

Supporting Information

DFT Study of the Mechanism and Stereochemistry of the Rh(I)–Catalyzed Diels–Alder Reactions between Electronically Neutral Dienes and Dienophiles

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1. Full Citation of 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, J. A. Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; 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.; Fox, D. J. *Gaussian 09*, Revision A.02; Gaussian Inc.: Wallingford CT, 2009.

2. Discussion of Different Calculation Methods

Recently Gellrich (Gellrich, U.; Himmel, D.; Meuwly, M.; Breit, B. *Chem. Eur. J.* **2013**, *19*, 16272) found that B3LYP functional with SDD-6-31G(d,p) basis set computed binding energy of Rh species with CO is very close to that obtained by CCSD(T) method, suggesting that B3LYP is a good method to investigate Rh-catalyzed reactions. Many other Rh-catalyzed reactions have been investigated by the B3LYP functional as well (see ref. 22 of the main text. One exception is found for underestimating the stability of oxonium ylide by B3LYP method, see Oku, A.; Sawada, Y.; Schroeder, M.; Higashikubo, I.; Yoshida, T.; Ohki, S. *J. Org. Chem.* **2004**, *69*, 1331). Here we further checked the reliability of the B3LYP functional in the calculations of Rh-catalyzed Diels–Alder reaction. We computed the activation free energies of the intermolecular [4+2] reaction of butadiene and acetylene (Table S1), finding that other DFT functionals underestimate the oxidative cyclization step’s activation free energy, while all tested functionals have similar activation free energies for the reductive elimination step. Pathway *b* involving transition state **3b-TS** is always disfavored compared to pathway *a* because **3-TS** is lower in **3b-TS** by about 5 kcal/mol (the oxidative cyclization step via **3-TS** is irreversible). In addition, we have computed the activation free energies of all steps for the Rh-catalyzed [4+2] reaction of butadiene and acetylene, showing that these computed values are only slightly affected by the choice of basis sets (Table S2). Houk and coworkers (Goldstein, E.; Beno, B.; Houk, K. N. *J. Am. Chem. Soc.* **1996**, *118*, 6036) have shown that B3LYP is a reasonable functional to investigate thermal Diels–Alder reaction. To compare the Rh-catalyzed Diels–Alder reaction and the thermal Diels–Alder reaction, together with a consideration that B3LYP calculations gave similar energy with that from CCSD(T) calculations, we chose B3LYP functional to investigate the reaction mechanism and stereochemistry of Rh-catalyzed Diels–Alder reactions.

Table S1. Calculated Activation Free Energies of Reaction 1 Using Different Methods in the Gas Phase (6-31G(d) for C, H, P and LANL2DZ for Rh).

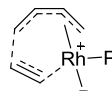
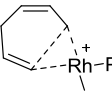
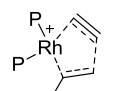
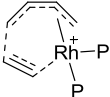
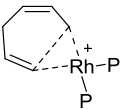
functional						
	2	3-TS	4	4-TS	2	3b-TS
B3LYP		19.3		22.7		24.0
M06//B3LYP		15.2		18.2		18.8
M06L//B3LYP		15.0		21.5		19.0
PBE1PBE//B3LYP		11.2		22.1		17.9
BP86//B3LYP		10.3		20.9		15.5
B97D//B3LYP		10.4		22.9		15.9

Table S2. Calculated Activation Free Energies of Reaction 1 Using Different Basis Sets in the Gas Phase (B3LYP//B3LYP Method).

basis set								
	2	3-TS	4	4-TS	2	3b-TS		
6-31G(d) for C, H, P LANL2DZ for Rh		19.3		22.7		24.0		
6-311+G(d,p) for C, H, P SDD for Rh		21.8		24.4		27.3		
Def2-TZVP for C, H, P, Rh		22.7		23.7		26.4		
cc-pVTZ for C, H cc-pV(T+d)Z for P cc-pVTZ-pp for Rh		21.9		23.8		26.0		

3. Energy Surface of Ene-Diene Substrate Catalyzed by Neutral Rh-Catalyst

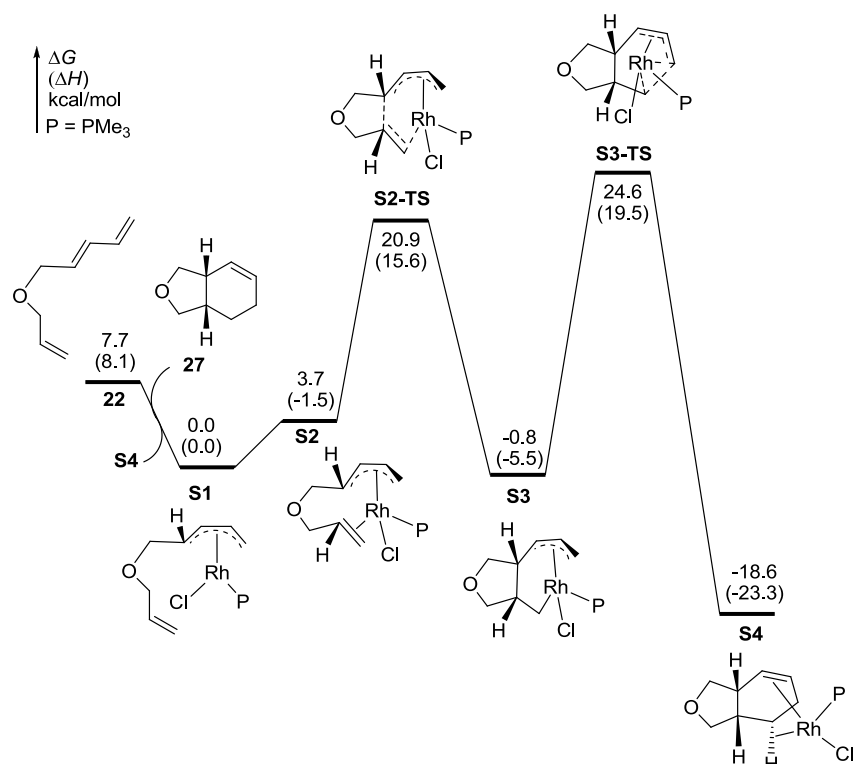


Figure S1. Potential energy surface of Rh-catalyzed intramolecular Diels–Alder reaction.

4. Calculated Energies of Ene–Diene Substrate Catalyzed by Cationic Rh-Catalyst

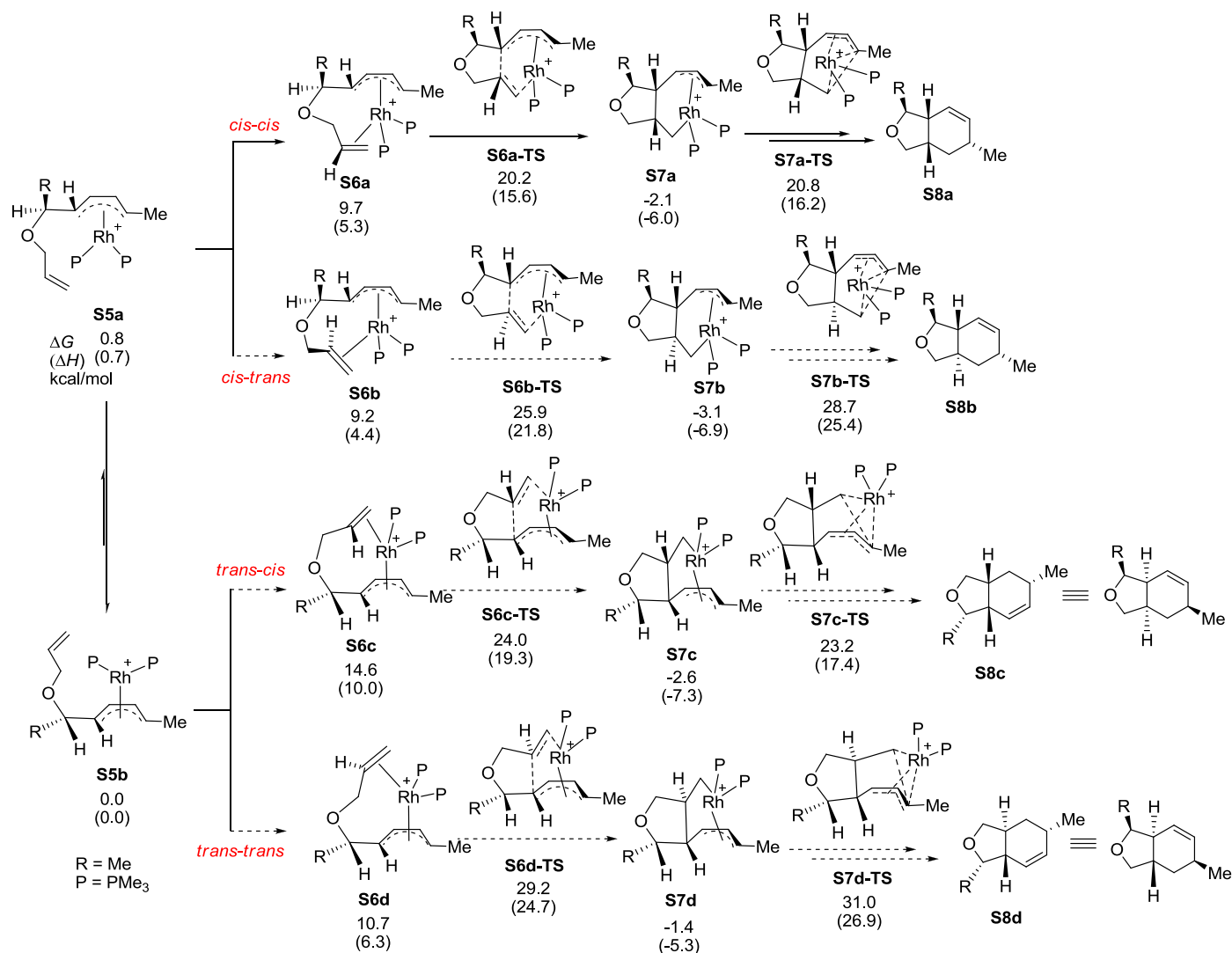


Figure S2. DFT-calculated energies for different pathways for ene–diene with a substituent adjacent to the diene moiety of the substrate.

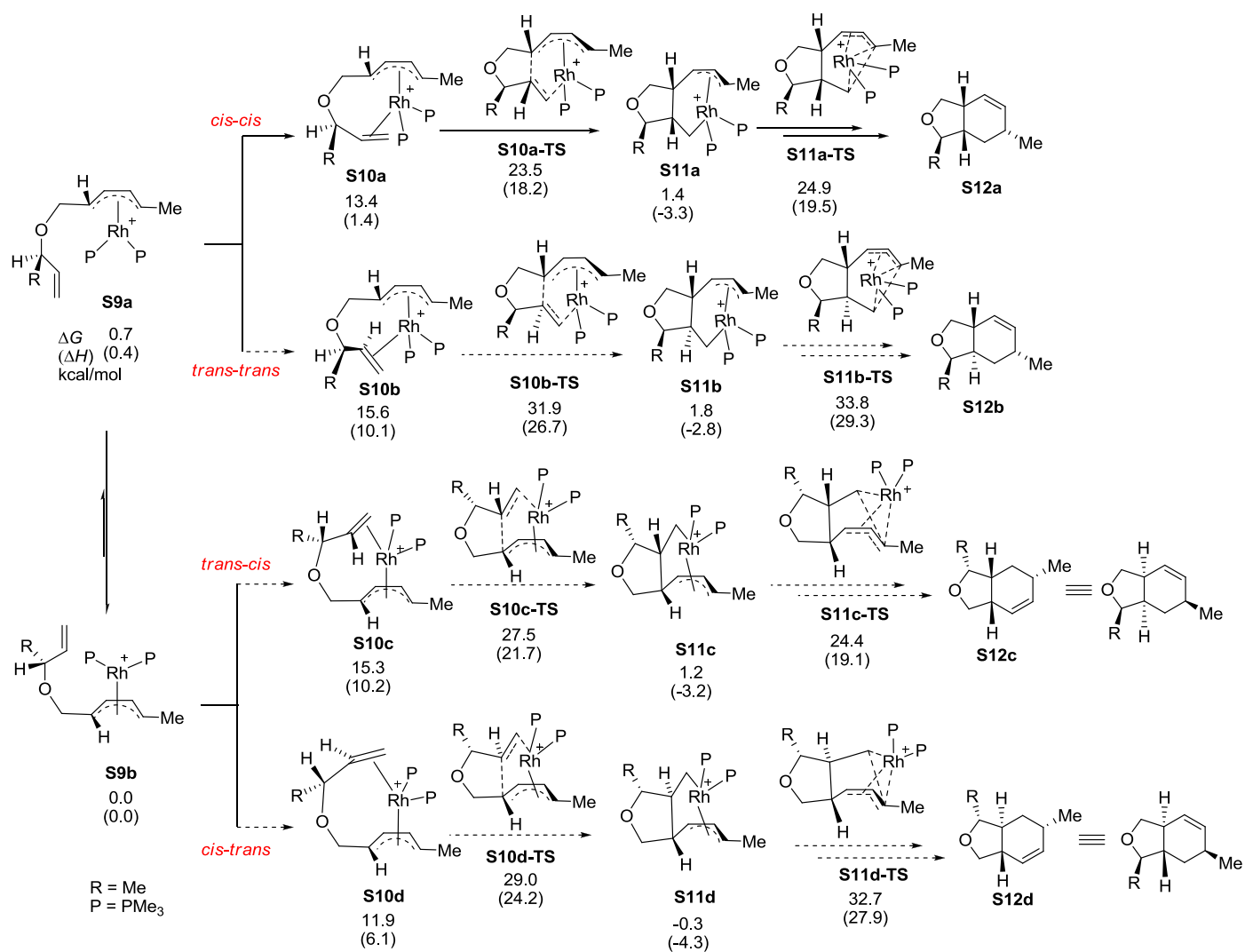
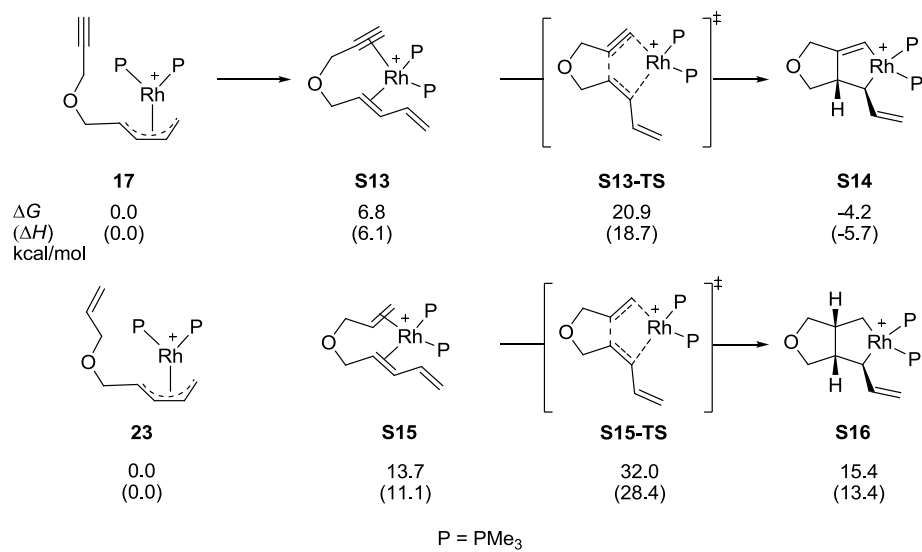


Figure S3. Calculated relative energies of ene–diene substrate with methyl group adjacent to the ene moiety of the substrate.

5. Other Oxidative Cyclization Steps for Substrates 16 and 22

Scheme S1. Other Oxidative Cyclization Possibilities of Substrates **16** and **22**



6. Calculated Energy Surface Using M06 Method

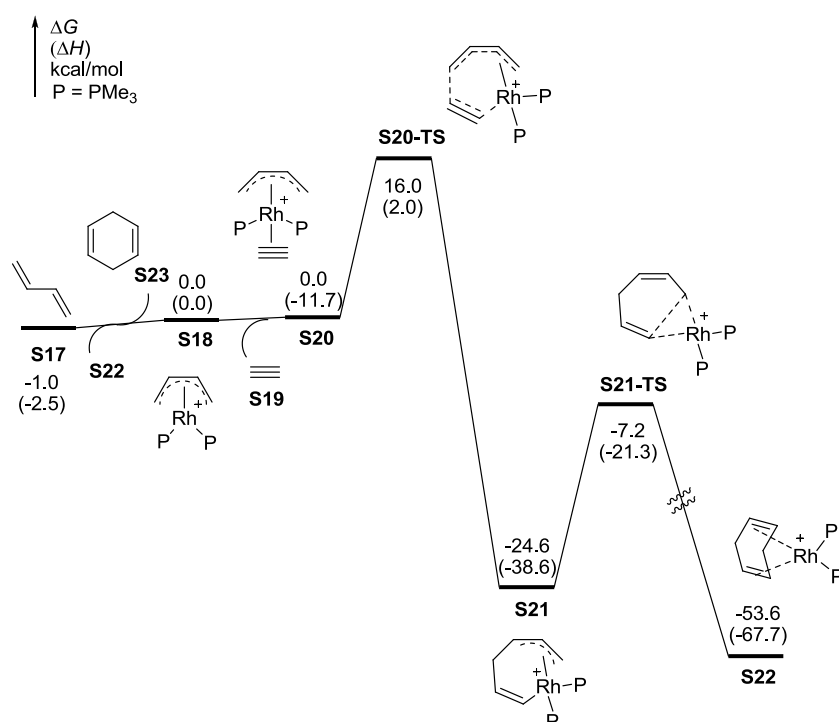


Figure S4. Energy surface of Rh-catalyzed Diels–Alder reaction using M06 method (6-31G(d) for C, H, P and LANL2DZ for Rh).

7. Calculated Energies of Oxidative Cyclization Step of Isoprene and Propyne Catalyzed by $\text{Rh}(\text{dppb})^+$ Catalyst

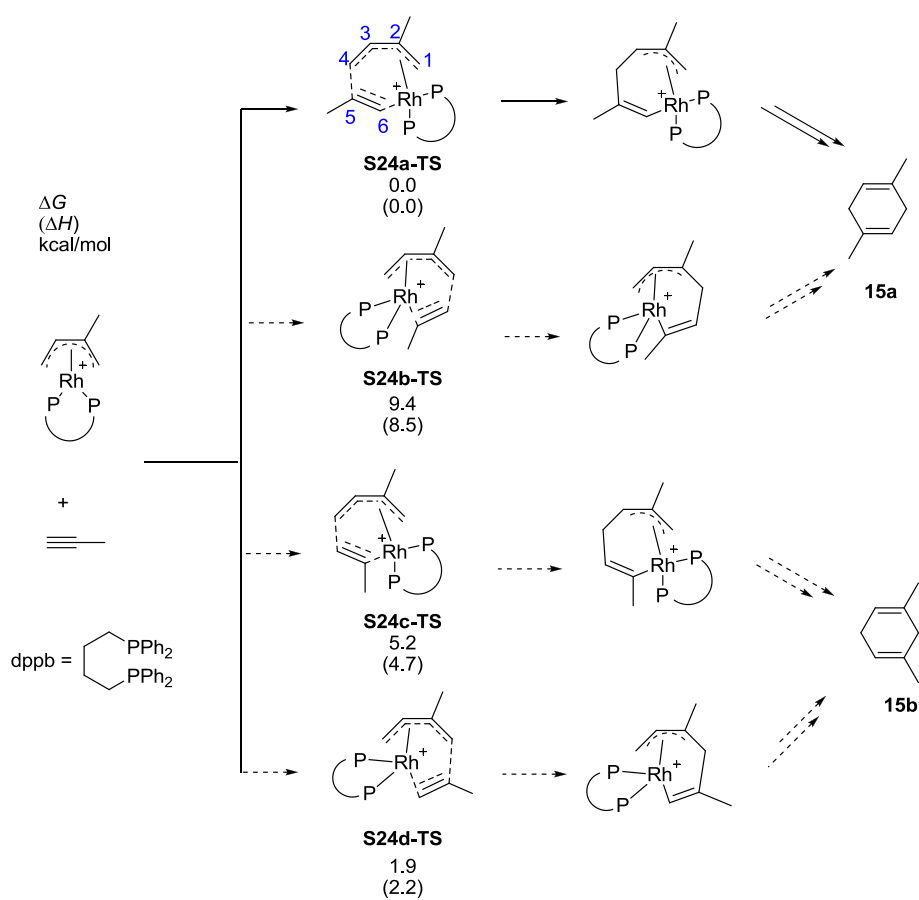


Figure S5. Computed energies of intermolecular Diels–Alder reaction using $\text{Rh}(\text{dppb})^+$ catalyst.

8. Energy Surface of Diels–Alder Reaction between Butadiene and Acetylene in Solution

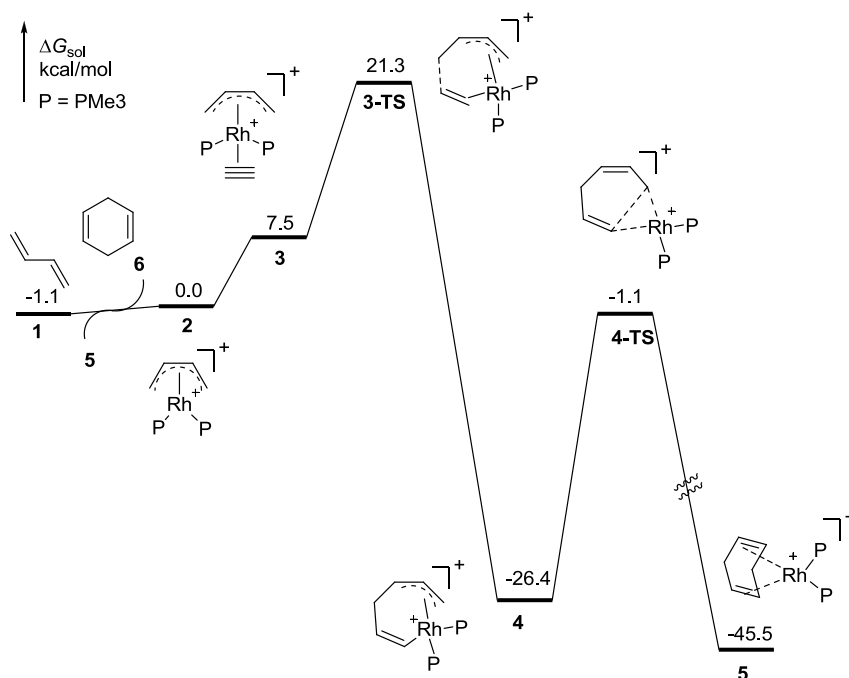
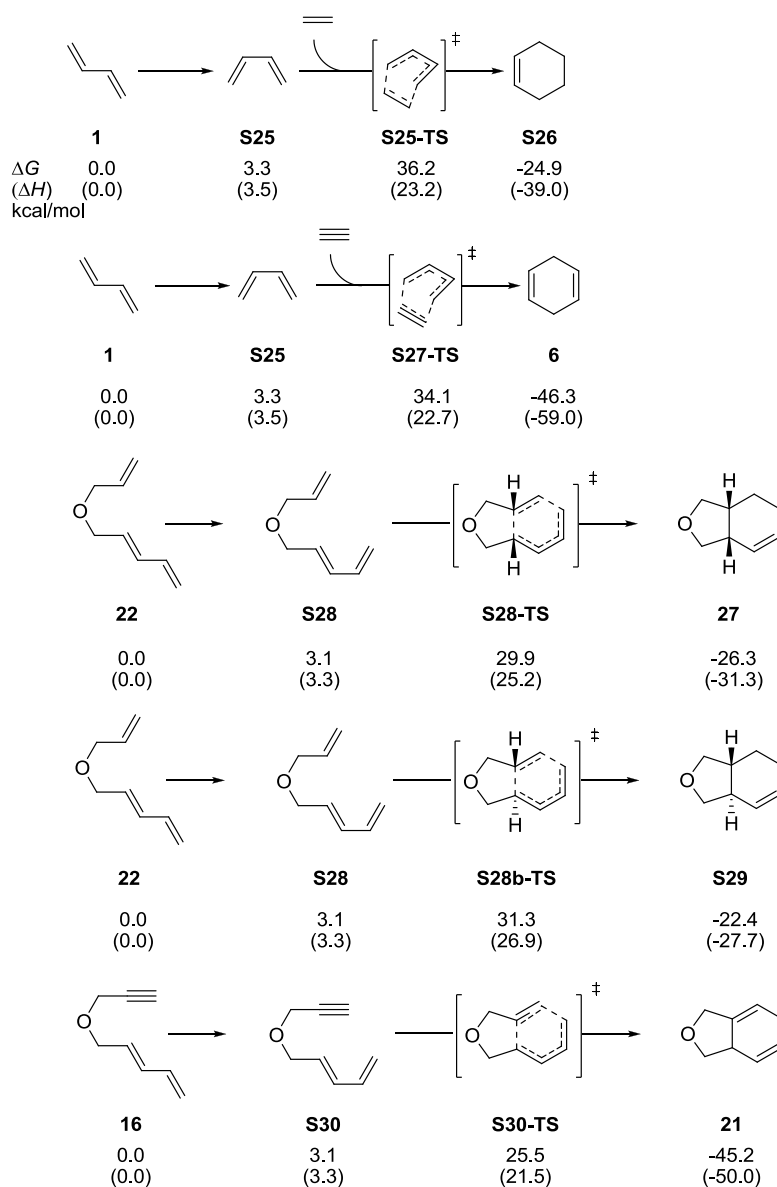


Figure S6. Energy surface of Diels–Alder reaction between butadiene and acetylene in solution (Solution energies in DCM were evaluated with B3LYP method by a self-consistent reaction field (SCRF) using the IEFPCM model, where UFF radii was used at the same level. Solvation energy calculations were carried out on the gas-phase optimized structures).

9. Calculated Energies of Thermal Diels–Alder Reaction

Scheme S2. Calculated Energies of Thermal Diels–Alder Reaction (B3LYP/6-31G(d) Method).



In the above calculations, we added key word “5d” to specify that all calculations used 5d orbitals instead of 6d orbitals.

10. Structures of Reductive Elimination Transition States.

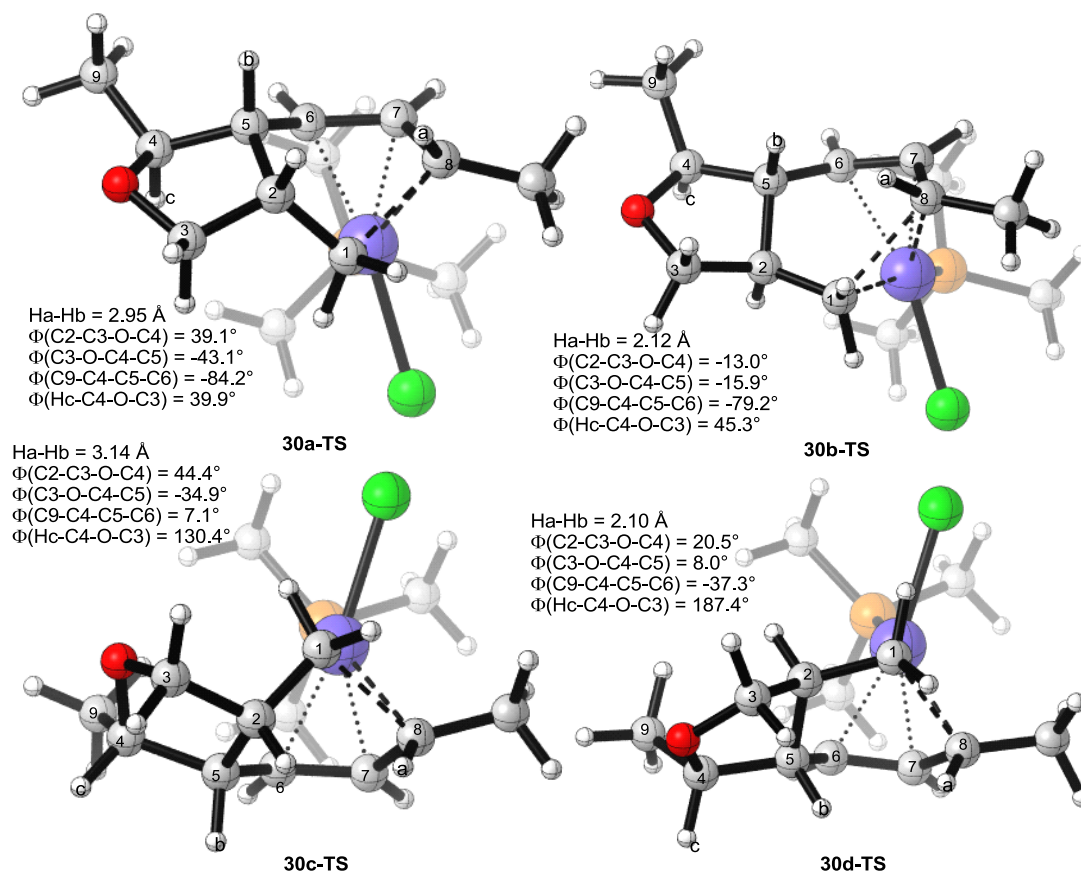


Figure S7. Structures of reductive elimination transition states in Figure 10.

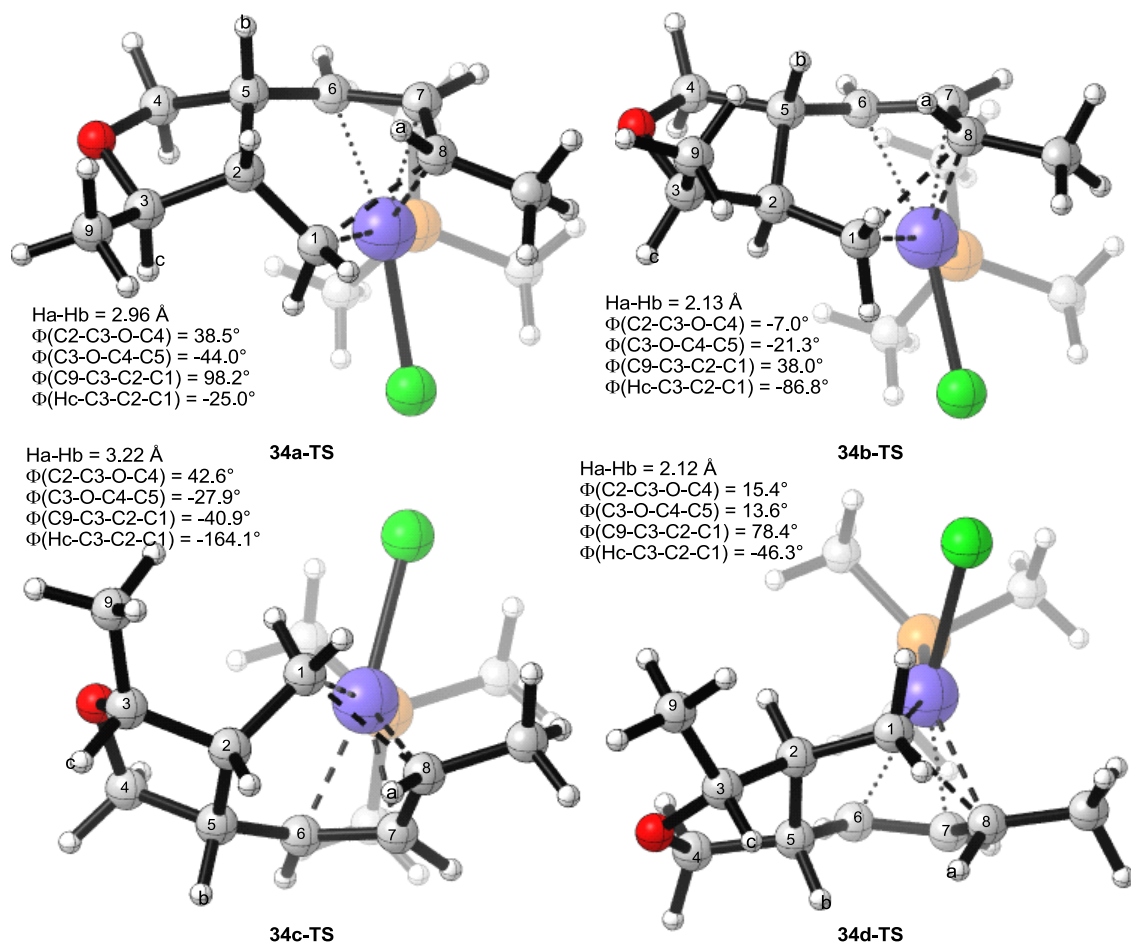
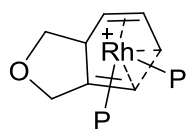
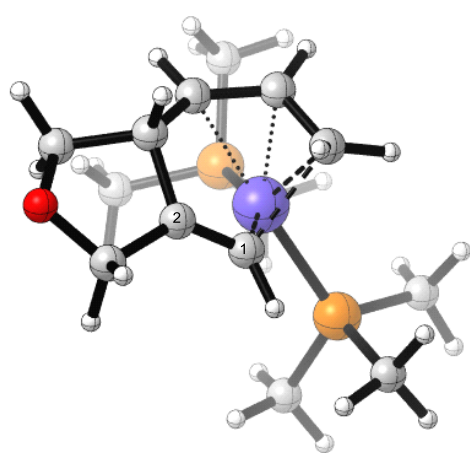
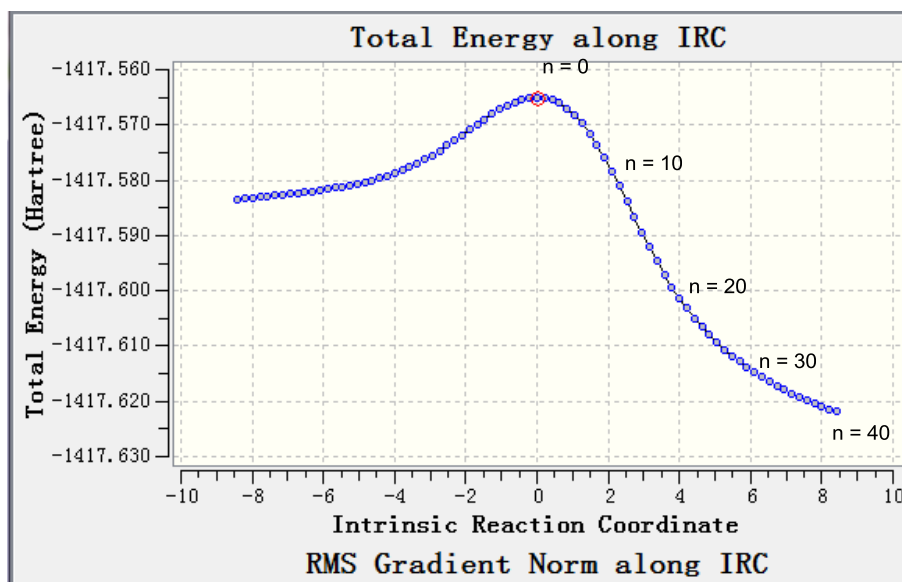


Figure S8. Structures of reductive elimination transition states in Figure 13.

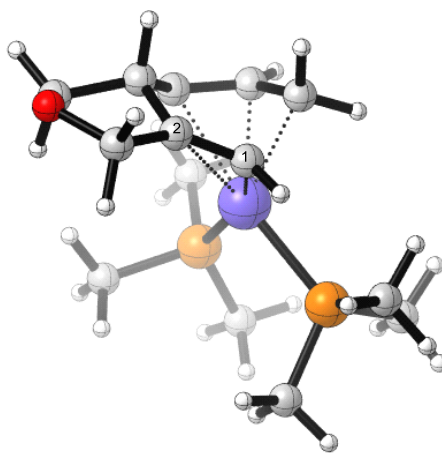
11. IRC Calculations



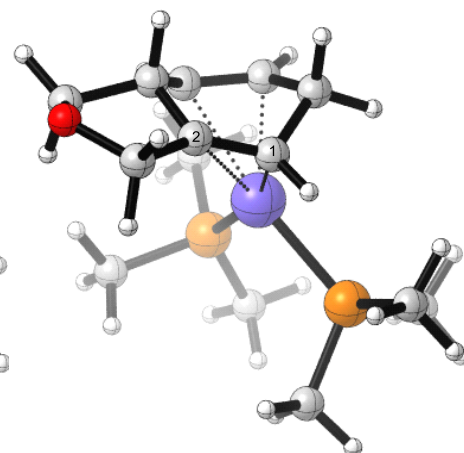
19-TS



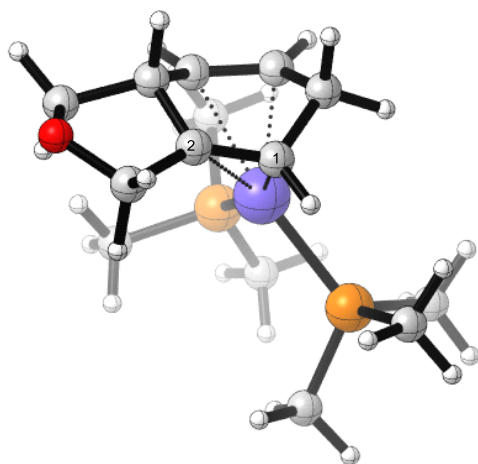
n = 0



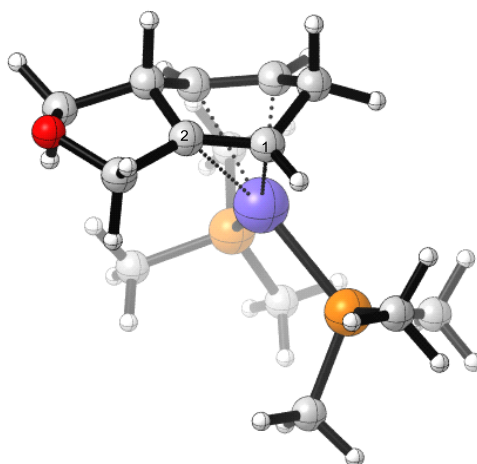
n = 10



n = 20

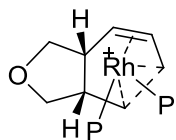


n = 30

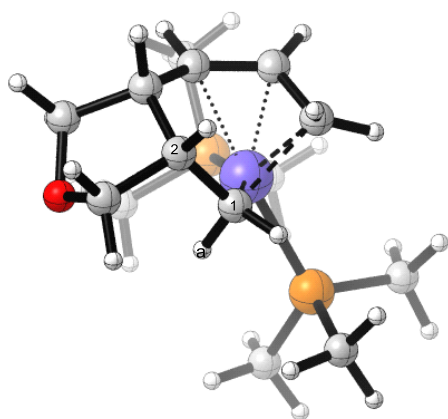
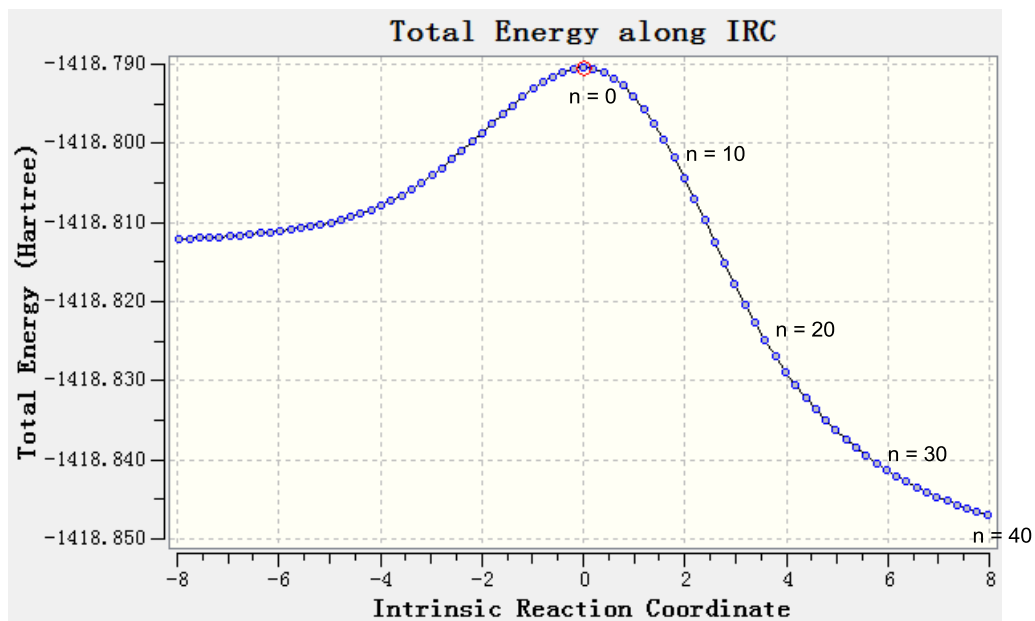


n = 40

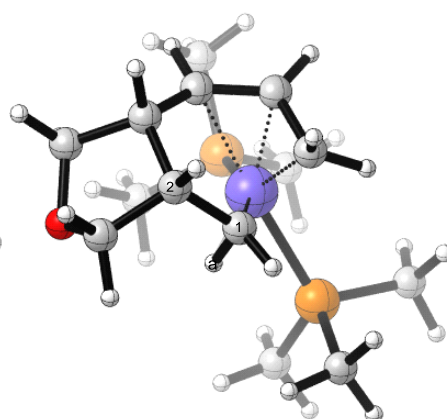
	Rh-C1	Rh-C2
n = 0	2.09 Å	2.85 Å
n = 10	2.15 Å	2.86 Å
n = 20	2.27 Å	2.86 Å
n = 30	2.43 Å	2.88 Å
n = 40	2.53 Å	2.86 Å



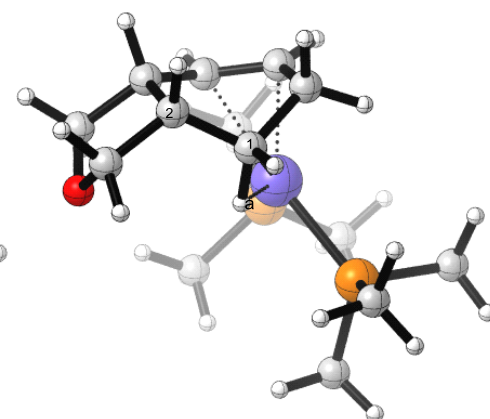
25-TS



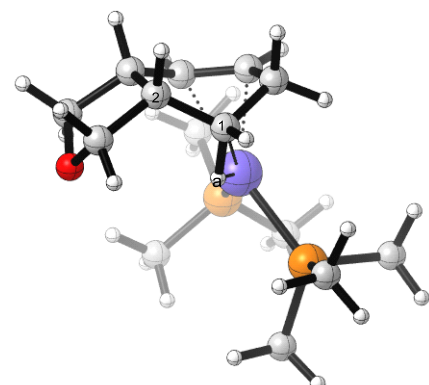
n = 0



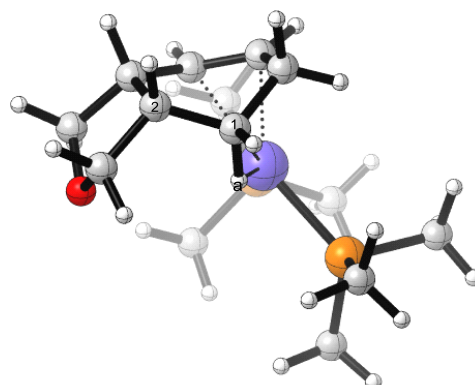
n = 10



n = 20



n = 30



n = 40

	Rh-C1	Rh-C2	Rh-Ha
n = 0	2.25 Å	3.20 Å	2.20 Å
n = 10	2.31 Å	3.25 Å	2.01 Å
n = 20	2.39 Å	3.30 Å	1.90 Å
n = 30	2.55 Å	3.38 Å	1.95 Å
n = 40	2.68 Å	3.45 Å	2.03 Å

12. Typical Gaussian Input Files

Attention: when computing species without Rh metal, a keyword 5d must be used to specify all elements used 5d instead of 6d orbitals.

Geometry optimization and frequency calculations of reactants, intermediates, and products:

```
%chk=name.chk  
%mem=2000MB  
%nprocshared=4  
#b3lyp/genecp opt freq
```

Title Card Required

```
0 1  
Coordinates
```

```
C H P Cl O O  
6-31G(d)  
*****
```

```
Rh 0  
LANL2DZ  
*****
```

```
Rh 0  
LANL2DZ
```

Geometry optimization and frequency calculations of transition states:

```
%chk=name.chk  
%mem=2000MB  
%nprocshared=4  
#b3lyp/genecp opt=(ts,noeigen,calcfc) freq
```

Title Card Required

```
0 1  
Coordinates
```

```
C H P Cl O O  
6-31G(d)  
*****
```

```
Rh 0  
LANL2DZ  
*****
```

```
Rh 0  
LANL2DZ
```

13. Computed Energies of All Stationary Points

Table S3. Sum of electronic and thermal Enthalpies (H , in Hartree, B3LYP), Sum of electronic and thermal Free Energies (G , in Hartree, B3LYP)

name	H	G
acetylene	-77.293276	-77.316171
1	-155.897781	-155.929811
2	-1187.253775	-1187.322387
3	-1264.552709	-1264.628818
3b	-1264.545608	-1264.625636
3-TS	-1264.534329	-1264.60777
3b-TS	-1264.523637	-1264.600326
4	-1264.605656	-1264.680559
4b	-1264.57644	-1264.652247
4-TS	-1264.570942	-1264.644382
5	-1264.642659	-1264.715547
6	-233.285105	-233.319768
7	-1226.544637	-1226.620947
8a	-1303.84133	-1303.920347
8b	-1303.842248	-1303.922201
8a-TS	-1303.823544	-1303.901104
8b-TS	-1303.82054	-1303.896054
9a	-1303.894744	-1303.972686
9b	-1303.891027	-1303.968079
propyne	-116.590016	-116.618145
11a	-1303.848316	-1303.928905
11b	-1303.847193	-1303.928288
11a-TS	-1303.827694	-1303.904817
11b-TS	-1303.824463	-1303.901297
12a	-1303.895686	-1303.973893
12b	-1303.890914	-1303.967788
13a	-1343.137155	-1343.220854
13b	-1343.136671	-1343.220771
13c	-1343.135804	-1343.22007
13d	-1343.137722	-1343.221247
13a-TS	-1343.116943	-1343.197604
13b-TS	-1343.110622	-1343.18932
13c-TS	-1343.113214	-1343.192854
13d-TS	-1343.113476	-1343.192876
14a	-1343.185005	-1343.266377
14b	-1343.176849	-1343.256941
14c	-1343.180365	-1343.261104
14d	-1343.180676	-1343.261588
16	-385.78295	-385.83075
17	-1417.140517	-1417.225354
18	-1417.134731	-1417.214217
18-TS	-1417.122129	-1417.20058
19	-1417.17894	-1417.259024
19-TS	-1417.14551	-1417.224464
20	-1417.215953	-1417.29423
21	-385.86257	-385.902764
22	-387.01727	-387.066066
23	-1418.376164	-1418.462457
24	-1418.368669	-1418.447886
24b	-1418.369899	-1418.448359
24-TS	-1418.3491	-1418.426805
24b-TS	-1418.340794	-1418.419491
25	-1418.385207	-1418.463007
25b	-1418.382665	-1418.463372
25-TS	-1418.346235	-1418.42563
26	-1418.412704	-1418.491984
27	-387.067225	-387.107948
28a	-1496.371621	-1496.450896
28b	-1496.367401	-1496.446043
29a	-1496.374268	-1496.447731
29b	-1496.36515	-1496.439312
29c	-1496.366274	-1496.439169
29d	-1496.362892	-1496.436124
29a-TS	-1496.349139	-1496.420924
29b-TS	-1496.338809	-1496.411377
29c-TS	-1496.342309	-1496.413019
29d-TS	-1496.33699	-1496.408712
30a	-1496.383637	-1496.458329
30b	-1496.384289	-1496.458193
30c	-1496.382387	-1496.456116
30d	-1496.381813	-1496.455863
30a-TS	-1496.347978	-1496.420785
30b-TS	-1496.335757	-1496.408067
30c-TS	-1496.344876	-1496.416584
30d-TS	-1496.333538	-1496.40591

32a	-1496.376432	-1496.456641
32b	-1496.376732	-1496.456718
33a	-1496.373557	-1496.446921
33b	-1496.357172	-1496.431514
33c	-1496.365225	-1496.438043
33d	-1496.364308	-1496.43854
33a-TS	-1496.349112	-1496.42134
33b-TS	-1496.335879	-1496.408243
33c-TS	-1496.341747	-1496.413106
33d-TS	-1496.339022	-1496.410649
34a	-1496.384172	-1496.458347
34b	-1496.381703	-1496.454871
34c	-1496.382162	-1496.456562
34d	-1496.384133	-1496.458534
34a-TS	-1496.347992	-1496.421632
34b-TS	-1496.33358	-1496.406319
34c-TS	-1496.34614	-1496.418539
34d-TS	-1496.335885	-1496.40845
S1	-1417.80169	-1417.876418
S2	-1417.804157	-1417.870502
S2-TS	-1417.776898	-1417.843056
S3	-1417.810439	-1417.877692
S3-TS	-1417.770672	-1417.837147
S4	-1417.838766	-1417.906071
S5b	-1496.9469	-1497.038689
S5a	-1496.945854	-1497.037415
S6a	-1496.938517	-1497.023309
S6b	-1496.939841	-1497.023978
S6c	-1496.931013	-1497.015443
S6d	-1496.936802	-1497.021676
S6a-TS	-1496.922118	-1497.006441
S6b-TS	-1496.912104	-1496.997483
S6c-TS	-1496.916127	-1497.00039
S6d-TS	-1496.907512	-1496.992152
S7a	-1496.956474	-1497.042042
S7b	-1496.957829	-1497.043618
S7c	-1496.958601	-1497.042885
S7d	-1496.955345	-1497.040844
S7a-TS	-1496.921089	-1497.005584
S7b-TS	-1496.906397	-1496.992915
S7c-TS	-1496.919161	-1497.001761
S7d-TS	-1496.904008	-1496.989222

S9a	-1496.950442	-1497.042709
S9b	-1496.951012	-1497.043794
S10a	-1496.937781	-1497.022442
S10b	-1496.934876	-1497.018933
S10c	-1496.934804	-1497.019435
S10d	-1496.941247	-1497.024822
S10a-TS	-1496.921981	-1497.006416
S10b-TS	-1496.908508	-1496.993027
S10c-TS	-1496.91637	-1496.999919
S10d-TS	-1496.912403	-1496.997537
S11a	-1496.956298	-1497.04149
S11b	-1496.955422	-1497.040987
S11c	-1496.956116	-1497.041827
S11d	-1496.957939	-1497.044265
S11a-TS	-1496.919939	-1497.00417
S11b-TS	-1496.904261	-1496.989939
S11c-TS	-1496.920507	-1497.004955
S11d-TS	-1496.906515	-1496.991682
S13	-1417.130761	-1417.214463
S13-TS	-1417.110761	-1417.192055
S14	-1417.149623	-1417.232082
S15	-1418.358506	-1418.440681
S15-TS	-1418.330976	-1418.411471
S16	-1418.35486	-1418.43797
S19	-77.226459	-77.249255
S24a-TS	-2187.183443	-2187.293734
S24b-TS	-2187.169834	-2187.278709
S24c-TS	-2187.175945	-2187.285421
S24d-TS	-2187.179934	-2187.290731
S25	-155.892216	-155.924575
ethylene	-78.530604	-78.55612
S25-TS	-234.391371	-234.428304
S26	-234.490519	-234.525593
S27-TS	-233.154946	-233.191641
S28	-387.011988	-387.061084
S28-TS	-386.974473	-387.016242
S28b-TS	-386.977046	-387.018377
S29	-387.061348	-387.101813
S30	-385.77767	-385.825763
S30-TS	-385.748749	-385.790055

Table S4. Sum of electronic and thermal Enthalpies (H , in Hartree, M06), Sum of electronic and thermal Free Energies (G , in Hartree, M06)

name	H	G
S17	-155.757443	-155.789632
S18	-1186.841559	-1186.91294
S20	-1264.086742	-1264.162147
S20b	-1264.076204	-1264.150163
S20-TS	-1264.064909	-1264.136659
S20b-TS	-1264.055261	-1264.129186
S21	-1264.129525	-1264.2014
S21b	-1264.095159	-1264.170048
S21-TS	-1264.101982	-1264.173696
S22	-1264.175918	-1264.247541
S23	-233.08786	-233.122616

Table S5. Thermal correction to Gibbs Free Energy ($TCGFE$ in Hartree, B3LYP), total free energy in solution (E_{sol} , in Hartree), and thermo corrected Gibbs free energy in DCM (G_{sol} , which equals to $E_{\text{sol}} + TCGFE$, in Hartree).

name	$TCGFE$	E_{sol}	G_{sol}
acetylene	0.007631	-77.32669249	-77.31906149
1	0.059068	-155.9905187	-155.9314507
2	0.273115	-1187.65031	-1187.377195
3	0.298808	-1264.983108	-1264.6843
3-TS	0.300444	-1264.962771	-1264.662327
4	0.302783	-1265.041156	-1264.738373
4-TS	0.303501	-1265.001529	-1264.698028
5	0.307337	-1265.076024	-1264.768687
6	0.094146	-233.41537	-233.321224

14. Coordinates of All Stationary Points Computed by B3LYP Method

acetylene				H	2.71057500	3.14454900	-0.40900400
C	0.00000000	0.00000000	0.60257900	H	1.20516700	2.88432600	-1.31879200
H	0.00000000	0.00000000	1.66907700	C	-1.70533600	2.71063400	-0.36520200
C	0.00000000	0.00000000	-0.60257900	H	-1.14485400	3.22017500	0.42243400
H	0.00000000	0.00000000	-1.66907700	H	-1.20592400	2.88277600	-1.32212000
				H	-2.71016400	3.14450900	-0.41083600
1				C	-3.06748400	0.37833400	-1.28330900
C	-0.00000600	-0.72893200	0.00000000	H	-3.37258700	-0.65853100	-1.12140600
H	-0.97806300	-1.21124400	0.00000000	H	-3.95569300	1.01807700	-1.23906400
C	1.10756500	-1.48482300	0.00000000	H	-2.62529000	0.45498300	-2.28117300
H	1.06043500	-2.56961100	0.00000000	C	-2.78651800	0.89295200	1.56794600
H	2.10032800	-1.03977800	0.00000000	H	-3.70170400	1.48665300	1.46802100
C	0.00000000	0.72892400	0.00000000	H	-3.05336900	-0.12952700	1.84670300
H	0.97806100	1.21123200	0.00000000	H	-2.17627100	1.31708900	2.37113400
C	-1.10756100	1.48483000	0.00000000				
H	-2.10033100	1.03979600	0.00000000	3			
H	-1.06041800	2.56961600	0.00000000	C	0.35199400	-2.06379200	-1.55586200
				H	0.67049300	-1.68409500	-2.52183900
2				C	1.27729000	-2.41164900	-0.54021100
C	0.72429200	-2.57217700	-0.63205400	H	2.33472900	-2.27327600	-0.73462600
H	1.22928500	-2.62246900	-1.59279900	H	1.05238900	-3.22035300	0.14809000
C	1.45197300	-2.34072800	0.52767000	C	-1.04203400	-2.10428700	-1.23609100
H	2.52906400	-2.22849500	0.45860000	H	-1.75601700	-1.73688800	-1.96834400
H	1.07264400	-2.57108200	1.51845900	C	-1.45084700	-2.42923100	0.07242300
C	-0.72574000	-2.57187200	-0.63120200	H	-0.92103800	-3.16110200	0.67182800
H	-1.23191100	-2.62203400	-1.59133100	H	-2.49333800	-2.29847700	0.34149600
C	-1.45189300	-2.34001600	0.52942900	P	-1.73802100	0.98706100	-0.09306200
H	-1.07145700	-2.57056500	1.51975200	P	1.77190100	0.92291800	-0.17642700
H	-2.52902600	-2.22735700	0.46172800	C	-0.14584200	-0.43368700	2.48450700
Rh	-0.00003600	-0.58945600	0.05263700	C	0.79272600	-1.20366100	2.28567500
P	-1.83134000	0.90247500	-0.01377700	Rh	0.00457200	-0.67640100	0.13110200
P	1.83155400	0.90227300	-0.01363300	H	-0.88468100	0.16235600	2.97822800
C	2.78795000	0.89063700	1.56733600	H	1.61767800	-1.87671900	2.39060400
H	3.05513500	-0.13220500	1.84442100	C	-2.14937700	1.49651100	-1.82341100
H	3.70299800	1.48456900	1.46750200	H	-2.45865300	0.62235400	-2.40434400
H	2.17830900	1.31358100	2.37160900	H	-2.96524700	2.22763900	-1.83274100
C	3.06658500	0.37926900	-1.28471100	H	-1.27550900	1.93510700	-2.31186300
H	3.95526200	1.01833100	-1.24001100	C	-1.56038800	2.61848600	0.76036400
H	3.37102500	-0.65807400	-1.12460300	H	-2.46271700	3.22255100	0.61733000
H	2.62383900	0.45776200	-2.28218700	H	-1.40630000	2.47341000	1.83392700
C	1.70568100	2.71090000	-0.36270100	H	-0.70773000	3.17559300	0.36395500
H	1.14629700	3.21966800	0.42624100	C	-3.38819800	0.43625700	0.53454200

H	-3.31882100	0.13539500	1.58402100	H	-2.52121000	2.08285300	1.15212000
H	-4.11998600	1.24615800	0.44508800	C	1.95056900	-1.45599600	-2.04565700
H	-3.74898800	-0.41951900	-0.04247400	H	1.55508300	-2.44742200	-1.80655600
C	1.63502100	2.14118800	-1.56151100	H	1.31830400	-1.00874300	-2.81856400
H	1.48287500	1.61011000	-2.50623200	H	2.96363700	-1.57373700	-2.44539700
H	0.79083500	2.81840500	-1.40681600	C	2.96050100	1.06365200	-1.08730000
H	2.54785000	2.74191400	-1.63792100	H	3.13516900	1.73745300	-0.24344700
C	3.43392000	0.18990700	-0.51819200	H	3.92845200	0.73248800	-1.47866500
H	4.18902800	0.98162900	-0.56645400	H	2.44351500	1.61556400	-1.87773800
H	3.71171100	-0.51146800	0.27367500	C	3.15734900	-1.26521000	0.58096000
H	3.43078100	-0.34376800	-1.47312200	H	4.09334100	-1.47694700	0.05198100
C	2.13671200	1.98922800	1.28615300	H	3.37142000	-0.63819200	1.45132800
H	2.39790400	1.36092300	2.14167900	H	2.73038400	-2.20806300	0.93446500
H	2.97118500	2.66471900	1.06988900				
H	1.26177000	2.58416300	1.55942900	3-TS			
				C	0.98203600	-2.04230300	-1.26572500
3b				H	1.66597900	-1.72043200	-2.04418800
C	-0.61426100	-2.58009000	0.59046600	C	1.50255600	-2.41094400	0.04854800
H	0.38351200	-2.99478500	0.48249500	H	2.57635000	-2.30378100	0.16480500
H	-1.10310500	-2.74935400	1.54458200	H	1.10691600	-3.33916400	0.45392700
C	-2.74354300	-1.83581500	-0.46908400	C	-0.40130400	-2.16820300	-1.52905900
H	-3.22616100	-1.83344800	0.50751500	H	-0.78306300	-1.92712300	-2.51707300
C	-3.47741700	-1.63054400	-1.57529000	C	-1.27490900	-2.37881200	-0.42541400
H	-3.03575400	-1.65882600	-2.56945800	H	-0.99929200	-3.04739200	0.38542800
H	-4.54864000	-1.46258700	-1.52556900	H	-2.34439700	-2.32749200	-0.60904100
P	-0.72801100	1.58810100	-0.42302700	P	-1.90066800	0.77781200	0.01933200
P	1.96901700	-0.39362600	-0.53197900	P	1.63952500	1.18829300	-0.16888300
C	0.12949200	0.86750500	2.58104500	C	0.13156700	-0.75296300	2.12248700
Rh	0.05723000	-0.14383300	0.79801800	C	1.04495700	-1.62722200	1.99790600
H	0.58865800	1.77811100	2.93448400	Rh	-0.03170300	-0.56287500	0.04201300
C	-0.67985600	-0.10261400	2.76366800	H	-0.39045700	-0.23029800	2.90905800
H	-1.33262400	-0.63581800	3.43639200	H	1.76224500	-2.27143800	2.47434800
C	-1.31713600	-2.13978300	-0.49157700	C	-2.65081300	0.93755300	-1.65719900
H	-0.83757600	-2.12986800	-1.46893900	H	-2.88483000	-0.05354400	-2.05571800
C	0.07400300	3.22759300	-0.16969400	H	-3.57127200	1.53012300	-1.61635600
H	1.11404500	3.21172200	-0.50314400	H	-1.94359300	1.42287600	-2.33627700
H	-0.46576100	3.99946400	-0.72977100	C	-1.78058600	2.53047100	0.58609200
H	0.05366000	3.48325900	0.89321700	H	-2.76296300	3.00968300	0.51433700
C	-0.83926400	1.43213200	-2.25623600	H	-1.45161500	2.56668800	1.62875400
H	-1.34927900	2.30789900	-2.67328300	H	-1.07428500	3.09763900	-0.02542800
H	0.15411700	1.36118200	-2.70742700	C	-3.29155000	0.15885400	1.06074800
H	-1.41115200	0.53668100	-2.51318600	H	-2.98136300	0.11684800	2.10891400
C	-2.47380500	1.88407400	0.07852700	H	-4.15880300	0.82249300	0.97468200
H	-2.88165800	2.74135700	-0.46931800	H	-3.58102900	-0.84819000	0.75213900
H	-3.07061800	0.99570700	-0.14281700	C	1.53091200	2.30111500	-1.64109900

H	1.59370900	1.70421500	-2.55624500	H	-2.21136500	3.18544800	1.28861100
H	0.57531400	2.83317200	-1.65050500	C	-0.06499700	3.01573900	-0.83580200
H	2.34218600	3.03733800	-1.64219500	H	0.28637300	2.79101900	-1.84702700
C	3.36882300	0.54506500	-0.30803100	H	-0.67137800	3.92763400	-0.86508500
H	4.08143000	1.37333000	-0.38427100	H	0.80250400	3.19844600	-0.19659300
H	3.61842100	-0.04641100	0.57815100	C	-2.55383800	1.68792700	-1.30298600
H	3.47537700	-0.08757900	-1.19408300	H	-2.98590700	2.69442600	-1.28251000
C	1.82094100	2.36288200	1.24642200	H	-2.26093100	1.44956900	-2.32995800
H	1.98970000	1.79419100	2.16598100	H	-3.31939600	0.97442100	-0.98567700
H	2.66990000	3.03576700	1.08511000				
H	0.91742200	2.96331900	1.37436600	4			
				C	1.93475100	-1.78212700	-0.66746300
3b-TS				H	2.73674900	-1.41082400	-1.30033800
C	-1.77433000	-2.05180700	-0.79040000	C	2.34852800	-2.20324500	0.73576500
H	-2.51091600	-1.81030300	-1.55174200	H	3.39146200	-1.90690200	0.90721400
H	-1.64466600	-3.11978300	-0.63479900	H	2.34514100	-3.30197900	0.79978600
C	-1.40123800	-1.88815700	1.70624400	C	0.79497600	-2.24506100	-1.35123800
H	-0.69074000	-2.71146600	1.62848000	H	0.78025100	-2.08773500	-2.43177300
C	-1.85770800	-1.53309200	2.91859000	C	-0.42990100	-2.57916200	-0.72889300
H	-2.59485500	-0.74410000	3.04907000	H	-0.45075900	-2.99629200	0.27348800
H	-1.52765900	-2.04092200	3.81916600	H	-1.27068300	-2.84423300	-1.36426900
P	1.99543100	0.17424500	0.40883600	P	-2.18684700	0.19136300	0.12609500
P	-1.07130800	1.60406900	-0.20393900	P	1.22382700	1.66458400	-0.09800300
C	0.93710200	-1.50635900	-1.93169700	C	0.46677100	-0.81247000	1.56811100
Rh	-0.04166300	-0.44894700	-0.47129900	C	1.48049400	-1.63305700	1.82964600
H	1.89993300	-1.50716300	-2.42213000	Rh	0.05793800	-0.40621700	-0.34160600
C	-0.14377500	-2.19784900	-2.00868100	H	-0.16900100	-0.35619600	2.32403300
H	-0.54467200	-3.03791100	-2.55420600	H	1.71005900	-1.90932800	2.86030900
C	-1.82697600	-1.27831100	0.44013600	C	-3.12183500	0.48777500	-1.43875700
H	-2.65221200	-0.57434600	0.51841700	H	-3.08068000	-0.40402000	-2.07132100
C	3.23573200	1.02599400	-0.65927500	H	-4.17058600	0.72068400	-1.22428800
H	2.86597800	2.00859800	-0.96480800	H	-2.68297900	1.32470500	-1.99121700
H	4.18217000	1.15495100	-0.12296800	C	-2.56905300	1.69252600	1.13209100
H	3.41723300	0.43587300	-1.56180600	H	-3.65218000	1.80630700	1.25078300
C	1.98397700	1.20015200	1.94379200	H	-2.11914700	1.60654000	2.12612200
H	2.99854300	1.28222100	2.34896400	H	-2.17684900	2.59098200	0.64668200
H	1.61176400	2.20836400	1.74227400	C	-3.16770900	-1.11033100	0.98671300
H	1.33860200	0.73157300	2.69261100	H	-2.71195900	-1.34070900	1.95446100
C	2.88470900	-1.34359900	0.96456100	H	-4.19772300	-0.77569400	1.14995400
H	3.84450400	-1.07951200	1.42247100	H	-3.17847300	-2.02490900	0.38832000
H	2.27561000	-1.87941200	1.69814600	C	0.69165900	2.91637700	-1.35014200
H	3.06205600	-2.00736600	0.11439600	H	0.82731500	2.51599900	-2.36006900
C	-1.69983600	2.22515800	1.41617100	H	-0.36592300	3.16362900	-1.21710000
H	-2.39956100	1.50663400	1.85098900	H	1.28089500	3.83527300	-1.25730800
H	-0.87093300	2.35624300	2.11681400	C	3.04935300	1.58615500	-0.35634800

H	3.49604300	2.58289500	-0.27353600	H	-2.59295100	2.65074800	-0.55009700
H	3.49934400	0.93309900	0.39689300	C	-3.29355500	-1.11406200	-1.01093400
H	3.27062800	1.17920400	-1.34713400	H	-4.36768500	-0.91687800	-0.92553300
C	1.10275400	2.56622300	1.50659300	H	-3.03544800	-1.19115900	-2.07222600
H	1.46494200	1.92113700	2.31223100	H	-3.07489100	-2.07452700	-0.53435200
H	1.71057400	3.47675900	1.48116700				
H	0.06687900	2.84057300	1.72132900	4-TS			
				C	2.68231200	0.18005700	-0.24660400
4b				H	3.00910400	1.21647900	-0.23733800
C	2.15419600	-2.26737800	-0.10892000	C	3.24660300	-0.69375300	0.85925700
H	2.23176500	-3.35722200	-0.24576000	H	3.45261400	-0.07635400	1.74316900
H	2.79228400	-2.04219400	0.75883200	H	4.22611000	-1.09672000	0.55253300
C	0.24869900	-2.04227600	1.57956000	C	2.07826900	-0.27925700	-1.41444900
H	0.90796500	-1.61708200	2.33746200	H	1.93095600	0.39740600	-2.25146700
C	-0.85387100	-2.69787100	1.97851700	C	1.50072400	-1.62005500	-1.46578500
H	-1.51744100	-3.18522900	1.26735900	H	2.14196800	-2.48604600	-1.34001700
H	-1.10538200	-2.80551700	3.02971200	H	0.75786700	-1.78779900	-2.24511400
P	1.25614400	1.39792800	0.54787600	P	-1.86372900	-1.06755800	0.03792700
P	-2.30391200	0.23208100	-0.21004300	P	-0.23047000	2.09130300	0.07081800
C	1.91175100	-0.42761800	-1.67200000	C	1.16943900	-2.02935900	0.55978100
Rh	0.17093100	-0.09878600	-0.72241100	C	2.31893900	-1.82891600	1.22151900
H	2.19111500	0.20509700	-2.51973300	Rh	0.34039700	-0.23141700	-0.10537600
C	2.61402100	-1.51685700	-1.32127600	H	0.56546100	-2.91996800	0.68896400
H	3.47502400	-1.87699600	-1.88585500	H	2.62025200	-2.49299300	2.03209100
C	0.69050200	-1.91581000	0.18169600	C	-2.98369200	-0.55836600	-1.33810400
H	0.02337900	-2.46234700	-0.51018500	H	-3.96975800	-1.02172100	-1.22343100
C	1.67287700	2.88033500	-0.46168900	H	-3.10370300	0.52642900	-1.35965200
H	0.77024400	3.29612100	-0.91948800	H	-2.55246600	-0.87475100	-2.29265700
H	2.13412000	3.64806700	0.16961300	C	-2.02873000	-2.90804500	-0.01822400
H	2.37152500	2.60183300	-1.25499000	H	-1.59061300	-3.36208700	0.87489300
C	0.29018500	2.06969200	1.96355100	H	-3.08735200	-3.18538700	-0.05922500
H	0.89622700	2.79780200	2.51473700	H	-1.52589900	-3.31351800	-0.90130900
H	-0.61478300	2.56539200	1.60310200	C	-2.81435500	-0.66187200	1.56957300
H	0.00361300	1.26119600	2.64174200	H	-3.81488100	-1.10665000	1.53517700
C	2.84798400	0.90906500	1.32445300	H	-2.28225200	-1.05473400	2.44153600
H	3.28302200	1.77384200	1.83716100	H	-2.91506100	0.41987600	1.69098700
H	2.68395200	0.11550000	2.05847100	C	0.20305000	2.69782700	1.76221700
H	3.53679200	0.54777500	0.55882300	H	1.24293700	2.44864000	1.99220400
C	-3.03661000	0.30276800	1.48564500	H	0.07159800	3.78300400	1.83353400
H	-2.72908900	-0.57950000	2.05392600	H	-0.43466200	2.21349300	2.50778600
H	-2.68366200	1.19249800	2.01509000	C	-1.92197200	2.79948800	-0.17918300
H	-4.13025800	0.33660600	1.43569700	H	-2.23469400	2.66686800	-1.21917400
C	-3.00807300	1.74862000	-1.01113200	H	-2.65545700	2.31663700	0.47178500
H	-2.75486900	1.76201500	-2.07623300	H	-1.91510700	3.87166900	0.04574300
H	-4.09856600	1.77775600	-0.91110900	C	0.76099700	3.19022900	-1.03776500

H	0.54819600	4.24264200	-0.82100700	H	-0.13875300	3.32672000	-1.55153800
H	1.83098100	3.01626100	-0.89911300				
H	0.50948700	2.98903100	-2.08357800	6			
5				C	-0.66751900	-1.25526400	-0.00010700
C	2.26691500	1.22467400	0.65479200	H	-1.20733800	-2.20124200	-0.00046500
H	2.03486100	2.14620700	1.18139600	C	-1.50094400	0.00000000	0.00019100
C	2.79685400	0.03960700	1.44219800	H	-2.17782700	0.00000000	0.87145900
H	2.43950000	0.06781600	2.47515200	H	-2.17872900	0.00000000	-0.87037900
H	3.89949600	0.04028700	1.48348700	C	0.66751900	-1.25526400	-0.00010900
C	2.26650800	1.18563700	-0.72161700	H	1.20733900	-2.20124000	-0.00046700
H	2.03211400	2.07527100	-1.29781400	C	1.50094400	0.00000000	0.00019100
C	2.79707700	-0.04127200	-1.44204200	H	2.17873400	0.00000000	-0.87037400
H	3.89973000	-0.04219300	-1.48311100	H	2.17782200	0.00000000	0.87146400
H	2.43993200	-0.06940700	-2.47506900	C	0.66751900	1.25526400	-0.00010900
P	-1.16970400	-1.73069000	0.00174600	C	-0.66751900	1.25526400	-0.00010700
P	-1.16842300	1.73139800	-0.00180700	H	1.20733900	2.20124000	-0.00046800
C	2.26673800	-1.22620600	-0.65470700	H	-1.20733800	2.20124100	-0.00046500
C	2.26610000	-1.18715400	0.72166300	7			
Rh	0.40797600	-0.00013600	-0.00012800	C	-1.60146000	-2.12027300	0.20317600
H	2.03430600	-2.14762600	-1.18133800	C	-2.17805700	-1.36514300	-0.81535000
H	2.03116600	-2.07668500	1.29780500	H	-1.93650800	-1.50795300	-1.86383900
C	-1.88617800	-2.10797100	-1.65927500	C	-0.26152200	-2.65684400	0.00933100
H	-2.55111900	-2.97708100	-1.60484200	H	0.22309500	-3.12022400	0.86507400
H	-2.45134600	-1.25274600	-2.03862900	C	0.45030200	-2.45790700	-1.16887200
H	-1.07921400	-2.32198200	-2.36631900	H	-0.02898600	-2.31383400	-2.13234900
C	-0.47484500	-3.36685100	0.50857500	H	1.48393700	-2.78142900	-1.21473100
H	-0.13939800	-3.32779600	1.54924500	Rh	-0.12359400	-0.46723900	-0.20826200
H	-1.23846200	-4.14674100	0.41745000	P	2.10199900	0.17503800	0.16222400
H	0.37596700	-3.63827300	-0.12300500	P	-1.11964000	1.69014700	-0.02444200
C	-2.65481900	-1.62704200	1.09719200	C	-1.82989400	2.19251400	-1.65472400
H	-3.25793500	-2.53703100	1.00745800	H	-2.50331800	1.41691500	-2.02845000
H	-2.33703300	-1.51672700	2.13851500	H	-2.38437600	3.13275600	-1.56080400
H	-3.28084800	-0.77035800	0.83472100	H	-1.02572800	2.32707300	-2.38427600
C	-1.88267000	2.11014200	1.65983400	C	-2.56886900	1.74079700	1.12107400
H	-1.07472800	2.32407700	2.36578500	H	-3.03703400	2.73103500	1.10057200
H	-2.54715000	2.97962200	1.60567900	H	-3.31248500	0.99416300	0.83265800
H	-2.44788400	1.25546900	2.04036700	H	-2.24087700	1.52528600	2.14248200
C	-2.65491400	1.62830200	-1.09540500	C	-0.22703100	3.22655200	0.49046100
H	-2.33848200	1.51714500	-2.13705200	H	0.66459600	3.39147700	-0.11985500
H	-3.28131100	0.77228100	-0.83166400	H	-0.88842600	4.09230300	0.37675000
H	-3.25718600	2.53882800	-1.00546200	H	0.07145800	3.15939000	1.54047400
C	-0.47285300	3.36669200	-0.51046800	C	2.43301200	1.00509900	1.77853700
H	-1.23568700	4.14729000	-0.41885000	H	1.87255400	1.93817300	1.85900400
H	0.37899300	3.63778600	0.11985700	H	2.12536200	0.34672000	2.59653600

H	3.50103600	1.22559800	1.88348900	H	3.01203400	-1.49497000	-1.69022300
C	3.33818400	-1.19861800	0.20576000	H	4.24708200	-0.31198500	-1.20907000
H	3.42515200	-1.66775200	-0.77802000	C	-0.51311900	3.08182000	0.58917900
H	4.32097400	-0.80799100	0.49072800	H	-0.23345500	2.98486000	1.64230400
H	3.03958700	-1.95854900	0.93408100	H	0.38733600	3.32608400	0.01877500
C	2.85206500	1.31188700	-1.08669800	H	-1.21880000	3.91316900	0.48801600
H	3.89274100	1.53794000	-0.82987200	C	-2.92537400	1.56087300	0.79714600
H	2.82579000	0.83910100	-2.07322600	H	-3.39107800	2.54292900	0.66278600
H	2.29284700	2.24936200	-1.14454700	H	-3.58773200	0.80373300	0.36883300
C	-2.26020400	-2.30076500	1.54577300	H	-2.82828400	1.35854800	1.86768600
H	-3.05007600	-1.56368500	1.71197000	C	-1.72394500	1.98056200	-1.76379700
H	-2.72263800	-3.29592600	1.58814600	H	-2.34674100	1.20331000	-2.21344100
H	-1.53787100	-2.23832500	2.36584200	H	-2.28102000	2.92377500	-1.77132900
H	-3.12361100	-0.86743200	-0.62356300	H	-0.82780700	2.09542300	-2.37823600
				H	1.62388000	-1.54603300	2.66275700
8a							
C	-0.21797000	-2.33850400	-0.96754400	8b			
C	0.66584400	-2.65184700	0.09506700	C	-0.80599200	-2.22495600	0.80771300
H	1.70510900	-2.84782000	-0.14381000	C	-1.62381900	-2.08682900	-0.35001800
H	0.30301300	-3.18077600	0.97131300	H	-2.66609100	-1.81913600	-0.20707200
C	-1.56269000	-1.94096600	-0.66645600	H	-1.44411300	-2.70526000	-1.22407100
C	-1.89385400	-1.78791500	0.70336100	C	0.59466600	-2.41388600	0.56092700
H	-1.51619600	-2.46735300	1.45987700	C	1.09604200	-2.43216100	-0.75799100
H	-2.85093600	-1.33806100	0.95064600	H	0.54015600	-2.88032500	-1.57450500
P	-1.27140000	1.51066400	-0.03181000	H	2.17051500	-2.41907100	-0.90425800
P	2.02336800	0.39100000	-0.46026100	P	1.92389600	0.68209200	0.36251200
C	0.03966000	0.09434800	2.65413500	P	-1.54480500	1.26496800	0.19125700
C	0.87192400	-0.79749100	2.53157200	C	0.42337600	0.30839700	-2.60682400
Rh	-0.05275700	-0.54655500	0.32047100	C	-0.64850300	-0.28774100	-2.68648600
H	-0.61066300	0.84417800	3.05194200	Rh	-0.03422400	-0.51248300	-0.41311300
C	-2.53158200	-1.63229300	-1.77682200	H	-1.55972200	-0.74105800	-3.01558900
H	-2.02840600	-1.27324600	-2.67975700	H	1.27128000	-2.39800500	1.41219900
H	-3.06840200	-2.55284100	-2.04091100	C	-1.34524000	-2.15661500	2.21269800
H	-3.28604700	-0.90296200	-1.46926300	H	-2.25256900	-1.54769400	2.26676300
H	0.11800200	-2.31840500	-2.00095500	H	-1.61746800	-3.16577400	2.54856800
C	2.01625000	1.42152400	-1.99741200	H	-0.60996900	-1.75813800	2.91881700
H	1.42827700	2.33197500	-1.85600200	C	2.10729800	2.48715500	-0.00382000
H	3.03680600	1.71128000	-2.27021800	H	1.33076800	3.06552000	0.50377500
H	1.57853700	0.85165700	-2.82277200	H	3.08320700	2.84710000	0.33889800
C	2.91068100	1.47470000	0.74622200	H	2.02556000	2.67080000	-1.07937300
H	3.85287200	1.83531800	0.32006400	C	3.52403700	0.02200000	-0.29011100
H	2.29249400	2.33386400	1.01839200	H	3.52305900	0.02159200	-1.38419100
H	3.12579100	0.91361800	1.65968400	H	4.36162800	0.63237700	0.06386800
C	3.34219200	-0.83516200	-0.88238600	H	3.67895000	-1.00536200	0.05099100
H	3.59076600	-1.44712900	-0.01082800	C	2.22432900	0.63356900	2.18822500

H	2.34340300	-0.40301400	2.51705900	C	-3.38933500	-0.37943700	0.61513900
H	3.13182100	1.18849100	2.45026500	H	-3.61467700	-0.83686900	-0.35293900
H	1.37637000	1.06484800	2.72671500	H	-3.19595200	-1.17350900	1.34237300
C	-1.52116900	2.74885000	-0.91105400	H	-4.26744400	0.18696900	0.94310800
H	-0.53996100	3.22982700	-0.90119900	C	0.90629700	3.05954600	-0.36466200
H	-1.73885700	2.44527800	-1.93854600	H	0.47976600	3.12515100	-1.36979400
H	-2.27321300	3.47634500	-0.58770900	H	0.13527500	3.32906600	0.36147700
C	-3.33923500	0.82138700	0.13686500	H	1.72397400	3.78377200	-0.28430800
H	-3.95051000	1.70210900	0.36039100	C	3.00081400	1.30265200	-1.18196900
H	-3.60660600	0.45268000	-0.85769800	H	3.64120900	2.17685300	-1.02214500
H	-3.57194200	0.04417900	0.87017500	H	3.58660800	0.39692500	-1.00907400
C	-1.40695800	2.00417000	1.88178000	H	2.66307200	1.29477500	-2.22237700
H	-2.20617500	2.73318300	2.05377800	C	2.31763000	1.52360500	1.61742800
H	-1.47924500	1.21630900	2.63774100	H	2.90085500	0.62936800	1.85306400
H	-0.44595700	2.51107500	2.00564800	H	2.98354000	2.39313500	1.64643300
H	1.30640600	0.85689400	-2.85931400	H	1.54411200	1.64023900	2.38199300
				H	-1.51436700	-1.88534300	-2.99173500

8a-TS

C	-0.37819200	-2.37234200	0.63977700
C	-0.93989200	-2.52708800	-0.69976600
H	-2.01453600	-2.67648900	-0.72882300
H	-0.38678400	-3.19474400	-1.35588400
C	1.01976100	-2.21927900	0.82188100
C	1.76261500	-1.90472200	-0.35977800
H	1.55828700	-2.41249900	-1.29879100
H	2.80757200	-1.63302700	-0.23287100
P	1.54480500	1.35634600	-0.04979900
P	-1.92004600	0.73388800	0.45734600
C	-0.24993900	-0.13401200	-2.33813100
C	-0.91634000	-1.21276200	-2.40329000
Rh	0.09603300	-0.41603200	-0.28713600
H	0.04785400	0.67889000	-2.98215700
C	1.64115600	-2.26572100	2.19323300
H	0.94098700	-1.95877100	2.97611100
H	1.95641600	-3.29431000	2.41178300
H	2.53616600	-1.64020200	2.25365900
H	-1.03549900	-2.43962500	1.50179700
C	-1.88172300	1.53828500	2.12281300
H	-1.12242300	2.32538500	2.15340100
H	-2.85244700	1.98146500	2.37069400
H	-1.62831400	0.79329000	2.88354600
C	-2.61077900	2.05807900	-0.63409300
H	-3.57479300	2.41100800	-0.25230900
H	-1.92843100	2.90888300	-0.69788100
H	-2.75535100	1.65729700	-1.64194000

8b-TS

C	1.39452600	-1.93677200	-0.73561400
C	1.82537200	-1.90134400	0.67345100
H	2.84736100	-1.56414900	0.82313400
H	1.58305500	-2.79859000	1.23932100
C	0.07679300	-2.37501700	-0.99586300
C	-0.83091900	-2.51310100	0.09892000
H	-0.50625100	-2.96166900	1.03464900
H	-1.87254300	-2.71508900	-0.13609800
P	-2.13738700	0.35788100	-0.21449800
P	1.25766700	1.59750400	-0.13399200
C	-0.02446200	-0.22260300	2.29967400
C	1.05932900	-0.88399600	2.38091500
Rh	-0.03049500	-0.45661000	0.22071400
H	1.85156600	-1.25076300	3.00935700
H	-0.26644300	-2.43928500	-2.02566100
C	2.38680500	-1.70400100	-1.84952400
H	3.07522700	-0.88494100	-1.62531900
H	2.99869100	-2.60347900	-1.99723700
H	1.88257900	-1.48463000	-2.79545800
C	-2.45224000	2.17450500	-0.26637400
H	-1.82079700	2.65925400	-1.01550800
H	-3.50083900	2.35939800	-0.52355200
H	-2.25056400	2.61947700	0.71162600
C	-3.43122600	-0.20050600	0.97622400
H	-3.20589300	0.18485100	1.97509700
H	-4.41809600	0.16449500	0.67177600

H	-3.45392000	-1.29159400	1.02981200	H	0.66595600	3.24013900	-1.05377000
C	-2.78923300	-0.19316900	-1.85061500	H	-0.72946700	2.72349300	-2.02249600
H	-2.79416500	-1.28457900	-1.91333400	C	-2.75164800	2.07933500	0.26235800
H	-3.81194300	0.17076500	-1.99832200	H	-3.15487700	1.67152700	-0.66912100
H	-2.15437100	0.19666200	-2.65187400	H	-3.18312700	1.52497300	1.10069900
C	0.80281600	3.08694500	0.86591500	H	-3.04301700	3.13205600	0.34504400
H	-0.16938300	3.48309400	0.56740600	C	2.98855900	1.59121300	-0.56338500
H	0.75813500	2.81532300	1.92518300	H	2.63712100	1.89152000	-1.55514600
H	1.55193400	3.87556000	0.73782900	H	2.69588700	2.35937700	0.15876500
C	3.03716100	1.43451600	0.34881900	H	4.08213800	1.53245100	-0.58635900
H	3.55681400	2.38944800	0.21701700	C	3.05818200	-1.18219000	-1.30859700
H	3.10197100	1.14215400	1.40118000	H	4.14209800	-1.02740600	-1.33477500
H	3.54577400	0.67839700	-0.25433100	H	2.85040400	-2.21941700	-1.03334700
C	1.37272000	2.27362600	-1.85209000	H	2.65121100	-1.00722000	-2.30893900
H	2.02705700	3.15134600	-1.89042700	C	3.13202800	-0.42753000	1.49009900
H	1.76906700	1.50655500	-2.52423100	H	2.89825300	-1.44861600	1.80483800
H	0.38069500	2.56035100	-2.21483000	H	4.21700800	-0.33554900	1.36842000
H	-0.70129200	0.30382200	2.95501700	H	2.80934200	0.26018800	2.27822400
				H	-1.73500800	-0.88776800	-3.36704200
9a							
C	-2.13969500	-1.40595600	0.11075700	9b			
C	-2.52777800	-1.50060200	-1.36177800	C	2.20195000	-1.47392300	-0.34662800
H	-3.51004100	-1.03067300	-1.50100600	C	2.36982800	-1.85619900	1.12159700
H	-2.67014200	-2.55608800	-1.63869900	H	3.33543800	-1.47621400	1.48002200
C	-1.15267400	-2.19560200	0.74958300	H	2.45045500	-2.95259600	1.18839200
C	0.02060100	-2.58146500	0.05417400	C	1.18351700	-1.99601200	-1.15102400
H	-0.00314900	-2.76887100	-1.01489400	C	-0.07167400	-2.48523100	-0.68514200
H	0.79193200	-3.11609000	0.60359600	H	-0.14948500	-2.96633800	0.28588800
P	2.26400100	-0.04289800	-0.09592800	H	-0.76575900	-2.85767500	-1.43489700
P	-0.91440000	1.90681400	0.26604500	P	-2.36652800	-0.18974300	-0.02681900
C	-0.42925400	-0.27701500	-1.83318200	P	0.77410600	1.94450600	0.00549800
C	-1.53113400	-0.86184500	-2.29512600	C	0.21306500	-0.69926800	1.66938000
Rh	-0.09051900	-0.33074300	0.13188300	C	1.28599800	-1.38216700	2.05896000
H	0.31809200	0.21271400	-2.45389700	Rh	-0.03272100	-0.32889900	-0.26796500
C	-1.21670100	-2.38000100	2.25291900	H	1.42159400	-1.61006700	3.11803900
H	-1.82164700	-1.60794100	2.73942300	H	1.28458600	-1.83127800	-2.22577300
H	-1.68729300	-3.34736600	2.47129100	C	3.43187900	-0.90082900	-1.01055100
H	-0.22261100	-2.39719300	2.71277400	H	3.81173500	-0.02102700	-0.48045600
H	-2.91952800	-1.02461700	0.76638600	H	4.24183300	-1.64438500	-0.99134100
C	-0.42787900	2.75353900	1.83668900	H	3.25404500	-0.63143800	-2.05604400
H	0.66074600	2.84722300	1.89911800	C	-3.10071300	1.02001600	1.15813200
H	-0.87000200	3.75435900	1.89175800	H	-2.86137900	2.04356500	0.86226800
H	-0.77298600	2.17175000	2.69744500	H	-4.18991200	0.90716900	1.18425900
C	-0.41827400	3.10491300	-1.04560600	H	-2.71105100	0.84894300	2.16649200
H	-0.89397400	4.07698800	-0.87821300	C	-3.19308900	-1.75959600	0.47274700

H	-2.80421900	-2.08795800	1.44128200	H	0.65462500	-0.63809300	-3.02166000		
H	-4.27602400	-1.61770000	0.55410600	C	2.87895200	-1.72560700	1.82552900		
H	-2.98893800	-2.54272400	-0.26152500	H	3.23418000	-1.94361600	2.84024900		
C	-3.17179400	0.24105100	-1.63187400	H	2.92603100	-2.65647300	1.25071200		
H	-2.90782600	-0.49776100	-2.39490300	H	3.57104300	-1.00957000	1.37032800		
H	-4.26181900	0.25937900	-1.52343500	C	0.17749600	2.96588200	-1.19588200		
H	-2.83611600	1.22579700	-1.97145500	H	-0.81936100	3.15021100	-0.78735300		
C	-0.36634900	3.32047800	0.48184100	H	0.73552400	3.90846500	-1.18601100		
H	-1.18403700	3.40658900	-0.24033600	H	0.06774300	2.63210500	-2.23231000		
H	-0.78950700	3.13529900	1.47328600	C	1.31233200	2.48928900	1.42118600		
H	0.17499000	4.27246900	0.50689400	H	1.76878600	3.47644600	1.29355600		
C	2.14618900	2.17108200	1.21800400	H	0.35888000	2.60535700	1.94230600		
H	2.46898400	3.21705500	1.24794700	H	1.96385900	1.87184900	2.04503700		
H	1.80979200	1.86765300	2.21311300	C	2.76070700	1.79686500	-0.94564600		
H	2.99944500	1.54534500	0.94465700	H	3.45874000	1.15652000	-0.39927200		
C	1.48638400	2.58248800	-1.57884800	H	2.75119500	1.48689700	-1.99476000		
H	1.88286300	3.59558800	-1.44934200	H	3.11711500	2.83107000	-0.89179600		
H	2.29362700	1.92841100	-1.92016700	C	-2.37536000	1.60791100	1.50254100		
H	0.71348100	2.60699900	-2.35413600	H	-1.94719000	1.34186000	2.47385000		
H	-0.54915900	-0.33544000	2.35582700	H	-1.91004900	2.53900100	1.16774900		
propyne				H	-3.44739300	1.78773400	1.63527600		
				C	-3.23747700	-1.05255300	0.93347300		
	C	0.00000000	0.00000000	0.21901200	H	-4.21707800	-0.62245700	1.16775500	
	C	0.00000000	0.00000000	1.42629700	H	-3.37730300	-1.84536200	0.19348100	
	H	0.00000000	0.00000000	2.49220100	H	-2.82044300	-1.50150400	1.84000400	
	C	0.00000000	0.00000000	-1.24156000	C	-3.04455800	0.86400600	-1.19254800	
	H	0.00000000	1.02249600	-1.63823300	H	-3.09889400	0.08051300	-1.95425300	
	H	0.88550800	-0.51124800	-1.63823300	H	-4.06421900	1.14741600	-0.90958500	
H	-0.88550800	-0.51124800	-1.63823300	H	-2.54564400	1.73121600	-1.63348700		
11a				H	-1.43250700	-1.77598600	-2.28822600		
	C	0.68184400	-1.29402900	-2.15645700	11b				
	C	1.83500400	-1.42200700	-1.34360200		C	0.69265900	-1.84815000	-1.87874900
	H	2.71025600	-0.83087100	-1.58923500		C	1.34000100	-2.38991900	-0.74575400
	H	2.05870700	-2.36894000	-0.86359900		H	2.42079600	-2.32416900	-0.68787200
	C	-0.51379500	-1.95933600	-1.73763700		H	0.91155700	-3.23168600	-0.21074300
	C	-0.52517000	-2.67833100	-0.52503900		C	-0.73928400	-1.79034100	-1.88486800
	H	0.34111500	-3.23683600	-0.18759500		C	-1.45837700	-2.23741600	-0.75977100
	H	-1.47161400	-3.04905700	-0.14665500		H	-1.11962800	-3.07797700	-0.16365400
P	-2.09979700	0.24918000	0.27472600	H	-2.52671600	-2.05375600	-0.71745600		
P	1.06564800	1.67130600	-0.21690300	P	-1.53541100	1.16999300	-0.39822200		
C	0.38836700	-0.79127900	2.17459000	P	1.90159400	0.83850600	0.15976300		
C	1.51528500	-1.19941400	1.89808600	C	-0.67785500	-1.08491100	2.39815400		
Rh	0.13907400	-0.53640200	-0.15037400	C	0.45045900	-1.44732700	2.09110200		
H	-0.43399000	-0.54546300	2.81343100	Rh	0.04183500	-0.63852000	-0.15155000		

H	1.42434800	-1.88315700	2.15185700	Rh	0.05486600	-0.42273500	-0.20381500
H	-1.23922900	-1.27567300	-2.70089200	H	0.13803600	-0.77238100	2.64186300
C	-1.99127400	-0.76438800	2.95528900	H	1.74203900	-0.32144300	-2.60548900
H	-2.20580200	0.30836600	2.91314700	C	3.19731200	-1.69988300	1.88012900
H	-2.78981800	-1.29867200	2.42992400	H	3.15063500	-1.84580300	2.96532300
H	-2.02199100	-1.06733700	4.00906400	H	3.50544700	-2.64729300	1.42415200
C	-1.47258900	2.63589500	0.73056100	H	3.97769800	-0.95841800	1.67189400
H	-0.53135000	3.17826200	0.60505900	C	-0.14384500	3.08259500	-1.26430900
H	-2.29750800	3.32336500	0.51495400	H	-1.20789600	3.12469500	-1.01347700
H	-1.54432700	2.31575200	1.77422500	H	0.27343100	4.09250100	-1.18443000
C	-3.32249800	0.70083700	-0.28648800	H	-0.05348400	2.74452000	-2.30133400
H	-3.54902700	0.25803800	0.68643200	C	0.72464500	2.77775700	1.48265800
H	-3.95608800	1.58267400	-0.42993600	H	1.14867100	3.78353900	1.39083400
H	-3.56902200	-0.02964300	-1.06222900	H	-0.29455400	2.86203700	1.86727600
C	-1.49912500	1.96990500	-2.06726600	H	1.31768800	2.20834200	2.20458600
H	-1.71926200	1.22333200	-2.83608600	C	2.50570100	2.18090600	-0.65717400
H	-2.24446600	2.77013900	-2.13418100	H	3.17868800	1.64158500	0.01613300
H	-0.51069200	2.38590100	-2.27551500	H	2.67310300	1.82488300	-1.67818100
C	2.00882200	1.66009500	1.81275400	H	2.75455900	3.24683400	-0.61491600
H	1.14102000	2.30231300	1.98227100	C	-2.66074500	1.34604700	1.32564700
H	2.02488100	0.90309000	2.60139700	H	-2.13032300	1.35818700	2.28213500
H	2.91712500	2.26826700	1.88149800	H	-2.43651400	2.27090200	0.78820600
C	3.56263100	0.03271700	0.04802500	H	-3.73761700	1.31261300	1.52274500
H	4.34896300	0.76403600	0.26277200	C	-2.89309500	-1.49995200	1.33055300
H	3.64259700	-0.78652700	0.76831100	H	-3.95258000	-1.30482800	1.52869500
H	3.72756000	-0.36893200	-0.95596200	H	-2.79827600	-2.44854200	0.79687600
C	2.12667800	2.25660500	-1.00783000	H	-2.36562400	-1.59304700	2.28438900
H	3.05957800	2.78767500	-0.78991800	C	-3.25313900	-0.02911300	-1.14033600
H	2.16312500	1.88933600	-2.03806500	H	-3.14221300	-0.93092700	-1.74875400
H	1.29954500	2.96648600	-0.92306000	H	-4.30257900	0.06802200	-0.84118200
H	1.24701600	-1.38518900	-2.68963400	H	-2.97442500	0.83401600	-1.75194500
				H	-0.44370900	-1.48399400	-2.96596100

11a-TS

C	1.37749100	-1.04104400	-1.87951400
C	2.20506900	-1.37721600	-0.71832200
H	3.15057600	-0.84638800	-0.67337700
H	2.29356600	-2.44510900	-0.53192800
C	0.15114400	-1.70954200	-2.08500100
C	-0.37858000	-2.47278200	-1.00523200
H	0.26982000	-3.09620000	-0.39503100
H	-1.38866800	-2.85971000	-1.10793000
P	-2.15654400	-0.12985900	0.33890600
P	0.74716200	1.90580900	-0.14799600
C	0.68882100	-0.87720500	1.71849200
C	1.86693100	-1.25303200	1.40188600

11b-TS

C	1.01672500	-1.93950500	-1.50813300
C	1.55037200	-2.36839500	-0.21364900
H	2.62302600	-2.24869400	-0.10175100
H	1.18413900	-3.33190400	0.13268400
C	-0.36483100	-2.06860900	-1.76129600
C	-1.22098200	-2.35763500	-0.65648400
H	-0.92948600	-3.08578800	0.09571900
H	-2.29315600	-2.31007800	-0.82473200
P	-1.87253800	0.78309500	-0.19087800
P	1.65848100	1.20526100	-0.19552900
C	0.16304200	-0.87960800	2.00576800

C	1.10265000	-1.69833700	1.73712500	C	0.85376200	-0.76951500	1.16671800
Rh	-0.00517700	-0.56582000	-0.09367300	C	2.09584800	-1.25444000	1.13149300
H	1.86198600	-2.33093300	2.16276900	Rh	-0.02798700	-0.21828600	-0.53977000
H	-0.76318300	-1.77593500	-2.72888400	H	0.26185800	-0.66807800	2.07464400
C	-0.55311900	-0.30635900	3.17895900	H	2.56642500	-0.12186100	-2.03347600
H	-0.59203100	0.78659400	3.12989100	C	2.82002400	-1.74619600	2.36346600
H	-1.58485400	-0.67296500	3.21283500	H	2.21100000	-1.63616700	3.26550600
H	-0.06472600	-0.59237300	4.11733500	H	3.08863300	-2.80568300	2.26239300
C	-1.79174700	2.52529700	0.41902300	H	3.75647800	-1.19272900	2.51379500
H	-1.04616700	3.10333300	-0.13272900	C	-0.54163300	3.25110400	-0.92516000
H	-2.76722200	3.00608300	0.28872200	H	-1.59030900	3.13624000	-0.63419500
H	-1.53460300	2.54404800	1.48200300	H	-0.23006600	4.27957300	-0.71256400
C	-3.36637300	0.16713200	0.70224900	H	-0.46280400	3.07898200	-2.00343600
H	-3.18337100	0.16031000	1.77987000	C	0.39909100	2.59630300	1.74409300
H	-4.22399500	0.81684600	0.49640400	H	0.70564600	3.64361700	1.83671500
H	-3.60761900	-0.85092200	0.38906400	H	-0.62377400	2.49513700	2.11577400
C	-2.48540300	0.99285300	-1.91931700	H	1.05580700	1.97923600	2.36403500
H	-2.71495800	0.01542500	-2.35318800	C	2.22450600	2.57493700	-0.46653900
H	-3.39076900	1.60931500	-1.93844900	H	2.95527700	1.96935700	0.07712600
H	-1.71544800	1.46933900	-2.53336100	H	2.38717900	2.43589700	-1.53914500
C	1.79177400	2.35284600	1.24839800	H	2.38210300	3.62987200	-0.21728800
H	0.87818600	2.93998100	1.36798400	C	-2.86065600	0.68443300	1.62378600
H	1.94947800	1.76870400	2.16019400	H	-2.24922700	0.60501100	2.52800400
H	2.63539600	3.03952800	1.12012200	H	-2.82733000	1.71887600	1.26925300
C	3.39441000	0.57263000	-0.29488100	H	-3.89599500	0.43736400	1.88272800
H	4.10539900	1.40553300	-0.31206000	C	-2.58771000	-2.11709600	1.05624600
H	3.61383100	-0.05378000	0.57493200	H	-3.62396200	-2.16820200	1.40714800
H	3.53600400	-0.02256700	-1.20203200	H	-2.42369800	-2.89744800	0.30872500
C	1.60067200	2.35196100	-1.64563300	H	-1.91755700	-2.30651700	1.90020400
H	2.42325000	3.07479600	-1.61291900	C	-3.47526100	-0.29843900	-1.02477300
H	1.67613900	1.77236000	-2.57093000	H	-3.28103200	-1.04021600	-1.80539000
H	0.65513300	2.90131600	-1.66768900	H	-4.48763100	-0.45229100	-0.63532100
H	1.69031800	-1.56662400	-2.27318700	H	-3.42009400	0.69823100	-1.47400900
				H	0.72313000	-1.22343000	-3.01867900
12a							
C	2.04896000	-0.83205300	-1.39356700	12b			
C	2.83807500	-1.31982000	-0.18719500	C	1.94881200	-1.59210500	-0.97926800
H	3.76483600	-0.73597600	-0.10524400	C	2.57996700	-2.04044500	0.32907300
H	3.16645000	-2.35556500	-0.36529000	H	3.59693200	-1.63180700	0.39601900
C	0.99246600	-1.53446300	-2.00728600	H	2.70951700	-3.13353500	0.31791900
C	0.07011300	-2.34686800	-1.31161700	C	0.77465300	-2.13852800	-1.54501400
H	0.36835200	-2.89371500	-0.42227800	C	-0.33414600	-2.59673100	-0.80708300
H	-0.76278500	-2.76974900	-1.86689000	H	-0.21413500	-3.03756000	0.17760300
P	-2.22452800	-0.46439600	0.32499000	H	-1.22412600	-2.89690000	-1.35292600
P	0.51766100	2.04144900	-0.01173400	P	-2.23063600	0.14545300	0.00783900

P	1.17565100	1.71016300	-0.14408600	P	-1.75861600	1.04010700	0.50829800
C	0.68027400	-0.89873000	1.49096300	P	1.49056600	1.19426400	-0.77963200
C	1.79106800	-1.63694300	1.54304200	C	0.51486700	-0.46420100	2.44046500
Rh	0.07482700	-0.39156500	-0.37730400	C	1.64100000	-0.88973600	2.21824400
H	2.15503400	-1.97669000	2.51512500	Rh	0.01775600	-0.51132600	0.04926000
H	0.61549200	-1.94243000	-2.60762500	H	-0.33686800	-0.16010300	3.00939700
C	-0.14763900	-0.50253700	2.67745500	C	-2.38095300	-1.90697900	-1.88838500
H	-0.32441600	0.57632400	2.72985300	H	-2.19112500	-1.20275300	-2.70435300
H	-1.12412200	-0.99978600	2.67980200	H	-2.65739200	-2.86969100	-2.33812100
H	0.37002100	-0.79942200	3.59912900	H	-3.24585300	-1.56612100	-1.31220500
C	-2.77794500	1.62843700	0.96529000	H	0.24915800	-1.67656800	-2.61413500
H	-2.35016000	2.53695100	0.53145500	C	3.00388000	-1.40257600	2.09847700
H	-3.86959500	1.71511400	0.94374600	H	3.44370200	-1.49707400	3.09894500
H	-2.45538400	1.55272800	2.00743100	H	3.02579100	-2.39116200	1.62880500
C	-3.33772300	-1.17745300	0.66599900	H	3.64437700	-0.73210000	1.51549900
H	-3.08135500	-1.41493400	1.70199800	C	0.79831500	2.44502700	-1.95429000
H	-4.38354700	-0.85345500	0.63020500	H	0.05510000	3.07724500	-1.46120800
H	-3.22455100	-2.08569800	0.06859900	H	1.59297000	3.08965700	-2.34501900
C	-2.95144600	0.46973700	-1.66650600	H	0.31439000	1.93114000	-2.79037700
H	-2.83618900	-0.41374400	-2.30211100	C	2.32802500	2.25620700	0.48180000
H	-4.01805100	0.70771700	-1.58881000	H	2.98503700	2.98731800	-0.00147900
H	-2.44106800	1.31032400	-2.14700500	H	1.59150500	2.78796000	1.08871900
C	0.87209300	2.77196200	1.33530300	H	2.92571700	1.63424300	1.15331900
H	-0.19461000	2.97393800	1.45965600	C	2.94211800	0.59136600	-1.75720300
H	1.23838000	2.26738700	2.23400800	H	3.57809000	-0.05370700	-1.14454900
H	1.40269700	3.72445000	1.23065600	H	2.60876000	0.02243600	-2.63019100
C	3.01931200	1.65731600	-0.18418500	H	3.54052100	1.44067300	-2.10416800
H	3.43740700	2.66430400	-0.07997600	C	-1.32168900	2.58790100	1.42658200
H	3.38375600	1.03427800	0.63762200	H	-0.75905200	2.34238300	2.33226900
H	3.36340600	1.22625900	-1.12828800	H	-0.70224800	3.24234500	0.80711500
C	0.76101400	2.83031800	-1.55643700	H	-2.22517400	3.13807800	1.70958400
H	1.34209700	3.75730000	-1.49912800	C	-3.10852900	0.36674700	1.58223700
H	0.98515500	2.33585700	-2.50693800	H	-3.84085600	1.14926600	1.80764900
H	-0.30334200	3.08552200	-1.54219100	H	-3.62451400	-0.45333500	1.07558700
H	2.63254500	-1.14207700	-1.69524200	H	-2.70608800	-0.01681000	2.52453700
				C	-2.74407500	1.70734200	-0.91014500
13a				H	-3.20591100	0.88719900	-1.46635300
C	0.14907500	-1.99771500	-1.58016500	H	-3.53523100	2.37232200	-0.54647500
C	1.27925300	-2.19483800	-0.75761200	H	-2.10550500	2.26635800	-1.59829200
H	2.26127500	-2.00050700	-1.17425100				
H	1.26431400	-2.93828100	0.03295000	13b			
C	-1.16906700	-2.10464900	-1.01712100	C	1.30817500	-2.21435100	-0.48318500
C	-1.25474600	-2.33573300	0.37738100	C	1.70446700	-1.93641600	0.85051800
H	-0.55468800	-2.98434600	0.89345300	H	2.72248800	-1.59835000	1.01838700
H	-2.23332800	-2.28094100	0.84505400	H	1.27458500	-2.48174900	1.68505200

C	-0.08699000	-2.50007800	-0.68611000	C	-0.34240600	2.60183200	-0.38153200
C	-0.98615600	-2.49265100	0.39720500	C	-0.91351300	2.47634300	0.89898900
H	-0.69342100	-2.82603300	1.38702000	H	-1.98734900	2.59150300	0.99774000
H	-2.04780500	-2.57332500	0.18970500	H	-0.34943200	2.71729900	1.79428300
P	-1.65271800	0.51330600	-1.07218700	C	1.05671100	2.32205800	-0.58071000
P	1.55437900	1.37193100	0.04930400	C	1.78393100	1.85421600	0.53626300
C	-1.18530400	0.11393900	2.61347100	H	1.58422200	2.21218200	1.54054800
C	0.02876100	-0.01758700	2.67121100	H	2.79977800	1.50579700	0.37702000
Rh	0.07614700	-0.50495800	0.26316600	P	1.24135200	-1.22228700	-0.85883800
H	1.02577100	-0.09689500	3.04686400	P	-2.12916400	-0.48618500	-0.25596100
H	-0.44874700	-2.59427500	-1.70749000	C	0.72717500	-0.59570400	2.81637200
C	2.25906500	-2.18243800	-1.65106600	C	-0.36971000	-0.08188900	2.67430600
H	3.11009900	-1.52226200	-1.46070500	Rh	-0.00793700	0.51437100	0.23797900
H	2.66529400	-3.18901400	-1.81661600	C	1.66750100	2.46759600	-1.94961600
H	1.76548500	-1.86691200	-2.57557800	H	0.94925900	2.25436900	-2.74738300
C	-2.63323000	0.27001900	2.73618700	H	2.00936200	3.50297600	-2.07866200
H	-3.01117900	1.09328100	2.12138800	H	2.54367900	1.82499300	-2.07494900
H	-3.15908000	-0.64689400	2.44993600	H	-0.95565500	2.81864500	-1.25265700
H	-2.88903400	0.49106700	3.77961000	H	-1.33535500	0.32851100	2.87067600
C	-2.12247300	2.28952000	-0.83352300	C	2.02166900	-1.20684500	3.10443500
H	-1.28058000	2.94689600	-1.06797000	H	2.84923500	-0.53518500	2.85194100
H	-2.95872000	2.55602900	-1.48885100	H	2.08908000	-1.42964300	4.17628500
H	-2.41829600	2.47162300	0.20394500	H	2.16011300	-2.14954200	2.56403100
C	-3.31275800	-0.30476300	-1.00331000	C	-2.43915900	-1.11509300	-1.96909800
H	-3.70792300	-0.29926100	0.01570200	H	-3.47762500	-1.44824200	-2.07179800
H	-4.01989700	0.21636300	-1.65754900	H	-2.24810500	-0.32379000	-2.70021800
H	-3.23697100	-1.34330600	-1.33750500	H	-1.78497500	-1.96145700	-2.19440700
C	-1.32347900	0.45361800	-2.89335200	C	-2.62629800	-1.94088700	0.77521500
H	-1.19744500	-0.58667500	-3.20746900	H	-2.65911400	-1.66150400	1.83172800
H	-2.15479400	0.89174300	-3.45671100	H	-3.61518900	-2.30448500	0.47566200
H	-0.40610800	0.99411500	-3.13787900	H	-1.90355300	-2.75368300	0.66830000
C	1.11183300	2.85920300	1.05555100	C	-3.59144400	0.62561500	-0.03261300
H	0.12975400	3.24128700	0.76704300	H	-3.50531000	1.50572100	-0.67682100
H	1.06833300	2.59110100	2.11443200	H	-4.51245300	0.09252600	-0.29113800
H	1.85504600	3.65182300	0.91793200	H	-3.66547200	0.96048400	1.00602800
C	3.29505600	1.07710800	0.60173900	C	0.83365100	-2.98677100	-0.47161200
H	3.87390500	2.00413500	0.53067900	H	0.86877400	-3.15424300	0.60890400
H	3.31683100	0.73115700	1.63915600	H	-0.17250300	-3.23437900	-0.82135700
H	3.77517400	0.32034200	-0.02504800	H	1.54295000	-3.66423300	-0.95900500
C	1.84181200	2.10297100	-1.62664000	C	3.06856800	-1.20186000	-0.56021600
H	2.61584800	2.87673500	-1.58059000	H	3.54462100	-2.04937200	-1.06475400
H	2.16150800	1.32469600	-2.32620300	H	3.50430400	-0.27942300	-0.95337700
H	0.92566100	2.55855300	-2.01207400	H	3.28814300	-1.25666300	0.50864200
				C	1.20729400	-1.21809700	-2.70998000
				H	1.60616300	-0.27073700	-3.08295900

13c

H	1.81675800	-2.03674400	-3.10854600	H	3.36201500	-1.91999300	-0.29507600
H	0.18619200	-1.32436500	-3.08205100	H	2.96750800	-1.32810200	-1.91801700
13d				C	2.98614700	0.56490100	1.43445500
				H	2.94391700	-0.32786300	2.06497400
C	-0.87998500	-1.54801300	1.74819000	H	4.03610800	0.84385400	1.29383500
C	-1.94577500	-1.46566600	0.80797700	H	2.47113800	1.37492600	1.95787900
H	-2.81869700	-0.87975600	1.07908600	13a-TS			
H	-2.16711900	-2.30746800	0.15971500				
C	0.31356700	-2.19678700	1.28442100	C	-1.13138300	-1.62569000	1.42811300
H	1.19183900	-2.17107400	1.92532600	C	-2.01841900	-1.68106300	0.26306300
C	0.39958100	-2.69143900	-0.03361400	H	-3.00795600	-1.27210400	0.44109200
H	-0.45244800	-3.14666300	-0.52738800	H	-2.02826100	-2.64456900	-0.24145500
H	1.36151400	-3.03697100	-0.39729300	C	0.16379800	-2.19477100	1.37795200
P	2.16911400	0.22074500	-0.19025700	C	0.64736300	-2.49962500	0.06436800
P	-0.98489500	1.72454500	0.22581100	H	0.00074700	-2.97666200	-0.66805100
C	-0.17867000	-0.34593000	-2.45458400	H	1.69164800	-2.79003600	-0.02608200
C	-1.31805900	-0.79436500	-2.35451600	P	2.06463800	0.36390400	-0.60362300
Rh	-0.13351100	-0.50324400	-0.08193300	P	-0.97160100	1.76720600	0.63282400
H	0.69662200	0.01694600	-2.95003700	C	-0.78133200	-0.31907900	-1.98478000
C	-0.95658700	-0.97773400	3.14038600	C	-1.89414800	-0.88885300	-1.73028800
H	-1.62695000	-0.11444600	3.18731900	Rh	-0.03515700	-0.38079200	-0.04569800
H	-1.36197100	-1.73523700	3.82398900	H	-0.31734700	0.10899800	-2.86135000
H	0.02699300	-0.68159500	3.51820900	C	1.01166400	-2.33284200	2.61553600
C	-2.67274900	-1.33250400	-2.47409400	H	0.73039000	-1.61363500	3.39073100
H	-2.94480800	-1.39282600	-3.53501500	H	0.88491300	-3.34059800	3.03209400
H	-2.74713000	-2.34186300	-2.05558400	H	2.07576200	-2.21242300	2.39309000
H	-3.41000500	-0.69986800	-1.96947200	H	-1.50796000	-1.21251200	2.35909400
C	-0.16619100	2.80649700	1.48405500	C	-3.22167800	-1.30922700	-2.23826600
H	0.86544500	3.02545300	1.19489700	H	-3.26102500	-1.12944900	-3.31862500
H	-0.70363400	3.75490100	1.59179400	H	-3.41321600	-2.37413000	-2.06525600
H	-0.15011400	2.29642900	2.45211100	H	-4.03633000	-0.74293000	-1.77135900
C	-1.00386700	2.79141900	-1.28345700	C	-0.05514500	2.74120900	1.91309400
H	-1.43390100	3.77305600	-1.05821000	H	0.95663700	2.97736500	1.57055200
H	0.00827000	2.93043600	-1.67104900	H	-0.57316600	3.67907500	2.14196500
H	-1.59980000	2.31009800	-2.06346700	H	0.02803000	2.15139900	2.83137400
C	-2.75189900	1.83823800	0.76184100	C	-1.28167300	3.01394400	-0.69709600
H	-3.39769000	1.31425400	0.05163800	H	-1.79349000	3.89536600	-0.29625600
H	-2.88708900	1.38882400	1.74974300	H	-0.34229300	3.33298200	-1.15481400
H	-3.06319700	2.88694000	0.81307700	H	-1.90495900	2.56409800	-1.47569400
C	2.62173600	1.73176200	-1.16206200	C	-2.65176300	1.65229400	1.40276800
H	2.29390400	1.63799200	-2.20195300	H	-3.36147200	1.21861100	0.69199500
H	2.15325000	2.62282300	-0.73526400	H	-2.62087600	1.01968800	2.29461400
H	3.70726500	1.87643700	-1.15519500	H	-3.01375500	2.64505700	1.69094300
C	3.31834600	-1.02795800	-0.92618800	C	2.25416000	2.07946100	-1.25941000
H	4.32991800	-0.61755900	-1.01375900	H	1.64761000	2.20693500	-2.16073700

H	1.93969000	2.81901300	-0.51897300	H	-3.46888000	-0.22215400	-2.53861100
H	3.30229500	2.26885100	-1.51501200	H	-1.73747100	-0.21264200	-2.96225300
C	2.91144400	-0.61618600	-1.91785800	C	0.73149900	3.14808000	0.48248000
H	3.90928500	-0.20969100	-2.11502800	H	-0.26730700	3.44477000	0.15778900
H	3.00580300	-1.66082000	-1.61252800	H	0.71460300	2.99889600	1.56629300
H	2.32648800	-0.58341300	-2.84172200	H	1.42907400	3.96025200	0.25164600
C	3.26913600	0.32884400	0.79254500	C	3.03003400	1.51960800	0.21180700
H	3.37823500	-0.69353400	1.16450200	H	3.52101300	2.48172500	0.03217700
H	4.25055600	0.69144400	0.46784700	H	3.06563100	1.29936600	1.28287000
H	2.90840100	0.95611000	1.61299000	H	3.58510100	0.74366900	-0.32158500
13b-TS				C	1.42899300	2.07497000	-2.11715800
				H	2.03325700	2.98226700	-2.22612000
				H	1.90279800	1.26512400	-2.68041100
				H	0.44232800	2.25587600	-2.55399000
				13c-TS			
C	1.51239600	-1.99246600	-0.57827100	C	-0.11165800	2.50832800	-0.50639300
C	1.88386800	-1.77942900	0.83569100	C	-0.79990200	2.54737800	0.78581600
H	2.88810100	-1.38964800	0.97676200	H	-1.85891100	2.77681300	0.72705600
H	1.66243300	-2.62345900	1.48580000	H	-0.27979300	3.10814400	1.55891600
C	0.21977000	-2.49470800	-0.83054400	C	1.27976700	2.25922300	-0.55899000
C	-0.72471500	-2.53591400	0.24540500	C	1.85644500	1.74550000	0.64998800
H	-0.42185500	-2.88669300	1.22912400	H	1.59289700	2.17095800	1.61480600
H	-1.75115900	-2.79384000	-0.00228000	H	2.88556200	1.39978800	0.60082600
P	-2.05812600	0.21623200	-0.57668200	P	1.43783600	-1.39319000	-0.27121000
P	1.26534700	1.58027400	-0.34204300	P	-1.93546700	-0.46878400	-0.74796400
C	-0.08438400	-0.00514800	2.24613500	C	-0.41983600	-0.04949200	2.24914600
C	1.02934600	-0.61984400	2.35580200	C	-1.01910900	1.07467100	2.28084500
Rh	0.01623600	-0.46125700	0.17471300	Rh	0.11099900	0.42802800	0.23859600
H	1.82445500	-0.86798700	3.03753400	C	2.06168100	2.42048400	-1.83607700
H	-0.08310600	-2.68174700	-1.85778400	H	1.44399200	2.26185300	-2.72542200
C	2.54258000	-1.85861900	-1.67341400	H	2.46137600	3.44177500	-1.88582400
H	3.19653400	-0.99533500	-1.52299300	H	2.92098900	1.74473500	-1.87396800
H	3.18743800	-2.74712100	-1.69084000	H	-0.66358500	2.73956700	-1.41283700
H	2.07156700	-1.76980600	-2.65709100	H	-1.64978500	1.71696700	2.87052900
C	-1.06111900	0.73948200	3.08896100	C	-0.17509600	-1.23703400	3.11392000
H	-1.33158000	1.69926300	2.63654200	H	0.89757300	-1.41475400	3.24385300
H	-1.98289800	0.15888400	3.20517200	H	-0.61728900	-1.09780200	4.10679700
H	-0.65699000	0.92981300	4.08985000	H	-0.60820700	-2.14152300	2.67327000
C	-2.42435400	2.00155600	-0.87556200	C	-1.87206800	-1.16289300	-2.46258700
H	-1.71339300	2.43388700	-1.58416500	H	-2.86599600	-1.48337500	-2.79316800
H	-3.43287300	2.10335200	-1.29056000	H	-1.50032000	-0.39876100	-3.15231500
H	-2.37886300	2.56407100	0.06096100	H	-1.19755800	-2.02272700	-2.51101600
C	-3.49982300	-0.26741000	0.47009000	C	-2.80507000	-1.79200900	0.20668200
H	-3.45990500	0.26183300	1.42572800	H	-3.00470600	-1.43001000	1.21970700
H	-4.43813800	-0.01139700	-0.03398400				
H	-3.48341700	-1.34117900	0.67077900				
C	-2.46931600	-0.53156100	-2.21430400				
H	-2.44407500	-1.62263500	-2.15025700				

H	-3.75515000	-2.05904700	-0.26834800	H	0.65449000	3.93153000	-1.55087100
H	-2.18479300	-2.68881000	0.27948500	H	0.68650300	2.42917600	-2.50715200
C	-3.28699800	0.78445700	-0.91642400	C	0.16253300	3.03370100	1.26917900
H	-2.97104300	1.60425900	-1.56831600	H	0.67118500	4.00114000	1.20001400
H	-4.18551000	0.32584700	-1.34300100	H	-0.91465000	3.20745600	1.24453000
H	-3.54100900	1.19433900	0.06560100	H	0.41782900	2.56975700	2.22699300
C	0.71438500	-3.08808500	-0.13170200	C	2.52758400	2.15494500	-0.00652000
H	0.36814500	-3.27377000	0.88828900	H	2.89909600	1.71251100	0.92278800
H	-0.12957400	-3.20994600	-0.81491200	H	3.03706800	1.67831100	-0.84758300
H	1.47302100	-3.83650000	-0.38460000	H	2.77838700	3.22110100	-0.01050300
C	2.97453400	-1.57454500	0.73573600	C	-3.00268300	1.56980500	0.50205300
H	3.51226100	-2.48234300	0.44205900	H	-2.69966600	1.89943000	1.49923200
H	3.63131700	-0.71433800	0.58891100	H	-2.66674900	2.30587200	-0.23347600
H	2.72519300	-1.63662900	1.79823500	H	-4.09641600	1.51984800	0.46987400
C	2.08811700	-1.39511400	-1.99865600	C	-3.12565200	-1.13296200	1.41694800
H	2.65765300	-0.48112800	-2.18398800	H	-4.21129700	-0.98977000	1.38828000
H	2.74082400	-2.25919100	-2.16504300	H	-2.89748200	-2.18894700	1.25259000
H	1.26076700	-1.43127600	-2.71261100	H	-2.76028800	-0.85654900	2.41056600
13d-TS				C	-3.18395500	-0.54228400	-1.42107800
				H	-2.96111600	-1.57293600	-1.70873300
				H	-4.26648300	-0.44066500	-1.28664000
				H	-2.86378700	0.11933200	-2.23148800
C	1.47475500	-1.32001300	-1.46705000	14a			
C	2.14523900	-1.42808100	-0.15419300				
H	3.09308000	-0.89942700	-0.10307200				
H	2.20498700	-2.44979600	0.21631100				
C	0.25437900	-2.00933600	-1.62897500	C	2.12876600	-0.86693300	-0.92235500
H	-0.24912000	-1.97800200	-2.59195700	C	2.87086500	-1.04845800	0.39710400
C	-0.39049700	-2.54114500	-0.46950300	H	3.76397500	-0.40885800	0.39208400
H	0.18764400	-3.05351600	0.29591200	H	3.25629400	-2.07758100	0.46402900
H	-1.39230800	-2.94420600	-0.59267100	C	1.17802300	-1.77350400	-1.45469200
P	-2.29747900	-0.09571800	0.13565800	C	0.29781600	-2.47364500	-0.59395200
P	0.69296600	1.92363800	-0.11331100	H	0.61066200	-2.76786100	0.40312900
C	0.38434900	-0.57524000	1.99741800	H	-0.47757400	-3.09175100	-1.04045100
C	1.59101700	-0.97134100	1.85284300	P	-2.25424500	-0.47491800	0.42858500
Rh	-0.02532700	-0.40801500	-0.02760400	P	0.34656600	2.10725000	-0.29078500
H	-0.25388600	-0.35436100	2.84072300	C	0.78599300	-0.34645800	1.49329600
C	2.18481800	-0.68409600	-2.63793400	C	2.05297900	-0.74010200	1.63306300
H	2.72306200	0.22374700	-2.35293900	Rh	-0.00820100	-0.25100500	-0.33792900
H	2.92999400	-1.38110000	-3.04365300	H	0.12887100	-0.08562700	2.32162400
H	1.48751300	-0.43679500	-3.44411400	C	0.91065600	-1.77075900	-2.94655900
C	2.86420800	-1.31205300	2.53381500	H	1.22249400	-0.83425200	-3.42050000
H	2.70042600	-1.28830000	3.61709800	H	1.48839700	-2.57953900	-3.41237300
H	3.22305000	-2.31243600	2.26702100	H	-0.14376000	-1.95462900	-3.17959000
H	3.66086600	-0.59707100	2.29625100	H	2.64951600	-0.26095300	-1.66064600
C	0.26499400	2.90989700	-1.61897900	C	2.72535400	-0.89248800	2.97724400
H	-0.82106300	2.95576300	-1.74447600	H	2.05679900	-0.62290500	3.80021100

H	3.05638500	-1.92731600	3.13431500	H	4.16232500	-1.60774700	-1.34833100
H	3.61987100	-0.25875700	3.04176000	H	3.06912900	-0.63613100	-2.34490600
C	-0.65277300	3.01081100	-1.55816800	C	-0.60004900	-0.19750300	2.71855100
H	-1.72201100	2.88244800	-1.36345200	H	-0.77726700	0.88244900	2.65420200
H	-0.42035400	4.08135700	-1.54590800	H	-1.57455700	-0.69427500	2.65166000
H	-0.43589600	2.61851800	-2.55689600	H	-0.19708400	-0.40787300	3.71768200
C	-0.01102400	3.02022800	1.27159900	C	-3.27223100	1.19905600	0.65161200
H	0.23239000	4.08217000	1.16127300	H	-2.94623000	2.17455500	0.28412900
H	-1.06602200	2.92670000	1.53954200	H	-4.34877900	1.10005300	0.47498800
H	0.59248300	2.60123700	2.08191600	H	-3.09035000	1.15403000	1.72847500
C	2.06828900	2.65556400	-0.66507800	C	-3.31425700	-1.64870000	0.31536700
H	2.75368800	2.23673300	0.07737000	H	-3.11892700	-1.86984900	1.36861000
H	2.36822400	2.29982200	-1.65471000	H	-4.38949600	-1.48462500	0.18525000
H	2.14365200	3.74809000	-0.64225500	H	-3.01123200	-2.51555900	-0.27675000
C	-3.08143600	0.87324100	1.38469600	C	-2.89880200	0.06926600	-1.97349700
H	-2.53543600	1.06763100	2.31297700	H	-2.54135400	-0.76420100	-2.58618400
H	-3.11277700	1.79586200	0.79761700	H	-3.99124800	0.11206500	-2.04360200
H	-4.10793400	0.58763300	1.63919700	H	-2.48693500	0.99931700	-2.37805700
C	-2.55852500	-1.94401400	1.50039900	C	-0.29514300	3.31440100	0.42812400
H	-3.61433700	-2.00589800	1.78506200	H	-1.09754900	3.43654600	-0.30554900
H	-2.27541600	-2.85690200	0.96998700	H	-0.74260800	3.11912800	1.40702900
H	-1.95058600	-1.87421600	2.40729800	H	0.26769500	4.25260200	0.48279700
C	-3.40933800	-0.73026000	-0.99213400	C	2.23542400	2.15009200	1.09247100
H	-3.10602500	-1.61215100	-1.56442000	H	2.59115200	3.18560600	1.07502800
H	-4.43525400	-0.87603600	-0.63653200	H	1.92442600	1.89348000	2.10873900
H	-3.38995800	0.13792600	-1.65861500	H	3.05755200	1.48590600	0.81503200
14b				C	1.48406400	2.55003400	-1.67988700
				H	1.88390700	3.56393700	-1.56828400
				H	2.28050200	1.89439200	-2.04193900
				H	0.68758800	2.57035700	-2.43091500
C	2.18700400	-1.44294200	-0.52378200	14c			
C	2.50081800	-1.80012900	0.92466500				
H	3.47892300	-1.37738000	1.19068100				
H	2.63318500	-2.89133900	0.99799400				
C	1.11923500	-2.02335500	-1.22446200	C	2.14254700	-1.36576900	-0.33230100
C	-0.07675700	-2.52393700	-0.64514500	C	2.74112700	-1.38882200	1.06771200
H	-0.07335700	-2.96439300	0.34777800	H	3.69529600	-0.84539000	1.05568800
H	-0.82791600	-2.92161900	-1.32258800	H	3.00233000	-2.42149800	1.34517500
P	-2.36543000	-0.15662100	-0.21616800	C	1.11612400	-2.23203900	-0.80167300
P	0.82052700	1.92474800	-0.06990700	C	0.05390700	-2.62115900	0.04372500
C	0.36514300	-0.68076200	1.67479900	H	0.19948000	-2.74286900	1.11237500
C	1.48909700	-1.34790300	1.94149400	H	-0.76361400	-3.19446000	-0.38620000
Rh	0.00320400	-0.33874300	-0.28245200	P	-2.27358000	-0.06399500	-0.01287600
H	1.72356900	-1.57508100	2.98395500	P	0.90082700	1.87568100	-0.44850100
H	1.12088500	-1.87951200	-2.30740600	C	0.64431400	-0.26577600	1.81557900
C	3.34384800	-0.87401100	-1.31261300	C	1.83397900	-0.79603000	2.10738600
H	3.75903800	0.02505700	-0.84424200	Rh	0.11760400	-0.35465800	-0.14293100

C	1.00847500	-2.48688200	-2.29210600	P	-2.39475400	-0.46702400	0.03238500
H	1.43882100	-1.67146800	-2.88370900	P	0.39440700	2.08676000	0.23509000
H	1.57452900	-3.39491800	-2.53727500	C	0.44218000	-0.88899600	1.31059600
H	-0.02498100	-2.65378700	-2.61259600	C	1.63766900	-1.46148000	1.45544400
H	2.81475800	-1.00370200	-1.10797000	Rh	-0.11034000	-0.17491700	-0.46441200
H	2.17020300	-0.81299400	3.14645200	H	-0.27441000	-0.79230800	2.12461000
C	-0.31877100	0.29807700	2.81721200	C	3.24822700	0.02053100	-1.63412100
H	-1.21432800	-0.32516400	2.91868500	H	3.55471000	0.82673900	-0.95831000
H	0.16331000	0.33576900	3.80312900	H	4.15684100	-0.55887000	-1.85318900
H	-0.64557100	1.31274700	2.56949800	H	2.90395400	0.46325300	-2.57373500
C	0.40369000	2.55345200	-2.09693900	C	2.09698200	-2.05275800	2.77035300
H	0.84341300	3.54403200	-2.25747700	H	1.34043700	-1.94203700	3.55259800
H	0.74374200	1.88740000	-2.89631600	H	2.31804800	-3.12275300	2.66240400
H	-0.68537500	2.64209200	-2.16128600	H	3.02005700	-1.56926300	3.11687000
C	0.38961000	3.21076900	0.71998900	C	0.86117200	3.13080300	-1.22023300
H	0.78596000	2.99868000	1.71703000	H	0.02476500	3.18942800	-1.92452900
H	0.78480400	4.17635100	0.38669500	H	1.12298700	4.14688900	-0.90481500
H	-0.69923200	3.27768400	0.78462900	H	1.71692700	2.69098300	-1.74000400
C	2.73449900	2.08136900	-0.45736900	C	-0.88255200	3.14261500	1.05684100
H	3.17759400	1.48094400	-1.25667100	H	-0.49575800	4.15408800	1.22192700
H	3.00650000	3.13139700	-0.60929800	H	-1.77921600	3.21148000	0.43290900
H	3.14232000	1.74287400	0.49946000	H	-1.15986800	2.71436300	2.02446100
C	-3.07040300	1.52876500	0.48325700	C	1.82832300	2.28289200	1.37903000
H	-2.82621300	1.77071600	1.52161700	H	1.61426900	1.78143000	2.32672100
H	-2.71934200	2.34328300	-0.15748600	H	2.71964400	1.82130600	0.94669900
H	-4.15941600	1.45756300	0.38935300	H	2.03063200	3.34228500	1.56871900
C	-3.24910200	-1.30098800	0.95104300	C	-3.11562700	0.29980000	1.54886900
H	-4.32214900	-1.15644900	0.78463800	H	-2.56740000	-0.02984000	2.43702800
H	-2.97301300	-2.31280700	0.64338400	H	-3.06307300	1.38883300	1.49223200
H	-3.04556600	-1.20124300	2.02066200	H	-4.16423800	0.00361700	1.65990200
C	-2.92716400	-0.30199100	-1.72999400	C	-2.93950500	-2.21990900	0.20619100
H	-2.66557800	-1.29892000	-2.09732400	H	-4.01395200	-2.27109200	0.41262900
H	-4.01791800	-0.19955700	-1.74466700	H	-2.72454700	-2.77457200	-0.71042400
H	-2.49864900	0.44016900	-2.41079400	H	-2.39722100	-2.69428900	1.02962400
14d				C	-3.46059900	0.18564900	-1.32755200
				H	-3.20666500	-0.30746400	-2.27102900
				H	-4.51909000	0.00413600	-1.11086100
C	2.20993500	-0.88115900	-1.00790400	H	-3.30568400	1.26232900	-1.44762700
C	2.62357500	-1.53619200	0.30694600				
H	3.57260400	-1.09342300	0.63880800				
H	2.85788600	-2.59435100	0.10846500	16			
C	1.18882000	-1.39698100	-1.81533700	C	-1.75105300	-0.28128500	0.42775500
H	1.12470300	-0.99906200	-2.83015200	O	-1.49058000	0.98463400	-0.16436300
C	0.09242000	-2.17875700	-1.35291100	C	-0.20274400	1.49645600	0.17144400
H	0.21223700	-2.85243700	-0.50885800	C	0.92435600	0.73699000	-0.47080500
H	-0.63519200	-2.50054100	-2.09395300	C	1.96723700	0.21248200	0.19496800

C	3.07580100	-0.49478400	-0.43131800	H	-2.36420500	2.45812700	-1.52375500
C	4.11769800	-1.00810300	0.23941000	C	-3.55028200	1.28454400	1.21864300
H	-1.66787900	-0.21112300	1.52681900	H	-3.62338600	0.58194300	2.05429900
H	-1.00886900	-1.02695600	0.10182200	H	-2.90354700	2.10938900	1.51996500
H	-0.22143800	2.53148300	-0.19081400	H	-4.54869500	1.67874500	0.99894100
H	-0.06985500	1.52521300	1.26616000	C	-0.46796800	3.12210600	0.82859000
H	0.86511400	0.63328500	-1.55491900	H	-1.23791300	3.38583600	0.09977500
H	2.01130500	0.31812700	1.28065900	H	-0.92611700	3.06133100	1.82017200
H	3.03195600	-0.60064700	-1.51542900	H	0.27800700	3.92411800	0.84523500
H	4.92321600	-1.53000600	-0.26809600	C	1.60928500	1.43314500	1.77554500
H	4.19766300	-0.92116900	1.32087200	H	2.37099300	0.70033000	1.50628900
C	-3.09413400	-0.72711200	0.06256500	H	2.08932700	2.40830200	1.91320900
C	-4.19746800	-1.12345800	-0.22253000	H	1.12553100	1.13949700	2.71170700
H	-5.17472900	-1.46239200	-0.48110300	C	1.37570400	1.97134600	-1.06891800
17				H	1.94266400	2.88985900	-0.88074200
				H	2.07654200	1.16121700	-1.28355300
				H	0.72579000	2.12485200	-1.93565300
				18			
O	3.26899600	-0.73476000	-0.13919000	O	-3.70269000	-0.91984300	0.84714400
C	4.69442800	-0.67847500	0.01031600	C	-2.91957100	-0.18828200	1.76719100
C	2.68724800	-1.82508700	0.55548900	C	-3.37054100	-0.72199300	-0.52399800
C	1.29044000	-2.04014200	0.05088800	C	-2.03670500	-1.33120700	-0.84802800
C	0.25766300	-2.43490900	0.86743500	C	-1.20362900	-1.00964100	-1.92848800
C	-1.09067800	-2.67413700	0.38317400	C	0.09217000	-1.62627700	-1.99494400
C	-1.42358600	-2.48764800	-0.95616800	C	0.47364600	-2.51687500	-0.94864600
H	5.14364700	-1.60177800	-0.38759600	H	-3.39996100	-0.33890100	2.74051000
H	4.95986800	-0.61960000	1.07787500	H	-2.95538900	0.89036500	1.54545200
H	3.26379000	-2.74587800	0.35600500	H	-4.15772900	-1.25528700	-1.07034700
H	2.70338300	-1.66068700	1.64466400	H	-3.43440000	0.33854900	-0.79964500
H	1.21310400	-2.11612900	-1.03069100	H	-1.92477900	-2.30559400	-0.38292000
H	0.42088500	-2.49184600	1.94151300	H	-1.46508300	-0.23319900	-2.64218500
H	-1.84938600	-2.94918300	1.11007800	H	0.76740700	-1.36045900	-2.80217300
H	-2.45089700	-2.63220300	-1.26697300	H	1.48828300	-2.90196200	-0.97792600
H	-0.69142700	-2.54976100	-1.75591100	H	-0.23439500	-3.21055700	-0.50462900
Rh	-0.79016800	-0.54252300	0.02296700	Rh	0.05259600	-0.48718600	-0.14687700
P	0.36912700	1.52409300	0.41171300	P	2.35673200	-0.27984200	0.32323600
P	-2.87400700	0.40617900	-0.25777800	P	-0.28752400	1.95396500	-0.27011800
C	5.21109700	0.48355700	-0.70184400	C	-1.51184300	-0.61886300	1.88798300
C	5.66846900	1.43572200	-1.28439000	C	-0.36831100	-0.98336800	2.15347400
H	6.08133600	2.27149000	-1.80428700	H	0.42732700	-1.39540800	2.73793000
C	-4.25916900	-0.76078200	-0.62960200	C	-0.24772100	2.93104100	1.30373100
H	-5.20873000	-0.21494700	-0.62532200	H	-0.42648700	3.99363300	1.10673800
H	-4.12724900	-1.21501900	-1.61513600	H	-1.02110800	2.56452700	1.98583900
H	-4.30969200	-1.55311700	0.12298400	H	0.71663300	2.82401400	1.80545500
C	-3.05023200	1.61650200	-1.64300400				
H	-2.81411200	1.11757200	-2.58789500				
H	-4.07521900	2.00062300	-1.69113400				

C	0.93082700	2.85230700	-1.34023800	H	0.10302200	4.02223900	1.29589600
H	0.86761100	2.46331100	-2.36163300	H	-0.54604700	2.57239400	2.10178900
H	0.71680600	3.92653700	-1.35978800	H	1.19995300	2.74308800	1.86278800
H	1.95458700	2.70945400	-0.98662900	C	1.30660500	2.92876600	-1.27498800
C	-1.86001200	2.60031900	-1.01596800	H	1.17960400	2.60651500	-2.31337600
H	-1.80281900	3.68967500	-1.11747800	H	1.18320400	4.01625100	-1.22619200
H	-2.02599900	2.17000900	-2.00819600	H	2.32597100	2.68104700	-0.96615600
H	-2.72012800	2.36217400	-0.38498300	C	-1.50688700	2.82619200	-0.84949700
C	2.95981400	1.09215000	1.40691400	H	-1.42450100	3.91841900	-0.87092200
H	2.78544500	2.07092000	0.95479800	H	-1.71661800	2.47263900	-1.86337200
H	2.44019500	1.05604900	2.36938500	H	-2.34864700	2.55770300	-0.20495800
H	4.03486700	0.98131900	1.58487200	C	3.16446700	0.70523300	1.37471800
C	3.08814800	-1.72893800	1.21126400	H	3.17204500	1.66664100	0.85602400
H	2.90665400	-2.65718700	0.66623900	H	2.62961400	0.82179200	2.32182700
H	4.16879300	-1.58924400	1.32288400	H	4.19976400	0.42014500	1.59040700
H	2.65062000	-1.82703900	2.20900100	C	2.75745200	-2.11314400	1.33051000
C	3.44856100	-0.15135100	-1.16129900	H	2.44207700	-3.01193300	0.79609000
H	4.50197300	-0.10661200	-0.86423000	H	3.83489700	-2.16938900	1.52036400
H	3.30409100	-1.02546800	-1.80304000	H	2.23129600	-2.08617400	2.28917700
H	3.20456600	0.74250400	-1.74146100	C	3.46153700	-0.72620300	-1.11708400
18-TS				H	4.50333600	-0.86341900	-0.80730100
				H	3.16353300	-1.57526400	-1.73869300
				H	3.38469600	0.18343200	-1.71966700
O	-4.12138900	-0.76484100	0.75627400	19			
C	-3.22507100	-0.37361200	1.77291400				
C	-3.59871900	-0.40585100	-0.50658200				
C	-2.23022200	-1.03405800	-0.64596200	O	-4.33563900	-0.65495400	1.15941200
C	-1.39242200	-0.78601600	-1.80587600	C	-3.14495900	-0.86681700	1.92556700
C	-0.27676600	-1.62560100	-2.03662700	C	-3.99507400	-0.18587300	-0.13935400
C	0.15832600	-2.46992500	-0.97076200	C	-2.66208400	-0.88799300	-0.45253600
H	-3.50516100	-0.91754400	2.68049400	C	-1.82738600	-0.36889800	-1.60269200
H	-3.32139600	0.70694300	1.97407800	C	-0.82698900	-1.13199500	-2.21141800
H	-4.28162600	-0.83380900	-1.24840300	C	-0.09520200	-2.13935100	-1.51884600
H	-3.57243400	0.68528000	-0.64797100	H	-3.23044300	-1.84286900	2.41854400
H	-2.26235200	-2.08205000	-0.35336000	H	-3.03888500	-0.09754400	2.70312900
H	-1.66629200	-0.01954100	-2.52492700	H	-4.81131100	-0.45419800	-0.81499300
H	0.31483900	-1.49662900	-2.93846800	H	-3.86990500	0.91095700	-0.15348400
H	1.09064700	-3.00901500	-1.11461500	H	-2.89245400	-1.94774800	-0.64442800
H	-0.55606900	-3.00617700	-0.35075600	H	-2.21185200	0.48537800	-2.15554700
Rh	0.13698500	-0.38987300	-0.18991600	H	-0.44008800	-0.78327300	-3.17026800
P	2.35494700	-0.60058800	0.35225000	H	0.69149200	-2.65823200	-2.06109200
P	0.05883300	2.06969800	-0.20963700	H	-0.57530300	-2.72704800	-0.73995000
C	-1.79614400	-0.65704500	1.42032700	Rh	0.36502700	-0.18910200	-0.56331000
C	-0.57274800	-0.65571800	1.77322600	P	2.31819000	-0.97049300	0.46246100
H	0.00984000	-0.69580300	2.68058100	P	0.33380200	2.16455400	-0.02275400
C	0.22274200	2.94007800	1.41509100	C	-2.00893900	-0.79929700	0.91547600

C	-0.72302000	-0.52289800	1.08518600	P	1.84943000	-1.60815500	0.23707300
H	-0.23553500	-0.38704100	2.04846800	P	1.34152700	1.90219900	0.26658600
C	0.33236000	2.67509100	1.75018700	C	-2.52945100	-0.96431300	0.13620300
H	0.29495300	3.76595400	1.83855400	C	-1.35261800	-1.52948000	-0.16189000
H	-0.54175300	2.25123400	2.25306700	H	-1.07858700	-2.54746700	0.09299000
H	1.23174600	2.31181400	2.25442700	C	3.41832100	-1.44204200	-0.72384300
C	1.77520800	3.08209400	-0.73302100	H	3.87764200	-0.46619700	-0.55601400
H	1.82699700	2.92024200	-1.81453800	H	4.12938000	-2.22193300	-0.42982200
H	1.68015800	4.15741400	-0.54674600	H	3.20554400	-1.54243400	-1.79249100
H	2.71190800	2.73294900	-0.28752800	C	2.41300700	-1.63995100	1.99811400
C	-1.10269400	3.10904300	-0.69827700	H	1.56105700	-1.85553500	2.65035900
H	-1.02309400	4.17249500	-0.44740300	H	3.17625400	-2.41171700	2.14619900
H	-1.14011600	3.00391300	-1.78669000	H	2.83104300	-0.67375900	2.29322600
H	-2.03367300	2.71485400	-0.28054200	C	1.44899700	-3.39185400	-0.04653600
C	3.03028600	-0.04395900	1.89094800	H	2.34314000	-4.00232800	0.11731800
H	3.28599800	0.97730700	1.59448100	H	0.67328100	-3.73137600	0.64549100
H	2.30759400	0.00047500	2.71157200	H	1.09932700	-3.54867900	-1.07125700
H	3.93699100	-0.53977300	2.25421800	C	3.16148000	1.99437800	0.58647800
C	2.20420500	-2.68790400	1.11698000	H	3.46783200	1.26859500	1.34431500
H	1.95447800	-3.37844800	0.30735900	H	3.71573400	1.79547700	-0.33544700
H	3.15292600	-2.99406700	1.57047400	H	3.42798200	2.99617300	0.94049400
H	1.41348800	-2.74380300	1.87088900	C	1.14315500	3.29614500	-0.93371000
C	3.71612500	-1.03957500	-0.74052600	H	0.08669800	3.49544000	-1.13215800
H	4.61610700	-1.44069700	-0.26151200	H	1.59809200	4.20937600	-0.53529100
H	3.44904800	-1.68291800	-1.58412300	H	1.63266500	3.04582400	-1.88009700
H	3.93853000	-0.03902400	-1.12435100	C	0.63665000	2.59321800	1.83005800
19-TS				H	1.08004900	3.56688700	2.06610300
				H	-0.44616200	2.70945600	1.72891900
				H	0.82780100	1.90637100	2.66016200
O	-4.40275000	-0.15427700	1.28190800	20			
C	-3.59252700	-1.32559500	1.15721300				
C	-3.70382000	0.96322900	0.74118700				
C	-2.94777600	0.36726300	-0.45801000	O	3.39690600	0.31931900	1.86931600
C	-1.77982000	1.11505500	-1.05766200	C	2.87828600	1.20910000	0.88801300
C	-0.98436200	0.55476400	-2.06131100	C	2.75840900	-0.94625500	1.72329400
C	-0.91901000	-0.89531600	-2.18332400	C	2.61317800	-1.11775500	0.20201000
H	-4.23533900	-2.15357500	0.83138900	C	1.44483900	-1.91234500	-0.33581000
H	-3.14558300	-1.59971200	2.12318800	C	1.02098000	-1.66374600	-1.63012900
H	-4.44726200	1.71755700	0.47274400	C	1.69698600	-0.57636500	-2.44908000
H	-3.00075300	1.39394500	1.47430800	H	3.69168800	1.86751300	0.56126100
H	-3.69875400	0.17064500	-1.24289300	H	2.08096800	1.83535800	1.31342500
H	-1.75311800	2.19260800	-0.91898100	H	3.39710300	-1.69385900	2.19803900
H	-0.34737900	1.17650700	-2.68323200	H	1.76986700	-0.95137100	2.21188600
H	-0.08882300	-1.29993100	-2.75863700	H	3.56896000	-1.48132600	-0.21184300
H	-1.83194700	-1.46190500	-2.33119100	H	1.10146300	-2.79110000	0.20363800
Rh	0.13832200	-0.07728400	-0.32594800	H	0.33162600	-2.34041400	-2.12562200

H	1.06635900	-0.28338800	-3.29256100	H	0.46507300	0.92556900	1.51637500
H	2.65660900	-0.92250600	-2.87016200	H	-1.04955000	2.52143400	0.04142600
Rh	-0.00391800	-0.12823400	-0.31721100	H	-3.09631400	1.27904200	-0.33644600
P	-1.02969800	1.98373000	-0.00494500	H	-2.83636500	-1.12478600	-0.92750200
P	-1.87221300	-1.36788100	0.32791100	H	-2.84553800	-1.07230400	0.81432000
C	2.36401000	0.32008100	-0.23024600	C	0.21781800	-0.73324300	0.17807600
C	1.89826400	0.59315300	-1.48916600	C	-0.89735600	-1.41971000	-0.06686100
H	1.84302700	1.60913100	-1.86841300	H	-0.85439300	-2.47851600	-0.32036900
C	-2.38569300	2.37705800	-1.19780600				
H	-3.20737500	1.66433000	-1.11104500	22			
H	-2.77129000	3.38661500	-1.01789600	O	-1.38751700	1.13017000	-0.23058200
H	-1.99469100	2.32472700	-2.21845600	C	-1.72981000	-0.07034700	0.45272700
C	-1.76708500	2.34686000	1.65063000	C	-3.17291100	-0.37717000	0.18066500
H	-0.98760900	2.29132600	2.41694400	C	-3.62487700	-1.56139000	-0.23064300
H	-2.20942200	3.34879600	1.66866000	C	-0.07958300	1.60319300	0.06798300
H	-2.54179400	1.61728100	1.90115700	C	1.01022200	0.74679900	-0.51539000
C	0.07015800	3.45119800	-0.24737100	C	2.03413800	0.23110400	0.18503600
H	-0.50145300	4.37338300	-0.09723200	C	3.10513000	-0.57222500	-0.38885300
H	0.90237300	3.44100500	0.46082300	C	4.13075200	-1.07651700	0.31313000
H	0.47459900	3.45658200	-1.26363300	H	-1.57209800	0.07154800	1.53850000
C	-3.61272200	-0.79242500	0.08562500	H	-1.08812000	-0.90755700	0.13989500
H	-3.80153100	0.14505600	0.61470000	H	-3.86485500	0.44489800	0.36105500
H	-3.81256400	-0.64192200	-0.97954700	H	-4.68440900	-1.74840400	-0.38308300
H	-4.30858300	-1.54778700	0.46645600	H	-2.95163200	-2.39346500	-0.42742700
C	-1.96325300	-3.03873300	-0.45797000	H	-0.04355500	2.60987000	-0.36762700
H	-1.03978700	-3.60005600	-0.29288500	H	0.05819800	1.70382300	1.15824900
H	-2.79647100	-3.60980900	-0.03477600	H	0.93765700	0.55924500	-1.58747500
H	-2.12152200	-2.93695700	-1.53598900	H	2.09126600	0.41969800	1.25875600
C	-1.82326300	-1.76097000	2.13276000	H	3.04598400	-0.76188100	-1.46085600
H	-2.65319200	-2.41988600	2.41119700	H	4.90753700	-1.67195200	-0.15693300
H	-0.87878300	-2.25490200	2.37835300	H	4.22578900	-0.90785900	1.38367000
H	-1.88740000	-0.84069700	2.72045500				
				23			
21				O	3.20367700	-0.79563800	-0.21553700
O	2.42035700	0.04139200	-0.08055400	C	4.63069600	-0.72423100	-0.05636600
C	1.66047700	-1.16907700	0.05113600	C	5.17193300	0.29549100	-1.01034800
C	1.52509900	1.12739700	-0.32722600	C	5.91007100	1.34199900	-0.63985000
C	0.24687900	0.75345400	0.44751700	C	2.60795500	-1.82630700	0.54860200
C	-1.04382600	1.43329300	0.08729700	C	1.20033400	-2.04817800	0.07713200
C	-2.17190500	0.74681700	-0.11754700	C	0.18040000	-2.40761600	0.92610200
C	-2.25608900	-0.76082600	-0.06555400	C	-1.17783300	-2.65701900	0.47582500
H	2.03270900	-1.70085000	0.93769900	C	-1.53672300	-2.51663300	-0.86180200
H	1.81522400	-1.82011300	-0.82198800	H	5.05700300	-1.71866300	-0.26801700
H	2.01231700	2.04242900	0.02291500	H	4.88501500	-0.46485600	0.98238600
H	1.30738900	1.22831900	-1.40302500	H	4.95185900	0.11950100	-2.06259700

H	6.31904100	2.03775300	-1.36678100	C	0.08299500	-1.43700400	-2.10366100
H	6.15172500	1.53264000	0.40385900	C	0.43430300	-2.42210200	-1.12914000
H	3.16409800	-2.76987500	0.40090000	H	-3.27009700	-0.64132700	2.70907300
H	2.63902200	-1.60002300	1.62667600	H	-2.61780200	0.64652100	1.68091200
H	1.10241500	-2.16275600	-0.99948900	H	-1.51580300	-2.24705400	1.62814500
H	0.36356500	-2.42798500	1.99825100	H	0.51762100	-1.30415200	2.55206400
H	-1.92432100	-2.89955200	1.22671300	H	-0.23050300	0.37930900	2.60433200
H	-2.57124100	-2.66478100	-1.14598000	H	-4.17990400	-0.99548400	-1.15928700
H	-0.82130800	-2.61019500	-1.67342500	H	-3.34809400	0.50685300	-0.72068100
Rh	-0.86651600	-0.53997400	0.03739100	H	-2.01624200	-2.26259400	-0.67517800
P	0.31524100	1.51882600	0.37400100	H	-1.42180600	0.05948800	-2.62176500
P	-2.94089700	0.42795600	-0.26190500	H	0.78236700	-1.10354000	-2.86422400
C	-3.09961800	1.62316300	-1.66272300	H	1.44345400	-2.82029700	-1.17616800
H	-2.86672900	1.11043200	-2.60100700	H	-0.29191200	-3.14762000	-0.77390100
H	-4.11996900	2.01842700	-1.71859700	Rh	0.01991600	-0.46975700	-0.15419400
H	-2.40459200	2.45850900	-1.55159300	P	2.34446800	-0.33951100	0.28543800
C	-4.33856200	-0.72678100	-0.62400200	P	-0.27630900	1.99281100	-0.19385200
H	-5.28099700	-0.16890400	-0.63844400	C	0.92972300	2.83462100	-1.32318700
H	-4.20322100	-1.20184800	-1.59926900	H	0.74703900	3.91420700	-1.35668500
H	-4.40540600	-1.50370500	0.14321200	H	1.95977300	2.66742700	-0.99916300
C	-3.61143200	1.33431800	1.20039800	H	0.82234100	2.42958900	-2.33454900
H	-3.69560600	0.64397900	2.04516100	C	-1.85328000	2.71871200	-0.85169100
H	-2.95508100	2.15487500	1.49274800	H	-1.75127000	3.80609500	-0.93780100
H	-4.60422500	1.73794400	0.97244400	H	-2.08743000	2.31636000	-1.84155000
C	-0.50233100	3.12468800	0.79861900	H	-2.68977500	2.50480000	-0.18124000
H	-1.28502700	3.38957100	0.08387200	C	-0.11164400	2.97569300	1.36947100
H	-0.94180900	3.07029300	1.79907100	H	-0.16454200	4.04905200	1.15760700
H	0.24840700	3.92242000	0.79704100	H	-0.92588100	2.72086100	2.05555400
C	1.59378300	1.43220300	1.70207400	H	0.83589200	2.76436200	1.87022500
H	2.35157400	0.70551200	1.40599300	C	3.04288300	1.00862200	1.34152000
H	2.07084200	2.41017400	1.82986500	H	2.88755000	1.99349600	0.89545000
H	1.14051800	1.13107800	2.65095000	H	2.56945200	0.99227800	2.32779800
C	1.29010500	1.94437500	-1.13416200	H	4.11960100	0.85592200	1.47165300
H	1.86660100	2.86184700	-0.97141100	C	3.03308900	-1.82064100	1.15263100
H	1.97993700	1.12476800	-1.34935300	H	4.12461900	-1.74676700	1.20730900
H	0.62389800	2.08879900	-1.98989800	H	2.64081000	-1.88196300	2.17150100
				H	2.76552100	-2.73966700	0.62739000
24				C	3.39989200	-0.25660300	-1.22960300
O	-3.69384700	-0.90032400	0.77915100	H	4.46166700	-0.25068900	-0.96027400
C	-2.77333900	-0.44188100	1.75131300	H	3.20892400	-1.12544300	-1.86695300
C	-1.44882000	-1.16870600	1.75731900	H	3.17491500	0.64586600	-1.80452300
C	-0.27479000	-0.63886500	2.22847100				
C	-3.35847600	-0.57858100	-0.56394300	24b			
C	-2.06186500	-1.21826200	-0.96724300	O	-3.13048700	-0.18615300	0.80104100
C	-1.19372400	-0.79562800	-1.99114700	C	-2.50710600	-0.90747600	1.86040400

C	-1.00103400	-0.72125100	1.98614500	H	0.22737300	2.68231600	1.99036000
C	-0.10338300	-1.75631000	1.85300200				
C	-3.21527800	-0.92108000	-0.42378800	24-TS			
C	-1.89049500	-1.47950000	-0.89074500	O	-4.05040600	-0.60906200	0.85845400
C	-1.16318700	-0.97464200	-1.98411700	C	-2.98065100	-0.32260500	1.73138900
C	0.19325700	-1.39560600	-2.17709400	C	-1.76211100	-1.14173300	1.33027300
C	0.74293600	-2.34219800	-1.26891100	C	-0.44841500	-0.70600100	1.78818500
H	-2.74638700	-1.97772700	1.78227200	C	-3.57553300	-0.46079400	-0.46218200
H	-2.97079000	-0.53395200	2.78024900	C	-2.23827400	-1.17639500	-0.61391700
H	-0.67893700	0.17675500	2.50612300	C	-1.41661600	-0.76338100	-1.76885300
H	0.87740900	-1.71024100	2.31064800	C	-0.28585700	-1.51646300	-2.14330100
H	-0.43872500	-2.75042500	1.56887900	C	0.27419200	-2.40631300	-1.18415700
H	-3.93165000	-1.74619300	-0.29577200	H	-3.31241900	-0.58766400	2.73994000
H	-3.63259500	-0.22169100	-1.15246600	H	-2.72837100	0.75216500	1.71945900
H	-1.68255900	-2.49465700	-0.56672200	H	-1.92061700	-2.21238000	1.45026300
H	-1.55906200	-0.16697900	-2.59371400	H	0.15651400	-1.48419300	2.25023700
H	0.79193600	-0.92827100	-2.95302000	H	-0.41535700	0.23294600	2.34085500
H	1.80182500	-2.56582400	-1.35851100	H	-4.32636000	-0.90378300	-1.12426200
H	0.15276200	-3.17722000	-0.90455800	H	-3.46760000	0.60336200	-0.72408700
Rh	0.05795300	-0.51806500	-0.15985300	H	-2.34096100	-2.26115000	-0.58606800
P	2.33757500	-0.00151000	0.27813700	H	-1.77720300	0.03523600	-2.41071200
P	-0.60202800	1.87035400	-0.19265100	H	0.25114700	-1.26214000	-3.05319400
C	2.78525500	1.37001600	1.43546600	H	1.22693000	-2.87212700	-1.42023900
H	3.87179200	1.40742100	1.56861300	H	-0.36993400	-3.01996200	-0.55852200
H	2.45131400	2.33848900	1.05738800	Rh	0.15219100	-0.36984300	-0.21328600
H	2.32171600	1.20002900	2.41218700	P	2.36935100	-0.53366900	0.35227700
C	3.32757900	-1.38356600	1.00941200	P	-0.04146100	2.05294500	-0.19594900
H	4.39135500	-1.12326100	0.99453400	C	1.23771700	2.88704900	-1.24475200
H	3.03387400	-1.56027800	2.04775700	H	1.09447700	3.97317600	-1.24405800
H	3.18075400	-2.30954600	0.44889700	H	2.24697100	2.67038000	-0.88449700
C	3.31762500	0.39228100	-1.23843800	H	1.15729700	2.52225600	-2.27361400
H	4.35997000	0.60761400	-0.97923800	C	-1.57835800	2.82556500	-0.88637000
H	3.29899000	-0.46332500	-1.92040300	H	-1.47455000	3.91583800	-0.91588200
H	2.89501400	1.25467000	-1.75968000	H	-1.76355500	2.46661600	-1.90291500
C	0.50408400	2.96375900	-1.20452600	H	-2.44398600	2.57802500	-0.26593100
H	1.52340900	2.98539200	-0.81171900	C	0.09878000	2.95967600	1.41222300
H	0.54191700	2.59194400	-2.23360900	H	0.07125000	4.04223400	1.24869000
H	0.12024300	3.98957300	-1.21888300	H	-0.73520800	2.68950200	2.06775300
C	-2.23890400	2.33374600	-0.92017400	H	1.03063000	2.70485500	1.92284400
H	-2.34745500	3.42364500	-0.90580500	C	3.11835600	0.73284300	1.46753700
H	-2.31745200	1.99598500	-1.95768600	H	3.06006500	1.73198700	1.02924100
H	-3.03755500	1.88296700	-0.32906800	H	2.59303300	0.73971000	2.42716600
C	-0.69823100	2.77965000	1.41713800	H	4.17228100	0.49537300	1.64802600
H	-0.89277700	3.84332400	1.24220100	C	2.86413700	-2.09312200	1.20803300
H	-1.52161100	2.37201200	2.01085600	H	3.94783300	-2.11009100	1.36641400

H	2.36972400	-2.16246200	2.18122100	H	2.55480100	2.57806600	-0.76884500	
H	2.57714400	-2.96316700	0.61281400	H	1.44299000	2.63164400	-2.14648700	
C	3.47187000	-0.50160600	-1.12664500	H	1.52130200	4.00343900	-1.01310600	
H	4.52035600	-0.61868300	-0.83081700	C	-1.25548200	3.02042500	-0.71983100	
H	3.20467400	-1.31488000	-1.80773100	H	-1.11860100	4.10288600	-0.62127800	
H	3.35665900	0.44497700	-1.66183100	H	-1.41771900	2.78593100	-1.77610000	
24b-TS				H	-2.15119600	2.73276900	-0.16097200	
				C	0.44759000	2.90974600	1.57119200	
	O	-4.20383900	-0.50720100	0.78220200	H	0.44281300	4.00170900	1.48466200
	C	-3.19972900	-0.98700600	1.66044300	H	-0.36919500	2.61292000	2.23739700
	C	-1.88752500	-0.30818000	1.32445600	H	1.39025500	2.60084400	2.03025200
	C	-0.59608500	-0.76841700	1.74969500				
	C	-3.69477000	-0.22738100	-0.51610100	25			
	C	-2.29894700	-0.79182700	-0.65854700	O	-3.75984100	0.26967500	0.59753600
	C	-1.49393400	-0.47337100	-1.83080100	C	-2.86997400	0.08224100	1.69474100
	C	-0.43071000	-1.32703900	-2.19432000	C	-1.95313500	-1.12594600	1.34245200
C	0.02261200	-2.30032400	-1.24688000	C	-0.45018500	-0.87696800	1.40373400	
H	-3.11072800	-2.08401600	1.62927600	C	-2.49265300	-1.58438000	-0.05215800	
H	-3.50858900	-0.70553200	2.67356300	C	-1.72233600	-1.03421200	-1.24495000	
H	-2.01525400	0.77417700	1.34050600	C	-0.64758400	-1.70704400	-1.85427800	
H	-0.03072100	-0.09999900	2.39550400	C	0.28720700	-2.48532200	-1.12833200	
H	-0.50296300	-1.82191900	2.01513700	H	-3.43927800	-0.12344100	2.61195400	
H	-4.35064500	-0.71489900	-1.25017700	H	-2.32319800	1.01718700	1.84277100	
H	-3.72496500	0.85422600	-0.71001900	H	-2.16459200	-1.93260700	2.05863400	
H	-2.29697900	-1.85898400	-0.44820200	H	0.09165700	-1.78988500	1.66189800	
H	-1.76593900	0.36371100	-2.46722700	H	-0.18235900	-0.08761600	2.11219400	
H	0.12696900	-1.12297700	-3.10436900	H	-2.50252900	-2.67896300	-0.10911500	
H	0.92270700	-2.85225500	-1.50528000	H	-2.26051800	-0.32223400	-1.86569600	
H	-0.69109600	-2.89969300	-0.68433100	H	-0.37430600	-1.39896700	-2.86571300	
Rh	0.14596800	-0.33940500	-0.24304300	H	1.13903000	-2.89635100	-1.66341200	
P	2.31508300	-0.78371000	0.32086600	H	-0.02441600	-3.05977200	-0.25964900	
P	0.23344000	2.11424600	-0.08853100	Rh	0.33596600	-0.33905200	-0.43923700	
C	3.19468900	0.36123000	1.47171900	P	2.54227100	-0.42949700	0.41518800	
H	4.20442400	-0.01341200	1.67162000	P	-0.17172900	2.00745900	-0.26858600	
H	3.27689100	1.36302700	1.04299400	C	1.01966500	2.93708200	-1.34065300	
H	2.65508100	0.42856200	2.42116400	H	0.75474100	3.99947100	-1.37927200	
C	2.58211600	-2.40773300	1.15492700	H	2.03986500	2.84553600	-0.95539200	
H	3.64929800	-2.57493500	1.33715900	H	0.99793200	2.53898800	-2.36046800	
H	2.05535200	-2.42253500	2.11369000	C	-1.80144300	2.55224200	-0.94132900	
H	2.19450300	-3.22116000	0.53704500	H	-1.93151500	3.63296400	-0.81778800	
C	3.44782800	-0.85550900	-1.13295200	H	-1.84300600	2.31615500	-2.00982200	
H	4.46993400	-1.09000200	-0.81579800	H	-2.61787500	2.02008500	-0.44386600	
H	3.11195700	-1.62433100	-1.83458000	C	-0.05294400	2.92310200	1.33280200	
H	3.44721200	0.10650500	-1.65329500	H	-0.21453500	3.99354400	1.16720900	
C	1.56607900	2.91188900	-1.09560700	H	-0.80736700	2.56693600	2.03954800	

H	0.93317500	2.78024700	1.78200500	H	2.29746200	-0.17732400	2.74405200
C	3.16785800	0.84640200	1.59617800	C	2.21495300	-2.78835300	1.05539500
H	3.11517200	1.84286000	1.14794600	H	3.18983000	-3.10272500	1.44311700
H	2.56513800	0.84198500	2.50977100	H	1.47556800	-2.87876000	1.85683000
H	4.20969100	0.64140600	1.86559500	H	1.92302300	-3.45333600	0.23859500
C	3.00161700	-1.99717500	1.27175700	C	3.67360500	-1.06491700	-0.76478800
H	4.06230300	-1.98999100	1.54444700	H	4.58556400	-1.46485300	-0.30802400
H	2.40929900	-2.11646200	2.18419400	H	3.40435000	-1.69036400	-1.62115500
H	2.80581800	-2.85141500	0.61820300	H	3.87586400	-0.05213800	-1.12623400
C	3.75320900	-0.33592100	-0.97757900	C	2.07162900	2.89048800	-0.70461700
H	4.78073700	-0.40028400	-0.60319400	H	2.93866000	2.45091400	-0.20248700
H	3.57913300	-1.16060300	-1.67539200	H	2.16130900	2.69726000	-1.77862400
H	3.63640200	0.60655600	-1.52158200	H	2.08816500	3.97393500	-0.54446800
C	-3.91892200	-1.00915500	-0.00860300	C	-0.76663100	3.22055800	-0.89049800
H	-4.57775600	-1.64981600	0.59761700	H	-0.57379100	4.28138300	-0.69612700
H	-4.37697700	-0.86469500	-0.98999200	H	-0.74227100	3.05010500	-1.97123400
25b				H	-1.76811600	2.97305700	-0.52650800
				C	0.43702000	2.76735900	1.68146300
O	-4.45729200	-0.42804300	1.10471800	H	0.53458300	3.85781400	1.71081800
C	-3.27101600	-0.57003500	1.88566000	H	-0.51680500	2.49276500	2.14313300
C	-2.12829700	-0.16925100	0.93074100	H	1.24450900	2.32691400	2.27329300
C	-0.72144500	-0.62684700	1.21824400	25-TS			
C	-4.14815300	-0.41934000	-0.29298400				
C	-2.66001300	-0.78661900	-0.38550100	O	-3.09884900	0.02708200	1.89429500
C	-1.88837800	-0.34602400	-1.59723200	C	-2.97320300	-0.98714800	-0.21097000
C	-0.89048900	-1.11384300	-2.19205000	C	-1.56642100	-1.57160300	-0.18364000
C	-0.15872500	-2.12925200	-1.49429200	C	-3.21118700	1.12981500	1.00206100
H	-3.15365900	-1.60944500	2.22932100	C	-2.97555500	0.55937900	-0.43246600
H	-3.35121100	0.07940300	2.76292700	C	-1.75779300	1.12936900	-1.12450200
H	-2.15281000	0.92416300	0.83185900	C	-1.00371800	0.48930200	-2.11417700
H	-0.23902000	-0.08811800	2.03758700	C	-0.97185800	-0.96643200	-2.14862800
H	-0.66365100	-1.70600400	1.39210700	H	-3.58535000	-1.49103800	-0.96600000
H	-4.79621000	-1.13482000	-0.80997600	H	-1.50687700	-2.62027000	-0.46959900
H	-4.34076800	0.58206000	-0.70726700	H	-1.13582400	-1.45759500	0.82679200
H	-2.57018700	-1.87625500	-0.28255000	H	-4.21214300	1.57849900	1.07815800
H	-2.25680300	0.51989400	-2.14373800	H	-2.47016900	1.87702900	1.29911000
H	-0.50099800	-0.77163500	-3.15180900	H	-3.84092500	0.81853900	-1.05936100
H	0.61855600	-2.64871500	-2.05092900	H	-1.69414200	2.21419100	-1.09499200
H	-0.65966800	-2.75453600	-0.75834300	H	-0.37657900	1.06463400	-2.78930900
Rh	0.35484700	-0.23077200	-0.52917100	H	-0.13406600	-1.41885800	-2.67745900
P	2.29027800	-1.04697900	0.45689200	H	-1.89357000	-1.50485700	-2.34628800
P	0.49886700	2.15466500	-0.06199200	Rh	0.08484300	-0.05066400	-0.35154300
C	3.00844500	-0.16753800	1.91206600	P	1.77805800	-1.62174100	0.26497500
H	3.93237900	-0.65703500	2.23869300	P	1.34503300	1.86659600	0.18870300
H	3.23414900	0.87190600	1.65895700	C	1.20543200	-3.37617200	0.36835100

H	2.04994500	-4.03829900	0.58719100	H	2.78646000	-1.93742400	-2.39103900
H	0.45924700	-3.48930200	1.16019600	Rh	-0.13867000	-0.17977400	-0.28775300
H	0.75526700	-3.68416100	-0.57983700	P	-1.14219000	1.96986100	-0.18766600
C	3.16002700	-1.75054400	-0.95402500	P	-1.98428400	-1.30780300	0.28137600
H	3.66488700	-0.78903400	-1.07007300	C	0.22621000	3.20750900	-0.10978700
H	3.89081800	-2.50063100	-0.63195000	H	-0.17612900	4.21685500	0.03014600
H	2.76001500	-2.04454500	-1.92927300	H	0.89685600	2.95436800	0.71597200
C	2.64300200	-1.43027700	1.88871000	H	0.79780000	3.18529600	-1.04312700
H	1.90914900	-1.45843400	2.70051700	C	-2.12749400	2.52910800	-1.64615300
H	3.36647100	-2.23879500	2.03958000	H	-3.03862900	1.93463800	-1.75171000
H	3.17282300	-0.47530400	1.94016200	H	-2.40278400	3.58450100	-1.54317200
C	3.16728800	1.92309000	-0.12639300	H	-1.53291400	2.40496400	-2.55617400
H	3.68745100	1.12989400	0.41622100	C	-2.18688500	2.45513000	1.25743100
H	3.36352200	1.79864200	-1.19590900	H	-1.63164300	2.27936900	2.18386500
H	3.57714300	2.88683700	0.19493800	H	-2.44555200	3.51798800	1.19935300
C	0.80965200	3.43137000	-0.63933400	H	-3.11440000	1.87632500	1.29125100
H	-0.20603700	3.69727400	-0.33493000	C	-3.58111900	-0.79102400	-0.48599000
H	1.47929100	4.25257900	-0.36259800	H	-3.84924900	0.22480300	-0.18574700
H	0.82992400	3.31541200	-1.72740000	H	-3.49414300	-0.82191700	-1.57601500
C	1.21950000	2.30877200	1.97952000	H	-4.38437100	-1.46802800	-0.17462100
H	1.74470400	3.24720200	2.18898000	C	-1.96130300	-3.11229000	-0.11070200
H	0.16686300	2.41900900	2.25668100	H	-1.09891400	-3.60435500	0.34687100
H	1.64957100	1.51594700	2.59803000	H	-2.87315000	-3.58251900	0.27337000
C	-3.62210800	-1.08785800	1.18892500	H	-1.92034500	-3.26347300	-1.19323500
H	-3.36384400	-1.99512800	1.74121100	C	-2.33997900	-1.29250400	2.09232300
H	-4.71939800	-1.02544300	1.10649700	H	-3.25199700	-1.85960400	2.31051900
				H	-1.50370900	-1.74347600	2.63448400
				H	-2.46303900	-0.26673400	2.44794200
26				C	3.54530400	1.10428800	0.57966700
O	2.42576800	1.15832200	1.46526900	H	3.53342900	2.00672300	-0.03743500
C	3.34780300	-0.20290100	-0.21631200	H	4.48193200	1.08418800	1.15629100
C	2.54384900	0.03460300	-1.50322100				
C	2.34284100	-0.15680800	2.01382700	27			
C	2.59935600	-1.11438800	0.81713600	O	2.38109900	0.15293500	-0.20291500
C	1.34796800	-1.78583500	0.27891100	C	1.73123400	-1.06316000	0.18057300
C	1.08132600	-1.92007500	-1.07511000	C	0.26871600	-0.71631200	0.56931700
C	1.97097800	-1.25710900	-2.10039700	C	-0.76891900	-1.34096400	-0.37813500
H	4.31003000	-0.65014400	-0.48709000	C	1.37612600	1.10329000	-0.52495300
H	3.15782700	0.56792600	-2.23826100	C	0.25311200	0.83286300	0.49501700
H	1.70358100	0.73579300	-1.28488700	C	-1.09114100	1.43305100	0.18530900
H	3.11297800	-0.28630400	2.78839000	C	-2.18806500	0.70966700	-0.06363900
H	1.35585900	-0.27102800	2.46753500	C	-2.18153500	-0.79815800	-0.12265800
H	3.26477300	-1.92677400	1.14012300	H	2.30405000	-1.49167600	1.01023600
H	0.85300400	-2.45225800	0.98387500	H	1.75397900	-1.78254700	-0.65315100
H	0.39929500	-2.69051400	-1.42198300	H	0.05108900	-1.04422900	1.59292900
H	1.40512500	-1.04300100	-3.01414800				

H	-0.75299200	-2.43419600	-0.28121200	H	1.21663400	3.60611800	-0.59554100
H	-0.48900500	-1.11572700	-1.41647500	H	1.45967900	2.00020000	-1.35095600
H	1.81909700	2.10087900	-0.44508200	H	-0.07131400	2.86502000	-1.59737200
H	1.00716800	0.96745700	-1.55577400	C	1.41408900	1.73743800	1.76358500
H	0.60316400	1.23168000	1.45830400	H	2.20037400	1.10543900	1.34929400
H	-1.15599600	2.52084500	0.20310700	H	1.81384300	2.74262500	1.94104800
H	-3.13733800	1.21484800	-0.23692200	H	1.08315800	1.31722900	2.71865600
H	-2.86150000	-1.14288100	-0.91309800	Cl	-2.68740600	1.37615400	-1.16493700
H	-2.58767500	-1.20959300	0.81546600				
				28b			
28a				C	0.86508600	-1.89408800	1.02413300
C	-0.72201900	-1.82423100	1.15016500	C	2.25999600	-1.91359600	0.63554400
C	-2.08793800	-2.03138100	0.71326100	C	2.67867200	-1.86857600	-0.67760700
C	-2.46094100	-2.06413600	-0.61701700	C	4.10157200	-1.61504100	-1.08058900
C	-3.88841700	-1.98351400	-1.07270900	C	-0.15192300	-1.80732300	0.04765600
C	0.31841700	-1.64790900	0.20674000	C	-1.62930100	-1.95987700	0.36907900
C	1.75885500	-1.57535100	0.66204400	C	-1.98830200	-2.05598300	1.85583500
C	2.33284300	-3.00121200	0.75578000	O	-2.34553000	-0.91446500	-0.30356100
O	2.46686000	-0.76187400	-0.27868400	C	-3.68166200	-1.24529000	-0.67355600
C	3.87126200	-0.65246400	-0.05761800	C	-4.19063200	-0.19529000	-1.61648800
C	4.41034000	0.45244700	-0.91844100	C	-5.32034800	0.48925500	-1.43719000
C	5.41731600	0.30386800	-1.77858300	H	0.62732800	-1.92511900	2.08243800
H	-0.52304100	-1.76645400	2.21754800	H	2.99873400	-1.79166400	1.42551000
H	-2.86562200	-1.96628000	1.47213700	H	2.00688800	-2.17231200	-1.47652700
H	-1.73211900	-2.32056200	-1.38250900	H	4.51023900	-2.46882300	-1.63745800
H	-4.02129700	-1.12460000	-1.74128900	H	4.15805700	-0.73140100	-1.72757100
H	-4.17595200	-2.88916600	-1.62312700	H	4.73878700	-1.42952300	-0.20981400
H	-4.57370200	-1.85616000	-0.22833300	H	0.05756900	-2.14772000	-0.96455400
H	0.23740800	-2.10640300	-0.77917200	H	-1.93496100	-2.91365500	-0.09745400
H	1.82042100	-1.10846900	1.65942900	H	-3.07493800	-2.09733700	1.98379600
H	3.35475000	-3.00742600	1.14910500	H	-1.57292600	-2.97319800	2.28769800
H	1.71571100	-3.60791700	1.42634800	H	-1.61282800	-1.20486900	2.42815300
H	2.33789100	-3.47611800	-0.23196700	H	-3.68541200	-2.23135000	-1.17105600
H	4.06159600	-0.42795600	1.00828900	H	-4.34050000	-1.31951600	0.20537800
H	4.38785500	-1.59368200	-0.29101800	H	-3.57615100	-0.02566800	-2.50005400
H	3.93686400	1.42542600	-0.79274400	H	-5.66819600	1.21996900	-2.16205600
H	5.79831000	1.13639900	-2.36351000	H	-5.94655600	0.33898400	-0.55984300
H	5.90251000	-0.65833900	-1.92992400	Rh	1.17230400	-0.03489800	0.00158100
Rh	-1.19319900	-0.08094600	0.02416400	P	-0.23791600	1.68093600	0.63640100
P	-0.00268800	1.80815500	0.57716200	C	0.69872400	3.04770000	1.45446800
C	-1.06423400	3.10094000	1.35819400	H	1.52093900	3.35148200	0.80377300
H	-1.44207800	2.73010700	2.31617300	H	0.04117500	3.90087500	1.66032100
H	-0.49758900	4.02433900	1.52765800	H	1.12069000	2.68533700	2.39731100
H	-1.91655200	3.29516200	0.70384600	C	-1.64346700	1.47259500	1.81780000
C	0.73002300	2.66585700	-0.88097700	H	-2.11528200	2.44508300	2.00080200

H	-2.37605600	0.78587400	1.39299300	H	-3.80313800	1.52617600	0.40614200
H	-1.28091100	1.07644700	2.77156300	C	-2.80058600	-2.15538100	0.37825800
C	-1.05510900	2.51149800	-0.79299300	H	-3.82122300	-2.40777600	0.06915500
H	-1.76581400	1.81378700	-1.24469600	H	-2.08680700	-2.83481700	-0.09222100
H	-1.58611700	3.41796600	-0.47893300	H	-2.72829400	-2.25565600	1.46557300
H	-0.28840000	2.76732000	-1.52887500	Cl	0.22396600	-1.99776100	-1.23232600
Cl	2.52730000	1.61795300	-1.08388600				
				29b			
29a				O	3.35185800	-0.88867000	0.78864700
O	3.45142500	-0.60244900	0.81791400	C	2.48138600	-0.67091200	1.88029000
C	2.42062300	-1.34534500	1.45434900	C	1.03814600	-1.08011000	1.70159900
C	1.24214900	-0.51449700	1.91487900	C	0.00070200	-0.39281200	2.29264900
C	-0.03289200	-1.01595600	2.07083100	C	3.09771700	-0.22235100	-0.47008200
C	3.11488200	-0.10700100	-0.48554200	C	2.03218900	0.83299700	-0.35882600
C	2.01112100	0.90974400	-0.34918500	C	1.18901700	1.19432600	-1.43554700
C	1.10865800	1.29238300	-1.37377000	C	0.03259000	1.98666600	-1.16142000
C	-0.03277200	2.06225000	-0.99952700	C	-0.23348000	2.36610800	0.19635200
C	-0.24773900	2.35364300	0.39268400	H	2.52784700	0.36694500	2.24853000
H	2.90379200	-1.77078000	2.34420400	H	2.90499400	-1.30259000	2.67328100
H	2.07287300	-2.16947000	0.81872700	H	0.87664400	-2.08674800	1.32408700
H	1.49952100	0.41882500	2.41323100	H	-0.93839000	-0.88673500	2.51674100
H	-0.73560600	-0.52767800	2.73950000	H	0.18695000	0.53301800	2.83284400
H	-0.25194000	-2.04097400	1.78705200	H	2.76055700	-0.98499100	-1.18066600
H	2.77855200	-0.93638900	-1.12116600	H	2.20771200	1.57468400	0.41818200
H	2.21184500	1.62915900	0.44173900	H	1.28195900	0.71338200	-2.40551200
H	1.16633900	0.86868500	-2.37267500	H	-0.67530100	2.19914900	-1.95909300
H	-0.77796000	2.31798200	-1.74958500	H	0.61688200	2.62892000	0.82410900
H	0.62637000	2.58331000	1.00071600	Rh	-0.08555900	0.15890000	0.01569100
Rh	-0.09439800	0.17410800	0.06673400	P	-2.37216100	-0.44387300	-0.03373400
P	-2.38644800	-0.42600700	-0.12295600	C	4.44391100	0.35180500	-0.92481300
C	4.40232700	0.49944400	-1.04671600	H	5.20139100	-0.43880800	-0.92599400
H	4.74187900	1.33297400	-0.42170000	H	4.36773400	0.76382000	-1.93773000
H	5.19124400	-0.25925100	-1.06774300	H	4.77823200	1.14629500	-0.24733700
H	4.24154900	0.86857000	-2.06527300	C	-1.47348900	3.15932900	0.53511400
C	-1.46692800	3.13592800	0.82372700	H	-1.83793100	2.92913900	1.54201600
H	-1.82135900	2.82753300	1.81364000	H	-1.26019900	4.23793400	0.50857100
H	-1.23208600	4.20854900	0.88709000	H	-2.28684300	2.97057500	-0.17383200
H	-2.29598000	3.02748800	0.11711000	C	-2.69835100	-2.18556700	0.48923100
C	-2.96978800	-0.37015400	-1.87416100	H	-2.05138800	-2.84574000	-0.09213100
H	-4.00753500	-0.71081500	-1.96609400	H	-2.46704400	-2.31289000	1.55173300
H	-2.89168100	0.65242900	-2.25708600	H	-3.75074600	-2.44554600	0.32668100
H	-2.31314600	-1.01479500	-2.46478500	C	-3.63824500	0.45834200	0.97857900
C	-3.72411800	0.49969600	0.76991500	H	-4.61221400	-0.03785800	0.89983800
H	-4.68989600	0.00189000	0.62643900	H	-3.33416700	0.47078900	2.03029800
H	-3.50113000	0.53305900	1.84109900	H	-3.74401100	1.49190100	0.64260600

C	-3.10108500	-0.39494500	-1.72785800	H	3.42953900	0.46872600	1.87449700
H	-4.12683700	-0.78101600	-1.73590800	H	4.60541400	-0.26297300	0.75588900
H	-3.10271200	0.63302200	-2.10437900	H	3.86373500	1.30584600	0.37567200
H	-2.46801100	-1.00533200	-2.37748200	Cl	-0.35126700	-2.05338100	-1.06019000
Cl	0.14920900	-1.96068300	-1.39296000				
				29d			
29c				O	-3.15029800	-0.87335900	0.78852100
C	-1.31999500	-0.24376700	1.95688500	C	-2.38909600	-0.69356700	1.96338500
C	-2.01089300	1.18708700	-0.34652900	C	-0.90045000	-0.94098800	1.81732100
O	-3.56853800	-0.10363800	0.97130100	C	0.04715100	-0.08131000	2.34146300
C	-0.09743700	-0.85385000	2.12375300	C	-3.28520100	0.27491100	-0.06703000
C	-3.32000700	0.43099500	-0.34193200	C	-2.03128000	1.13476000	-0.13399300
C	-2.57207000	-0.96398900	1.50994800	C	-1.27374800	1.37334700	-1.29717300
C	-1.11678200	1.34723400	-1.42589200	C	0.00093500	2.01598800	-1.19621600
C	0.13315100	1.99694900	-1.17998200	C	0.47007300	2.41437700	0.09451300
C	0.44813700	2.39868300	0.16434200	H	-2.56600600	0.29705100	2.41327200
H	-3.05377700	-1.39264700	2.39909600	H	-2.77656700	-1.44158000	2.66876300
H	-2.31187500	-1.78511000	0.83138200	H	-0.62807600	-1.96159600	1.56137600
H	-1.48846700	0.72675900	2.42193900	H	1.03812800	-0.42980200	2.61463900
H	0.65144200	-0.40702800	2.77111200	H	-0.25533900	0.85812500	2.79959400
H	0.02864000	-1.90157800	1.86918600	H	-1.96461000	1.86628400	0.66720400
H	-2.00779100	1.95871100	0.41748900	H	-1.53765800	0.89732100	-2.23590700
H	-1.28334500	0.85384800	-2.37862500	H	0.62569000	2.10575400	-2.08094000
H	0.85271900	2.10253900	-1.98772900	H	-0.26451200	2.79224100	0.80429100
H	-0.36487600	2.77789600	0.78143400	Rh	0.05055900	0.22339300	0.05168300
Rh	0.07270500	0.22597900	0.05052300	P	2.24078900	-0.63276600	-0.06088500
P	2.30273400	-0.56584400	-0.04489300	C	1.81845300	3.07553900	0.24664800
C	1.75205900	3.10364400	0.45645600	H	2.24840600	2.89413500	1.23710300
H	2.12118100	2.88136700	1.46335900	H	1.72375700	4.16555400	0.13370700
H	1.61588500	4.19354200	0.39857200	H	2.53248300	2.73065700	-0.50892700
H	2.53378900	2.83703100	-0.26190000	H	-4.06993000	0.91399300	0.37844200
H	-4.11065800	1.19124100	-0.42397800	C	-3.78829300	-0.26026900	-1.40251500
C	-3.54153600	-0.59262000	-1.45405300	H	-4.04388700	0.56193300	-2.08092100
H	-2.75847200	-1.35277400	-1.48074300	H	-4.68917800	-0.85713400	-1.23029300
H	-3.56374200	-0.09089300	-2.42942500	H	-3.03418100	-0.90226400	-1.86591800
H	-4.51355800	-1.07333200	-1.30237500	C	2.36367800	-2.37821900	0.52674100
C	2.58360800	-2.27088900	0.60855800	H	2.10857800	-2.43368000	1.59018400
H	1.85645000	-2.94827500	0.15737500	H	1.65112800	-2.98141700	-0.03957900
H	3.60214300	-2.59922300	0.37221400	H	3.38048500	-2.76249300	0.38809200
H	2.45552800	-2.27863400	1.69529200	C	2.94965500	-0.70840500	-1.76217400
C	2.94117500	-0.69591900	-1.77334700	H	3.08614900	0.30513100	-2.15280600
H	3.00358000	0.29832900	-2.22680700	H	3.91563400	-1.22666700	-1.76916700
H	3.93369300	-1.16089300	-1.79826800	H	2.23562600	-1.23849300	-2.39739200
H	2.23452500	-1.30121600	-2.34733700	C	3.61433300	0.15715200	0.90450600
C	3.68315600	0.32542600	0.81935700	H	4.52787000	-0.44300800	0.82583200

H	3.82276600	1.16194300	0.53146900	H	-2.57333400	-2.12127800	1.79230200
H	3.33686100	0.23605400	1.96029900	Cl	0.08022000	-2.02783700	-1.28087200
Cl	-0.39208800	-1.82248400	-1.42034600				
29a-TS				29b-TS			
O	3.72532000	-0.88834600	0.79448500	O	3.91629100	-0.73811500	0.87267100
C	2.56404400	-1.40580700	1.42067500	C	2.86706000	-0.88456100	1.82282600
C	1.55501300	-0.28249400	1.59579300	C	1.54811400	-1.06430300	1.10820200
C	0.14871000	-0.64364200	1.79425600	C	0.26380400	-0.86500600	1.73768500
C	3.30318400	-0.19164500	-0.37174400	C	3.44074500	-0.24604300	-0.38757900
C	2.13448400	0.72309900	0.00575800	C	2.11815900	0.45656300	-0.14074900
C	1.33096100	1.19414600	-1.15344800	C	1.36191100	0.99147800	-1.27399400
C	0.30956800	2.14096300	-0.99500400	C	0.39075400	1.98737800	-1.06011900
C	-0.23978000	2.33585700	0.31765900	C	-0.06042300	2.23783300	0.28379600
H	2.87754500	-1.80573000	2.39109200	H	2.83903000	-0.02980200	2.51807700
H	2.11593000	-2.21203300	0.82273500	H	3.08744700	-1.78363700	2.41217400
H	1.89865000	0.48467600	2.29002100	H	1.56547900	-1.91348100	0.42616700
H	-0.36241900	-0.12833200	2.60815900	H	-0.36310900	-1.75129300	1.80117900
H	-0.07079700	-1.71093500	1.75255900	H	0.22309000	-0.22521900	2.62148400
H	2.93704100	-0.91420800	-1.11772600	H	3.29198200	-1.08801800	-1.08055800
H	2.45179600	1.57503700	0.61081700	H	2.23644900	1.19748400	0.65073900
H	1.59351500	0.83122400	-2.14290700	H	1.56377300	0.62587600	-2.27631400
H	-0.20494200	2.52864800	-1.87233300	H	-0.12980400	2.41810400	-1.91303700
H	0.47065200	2.36534000	1.14572500	H	0.69815800	2.25823100	1.06812600
Rh	-0.29681300	0.14911600	-0.08069700	Rh	-0.30359400	0.07621600	-0.09606200
P	-2.47855400	-0.43611400	0.02657200	P	-2.53091000	-0.24772800	0.15078700
C	4.50779000	0.56677200	-0.91888700	C	4.51408700	0.68622700	-0.94754500
H	4.86783200	1.29772300	-0.18609000	H	5.47029400	0.15575700	-0.99920200
H	5.32082300	-0.13433400	-1.13216900	H	4.25002100	1.02498600	-1.95505700
H	4.25233400	1.09325600	-1.84439100	H	4.64145700	1.56159100	-0.30122000
C	-1.41341800	3.26805400	0.51552100	C	-1.15440700	3.25669300	0.51776900
H	-1.94647700	3.05015600	1.44669700	H	-1.61296700	3.13403400	1.50404000
H	-1.07874000	4.31430100	0.57494200	H	-0.75027300	4.27920000	0.47834000
H	-2.13098500	3.20179700	-0.31084100	H	-1.94511500	3.18993600	-0.23852200
C	-3.23671600	-0.52573400	-1.65223400	C	-3.01827800	-1.93120800	0.72960200
H	-4.27426800	-0.87744600	-1.60465000	H	-2.49280700	-2.67049300	0.12037200
H	-3.21294400	0.46250700	-2.12215000	H	-2.73147800	-2.06325600	1.77768500
H	-2.63613700	-1.21275100	-2.25430800	H	-4.10176000	-2.07025200	0.64097400
C	-3.67837000	0.60936000	0.96931700	C	-3.52352200	0.82158000	1.28857100
H	-4.68346100	0.17488300	0.92318700	H	-4.56326200	0.47667500	1.32081700
H	-3.36957700	0.67609900	2.01735600	H	-3.10267300	0.77265000	2.29770600
H	-3.71038700	1.62000900	0.55586200	H	-3.50777700	1.86200900	0.95827900
C	-2.80907300	-2.11080300	0.72359800	C	-3.41956100	-0.09120600	-1.45716400
H	-3.86024700	-2.38914100	0.58862300	H	-4.48911900	-0.30521300	-1.34716800
H	-2.16121100	-2.82671500	0.21168300	H	-3.29243500	0.92150900	-1.85233100
				H	-2.96630700	-0.79800100	-2.15750800

Cl	-0.32317200	-2.06593000	-1.45432000
29c-TS			
C	-1.61502400	0.06272400	1.62772200
C	-2.13293800	1.01356900	-0.05049500
O	-3.87955700	-0.28815500	0.98151200
C	-0.25443800	-0.42574700	1.84033100
C	-3.49436800	0.31885400	-0.25437000
C	-2.75311900	-0.93276000	1.55329600
C	-1.30541000	1.26082400	-1.25266700
C	-0.18281400	2.09976900	-1.19057600
C	0.40160900	2.37819100	0.09038100
H	-3.05997000	-1.25049900	2.55603100
H	-2.44195100	-1.81750200	0.98043500
H	-1.86003900	0.92339700	2.25025500
H	0.31500600	0.09221200	2.61285600
H	-0.14197700	-1.50970100	1.86928900
H	-2.25278500	1.94409200	0.50447700
H	-1.60894500	0.83641500	-2.20226200
H	0.35871700	2.33642600	-2.10441600
H	-0.28787700	2.56056200	0.91674000
Rh	0.26902300	0.16416200	-0.09238600
P	2.40196800	-0.55628100	0.09922900
C	1.65333400	3.22238300	0.17837100
H	2.18549200	3.05774800	1.12066600
H	1.40594700	4.29328000	0.13316000
H	2.34502400	3.01326700	-0.64589800
H	-4.24030600	1.10900800	-0.41291500
C	-3.58690100	-0.67908000	-1.41258700
H	-2.78010800	-1.41679400	-1.39223000
H	-3.55722000	-0.16657900	-2.38086000
H	-4.54997600	-1.19442400	-1.33987100
C	2.62552000	-2.16355600	0.97650100
H	1.94040100	-2.89274100	0.53763100
H	3.65961500	-2.51414900	0.88356800
H	2.38507700	-2.04371700	2.03738800
C	3.14865400	-0.87601000	-1.55593600
H	3.18318600	0.05465400	-2.13092800
H	4.16260200	-1.28263000	-1.46373800
H	2.50551500	-1.58691200	-2.08111100
C	3.67833900	0.49372300	0.93007100
H	3.36751400	0.71993800	1.95465900
H	4.63875500	-0.03336600	0.96019200
H	3.81084200	1.43587700	0.39383000
Cl	-0.21625300	-2.12017600	-1.03649300

29d-TS

O	-3.99777200	-0.08874200	0.97392700
C	-2.96215800	-0.09320300	1.94334400
C	-1.67555600	-0.55332300	1.29974900
C	-0.36693100	-0.36143200	1.87629400
C	-3.52294300	0.24961100	-0.34021800
C	-2.10004900	0.77861600	-0.21562500
C	-1.30708400	1.03215400	-1.41812600
C	-0.21592000	1.91881700	-1.36602000
C	0.29686200	2.32231600	-0.08304600
H	-2.84526900	0.89174700	2.42632000
H	-3.26478700	-0.80797400	2.71822900
H	-1.79157500	-1.51677300	0.80733900
H	0.16829900	-1.27516200	2.12264700
H	-0.24364300	0.43865900	2.60908400
H	-2.09013900	1.64083700	0.45021800
H	-1.56779800	0.54458500	-2.35127100
H	0.33346600	2.14034100	-2.27866300
H	-0.43311700	2.56030800	0.69285600
Rh	0.27951000	0.12289200	-0.10470600
P	2.45591700	-0.42931700	0.20237700
C	1.50518800	3.23098600	-0.02476200
H	1.98371400	3.20069700	0.95900400
H	1.21468000	4.27619800	-0.20747300
H	2.25476000	2.96512200	-0.77891700
H	-4.14408300	1.09423400	-0.67758100
C	-3.73002500	-0.92383300	-1.29623700
H	-3.62100400	-0.60282900	-2.33860400
H	-4.74626000	-1.30926700	-1.16685100
H	-3.01512800	-1.73129200	-1.11401600
C	2.73947100	-1.99284600	1.14059900
H	2.46983900	-1.85139700	2.19207800
H	2.10404500	-2.77051000	0.71000000
H	3.79220400	-2.29183700	1.08374300
C	3.30430900	-0.74859800	-1.40333500
H	3.29451500	0.16087900	-2.01200800
H	4.34086500	-1.07091500	-1.24997500
H	2.74261400	-1.52571900	-1.92809900
C	3.62118600	0.72243800	1.06303800
H	4.60569800	0.25261900	1.16823500
H	3.73370900	1.65200100	0.50129100
H	3.23648600	0.96474000	2.05843900
Cl	0.03148700	-2.22941000	-1.03325000

30a				O	4.14023200	-1.15101800	0.91314200
O	3.84921000	-1.40648100	0.46708000	C	2.90057500	-1.59408600	1.48334300
C	2.49620600	-1.74425600	0.75859700	C	1.79823600	-1.04991700	0.55614700
C	1.89058500	-0.42228200	1.24517500	C	0.42102800	-0.78291400	1.12005900
C	0.37454600	-0.36549700	1.37903800	C	3.90372000	-0.22704400	-0.16445200
C	3.85535500	-0.12274300	-0.16505100	C	2.46454500	0.25409600	0.06437600
C	2.51864400	0.58679800	0.23507600	C	1.72324000	0.87586900	-1.08369200
C	1.64274300	0.88788900	-0.96973000	C	0.78299500	1.88438500	-0.93992900
C	0.67830700	1.89950900	-1.01980600	C	0.05138000	2.13543200	0.28125200
C	-0.10005600	2.29663100	0.11383000	H	2.80486900	-1.19369600	2.50443600
H	2.50667800	-2.52497700	1.52569900	H	2.90215000	-2.68872600	1.54133300
H	1.96809900	-2.12194900	-0.12881100	H	1.69592600	-1.72530200	-0.30154500
H	2.33143300	-0.21632900	2.23304900	H	-0.13221100	-1.70494200	1.31280700
H	0.06163100	0.33896800	2.15643700	H	0.44330800	-0.15630800	2.01998900
H	-0.03578700	-1.35545800	1.60342200	H	3.95393300	-0.77169600	-1.12310900
H	3.87437700	-0.26741800	-1.25698900	H	2.47993500	0.95747800	0.91047100
H	2.73432700	1.53172800	0.74972800	H	2.03008700	0.60188000	-2.09105300
H	1.98485500	0.49937300	-1.92585100	H	0.40751000	2.34946200	-1.85414400
H	0.31961700	2.20091700	-2.00742400	H	0.59302800	1.98865100	1.21705000
H	0.39203700	2.28051600	1.08662000	Rh	-0.56790400	0.18458100	-0.42132200
Rh	-0.50288600	0.18722200	-0.39346300	P	-2.61135400	-0.23717100	0.53070400
P	-2.62677800	-0.32360300	0.43593500	C	4.97951900	0.84789500	-0.13726300
C	5.11603900	0.61746900	0.26232200	H	5.97300800	0.39449500	-0.21480400
H	5.10137700	0.81321300	1.34067200	H	4.85230700	1.54285500	-0.97571900
H	6.00254600	0.01531500	0.03780000	H	4.93455100	1.41444700	0.79958900
H	5.20415400	1.57343500	-0.26703200	C	-0.90160800	3.31444800	0.32284100
C	-1.14119900	3.38603800	-0.02716400	H	-1.58218100	3.24909500	1.17813200
H	-1.88072300	3.33893400	0.77913700	H	-0.35699800	4.26548500	0.42072200
H	-0.68139000	4.38444000	0.01998900	H	-1.51031500	3.37996300	-0.58752500
H	-1.67679900	3.31630400	-0.98146900	C	-2.92680800	-1.97280800	1.06410600
C	-3.84880600	-0.34815300	-0.94648900	H	-2.62814200	-2.63888200	0.25039200
H	-4.84522800	-0.63868400	-0.59481000	H	-2.32923200	-2.20742700	1.95031600
H	-3.90926700	0.64203200	-1.40976000	H	-3.98591900	-2.11868400	1.30361400
H	-3.49763600	-1.06328900	-1.69586100	C	-3.16585000	0.74039500	1.99814800
C	-3.41950900	0.77814400	1.69156800	H	-4.16079000	0.42170700	2.32935400
H	-4.40917200	0.40470500	1.97815500	H	-2.45759400	0.60314500	2.82119700
H	-2.78867600	0.83023200	2.58470700	H	-3.19938300	1.80441600	1.74921100
H	-3.52514800	1.78932800	1.28836100	C	-3.93439500	0.06628000	-0.71882200
C	-2.81620500	-1.99457700	1.19123200	H	-4.92614500	-0.16051700	-0.31086500
H	-3.87084000	-2.22857500	1.37442300	H	-3.91218300	1.11195500	-1.04241700
H	-2.38075000	-2.72615000	0.50541100	H	-3.73421400	-0.57223200	-1.58397500
H	-2.27441100	-2.03852100	2.14132300	Cl	-0.89003800	-1.80230900	-1.85919600
Cl	-0.52631200	-1.98982300	-1.54107900				
				30c			
30b				C	-1.79708400	-0.48084200	1.45930800

C	-2.49127200	0.62900600	0.62448800	C	-1.86904600	-0.75625100	0.79358800
O	-3.61499000	-1.37875600	0.18175800	C	-0.43682800	-0.59020500	1.24874200
C	-0.27781100	-0.39259400	1.49800400	C	-3.95358700	0.26857700	0.17896500
C	-3.88940600	-0.01104600	0.47369600	C	-2.43923700	0.57689200	0.25518700
C	-2.40162100	-1.76798600	0.84627300	C	-1.71418100	1.05865000	-0.97030100
C	-1.79316300	0.87772400	-0.69793700	C	-0.67668400	1.97844100	-0.93904700
C	-0.82407700	1.86168900	-0.88734400	C	0.15129000	2.22415400	0.21920200
C	0.07772900	2.27744100	0.15026900	H	-2.77328900	-0.55802600	2.77601700
H	-2.62909100	-2.50804700	1.62617400	H	-3.01547600	-2.16950500	2.05406700
H	-1.73587200	-2.22200400	0.10651200	H	-1.89824800	-1.50384300	-0.00713400
H	-2.16153100	-0.38727800	2.49543000	H	0.03646600	-1.55039600	1.46851000
H	0.06221700	0.32791400	2.24990900	H	-0.34032000	0.08497300	2.10790200
H	0.17074800	-1.36989100	1.70489800	H	-2.30188300	1.31878500	1.05452300
H	-2.54485300	1.56394900	1.19629600	H	-2.09786800	0.76219700	-1.94227700
H	-2.23482500	0.43319600	-1.58421200	H	-0.31651000	2.35321600	-1.89972500
H	-0.56871300	2.12969600	-1.91576900	H	-0.33753500	2.17898300	1.19304500
H	-0.31248600	2.29708100	1.16832600	Rh	0.53741800	0.18430200	-0.40510200
Rh	0.44592000	0.17374400	-0.34029000	P	2.58138700	-0.38967900	0.45903800
P	2.62814500	-0.29567000	0.31519600	C	1.21431200	3.30194300	0.13337600
C	1.09407800	3.36402800	-0.13219700	H	1.94177700	3.21256500	0.94686300
H	1.90865800	3.35059000	0.59962400	H	0.77252100	4.30675600	0.21014400
H	0.63476500	4.36247000	-0.07933800	H	1.76320900	3.25917700	-0.81552600
H	1.53586900	3.26021800	-1.13066800	H	-4.53637600	1.16919900	0.41605900
H	-4.38472800	0.06788500	1.45967400	C	-4.45895500	-0.31511800	-1.13813000
C	-4.83910100	0.54579100	-0.57616800	H	-4.46635900	0.44243000	-1.93085500
H	-4.41604000	0.48192600	-1.58263500	H	-5.48438700	-0.67262100	-1.00132500
H	-5.07854500	1.59336600	-0.36011900	H	-3.84652200	-1.16125900	-1.46828100
H	-5.77139700	-0.02802600	-0.56911200	C	2.77508500	-2.14211200	0.99561200
C	2.91622900	-1.97060200	1.02857000	H	2.20223700	-2.31830800	1.91123700
H	2.44874700	-2.70544900	0.36795600	H	2.37948100	-2.78496200	0.20484400
H	3.98759000	-2.17711800	1.12801800	H	3.82787200	-2.37752700	1.18683800
H	2.45003300	-2.03980300	2.01640700	C	3.87181600	-0.20123800	-0.84604600
C	3.74253500	-0.26615800	-1.15566400	H	3.92253300	0.84160600	-1.17517100
H	3.73670400	0.73024200	-1.60937900	H	4.85766900	-0.50815300	-0.47844400
H	4.77145000	-0.52882600	-0.88430900	H	3.58538900	-0.82373500	-1.69867800
H	3.35760900	-0.98416300	-1.88547200	C	3.26747100	0.55065100	1.89433200
C	3.48257000	0.80814200	1.52750700	H	4.24238600	0.15103000	2.19589400
H	2.92250100	0.82552300	2.46807400	H	3.38164400	1.60581900	1.63167000
H	4.50189700	0.45985800	1.72943900	H	2.57808100	0.48116300	2.74164500
H	3.52697200	1.82853900	1.13686500	Cl	0.57444800	-1.87254700	-1.77567900
Cl	0.42682600	-1.99781200	-1.51025600				
				30a-TS			
30d				O	-3.83803600	0.81390600	1.06302500
O	-4.18110600	-0.68553700	1.23854700	C	-3.28103300	-0.42326500	1.48250100
C	-2.94776700	-1.09945100	1.83124400	C	-2.55046600	-1.02407900	0.24631100

C	-1.24290900	-1.73221100	0.59591900	C	3.23397700	1.37299000	-0.26001700
C	-2.86590100	1.40456400	0.20541600	C	2.30025100	0.32564900	0.34819400
C	-2.37745300	0.23242400	-0.68023900	C	0.99897300	0.72576100	1.02126500
C	-0.99307100	0.43818000	-1.26542000	C	0.32553700	-0.20841000	1.85536000
C	-0.23801700	-0.59135600	-1.89103700	C	0.62883500	-1.61216600	1.62378700
C	-0.45365800	-1.95300600	-1.42944100	H	4.06800700	-1.46271600	-0.88569600
H	-4.09532300	-1.05061900	1.85570200	H	3.54663900	-0.88502900	-2.48877800
H	-2.56459200	-0.25728400	2.30307000	H	1.49628300	0.02382500	-1.60429700
H	-3.22579600	-1.72865900	-0.25192100	H	0.56162600	-2.14611800	-1.34250200
H	-1.29600000	-2.82076100	0.60842600	H	1.77023700	-2.64787300	-0.14556700
H	-0.83756800	-1.42411000	1.56742000	H	2.90973300	-0.24346600	1.06943100
H	-3.09229700	0.14410900	-1.51363100	H	0.81795900	1.78645000	1.18068200
H	-0.80699700	1.45298800	-1.61538200	H	-0.36473300	0.09248500	2.64083400
H	0.49722900	-0.37942500	-2.66455600	H	1.68252700	-1.86612100	1.67362500
H	-1.47307900	-2.32290100	-1.50316300	Rh	-0.60487800	-0.40736500	0.00889200
Rh	0.51461000	-0.42697500	0.03308900	C	-0.25485700	-2.69534100	2.19385400
P	2.11445500	1.24566800	-0.07694000	H	-1.30974400	-2.40969500	2.18437300
C	3.82796700	0.62856300	-0.37225300	H	0.04416900	-2.91217100	3.23087400
H	4.04325500	-0.13738200	0.37701400	H	-0.15275700	-3.62413900	1.62354100
H	3.88985800	0.17055000	-1.36459300	H	2.64472900	2.09527900	-0.85133100
H	4.56288800	1.43910600	-0.30402000	C	4.12355500	2.12752500	0.71683100
C	1.93601000	2.56746600	-1.36210700	H	4.82377400	2.77238500	0.17597600
H	1.00354900	3.11877000	-1.20572300	H	3.52164200	2.75811100	1.38262200
H	2.77225600	3.27446400	-1.32008900	H	4.70538800	1.42795100	1.32733600
H	1.90718300	2.12029000	-2.36121800	Cl	-1.98140600	-1.58079800	-1.61444300
C	2.28491100	2.22210200	1.48039300	P	-2.24683100	1.19525900	-0.00521600
H	3.11119600	2.93969800	1.41701500	C	-2.53582300	1.98289200	-1.64898500
H	1.35431600	2.76215300	1.68192300	H	-2.74049900	1.19001500	-2.37303100
H	2.46207200	1.52077100	2.30008800	H	-3.37752900	2.68441300	-1.61356800
Cl	1.85559500	-1.35571800	1.84951200	H	-1.63492500	2.51759000	-1.96603500
C	0.56515200	-3.02893300	-1.72498000	C	-2.04416100	2.66029600	1.10940800
H	0.35001500	-3.48409600	-2.70367100	H	-1.15346300	3.22847100	0.82399200
H	1.58533900	-2.63711900	-1.73340400	H	-2.91589300	3.32133100	1.04878800
H	0.51864500	-3.82535200	-0.97547000	H	-1.92505900	2.33142500	2.14684900
H	-2.01608500	1.76806600	0.81197700	C	-3.91832000	0.56756600	0.45973600
C	-3.50498300	2.56632800	-0.53723900	H	-4.68250800	1.34492700	0.34288100
H	-4.35597500	2.21580200	-1.13190400	H	-4.14946100	-0.28590900	-0.18226200
H	-3.86614700	3.32184400	0.16789500	H	-3.90855200	0.22686900	1.49991000
H	-2.78235000	3.04327900	-1.20953100				
				30c-TS			
30b-TS				O	3.05326900	1.31347200	1.17659900
O	4.06944700	0.60834200	-1.15654700	C	2.81324700	-0.70254800	-0.00219500
C	3.49390700	-0.68458000	-1.41316700	C	1.60950200	-1.38915200	0.63881800
C	2.05763300	-0.58227700	-0.88176900	C	2.76672600	1.75642800	-0.15064200
C	1.21928100	-1.79805600	-0.54493500	C	2.39061200	0.46178800	-0.96169800

C	0.95361800	0.38309100	-1.45698100	C	0.94998200	0.47151700	-1.30538400
C	0.30770800	-0.82071100	-1.85720700	C	0.24775500	-0.63085200	-1.86719000
C	0.68955400	-2.06372700	-1.20076200	C	0.61552300	-1.94846900	-1.37510400
H	3.42819200	-1.43485700	-0.53837100	H	4.23632400	-1.19678200	0.67224500
H	1.76892400	-2.43326500	0.91009400	H	3.85559800	-0.38350600	2.21281400
H	1.28401300	-0.85852200	1.54449900	H	1.69165800	0.34059600	1.37682400
H	3.03688600	0.43595900	-1.85226900	H	0.80265600	-1.84340200	1.63246200
H	0.61435000	1.28662400	-1.96021800	H	1.92884400	-2.56402100	0.46790300
H	-0.48489300	-0.81660700	-2.60276400	H	3.92030400	1.59550400	-1.29039100
H	1.72683300	-2.36974100	-1.30895500	H	2.86639400	-0.46889500	-1.30062400
Rh	-0.34823200	-0.43562200	0.06909400	H	0.71474800	1.46928100	-1.66607000
C	-0.24467500	-3.25311500	-1.23449400	H	-0.51312600	-0.51308700	-2.63589700
H	-0.03997200	-3.86001600	-2.12961000	H	1.66993600	-2.18996800	-1.45888400
H	-1.29496500	-2.95161700	-1.24106600	Rh	-0.52490500	-0.44808100	0.05241200
H	-0.08765600	-3.89308100	-0.36050400	P	-2.22180400	1.08625000	-0.14692600
H	3.69795600	2.15946100	-0.58578900	C	-3.90156200	0.33586100	-0.28282600
C	1.74258000	2.87685000	-0.06807700	H	-4.04297100	-0.33643500	0.56688200
H	1.56033600	3.31643000	-1.05557800	H	-3.96677500	-0.25175300	-1.20393300
H	0.79727200	2.50423600	0.33816800	H	-4.68293200	1.10488300	-0.28951500
H	2.11876200	3.66611600	0.59051600	C	-2.18481100	2.24493100	-1.59107200
Cl	-1.43289400	-1.27503300	2.08622900	H	-1.29264900	2.87697100	-1.54393200
P	-2.19664000	0.94090600	-0.17340700	H	-3.07061600	2.88988200	-1.59861300
C	-2.50018500	2.08253300	1.24504000	H	-2.15679500	1.67908000	-2.52797400
H	-3.43448400	2.64171400	1.11760300	C	-2.38624900	2.23692700	1.28578500
H	-2.54567400	1.48126100	2.15686600	H	-3.24859400	2.90339900	1.16783600
H	-1.66877900	2.78836500	1.33785700	H	-1.47609700	2.83722900	1.38115200
C	-2.26728300	2.08247000	-1.63053300	H	-2.50002200	1.63558100	2.19145400
H	-3.21051300	2.63994800	-1.65094900	Cl	-1.70157600	-1.23317400	2.02915200
H	-1.43897300	2.79648700	-1.58608300	C	-0.27160800	-3.14325600	-1.62978500
H	-2.17820000	1.51106900	-2.56049700	H	-1.33226200	-2.88180800	-1.59427900
C	-3.79040100	0.02018500	-0.30998300	H	-0.04538500	-3.57030800	-2.61885700
H	-3.86420500	-0.65479600	0.54655600	H	-0.09335300	-3.92771100	-0.88724800
H	-4.64806000	0.70282100	-0.32538000	C	2.67343100	2.72659700	0.04464100
H	-3.79220800	-0.57940100	-1.22586800	H	2.14645900	3.21725400	-0.78318400
C	3.66625700	0.04329200	1.04463600	H	1.96829900	2.58089000	0.87002700
H	4.70759800	0.14860000	0.69134000	H	3.46382300	3.40113300	0.38900800
H	3.67696400	-0.43431800	2.02808500				
				32a			
30d-TS				O	-2.40903800	-0.51237700	0.60603400
O	4.16240000	0.89691600	0.63241800	C	-3.80894300	-0.71336000	0.84890000
C	3.68427900	-0.36022000	1.13197600	C	-4.65658300	-0.20938700	-0.29388200
C	2.20437000	-0.38664400	0.73660200	C	-5.48867900	-0.96463300	-1.01169900
C	1.38203200	-1.65901500	0.72704100	C	-1.86327700	-1.29056300	-0.45454700
C	3.29421700	1.40663800	-0.40772500	C	-0.41088700	-1.57838300	-0.18386200
C	2.31462100	0.24841000	-0.67342400	C	0.48716800	-1.78877700	-1.25754700

C	1.86105700	-2.17320000	-1.00391700	C	4.57855300	-1.18840100	-0.68300200
C	2.37841700	-2.34136300	0.26640100	C	5.48913500	-1.85741500	0.02538600
H	-3.99306900	-1.79317800	0.97559400	C	4.23912400	1.25189100	-1.17550400
H	-4.56250600	0.85578400	-0.51097700	H	4.24384800	0.33608300	0.78218200
H	-6.09213100	-0.55148400	-1.81555100	H	2.62545600	-1.76154700	0.89517700
H	-5.60622000	-2.02891400	-0.81566400	H	1.93432000	-0.35670300	1.73033000
H	-2.40211300	-2.25204000	-0.51029000	H	0.62246800	-1.98030200	-0.53699200
H	-2.00192400	-0.78978500	-1.42282800	H	-0.17075800	-1.46660300	2.42644100
H	-0.27118400	-2.11936600	0.75173900	H	-2.40260600	-2.30756900	1.80105900
H	0.17542800	-1.62675000	-2.28651300	H	-1.25238500	-2.71723200	-1.03919500
H	2.54878400	-2.13730800	-1.84692500	H	-3.76703000	-2.14800000	-1.43491400
H	1.71697000	-2.56861000	1.09935400	H	-3.49266200	-3.87237700	-1.11477300
Rh	1.27498700	-0.19344100	-0.08972200	H	-4.10670000	-2.80589900	0.17204000
P	0.23649700	1.83979300	-0.37973600	H	4.27203600	-1.54904700	-1.66576300
C	1.33213500	3.05959700	-1.22836800	H	5.95882000	-2.76241000	-0.35066000
H	0.85228000	4.04389900	-1.28715000	H	5.80893000	-1.51861200	1.00933300
H	2.27096400	3.12993600	-0.67486900	H	5.31942500	1.42639600	-1.20172500
H	1.55382300	2.70673400	-2.24046500	H	3.74185300	2.16755900	-0.83927600
C	-1.32035200	1.98460700	-1.36534000	H	3.89818100	1.02919800	-2.19250700
H	-1.60979500	3.03693900	-1.46727400	Rh	-1.24273400	-0.26491300	0.08058000
H	-1.17454100	1.56233400	-2.36463500	P	-0.50814400	1.89715900	0.37131600
H	-2.11729200	1.43790900	-0.85736800	C	-1.84002700	3.00844400	1.00411500
C	-0.21426200	2.68121600	1.19832300	H	-1.49244900	4.04742100	1.05242700
H	-0.59895400	3.69231700	1.01925200	H	-2.70466300	2.92978900	0.34181100
H	-0.97603400	2.08599600	1.71060300	H	-2.14111400	2.68348200	2.00498600
H	0.67684900	2.73004200	1.82941800	C	0.87860900	2.28844600	1.53098200
C	-4.12079300	0.01208700	2.15642500	H	1.02008500	3.37314700	1.60122900
H	-3.46588400	-0.35278100	2.95383600	H	0.65586600	1.89779100	2.52897800
H	-3.96003200	1.09031000	2.04561200	H	1.79684400	1.82866500	1.16082800
H	-5.16324200	-0.15380900	2.44647600	C	0.03438900	2.71176200	-1.19103600
C	3.84849400	-2.44871000	0.54832400	H	0.26652300	3.77181900	-1.03399700
H	4.15833600	-1.65243900	1.23579000	H	0.92153500	2.19342500	-1.56602900
H	4.08858700	-3.41262000	1.01630300	H	-0.76856400	2.61288700	-1.92619300
H	4.44189600	-2.34841000	-0.36643500	Cl	-3.03184100	0.65036500	-1.23459200
Cl	3.04238100	1.01455900	0.99723400				
				33a			
32b				O	-3.59296000	0.21755200	0.11880900
O	2.47963800	-0.04695000	-0.25372300	C	-2.90458300	-0.81861400	-0.58488000
C	3.90969600	0.08991100	-0.23952100	C	-1.71668400	-0.30151700	-1.37553600
C	1.96036900	-0.89281200	0.76876700	C	-0.61570700	-1.06695400	-1.69794100
C	0.59611000	-1.39602800	0.38253300	C	-2.87362600	0.76717800	1.22012800
C	-0.36069400	-1.69934200	1.38156800	C	-1.66514200	1.51644700	0.73084100
C	-1.64063300	-2.27599400	1.02420600	C	-0.50558200	1.80694900	1.49385300
C	-2.01149500	-2.55248500	-0.27803900	C	0.65170000	2.25723900	0.79102300
C	-3.42278400	-2.86601800	-0.68091800	C	0.60989800	2.32276300	-0.64600200

H	-2.55428300	-1.58107600	0.12284000	H	-0.26543300	-0.86282600	2.44325400
H	-1.91056500	0.60282000	-1.95147000	H	0.74015500	0.67223300	2.56597700
H	-0.00252900	-0.81332700	-2.55770000	H	3.71486000	-0.32490400	-1.96181000
H	-0.52564000	-2.07733500	-1.31061200	H	2.44421600	-1.47634200	-1.48620300
H	-3.58552500	1.45115300	1.70076000	H	2.28269800	1.47016400	-0.67299100
H	-2.59049600	-0.01245200	1.93845500	H	0.67470400	0.03820400	-2.89124200
H	-1.89252900	2.16800100	-0.10943400	H	-1.09047700	1.71915700	-2.31921500
H	-0.42326700	1.52634600	2.54030700	H	0.86446200	2.64535000	-0.09938300
H	1.57778100	2.42772100	1.33537500	Rh	-0.04852000	0.10451200	-0.17320700
H	-0.31404700	2.66657500	-1.10818900	P	-2.30681200	-0.32143300	0.41527000
Rh	0.11260900	0.28967800	0.04771100	C	-2.61581600	-1.94337100	1.24596700
P	2.22848200	-0.78625900	-0.10758200	H	-3.69316700	-2.12549000	1.33174300
C	2.17663200	-2.60260100	-0.44258400	H	-2.14350100	-2.73192900	0.65672500
H	1.46945700	-3.06709600	0.24768900	H	-2.18282500	-1.94716200	2.25133500
H	1.84603400	-2.78310500	-1.47017500	C	-3.24085000	0.81365500	1.54728400
H	3.17243600	-3.04089900	-0.31158400	H	-4.23604800	0.40668600	1.75978400
C	3.51027500	-0.26912900	-1.34621600	H	-2.69670900	0.92131500	2.49138200
H	4.36335100	-0.95650900	-1.31658800	H	-3.35458800	1.80544700	1.10537500
H	3.08150000	-0.28357300	-2.35307400	C	-3.41110800	-0.42669400	-1.06046400
H	3.86970700	0.74153100	-1.14235800	H	-4.43380500	-0.70440000	-0.78079400
C	3.16650600	-0.70444200	1.48121700	H	-3.43204900	0.53574400	-1.58146700
H	4.09799500	-1.28000000	1.42986600	H	-2.99420500	-1.18062000	-1.73411500
H	3.40236400	0.33763500	1.71932600	C	-1.22250700	3.23409200	0.01744400
H	2.52303800	-1.10648000	2.26825200	H	-1.32139000	3.25294200	1.10812400
C	-3.94424900	-1.42575200	-1.53352200	H	-1.01121900	4.26458100	-0.30401500
H	-4.80432500	-1.77916800	-0.95621800	H	-2.19184300	2.95408500	-0.40908200
H	-4.29730900	-0.67673000	-2.25147700	H	3.52936000	-1.17506100	1.92093400
H	-3.51645700	-2.26767500	-2.08663500	C	3.30519800	0.93739800	1.83394800
C	1.83322000	2.75795100	-1.41878500	H	4.35986100	1.16752200	1.65723900
H	1.89543500	2.26556000	-2.39537800	H	3.12590900	0.96464200	2.91488700
H	1.80293900	3.84114900	-1.60701400	H	2.69912800	1.72263300	1.37149500
H	2.75906000	2.54937100	-0.87356800	Cl	-0.18977100	-2.28121600	-1.12024200
Cl	-0.32535600	-1.60421200	1.70501600				
				33c			
33b				O	3.66552300	0.36883700	-0.33289100
O	3.66096100	-0.65697200	0.00797500	C	2.99351200	-0.58228400	-1.16988100
C	3.00587200	-0.45766600	1.26895100	C	1.62129400	-0.11305600	-1.64026400
C	1.55914600	-0.89995300	1.34219000	C	0.52595500	-0.91737200	-1.87109800
C	0.57345300	-0.28287300	2.07771800	C	3.02745500	0.69596500	0.90205700
C	2.93335200	-0.53213500	-1.21761000	C	1.77036300	1.47169400	0.63200700
C	1.92524600	0.57634700	-1.17515600	C	0.69954200	1.67498700	1.53715400
C	0.83602700	0.72395000	-2.06427700	C	-0.52931500	2.17617100	1.00985500
C	-0.20669700	1.63040300	-1.69189200	C	-0.64206200	2.38177100	-0.40941500
C	-0.11685700	2.30440600	-0.42506900	H	1.64421200	0.86149100	-2.12532200
H	1.38916300	-1.92245300	1.01341900	H	-0.22805400	-0.61293000	-2.59059800

H	0.54136700	-1.96565400	-1.59186900	H	-0.80018300	0.14868800	2.61264500
H	3.76613500	1.31912900	1.42309900	H	-3.65654800	1.32520700	-1.61997200
H	2.82400500	-0.18973100	1.51572200	H	-2.51838400	0.04318100	-2.10726800
H	1.90269200	2.19953900	-0.16510700	H	-1.96943700	2.01457100	0.19687300
H	0.72763700	1.28865200	2.55191400	H	-0.54293600	1.59147600	-2.51495900
H	-1.38978900	2.28243800	1.66614200	H	1.45547300	2.51957500	-1.33949300
H	0.22402600	2.78424800	-0.93294600	H	-0.37554500	2.61075700	1.15744800
Rh	-0.06822500	0.29239500	0.03996300	Rh	0.10052500	0.27386100	-0.08499500
P	-2.18679100	-0.76773100	-0.10632900	P	2.20620200	-0.78024900	0.17353400
C	-2.14469300	-2.59252200	-0.38738700	C	2.10497400	-2.61814700	0.33301000
H	-1.46536000	-3.04305400	0.33872700	H	3.10779600	-3.06021200	0.33413600
H	-1.77882800	-2.80500200	-1.39666100	H	1.52146700	-3.00564400	-0.50466700
H	-3.14986000	-3.01607100	-0.28120500	H	1.60225300	-2.88917300	1.26720600
C	-3.41474900	-0.26991500	-1.40594500	C	3.32535200	-0.37803400	1.59821500
H	-4.28669900	-0.93331800	-1.38056000	H	4.19914400	-1.03949800	1.59471300
H	-2.95065000	-0.33897600	-2.39538500	H	2.78802100	-0.51118400	2.54278700
H	-3.75182700	0.75786000	-1.25939400	H	3.66971700	0.65692000	1.54570400
C	-3.16712700	-0.62951900	1.45237500	C	3.31593400	-0.55932700	-1.28368300
H	-4.10537400	-1.19288600	1.39128400	H	4.23602000	-1.14630300	-1.18210900
H	-3.39328400	0.42143400	1.65835000	H	3.57527500	0.49848600	-1.39470300
H	-2.55257200	-1.02117800	2.26773200	H	2.76367000	-0.87961200	-2.17113700
C	-1.94655500	2.86316200	-1.00096900	C	1.78084900	2.74536000	1.41789800
H	-2.08663000	2.49786600	-2.02428600	H	1.85660600	2.24530500	2.38939400
H	-1.96729800	3.96198900	-1.04648800	H	1.75322400	3.82720300	1.61412400
H	-2.80935300	2.54666000	-0.40496000	H	2.69780400	2.53943100	0.85526500
H	3.60958300	-0.54443000	-2.08103300	C	-3.94103200	-1.35680300	1.68221300
C	3.07353600	-2.00676500	-0.61895700	H	-4.94643600	-0.92492600	1.65551900
H	2.41553700	-2.15978800	0.23955600	H	-3.64402900	-1.50883200	2.72480400
H	2.80177800	-2.73185100	-1.39486900	H	-3.97208300	-2.32810700	1.17742300
H	4.10838000	-2.20484100	-0.32135300	Cl	-0.11721700	-1.41545300	-1.99063900
Cl	0.39383000	-1.62753000	1.68365000				
				33a-TS			
33d				O	3.92171600	-0.04947600	-0.13664100
O	-3.51885100	-0.23165700	-0.32435400	C	3.03447200	-0.87953800	0.60894300
C	-2.96020400	-0.41691600	0.96811100	C	1.87480600	-0.01285700	1.09851300
C	-1.57280300	-1.02638800	0.99095400	C	0.62056900	-0.68087100	1.45823800
C	-0.61942600	-0.67168300	1.92110100	C	3.13978900	0.65098500	-1.08398100
C	-2.87050000	0.64226900	-1.26148400	C	1.93910800	1.27428600	-0.38269300
C	-1.72800200	1.42843900	-0.68680100	C	0.86079600	1.71901300	-1.30627900
C	-0.60971000	1.82901400	-1.45676900	C	-0.26229600	2.41287100	-0.83545400
C	0.55470100	2.29381900	-0.77385900	C	-0.57552700	2.33290200	0.56351000
C	0.54718500	2.31372900	0.66105600	H	2.62180400	-1.66206600	-0.04592900
H	-2.93486100	0.53538800	1.52304200	H	2.19439400	0.71612500	1.84514900
H	-1.46574300	-1.95348100	0.43207600	H	0.19020200	-0.39598300	2.41919800
H	0.16267300	-1.36529600	2.20880500	H	0.59585900	-1.75531400	1.27404100

H	3.78165100	1.42223400	-1.52438400	H	2.29241900	1.34858900	-0.17807900
H	2.78788600	-0.02315500	-1.87890900	H	1.09731300	0.30569400	-2.78753000
H	2.21669900	2.08906100	0.28771100	H	-0.58896300	2.09747500	-2.37624000
H	0.99032100	1.54300700	-2.37025000	H	0.79587400	2.43243200	0.37369900
H	-0.99508400	2.79195300	-1.54534900	Rh	-0.28292000	0.06791000	-0.23203100
H	0.26318100	2.41035300	1.25791800	P	-2.41185900	-0.27369100	0.47477100
Rh	-0.31498600	0.24009000	-0.15986800	C	-2.68807700	-1.84783700	1.39761200
P	-2.29993400	-0.77855800	0.20386500	H	-3.75981400	-2.02765900	1.53923300
C	-2.20378500	-2.56739700	0.64091500	H	-2.24247500	-2.66488500	0.82500900
H	-1.56011200	-3.06355300	-0.08945200	H	-2.20740800	-1.79574300	2.37963000
H	-1.76308500	-2.68201100	1.63607800	C	-3.25215800	0.94559200	1.58403000
H	-3.20033600	-3.02332600	0.63785300	H	-4.24737000	0.58133500	1.86316200
C	-3.45473000	-0.13990000	1.49989700	H	-2.65871400	1.08690900	2.49262300
H	-4.35853000	-0.75817700	1.54516100	H	-3.35775800	1.91227200	1.08782500
H	-2.96210800	-0.16181800	2.47708600	C	-3.58083700	-0.42108600	-0.94391500
H	-3.74227200	0.89125600	1.28261000	H	-4.59630500	-0.65570200	-0.60368100
C	-3.33958700	-0.77548200	-1.31908000	H	-3.59679300	0.51626300	-1.50874300
H	-4.27741900	-1.32214400	-1.16515300	H	-3.21151000	-1.21597100	-1.59735700
H	-3.56606800	0.25545500	-1.60880400	C	-1.18173900	3.27807700	0.05605900
H	-2.76017600	-1.24305400	-2.11975600	H	-1.44985700	3.28728800	1.11722600
C	3.83175400	-1.50735500	1.74653600	H	-0.84573300	4.29435400	-0.19827500
H	4.67515800	-2.07460800	1.33995900	H	-2.09016800	3.08039800	-0.52494300
H	4.22809400	-0.73399100	2.41425100	H	3.58513700	-1.54709600	1.64606400
H	3.20293800	-2.18795600	2.32963400	C	3.54229800	0.53291500	2.15001200
C	-1.84039300	2.96927200	1.09315500	H	4.62349000	0.62810800	2.29041700
H	-2.13124300	2.54039200	2.05756300	H	3.08504300	0.32937600	3.12458200
H	-1.70207500	4.04920800	1.25078400	H	3.16561100	1.49495700	1.78624600
H	-2.67942200	2.84526000	0.39853000	Cl	-0.43340600	-2.26375800	-1.23041700
Cl	0.20585500	-1.64544600	-1.73939100				
				33c-TS			
33b-TS				O	4.00373100	0.11113800	-0.31233100
O	4.08419600	-0.45792000	-0.00243500	C	3.13697900	-0.62823500	-1.17818100
C	3.26762400	-0.60712100	1.17009900	C	1.81887700	0.15923500	-1.32959400
C	1.81983300	-0.83759600	0.74844800	C	0.55647600	-0.53045800	-1.60987300
C	0.66356400	-0.58777400	1.57620200	C	3.26320700	0.55938600	0.80823100
C	3.31573600	-0.24719900	-1.17941600	C	2.00583200	1.24328300	0.30852400
C	2.05199000	0.48861700	-0.80022600	C	1.00266400	1.57843500	1.35246000
C	1.06914100	0.82161400	-1.83235300	C	-0.14012500	2.32818300	1.03723400
C	0.10539800	1.81810100	-1.58658100	C	-0.54898800	2.39618400	-0.33670800
C	-0.09538500	2.26570400	-0.23279100	H	1.95948000	1.01555400	-1.98911900
H	1.72827900	-1.76434900	0.18335500	H	0.02130000	-0.17605200	-2.49168900
H	0.09807300	-1.47375900	1.85509400	H	0.56521500	-1.61483100	-1.52206600
H	0.74057300	0.15880100	2.36672500	H	3.90888300	1.26474400	1.34358900
H	3.93279100	0.36700900	-1.84694800	H	2.99769900	-0.26263100	1.48813200
H	3.08753900	-1.19147000	-1.69574400	H	2.23145200	2.13139200	-0.28383900

H	1.20477000	1.28628700	2.37870500	H	1.00313600	1.43131700	2.47832900
H	-0.81778800	2.63516800	1.83172900	H	-0.88303900	2.77315300	1.54543500
H	0.23848000	2.54205700	-1.07821700	H	0.48136700	2.32524400	-1.19940500
Rh	-0.26466400	0.23356200	0.15312900	Rh	-0.32125600	0.19404100	0.18230600
P	-2.28028300	-0.72795700	-0.21228000	P	-2.37608700	-0.61524600	-0.32301000
C	-2.22694400	-2.49636900	-0.73124600	C	-2.43011500	-2.41861600	-0.71105700
H	-1.57659700	-3.03558300	-0.03834100	H	-3.46622700	-2.77232200	-0.75566400
H	-1.80913100	-2.57290300	-1.73990900	H	-1.88336800	-2.95491100	0.06824500
H	-3.23138400	-2.93465000	-0.72752100	H	-1.95217300	-2.60673700	-1.67759400
C	-3.44356500	-0.00798300	-1.45780600	C	-3.35053600	0.08603000	-1.73063400
H	-4.36444800	-0.60017700	-1.50762400	H	-4.28131300	-0.47686600	-1.86417200
H	-2.97235600	-0.00502000	-2.44591900	H	-2.76299300	0.02533400	-2.65202600
H	-3.69859300	1.02119200	-1.19485200	H	-3.59568200	1.13411300	-1.54727600
C	-3.29126500	-0.77068400	1.32877200	C	-3.53430400	-0.46455000	1.10430800
H	-4.24603600	-1.28504800	1.16837800	H	-4.50429000	-0.92625100	0.88530400
H	-3.48401100	0.25100500	1.67068300	H	-3.68425700	0.59166800	1.34902600
H	-2.70958900	-1.29020700	2.09508000	H	-3.06902100	-0.95843400	1.96150000
C	-1.84402400	3.08315100	-0.70589800	C	-1.57912400	3.00885700	-1.12395300
H	-2.18397200	2.78545800	-1.70301900	H	-1.84096100	2.62969700	-2.11666900
H	-1.72066500	4.17619800	-0.72281500	H	-1.35445900	4.07953000	-1.24014900
H	-2.64275300	2.85482400	0.00954600	H	-2.46458800	2.93091600	-0.48241300
H	3.64179100	-0.59952200	-2.15254500	C	3.96472400	-1.61421600	-1.64999600
C	3.01388900	-2.08860600	-0.73778900	H	4.99597200	-1.36220700	-1.91872200
H	2.40040900	-2.20792100	0.15930900	H	3.44069400	-1.95590800	-2.54881400
H	2.57167600	-2.69812600	-1.53396500	H	3.98846600	-2.43025700	-0.92053300
H	4.02029300	-2.47246000	-0.54085900	Cl	-0.19372300	-1.69389400	1.87143500
Cl	0.23306300	-1.74364100	1.63708400				
				34a			
33d-TS				O	3.92124500	-0.46507200	-0.34003900
O	4.07628800	0.07518500	0.03446800	C	2.82143000	-1.16643700	0.28559000
C	3.27484700	-0.38626400	-1.05885100	C	2.06605100	-0.10696000	1.12044400
C	1.88766100	-0.70724500	-0.53558900	C	0.56959300	-0.32490100	1.29976300
C	0.71882600	-0.84426800	-1.37141000	C	3.88820400	0.91136000	0.00904100
C	3.28727400	0.64332700	1.07647100	C	2.43491000	1.21485300	0.39746600
C	1.94626900	1.05119300	0.51209000	C	1.56236000	1.48798300	-0.81280200
C	0.92228700	1.59225300	1.40749600	C	0.41162200	2.27292600	-0.77494300
C	-0.15130000	2.32910400	0.87371900	C	-0.43004800	2.36100200	0.38638100
C	-0.39041300	2.27319200	-0.54480600	H	2.17345700	-1.54206100	-0.51425800
H	3.21725000	0.39643500	-1.83465000	H	2.52509000	-0.07608400	2.12362900
H	1.92665900	-1.44016300	0.27079300	H	0.18945400	0.21192800	2.17575800
H	0.27237000	-1.83563700	-1.38609600	H	0.33290400	-1.38930700	1.39766600
H	0.72173100	-0.34273600	-2.34140900	H	4.55782700	1.11996200	0.86026800
H	3.82537800	1.52592800	1.44712500	H	4.24101700	1.49526100	-0.84879600
H	3.17016900	-0.06179600	1.91163700	H	2.37462500	2.06272600	1.09117000
H	2.08341400	1.67965700	-0.36728500	H	1.99496600	1.26924600	-1.78600200

H	0.00031700	2.61637900	-1.72732600	Rh	-0.56354100	0.34247700	-0.42150200
H	0.06341900	2.33348200	1.35845600	P	-2.41435700	-0.60410800	0.54948400
Rh	-0.45133300	0.30933200	-0.37172900	C	-2.47306500	-2.44601100	0.56811700
P	-2.42037400	-0.67242900	0.38852800	H	-3.47388700	-2.80149700	0.83713500
C	-2.29193100	-2.43850400	0.90003100	H	-2.19837300	-2.80377300	-0.42764900
H	-1.76582600	-2.98152600	0.11050200	H	-1.75326100	-2.83621800	1.29419400
H	-1.71465900	-2.51769600	1.82655100	C	-2.86687800	-0.16927600	2.28787300
H	-3.28376400	-2.87464400	1.06286900	H	-3.75800400	-0.71900300	2.61169300
C	-3.34579400	0.08884100	1.79696700	H	-2.03588400	-0.41484400	2.95685600
H	-4.24182700	-0.49279300	2.04161700	H	-3.06548600	0.90289000	2.36664400
H	-2.70100100	0.13397800	2.68037300	C	-3.91438800	-0.14321200	-0.42035800
H	-3.64551300	1.10868800	1.53963100	H	-4.81592400	-0.60522600	-0.00203800
C	-3.66891400	-0.71826200	-0.96945000	H	-4.03889400	0.94448000	-0.42288600
H	-4.58685600	-1.22465500	-0.64982600	H	-3.76850300	-0.48143100	-1.45028300
H	-3.91572900	0.30041600	-1.28593200	C	-1.19194600	3.09183500	1.15347800
H	-3.22706500	-1.25017500	-1.81673500	H	-1.75871300	2.70990600	2.00888100
C	3.36008600	-2.33527500	1.10233100	H	-0.76354100	4.05778200	1.46025300
H	3.92563000	-3.01917200	0.46146000	H	-1.90211400	3.29373000	0.34202700
H	4.02496800	-1.98361100	1.90075400	H	3.42730500	-2.40682300	0.23249400
H	2.53759700	-2.90141000	1.55731300	C	3.39584100	-1.40750600	2.13656500
C	-1.65808500	3.24657900	0.35378700	H	4.39593700	-1.73559500	2.43815900
H	-2.36301100	2.98152100	1.14864300	H	2.66280900	-2.10307500	2.56239800
H	-1.39139300	4.30349700	0.50348100	H	3.22526700	-0.41437300	2.56717900
H	-2.18660700	3.17519700	-0.60445800	Cl	-0.82246000	-1.21700800	-2.32498000
Cl	-0.17584000	-1.64301700	-1.85613300				
				34c			
34b				O	3.66966700	-1.04868500	0.29449200
O	4.39770400	-0.59008700	0.09368300	C	3.39913600	-0.69362300	-1.06067400
C	3.30745900	-1.38367100	0.61288100	C	2.14197700	0.20938400	-0.98585700
C	2.03030100	-0.74063100	0.00342800	C	0.83799800	-0.56407000	-0.79898500
C	0.70354900	-0.82929500	0.72531700	C	3.19968900	-0.01377300	1.16623000
C	3.90773600	0.51419400	-0.66761000	C	2.48561600	1.03438200	0.27419000
C	2.47514600	0.72891900	-0.17714200	C	1.32747700	1.71538500	0.96513300
C	1.53275000	1.50405900	-1.05282500	C	0.29766200	2.46102400	0.37527100
C	0.50214800	2.29592000	-0.57089900	C	-0.30157700	2.19556900	-0.90166600
C	-0.10956100	2.11904400	0.72699200	H	2.09293000	0.84522100	-1.87579800
H	1.89448200	-1.16721700	-0.99766900	H	0.38218300	-0.81652000	-1.76144400
H	0.29205200	-1.84148000	0.70367500	H	0.98606000	-1.46831400	-0.20231500
H	0.74040000	-0.45543700	1.75389500	H	4.04704400	0.42749400	1.70837300
H	4.57031700	1.36867200	-0.49249600	H	2.50865700	-0.45771600	1.89159800
H	3.91839800	0.28202900	-1.74533700	H	3.21748500	1.80513400	-0.01331800
H	2.51634600	1.19644000	0.81591200	H	1.47406600	1.88964600	2.02988600
H	1.75000900	1.54059800	-2.11834500	H	-0.28370400	3.08678100	1.05752600
H	-0.02959400	2.91662900	-1.29533700	H	0.34178700	1.90354200	-1.72675800
H	0.54919200	1.82659400	1.54625900	Rh	-0.50928900	0.44050900	0.40268100

P	-2.26914500	-0.84801100	-0.43665600	P	-2.39518200	-0.69821000	-0.51577600
C	-1.97445500	-2.66677800	-0.41642300	C	-2.34907600	-2.54025400	-0.56309700
H	-1.65704300	-2.94512900	0.59199700	H	-3.33142000	-2.94867100	-0.82518300
H	-1.17051000	-2.91945200	-1.11475100	H	-2.03740400	-2.89799600	0.42161900
H	-2.87805100	-3.21974100	-0.69604400	H	-1.61795700	-2.87643600	-1.30480800
C	-2.88603500	-0.55264200	-2.15445000	C	-2.91175200	-0.26648400	-2.23703600
H	-3.71154300	-1.22920300	-2.40316300	H	-3.78753900	-0.85051700	-2.54208900
H	-2.07304900	-0.70901700	-2.87066400	H	-2.08933000	-0.47455000	-2.92899500
H	-3.23152300	0.48057200	-2.25146700	H	-3.15493100	0.79737000	-2.30318500
C	-3.78468600	-0.65471900	0.59879600	C	-3.89488600	-0.33755900	0.49653500
H	-4.59363500	-1.30566200	0.24789300	H	-4.77979500	-0.83900900	0.08833300
H	-4.12641900	0.38516400	0.57158700	H	-4.07758400	0.74138700	0.52474100
H	-3.52646300	-0.90991000	1.63054600	H	-3.71098000	-0.68803600	1.51634800
C	-1.49969500	3.01540900	-1.33436400	C	-1.52766700	3.09884300	-0.95595300
H	-2.08030700	2.49652300	-2.10497200	H	-2.12047600	2.72126000	-1.79550600
H	-1.18947600	3.97991000	-1.76365000	H	-1.20104600	4.11385200	-1.22749800
H	-2.17188500	3.23056900	-0.49496400	H	-2.19288900	3.19175800	-0.08857500
H	4.22558100	-0.06949600	-1.44881900	C	3.64081600	-2.44396400	-0.92195400
C	3.32118400	-1.96027300	-1.90060000	H	4.59563400	-2.65791100	-1.41364000
H	2.51506400	-2.61663700	-1.55991700	H	2.86147000	-3.04003000	-1.41152200
H	3.15596500	-1.71320300	-2.95592200	H	3.71507700	-2.75666300	0.12499600
H	4.26252600	-2.51363600	-1.82248800	Cl	-0.59891000	-1.31333200	2.25058100
Cl	-0.48845000	-1.02951900	2.37945100				
				34a-TS			
34d				O	3.58857100	-1.83491800	0.21828100
O	4.39607400	-0.20371100	-0.42956800	C	3.39521200	-0.56805400	0.84991200
C	3.31747800	-0.96061100	-1.01596600	C	2.62943500	0.31196000	-0.19024800
C	2.06365300	-0.49943900	-0.24570900	C	1.56378100	1.20726300	0.43867900
C	0.70155100	-0.65683300	-0.88203100	C	2.39697700	-2.08704600	-0.50511100
C	3.88814200	0.88956100	0.34263100	C	2.06009000	-0.75026500	-1.19674400
C	2.40232800	0.99088500	-0.01677600	C	0.59790700	-0.60035000	-1.57261100
C	1.47427100	1.64811000	0.96390900	C	0.00392300	0.63296000	-1.95758700
C	0.34615600	2.36395900	0.59866600	C	0.56739400	1.85045000	-1.39664200
C	-0.34329700	2.19794600	-0.66231900	H	2.74694700	-0.71166700	1.73099600
H	3.22396800	-0.67156700	-2.07706400	H	3.36284700	0.93247200	-0.71953400
H	2.05713600	-1.00477200	0.72870800	H	1.84913900	2.25264300	0.55668400
H	0.37478200	-1.69972800	-0.90090200	H	1.23822300	0.85461000	1.42498000
H	0.65069900	-0.22601200	-1.88948800	H	2.59009800	-2.90816800	-1.20201900
H	4.45606200	1.79368700	0.09320600	H	1.57952500	-2.38248100	0.17532600
H	4.02191900	0.68433400	1.41618200	H	2.65858700	-0.70093300	-2.11879100
H	2.31757500	1.49745700	-0.98877600	H	0.15330500	-1.50322600	-1.99078200
H	1.76883200	1.65469300	2.01129000	H	-0.85975200	0.67641000	-2.61776100
H	-0.18045800	2.90136600	1.39022600	H	1.62204200	2.02136700	-1.59646900
H	0.27471100	2.00109100	-1.53950200	Rh	-0.49503200	0.36050200	0.03565600
Rh	-0.57648400	0.33462600	0.40953300	P	-2.42224900	-0.92391600	0.00029100

C	-3.98026900	0.06327000	0.05704600	H	4.02840100	0.92868300	-0.53285200
H	-3.92935300	0.72573000	0.92483800	H	3.99457800	0.64345600	1.21837900
H	-4.05873300	0.67899600	-0.84463100	H	4.92640800	-0.45814000	0.16632500
H	-4.86206500	-0.58409500	0.12887600	C	2.69033500	-2.16417600	1.31828000
C	-2.71057500	-2.04749200	-1.44396600	H	1.92442800	-2.93588900	1.19368400
H	-1.91630200	-2.79860300	-1.49754900	H	3.67682700	-2.63748700	1.25822100
H	-3.67441400	-2.56157900	-1.35718400	H	2.57477300	-1.72208900	2.31327900
H	-2.70330300	-1.47291000	-2.37602800	C	2.84736800	-1.80018700	-1.53746600
C	-2.60068000	-2.06710100	1.43815100	H	3.82284600	-2.29846700	-1.49308400
H	-3.56296100	-2.59179400	1.41688600	H	2.06698000	-2.55037400	-1.69938300
H	-1.78966400	-2.80213800	1.42881900	H	2.82605200	-1.09359900	-2.37116400
H	-2.51891300	-1.47403900	2.35286500	Cl	1.52288400	1.53057300	-1.91335200
Cl	-1.33100100	1.26801300	2.14147500	C	-4.66664200	0.56653200	-0.59515800
C	4.74268600	-0.02275300	1.29200500	H	-4.56307800	1.52526500	-1.11695000
H	4.61798200	0.94109900	1.79807700	H	-5.66282600	0.16607400	-0.80955100
H	5.22902800	-0.71539500	1.98645300	H	-4.60569500	0.74840800	0.48416500
H	5.40138500	0.11700000	0.42748300	C	-0.10125000	2.83167400	1.87068800
C	-0.22863600	3.13470000	-1.40589200	H	-0.35009100	3.13543900	2.89914400
H	-0.05016100	3.67532100	-2.34776500	H	0.98556900	2.76792700	1.77574400
H	-1.30132600	2.95469600	-1.29894300	H	-0.45112600	3.62497700	1.20237300
H	0.08300400	3.79072500	-0.58697100				
				34c-TS			
34b-TS				O	-2.86531300	-1.83537700	0.61963200
O	-3.88532000	-1.73350400	-0.50546600	C	-3.65313900	-0.67510800	0.36229700
C	-3.60671600	-0.42493500	-1.06442300	C	-2.71114500	0.23751400	-0.46594000
C	-2.14979700	-0.13793000	-0.62400600	C	-1.70584100	1.01606300	0.37594900
C	-1.56043800	1.25662300	-0.54700800	C	-2.18607400	-2.15025800	-0.59007100
C	-2.81582700	-2.16704000	0.34354000	C	-2.00252400	-0.81418600	-1.37634900
C	-2.09571100	-0.88106700	0.73364300	C	-0.55089100	-0.51263300	-1.70754500
C	-0.68791700	-0.90831000	1.30238200	C	-0.02257600	0.78493100	-1.95588200
C	-0.16198100	0.25574600	1.92744400	C	-0.64749200	1.92251800	-1.29441900
C	-0.77456600	1.51962900	1.54887700	H	-3.31282700	0.92447700	-1.07328100
H	-3.66266000	-0.51610400	-2.15679700	H	-2.02599900	2.01277000	0.67959300
H	-1.51362100	-0.72132300	-1.30183900	H	-1.42194200	0.46638000	1.28213500
H	-1.05394200	1.59478800	-1.45229800	H	-2.77712000	-2.86898000	-1.17942700
H	-2.23551700	2.03881700	-0.20784100	H	-1.23261100	-2.61663800	-0.32451600
H	-3.25460700	-2.70980700	1.18798000	H	-2.55674000	-0.89000000	-2.32420000
H	-2.14096300	-2.85234600	-0.19639600	H	-0.03671100	-1.33913300	-2.19767800
H	-2.75219700	-0.35534600	1.44308300	H	0.85364500	0.93044100	-2.58453200
H	-0.27304000	-1.87567200	1.57697200	H	-1.69359600	2.10253200	-1.52571700
H	0.63718600	0.21892000	2.66474000	Rh	0.42406300	0.35144500	0.02207900
H	-1.85107100	1.56065300	1.67871100	P	2.41183200	-0.83146500	-0.01709400
Rh	0.55521900	0.35463800	-0.01895800	C	3.92317300	0.20057600	0.21589900
P	2.49933000	-0.86320400	0.01356700	H	3.79030400	0.79209200	1.12524300
C	4.02066700	0.15525400	0.23915400	H	4.03518700	0.88614400	-0.63011300

H	4.82322200	-0.41989000	0.29818000	C	2.70464900	-1.98895400	-1.52680100
C	2.82767800	-1.81497200	-1.53099100	H	1.89010700	-2.70872600	-1.65361500
H	2.06665100	-2.58318000	-1.70061600	H	3.64873500	-2.53960400	-1.44829400
H	3.80306400	-2.30380700	-1.42855800	H	2.74358700	-1.35285800	-2.41703500
H	2.85460000	-1.15996200	-2.40805600	C	2.49585000	-2.20276600	1.34123100
C	2.55459600	-2.08728600	1.32878900	H	3.43243900	-2.77145200	1.30751200
H	3.53873500	-2.57034900	1.32477300	H	1.65080400	-2.89328500	1.25733800
H	1.77833000	-2.84969700	1.20860000	H	2.41501400	-1.67247300	2.29361900
H	2.39205500	-1.57848400	2.28274400	Cl	1.35506800	1.13580900	2.19397200
Cl	1.11801500	1.14931900	2.21927800	C	-4.18126900	-0.35795600	1.98786800
H	-4.50197400	-0.95291000	-0.29142300	H	-4.04044500	0.59559400	2.51008400
C	-4.20381400	-0.13540700	1.67207800	H	-5.24252300	-0.62360500	2.03530800
H	-4.82069600	0.75193000	1.48992100	H	-3.61029000	-1.13187700	2.51241600
H	-4.82919100	-0.89424600	2.15307400	H	-4.29755800	0.55196700	0.03651200
H	-3.40089800	0.13303500	2.36454300	C	0.20300700	3.14228100	-1.51918400
C	0.11624400	3.21912000	-1.14161800	H	1.27294400	2.99768900	-1.34928300
H	1.18718900	3.05407300	-1.00103000	H	0.06180700	3.61010900	-2.50563300
H	-0.03520000	3.84411400	-2.03503900	H	-0.16449700	3.84845100	-0.76770300
H	-0.25068900	3.78561000	-0.27972600				
				S1			
34d-TS				O	3.81057000	0.36254300	-0.05493700
O	-3.98410300	-1.49935500	-0.13308900	C	4.86229400	-0.54839700	-0.34205500
C	-3.72602700	-0.24553400	0.54208000	C	6.15455000	0.03478600	0.14819300
C	-2.22018200	-0.02077700	0.32441100	C	7.02424500	-0.61146100	0.92391400
C	-1.56098300	1.33140400	0.50277900	C	2.55270200	-0.08864300	-0.54068200
C	-2.89723000	-1.84093500	-1.00658300	C	1.49462400	0.85355100	-0.04641800
C	-2.07082900	-0.56237800	-1.11889500	C	0.71713000	1.61806500	-0.89803000
C	-0.62000100	-0.59641300	-1.56743400	C	-0.49154000	2.28509000	-0.46052800
C	0.01972200	0.61072500	-1.96452700	C	-0.90472400	2.19103700	0.88994400
C	-0.56213100	1.84255000	-1.45652300	H	4.91554000	-0.71793600	-1.43380600
H	-1.70339600	-0.73647000	0.97837600	H	4.67206100	-1.52686400	0.12888000
H	-1.12973700	1.51208000	1.48817700	H	6.36452900	1.04897300	-0.19013800
H	-2.16962000	2.18844100	0.21925800	H	7.96472900	-0.16038900	1.22871500
H	-3.31171800	-2.18233700	-1.96246700	H	6.83102000	-1.62092600	1.28150800
H	-2.30760500	-2.66429400	-0.57232500	H	2.55060400	-0.13509900	-1.64300400
H	-2.62821100	0.11346700	-1.78615500	H	2.33685800	-1.10412000	-0.17302500
H	-0.22997800	-1.53844300	-1.94685300	H	1.52317300	1.04881500	1.02252300
H	0.88470200	0.62986800	-2.62414600	H	0.89079700	1.55266700	-1.97057500
H	-1.61768200	1.97146100	-1.67170800	H	-1.10618300	2.78109800	-1.20645100
Rh	0.54667700	0.37623800	0.03073000	H	-1.86293500	2.62705600	1.15809500
P	2.41349700	-0.95638300	-0.01671900	H	-0.18840600	2.15984300	1.70820500
C	4.00537600	-0.03983400	0.15179400	Rh	-0.81706200	0.23017600	-0.01717200
H	3.95385500	0.56603100	1.05965900	P	-3.05195500	-0.27285900	0.14315100
H	4.13542600	0.62996800	-0.70399700	C	-3.48561000	-1.39744900	1.53934600
H	4.85789200	-0.72708000	0.20476100	H	-3.26411000	-0.90315700	2.49036300

H	-4.54538400	-1.67675100	1.51557600	H	4.05733300	-0.17463800	1.61009200
H	-2.86200000	-2.29184700	1.46222000	H	2.91547600	1.17672400	1.84076600
C	-4.26379100	1.11113100	0.34567200	H	2.43973500	-0.46302200	2.33034900
H	-5.29147600	0.73058000	0.35108800	Cl	-0.17811900	-1.52501200	1.64973100
H	-4.08106800	1.63755900	1.28732300				
H	-4.15678100	1.82566600	-0.47658200	S2-TS			
C	-3.69498400	-1.16081900	-1.33914000	O	3.94559700	-0.75291900	0.36288300
H	-3.61149400	-0.51447600	-2.21822600	C	2.83793500	-1.36471900	1.00673100
H	-3.07488900	-2.04596200	-1.50163900	C	1.83510600	-0.28491900	1.38883800
H	-4.74251000	-1.45508400	-1.20448800	C	0.44799900	-0.69145400	1.65090400
Cl	-0.41111300	-2.12625800	-0.22781700	C	3.41098800	0.07012000	-0.65714900
S2				C	2.28050100	0.91800300	-0.08264200
O	-3.67217000	-0.51846000	-0.23586400	C	1.40111500	1.52948000	-1.11918300
C	-2.72490300	-1.44277000	-0.75974700	C	0.36714600	2.40549800	-0.77418300
C	-1.61194100	-0.80184900	-1.55835400	C	-0.10818100	2.37399900	0.58663100
C	-0.35955800	-1.35685300	-1.72897000	H	3.22755700	-1.87120200	1.89594600
C	-3.16759600	0.29638500	0.82125200	H	2.35447000	-2.10202700	0.34984400
C	-2.09245600	1.21431900	0.30942900	H	2.22350800	0.38918600	2.15259700
C	-1.07392200	1.80534300	1.09790400	H	0.00549800	-0.28899400	2.56299300
C	0.04627500	2.37523700	0.42077800	H	0.23188600	-1.74859700	1.49390800
C	0.11106700	2.24352200	-1.01537200	H	4.22943400	0.69841600	-1.02512900
H	-3.31327300	-2.07323100	-1.43949200	H	3.02139800	-0.53817100	-1.48739100
H	-2.30606700	-2.07666000	0.03188800	H	2.63597000	1.69117200	0.60017700
H	-1.93246300	-0.02334000	-2.24925400	H	1.61831300	1.32150800	-2.16320300
H	0.24915400	-1.07395400	-2.58264700	H	-0.21031700	2.88636300	-1.56040100
H	-0.09664200	-2.27848100	-1.21855700	H	-1.02343000	2.91840800	0.80838600
H	-4.03925700	0.86715700	1.16659900	H	0.61549500	2.41021800	1.40161800
H	-2.79403500	-0.31804100	1.65105400	Rh	-0.15493000	0.30645700	-0.07031000
H	-2.36039800	1.70588900	-0.62272700	P	-2.33031300	-0.19822100	0.17270900
H	-1.03024500	1.66241600	2.17438400	C	-2.70373200	-1.87610900	0.83510300
H	0.87450300	2.77112300	1.00286900	H	-2.15605800	-2.60536600	0.23195800
H	1.03968700	2.53980000	-1.49702200	H	-2.36420600	-1.95154000	1.87264900
H	-0.76724700	2.45067200	-1.62392600	H	-3.77828100	-2.08642200	0.79367200
Rh	-0.06119500	0.28783500	-0.12352200	C	-3.35344500	0.90950700	1.24147500
P	2.24371700	-0.20061100	-0.06308500	H	-4.39758600	0.57741200	1.26722300
C	2.73782200	-1.94529600	-0.39883700	H	-2.95296600	0.91102300	2.25976200
H	2.16694100	-2.59637800	0.26814300	H	-3.31630600	1.93404900	0.85928800
H	2.50612000	-2.20840400	-1.43520400	C	-3.21948000	-0.17508100	-1.44130300
H	3.81074600	-2.08706100	-0.22726600	H	-4.26891600	-0.47074800	-1.32513100
C	3.35811400	0.74642700	-1.19968800	H	-3.17305300	0.83002800	-1.87206900
H	4.40443800	0.45034600	-1.06387100	H	-2.70629800	-0.86556200	-2.11590000
H	3.06912100	0.56404800	-2.23953900	Cl	0.08058500	-1.74817800	-1.47893300
H	3.27173400	1.81994600	-1.00503100	S3			
C	3.00010600	0.11462900	1.59071400	O	-3.81955700	1.14938700	0.11042100

C	-2.63820700	1.47664900	0.86153200	C	0.87082600	-1.09710400	2.07129400
C	-2.03611300	0.14010300	1.35533800	H	4.69619700	-0.66704800	-1.03817600
C	-0.51731100	0.07152100	1.44343300	H	3.16142100	-0.75319900	-1.93366800
C	-4.06688500	-0.24425000	0.21550600	H	3.55115900	-0.74845900	1.02666200
C	-2.68366000	-0.88685300	0.38475600	H	1.96079400	-2.45412000	0.42597100
C	-1.95539200	-0.99616400	-0.94084000	H	1.33401800	-1.50388100	-0.91586500
C	-0.94621300	-1.91791000	-1.20020900	H	2.75796500	2.79800200	-0.75748200
C	-0.05729000	-2.39676500	-0.17716400	H	1.74710700	1.53211500	-1.51399200
H	-2.90770400	2.12498100	1.70672600	H	3.07035700	1.48316800	1.23270200
H	-1.95157500	2.01668900	0.20310100	H	0.56689900	2.15417800	1.03357500
H	-2.43508600	-0.06888100	2.36155900	H	-0.36410500	0.62583000	2.73093700
H	-0.19143700	-0.71985400	2.12690800	H	0.18989100	-1.82876400	2.50460800
H	-0.09306600	1.02802000	1.76424200	H	1.90645300	-1.32228900	2.30733600
H	-4.70216000	-0.47649700	1.08781300	Rh	-0.28855300	-0.44254500	0.25040200
H	-4.59615500	-0.56492300	-0.68800900	P	-2.21978000	0.77642400	-0.18786000
H	-2.74692300	-1.87516700	0.85705000	C	-3.76510500	-0.04769800	0.39095700
H	-2.40849000	-0.48762900	-1.78830000	H	-3.78835400	-1.05516000	-0.03203500
H	-0.65683300	-2.06848200	-2.24191200	H	-3.75200500	-0.13122100	1.48221700
H	0.73168000	-3.08136100	-0.48347400	H	-4.65618300	0.51139600	0.08236900
H	-0.44260000	-2.59797500	0.82107600	C	-2.37167300	2.47678300	0.53151200
Rh	0.28694000	-0.27997300	-0.41562900	H	-1.58447300	3.12355800	0.13159500
P	2.43636300	0.01922400	0.37576900	H	-3.34500900	2.92009600	0.29317300
C	2.75064300	1.52662500	1.38746500	H	-2.26249800	2.43651800	1.62042200
H	2.36171200	2.38938000	0.83994300	C	-2.54575300	1.06584700	-1.98096700
H	2.22318700	1.45183200	2.34350000	H	-3.51134500	1.55998300	-2.13932300
H	3.82132400	1.65447300	1.58193200	H	-1.75043700	1.68593300	-2.40636700
C	3.18871200	-1.33164000	1.38753300	H	-2.53603000	0.09627500	-2.48590200
H	4.21902900	-1.09098200	1.67322000	Cl	-1.31978200	-2.22749700	-1.04158300
H	2.59576100	-1.48512000	2.29486600				
H	3.18349700	-2.26505900	0.81687400	S4			
C	3.60522700	0.20881800	-1.03880700	O	3.60863000	0.45697000	1.80954300
H	4.62853900	0.38610400	-0.68875900	C	3.77031400	0.80681700	0.43974600
H	3.59149600	-0.69310800	-1.65931000	C	3.10942500	-0.32661200	-0.38755500
H	3.26826400	1.05416200	-1.64543600	C	2.30637600	0.15975000	-1.59996100
Cl	0.33795300	2.03435000	-1.24538100	C	2.32214500	-0.13967400	1.90095200
				C	2.23235300	-1.07075000	0.67134100
S3-TS				C	0.83337900	-1.44480300	0.20961300
O	3.79074900	1.13773800	-1.34166600	C	0.48407400	-1.48993900	-1.16083500
C	3.68200800	-0.26149100	-1.09708300	C	1.45813300	-0.97469600	-2.20352700
C	2.87134800	-0.43581500	0.22700700	H	4.84112100	0.92272800	0.25005000
C	1.72604800	-1.43909900	0.10711900	H	3.27500300	1.77075200	0.23272200
C	2.59914800	1.71841300	-0.83768900	H	3.88037600	-1.01518000	-0.75320300
C	2.37567700	1.01945800	0.51574700	H	2.97271700	0.59163600	-2.35725300
C	0.97043700	1.14273300	1.06916400	H	1.64819800	1.00367600	-1.30080100
C	0.42038800	0.28643900	2.05982200	H	2.26086700	-0.66435700	2.85889100

H	1.52877700	0.62586600	1.86381200	H	4.61083100	0.60091900	-1.67555100	
H	2.74340400	-2.00803300	0.93460000	H	5.23047800	0.95503000	-0.04675800	
H	0.30920800	-2.10919000	0.89455300	H	4.37130300	-1.84836300	-1.03478500	
H	-0.26368600	-2.20209100	-1.50610200	H	6.19148900	-2.58398300	0.43341400	
H	0.91108300	-0.61460000	-3.08325100	H	6.49484300	-0.83705600	0.95609100	
H	2.11738700	-1.78668000	-2.55238800	Rh	-0.86479900	0.33533000	-0.03098800	
Rh	-0.35653600	0.27397900	-0.31233800	P	0.26564500	-1.72073500	0.43118500	
P	-2.31910800	-0.46914300	0.36544700	P	-2.90084600	-0.59181700	-0.50756900	
C	-3.68026200	-0.06169000	-0.80744100	C	-0.65680800	-3.19355600	1.06843100	
H	-3.68091800	1.01896300	-0.96877600	H	-1.39225300	-3.55945800	0.34790400	
H	-3.49693500	-0.55434500	-1.76682400	H	0.04514900	-4.00612000	1.28546100	
H	-4.65051600	-0.38532500	-0.41185600	H	-1.17580200	-2.92822000	1.99455300	
C	-2.53511900	-2.28480900	0.63587300	C	1.50005400	-1.47774100	1.78103200	
H	-1.88263800	-2.63116200	1.44234400	H	1.98604400	-2.43070500	2.01971200	
H	-3.57436200	-2.50049200	0.90838200	H	2.25505200	-0.75930300	1.45515400	
H	-2.28746800	-2.83874900	-0.27441200	H	0.99720200	-1.10413000	2.67865800	
C	-2.87495900	0.25986600	1.96308200	C	1.25846500	-2.41425500	-0.95941500	
H	-3.88363400	-0.08361800	2.22166800	H	1.95669700	-1.64182600	-1.28987900	
H	-2.17942400	-0.02348600	2.75845700	H	1.81938800	-3.29877600	-0.63760500	
H	-2.86119100	1.34797500	1.86396700	H	0.60749000	-2.68822000	-1.79506200	
Cl	-1.19534300	2.50513500	-0.30147900	C	-3.93892900	-1.37805700	0.80004800	
S5a				H	-4.88610300	-1.73227100	0.37841400	
				H	-3.41325800	-2.22369200	1.25001700	
	C	0.14649400	2.33159700	-0.64872800	H	-4.15417800	-0.64959800	1.58697000
	C	-1.19823600	2.50214800	-0.14518700	C	-2.77918100	-1.88741200	-1.82061200
	C	-1.55021100	2.12015300	1.16046100	H	-3.77823400	-2.23554500	-2.10504000
	C	-2.90756400	2.35128500	1.75944900	H	-2.29001400	-1.46306500	-2.70272500
	C	1.21269300	1.81586400	0.05776000	H	-2.19369100	-2.74534600	-1.48316500
	C	2.58811300	1.73171200	-0.56712400	C	-4.08342100	0.58288700	-1.30845500
	C	3.40218600	2.96572600	-0.13504100	H	-3.61493900	1.03594500	-2.18708000
	O	3.19137800	0.50153600	-0.16310800	H	-4.98603200	0.04937800	-1.62632200
C	4.54452600	0.31333000	-0.61321400	H	-4.37592500	1.37765600	-0.61977700	
C	4.92831500	-1.12577800	-0.44005900	S5b				
C	5.91492200	-1.53617900	0.35728500					
H	0.28761400	2.52168200	-1.71187100		C	-0.04088000	-2.43308600	0.41928300
H	-1.94920000	2.90745400	-0.81744400		C	1.26877200	-2.49208800	-0.18790000
H	-0.76167900	2.02571000	1.90656000		C	1.52329500	-1.92667100	-1.45083500
H	-3.19381600	1.53635900	2.43266600		C	2.85192800	-2.01388000	-2.14592200
H	-2.87732100	3.26524100	2.36922200		C	-1.16213400	-1.87245600	-0.15987800
H	-3.68726500	2.48668800	1.00618300		C	-2.50863400	-1.80515800	0.53058300
H	1.20026600	1.77243800	1.14513300		C	-2.45806700	-1.77893000	2.06034900
H	2.49243400	1.73753200	-1.66582700		O	-3.18926400	-0.66561700	-0.00130600
H	4.38094500	2.99231500	-0.62290000	C	-4.62333700	-0.74387300	0.05000000	
H	2.87159200	3.88296600	-0.40903300	C	-5.19948200	0.38923900	-0.74370100	
H	3.55537500	2.96416700	0.95000100	C	-6.03528600	1.29800400	-0.24077700	

H	-0.09358000	-2.74491000	1.45924800	O	-3.50923200	-0.45821600	1.23709000
H	2.07637600	-2.94876100	0.37738600	C	-2.51242000	0.11844100	2.05666600
H	0.68874100	-1.77351400	-2.13421200	C	-1.20876500	-0.64528000	2.10244300
H	2.80532200	-2.80284300	-2.90940500	C	0.00532700	-0.08320000	2.40015200
H	3.09101800	-1.08340700	-2.67195500	C	-3.27763800	-0.37315900	-0.17107500
H	3.67061900	-2.26379600	-1.46649700	C	-2.01347100	-1.11424500	-0.51534400
H	-1.21815400	-1.73131700	-1.23677900	C	-1.19083800	-0.94116100	-1.64640600
H	-3.06530100	-2.70724100	0.21613800	C	0.02101900	-1.70715700	-1.72561300
H	-3.46302900	-1.65005900	2.47142800	C	0.36965500	-2.58300000	-0.66925700
H	-2.06772700	-2.71881200	2.46449900	H	-2.94609200	0.10386100	3.06466300
H	-1.83034500	-0.95450300	2.41541200	H	-2.33111200	1.17261400	1.79238300
H	-4.93813300	-1.71073800	-0.37638900	H	-1.30983100	-1.72685100	2.16493600
H	-4.98107500	-0.70311000	1.08756100	H	0.80737100	-0.70910500	2.77455600
H	-4.91971000	0.42210400	-1.79617600	H	0.09619400	0.98231000	2.59255400
H	-6.46469100	2.08288800	-0.85684900	H	-3.20975800	0.67981800	-0.46734800
H	-6.33755600	1.28168800	0.80436200	H	-2.00689900	-2.09400600	-0.04779500
Rh	0.85267200	-0.34473800	-0.00121600	H	-1.41027500	-0.20716800	-2.41615100
P	-0.37048400	1.70705700	-0.24053400	H	0.68053000	-1.56931400	-2.57864300
P	2.88780100	0.58688500	0.48720000	H	-0.42927200	-3.01630400	-0.07607800
C	0.47818300	3.32084200	-0.56690200	Rh	0.13444700	-0.33031900	0.00305700
H	1.10832400	3.24035000	-1.45751800	P	2.48568800	-0.05712400	0.27581600
H	-0.27197100	4.09894800	-0.74541300	P	-0.16260300	2.07037300	-0.50436300
H	1.09836400	3.63336500	0.27721100	C	-4.50242100	-1.00693300	-0.83695900
C	-1.57747100	2.15549200	1.08255100	H	-4.58602400	-2.06344900	-0.56343500
H	-2.08513200	3.09456100	0.83551800	H	-5.40742100	-0.49185700	-0.50172900
H	-2.31909400	1.35620400	1.15374900	H	-4.43402400	-0.92991400	-1.92672100
H	-1.06920300	2.26834600	2.04508400	C	1.57692400	-3.48279800	-0.75774400
C	-1.42504900	1.55806600	-1.74864300	H	1.89148400	-3.83755200	0.22810600
H	-2.13430500	0.74109800	-1.60308000	H	1.31863100	-4.37869100	-1.34036000
H	-1.97669000	2.48992400	-1.91717100	H	2.43306400	-3.01544300	-1.25285700
H	-0.79872800	1.35223400	-2.62202300	C	3.49415400	-0.14602600	-1.27288000
C	2.79425400	1.66094000	1.98853300	H	4.55623500	0.00048700	-1.04795200
H	3.79520400	2.00599100	2.27083900	H	3.37097600	-1.12116200	-1.75050200
H	2.15856200	2.53207900	1.81857500	H	3.17215500	0.62078900	-1.98171600
H	2.37341400	1.08536100	2.81870200	C	3.31520700	-1.30980000	1.35435800
C	3.82327700	1.60744400	-0.73355300	H	4.39667700	-1.13558900	1.35655400
H	4.77752600	1.93543400	-0.30691300	H	2.95067900	-1.22213200	2.38146100
H	4.02370100	1.01871600	-1.63373300	H	3.12378400	-2.32377800	1.00485100
H	3.24365800	2.48761700	-1.02019100	C	3.14761100	1.48201100	1.06720500
C	4.16280500	-0.63413300	1.03668000	H	4.23321900	1.39447100	1.18293000
H	4.48421400	-1.26887800	0.20878600	H	2.94054400	2.37173300	0.46952400
H	5.03907300	-0.10600200	1.42859100	H	2.70493100	1.61460000	2.05906900
H	3.75136800	-1.26848600	1.82718800	C	0.99530900	2.70929200	-1.80600300
				H	2.03913200	2.61613700	-1.49943900
				H	0.85856200	2.13149700	-2.72574300

S6a

H	0.79207000	3.76403800	-2.02110800	C	-0.63756300	3.13412700	0.89731400
C	0.03164500	3.31768100	0.85545800	H	-0.76489200	4.16424100	0.54770900
H	-0.03850800	4.33517900	0.45565100	H	-1.53814000	2.83569900	1.44108400
H	-0.76712300	3.18171800	1.59157200	H	0.21370700	3.09773300	1.58119600
H	0.98941900	3.20851100	1.36782600	C	-1.96441500	2.39544500	-1.47666500
C	-1.75914500	2.68581100	-1.22877300	H	-1.97836200	3.46921700	-1.69320700
H	-1.63082400	3.72402100	-1.55401000	H	-2.01761100	1.85622700	-2.42639100
H	-2.06442700	2.08981000	-2.09323300	H	-2.83434400	2.15050000	-0.86571400
H	-2.55953100	2.65919000	-0.48527900	C	2.77548500	1.72145500	1.38753200
S6b				H	2.42159700	2.62970500	0.89628300
				H	2.28031700	1.63929800	2.36047300
				H	3.85367900	1.81682500	1.55517400
O	-3.00495100	0.34605900	0.86268100	C	3.42507000	-1.01719000	1.34801000
C	-2.39555000	-0.22715500	2.01761400	H	4.46152900	-0.66793300	1.40709800
C	-0.87889800	-0.11802600	2.09427900	H	3.04012700	-1.11802600	2.36619600
C	-0.05712800	-1.22292900	2.16211700	H	3.41350300	-1.99900500	0.87428900
C	-3.15397600	-0.54906200	-0.26054300	C	3.48841000	0.43600200	-1.11034400
C	-1.87022300	-1.29028200	-0.56918500	H	4.50855200	0.70589700	-0.81616500
C	-1.10319000	-1.07263400	-1.73098000	H	3.52578900	-0.49511600	-1.68299700
C	0.18519000	-1.68889100	-1.86142800	H	3.08697400	1.21696000	-1.75933100
C	0.64813100	-2.56192300	-0.85929500	S6c			
H	-2.69115600	-1.27744500	2.13226300				
H	-2.81739200	0.32113300	2.86747500				
H	-0.49116200	0.83623600	2.44045500	O	3.03870500	0.04139700	0.88710600
H	0.93152400	-1.16219800	2.60016900	C	2.42348400	-0.10739900	2.16197900
H	-0.46706700	-2.22627600	2.07871000	C	1.04669700	-0.75853900	2.19804400
H	-3.39348000	0.12001100	-1.09090900	C	-0.11085000	-0.07966300	2.46687900
H	-1.77827000	-2.24997100	-0.06701100	C	3.14077800	-1.17973900	0.14653500
H	-1.42546900	-0.36491100	-2.48898000	C	1.76590400	-1.66796900	-0.29694900
H	0.81100100	-1.43417500	-2.71250300	C	1.07434800	-1.36085000	-1.48276900
H	-0.08598500	-3.10469200	-0.27259500	C	-0.27580600	-1.84284500	-1.62310500
Rh	0.13630900	-0.36861400	-0.03701900	C	-0.88163600	-2.58876300	-0.58752600
P	2.42256500	0.20506600	0.38401100	H	2.36377600	0.90467700	2.57059500
P	-0.41556600	1.99162500	-0.54235100	H	3.08543600	-0.69742500	2.81658700
C	-4.33675300	-1.50173700	-0.05733300	H	1.02605100	-1.84179400	2.28848400
H	-5.24034700	-0.92864000	0.16953600	H	-0.98987300	-0.61472200	2.80865700
H	-4.51490900	-2.08598800	-0.96695500	H	-0.10119000	0.99453300	2.62879700
H	-4.16226400	-2.20792000	0.76208400	H	3.54450900	-1.94865600	0.82422800
C	1.97237000	-3.26934700	-0.97261800	H	1.46803500	-2.58536600	0.19723300
H	2.33444000	-3.61293600	0.00054300	H	1.50055200	-0.73316100	-2.25791000
H	1.84983700	-4.16884800	-1.59275700	H	-0.83100500	-1.59675300	-2.52472100
H	2.74636200	-2.65515200	-1.44304400	H	-0.24795700	-3.15755200	0.08538800
C	0.80030500	2.91023800	-1.60343100	Rh	-0.18871900	-0.38562700	0.04078800
H	0.43980200	3.92552600	-1.80132600	P	-2.42807800	0.37284600	0.21475300
H	1.78215300	2.98422600	-1.13189200	P	0.59732900	1.87902800	-0.56500100
H	0.91708000	2.39004100	-2.55973200	C	4.14887000	-0.98075500	-0.98292300

H	5.09721500	-0.62710400	-0.56861300	H	-1.08494400	-1.26070700	2.59993800
H	4.32798100	-1.93149600	-1.49488100	H	0.46674100	-2.14293300	2.24312900
H	3.80624900	-0.25300300	-1.72213700	H	1.41418100	-2.60248400	0.27173600
C	-2.24516100	-3.20972300	-0.76461200	H	1.78659100	-0.61869700	-2.05156000
H	-2.14324900	-4.15554000	-1.31595500	H	-0.46592000	-1.32826100	-2.75475700
H	-2.70722100	-3.46327100	0.19403900	H	-0.40916200	-3.14617700	-0.25414700
H	-2.93804300	-2.58283700	-1.33368100	Rh	-0.14045100	-0.38069600	0.08778300
C	-3.52675600	-0.66876400	1.27639100	P	-2.35947400	0.36201500	0.43151200
H	-3.19089300	-0.62787300	2.31631500	P	0.54579800	1.85205700	-0.76742400
H	-4.55294300	-0.28825700	1.22998500	C	-2.22598900	-3.01942700	-1.47945600
H	-3.52159500	-1.70846800	0.95154400	H	-2.95031800	-3.02434900	-0.65792500
C	-3.37021500	0.45650600	-1.37362900	H	-2.16011400	-4.05752600	-1.83390600
H	-3.38533300	-0.52608200	-1.85090200	H	-2.62700800	-2.41703100	-2.30018900
H	-4.40248600	0.77639800	-1.19414400	H	3.35763800	-1.84448500	1.23731300
H	-2.89400600	1.15949400	-2.06104400	C	4.23200800	-1.04869400	-0.54580900
C	-2.78416700	2.02316200	0.97609000	H	4.46420900	-2.03754700	-0.95397700
H	-2.40147000	2.04622400	2.00053900	H	5.11719200	-0.66925600	-0.02774300
H	-2.33217900	2.84472600	0.41839700	H	4.01288700	-0.37851600	-1.38213500
H	-3.86696800	2.18392800	1.00931400	C	2.13775100	2.00793400	-1.69784100
C	-0.43374800	2.75850500	-1.83549500	H	2.34526700	3.06557600	-1.89353800
H	-0.45715200	2.16028000	-2.75229900	H	2.94746400	1.59154500	-1.09650800
H	-1.46207100	2.91558000	-1.50548300	H	2.08807800	1.48696600	-2.65890800
H	0.00418400	3.73481300	-2.07029800	C	-0.57671200	2.77999900	-1.91898400
C	0.74194100	3.14825400	0.77825900	H	-0.76381800	2.18066600	-2.81573300
H	1.52702300	2.84499300	1.47709000	H	-1.53750300	3.00438300	-1.44882400
H	1.01385500	4.12262000	0.35768800	H	-0.11558800	3.72633700	-2.22230300
H	-0.19280900	3.25615900	1.33370600	C	0.84228600	3.09870600	0.56860100
C	2.24752800	2.09333800	-1.37546100	H	1.70609100	2.78121400	1.15817400
H	2.40428300	3.15388800	-1.60102700	H	1.05657400	4.08167800	0.13501500
H	3.03425600	1.74102700	-0.70866300	H	-0.01994400	3.18821000	1.23372000
H	2.29174300	1.53538300	-2.31565900	C	-2.66335100	1.97766500	1.27907300
S6d				H	-2.17539600	1.98579200	2.25884100
				H	-2.27631300	2.81406700	0.69287000
O	2.88407600	0.14324700	1.03655000	H	-3.73876000	2.12558600	1.42583300
C	2.13634800	0.11328500	2.25188800	C	-3.36943900	0.50333300	-1.10814600
C	0.60749400	0.01591500	2.14860800	H	-3.45233500	-0.47933000	-1.57771600
C	-0.08201500	-1.20587500	2.19502800	H	-4.37553200	0.86531000	-0.86997000
C	3.06693400	-1.14580900	0.43807300	H	-2.90429800	1.18672500	-1.82120700
C	1.77254500	-1.67774200	-0.16802800	C	-3.40979700	-0.75672000	1.46552300
C	1.24501700	-1.29624600	-1.40277200	H	-4.46440300	-0.48412900	1.35190800
C	-0.07420100	-1.72071300	-1.81953200	H	-3.27522200	-1.79904100	1.16800300
C	-0.86430500	-2.55709500	-1.04347300	H	-3.14487500	-0.66170700	2.52207700
H	2.50700500	-0.71597400	2.87383200	S6a-TS			
H	2.39157500	1.04562600	2.76279200				
H	0.08532200	0.90163800	2.50538700	O	-3.84278600	-0.14753900	1.31620300

C	-2.71851900	0.27597100	2.04922300	C	0.26421100	3.33134200	0.81187600
C	-1.52890400	-0.62151700	1.74596300	H	0.27634200	4.35834400	0.43123500
C	-0.19504400	-0.11901100	2.00871000	H	-0.59612800	3.22158500	1.48017100
C	-3.47804600	-0.23331700	-0.05071500	H	1.17222800	3.16262900	1.39556200
C	-2.15728000	-0.99518200	-0.16504000	C	-1.37475100	2.78135400	-1.44187600
C	-1.39630200	-0.80166000	-1.40368500	H	-1.24759700	3.84892900	-1.65273000
C	-0.35461700	-1.69962400	-1.75854300	H	-1.53838100	2.25913400	-2.38895100
C	0.20235900	-2.55933400	-0.79633900	H	-2.26254600	2.65554800	-0.81632600
H	-2.98596700	0.21303800	3.10907900				
H	-2.46255600	1.32529000	1.81936100	S6b-TS			
H	-1.68218600	-1.65233200	2.06086300	O	-3.95629900	-0.11729400	1.29360700
H	0.44553700	-0.78945300	2.57862100	C	-2.88102900	-0.44561700	2.15711300
H	-0.12016900	0.91738200	2.33786100	C	-1.59852000	0.14096400	1.61132900
H	-3.33397000	0.78341800	-0.45302300	C	-0.28523400	-0.27549300	1.99614500
H	-2.27410300	-2.05220800	0.07529100	C	-3.56402900	-0.00450100	-0.07711800
H	-1.76085900	-0.08704800	-2.13501900	C	-2.20079300	-0.65021800	-0.24592600
H	0.10827200	-1.61088900	-2.73903700	C	-1.47133000	-0.54184600	-1.49646900
H	-0.42186800	-2.88358200	0.03359500	C	-0.49953400	-1.51890500	-1.83083100
Rh	0.25938900	-0.24061600	-0.06782500	C	-0.02896000	-2.43340200	-0.85530200
P	2.50430000	-0.28960800	0.47136300	H	-2.79495300	-1.53232000	2.31223800
P	0.13008000	2.12017200	-0.58415400	H	-3.10438300	0.01061800	3.12900700
C	-4.61634100	-0.92385300	-0.79729600	H	-1.70829200	1.21148600	1.44182000
H	-4.76226200	-1.94047800	-0.41827700	H	0.35217000	0.48051300	2.44925600
H	-5.54452000	-0.36502900	-0.64672200	H	-0.18251800	-1.26656200	2.43892100
H	-4.40942400	-0.97329500	-1.87091600	H	-3.52082300	1.06092200	-0.35154800
C	1.31525200	-3.51159900	-1.15359400	H	-2.22406300	-1.67078900	0.13034600
H	1.94855800	-3.76021200	-0.29710200	H	-1.75258100	0.21158300	-2.22534900
H	0.88894500	-4.46150900	-1.50542200	H	-0.02543700	-1.47315800	-2.80875600
H	1.95072100	-3.12430000	-1.95648100	H	-0.71780200	-2.76761500	-0.08206700
C	3.62414100	-0.49664500	-0.98122800	Rh	0.27039600	-0.23939400	-0.11030900
H	4.67165100	-0.48855100	-0.66028000	P	2.47976000	-0.52739600	0.45014600
H	3.41802400	-1.44527600	-1.48252500	P	0.37813400	2.19379100	-0.45947300
H	3.46420200	0.31297400	-1.69827900	C	-4.63182600	-0.69221100	-0.93106200
C	3.04831900	-1.64015500	1.60985700	H	-5.60995800	-0.26061200	-0.69950400
H	4.13837300	-1.62632300	1.71718300	H	-4.43307600	-0.55180100	-1.99871800
H	2.60121400	-1.50098900	2.59831400	H	-4.67064800	-1.76460900	-0.71394400
H	2.74294100	-2.61574000	1.22804700	C	0.99189100	-3.47865400	-1.24129400
C	3.23395600	1.17307700	1.33564700	H	1.56003500	-3.84918300	-0.38375500
H	4.28840100	0.98264500	1.56283800	H	0.48145100	-4.35127600	-1.67205400
H	3.17264400	2.07289900	0.71915900	H	1.69774600	-3.11359900	-1.99409600
H	2.70298200	1.35453200	2.27497400	C	1.70872800	2.78284600	-1.60643700
C	1.43915800	2.70617200	-1.75798200	H	1.64755100	3.86736600	-1.75041000
H	2.43893100	2.54421300	-1.34727300	H	2.70181700	2.53999800	-1.21868800
H	1.36104100	2.14458800	-2.69430600	H	1.59334400	2.29059400	-2.57717800
H	1.32005700	3.77354600	-1.97499200	C	0.59036400	3.30745500	1.00864300

H	0.58440200	4.35899400	0.70167500	H	4.35748100	-1.89482300	-1.46271700
H	-0.22924000	3.15050800	1.71771800	H	3.95766600	-0.17363900	-1.66377900
H	1.53077800	3.10137200	1.52574100	C	-1.88922600	-3.33797800	-1.00539500
C	-1.10287400	2.97761500	-1.25539900	H	-1.63535400	-4.36304400	-1.30963100
H	-0.95013100	4.05670200	-1.36766100	H	-2.58486000	-3.43118600	-0.16647700
H	-1.27219800	2.54739700	-2.24677700	H	-2.41622400	-2.87305200	-1.84483500
H	-1.99982300	2.81656500	-0.64991100	C	-3.39200500	-1.00288600	1.50785300
C	3.32788600	0.83608400	1.36772600	H	-2.99927100	-0.86686100	2.51972200
H	3.36308500	1.75219000	0.77441900	H	-4.46519700	-0.78411200	1.51943200
H	2.80243000	1.04414500	2.30461300	H	-3.24571100	-2.04463700	1.21817300
H	4.35507000	0.53938200	1.60565900	C	-3.56323800	0.05852200	-1.18066300
C	2.83456600	-1.94006200	1.58473300	H	-3.51729900	-0.94198100	-1.61669900
H	3.91430100	-2.04870000	1.73407300	H	-4.60706100	0.29239900	-0.94346300
H	2.36372600	-1.75411500	2.55473800	H	-3.19737700	0.77342600	-1.92228700
H	2.43594900	-2.87306300	1.18396900	C	-3.00596200	1.76295600	1.07412100
C	3.62191100	-0.80706200	-0.97153200	H	-2.51341900	1.89678800	2.04155300
H	4.65085400	-0.93394500	-0.61740400	H	-2.73235100	2.59611700	0.42340300
H	3.32539900	-1.70204500	-1.52279300	H	-4.08986500	1.78823000	1.22942900
H	3.58267400	0.04624000	-1.65454900	C	-0.73476200	2.78074400	-1.87327400
S6c-TS				H	-0.71018600	2.17197000	-2.78261100
O	3.34509500	0.25888600	0.89412000	H	-1.77348500	2.85481900	-1.54162100
C	2.55329900	0.15044600	2.06731100	H	-0.37566900	3.78722900	-2.11550900
C	1.37029000	-0.80351900	1.87187800	C	0.35927800	3.27438400	0.75739400
C	0.02668700	-0.30258400	2.08093800	H	1.16104400	3.05211700	1.46804700
C	3.39610700	-1.01600600	0.26951100	H	0.54031100	4.26980000	0.33762200
C	1.95272600	-1.49073500	0.01948300	H	-0.58768900	3.29007400	1.30206100
C	1.29894500	-1.20689200	-1.26086000	C	2.00681800	2.28017900	-1.34294500
C	0.11554200	-1.90669200	-1.61477100	H	2.16195500	3.34960500	-1.52362800
C	-0.63134700	-2.59133600	-0.63526100	H	2.78510300	1.90321700	-0.67533600
H	2.21638300	1.15892000	2.31938100	H	2.07508800	1.75635600	-2.30160200
H	3.17171100	-0.22245000	2.89844000	S6d-TS			
H	1.52786900	-1.79877400	2.28430300	O	3.98792600	-0.94460500	1.14211700
H	-0.66411700	-0.98653000	2.57126900	C	2.87545200	-1.20600300	1.97428200
H	-0.05884400	0.72245100	2.44056000	C	1.71262700	-0.32718100	1.57305800
H	3.83918700	-1.73715600	0.97724500	C	0.35811100	-0.58543500	1.92593800
H	1.79800400	-2.52860400	0.30976200	C	3.63765400	-0.67962700	-0.22079700
H	1.80754800	-0.60545400	-2.00417700	C	2.16117600	-0.98934500	-0.42761900
H	-0.29006100	-1.78327600	-2.61682000	C	1.43223000	-0.61391200	-1.61507700
H	-0.10780400	-2.99928900	0.22639800	C	0.30976900	-1.38354600	-2.02479100
Rh	-0.29377200	-0.29682300	-0.02595200	C	-0.27490900	-2.34543800	-1.16628900
P	-2.52220400	0.13596800	0.34120700	H	2.59039200	-2.27031500	1.97372700
P	0.34388300	1.99647300	-0.58455100	H	3.19022700	-0.95004900	2.99308400
C	4.30276500	-0.92837500	-0.95187000	H	1.99537600	0.72328800	1.52965500
H	5.31079600	-0.65068900	-0.63129200	H	-0.16416100	0.19950200	2.46840800

H	0.10975300	-1.59586900	2.25161200	C	-1.90028700	-0.57241000	1.47456400
H	1.97544400	-2.02153500	-0.14443200	C	-0.39131400	-0.36676100	1.53524700
H	1.80107400	0.17764000	-2.25841300	C	-3.83257400	-0.25627000	-0.00240600
H	-0.16969600	-1.13904500	-2.97010500	C	-2.48135400	-1.04070300	0.09789100
H	0.36311500	-2.87386100	-0.46080700	C	-1.58784800	-0.81126600	-1.11197100
Rh	-0.26057800	-0.23521800	-0.15063500	C	-0.60638500	-1.73060700	-1.54688600
P	-2.45071300	-0.37228800	0.53006700	C	0.17308400	-2.52464100	-0.68286900
P	-0.19147000	2.21804700	-0.30262200	H	-2.86486300	0.86225200	2.86066600
C	-1.44365600	-3.16811300	-1.65835900	H	-2.34867100	1.56550700	1.30740200
H	-2.09325600	-3.51350000	-0.84892000	H	-2.16129000	-1.34050000	2.21457100
H	-1.07280300	-4.07150500	-2.16187900	H	0.11288500	-1.22664300	1.98145700
H	-2.05571400	-2.62204200	-2.38344200	H	-0.11337000	0.53655500	2.08688800
H	4.16640100	-1.42834600	-0.83240700	H	-3.71826900	0.54412300	-0.75456600
C	4.15025200	0.70235800	-0.60704500	H	-2.69407300	-2.11493300	0.15710200
H	4.00311100	0.90796700	-1.67272600	H	-2.00609100	-0.17632800	-1.89006600
H	5.22314700	0.74967700	-0.40038800	H	-0.26952300	-1.64519700	-2.58359100
H	3.66538900	1.48580600	-0.01696400	H	-0.25441900	-2.80682900	0.27832100
C	1.18254500	2.99319800	-1.27669500	Rh	0.47672200	-0.22808300	-0.34434700
H	1.04631500	4.07927700	-1.32472200	P	2.65676000	-0.35447300	0.62260400
H	2.15328200	2.78467400	-0.82222400	P	0.22073600	2.14352500	-0.57346800
H	1.18691300	2.59892200	-2.29753900	C	-5.04595200	-1.10358900	-0.34708400
C	-1.63161500	2.96798000	-1.19925500	H	-5.17269900	-1.90631600	0.38712500
H	-1.68173700	2.54837100	-2.20905800	H	-5.95156400	-0.48973500	-0.34407700
H	-2.57722500	2.75498400	-0.69551600	H	-4.93613100	-1.55073100	-1.34124800
H	-1.51690500	4.05501800	-1.27525500	C	1.22204800	-3.46701800	-1.22244500
C	-0.11900700	3.22859300	1.25098700	H	2.03353400	-3.63796200	-0.50757600
H	0.80057100	2.99993200	1.79976000	H	0.77825700	-4.45025600	-1.43081100
H	-0.12820600	4.29999900	1.02248400	H	1.65968500	-3.09983000	-2.15744900
H	-0.96750700	3.00292200	1.90248600	C	3.93013100	-0.69030600	-0.67470600
C	-3.09649500	0.93465600	1.67037900	H	4.92666900	-0.77916800	-0.22844900
H	-2.48969400	0.97291300	2.57999300	H	3.69414000	-1.62034300	-1.19929900
H	-3.08518800	1.92128100	1.20302700	H	3.94595500	0.12377300	-1.40644100
H	-4.12799100	0.69908400	1.95381300	C	2.91853100	-1.71123500	1.84775400
C	-3.70800900	-0.37853100	-0.81921200	H	3.97516800	-1.77684900	2.12787200
H	-3.54594400	-1.23384200	-1.47869800	H	2.33210500	-1.51605700	2.75083400
H	-4.71838000	-0.44051000	-0.40028400	H	2.60004500	-2.67019800	1.43171500
H	-3.62312100	0.53543700	-1.41318200	C	3.38262100	1.08393000	1.53054100
C	-2.86919800	-1.87414400	1.52295600	H	4.38983300	0.84199300	1.88679400
H	-3.94709900	-1.91644700	1.71350000	H	3.44767000	1.96154200	0.88115500
H	-2.56406900	-2.78560400	1.00670200	H	2.75998700	1.33467100	2.39494000
H	-2.34799500	-1.83201200	2.48389800	C	1.55472900	2.77048600	-1.69606600
				H	2.54142000	2.61426300	-1.25048500
S7a				H	1.51976700	2.23800200	-2.65224300
O	-4.03725600	0.34777400	1.27439400	H	1.42427000	3.84072400	-1.89074800
C	-2.76280300	0.66222500	1.79048700	C	0.34240500	3.27088600	0.88555100

H	0.29591100	4.31682800	0.56385900	H	-0.10808800	3.10103600	1.62734000	
H	-0.48617900	3.08437600	1.57490900	H	1.65049700	2.87929800	1.69291600	
H	1.28078500	3.10866000	1.42167600	C	-0.52799800	3.13458700	-1.47083700	
C	-1.29102800	2.78000500	-1.42638900	H	-0.28819700	4.20260600	-1.51817300	
H	-1.21787400	3.86252900	-1.57808200	H	-0.56958000	2.73814800	-2.48998300	
H	-1.39877500	2.29488400	-2.40121300	H	-1.51560800	3.01635600	-1.01560200	
H	-2.18520800	2.56661000	-0.83479500	C	3.30040800	0.37712300	1.82906300	
S7b				H	3.59320700	1.27044300	1.27094500	
				H	2.63503000	0.67617700	2.64480600	
	O	-4.23421700	0.21509600	1.41550300	H	4.20030600	-0.07238700	2.26255600
	C	-3.02014100	0.25183900	2.16770600	C	2.28899100	-2.29210100	1.84699300
	C	-1.90130800	0.35680500	1.11114800	H	3.26579500	-2.56686200	2.25903600
	C	-0.51318500	-0.12846100	1.43722600	H	1.61631700	-2.05100300	2.67562900
	C	-3.98057500	0.00129300	0.01504200	H	1.87631000	-3.14688000	1.30593700
	C	-2.52058500	-0.48318000	-0.02613900	C	3.77321100	-1.32405600	-0.45893200
	C	-1.75126500	-0.36693300	-1.31177900	H	4.67419500	-1.63831500	0.07923600
	C	-0.86302600	-1.34227500	-1.77075900	H	3.42921900	-2.15142400	-1.08557400
C	-0.18672100	-2.27727100	-0.92814800	H	4.02860200	-0.48074100	-1.10812000	
H	-2.91941300	-0.66447500	2.76827800					
H	-3.04459300	1.10964200	2.84845700	S7c				
H	-1.85684700	1.40181500	0.77719600	O	3.64286600	0.57071800	0.76320000	
H	0.04451400	0.53446200	2.10375400	C	2.66620800	0.66035100	1.79567700	
H	-0.51109300	-1.14942500	1.83198700	C	1.77091700	-0.60890200	1.69462800	
H	-4.05748300	0.96871500	-0.51080600	C	0.26666900	-0.37838900	1.64961800	
H	-2.51306700	-1.53137100	0.30373900	C	3.80609000	-0.82222100	0.47036700	
H	-2.06575400	0.39773800	-2.01917500	C	2.34986500	-1.35079700	0.45153300	
H	-0.49839400	-1.23918100	-2.79536200	C	1.61193100	-1.03891900	-0.84351400	
H	-0.70487300	-2.61694500	-0.03200400	C	0.59265300	-1.86698000	-1.36653300	
Rh	0.49492700	-0.20103200	-0.39603500	C	-0.34212100	-2.56688800	-0.57683800	
P	2.44483100	-0.83455600	0.72697600	H	2.11254500	1.59186400	1.65065100	
P	0.74706100	2.21506700	-0.49362900	H	3.15565200	0.71017800	2.77811300	
C	-5.01635000	-0.96210300	-0.54246900	H	1.96809600	-1.23390500	2.57768900	
H	-6.02343900	-0.56769100	-0.37854800	H	-0.27769600	-1.23506900	2.05598900	
H	-4.87513600	-1.10318500	-1.62030400	H	-0.03709500	0.52658500	2.18432700	
H	-4.94640000	-1.93582500	-0.04582300	H	4.31265900	-1.30837800	1.32171200	
C	0.72142800	-3.31517500	-1.55251900	H	2.33111200	-2.43415400	0.61874200	
H	1.44422700	-3.71669100	-0.83481500	H	2.15205600	-0.44322400	-1.57161500	
H	0.13511000	-4.16955400	-1.91777100	H	0.36387900	-1.76295400	-2.43083900	
H	1.27784100	-2.91261300	-2.40690200	H	-0.04030700	-2.87320300	0.42386800	
C	2.29769100	2.71128900	-1.37684400	Rh	-0.44836400	-0.24571900	-0.29022800	
H	2.34243600	3.79894700	-1.49931000	P	-2.70283300	-0.14280500	0.49665600	
H	3.18327800	2.38745600	-0.82223400	P	0.05919500	2.07765500	-0.57760300	
H	2.32541600	2.24865200	-2.36881800	C	4.67796200	-0.98852800	-0.76199100	
C	0.82240200	3.21299300	1.06170900	H	5.67316300	-0.57995600	-0.56386100	
H	0.96146900	4.27485400	0.83209500	H	4.78794500	-2.04930600	-1.01089300	

H	4.27167500	-0.46531100	-1.63247800	H	2.16671400	-2.02899900	0.27001700	
C	-1.42469800	-3.40920800	-1.20835500	H	2.13158800	0.05036600	-1.96187100	
H	-1.06483500	-4.43452300	-1.37096000	H	0.33575500	-1.26349600	-2.83308900	
H	-2.31135800	-3.48849500	-0.57082300	H	0.24414700	-2.77953800	-0.13580200	
H	-1.73623900	-3.01267100	-2.18117800	Rh	-0.50793100	-0.18466000	-0.39488900	
C	-3.17318200	-1.43816200	1.72567200	P	-2.55575700	-0.51954300	0.68191800	
H	-2.60579400	-1.29882200	2.65110400	P	-0.33969700	2.23810500	-0.39164200	
H	-4.24130200	-1.37848800	1.96003800	C	-1.23820400	-3.16236100	-1.71472800	
H	-2.95070000	-2.43311900	1.33217900	H	-2.05355900	-3.43797800	-1.03879700	
C	-3.91187600	-0.40372900	-0.87805000	H	-0.80163300	-4.10259700	-2.07864300	
H	-3.72649800	-1.36582200	-1.36386300	H	-1.67291800	-2.64918200	-2.58022000	
H	-4.93911200	-0.39243700	-0.49746000	H	4.42187700	-1.81411700	-0.14566100	
H	-3.80862900	0.38666100	-1.62809900	C	4.58945300	0.22792600	-0.79147700	
C	-3.36069900	1.37968400	1.31526000	H	4.55810200	-0.04524700	-1.85236600	
H	-2.78243300	1.60119000	2.21773900	H	5.63852600	0.34280100	-0.50395900	
H	-3.29976500	2.23916900	0.64132400	H	4.10190900	1.20118200	-0.65948800	
H	-4.40870400	1.23758200	1.60058700	C	1.05567200	2.95684600	-1.37191100	
C	-1.07654700	2.73796200	-1.88394200	H	0.99316400	4.05038200	-1.39714300	
H	-1.00144300	2.12822900	-2.79037400	H	2.01579400	2.66941500	-0.93380300	
H	-2.11486400	2.71985100	-1.53996000	H	1.02089200	2.57828300	-2.39827600	
H	-0.81106600	3.76991000	-2.13909200	C	-1.79818800	3.02377700	-1.22128200	
C	-0.14832500	3.31379900	0.78277800	H	-1.91795800	2.61502900	-2.22996700	
H	0.55558200	3.11712800	1.59590300	H	-2.71657800	2.82843200	-0.65986600	
H	0.03720300	4.32471300	0.40410400	H	-1.66233100	4.10804300	-1.29987900	
H	-1.16186900	3.27032600	1.18932400	C	-0.21454200	3.18067800	1.19412400	
C	1.71698800	2.49847900	-1.27483800	H	0.68463900	2.87964500	1.74036900	
H	1.83642500	3.58431000	-1.35725900	H	-0.15758200	4.25658400	0.99768800	
H	2.51959400	2.08262800	-0.65837800	H	-1.08376400	2.98600700	1.82822200	
H	1.79914200	2.06307600	-2.27625700	C	-3.16827600	0.75167300	1.87512500	
S7d				H	-2.46288700	0.85863900	2.70506600	
				H	-3.27842000	1.72228000	1.38403300	
	O	4.20119100	-0.53407300	1.46360600	H	-4.14083200	0.45588800	2.28332900
	C	2.99166600	-0.49833400	2.21144300	C	-3.93984800	-0.64945900	-0.53328500
	C	1.92597900	-0.11555600	1.16711600	H	-3.75154600	-1.47235700	-1.22864400
C	0.46806900	-0.36624300	1.44981900	H	-4.89003600	-0.83068300	-0.01903900	
C	3.94958800	-0.84862800	0.07736500	H	-4.02314600	0.27768800	-1.10875800	
C	2.40455200	-0.99488700	-0.01033400	C	-2.70272000	-2.05790300	1.68979200	
C	1.68671700	-0.68263300	-1.29482400	H	-3.71851700	-2.16134500	2.08588900	
C	0.65772700	-1.47567600	-1.81094200	H	-2.46499000	-2.93721500	1.08672900	
C	-0.18396200	-2.32162900	-1.02678300	H	-2.00358300	-2.01707100	2.53049500	
H	2.76572000	-1.47912200	2.66036200	S7a-TS				
H	3.11027900	0.23423600	3.01513200		O	3.03100500	-0.27593100	-1.81066500
H	2.08511500	0.93966600	0.91100500		C	2.58626200	-1.48232100	0.14849000
H	0.02000400	0.35112300	2.14213200		C	1.11083200	-1.83058300	-0.01083400
H	0.28312800	-1.38843600	1.79649300					

C	3.14991200	0.72817100	-0.79318600	H	-1.54172000	-1.41416100	2.71564600
C	2.79672600	0.00823100	0.55373700	H	2.39543800	1.48593200	-1.03371600
C	1.64331200	0.65579900	1.28831000	C	4.53624200	1.36976200	-0.80133900
C	0.74600500	0.01052000	2.15130400	H	4.60200600	2.16178800	-0.04531800
C	0.52567000	-1.42399500	2.02580500	H	4.74390500	1.81109400	-1.78054800
H	3.06487700	-2.15449000	0.86889600	H	5.31900200	0.63376000	-0.58530800
H	0.87428200	-2.88531800	0.12649500				
H	0.76796200	-1.52514300	-1.01368600	S7b-TS			
H	3.67155100	0.06649900	1.21860900	O	4.23968200	-0.49299600	-1.47920900
H	1.74399200	1.73083300	1.41225600	C	3.30818100	-1.57944900	-1.50043300
H	0.17209500	0.57943800	2.87906000	C	2.04978200	-1.01944400	-0.81509900
H	1.41188300	-2.04293900	2.12666500	C	0.97993400	-1.92707000	-0.25597700
Rh	-0.27935600	-0.06141600	0.27918300	C	3.81289400	0.54859800	-0.57852500
P	-2.11470200	-1.17801500	-0.81114900	C	2.71766700	-0.12214800	0.25841900
P	-1.17746600	2.09726600	0.06362700	C	1.71017500	0.70203000	1.01608000
C	-1.82502000	-2.96331800	-1.19864400	C	0.84837400	0.08678000	1.92670700
H	-2.71488000	-3.39952500	-1.66458000	C	0.72316200	-1.36366700	1.86667200
H	-0.98119100	-3.07407600	-1.88589300	H	3.71364500	-2.44234900	-0.95047000
H	-1.60139000	-3.51960300	-0.28368300	H	3.13643300	-1.87899200	-2.53935100
C	-3.68228300	-1.26466300	0.16342500	H	1.57662000	-0.33692800	-1.53371500
H	-4.04857800	-0.26358700	0.39983500	H	0.19519000	-2.16572100	-0.97412100
H	-4.45428200	-1.80263400	-0.39748500	H	1.32790500	-2.86260000	0.17747700
H	-3.49870600	-1.79260100	1.10367900	H	3.37339900	1.37018300	-1.17104700
C	-2.66708000	-0.54437300	-2.45983000	H	3.23152200	-0.78463800	0.97328000
H	-1.82581400	-0.56330100	-3.15993300	H	1.82970500	1.78190200	1.04138800
H	-3.47473300	-1.16497400	-2.86297400	H	0.29710200	0.65318100	2.67336700
H	-3.02553900	0.48592400	-2.38489900	H	1.67869800	-1.87742600	1.86667100
C	-3.00072200	2.39253800	0.19351600	Rh	-0.43006500	-0.06175800	0.19142300
H	-3.54855700	1.83419700	-0.56963100	P	-2.39951100	-1.13958500	-0.55623500
H	-3.36163000	2.08204800	1.17887400	P	-1.18237600	2.12307400	-0.05630400
H	-3.21769900	3.45802900	0.06210600	C	-3.93105800	-0.80264700	0.42094900
C	-0.55959200	3.35580000	1.27197700	H	-4.20683700	0.25182600	0.36605900
H	0.51839600	3.50140500	1.16444100	H	-4.76424400	-1.40413700	0.04115200
H	-1.05533200	4.31698500	1.09917100	H	-3.75896300	-1.05967400	1.47044800
H	-0.76838100	3.03606100	2.29768300	C	-2.35330900	-2.99038700	-0.49739900
C	-0.76262900	2.88127600	-1.55975100	H	-2.10723500	-3.33322800	0.51135400
H	-1.14722100	3.90610000	-1.60835500	H	-3.33109000	-3.39584400	-0.77851100
H	0.32298800	2.90205300	-1.69359700	H	-1.60517000	-3.38612200	-1.19009100
H	-1.19221000	2.30141300	-2.38166600	C	-2.92932900	-0.85753400	-2.30703800
C	3.31979300	-1.52837400	-1.20797500	H	-2.12593200	-1.16187900	-2.98528100
H	2.96843900	-2.31654500	-1.87966200	H	-3.82672500	-1.44130200	-2.53963900
H	4.40160700	-1.66339700	-1.05331700	H	-3.14223500	0.19926700	-2.48717500
C	-0.66459900	-2.06577100	2.70291400	C	-2.91699400	2.61738000	-0.46874700
H	-0.39870800	-2.31132700	3.74122000	H	-3.26892400	2.12128500	-1.37684500
H	-0.93332400	-3.00974500	2.21699700	H	-3.59017900	2.36646100	0.35559400

H	-2.96054200	3.70012900	-0.62918900	H	3.16604400	-2.17713500	1.14940100
C	-0.88416000	3.19531200	1.42068400	C	2.80548700	-0.54932700	-2.32744200
H	0.16345100	3.15701600	1.73018400	H	2.04260600	-0.38204600	-3.09419400
H	-1.14115800	4.23535000	1.19234000	H	3.56226800	-1.23323600	-2.72675300
H	-1.50422600	2.85671100	2.25666300	H	3.28851100	0.40665900	-2.10636600
C	-0.22704900	2.96596500	-1.39718300	C	3.00595000	2.15255500	0.60551300
H	-0.48738900	4.02896600	-1.44972900	H	3.63925700	1.56714900	-0.06603100
H	0.84666800	2.87107700	-1.21397900	H	3.13616700	1.77255100	1.62335300
H	-0.45142900	2.49876800	-2.36084100	H	3.33936900	3.19533300	0.57241400
C	5.01687700	1.06831400	0.19155400	C	0.48470500	3.34385000	1.18156700
H	5.78002700	1.43111800	-0.50312600	H	-0.53595100	3.56639500	0.85929900
H	4.73153800	1.89864700	0.84868500	H	1.07671800	4.26250900	1.11149000
H	5.46013800	0.27316400	0.80048500	H	0.46040700	3.02547800	2.22831100
C	-0.30107300	-2.08248300	2.71164500	C	1.20716700	2.84294100	-1.54558000
H	0.09479300	-2.20619000	3.73001700	H	1.69017300	3.82544400	-1.49960900
H	-1.24597600	-1.53675700	2.77514100	H	0.17504400	2.97337200	-1.88320100
H	-0.49925700	-3.08782200	2.32666900	H	1.72813200	2.22721000	-2.28312300
S7c-TS				C	-3.41581800	-1.46291600	-1.25300400
O	-3.18588900	-0.16757100	-1.77761600	H	-3.01687200	-2.19815900	-1.95656600
C	-2.70598500	-1.45445900	0.12229600	H	-4.49477400	-1.64777800	-1.12525700
C	-1.23294300	-1.81318400	-0.03036000	C	0.51481000	-2.06973500	2.70919400
C	-3.48204000	0.73066300	-0.70737300	H	0.22650200	-2.30693400	3.74341700
C	-2.91977000	0.02792400	0.58196600	H	0.77283500	-3.02075700	2.23074700
C	-1.71647300	0.68336600	1.23144900	H	1.40448900	-1.43619900	2.73508400
C	-0.82928200	0.03609200	2.10686800	C	-2.96035900	2.10999600	-1.06680400
C	-0.64981400	-1.40404800	2.01277600	H	-3.22749900	2.84490500	-0.29924500
H	-3.19656100	-2.14981900	0.81168000	H	-1.87247000	2.09301900	-1.18674600
H	-1.00812500	-2.87055600	0.10610500	H	-3.40581000	2.43358700	-2.01196400
H	-0.88334100	-1.51113300	-1.03344500	S7d-TS			
H	-4.57740800	0.78386300	-0.59773800	O	-4.38986500	-0.49193500	-1.20638300
H	-3.71348300	0.04520700	1.34333500	C	-3.48563300	-1.59402500	-1.25588600
H	-1.79095900	1.76135000	1.33474800	C	-2.18270300	-1.02876000	-0.67028100
H	-0.24085700	0.60177900	2.82568300	C	-1.05553400	-1.93047100	-0.22820600
H	-1.55414000	-1.99704400	2.10829800	C	-3.99904200	0.46694000	-0.19810100
Rh	0.18972400	-0.07961500	0.23806600	C	-2.78222000	-0.19019200	0.49003400
P	2.02321300	-1.26066100	-0.80798200	C	-1.73289300	0.61817300	1.20800100
P	1.22651600	2.02669000	0.11499500	C	-0.80035300	-0.02561600	2.02390500
C	1.62177600	-2.97064700	-1.38836500	C	-0.65912300	-1.47080600	1.88893800
H	2.51240500	-3.44318600	-1.81570400	H	-3.85240200	-2.44041900	-0.65279000
H	0.83924400	-2.94287100	-2.15245100	H	-3.40071100	-1.91799700	-2.29720600
H	1.26863000	-3.58335000	-0.55396200	H	-1.78604400	-0.31737900	-1.40534000
C	3.47874600	-1.58211000	0.28679400	H	-0.32486600	-2.11144000	-1.01666400
H	3.90392600	-0.64518400	0.65415800	H	-1.34962600	-2.89812000	0.17419000
H	4.25217900	-2.13335600	-0.25934700	H	-3.19675100	-0.90964800	1.21220200

H	-1.85541200	1.69414800	1.28297900	C	2.43769500	1.39168300	-0.12922900
H	-0.20424200	0.51560200	2.75447800	C	0.97012500	1.70861800	-0.05249400
H	-1.60433600	-2.00147700	1.93403300	C	0.22666700	2.04874500	-1.18236100
Rh	0.37724100	-0.08897300	0.20875700	C	-1.15493300	2.48396100	-1.10848600
P	2.29185400	-1.13009000	-0.71917300	C	-1.85907700	2.68561400	0.05722100
P	1.17308600	2.08994200	0.06165700	H	4.37063100	1.35591700	1.59743400
C	3.85433400	-0.95647200	0.25287000	H	4.96728400	-0.99290300	-0.32327700
H	4.16694800	0.08703400	0.31749700	H	6.68885100	0.53468800	-1.17548800
H	4.65775000	-1.53609000	-0.21480200	H	6.16059800	1.82845500	0.03370300
H	3.69439100	-1.33068800	1.26848300	H	2.97797800	2.31158700	0.15448300
C	2.19101300	-2.97317500	-0.87235700	H	2.74520600	1.15153800	-1.15579200
H	1.94189500	-3.42268400	0.09304600	H	0.65122000	2.02755200	0.93816900
H	3.15458000	-3.37117900	-1.20776200	H	0.67339900	1.95292700	-2.16872800
H	1.42736500	-3.26615200	-1.59854300	H	-1.68769400	2.57019800	-2.05376200
C	2.79200400	-0.66518100	-2.43957600	H	-1.32692300	2.78454700	1.00132400
H	1.96992100	-0.88233900	-3.12890300	Rh	-0.85747000	0.34132400	-0.30060900
H	3.67476000	-1.23282600	-2.75398800	P	-2.68835900	-0.73842200	0.76090800
H	3.01919600	0.40157800	-2.51047200	P	0.22286900	-1.58291800	-0.92574700
C	2.94709700	2.54205200	-0.20557200	C	-0.83339000	-2.63715000	-2.01942300
H	3.35356000	2.06696100	-1.10177900	H	-0.29497700	-3.54733900	-2.30666800
H	3.54516700	2.23780400	0.65820000	H	-1.76642900	-2.92121300	-1.52879700
H	3.03702500	3.62763400	-0.32091300	H	-1.08291100	-2.07641700	-2.92552400
C	0.80513300	3.13317700	1.54424800	C	1.70696500	-1.36568400	-2.00110700
H	-0.26290200	3.13022100	1.77461500	H	1.98798100	-2.33227400	-2.43353200
H	1.11783000	4.16748000	1.36521000	H	1.49650800	-0.66568500	-2.81461000
H	1.34866500	2.74971700	2.41344200	H	2.53800200	-0.99103500	-1.40216700
C	0.33009700	2.99266000	-1.31283100	C	0.86892500	-2.73773400	0.35900800
H	0.61094400	4.05169100	-1.31671500	H	1.39029500	-3.57904700	-0.11144000
H	-0.75413200	2.91079900	-1.20047100	H	1.56885600	-2.18460600	0.99087000
H	0.60750600	2.54854100	-2.27346800	H	0.06240600	-3.12906100	0.98234000
C	0.43077100	-2.21052500	2.62831600	C	-2.70684900	-2.51284200	1.28906500
H	0.10155700	-2.40180400	3.65981700	H	-2.58232000	-3.19330200	0.44322200
H	1.36562200	-1.64580400	2.66553500	H	-1.90385700	-2.69612500	2.00871100
H	0.62733200	-3.18743200	2.17454800	H	-3.66251800	-2.73945000	1.77425800
H	-4.82869800	0.55860200	0.51419000	C	-3.01759300	0.07514100	2.38914900
C	-3.76493000	1.82088900	-0.86020400	H	-3.90560000	-0.35846000	2.86245100
H	-4.64321900	2.08701500	-1.45552700	H	-2.15683300	-0.07573100	3.04782700
H	-3.61673100	2.60959600	-0.11252000	H	-3.17081600	1.14887400	2.26635000
H	-2.90107400	1.79856800	-1.53463400	C	-4.28995600	-0.59975800	-0.15069100
S9a				H	-5.12020200	-0.97710900	0.45648300
				H	-4.48489600	0.44262900	-0.41540300
				H	-4.23537200	-1.18121300	-1.07621300
O	2.75657500	0.34891500	0.77531600	C	4.21172500	-0.65422000	2.36999500
C	4.13527100	0.34771800	1.22270400	H	3.48923900	-0.39690800	3.15094400
C	5.07752300	0.00837200	0.09634900	H	3.99776900	-1.66905800	2.01572700

H	5.21574000	-0.65164100	2.80484800	C	-1.09159200	1.75756200	1.78894200	
C	-3.29866600	3.12002500	0.06130500	H	-1.46073300	2.76502600	2.01323800	
H	-3.88818000	2.61488800	0.83361100	H	-1.93619000	1.11038400	1.54461700	
H	-3.35842600	4.19439700	0.28282200	H	-0.57129300	1.36935700	2.67003500	
H	-3.77853600	2.95149700	-0.90789800	C	4.13915700	0.96008200	0.92324500	
S9b				H	3.70194000	1.88648100	1.30222600	
				H	4.20285200	0.24669800	1.75041500	
	O	-3.18509000	0.05811900	-0.11648800	H	5.15075400	1.16909800	0.55836100
	C	-4.59698500	0.25657900	-0.38610400	C	4.18717500	-1.08738900	-1.08912800
	C	-2.65103500	-1.11553600	-0.70671500	H	5.13463100	-0.65589100	-1.43042500
	C	-1.35132000	-1.49554700	-0.05031200	H	4.40589800	-1.83394900	-0.32337600
	C	-0.36436600	-2.14213200	-0.76635400	H	3.70126200	-1.58204000	-1.93514400
	C	0.91024700	-2.57114300	-0.23512800	C	3.22870700	1.48633900	-1.79547100
	C	1.28380200	-2.30457700	1.08983500	H	4.27919600	1.72934700	-1.99072100
	C	2.56929500	-2.78093000	1.70253000	H	2.79080100	1.06200700	-2.70416200
C	-5.42819500	-0.77378400	0.33396700	H	2.69356300	2.40713200	-1.55662500	
C	-6.26160300	-1.62507300	-0.26634500					
C	-4.92742200	1.67712100	0.06186500	S10a				
H	-4.75988500	0.16501900	-1.47102400	O	-3.63660400	-0.96880900	0.02037000	
H	-3.35610300	-1.95084100	-0.56695900	C	-2.99593400	-0.39834100	1.15637400	
H	-2.51746500	-0.97876300	-1.79173300	C	-1.64964400	-1.02860200	1.45276600	
H	-1.37509400	-1.53223500	1.03648600	C	-0.61662500	-0.39374900	2.09141100	
H	-0.49763900	-2.24499100	-1.84229500	C	-3.02833400	-0.68840100	-1.23085000	
H	1.60416500	-3.06910700	-0.90628900	C	-1.64633700	-1.27117600	-1.30170700	
H	0.50729600	-2.08801200	1.82233200	C	-0.59817700	-0.88966100	-2.16394800	
H	3.01496300	-2.01845500	2.35055000	C	0.68106300	-1.51830200	-1.99062500	
H	2.35921400	-3.64983300	2.34149100	C	0.86451200	-2.47090000	-0.96048400	
H	3.30267100	-3.09267100	0.95495700	H	-2.86636100	0.68730200	1.01077000	
H	-5.32603100	-0.77724800	1.41986500	H	-1.63437800	-2.11549200	1.39443700	
H	-6.86476300	-2.33116400	0.29739600	H	0.13558200	-0.98117000	2.60516500	
H	-6.38765900	-1.63564700	-1.34744500	H	-0.69918300	0.64900300	2.38448400	
H	-5.97795200	1.90016500	-0.14663000	H	-3.67389800	-1.18154000	-1.96846300	
H	-4.30533900	2.40589300	-0.46768100	H	-3.03897400	0.38581900	-1.44530500	
H	-4.76077300	1.79150500	1.13865900	H	-1.63766000	-2.29217500	-0.93493900	
Rh	0.92041600	-0.37654400	-0.05963900	H	-0.71407900	-0.10238700	-2.90311900	
P	0.06750000	1.81815300	0.35320000	H	1.51077600	-1.21534800	-2.62401500	
P	3.09655500	0.25163000	-0.42574000	H	0.00537100	-3.04916200	-0.63549400	
C	1.16065800	3.22348200	0.86600000	Rh	0.17189800	-0.33973500	-0.18068500	
H	0.54783500	4.11072800	1.05992200	P	2.31150100	0.12423200	0.75717500	
H	1.68921300	2.96358300	1.78811500	P	-0.28031500	2.06448100	-0.53826800	
H	1.89641700	3.47819500	0.09897500	C	1.09405700	2.94858100	-1.41711500	
C	-0.94421300	2.56561400	-0.99736900	H	0.83219900	3.99824600	-1.58954800	
H	-1.32616900	3.54741500	-0.69536500	H	2.02443400	2.91471900	-0.84650700	
H	-0.34558300	2.68106800	-1.90596400	H	1.27159200	2.46771800	-2.38431800	
H	-1.78670000	1.90053500	-1.20280300	C	-1.69190900	2.60312300	-1.61969900	

H	-1.61116700	3.67948700	-1.80788600	H	1.25766700	-0.84161100	-2.89062100
H	-1.68087400	2.08439200	-2.58241900	H	0.28644700	-3.01457200	-0.92085500
H	-2.65078600	2.41562500	-1.13050500	Rh	0.13496300	-0.35939800	-0.17938200
C	-0.60013900	3.16518700	0.92021500	P	2.24367800	0.29484200	0.74417000
H	-0.68882900	4.20879000	0.59931400	P	-0.53594000	2.01325400	-0.46340700
H	-1.53917000	2.87223300	1.40054200	C	2.27924600	1.65840600	1.99664100
H	0.19800400	3.09430300	1.66167500	H	3.29463500	1.77514800	2.39049100
C	2.56044500	1.61852200	1.82340900	H	1.96381700	2.61186200	1.56858700
H	2.41651300	2.54726000	1.26776500	H	1.61175700	1.41488900	2.82943100
H	1.85930900	1.60002700	2.66295600	C	3.14556000	-1.00812000	1.70038900
H	3.57952800	1.61406800	2.22455600	H	4.16081400	-0.66310500	1.92353800
C	2.95471400	-1.16467800	1.91758700	H	2.63768300	-1.20656500	2.64838100
H	3.97886000	-0.91634400	2.21634700	H	3.20465300	-1.93978600	1.13627000
H	2.33386200	-1.20391500	2.81715300	C	3.53794900	0.82600400	-0.46557200
H	2.95133500	-2.15015700	1.45273000	H	4.44270600	1.14839500	0.06134700
C	3.69622300	0.29331500	-0.45730600	H	3.79734900	-0.00816300	-1.12250900
H	4.64707800	0.46042300	0.06028200	H	3.17502300	1.64820300	-1.08541400
H	3.78056500	-0.61305600	-1.06106600	C	0.74786000	3.16301800	-1.15568100
H	3.50705100	1.13201000	-1.13213200	H	1.62526100	3.22927700	-0.50848800
C	-3.95315000	-0.63624600	2.33094900	H	1.07165400	2.80320200	-2.13772000
H	-4.92956500	-0.20259400	2.09678700	H	0.33354400	4.17038500	-1.27290100
H	-4.08709100	-1.70888800	2.50348000	C	-1.94387800	2.43584200	-1.59090600
H	-3.56746500	-0.17811500	3.24631300	H	-2.06267900	3.52442300	-1.62074500
C	2.16130900	-3.22601900	-0.80698400	H	-1.76291400	2.08506200	-2.61094900
H	2.26262900	-3.66247400	0.19108800	H	-2.86342100	1.99229200	-1.20699700
H	2.17515600	-4.06775800	-1.51417300	C	-1.08535900	2.90307100	1.06223200
H	3.04684400	-2.61893200	-1.01567500	H	-1.24488600	3.96519300	0.84691700
				H	-2.03045000	2.46774300	1.39670500
S10b				H	-0.35127100	2.81334100	1.86591400
O	-3.07958400	0.08358500	0.30091000	C	2.41949100	-2.84351100	-1.35302200
C	-2.66449400	-0.50468700	1.54676900	H	2.72111600	-3.28480700	-0.39856800
C	-1.13669900	-0.52865400	1.76649100	H	2.47522300	-3.65123200	-2.09676300
C	-0.33092300	-1.65431600	1.68311600	H	3.15454200	-2.08619100	-1.64144700
C	-3.02585900	-0.74917200	-0.86159200	H	-3.04908900	0.21737000	2.27490800
C	-1.66055900	-1.33541600	-1.14151300	C	-3.35452900	-1.84250800	1.83532700
C	-0.78638400	-0.84422700	-2.13194900	H	-4.43587200	-1.73497500	1.70649100
C	0.56966700	-1.31105500	-2.19289500	H	-3.16239200	-2.14231800	2.87005400
C	1.01334700	-2.30844500	-1.30853700	H	-3.01331400	-2.65764300	1.18897900
H	-0.77046500	0.29571000	2.37407900				
H	0.58754900	-1.72190700	2.25314800	S10c			
H	-0.72739900	-2.60928400	1.35189100	C	2.91655500	-1.17220800	1.19184300
H	-3.76116600	-1.55869800	-0.77772600	C	1.43565200	-1.31892500	1.57696700
H	-3.34880300	-0.10050700	-1.68009000	C	0.65306900	-0.33489500	2.11032600
H	-1.52783500	-2.35911300	-0.80643100	C	1.46119300	-1.54100300	-1.24383500
H	-1.08881000	-0.03664200	-2.79120900	C	0.44858200	-1.11718600	-2.12887400

C	-0.88800800	-1.59722500	-1.91017100	O	3.14862500	-0.34725400	0.04822700
C	-1.16805300	-2.46409400	-0.83476000	C	2.86920600	-1.00998600	-1.18738000
H	1.06858700	-2.34194300	1.64428500	H	3.06361600	-0.27932900	-1.97312200
H	-0.24283800	-0.59911400	2.66081600	H	3.57800300	-1.84279000	-1.31547800
H	1.03411600	0.66852000	2.26219100				
H	1.35231200	-2.53220800	-0.81651600	S10d			
H	0.63680600	-0.39243900	-2.91526900	O	3.10140500	-0.49805400	0.11412100
H	-1.68814900	-1.23687800	-2.55145600	C	2.64523900	-0.97551900	1.38677900
H	-0.37401300	-3.10314900	-0.46247500	C	1.22428600	-0.53421300	1.73525800
Rh	-0.20847800	-0.36114700	-0.17639800	C	0.19236700	-1.42480900	1.94481300
P	-2.26141600	0.44424900	0.72341800	C	2.80602200	-1.37968200	-0.97045800
P	0.58314100	1.91034500	-0.62128500	C	1.34591400	-1.76321100	-1.06817400
C	-0.63365600	2.97974100	-1.52627200	C	0.46480400	-1.28700000	-2.05936000
H	-0.21262500	3.97503200	-1.70593700	C	-0.93995200	-1.55765300	-1.94972700
H	-1.56766800	3.09524200	-0.97298800	C	-1.42400800	-2.35071500	-0.89250700
H	-0.86666200	2.52070100	-2.49269000	H	2.67426700	-2.07546600	1.38001700
C	2.05893600	2.17454800	-1.70906300	H	1.14482400	0.46003300	2.16963700
H	2.19933200	3.24913000	-1.86914800	H	-0.65147600	-1.16764300	2.57231500
H	1.92496900	1.69867600	-2.68445400	H	0.33342900	-2.48849400	1.77067900
H	2.94796800	1.76846100	-1.22370700	H	3.40883800	-2.29408600	-0.86321800
C	1.08930600	2.97874400	0.80641100	H	3.14464700	-0.86190000	-1.87109600
H	1.29161400	3.99872000	0.46186200	H	1.09742100	-2.69847000	-0.57639900
H	2.00888800	2.57556400	1.24129400	H	0.81400400	-0.63146500	-2.85135500
H	0.32341900	3.01753600	1.58376200	H	-1.62246900	-1.10316900	-2.66296100
C	-2.28862700	1.99750200	1.73274400	H	-0.76379400	-3.09887700	-0.46539900
H	-1.97347200	2.86783500	1.15423300	Rh	-0.22019400	-0.41076100	-0.14752600
H	-1.62485300	1.89348800	2.59643500	P	-2.16743700	0.66647700	0.74557000
H	-3.30438900	2.17956000	2.09961900	P	0.77567500	1.77128400	-0.75574200
C	-3.09017900	-0.69587700	1.92192800	C	-1.93181100	2.16991400	1.80138000
H	-4.01211400	-0.23598300	2.29393200	H	-2.89411300	2.49037800	2.21453700
H	-2.43436700	-0.89514400	2.77444000	H	-1.50617700	3.00101400	1.23560300
H	-3.33882400	-1.64630000	1.45031800	H	-1.25882400	1.93565000	2.63243500
C	-3.60440200	0.75817800	-0.50865700	C	-3.21547400	-0.33691500	1.89496700
H	-4.52298600	1.08027800	-0.00621200	H	-4.11262300	0.23378600	2.15793400
H	-3.81471400	-0.15450500	-1.07234500	H	-2.67246500	-0.56206100	2.81667100
H	-3.29809700	1.53132600	-1.21841900	H	-3.52108300	-1.27646400	1.43350400
C	-2.54272900	-3.04756600	-0.62915800	C	-3.42681600	1.22982900	-0.48733800
H	-2.69167000	-3.38540600	0.40060900	H	-4.26027100	1.73006000	0.01806300
H	-2.66062600	-3.93589500	-1.26616700	H	-3.81937400	0.37006600	-1.03701100
H	-3.34821600	-2.35533800	-0.89306400	H	-2.98284800	1.91951700	-1.20781400
H	3.29635500	-2.18146500	0.97087400	C	-0.36154200	2.98003900	-1.58744300
C	3.74315100	-0.58580900	2.33802000	H	-1.18361100	3.27623500	-0.93249100
H	3.43111600	0.44040300	2.55736300	H	-0.78604600	2.52484400	-2.48789600
H	3.62538900	-1.18270300	3.24742800	H	0.18655000	3.88305900	-1.87743700
H	4.80046400	-0.57278900	2.05968500	C	2.18411600	1.81370500	-1.95854400

H	2.45049600	2.85656800	-2.16239700	H	-1.12908500	2.29399000	-2.75145500	
H	1.91845200	1.33750400	-2.90666900	H	-2.28699800	2.44559900	-1.41376000	
H	3.04608500	1.30652000	-1.52304300	C	-0.37534500	3.20777900	0.88922300	
C	1.51119200	2.78794000	0.60447900	H	-0.38265100	4.26566400	0.60558700	
H	1.79155100	3.77795400	0.22897700	H	-1.36350400	2.94988400	1.28373100	
H	2.41140800	2.28592200	0.96841800	H	0.35861800	3.06155900	1.68542600	
H	0.81772700	2.91078300	1.43935200	C	2.65709600	1.29946700	2.00047000	
C	-2.88469800	-2.69388100	-0.76457300	H	2.63313500	2.24783600	1.45914800	
H	-3.14463600	-2.99690600	0.25370500	H	1.90614900	1.33158700	2.79550500	
H	-3.11212800	-3.55401300	-1.41043200	H	3.64553100	1.18870800	2.45918800	
H	-3.54447800	-1.87662200	-1.07088800	C	2.71004700	-1.53110600	2.02019300	
C	3.63157700	-0.46316800	2.43700900	H	3.74122900	-1.45004000	2.38059500	
H	4.63839600	-0.82697700	2.21436900	H	2.03892300	-1.50630100	2.88347900	
H	3.34695000	-0.80532900	3.43725500	H	2.58502400	-2.49034000	1.51496900	
H	3.65799400	0.63232000	2.44196500	C	3.77047600	-0.10581600	-0.26166100	
S10a-TS				H	4.70540300	-0.05313600	0.30716600	
				H	3.78008000	-1.01169200	-0.87223400	
	O	-4.01120300	-0.69067800	0.11335000	H	3.71004700	0.75768600	-0.92928100
	C	-3.17685300	-0.23805900	1.16512000	C	-3.89934700	-0.50039100	2.48293900
	C	-1.83371900	-0.96274000	1.07801300	H	-4.87172600	0.00065200	2.47513900
	C	-0.67269200	-0.34876000	1.69370200	H	-4.06751400	-1.57347300	2.62016100
	C	-3.29831900	-0.57727900	-1.09514600	H	-3.31725800	-0.12311000	3.32931200
	C	-1.91925100	-1.20315400	-0.94655500	C	1.95030100	-3.27471400	-1.24017300
	C	-0.91656900	-0.81611400	-1.94628100	H	2.40170500	-3.52064700	-0.27452200
	C	0.27476200	-1.57536100	-2.10106000	H	1.73063800	-4.23391900	-1.72944300
C	0.68057100	-2.47415100	-1.10238800	H	2.69798300	-2.76112200	-1.85327400	
H	-2.99019400	0.84574700	1.04978300	S10b-TS				
H	-1.92224800	-2.03075600	1.27516100		O	-4.17972200	0.20051400	0.33335200
H	-0.11241600	-0.99757000	2.36458400		C	-3.35274100	-0.26765800	1.40755900
H	-0.80648500	0.65537300	2.09661300		C	-1.91206500	0.16965700	1.15679300
H	-3.87499100	-1.10811500	-1.86008000		C	-0.74316500	-0.44789800	1.70580800
H	-3.20806600	0.47662900	-1.40249200		C	-3.45876000	0.55903500	-0.83017700
H	-1.96838200	-2.28457700	-0.82261800		C	-2.18345900	-0.24713100	-0.89246700
H	-1.17698200	-0.06908600	-2.68937100		C	-1.20892500	-0.05165400	-1.95139600
H	0.94433200	-1.34582100	-2.92715400		C	-0.29341100	-1.09058400	-2.25927000
H	-0.07999400	-2.92861500	-0.47160300		C	-0.13234600	-2.19016200	-1.37963300
Rh	0.28334400	-0.23398700	-0.20477000	C	-0.13234600	-2.19016200	-1.37963300	
P	2.31994900	-0.13074400	0.87880900	H	-1.86178200	1.25780300	1.12798600	
P	0.00966200	2.14090900	-0.57483700	H	-0.13955300	0.16141200	2.37525600	
C	1.49315300	2.97554200	-1.30786400	H	-0.81209800	-1.49272900	2.00405700	
H	1.30203300	4.04332800	-1.46220500	H	-4.09483300	0.30567300	-1.68770100	
H	2.36796400	2.86864500	-0.66174700	H	-3.26440500	1.64179000	-0.87126600	
H	1.72563200	2.51643900	-2.27399900	H	-2.40084700	-1.29740500	-0.72128500	
C	-1.28947700	2.72845700	-1.76045200	H	-1.25897600	0.82990600	-2.58251200	
H	-1.24998100	3.81977200	-1.85049300	H	0.37481000	-0.96719600	-3.10852700	

H	-0.99767800	-2.53590800	-0.81888300	C	-1.06954500	-2.52060800	-0.78897100
Rh	0.21847500	-0.18200800	-0.23585400	H	1.37849700	-2.38793100	1.45442100
P	2.24000600	-0.81696800	0.65576400	H	-0.15809000	-0.93875300	2.40532500
P	0.64405700	2.24324500	-0.17819200	H	0.86934100	0.51893600	2.09514500
C	3.01217400	0.28723400	1.92291300	H	1.65551800	-2.71305100	-0.63494100
H	3.93485600	-0.16881300	2.29747600	H	1.07694800	-0.63848700	-2.68050100
H	3.25781000	1.26483900	1.50230300	H	-1.21215700	-1.60546000	-2.74327600
H	2.32979200	0.42935600	2.76626900	H	-0.36551000	-3.00231100	-0.11455700
C	2.24150400	-2.41311000	1.58452000	Rh	-0.31566800	-0.26991400	-0.18822400
H	3.25506800	-2.65730800	1.92060000	P	-2.31555300	0.36953200	0.76131400
H	1.59305100	-2.32541000	2.46118500	P	0.47698500	1.94845800	-0.71949800
H	1.86918500	-3.22790300	0.96203100	C	-0.72149900	2.97563500	-1.69146900
C	3.61001600	-1.02055100	-0.56361400	H	-0.30972400	3.97253800	-1.88436000
H	4.53492900	-1.31505400	-0.05543500	H	-1.67334400	3.08846800	-1.16602600
H	3.35291400	-1.78702500	-1.29810300	H	-0.91960200	2.48746600	-2.65107700
H	3.77857300	-0.07903200	-1.09390000	C	1.99404300	2.14157100	-1.76227200
C	2.23062200	2.78275800	-0.96754300	H	2.18397200	3.20464700	-1.94666800
H	3.09519100	2.36773500	-0.44262300	H	1.87005700	1.64129500	-2.72696700
H	2.25778900	2.42646000	-2.00214300	H	2.85193800	1.71306900	-1.23862200
H	2.31555800	3.87508200	-0.96689600	C	0.93107200	3.05620800	0.69210500
C	-0.55386100	3.32028500	-1.09744900	H	1.17495500	4.05956300	0.32640400
H	-0.26323400	4.37314300	-1.01230900	H	1.81409400	2.65093500	1.19569200
H	-0.57103900	3.05131300	-2.15756500	H	0.12144300	3.13511500	1.42041000
H	-1.56478800	3.20727900	-0.69458800	C	-2.42335600	1.98297900	1.65631900
C	0.68752900	3.12337900	1.45420600	H	-2.19116100	2.82358500	0.99900500
H	0.90936900	4.18730100	1.31580000	H	-1.72207100	1.98955600	2.49583200
H	-0.28442200	3.03712800	1.95119300	H	-3.43667900	2.12069800	2.04841300
H	1.44458300	2.69172700	2.11332800	C	-3.02027100	-0.75391100	2.04852600
C	0.83585100	-3.29586500	-1.72969400	H	-4.01779300	-0.41043300	2.34321100
H	1.16033200	-3.86257500	-0.85269800	H	-2.37910400	-0.75542200	2.93484200
H	0.34558400	-4.01751100	-2.39795500	H	-3.09524500	-1.77647600	1.67441000
H	1.72314500	-2.92407700	-2.25181600	C	-3.67879200	0.49997700	-0.47502200
H	-3.66969000	0.29776100	2.29619800	H	-4.61318600	0.80269200	0.01047600
C	-3.60398700	-1.74921900	1.67974700	H	-3.83141500	-0.46491200	-0.96457500
H	-4.68239900	-1.91075400	1.76265800	H	-3.41937400	1.23586000	-1.24091300
H	-3.13954100	-2.05874300	2.62206300	C	-2.44463600	-3.13764900	-0.80465400
H	-3.23165200	-2.39728000	0.87900200	H	-2.87200600	-3.22934400	0.19794900
				H	-2.38833400	-4.15811700	-1.20902900
S10c-TS				H	-3.14559500	-2.57900300	-1.43327400
C	3.07711600	-0.98486800	1.31174000	H	3.62388000	-1.94269600	1.33251700
C	1.57551800	-1.34485600	1.20962100	C	3.48703600	-0.16746200	2.52996400
C	0.55156800	-0.45683300	1.73492900	H	3.02719500	0.82512500	2.52103500
C	1.69424000	-1.63649100	-0.80574200	H	3.19984300	-0.67720200	3.45466900
C	0.72719300	-1.23989000	-1.84804700	H	4.57285800	-0.03687700	2.52919000
C	-0.56197900	-1.82862000	-1.89998100	O	3.46317700	-0.27689900	0.14169300

C	3.11278400	-1.08189800	-0.96953700	H	0.97887500	2.57007600	-2.52151100
H	3.20694500	-0.45879100	-1.86061700	H	2.06052500	2.64472200	-1.11567700
H	3.81815400	-1.92251300	-1.05933200	C	-0.05605600	3.23431500	1.10026800
S10d-TS				H	-0.04133100	4.30221700	0.85659200
				H	0.88916800	2.97854600	1.59036700
				H	-0.86680200	3.04843700	1.80836600
O	4.13287700	-0.47600300	0.07639200	C	-1.56232900	-3.33774700	-1.29142400
C	3.29718500	-0.83925800	1.17409300	H	-1.94319300	-3.70801100	-0.33566600
C	1.95972800	-0.14093000	0.99146900	H	-1.24594500	-4.22324400	-1.86003300
C	0.74371300	-0.50056200	1.65352300	H	-2.39027400	-2.87973900	-1.84180400
C	3.41333400	-0.28586900	-1.13303200	C	4.00705500	-0.39749000	2.45230600
C	2.00940900	-0.82833600	-0.99595700	H	5.00661400	-0.84168300	2.47958700
C	1.01493100	-0.58666600	-2.02665300	H	3.45332700	-0.72660800	3.33706600
C	-0.09159900	-1.46382600	-2.15073900	H	4.11719400	0.69144600	2.48147700
C	-0.39166200	-2.39653800	-1.12641900	S11a			
H	3.15339700	-1.93161400	1.20506600				
H	2.11457000	0.93227900	0.87574700				
H	0.30462600	0.25092500	2.30646800	O	-4.22241900	-0.48270300	0.47778800
H	0.65773800	-1.51976200	2.03194000	C	-3.12550400	0.07527600	1.18535100
H	3.93027100	-0.84323700	-1.92657300	C	-2.01783800	-0.99231000	1.04699400
H	3.42063100	0.77569500	-1.41826300	C	-0.59564400	-0.51848800	1.32163800
H	2.03506400	-1.87036900	-0.68672900	C	-3.70593000	-1.06347800	-0.70762900
H	1.18064600	0.18523700	-2.77166100	C	-2.27628500	-1.58992000	-0.37762100
H	-0.78237700	-1.32193200	-2.97883600	C	-1.26175200	-1.22231900	-1.45099500
H	0.43209900	-2.82784100	-0.56090800	C	-0.07300900	-1.94802500	-1.68937800
Rh	-0.30295200	-0.23821600	-0.24040300	C	0.69609900	-2.56294100	-0.68151200
P	-2.33241500	-0.38406800	0.82772700	H	-2.79536100	1.00502200	0.68403400
P	-0.26453500	2.21180400	-0.43225200	H	-2.25225600	-1.77911500	1.77795000
C	-2.82545100	0.98729600	1.96711000	H	-0.02373600	-1.26650100	1.87490100
H	-3.77193700	0.73488800	2.45723100	H	-0.56723000	0.42847400	1.86859100
H	-2.96063300	1.92699800	1.42652600	H	-4.39370800	-1.85252800	-1.02157500
H	-2.06401700	1.13135200	2.73914100	H	-3.65879500	-0.31181500	-1.51272000
C	-2.53701500	-1.82713100	1.96185800	H	-2.29524200	-2.68266400	-0.29737400
H	-3.55877400	-1.86101000	2.35518200	H	-1.66405600	-0.69484700	-2.31320800
H	-1.84187700	-1.73353600	2.80149600	H	0.39919200	-1.82043600	-2.66725900
H	-2.32503400	-2.76333500	1.44352700	H	0.18414900	-2.90555100	0.21660200
C	-3.79494000	-0.49301400	-0.29159300	Rh	0.51480500	-0.24784100	-0.41089500
H	-4.72230200	-0.53648100	0.29020100	P	2.49986600	0.06295000	0.87765700
H	-3.72841300	-1.38686200	-0.91553400	P	-0.13592000	2.03236700	-0.78477100
H	-3.82467400	0.38239600	-0.94656700	C	1.21429600	2.88312800	-1.72681100
C	-1.75535700	2.96927900	-1.22926100	H	0.91598900	3.90387300	-1.99017800
H	-2.65969500	2.76376100	-0.65024000	H	2.13264400	2.93010400	-1.13459700
H	-1.88668700	2.54005600	-2.22753700	H	1.42750600	2.33598300	-2.65103800
H	-1.64099700	4.05496200	-1.32317700	C	-1.58737800	2.35324400	-1.88407600
C	1.07465300	2.93116500	-1.49342700	H	-1.69586300	3.42732500	-2.07097700
H	1.01070900	4.02483200	-1.50314300	H	-1.44798400	1.84268900	-2.84178200

H	-2.50679600	1.98035500	-1.42527800	Rh	0.50684100	-0.11611900	-0.48695500
C	-0.45570100	3.19275500	0.61744000	P	2.26528800	-0.87885400	0.85325600
H	-0.65977500	4.19944600	0.23720100	P	0.67120100	2.28979700	-0.19271700
H	-1.32410500	2.85694900	1.19118800	C	2.85807300	0.16395500	2.25897800
H	0.40586400	3.23815000	1.28825700	H	3.68354600	-0.33133300	2.78167300
C	2.78513100	1.63068500	1.81655100	H	3.20837200	1.13604600	1.90088900
H	2.79066900	2.49225300	1.14262300	H	2.04427500	0.32647800	2.97236500
H	1.99335200	1.77323600	2.55855300	C	1.99556900	-2.49827000	1.69494700
H	3.74755400	1.59398000	2.33836800	H	2.89983600	-2.80850600	2.22929000
C	2.82311500	-1.19785500	2.18693300	H	1.17768100	-2.41024900	2.41646200
H	3.80882500	-1.04012400	2.63726100	H	1.73145200	-3.26848500	0.96638800
H	2.06647300	-1.12379300	2.97410100	C	3.79909500	-1.14711600	-0.13928400
H	2.78276600	-2.20469200	1.76421200	H	4.60698600	-1.52846200	0.49469300
C	4.00215700	-0.03903000	-0.19474100	H	3.60599400	-1.86865000	-0.93794400
H	4.91356900	0.08303300	0.40072100	H	4.12384600	-0.20567700	-0.59343400
H	4.03748300	-1.00904600	-0.69889600	C	2.33504600	2.92624500	-0.69798500
H	3.97495400	0.74534300	-0.95779700	H	3.11822500	2.52264300	-0.04975000
C	-3.56327000	0.39004800	2.60634300	H	2.55188300	2.62378500	-1.72775400
H	-4.39259700	1.10354700	2.60064300	H	2.36563900	4.01985600	-0.64317900
H	-3.90015200	-0.52199100	3.11016600	C	-0.44318800	3.32606600	-1.24676800
H	-2.74048500	0.82546800	3.18524900	H	-0.22583100	4.39165900	-1.11323400
C	1.97189400	-3.29836400	-1.01517300	H	-0.30393100	3.06784400	-2.30110200
H	2.67813400	-3.30488300	-0.17860700	H	-1.48982200	3.14634300	-0.98436900
H	1.75451400	-4.34998500	-1.24746300	C	0.42584900	3.05104300	1.47484200
H	2.47618300	-2.86700200	-1.88705700	H	0.55756200	4.13732300	1.42632500
S11b				H	-0.58469500	2.84122400	1.83959700
				H	1.14138800	2.64285600	2.19359600
O	-4.48022100	-0.06935900	0.50410100	C	1.05430600	-3.02184400	-2.02735700
C	-3.42715300	-0.06583900	1.48773300	H	1.66565100	-3.51094200	-1.26209600
C	-2.13304700	0.16189500	0.64979700	H	0.57182700	-3.82428400	-2.60223600
C	-0.79766600	-0.33878900	1.13491400	H	1.72632100	-2.49025100	-2.71112100
C	-3.96233000	-0.01647800	-0.82313800	H	-3.59199400	0.79130100	2.15346300
C	-2.51433300	-0.50070600	-0.69274600	C	-3.49194600	-1.35154800	2.30594800
C	-1.53839300	-0.17789800	-1.78974000	H	-4.50090500	-1.46592700	2.71303400
C	-0.54731100	-1.06044300	-2.22670400	H	-2.78751900	-1.32240500	3.14580400
C	0.01356700	-2.10166800	-1.42599500	H	-3.27857100	-2.23648400	1.69609900
H	-2.06450400	1.24326400	0.47151800	S11c			
H	-0.38941400	0.23115900	1.97374300				
H	-0.80596600	-1.40568100	1.37167800	C	3.32072900	-0.93352100	1.39037400
H	-4.58414900	-0.65126000	-1.46143200	C	1.96633300	-1.37222600	0.75184900
H	-3.99789600	1.01245400	-1.21824300	C	0.83135600	-0.41688200	1.10857900
H	-2.53309800	-1.58640000	-0.53547600	C	2.33779800	-1.35054700	-0.76463900
H	-1.75996700	0.67915400	-2.42249200	C	1.23173600	-0.88951200	-1.70365600
H	-0.01891400	-0.79733700	-3.14584300	C	0.06799900	-1.65871200	-1.96658700
H	-0.63352400	-2.57659800	-0.68947900	C	-0.60843600	-2.44198800	-1.01828000

H	1.71061900	-2.38829600	1.06892900	H	3.56700200	0.35522500	-1.52061500
H	0.22622800	-0.79512800	1.93538100	H	4.49812000	-1.08457500	-1.05962000
H	1.20968300	0.57137700	1.36476900				
H	2.60844800	-2.37185800	-1.06266600	S11d			
H	1.56364800	-0.26657100	-2.53221200	O	4.40280200	-0.65923400	0.49406700
H	-0.46464600	-1.44425400	-2.89699500	C	3.37311300	-0.45616200	1.47388000
H	-0.04847800	-2.84515800	-0.17818900	C	2.12423700	-0.14911100	0.61488100
Rh	-0.49346300	-0.12836500	-0.47128800	C	0.74373400	-0.30253400	1.19517000
P	-2.46500400	-0.12786500	0.91269600	C	3.84803400	-0.99789700	-0.78092600
P	0.07852900	2.17698700	-0.54755400	C	2.33763700	-1.14837700	-0.54313900
C	-1.03471900	3.06325400	-1.72753400	C	1.39695300	-0.91483000	-1.69245300
H	-0.75598500	4.12007200	-1.80233100	C	0.25893600	-1.69011400	-1.92925200
H	-2.07513000	2.99755000	-1.39460200	C	-0.44272600	-2.42056000	-0.92255900
H	-0.96113700	2.61143500	-2.72180800	H	3.20797500	-1.39374800	2.03101400
C	1.76750500	2.61362400	-1.14569500	H	2.25270000	0.86912400	0.22267300
H	1.90273200	3.70072100	-1.14778900	H	0.46178000	0.49312700	1.88944700
H	1.91927800	2.23763700	-2.16113900	H	0.59281700	-1.28165200	1.66092200
H	2.51419400	2.16112100	-0.48585200	H	4.31200200	-1.91978400	-1.14845000
C	-0.01789800	3.20655000	0.98431000	H	4.06605000	-0.19398300	-1.49985800
H	0.29490400	4.23336000	0.76676600	H	2.15506900	-2.15090100	-0.13451100
H	0.64784400	2.80006100	1.75211200	H	1.73896200	-0.26791400	-2.49744600
H	-1.03413000	3.22441400	1.38204100	H	-0.24708600	-1.54733400	-2.88677400
C	-2.92679800	1.30657800	1.98629400	H	0.13716100	-2.82730500	-0.09477100
H	-3.08786100	2.20164900	1.37815200	Rh	-0.55997000	-0.22280900	-0.44304100
H	-2.13501100	1.51284200	2.71259600	P	-2.37402900	-0.36063900	1.02437100
H	-3.85211100	1.08940100	2.53094000	P	-0.29592100	2.17977000	-0.68817700
C	-2.58022100	-1.52081600	2.12275500	C	-2.73871800	1.04932600	2.16201600
H	-3.55780500	-1.51998800	2.61661800	H	-3.61586100	0.82505700	2.77872400
H	-1.80618400	-1.41553600	2.88947200	H	-2.93793100	1.96384900	1.59624300
H	-2.43607100	-2.48040100	1.62010000	H	-1.88612100	1.22712900	2.82460200
C	-3.99105000	-0.32455600	-0.11401300	C	-2.34917100	-1.77948600	2.20365600
H	-4.88223600	-0.37910700	0.52075100	H	-3.27580100	-1.81101700	2.78659300
H	-3.92984800	-1.23473600	-0.71623200	H	-1.50675000	-1.67316000	2.89384800
H	-4.09721600	0.52959400	-0.79068900	H	-2.23554900	-2.72313700	1.66458300
C	-1.86398800	-3.19802800	-1.37743400	C	-3.96481600	-0.57199300	0.11086800
H	-2.54092900	-3.30817500	-0.52419100	H	-4.80191000	-0.66409200	0.81154700
H	-1.61033700	-4.21530300	-1.70610500	H	-3.92398600	-1.47038400	-0.51102400
H	-2.41353600	-2.71726200	-2.19424200	H	-4.14394200	0.29100100	-0.53802400
H	4.00169700	-1.80034200	1.32510300	C	-1.84542400	2.97379900	-1.31878100
C	3.33447400	-0.41724100	2.81913700	H	-2.66158200	2.85414600	-0.60060900
H	2.71052100	0.47282100	2.94376200	H	-2.14624000	2.50501800	-2.26149200
H	2.98154400	-1.19179400	3.50844600	H	-1.69026000	4.04350000	-1.49666000
H	4.35695900	-0.15094500	3.10212700	C	0.93495000	2.74935000	-1.94829200
O	3.77895000	0.08138100	0.49688600	H	0.90471300	3.83927100	-2.05707100
C	3.62294200	-0.46953000	-0.80663100	H	0.71209500	2.29259600	-2.91751800

H	1.94637500	2.45436500	-1.65379300	H	-2.80211100	-2.39286800	-2.76957700
C	0.14475800	3.22909700	0.76917500	H	-2.77880000	-0.62285100	-2.60029800
H	0.19405400	4.28495800	0.48244800	C	-3.59267800	1.56012000	-0.43573500
H	1.12097000	2.93180700	1.16473100	H	-3.79300400	0.86795800	-1.25728400
H	-0.59693400	3.11555800	1.56431100	H	-4.04631400	1.16173600	0.47675600
C	-1.64159300	-3.25856200	-1.31298800	H	-4.06690400	2.51952600	-0.66933500
H	-2.29912500	-3.45954100	-0.46138300	C	-1.80768900	3.12680700	1.10205200
H	-1.31819800	-4.23623100	-1.69608400	H	-0.80712400	3.52599200	1.28593600
H	-2.23835100	-2.78184300	-2.09927200	H	-2.45379500	3.94957800	0.77773000
C	3.81275400	0.63720500	2.43376400	H	-2.19956900	2.72623500	2.04228300
H	4.76550600	0.36649600	2.89840500	C	-1.29032000	2.71791400	-1.71408100
H	3.07374000	0.77702700	3.23137100	H	-1.93324800	3.59204100	-1.86559600
H	3.95319100	1.58641200	1.90459000	H	-0.25120800	3.04996900	-1.63550300
S11a-TS				H	-1.36982000	2.06221900	-2.58645100
O	3.01125900	0.46710600	-1.77044600	C	3.61310500	-0.58872600	-1.01592500
C	2.84270100	-0.54752200	0.33215100	H	3.40681300	-1.51046600	-1.57093800
C	1.52693500	-1.30873100	0.22454000	C	5.12697600	-0.42149500	-0.86834900
C	2.83467200	1.57452800	-0.89387100	H	5.56241600	-1.29569800	-0.37150000
C	2.61251900	0.98300100	0.53216700	H	5.58577000	-0.32412900	-1.85679200
C	1.28504900	1.37349900	1.14842800	H	5.39142300	0.46521900	-0.28143500
C	0.57140200	0.62946500	2.10086300	C	-0.21022900	-1.66391200	2.95670200
C	0.77290600	-0.81019500	2.18793800	H	-0.16858200	-2.70773500	2.62878000
H	3.45833300	-0.95754100	1.13983300	H	0.06579600	-1.65836400	4.02119200
H	1.58192900	-2.36068200	0.50255100	H	-1.23905400	-1.30734400	2.86459200
H	1.15351600	-1.23980200	-0.81156400	S11b-TS			
H	3.71392600	2.23224800	-0.91235200	O	4.31597300	0.84369600	-1.18185300
H	1.97424300	2.14404100	-1.25660000	C	3.71090000	-0.46439000	-1.27051300
H	3.39331300	1.37129500	1.20160000	C	2.31026100	-0.26266400	-0.62755200
H	1.08033800	2.44122600	1.11102400	C	1.49970500	-1.41123800	-0.07469900
H	-0.16719100	1.10784400	2.73947200	C	3.51333200	1.74389900	-0.41739400
H	1.79439300	-1.12825000	2.37227100	C	2.62260600	0.83372800	0.42494700
Rh	-0.31763400	0.01329500	0.26368300	C	1.37301400	1.36275900	1.07812900
P	-1.70847400	-1.71716400	-0.66908700	C	0.66509100	0.56460600	1.98104500
P	-1.77477000	1.79751500	-0.18504000	C	0.96152000	-0.86133500	1.99910800
C	-0.95122400	-3.40462800	-0.68126200	H	3.60229700	-0.70829700	-2.33466500
H	-1.65204700	-4.13027700	-1.10749800	H	1.69925200	0.23296000	-1.39429600
H	-0.03640300	-3.41036000	-1.28057000	H	0.85714900	-1.88316400	-0.81883300
H	-0.70136400	-3.71750900	0.33674900	H	2.05535000	-2.19812400	0.42878200
C	-3.30779400	-2.04459100	0.19661300	H	4.18076200	2.37978500	0.17219500
H	-3.95149600	-1.16311000	0.17104100	H	2.91110700	2.39048800	-1.07783300
H	-3.83464500	-2.88118900	-0.27528000	H	3.26060400	0.38991400	1.20309100
H	-3.11181800	-2.29735000	1.24297300	H	1.17861200	2.43157900	1.04369300
C	-2.20029600	-1.53742600	-2.44389400	H	-0.07002100	0.98023200	2.66584600
H	-1.30181200	-1.48064500	-3.06650900	H	2.02157900	-1.07986800	2.07240700

Rh	-0.40088400	-0.00766800	0.19419100	C	0.83525800	0.40170300	2.32281700
P	-1.94406900	-1.63197500	-0.57873800	H	3.54962900	0.32451500	1.35765500
P	-1.74489000	1.85596700	-0.15530100	H	1.88273400	2.00764600	0.82044200
C	-3.51536200	-1.75269300	0.38552000	H	1.36169700	1.08372900	-0.60758200
H	-4.09366300	-0.82997100	0.31062800	H	3.51216700	-2.61957000	-1.02490900
H	-4.12731200	-2.58237800	0.01516200	H	1.79925300	-2.31146800	-1.40252500
H	-3.28154200	-1.92765100	1.43980900	H	3.20366700	-1.97146400	1.15952200
C	-1.35093600	-3.38456900	-0.49420000	H	0.77943000	-2.72987700	0.90344400
H	-1.01110300	-3.62348300	0.51739600	H	-0.34968100	-1.43025800	2.64249000
H	-2.16444900	-4.06683100	-0.76304500	H	1.88011100	0.57416500	2.56078700
H	-0.52023600	-3.55041600	-1.18638900	Rh	-0.27839200	-0.07021200	0.29748700
C	-2.51689300	-1.54418700	-2.33672500	P	-1.40769100	1.90386800	-0.49415900
H	-1.65256600	-1.60080800	-3.00583700	P	-1.92999100	-1.59292000	-0.38664400
H	-3.19416000	-2.37467600	-2.56454500	C	-0.44374700	3.47344700	-0.32741900
H	-3.03799000	-0.60428700	-2.53503900	H	-1.03188600	4.31998000	-0.69729400
C	-3.53089300	1.80990400	-0.63645600	H	0.48500700	3.41659000	-0.90207500
H	-3.68172200	1.24095500	-1.55725800	H	-0.19134900	3.65368000	0.72167500
H	-4.12870700	1.35865900	0.16025100	C	-2.98394600	2.36150300	0.35581400
H	-3.89227200	2.83104700	-0.80005900	H	-3.73203700	1.57458500	0.24369300
C	-1.83545500	2.98636600	1.30566100	H	-3.38486000	3.29232500	-0.05999100
H	-0.83719000	3.25883600	1.65799900	H	-2.79487500	2.50637600	1.42373800
H	-2.37396900	3.90348600	1.04381300	C	-1.84955900	1.94698600	-2.29025800
H	-2.36689900	2.48955600	2.12349700	H	-0.94205300	1.82885500	-2.89084300
C	-1.02714300	2.92410200	-1.48345200	H	-2.32524700	2.89832100	-2.55211100
H	-1.58349100	3.86399200	-1.57016700	H	-2.53225600	1.13204000	-2.54562100
H	0.01994200	3.14803900	-1.26212800	C	-3.70549800	-1.10543700	-0.57533300
H	-1.06835500	2.39877500	-2.44251000	H	-3.82100300	-0.30096500	-1.30630800
C	4.61512200	-1.49801900	-0.60877600	H	-4.10530600	-0.76664400	0.38528200
H	4.24993800	-2.51584400	-0.79002300	H	-4.29472800	-1.96456700	-0.91387800
H	5.62127100	-1.41923500	-1.03104600	C	-2.12434200	-3.09010000	0.68346100
H	4.69739900	-1.34024400	0.47292600	H	-1.18103800	-3.63420500	0.77522900
C	0.13337100	-1.80979600	2.83247400	H	-2.87140400	-3.76553300	0.25316600
H	0.49379700	-1.78534800	3.87101600	H	-2.45567300	-2.79780700	1.68481300
H	-0.92771400	-1.54777400	2.83226000	C	-1.55096000	-2.32557900	-2.04225700
H	0.24126400	-2.84312300	2.48700600	H	-2.30647600	-3.06681500	-2.32551600
				H	-0.57020800	-2.80945600	-2.02013600
				H	-1.52135400	-1.53846300	-2.80170600
S11c-TS				C	4.04395400	1.46392300	-1.46053600
O	3.03644200	-0.71525300	-1.70069600	H	3.11852000	1.97469300	-1.74475600
C	3.77231000	0.11943700	-0.80775300	H	4.60845600	2.11240700	-0.78193100
C	2.92141200	0.08031600	0.49405300	H	4.63902900	1.31955600	-2.36683800
C	1.71287000	1.00353000	0.43443100	H	4.73871100	-0.36255200	-0.57618600
C	2.70083300	-1.88059200	-0.95889400	C	-0.06843600	1.28408000	3.15442600
C	2.49700500	-1.42095100	0.52174400	H	0.18222700	1.15563100	4.21736000
C	1.11291000	-1.70704300	1.06302300	H	0.08796200	2.34248000	2.92115400
C	0.46501800	-0.98482700	2.07656600				

H	-1.12634700	1.04706400	3.01713700	H	1.14439700	3.79016700	-1.89486900	
S11d-TS				H	-0.36727800	2.98907200	-1.39533400	
				H	0.66794700	2.23465400	-2.61907700	
	O	-4.40731900	0.54791000	-0.85283300	H	-4.30828400	-1.34003800	0.01998100
	C	-3.79870600	-0.75343100	-0.76320600	C	-3.93673000	-1.45886300	-2.10169700
	C	-2.35920400	-0.43612200	-0.30580600	H	-3.53737400	-2.47837800	-2.04694100
	C	-1.45162500	-1.49967800	0.26125500	H	-4.99147900	-1.52215900	-2.38525600
	C	-3.66645600	1.52285300	-0.10989600	H	-3.40637300	-0.90908600	-2.88717200
	C	-2.64331200	0.71604800	0.69200400	C	0.19166700	-1.60600700	3.04701900
	C	-1.37664600	1.35868000	1.19467900	H	1.23302000	-1.30414500	2.91016100
	C	-0.54834500	0.66699900	2.08243600	H	-0.05972500	-1.50413100	4.11264400
C	-0.76207200	-0.76669800	2.23114000	H	0.09740200	-2.66874800	2.80205700	
H	-1.85793400	0.01900600	-1.17193300					
H	-0.85195500	-2.00599300	-0.49559000	S13				
H	-1.93256800	-2.26381000	0.86880400	O	3.48790000	-0.65548800	-0.16086700	
H	-4.35705600	2.09117800	0.52230100	C	3.19793400	0.17996800	0.96339900	
H	-3.17542800	2.22468500	-0.80217100	C	1.77807800	0.09490400	1.48977700	
H	-3.17650100	0.28232100	1.55140500	C	0.87872800	1.17823900	1.57421500	
H	-1.24544500	2.42982800	1.06603900	C	-0.11489700	1.30658200	2.64134300	
H	0.22113300	1.16914200	2.66375700	C	-0.72702600	2.45388500	2.97820000	
H	-1.79688700	-1.02967900	2.42292300	H	3.88431200	-0.08327700	1.78377300	
Rh	0.38834000	0.01089400	0.25071600	H	3.43951200	1.19342600	0.63654100	
P	1.95117700	-1.58753600	-0.53372700	H	1.63047300	-0.68716300	2.23770300	
P	1.57954700	1.90587000	-0.37139300	H	1.16012000	2.11133100	1.08810200	
C	3.61907500	-1.51886400	0.25838300	H	-0.32082000	0.40316000	3.21538200	
H	4.11769400	-0.57407300	0.03518600	H	-1.42765900	2.50226200	3.80563400	
H	4.24742600	-2.34153700	-0.10003500	H	-0.52364700	3.38800900	2.45887100	
H	3.51061800	-1.60263200	1.34384200	Rh	0.14558500	-0.42831200	0.07880200	
C	1.49335300	-3.35574200	-0.22806500	P	-2.23978500	-0.69653100	0.07358200	
H	1.30282800	-3.52131700	0.83595200	P	0.14533300	1.24165500	-1.44056600	
H	2.31044100	-4.01227600	-0.54564100	C	1.53776400	-2.06846900	-0.20238100	
H	0.59473600	-3.63005000	-0.78811200	C	0.39694200	-2.51991800	-0.48418600	
C	2.32916500	-1.63545800	-2.34502700	H	-0.23836400	-3.32274900	-0.81304200	
H	1.40859800	-1.82946700	-2.90442800	C	-0.42345600	0.60886700	-3.07359500	
H	3.05120100	-2.42848300	-2.56872100	H	-0.26982100	1.37292600	-3.84391900	
H	2.73892300	-0.68240600	-2.68855900	H	0.14486000	-0.28702100	-3.33788300	
C	3.30769600	1.90959200	-1.03141900	H	-1.48481000	0.35153000	-3.03984100	
H	3.40502600	1.24351200	-1.89197700	C	-0.80196100	2.80601600	-1.21763100	
H	4.01190400	1.59203000	-0.25734800	H	-0.54147900	3.27607100	-0.26570500	
H	3.57785800	2.92337500	-1.34598800	H	-0.56677400	3.49889700	-2.03311700	
C	1.74636400	3.16036200	0.97787200	H	-1.87607500	2.61105200	-1.22015200	
H	0.77104700	3.42301000	1.39561500	C	1.85391500	1.83254200	-1.79553000	
H	2.21506300	4.07231600	0.59235200	H	1.85540300	2.39305200	-2.73705400	
H	2.37058200	2.75889600	1.78233000	H	2.20335400	2.49561500	-0.99974600	
C	0.67058400	2.82244700	-1.69616100	H	2.53709600	0.98285500	-1.86838700	

C	-3.08748800	-1.66953200	-1.24980300	H	0.02118100	3.57414000	-2.25500800
H	-3.09371100	-1.11394200	-2.19224500	H	1.20923400	3.13167100	-1.01215600
H	-2.56652900	-2.61623300	-1.41645000	H	1.00741100	2.10218900	-2.44506000
H	-4.12393500	-1.88151700	-0.96521200	C	-2.81293400	-2.19271400	-1.16357100
C	-2.56900100	-1.70886400	1.58585800	H	-3.09867200	-1.48149900	-1.94337500
H	-2.24748400	-1.16271500	2.47716200	H	-2.13037300	-2.92419300	-1.60507100
H	-3.63994000	-1.92500600	1.67242000	H	-3.71090600	-2.71333600	-0.81268800
H	-2.01699100	-2.65160100	1.53871300	C	-1.75318300	-2.65109300	1.48705100
C	-3.40066300	0.72400400	0.30681100	H	-1.37300900	-2.22205400	2.41868600
H	-4.38146200	0.36031900	0.63242300	H	-2.70569200	-3.15297100	1.69124000
H	-3.00297500	1.40802600	1.06158500	H	-1.02890500	-3.38524700	1.12434400
H	-3.53706500	1.27194400	-0.63015600	C	-3.35184000	-0.32595300	0.97490300
C	3.00917900	-1.97955400	-0.03268100	H	-4.17525800	-0.98540300	1.27032900
H	3.48829500	-2.55481300	-0.83178600	H	-2.98429100	0.20303100	1.85902600
H	3.31008400	-2.42540700	0.92923000	H	-3.73857600	0.40795900	0.26265700
S13-TS				C	3.42924900	-1.78569300	-0.75474600
				H	3.58186800	-2.38035100	-1.65896300
				H	3.88898000	-2.31201800	0.09879300
O	4.01014100	-0.52046700	-0.96696800	S14			
C	3.56993000	0.39427600	0.02876900				
C	2.29537200	-0.09340700	0.71747600				
C	1.33218500	0.91423800	1.17420300	O	-4.24862700	-1.44268300	-0.67475500
C	0.80378200	0.84501300	2.54349200	C	-3.62104300	-1.54134300	0.60261800
C	0.50328500	1.91455400	3.29845100	C	-2.44916400	-0.50502300	0.60128200
H	4.34758700	0.51030800	0.79903800	C	-1.02897500	-1.06716800	0.63428700
H	3.41968100	1.36300500	-0.45661500	C	-0.45721300	-1.32901700	1.96463300
H	2.48935000	-0.82338200	1.50567100	C	0.12981800	-2.47994200	2.33275400
H	1.52544200	1.92517600	0.81752400	H	-4.33390500	-1.30100200	1.40451700
H	0.69133900	-0.15291000	2.96764900	H	-3.29203100	-2.57639200	0.73193300
H	0.13326000	1.80702600	4.31304900	H	-2.58031200	0.18497400	1.44523100
H	0.64631400	2.93135000	2.93914600	H	-0.94211300	-1.93751000	-0.03869300
Rh	0.05007500	-0.27254600	-0.10829000	H	-0.58907700	-0.54571900	2.71242100
P	-1.98224200	-1.31667700	0.23254800	H	0.47992600	-2.64246900	3.34808400
P	-0.81494500	1.73833900	-0.85894700	H	0.24145900	-3.31227600	1.64126700
C	1.96044200	-1.57469500	-0.52550000	Rh	0.19205800	0.11533200	-0.62090600
C	0.79642900	-2.02763400	-0.85410400	P	0.35384800	2.06380600	0.48165300
H	0.43733600	-2.89949800	-1.38288600	P	2.45640600	-1.00011900	-0.42208800
C	-2.04934400	1.49467600	-2.20912000	C	-2.65655700	0.20717600	-0.71202000
H	-2.32829700	2.45893900	-2.64794900	C	-1.59086900	0.72885000	-1.33408500
H	-1.61573800	0.86160200	-2.98887000	H	-1.64966900	1.25634800	-2.29076000
H	-2.95357700	1.01119300	-1.83051400	C	3.70546300	-0.21607500	-1.54563700
C	-1.62819100	2.96001400	0.25668000	H	4.63380800	-0.79688900	-1.57096400
H	-0.97530700	3.18321100	1.10448300	H	3.30701100	-0.15234600	-2.56351700
H	-1.85064800	3.88737500	-0.28197200	H	3.93892200	0.79822800	-1.20590500
H	-2.56037800	2.54638800	0.65079600	C	3.41143200	-1.21480000	1.14610200
C	0.48047400	2.73369500	-1.72340300	H	2.78329000	-1.70762200	1.89364400

H	4.30836000	-1.81949300	0.97403800	C	0.62284200	2.07216300	-2.31080200
H	3.71777700	-0.24196700	1.54156300	H	0.21861700	2.81598200	-3.00647200
C	2.38864500	-2.73044000	-1.08091900	H	1.39715800	2.54804500	-1.70371200
H	3.39030500	-3.17094300	-1.13458400	H	1.08008100	1.26241100	-2.88664000
H	1.76629100	-3.35496800	-0.43287500	C	-1.96906700	0.89195900	-2.53041800
H	1.95075200	-2.73426900	-2.08450200	H	-2.13241700	1.70737600	-3.24353300
C	0.72177000	3.41255900	-0.71820400	H	-1.60181200	0.01559000	-3.07187400
H	1.61821900	3.17370300	-1.29839200	H	-2.92911000	0.64328000	-2.07036300
H	-0.11836300	3.53493700	-1.40704000	C	-2.82506300	-2.24837100	-0.73776200
H	0.88899800	4.35513100	-0.18507400	H	-3.11397200	-1.67314600	-1.62098200
C	-1.09073600	2.68341800	1.43397100	H	-2.21798100	-3.09544100	-1.06694300
H	-1.32624300	1.99912600	2.25353000	H	-3.73119100	-2.63064300	-0.25517900
H	-0.85572100	3.66635600	1.85652500	C	-1.62737000	-2.29951200	1.89896700
H	-1.96010900	2.76191400	0.77832300	H	-2.58467500	-2.73343400	2.20918600
C	1.72995900	2.15932100	1.70166200	H	-0.93573200	-3.11059200	1.65662200
H	1.73621100	3.14400600	2.18296900	H	-1.21295700	-1.72720800	2.73403500
H	1.60862500	1.39053400	2.46966100	C	-3.17232400	-0.02897300	1.06663900
H	2.68889700	2.00626700	1.19963000	H	-4.00194500	-0.59050000	1.51036700
C	-4.06238900	-0.11360500	-1.16207700	H	-2.73886100	0.63138000	1.82297900
H	-4.20005300	-0.12302500	-2.24530600	H	-3.57129300	0.58269100	0.25290900
H	-4.79951700	0.57811200	-0.71660400	C	3.05077100	-1.53870300	-0.94190000
S15				H	2.75254100	-1.00779300	-1.86213400
				H	3.65783900	-2.40137900	-1.24288000
	O	3.91672400	-0.74895700	C	3.39465300	0.51917300	0.18774500
	C	1.83032200	-2.05420200	H	4.20846400	1.01724200	0.72858700
C	0.66113500	-2.38615000	-0.86534500	H	3.18031200	1.11607700	-0.71425400
C	2.18586300	0.43085700	1.08703800	S15-TS			
C	1.25038500	1.44000300	1.25744700				
C	0.45002600	1.56171500	2.47978600		O	4.28179600	-0.91309500
C	-0.15366400	2.68580900	2.89683800		C	2.00647100	-1.60579600
H	2.02247700	-2.47535200	0.77489900	C	0.71923200	-1.82320800	-1.00315500
H	0.00215400	-3.13663200	-0.44248200	C	2.39898700	-0.05264400	0.62963000
H	0.55792200	-2.22507400	-1.93676400	C	1.50214100	1.12992000	0.78095600
H	2.28732600	-0.29746300	1.89068000	C	1.12188100	1.53860200	2.14306300
H	1.32962100	2.33250500	0.63801500	C	0.98478200	2.81139700	2.55486900
H	0.41340300	0.67504900	3.11264800	H	2.14853600	-2.33234300	0.50438500
H	-0.68314700	2.72564400	3.84347700	H	0.27049100	-2.79770200	-0.81481200
H	-0.10824000	3.61211600	2.32928100	H	0.69645400	-1.56984600	-2.06612800
Rh	0.18089400	-0.29571600	-0.00292300	H	2.58457800	-0.51876000	1.59802700
P	-1.87773000	-1.18926000	0.44380600	H	1.75602200	1.96567600	0.12816000
P	-0.73505300	1.40012700	-1.25209800	H	0.97451000	0.73596200	2.86675700
C	-1.50536100	2.92633200	-0.55459000	H	0.71894800	3.05027700	3.57975300
H	-1.83380300	3.58631800	-1.36486600	H	1.16885500	3.65352300	1.89068900
H	-2.36563900	2.67265800	0.06970200	Rh	0.00635900	-0.17645500	0.01464600
H	-0.78630100	3.46356000	0.06744700	P	-1.84578300	-1.53483600	0.43141100

P	-1.14274800	1.68057500	-0.85692200	H	-1.52032700	0.69805200	-2.78132100
C	-2.00148400	2.82546300	0.30548600	H	-1.78289000	3.07404400	-3.19690500
H	-2.37025900	3.71133100	-0.22268200	H	-2.10716300	3.38947400	-1.40481300
H	-2.84596100	2.31709400	0.77841400	Rh	0.18879600	0.00048900	-0.26832500
H	-1.30598600	3.13471500	1.09190400	P	2.22051900	-1.49165800	-0.37829400
C	-0.08549300	2.82715300	-1.85107400	P	0.90040700	1.88362100	0.73351100
H	-0.71024100	3.58154500	-2.34191600	C	1.67355700	2.99512100	-0.51405000
H	0.63673300	3.33998300	-1.21082600	H	2.02610200	3.91666300	-0.03737200
H	0.46156600	2.26999800	-2.61751300	H	2.52159500	2.49550900	-0.99168900
C	-2.45211300	1.24790000	-2.08729600	H	0.93659800	3.24733500	-1.28293100
H	-2.85467600	2.15710700	-2.54720700	C	-0.31491400	2.96367100	1.59816000
H	-2.02907200	0.61426000	-2.87270700	H	0.20292100	3.81951500	2.04391300
H	-3.27583700	0.70916800	-1.61159400	H	-1.06220600	3.33325600	0.89243100
C	-2.72662900	-2.46000800	-0.90156800	H	-0.82379600	2.40938800	2.39186700
H	-3.13795400	-1.76184700	-1.63560600	C	2.20161600	1.62498400	2.01017000
H	-2.03496500	-3.13026000	-1.41961800	H	2.52779800	2.58800900	2.41851000
H	-3.54389600	-3.05514100	-0.48009700	H	1.80857900	1.01028400	2.82525900
C	-1.39525100	-2.86149600	1.63755300	H	3.06492100	1.11742500	1.57246900
H	-2.27592600	-3.45714600	1.90202600	C	2.89196100	-2.19381400	1.19653000
H	-0.63668500	-3.52627800	1.21418000	H	3.28400400	-1.39748000	1.83602100
H	-0.98907900	-2.40989000	2.54780600	H	2.09698500	-2.71034400	1.74375000
C	-3.21608100	-0.66768200	1.31353000	H	3.69646300	-2.90874900	0.99335700
H	-3.94848500	-1.39350900	1.68354100	C	1.85171800	-3.02627800	-1.35153400
H	-2.81515200	-0.10493100	2.16164300	H	2.72613800	-3.68506000	-1.39791200
H	-3.72810100	0.02827900	0.64386600	H	1.02584300	-3.57572400	-0.88785600
C	3.23517200	-1.56847300	-1.23223800	H	1.55764200	-2.76336400	-2.37281100
H	2.96688900	-1.04172300	-2.16366400	C	3.74272400	-0.85866900	-1.22163100
H	3.56522000	-2.58131600	-1.47687700	H	4.50979800	-1.63798200	-1.28741700
C	3.72208700	0.28321500	-0.08606400	H	3.49500200	-0.52419300	-2.23416000
H	4.43216300	0.74053900	0.60758900	H	4.15696700	-0.00745700	-0.67164900
H	3.52654700	0.98431800	-0.91489000	C	-3.13198700	-1.82292600	1.48428000
S16				H	-3.27376700	-1.03982300	2.24826900
				H	-3.12946600	-2.80002500	1.97154200
				C	-3.94411300	-0.67232100	-0.28229200
O	-4.17845200	-1.80042400	0.53701100	H	-4.54452400	-0.77513900	-1.18820500
C	-1.84295100	-1.53293200	0.65339300	H	-4.23560900	0.25466300	0.23783600
C	-0.73765800	-0.78886800	1.38800000				
C	-2.40246000	-0.66886100	-0.54885600				
C	-1.76058900	0.72312800	-0.60818700	S17			
C	-1.70874000	1.36304600	-1.93483900	C	-0.00000100	-0.72594800	0.00000000
C	-1.85985600	2.67698200	-2.18929800	H	-0.98068900	-1.20957400	0.00000000
H	-1.46393100	-2.48644400	0.27048600	C	1.10811000	-1.47307500	0.00000000
H	-0.04353100	-1.42433900	1.94305500	H	1.07087600	-2.55984400	0.00000000
H	-1.12316200	-0.00078900	2.04085500	H	2.09833900	-1.01665500	0.00000000
H	-2.21467000	-1.19714800	-1.49214700	C	0.00000000	0.72594700	0.00000000
H	-2.14427600	1.38881800	0.16878800	H	0.98068900	1.20957200	0.00000000

C	-1.10810900	1.47307600	0.00000000	C	0.00000000	0.00000000	-0.60247300
H	-2.09834000	1.01665900	0.00000000	H	0.00000000	0.00000000	-1.67163600
H	-1.07087200	2.55984500	0.00000000				
S18				S20			
C	0.72254200	-2.57423100	-0.59923900	C	0.38668000	-2.06372300	-1.53494700
H	1.22737400	-2.64466800	-1.56308600	H	0.72466200	-1.67563800	-2.49548300
C	1.45220600	-2.29022100	0.54433500	C	1.29167800	-2.40417200	-0.50557500
H	2.53183000	-2.17527800	0.46313000	H	2.35657700	-2.26899400	-0.68357100
H	1.08212400	-2.48894300	1.54969800	H	1.05512900	-3.20782900	0.19110400
C	-0.72325100	-2.57412500	-0.59869000	C	-1.01040200	-2.09343600	-1.23295800
H	-1.22883900	-2.64452400	-1.56214200	H	-1.71857300	-1.72207700	-1.97470600
C	-1.45196400	-2.28997300	0.54546900	C	-1.43139400	-2.40893900	0.07235800
H	-1.08110900	-2.48874700	1.55053800	H	-0.91515600	-3.14865900	0.68179300
H	-2.53163800	-2.17489100	0.46514000	H	-2.47949300	-2.27128500	0.33155900
Rh	-0.00003900	-0.59494600	0.03387000	P	-1.69903900	0.96988300	-0.08855700
P	-1.80421900	0.89609000	-0.00849500	P	1.71806400	0.92870500	-0.17492000
P	1.80427000	0.89601300	-0.00841100	C	-0.17034900	-0.45243000	2.47446400
C	2.77439300	0.88415200	1.54600200	C	0.82159800	-1.15067800	2.27317100
H	3.05320300	-0.13831200	1.82254500	Rh	0.00357300	-0.68256300	0.12094800
H	3.68705200	1.48399000	1.42992300	H	-0.96620800	0.08973400	2.94975700
H	2.17585700	1.30606000	2.36164500	H	1.70092700	-1.76332800	2.33740100
C	3.01783200	0.38259600	-1.28189900	C	-2.08033100	1.52771500	-1.79458000
H	3.90605000	1.02774100	-1.24627700	H	-2.39752000	0.67314100	-2.40386700
H	3.33147300	-0.65552100	-1.12538200	H	-2.89047500	2.26949600	-1.78796000
H	2.56478800	0.45778700	-2.27741600	H	-1.19841200	1.97138700	-2.26930400
C	1.68126500	2.69238800	-0.34468300	C	-1.53243200	2.56313800	0.80675200
H	1.13710700	3.20459600	0.45650200	H	-2.42155900	3.18561500	0.64058100
H	2.69119700	3.12035800	-0.40171300	H	-1.42571600	2.39081500	1.88489300
H	1.17078900	2.87537200	-1.29661800	H	-0.65354400	3.12043200	0.46116200
C	-1.68094000	2.69215600	-0.34632300	C	-3.35409300	0.41393000	0.47490100
H	-1.13647500	3.20491700	0.45429600	H	-3.31612400	0.05384900	1.51019900
H	-1.17062900	2.87421800	-1.29852900	H	-4.07727800	1.23755000	0.40996300
H	-2.69078700	3.12031100	-0.40349000	H	-3.71110600	-0.40596400	-0.16009700
C	-3.01841400	0.38188800	-1.28106500	C	1.55211000	2.15529000	-1.52918400
H	-3.33238400	-0.65596400	-1.12345400	H	1.38683400	1.63341700	-2.48050800
H	-3.90639600	1.02737300	-1.24573900	H	0.70707500	2.83175600	-1.35413800
H	-2.56568500	0.45599000	-2.27680900	H	2.46393500	2.76168900	-1.61263500
C	-2.77370800	0.88568800	1.54631700	C	3.36921000	0.22819500	-0.55047500
H	-3.68628600	1.48562700	1.43012600	H	4.11225900	1.03336400	-0.62229300
H	-3.05263800	-0.13648600	1.82381700	H	3.67926000	-0.46297900	0.24297200
H	-2.17474500	1.30812700	2.36137200	H	3.35160400	-0.31371200	-1.50410900
				C	2.09903300	1.96738000	1.28530200
S19				H	2.43972800	1.33072300	2.10994200
C	0.00000000	0.00000000	0.60247300	H	2.88885600	2.69083000	1.04396900
H	0.00000000	0.00000000	1.67163600	H	1.21031300	2.50954700	1.62749600

S20-TS				C	1.92809200	-1.73917200	-0.63417100
				H	2.73615500	-1.36317500	-1.26353800
C	0.97346000	-2.01238900	-1.24128800	C	2.32631900	-2.15398100	0.76752600
H	1.66446000	-1.68916200	-2.01820100	H	3.38366100	-1.90487000	0.93845400
C	1.47858500	-2.36230600	0.08418000	H	2.27504100	-3.25264900	0.84995700
H	2.55630200	-2.25121000	0.20251500	C	0.81003300	-2.24317900	-1.32623700
H	1.09524600	-3.30419000	0.48296200	H	0.79999100	-2.09999100	-2.41159300
C	-0.40657300	-2.15679500	-1.51465300	C	-0.41001700	-2.57780200	-0.70435500
H	-0.78904200	-1.91133900	-2.50467700	H	-0.43211300	-2.97272500	0.31273900
C	-1.27610900	-2.37329200	-0.41494300	H	-1.25249200	-2.86277500	-1.33467300
H	-0.99858900	-3.04261100	0.40031800	P	-2.14801300	0.17128500	0.13011000
H	-2.34970600	-2.32189000	-0.59661900	P	1.17906600	1.64649800	-0.10949100
P	-1.86509100	0.77699900	0.01336400	C	0.47737100	-0.72379900	1.56648300
P	1.60518500	1.16388600	-0.17619600	C	1.48755000	-1.53870800	1.84554600
C	0.10429000	-0.70581500	2.12413400	Rh	0.06964500	-0.41405300	-0.36134000
C	1.02418100	-1.57098400	1.97214300	H	-0.15575100	-0.21904300	2.30065100
Rh	-0.02792400	-0.57785400	0.03822300	H	1.71833200	-1.78220700	2.88646400
H	-0.41752800	-0.17435000	2.90976200	C	-3.10902400	0.43888800	-1.40423300
H	1.75856400	-2.20024700	2.45123500	H	-3.07453300	-0.46548800	-2.02415600
C	-2.58725400	0.97873800	-1.65290400	H	-4.15730200	0.67106600	-1.17303300
H	-2.88426900	-0.00008600	-2.04822900	H	-2.68149700	1.26972100	-1.97934700
H	-3.47179800	1.62887300	-1.61913200	C	-2.52880600	1.66468300	1.12207500
H	-1.84671700	1.41349500	-2.33506300	H	-3.61524900	1.76972500	1.24519600
C	-1.71879500	2.49638100	0.62381300	H	-2.07666100	1.58780900	2.11917400
H	-2.68831100	3.00492800	0.53651400	H	-2.14884000	2.56857800	0.63013800
H	-1.42414600	2.48996000	1.68106900	C	-3.09307100	-1.11907600	1.01607100
H	-0.97575900	3.06638300	0.05410800	H	-2.59581200	-1.36614000	1.96224400
C	-3.26798400	0.17220600	1.01813100	H	-4.11467700	-0.77747100	1.22836500
H	-2.96816300	0.09886500	2.07018300	H	-3.14096800	-2.02968900	0.40832700
H	-4.11978700	0.86088100	0.93903100	C	0.61643600	2.85729200	-1.36474600
H	-3.58254900	-0.82219700	0.68507300	H	0.77267000	2.45158400	-2.37177300
C	1.49461400	2.26378600	-1.63860600	H	-0.45391300	3.06395900	-1.24094800
H	1.54136800	1.65657800	-2.55139900	H	1.17047500	3.80159500	-1.27715100
H	0.54345400	2.80933500	-1.64716000	C	2.99103200	1.60759500	-0.35695700
H	2.31684300	2.99176400	-1.65262600	H	3.41509200	2.61785800	-0.28221900
C	3.33072600	0.55059900	-0.30962300	H	3.45201400	0.97458400	0.41134700
H	4.02895400	1.39548700	-0.37816200	H	3.22960100	1.19242800	-1.34277200
H	3.58934300	-0.03656300	0.58063200	C	1.04799900	2.56534200	1.46760300
H	3.46092200	-0.07631100	-1.19959200	H	1.46521200	1.95959800	2.28077800
C	1.78824800	2.32491700	1.23138200	H	1.61329100	3.50429800	1.40341700
H	2.00438300	1.74883200	2.13992200	H	0.00494700	2.80057700	1.70735500
H	2.61540900	3.02403200	1.05086300				
H	0.87195800	2.90062200	1.39852000	S21-TS			
				C	2.66531600	0.18391100	-0.27208800
S21				H	2.99317900	1.22415300	-0.31118600

C	3.17916500	-0.61140900	0.90198100	H	-3.88078900	0.00010700	1.46222800
H	3.33410600	0.06431200	1.75691500	C	-2.23729200	-1.19919400	-0.68586200
H	4.18303500	-1.00708600	0.66740600	H	-1.98952600	-2.10494400	-1.23802100
C	2.10333500	-0.33222100	-1.43188300	C	-2.77606100	-0.00172300	-1.43201200
H	1.98417900	0.31512300	-2.30128900	H	-3.88103500	-0.00089400	-1.46193800
C	1.48191900	-1.65077300	-1.42313200	H	-2.42997300	-0.00407500	-2.47160300
H	2.08831100	-2.53162300	-1.22005200	P	1.16093800	1.70148000	0.00216200
H	0.76570400	-1.84339000	-2.22816700	P	1.16143000	-1.70110200	-0.00224000
P	-1.83390900	-1.04553100	0.03457700	C	-2.23720900	1.19722500	-0.68970100
P	-0.24479600	2.05095300	0.05983100	C	-2.23736800	1.19869200	0.68587100
C	1.12399200	-1.97349700	0.63832900	Rh	-0.41351800	0.00003200	-0.00011800
C	2.26519100	-1.73680700	1.29256400	H	-1.98901000	2.10113400	-1.24691000
Rh	0.34011100	-0.24097600	-0.17643800	H	-1.98974000	2.10452200	1.23796100
H	0.52088400	-2.86704600	0.79117400	C	1.81812400	2.09844000	-1.66058100
H	2.56403500	-2.36819800	2.13215500	H	2.49054200	2.96583300	-1.61517800
C	-3.02380600	-0.45628900	-1.22349000	H	2.36384400	1.24691800	-2.08237500
H	-4.01746100	-0.89040500	-1.04866700	H	0.98270000	2.33092200	-2.33241900
H	-3.10499400	0.63485000	-1.20611300	C	0.49510300	3.32242300	0.54281200
H	-2.67479700	-0.75802400	-2.21824500	H	0.19615000	3.27702500	1.59689800
C	-2.03936800	-2.86122500	-0.10204700	H	1.26210800	4.10044900	0.43141000
H	-1.57266000	-3.37497000	0.74597600	H	-0.37755000	3.60809300	-0.05660500
H	-3.10749200	-3.11510700	-0.10661900	C	2.66040600	1.59104200	1.04998900
H	-1.58590000	-3.22996500	-1.03022900	H	3.26427000	2.50215100	0.94391200
C	-2.64272700	-0.69774600	1.63988300	H	2.36675300	1.48512900	2.10150500
H	-3.65777900	-1.11604500	1.66748700	H	3.28163500	0.73098500	0.77657000
H	-2.04902900	-1.14999100	2.44407700	C	1.81643500	-2.09930800	1.66109800
H	-2.69813400	0.38109900	1.82743000	H	0.98006300	-2.33272800	2.33143500
C	0.26289100	2.56056700	1.74606500	H	2.48916500	-2.96646900	1.61585600
H	1.31721300	2.30569800	1.90913600	H	2.36126500	-1.24808700	2.08464400
H	0.12786100	3.64084100	1.89141000	C	2.66223500	-1.59026400	-1.04813500
H	-0.33324100	2.02160900	2.49267300	H	2.36989900	-1.48375600	-2.09996200
C	-1.92384400	2.77981900	-0.07885700	H	3.28341500	-0.73054700	-0.77349200
H	-2.28176000	2.71514500	-1.11345600	H	3.26574400	-2.50158100	-0.94182700
H	-2.64366700	2.27425600	0.57532800	C	0.49613800	-3.32172300	-0.54461500
H	-1.88834600	3.83980000	0.20640000	H	1.26312600	-4.09977200	-0.43324600
C	0.70113800	3.18494600	-1.02688600	H	-0.37687200	-3.60789700	0.05405100
H	0.47019000	4.23043600	-0.78227900	H	0.19784500	-3.27559300	-1.59885300
H	1.77849700	3.02866300	-0.90314000				
H	0.44446000	3.00280200	-2.07715400	S23			
				C	-0.00009500	0.66610300	1.24679700
S22				H	-0.00030400	1.20467500	2.19581800
C	-2.23690100	-1.19773400	0.68969100	C	0.00015900	1.49464800	0.00000000
H	-1.98845200	-2.10160900	1.24684700	H	0.87153600	2.17349900	0.00000000
C	-2.77581900	0.00113000	1.43210600	H	-0.87074900	2.17408700	0.00000000
H	-2.42955000	0.00352900	2.47163700	C	-0.00009500	-0.66610300	1.24679700

H	-0.00030400	-1.20467500	2.19581800	C	3.41529100	-0.56458600	0.28552300
C	0.00016000	-1.49464800	0.00000000	C	4.22980800	0.14440800	-0.61352000
H	-0.87074700	-2.17408900	0.00000000	C	3.84671700	-1.82402200	0.73540000
H	0.87153800	-2.17349800	0.00000000	C	5.44372200	-0.39068800	-1.04798800
C	-0.00009500	-0.66610300	-1.24679700	H	3.92825100	1.12819700	-0.96128500
C	-0.00009500	0.66610300	-1.24679700	C	5.06446300	-2.35461000	0.30287700
H	-0.00030400	-1.20467500	-2.19581800	H	3.24132700	-2.39806400	1.42950500
H	-0.00030400	1.20467500	-2.19581800	C	5.86484300	-1.64154100	-0.59180900
S24a-TS				H	6.06505800	0.17648900	-1.73529200
				H	5.39043500	-3.32242400	0.67414900
				H	6.81288500	-2.05389700	-0.92444300
C	1.08677300	-0.43131200	-2.60909400	C	2.09243600	1.92572900	0.86378200
C	1.42493000	-1.80883400	-2.25155200	C	2.93867800	2.48377400	1.83830200
H	2.48275200	-1.97556800	-2.07838400	C	1.52490300	2.77132900	-0.10126000
H	0.94542200	-2.56008900	-2.87472400	C	3.19522000	3.85449000	1.85248600
C	-0.24775300	-0.06801600	-2.91178900	H	3.41201500	1.85099100	2.58340100
C	-1.24528800	-1.01975300	-2.51438200	C	1.79053700	4.14363400	-0.09233800
H	-1.09720400	-2.07982400	-2.70858300	H	0.87621200	2.34988000	-0.86426800
H	-2.28323900	-0.70201700	-2.56924800	C	2.62171600	4.68730800	0.88754000
P	-1.79334800	0.14134400	0.50530500	H	3.84859400	4.27178700	2.61326300
P	1.76951800	0.11247600	0.78627600	H	1.34969500	4.78438300	-0.85100800
C	-0.00548300	-2.58464900	0.15989700	H	2.82723900	5.75373500	0.89829600
C	0.84458800	-3.11080500	-0.63036400	C	-2.74023400	1.44176300	-0.39996700
Rh	-0.00744200	-0.68990400	-0.69868800	C	-2.25205900	2.75869000	-0.45549600
H	-0.59093500	-2.90022800	1.00991100	C	-3.93822100	1.13592100	-1.06601500
C	-0.59230500	1.27919300	-3.48889200	C	-2.94984200	3.74445700	-1.15461200
H	0.20643600	2.01043600	-3.32755700	H	-1.32813600	3.02689300	0.04713800
H	-0.73526400	1.17996100	-4.57308100	C	-4.62891900	2.12329100	-1.77186100
H	-1.52341000	1.67314900	-3.07356100	H	-4.34560100	0.13097100	-1.02219300
H	1.88796500	0.29617800	-2.70085100	C	-4.13800200	3.42913500	-1.81771900
C	1.64863300	-4.30048000	-0.99449800	H	-2.56593500	4.76053300	-1.17760600
H	1.38416800	-5.12599000	-0.32341800	H	-5.55636500	1.87071600	-2.27777700
H	1.45831100	-4.62796500	-2.02300100	H	-4.67983400	4.19750100	-2.36138900
H	2.72247100	-4.10765700	-0.89489700	C	-3.09336700	-1.07675600	0.98400900
C	1.68039100	-0.43460300	2.57501400	C	-3.96638400	-0.82050700	2.05657400
H	2.69146100	-0.35040100	2.98952000	C	-3.27355000	-2.25110600	0.23584500
H	1.44518800	-1.50533400	2.54427400	C	-4.98195700	-1.72128200	2.37624300
C	-1.36935300	0.99989700	2.09897800	H	-3.86850000	0.08471100	2.64684400
H	-0.65116900	1.78631500	1.84753400	C	-4.29690400	-3.14762200	0.55230800
H	-2.27361100	1.51881400	2.43359100	H	-2.61031000	-2.46270200	-0.59608100
C	0.69281500	0.27386600	3.51795600	C	-5.14975100	-2.88702100	1.62542900
H	0.92969200	1.34338200	3.57658400	H	-5.64428100	-1.50935300	3.21061800
H	0.88798900	-0.13110900	4.51915500	H	-4.42363800	-4.04989100	-0.03922200
C	-0.80554400	0.09497000	3.22411500	H	-5.94242100	-3.58621300	1.87529200
H	-1.35133100	0.33335300	4.14371500				
H	-1.01932300	-0.96325800	3.02760500				

S24b-TS				H	-4.15780500	3.54331900	3.14822200
C	-0.92453000	0.32964100	-2.75771300	H	-3.07602500	5.35631500	1.83420200
C	-1.40454500	-1.06009000	-2.75206100	C	-3.38670200	-0.85677100	0.29509100
H	-2.48152600	-1.16399900	-2.64877100	C	-3.60573000	-2.24268200	0.39065700
H	-0.98168900	-1.68388300	-3.53670500	C	-4.40335200	-0.05570100	-0.25265600
C	0.47156800	0.52262600	-2.81288000	C	-4.81030900	-2.80601000	-0.03263900
C	1.32991600	-0.61301900	-2.66130900	H	-2.83905900	-2.89464700	0.79744400
H	1.09680100	-1.54770400	-3.16591400	C	-5.60485600	-0.62300700	-0.68341300
H	2.39320500	-0.41812300	-2.56701700	H	-4.27257400	1.01915100	-0.32181300
P	1.75703000	0.16374200	0.44529300	C	-5.81298500	-1.99845500	-0.57374600
P	-1.75185900	-0.13814200	0.77646500	H	-4.96563200	-3.87693500	0.06417800
C	-0.08413500	-2.74575100	-0.59856600	H	-6.38174100	0.01567500	-1.09407500
C	-0.96174600	-2.71290300	-1.52172100	H	-6.75079700	-2.43766100	-0.90097300
Rh	0.01094300	-0.60976500	-0.90121700	C	2.60793400	1.61209200	-0.33439400
H	-1.70453000	-3.28618600	-2.04675900	C	3.78334600	1.43560600	-1.08281000
H	0.87265500	1.53250000	-2.79922200	C	2.07802500	2.90787900	-0.20883100
C	-1.91206300	1.46153600	-2.88813000	C	4.40346700	2.52383900	-1.70025400
H	-2.77425900	1.32817300	-2.22902900	H	4.23324300	0.45171100	-1.16872900
H	-2.29385200	1.49497700	-3.91730600	C	2.70444700	3.99427000	-0.82130600
H	-1.45153400	2.43001200	-2.67486500	H	1.18266300	3.08329100	0.37775900
C	0.48777400	-3.77066400	0.32742300	C	3.86553100	3.80505300	-1.57384800
H	1.48202800	-3.50806500	0.69226000	H	5.31394500	2.36783200	-2.27171600
H	0.55170100	-4.74194300	-0.17651000	H	2.28824400	4.99082200	-0.70276700
H	-0.16416500	-3.89669300	1.20032600	H	4.35220800	4.65155000	-2.04928400
C	1.27018000	0.86838700	2.10601900	C	3.16778400	-0.96903000	0.79346200
H	0.42100500	1.52935400	1.90981900	C	4.05440900	-0.70816400	1.85364400
H	2.08696000	1.52021800	2.43619800	C	3.43136300	-2.05480200	-0.05527800
C	-1.48194200	-0.86965900	2.49329900	C	5.16136100	-1.52861400	2.06961500
H	-1.90168300	-0.16878600	3.22315100	H	3.89812300	0.14352700	2.50812200
H	-2.10903000	-1.76552800	2.53647300	C	4.54644100	-2.86955000	0.15696800
C	-0.04995800	-1.25887100	2.89485200	H	2.76179000	-2.25867400	-0.88492300
H	0.38954600	-1.89375200	2.12124600	C	5.40905900	-2.61191100	1.22303600
H	-0.13150800	-1.88953100	3.78984300	H	5.83379400	-1.31683900	2.89586600
C	0.92535900	-0.12447200	3.23074200	H	4.73766100	-3.70506600	-0.51043500
H	1.85015200	-0.58614000	3.59363100	H	6.27323200	-3.24781400	1.39149900
H	0.52970900	0.46351500	4.06978700				
C	-2.18043200	1.62622400	1.13040100	S24c-TS			
C	-1.58687800	2.65730800	0.39007600	C	1.04441800	0.00490400	-2.70020600
C	-3.11583400	1.96460500	2.12547200	C	1.46055300	-1.38690400	-2.59936000
C	-1.90507700	3.99528000	0.64057600	H	2.52476700	-1.53584000	-2.45113400
H	-0.87207700	2.40650900	-0.38643500	H	1.01131000	-2.05831200	-3.32679600
C	-3.43334700	3.29886900	2.37674000	C	-0.31675300	0.32860700	-2.90714600
H	-3.61547700	1.18739500	2.69686300	C	-1.24629800	-0.74295500	-2.67815000
C	-2.82648200	4.31789200	1.63667700	H	-1.04695100	-1.73767900	-3.07065000
H	-1.43606700	4.78165400	0.05557100	H	-2.30078800	-0.47891600	-2.67146700

P	-1.71098300	0.11731800	0.48068700	C	-3.86881900	3.84439100	-1.31208600
P	1.84001700	-0.12670800	0.70719600	H	-2.25276200	4.98394200	-0.45084200
C	0.05465100	-2.77418300	-0.28095900	H	-5.34509400	2.44365200	-2.02676500
C	0.93737000	-2.90178700	-1.18636100	H	-4.37028100	4.71331300	-1.72803400
Rh	0.01855800	-0.68924100	-0.85245000	C	2.23560200	1.64899300	1.00931600
C	-0.74885300	1.72807000	-3.25088200	C	1.66194100	2.63827100	0.19768300
H	-0.02118300	2.47699000	-2.92237200	C	3.14697500	2.03736900	2.00766000
H	-0.83696400	1.81003200	-4.34258400	C	1.98237200	3.98661200	0.38104900
H	-1.72507200	1.96958000	-2.82712600	H	0.96430400	2.34737200	-0.58228700
H	1.79665900	0.78771700	-2.66345500	C	3.46004100	3.38318700	2.19550800
H	1.65482000	-3.55931600	-1.64218100	H	3.62707600	1.29077500	2.63378200
C	-0.61362600	-3.60971700	0.75798100	C	2.87783100	4.36066800	1.38321900
H	-1.69294400	-3.65818200	0.59592600	H	1.53435000	4.74089800	-0.25991700
H	-0.21490200	-4.63051900	0.74219700	H	4.16355300	3.66887300	2.97218700
H	-0.46242500	-3.19855500	1.76118600	H	3.12689100	5.40769500	1.52926200
C	1.74896800	-0.88236400	2.41733800	C	3.45641500	-0.78926300	0.10468700
H	1.47117600	-1.93085800	2.26287300	C	3.84398400	-2.11264600	0.37582000
H	2.76766800	-0.89080200	2.82166000	C	4.29251800	0.00652000	-0.69739100
C	-1.22444100	0.74342400	2.16448600	C	5.04010400	-2.62148000	-0.13536600
H	-0.46759500	1.51590200	1.99944100	H	3.22323100	-2.75439400	0.99242400
H	-2.09680700	1.26814900	2.56775700	C	5.48455600	-0.50680200	-1.21097000
C	-0.70237700	-0.30761500	3.17509400	H	4.02571900	1.03832300	-0.90596000
H	-0.98824900	-1.32239200	2.87478000	C	5.86186400	-1.82221900	-0.93191100
H	-1.21701400	-0.13315300	4.12671500	H	5.33071000	-3.64258200	0.09540200
C	0.80791500	-0.24958500	3.45718900	H	6.12301200	0.12619700	-1.82077200
H	0.99333200	-0.78404100	4.39770800	H	6.79273300	-2.21879100	-1.32650600
H	1.10277300	0.79069400	3.64178800				
C	-3.11726900	-1.03385200	0.80842500	S24d-TS			
C	-3.46611700	-2.00163900	-0.14739500	C	0.96967900	-0.45122300	-2.73250500
C	-3.90988300	-0.91367500	1.96260700	C	1.28546100	-1.83310800	-2.33221800
C	-4.57851600	-2.82436400	0.04179800	H	2.34773000	-2.02589400	-2.21114600
H	-2.85753300	-2.11550200	-1.03835500	H	0.76486200	-2.58795200	-2.91773500
C	-5.01263600	-1.74657000	2.15760100	C	-0.39117500	-0.11544700	-2.90452800
H	-3.68202000	-0.16896700	2.71768500	H	-0.66031700	0.89281500	-3.20883100
C	-5.35163000	-2.70180600	1.19771100	C	-1.38459900	-1.04223400	-2.46143600
H	-4.83537700	-3.56416000	-0.71114200	H	-1.26525100	-2.10537500	-2.66024700
H	-5.60899600	-1.64366100	3.05955200	H	-2.41620500	-0.70424400	-2.46286500
H	-6.21283500	-3.34581000	1.34968300	P	-1.86101200	0.21400800	0.43952700
C	-2.57516000	1.59320900	-0.22335200	P	1.69906300	0.13900700	0.78405800
C	-2.03369900	2.88007400	-0.06114500	C	-0.07930400	-2.55756000	0.14626100
C	-3.77666800	1.45352400	-0.93786200	C	0.73513900	-3.09665400	-0.67418500
C	-2.67922200	3.99543400	-0.59680500	Rh	-0.07441700	-0.67323400	-0.72358700
H	-1.10810100	3.02576400	0.48540400	H	-0.63317200	-2.87345200	1.01776600
C	-4.41442300	2.57081700	-1.48117200	C	2.08507300	0.48392000	-3.12729500
H	-4.23092000	0.47534900	-1.05695900	H	2.94567200	0.38905900	-2.46039100

H	2.43165400	0.23367200	-4.13894300	C	4.83536500	-2.54667600	0.55428200
H	1.75700200	1.52740700	-3.13735600	H	2.83813600	-2.52533800	1.33291100
C	1.51463100	-4.29921100	-1.05002900	C	5.83736700	-1.82984000	-0.10425300
H	1.24992200	-5.11604300	-0.36843100	H	6.37766700	0.06178900	-0.98660200
H	1.29930200	-4.62998500	-2.07237500	H	5.01582400	-3.57050000	0.87066100
H	2.59305700	-4.12297300	-0.97104500	H	6.79707900	-2.29496000	-0.30938100
C	1.50871500	-0.31304000	2.59619700	C	2.06852400	1.94459000	0.80437600
H	2.51188700	-0.27383600	3.03526600	C	2.91445000	2.51689600	1.77131500
H	1.20597500	-1.36695000	2.61130700	C	1.51893200	2.77317900	-0.18495600
C	-1.47047500	1.19406600	1.97231300	C	3.18926500	3.88415000	1.75237600
H	-0.74455700	1.95949000	1.67962000	H	3.37216200	1.89691200	2.53680100
H	-2.38474700	1.73801500	2.23163400	C	1.80086700	4.14191900	-0.20868100
C	0.55183700	0.50938500	3.47493500	H	0.87002500	2.33858900	-0.94022700
H	0.72014400	0.16922000	4.50489200	C	2.63279900	4.69951100	0.76275600
H	0.84244800	1.56698100	3.45860200	H	3.84181000	4.31250800	2.50771100
C	-0.95211500	0.38716900	3.18836300	H	1.37291400	4.76933000	-0.98564000
H	-1.48155400	0.75633800	4.07418000	H	2.85142700	5.76328300	0.74840100
H	-1.22956700	-0.67132900	3.10728900				
C	-2.80374100	1.44299800	-0.56751800	S25			
C	-4.05662800	1.13261100	-1.11973500	C	1.54389000	-0.49371800	-0.07490500
C	-2.25159100	2.71274700	-0.81047300	H	1.17459700	-1.45589000	-0.42119700
C	-4.73928700	2.07060900	-1.89783300	H	2.61124100	-0.41875800	0.11212500
H	-4.50988100	0.16407400	-0.93475700	C	0.72843800	0.55457200	0.09962100
C	-2.94041100	3.64920000	-1.58150000	H	1.16411100	1.50952700	0.39550700
H	-1.28635100	2.98264300	-0.39339500	C	-0.72843800	0.55457200	-0.09962100
C	-4.18457100	3.32942700	-2.13049000	H	-1.16411100	1.50952700	-0.39550700
H	-5.70902000	1.81570900	-2.31557400	C	-1.54389000	-0.49371800	0.07490500
H	-2.50669300	4.63095900	-1.75024300	H	-1.17459800	-1.45589000	0.42119700
H	-4.71915500	4.05919200	-2.73149000	H	-2.61124100	-0.41875800	-0.11212500
C	-3.15794800	-0.97732400	0.99166000				
C	-4.03159900	-0.66088500	2.04787500	ethylene			
C	-3.33632800	-2.19507400	0.31558000	C	0.00000000	0.66561600	0.00000000
C	-5.04463700	-1.54373600	2.42148800	H	0.92378900	1.23960300	0.00000000
H	-3.93694000	0.27745800	2.58418400	H	-0.92375100	1.23964700	0.00000000
C	-4.35676300	-3.07401700	0.68578700	C	0.00000000	-0.66561600	0.00000000
H	-2.67493400	-2.45505800	-0.50367000	H	-0.92378900	-1.23960300	0.00000000
C	-5.20972200	-2.75273400	1.74216400	H	0.92375100	-1.23964700	0.00000000
H	-5.70702300	-1.28376600	3.24210400				
H	-4.48121800	-4.01008400	0.14878400	S25-TS			
H	-6.00019000	-3.43806500	2.03388100	C	-0.44848500	-1.43702400	0.49042700
C	3.35261900	-0.61762500	0.44253600	H	-0.12796700	-1.06815200	1.45801000
C	4.37053700	0.09491900	-0.21266800	H	-0.39594500	-2.51742300	0.37976600
C	3.60240000	-1.94900800	0.82131200	C	-1.32296700	-0.70299400	-0.29042400
C	5.60081600	-0.50880400	-0.48550500	H	-1.87031200	-1.21252000	-1.08216400
H	4.21657900	1.13207900	-0.49257700	C	-1.32190600	0.70462700	-0.29065900

H	-1.86855200	1.21476700	-1.08248300	S28			
C	-0.44655300	1.43756400	0.49028400	C	-1.75973300	0.06070500	0.42928500
H	-0.12649200	1.06808700	1.45782300	C	-3.16923400	-0.27091700	0.03678300
H	-0.39236900	2.51787700	0.37960700	O	-1.25994000	1.04328400	-0.47036900
C	1.57636500	-0.69398300	-0.22775200	C	0.02007600	1.54666800	-0.10970800
H	2.07397200	-1.23806900	0.56996900	C	1.12869000	0.54691000	-0.29192200
H	1.47194600	-1.23641900	-1.16065900	C	2.02632900	0.23155000	0.65490800
C	1.57775700	0.69210400	-0.22714200	C	3.15934900	-0.68962800	0.49952600
H	1.47397900	1.23569200	-1.15938800	C	3.80761200	-0.95594900	-0.64270100
H	2.07647100	1.23439800	0.57111000	C	-3.63166300	-1.50961100	-0.12949500
				H	-1.74010800	0.46621500	1.45850300
S26				H	-1.13174600	-0.84271300	0.42590200
C	-0.66630700	1.30627200	0.05701500	H	-3.82923100	0.58622600	-0.09295800
C	0.66608800	1.30630100	-0.05724600	H	0.17584200	2.40717700	-0.77312000
C	1.49918100	0.04799600	-0.11042900	H	0.01264700	1.92130300	0.92842800
C	0.69832600	-1.19253100	0.31871500	H	1.17593200	0.06987500	-1.27108200
C	-0.69829200	-1.19233600	-0.31925300	H	1.91273500	0.68110700	1.64317600
C	-1.49909000	0.04775300	0.11115900	H	3.49780900	-1.17613600	1.41481400
H	-1.19987600	2.25484500	0.11155100	H	4.62436500	-1.67108300	-0.67603400
H	1.19956000	2.25488500	-0.11279400	H	3.55202600	-0.46252800	-1.57712900
H	1.88956400	-0.09009300	-1.13173400	H	-4.67064900	-1.70386600	-0.38169500
H	2.38669600	0.16401300	0.52729000	H	-2.98864400	-2.38021400	-0.01590900
H	1.24489700	-2.10603700	0.05372000				
H	0.59288800	-1.19313200	1.41271600	S28-TS			
H	-0.59299400	-1.19188900	-1.41326700	O	-2.39227900	-0.13471800	-0.03960000
H	-1.24471700	-2.10613200	-0.05497300	C	-1.68884200	1.09214200	0.11532100
H	-2.38752700	0.16365600	-0.52526700	C	-0.33495000	1.04793900	-0.55002600
H	-1.88793400	-0.09084000	1.13298900	C	0.76980800	1.80106100	-0.17605900
				C	-1.57220000	-1.29661600	0.17807200
S27-TS				C	-0.13517200	-0.90652200	0.35608600
C	-0.38125500	1.44568500	0.47272000	C	0.95322800	-1.43599100	-0.32036800
H	-0.01234500	1.07804700	1.42363700	C	2.21175400	-0.81195800	-0.22460300
H	-0.32460100	2.52451200	0.34773400	C	2.42543300	0.30739800	0.56198100
C	-1.24945400	0.70659400	-0.29877400	H	-1.58138700	1.37427000	1.17735700
H	-1.80499300	1.21176300	-1.08717900	H	-2.33499400	1.84160100	-0.35813200
C	-1.24950300	-0.70651700	-0.29877100	H	-0.37804200	0.71361500	-1.58557700
H	-1.80509000	-1.21164900	-1.08716700	H	1.46800300	2.15189000	-0.92610400
C	-0.38134900	-1.44567200	0.47271400	H	0.75292500	2.36989700	0.75135500
H	-0.01240100	-1.07806100	1.42362900	H	-1.94805800	-1.81611600	1.07288200
H	-0.32478000	-2.52450300	0.34772900	H	-1.70391800	-1.96749800	-0.68061600
C	1.64416900	0.61830300	-0.22837400	H	0.06748500	-0.41414700	1.30368900
H	2.06191900	1.59453400	-0.35759700	H	0.78735500	-2.16223400	-1.11504100
C	1.64413900	-0.61839200	-0.22837800	H	2.96929300	-1.08599200	-0.95728000
H	2.06181100	-1.59465500	-0.35760800	H	3.36633800	0.84710200	0.49210100
				H	1.89888000	0.44062700	1.49974800

S28b-TS

O	-2.34192100	0.10403000	0.03025600
C	-1.45562000	1.04424100	-0.56293600
C	-0.25271500	1.29156400	0.30937100
C	1.00594200	1.69499500	-0.11437800
C	-1.70705700	-1.16802900	0.24702900
C	-0.23978700	-1.00325600	0.53084200
C	0.71136600	-1.43016800	-0.38202300
C	2.02632400	-0.93777800	-0.41418800
C	2.44273600	0.09270400	0.41661800
H	-2.06120600	1.95502300	-0.65922700
H	-1.14146900	0.74114100	-1.57600600
H	-0.51743200	1.50138900	1.34652900
H	1.58270200	2.37930300	0.50069500
H	1.23435700	1.73055200	-1.17626400
H	-2.25614500	-1.62867500	1.07566900
H	-1.83888400	-1.79933500	-0.64633400
H	0.05544400	-0.75723300	1.54626800
H	0.36510300	-1.98602800	-1.25367500
H	2.63746100	-1.18541400	-1.28047400
H	3.42491200	0.53649600	0.26948000
H	2.06339200	0.17490700	1.42928500

S29

C	-0.28846700	0.71139200	0.39055800
C	-0.20196000	-0.68086900	-0.24995400
C	-1.61601200	-1.19409500	0.00711100
O	-2.46057900	-0.03304700	-0.10104400
C	-1.65868500	1.15954700	-0.12169500
C	0.95745000	1.50584500	0.11236900
C	2.11884000	0.88069400	-0.12077400
C	2.29450300	-0.62438000	-0.16098000
C	1.03228700	-1.42081300	0.25505100
H	-0.38821800	0.57673100	1.48139300
H	-0.09216600	-0.53148600	-1.33528900
H	-1.95280400	-1.93937600	-0.72291600
H	-1.71314700	-1.63069700	1.01394600
H	-2.14510600	1.91120300	0.51020400
H	-1.59389800	1.55753900	-1.14684100
H	0.91526400	2.59382700	0.14207100
H	3.01629700	1.47035300	-0.30608600
H	3.14449200	-0.90974200	0.47461300
H	2.59078900	-0.91082000	-1.18231100
H	1.09072100	-2.44263200	-0.14006600
H	0.98466800	-1.50444700	1.34951300

S30

C	-1.78733900	-0.11168000	0.47821000
O	-1.37097200	0.88157300	-0.44941300
C	-0.10730600	1.45109600	-0.11733300
C	1.04237200	0.49976100	-0.29887400
C	1.96392800	0.23987900	0.64234200
C	3.13778300	-0.62840400	0.48628200
C	3.78524100	-0.87709200	-0.66032400
H	-1.84297700	0.31646500	1.49482700
H	-1.05882900	-0.93658700	0.52246000
H	-0.00773900	2.30312500	-0.80101200
H	-0.11783300	1.84681200	0.91246000
H	1.10200300	0.01249100	-1.27222200
H	1.84029400	0.69805300	1.62549900
H	3.50881700	-1.08636700	1.40352100
H	4.63519700	-1.55229300	-0.69492000
H	3.49603500	-0.40760200	-1.59724000
C	-3.09798200	-0.62841700	0.08926800
C	-4.17881600	-1.07580600	-0.20626300
H	-5.13447300	-1.46270100	-0.47792200

S30-TS

O	2.32310600	-0.04823600	-0.33017100
C	1.75062200	1.03988700	0.38261300
C	1.56301700	-1.24435800	-0.13940000
C	0.11554500	-0.94593700	-0.38643400
C	-0.92788600	-1.34256400	0.42074000
C	-2.20102000	-0.73750500	0.33332000
C	-2.46082700	0.31371600	-0.52069100
H	2.32163800	1.92188300	0.07341900
H	1.89546400	0.90580900	1.46914300
H	1.97947100	-1.95913400	-0.85837700
H	1.71117400	-1.64558700	0.87719300
H	-0.09561900	-0.56546300	-1.38269600
H	-0.71158700	-1.95049300	1.29897000
H	-2.91331700	-0.94830600	1.12908100
H	-3.40305900	0.85134200	-0.44655800
H	-1.95465100	0.41473100	-1.47392100
C	0.30159400	1.23570900	0.13444500
C	-0.80116700	1.80007900	0.07980700
H	-1.45364000	2.64694300	0.12871400