800	H	-1.92002000	6.39715300	3.30323500
H	1.41008200	-2.60490900	-0.54411000	C	-3.06427300	-2.16733200	-2.19200700
H	3.01572600	-1.53219000	0.71196200	C	-2.80596700	-0.86446800	-2.65850300
O	-0.13600200	-1.70360200	-1.50392700	C	-3.82211700	0.25666400	-2.76187900
C	1.64245000	-0.44166400	-0.51932400	C	-4.69556600	0.38462100	-1.49615300
C	1.17482900	0.73497100	-1.02527000	C	-3.93832400	-0.00948300	-0.22680500
H	0.44963200	0.74455000	-1.82645000	C	-3.94776300	-1.29800400	0.34559500
H	1.62778700	1.68218100	-0.74770200	C	-4.62650500	-2.53133300	-0.22328500
C	-0.83680000	-0.29743000	1.03022400	C	-4.43199500	-2.67882600	-1.75013900
C	-1.03308600	0.79798900	0.38371400	H	-2.33524200	-2.93103800	-2.45642400
				H	-1.90888000	-0.72925500	-3.26100200

H	-4.45182000	0.13333500	-3.65831800	H	-4.52411900	-3.73683000	-2.02067600
H	-3.26188700	1.18687800	-2.89483500	H	-5.22771600	-2.15927700	-2.29530100
H	-5.03634600	1.42145200	-1.39503500	H	0.75456500	-0.35385200	3.47865200
H	-5.60330900	-0.22213700	-1.58522800	H	1.59219000	-1.77993800	2.90382800
H	-3.71893800	0.81354400	0.44721500	H	3.01064500	0.16739800	2.59092500
H	-3.72923700	-1.36302700	1.41122000	H	1.75725100	1.05449500	1.72952900
H	-5.69680800	-2.53597500	0.03988000				
H	-4.17704900	-3.39654400	0.27509100				

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