

*Supplementary Information*

DFT Computational Insight into Pd(0)-Catalyzed Oxidative Cross-Couplings of 1,2-  
Allenyl Ketones and Aryl Boronic Acid: Pd(II)-Carbenoid Intermediate versus  $\pi$ -  
Allyl-Pd(II) Intermediate

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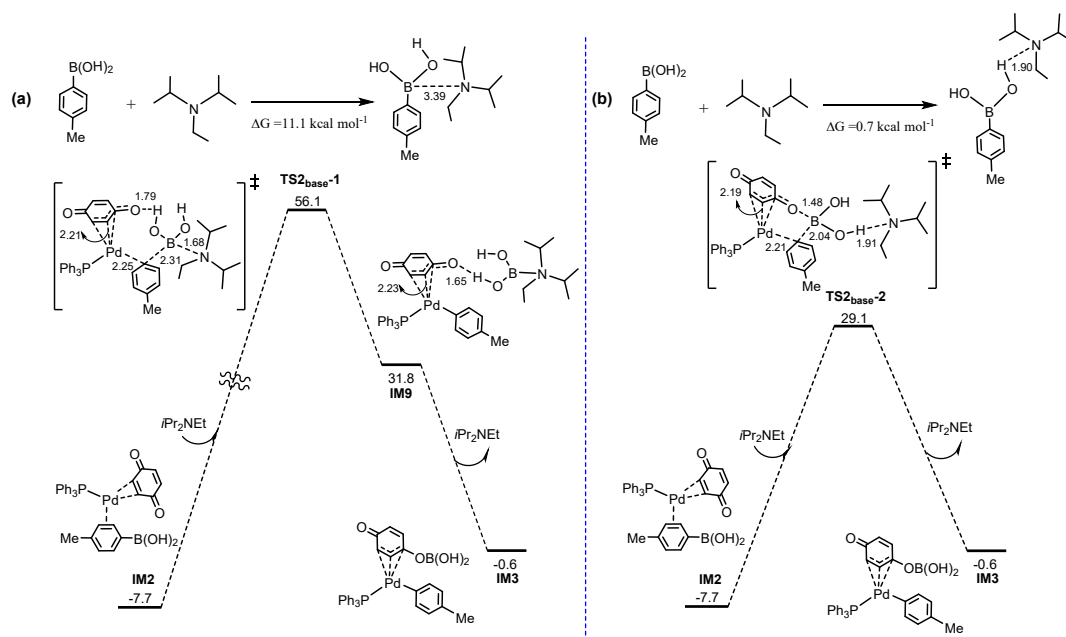
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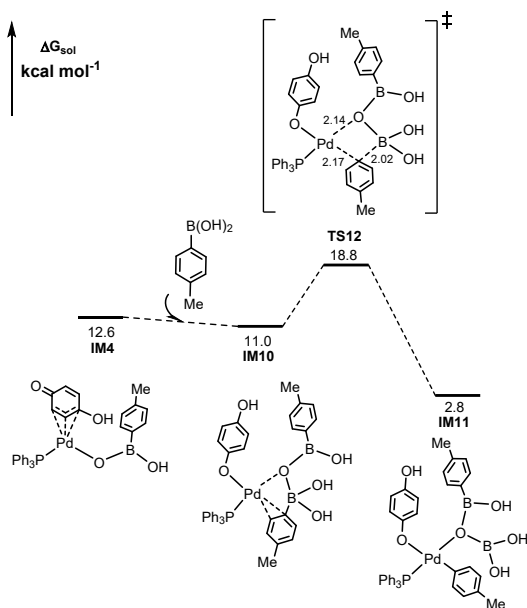
## 1. *iPr*<sub>2</sub>NEt assisted oxidative transmetalation



**Fig. S1** Calculated energy profile of *iPr*<sub>2</sub>NEt-assisted oxidative transmetalation processes. Selected bond distances are in Å.

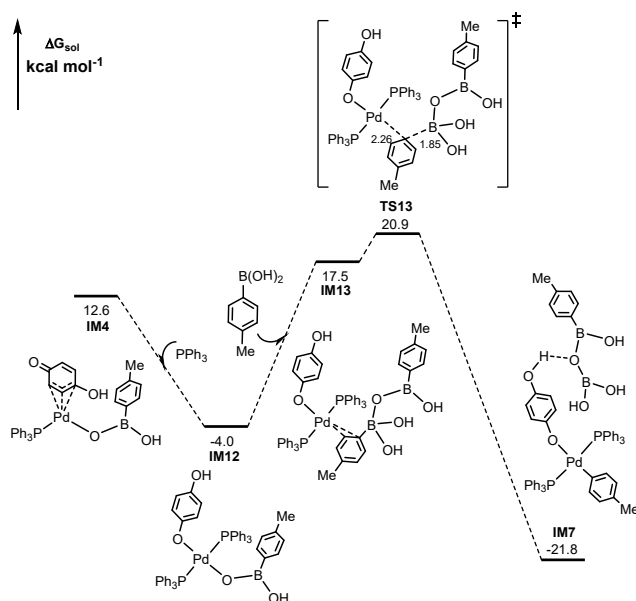
Fig. S1a describes the pathway where *iPr*<sub>2</sub>NEt assists the oxidative transmetalation by forming a hypothetical acid-base adduct with aryl boronic acid. The calculated results indicate that the expected adduct cannot be formed due to the steric effect of two *iPr* groups and in this way the transmetalation barrier is found to be as high as 71.9 kcal mol<sup>-1</sup>. Fig. S1b shows the pathway where *iPr*<sub>2</sub>NEt assists the reaction by forming an H-bond complex with aryl boronic acid. The calculated barrier of the transmetalation process is 2.0 kcal mol<sup>-1</sup> higher than that (42.9 kcal/mol) without the *iPr*<sub>2</sub>NEt (TS2 relative to A' in Fig. 1).

## 2. Other possible transmetalation processes



**Fig. S2** Calculated energy profile of transmetalation process followed by isomerization.

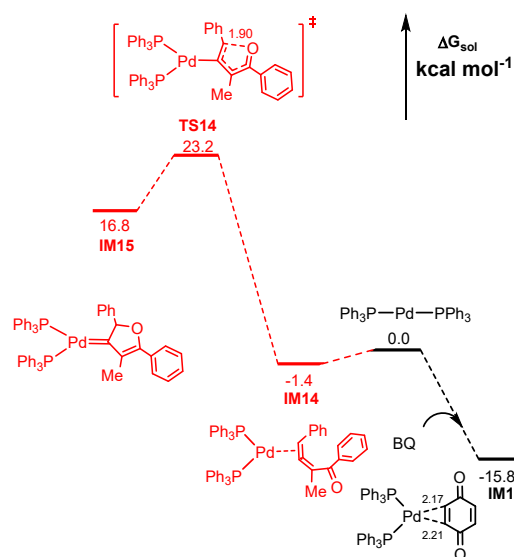
Selected bond distances are in Å.



**Fig. S3** Calculated energy profile of transmetalation process followed by isomerization

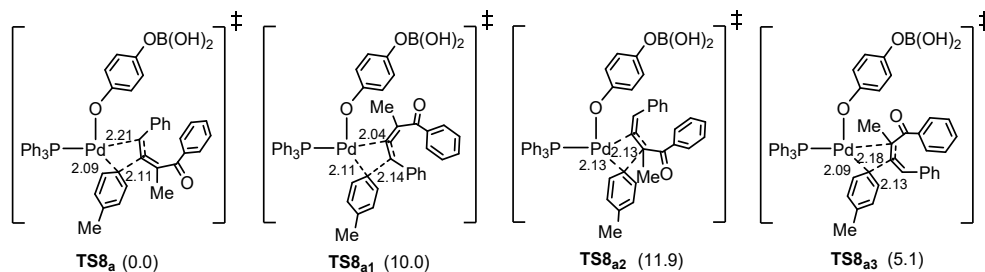
with the addition of a  $\text{PPh}_3$ . Selected bond distances are in Å.

### 3. Pd(0)-catalyzed nucleophilic cyclization



**Fig. S4** Calculated energy profiles of Pd(0)-catalyzed nucleophilic cyclization (red line) and the coordination of Pd(0) by BQ (black line). Selected bond distances are in Å.

### 4. Possible migratory insertions of the phenyl group to the 1,2-allenyl ketone



**Fig. S5** Calculated relative energies of several migratory-insertion transition states of the phenyl group to the allenyl ketone **1<sub>a</sub>**. The numbers in parenthesis are  $\Delta\Delta G^\ddagger$  (in kcal mol<sup>-1</sup>). Selected bond distances are in Å.



<b>IM1</b>	0.792392	0.84524	0.707391	-3028.619643	-3027.774403	-3027.912252	
<b>IM2</b>	0.517051	0.553588	0.447917	-1992.685919	-1992.132331	-1992.238002	
<b>TS2</b>	0.515092	0.550755	0.449699	-1992.632239	-1992.081484	-1992.18254	-371.71
<b>IM3</b>	0.51707	0.553353	0.449096	-1992.675749	-1992.122396	-1992.226653	
<b>TS3</b>	0.511452	0.547247	0.443588	-1992.648525	-1992.101278	-1992.204937	-544.45
<b>IM4</b>	0.515046	0.55141	0.446481	-1992.652107	-1992.100697	-1992.205626	
<b>IM5</b>	0.67161	0.717673	0.594921	-2440.098466	-2439.380793	-2439.503545	
<b>TS4</b>	0.670956	0.717188	0.59321	-2440.088152	-2439.370964	-2439.494942	-271.34
<b>IM6</b>	0.673439	0.719827	0.593837	-2440.121282	-2439.401455	-2439.527445	
<b>IM7</b>	0.947733	1.011748	0.846497	-3476.088788	-3475.07704	-3475.242291	
<b>TS5</b>	0.941263	1.005076	0.838009	-3476.029668	-3475.024592	-3475.191659	-1193.37
<b>B</b>	0.791754	0.844632	0.702903	-3028.642274	-3027.797642	-3027.939371	
<b>C<sub>a</sub></b>	0.773166	0.827158	0.681273	-2723.761103	-2722.933945	-2723.07983	
<b>TS6<sub>a</sub></b>	0.774259	0.827143	0.682959	-2723.744228	-2722.917085	-2723.061269	-100.70
<b>D<sub>a</sub></b>	0.776494	0.829193	0.684507	-2723.764737	-2722.935544	-2723.08023	
<b>TS7<sub>a</sub></b>	0.775896	0.827922	0.686321	-2723.747016	-2722.919094	-2723.060695	-300.06
<b>E<sub>a</sub></b>	0.777388	0.830131	0.683091	-2723.809943	-2722.979812	-2723.126852	
<b>TS8<sub>a</sub></b>	0.774438	0.827071	0.684532	-2723.747261	-2722.92019	-2723.062729	-262.41
<b>TS8<sub>r-1</sub></b>	0.774704	0.82722	0.686097	-2723.732952	-2722.905732	-2723.046855	-282.20
<b>TS8<sub>r-2</sub></b>	0.773792	0.826683	0.682693	-2723.726526	-2722.899843	-2723.043833	-258.34
<b>TS8<sub>r-3</sub></b>	0.774412	0.827002	0.685996	-2723.740533	-2722.913531	-2723.054537	-251.76
<b>G<sub>a</sub></b>	0.77747	0.830154	0.688611	-2723.818815	-2722.988661	-2723.130204	
<b>TS9<sub>a</sub></b>	0.775619	0.828033	0.686578	-2723.772169	-2722.944136	-2723.085591	-263.00
<b>TS10<sub>a</sub></b>	0.773268	0.825398	0.683812	-2723.784322	-2722.958924	-2723.10051	-412.98
<b>IM8</b>	0.6814	0.727626	0.59946	-2758.419013	-2757.691387	-2757.819553	
<b>F</b>	0.681079	0.72836	0.596104	-2758.410102	-2757.681742	-2757.813998	
<b>TS11</b>	0.678298	0.724598	0.59666	-2758.382545	-2757.657947	-2757.785885	-998.62
<b>TS2<sub>basic-1</sub></b>	0.783589	0.830491	0.707882	-2363.46111	-2362.630619	-2362.753228	-373.16
<b>IM9</b>	0.785073	0.832488	0.707662	-2363.499528	-2362.66704	-2362.791866	
<b>TS2<sub>basic-2</sub></b>	0.77961	0.828278	0.698456	-2363.494656	-2362.666378	-2362.7962	-357.14
<b>IM10</b>	0.670616	0.716549	0.592531	-2440.096083	-2439.379534	-2439.503552	
<b>TS12</b>	0.668913	0.715702	0.588411	-2440.079576	-2439.363874	-2439.491165	-198.42
<b>IM11</b>	0.671805	0.71864	0.591978	-2440.108562	-2439.389922	-2439.516584	
<b>IM12</b>	0.790768	0.845013	0.697845	-3028.616394	-3027.771381	-3027.918549	
<b>IM13</b>	0.946912	1.010085	0.851163	-3476.03075	-3475.020665	-3475.179587	
<b>TS13</b>	0.945214	1.008752	0.847891	-3476.02219	-3475.013438	-3475.174299	-156.48
<b>IM14</b>	0.808699	0.860996	0.721013	-2930.925966	-2930.06497	-2930.204953	
<b>TS14</b>	0.807387	0.859254	0.718451	-2930.884169	-2930.024915	-2930.165718	-430.30
<b>IM15</b>	0.809883	0.861539	0.721156	-2930.897146	-2930.035607	-2930.17599	
<b>TS15</b>	0.77239	0.824706	0.683864	-2723.731453	-2722.906747	-2723.047589	-807.65
<b>3<sub>a</sub></b>	0.367949	0.390002	0.316018	-1001.33305	-1000.943048	-1001.017032	
<b>3<sub>a</sub>'</b>	0.259584	0.275113	0.216498	-731.1054366	-730.8303236	-730.8889386	
<b>1<sub>b</sub></b>	0.147172	0.157681	0.111644	-460.8312447	-460.6735637	-460.7196007	
<b>C<sub>b</sub></b>	0.663839	0.711835	0.576778	-2453.527033	-2452.8152	-2452.95026	

<b>TS6<sub>b</sub></b>	0.663019	0.710257	0.577073	-2453.508192	-2452.797935	-2452.931119	-283.41
<b>D<sub>b</sub></b>	0.667958	0.714354	0.584937	-2453.537567	-2452.823213	-2452.95263	
<b>TS7<sub>b</sub></b>	0.666607	0.712715	0.582739	-2453.522015	-2452.8093	-2452.939276	-290.66
<b>E<sub>b</sub></b>	0.669708	0.71479	0.589664	-2453.587654	-2452.872864	-2452.99799	
<b>TS8<sub>b</sub></b>	0.66442	0.711217	0.580466	-2453.510861	-2452.799644	-2452.930395	-345.76
<b>G<sub>b</sub></b>	0.667675	0.714506	0.582264	-2453.600518	-2452.886012	-2453.018254	
<b>TS9<sub>b</sub></b>	0.666779	0.712798	0.585075	-2453.53761	-2452.824812	-2452.952535	-463.85
<b>TS10<sub>b</sub></b>	0.664006	0.709885	0.582178	-2453.558193	-2452.848308	-2452.976015	-570.84
<b>3<sub>b</sub></b>	0.258839	0.2737520	0.216663	-731.1002944	-730.8265424	-730.8836314	

## 7. Cartesian coordinates of all structures involved in this work

### PPh<sub>3</sub>

P	-0.00103600	-0.00127200	-1.27980700
C	0.36221100	1.60166800	-0.44680800
C	1.38325100	2.38096500	-1.00236600
C	-0.29728200	2.06821100	0.69362600
C	1.74930700	3.59092600	-0.42455700
H	1.89626200	2.02951500	-1.89942600
C	0.06111800	3.28564100	1.26591300
H	-1.09552600	1.47360600	1.13908700
C	1.08510700	4.04702000	0.71094700
H	2.54892500	4.18405300	-0.86605000
H	-0.46128200	3.63929200	2.15390200
H	1.36400300	4.99842600	1.16146800
C	-1.57120900	-0.48655100	-0.44694200
C	-2.75430800	0.02739200	-0.99000100
C	-1.64871400	-1.30908800	0.68007800
C	-3.98556600	-0.25863700	-0.41223300
H	-2.70449000	0.66171200	-1.87691300
C	-2.88287900	-1.60551500	1.25217700
H	-0.73668400	-1.71827700	1.11562300
C	-4.05163800	-1.07982600	0.71029500
H	-4.89697200	0.15289000	-0.84359500
H	-2.93012100	-2.24886100	2.12985600
H	-5.01537400	-1.31232600	1.16097700
C	1.20505200	-1.11817900	-0.44724900
C	1.97196900	-0.76587500	0.66636200
C	1.34068900	-2.40548500	-0.97996200
C	2.85255100	-1.68276500	1.23421000
H	1.87889600	0.23254000	1.09431100
C	2.20988900	-3.32526100	-0.40549500
H	0.75334700	-2.68652300	-1.85610500
C	2.97155200	-2.96286400	0.70248400
H	3.44651300	-1.39500500	2.10073600



H	2.30094400	-4.32450900	-0.82889300
H	3.66050600	-3.67811600	1.14926200
<b>BQ</b>			
C	-0.66937700	1.26411600	0.00028400
C	0.66931600	1.26402000	0.00014900
C	1.44135700	-0.00003800	0.00001100
C	0.66939200	-1.26413100	0.00029200
C	-0.66933600	-1.26402300	0.00006600
C	-1.44136100	0.00005000	-0.00001900
H	1.26189300	2.17767000	-0.00004300
O	-2.66020900	-0.00006000	-0.00033100
H	-1.26172900	2.17790300	0.00035300
O	2.66020800	0.00005400	-0.00036700
H	-1.26197800	-2.17764100	0.00003600
H	1.26187100	-2.17784100	0.00053400
<b>2</b>			
B	-2.21540100	0.00002100	0.00302600
O	-2.86285000	-1.20818200	0.00461400
H	-3.82447700	-1.15394800	0.00762200
O	-2.86280100	1.20824100	0.00528500
H	-3.82443000	1.15404400	0.00814600
C	-0.66055500	-0.00000600	-0.00072000
C	0.06458400	-1.19817500	-0.00445500
C	0.06466300	1.19814300	-0.00487600
C	1.45297100	-1.19933500	-0.01085300
H	-0.47660400	-2.14446000	-0.00640800
C	1.45301800	1.19926700	-0.01112500
H	-0.47651400	2.14443800	-0.00719900
C	2.16923400	-0.00006800	-0.01027500
H	1.99868600	-2.14433600	-0.01790700
H	1.99876000	2.14426400	-0.01809400
C	3.66854400	0.00002000	0.01670000
H	4.04801300	0.00610300	1.04874700
H	4.08194600	-0.89092000	-0.47264000
H	4.08208600	0.88516100	-0.48297300
<b>1<sub>a</sub></b>			
C	-0.69341100	1.90532300	-0.49493300
C	0.26774100	1.10521900	-0.90085600
C	1.24913600	0.32270400	-1.28172100
H	1.21381200	-0.08589600	-2.29700500
C	-1.87598000	1.39212900	0.26979500

O	-2.46126700	2.15401000	1.02254500
C	2.40459700	-0.07735100	-0.47046000
C	3.33884100	-0.96771100	-1.00791000
C	2.60311100	0.40519400	0.82912700
C	4.44404800	-1.37037200	-0.26726100
H	3.19053000	-1.34745700	-2.01940500
C	3.70640700	0.00349800	1.56712400
H	1.88014400	1.10173400	1.25393000
C	4.63141600	-0.88624300	1.02284700
H	5.16141600	-2.06583600	-0.70007200
H	3.84819500	0.38808500	2.57593700
H	5.49686700	-1.19847300	1.60480300
C	-2.31735300	-0.02271800	0.12810200
C	-2.11719500	-0.77532400	-1.03258500
C	-3.02899500	-0.58431900	1.19316500
C	-2.60584500	-2.07374600	-1.11754200
H	-1.60184300	-0.33222300	-1.88223500
C	-3.49973000	-1.88651200	1.11508500
H	-3.20100600	0.02725800	2.07679500
C	-3.28766500	-2.63391200	-0.04180000
H	-2.45667800	-2.64924000	-2.02951700
H	-4.03943700	-2.32180900	1.95434300
H	-3.66319400	-3.65393500	-0.10781200
C	-0.60854400	3.40199800	-0.62230600
H	-0.60792800	3.86121000	0.37331300
H	0.29434100	3.70292000	-1.16244500
H	-1.48857000	3.79444700	-1.14821900

***i*Pr<sub>2</sub>NEt**

N	0.01610600	0.26094400	0.11917000
C	0.45761800	1.37461500	-0.69969700
C	0.20863700	2.71476500	-0.02680700
H	-0.01165400	1.35912800	-1.70553100
H	1.53675300	1.27374400	-0.87863700
H	0.54369000	3.54814600	-0.65862400
H	-0.85709100	2.87050600	0.18853700
H	0.74806900	2.75702400	0.92841300
C	-1.41606500	-0.01601200	0.04475100
C	-1.94281000	-0.54727000	1.37162000
C	-1.83679600	-0.91966700	-1.11455300
H	-1.89194900	0.96546700	-0.11731800
H	-1.64828900	0.11858500	2.19205300
H	-3.03813300	-0.62645800	1.35411200
H	-1.55025400	-1.55025200	1.59158200

H	-1.47444400	-0.53594000	-2.07834900
H	-1.44785200	-1.93996400	-0.98453900
H	-2.93135300	-0.99256000	-1.17438000
C	0.92139700	-0.88284000	0.22294600
C	2.01384000	-0.58044700	1.24149500
C	1.53020400	-1.37107200	-1.09408000
H	0.31883500	-1.71223400	0.62556900
H	1.56872300	-0.33547800	2.21391800
H	2.69683900	-1.43211800	1.36708600
H	2.61737700	0.28306000	0.92343100
H	0.76559400	-1.54922900	-1.86029600
H	2.25145900	-0.64878700	-1.50122000
H	2.07478100	-2.31167900	-0.93405800

**Pd(PPh<sub>3</sub>)<sub>2</sub>**

Pd	0.00215800	0.01107600	0.57829300
P	-2.29020400	-0.01608800	0.21694600
P	2.29238400	0.01574900	0.21301000
C	2.90691800	1.57661300	-0.53314800
C	2.33391100	2.77000000	-0.08140800
C	3.91343000	1.62833800	-1.50138400
C	2.77376100	3.99415600	-0.57200100
H	1.52795600	2.72456500	0.65400900
C	4.34548100	2.85408300	-1.99997600
H	4.35915600	0.70348600	-1.87008300
C	3.77996400	4.03702800	-1.53344900
H	2.32360000	4.91722300	-0.20973500
H	5.12755000	2.88502200	-2.75730400
H	4.12046100	4.99444300	-1.92516500
C	2.78976500	-1.25309300	-1.01958600
C	3.98791900	-1.96848100	-0.95910000
C	1.90028700	-1.50194800	-2.07117500
C	4.28905100	-2.91635000	-1.93426100
H	4.68826500	-1.78809800	-0.14289000
C	2.20595500	-2.44125800	-3.04816000
H	0.95439200	-0.95618100	-2.10521400
C	3.40135800	-3.15319200	-2.97869900
H	5.22292800	-3.47371900	-1.87521200
H	1.50354400	-2.62346000	-3.86048900
H	3.63799200	-3.89803400	-3.73713500
C	3.47096300	-0.27184400	1.59036800
C	3.08347100	-1.18337300	2.57808600
C	4.71767900	0.35116800	1.69023300
C	3.93325300	-1.48113700	3.63663700

H	2.09953000	-1.65159600	2.50978800
C	5.56372500	0.05980300	2.75635000
H	5.02726400	1.07085700	0.93128800
C	5.17490000	-0.85747100	3.72792800
H	3.62097300	-2.19328900	4.39894000
H	6.53187900	0.55339900	2.82920900
H	5.83779900	-1.08207200	4.56217100
C	-3.03239000	1.61876100	-0.17376800
C	-2.23424500	2.53240600	-0.87097600
C	-4.33898600	1.97803900	0.16680500
C	-2.74042700	3.77310400	-1.23976200
H	-1.20439200	2.25863300	-1.11326000
C	-4.84110300	3.22536800	-0.19416800
H	-4.96795000	1.27982700	0.72021100
C	-4.04542900	4.12150700	-0.90072200
H	-2.11112500	4.47417200	-1.78599600
H	-5.85991400	3.49727500	0.07856800
H	-4.44039900	5.09650400	-1.18244200
C	-3.42888500	-0.67666200	1.49667200
C	-4.57275600	-1.42695600	1.21276500
C	-3.12453100	-0.37549300	2.82813400
C	-5.40226200	-1.85846300	2.24403000
H	-4.81571600	-1.67572400	0.17917100
C	-3.95913300	-0.79747800	3.85623600
H	-2.21730400	0.18967700	3.05049400
C	-5.09940800	-1.54138800	3.56459500
H	-6.28977600	-2.44603100	2.01303600
H	-3.71388100	-0.55455000	4.88902600
H	-5.74982900	-1.88086600	4.36933300
C	-2.70386600	-1.00870600	-1.27414100
C	-1.89893000	-2.11893100	-1.55079300
C	-3.76683700	-0.71050200	-2.13142100
C	-2.15733400	-2.92237700	-2.65588400
H	-1.05198100	-2.33328000	-0.89475100
C	-4.02273900	-1.51271800	-3.23965600
H	-4.39521700	0.15897800	-1.93435700
C	-3.22017500	-2.61903800	-3.50259400
H	-1.52019100	-3.78181300	-2.86105500
H	-4.85127400	-1.26914600	-3.90325400
H	-3.42042000	-3.24170500	-4.37334300
A			
P	-1.86001000	0.28360500	-0.11395600
Pd	0.02517400	-1.12487900	-0.67048900

P	1.91163400	0.22805700	-0.04309100
C	1.56491700	1.28556400	1.41511400
C	1.10357600	0.61996300	2.55834000
C	1.70708000	2.67226700	1.45596900
C	0.79392600	1.32175400	3.71546600
H	0.99447500	-0.46667100	2.53924300
C	1.39128200	3.37708900	2.61533900
H	2.04888100	3.21454300	0.57509300
C	0.93800000	2.70707300	3.74587600
H	0.43198400	0.78581000	4.59187300
H	1.49246500	4.46170600	2.62587000
H	0.68991200	3.26297800	4.64874900
C	2.46762300	1.35751200	-1.37774600
C	3.56613700	2.21057000	-1.22505600
C	1.80292900	1.32013100	-2.60538000
C	3.95763700	3.04450600	-2.26552200
H	4.12453700	2.21255300	-0.28781900
C	2.19892200	2.14923200	-3.65139400
H	0.97242900	0.62114100	-2.73410400
C	3.27008200	3.01920000	-3.47726500
H	4.80977300	3.70975800	-2.13585900
H	1.67415600	2.10918800	-4.60460700
H	3.58228100	3.66894800	-4.29340800
C	3.50441500	-0.55535100	0.42972700
C	4.01578400	-1.52870600	-0.43217200
C	4.23043900	-0.20329200	1.57195700
C	5.23011400	-2.14549100	-0.15713100
H	3.44951600	-1.82854200	-1.31407100
C	5.44855100	-0.81864100	1.84179100
H	3.84536200	0.55500700	2.25345700
C	5.94939200	-1.78959600	0.97955500
H	5.59956700	-2.91964100	-0.82711400
H	6.00881100	-0.53742100	2.73252500
H	6.89908200	-2.27556600	1.19849600
C	-2.66175200	-0.20738800	1.45777900
C	-3.92700500	0.25810700	1.83190100
C	-1.98534600	-1.09007400	2.30069500
C	-4.48793700	-0.13492900	3.04122900
H	-4.47691100	0.92632100	1.16728700
C	-2.54731100	-1.48835100	3.50904000
H	-1.01684200	-1.47934000	1.98029800
C	-3.79717900	-1.00552700	3.88184800
H	-5.47289600	0.23131100	3.32635700
H	-2.01325900	-2.18467800	4.15392400

H	-4.24297200	-1.31852600	4.82475200
C	-1.51690500	2.07664500	0.07297500
C	-0.85913300	2.70419300	-0.99135400
C	-1.87089800	2.83645000	1.18807800
C	-0.56782700	4.06113700	-0.95080400
H	-0.57755200	2.11921600	-1.86802800
C	-1.57858800	4.19787500	1.23025000
H	-2.37314300	2.36454400	2.03200700
C	-0.93136300	4.81336700	0.16460600
H	-0.05087300	4.52876800	-1.78854200
H	-1.85614900	4.77875800	2.10912600
H	-0.70483200	5.87794800	0.20361500
C	-3.28466700	0.29099900	-1.28198200
C	-3.84004200	-0.94827300	-1.62748000
C	-3.84214900	1.45879100	-1.80970500
C	-4.92672900	-1.00931200	-2.49146400
H	-3.44098900	-1.87500500	-1.20639500
C	-4.92604000	1.38922000	-2.68156500
H	-3.43582100	2.43235600	-1.53866500
C	-5.46825400	0.15679900	-3.02654300
H	-5.35284300	-1.97850100	-2.74587900
H	-5.34897000	2.30748200	-3.08692300
H	-6.31667200	0.10454600	-3.70732600
C	1.39949300	-3.78978200	-0.69522300
C	0.58490300	-3.02591100	-1.64542300
C	-0.81853500	-2.94961300	-1.50405800
C	-1.49061700	-3.59976900	-0.36802100
C	-0.61767100	-4.19456100	0.67550000
C	0.71230200	-4.27529400	0.52992100
H	1.06073900	-2.82710100	-2.60697200
H	-1.45638100	-2.70739400	-2.35544500
H	-1.14129700	-4.59796300	1.54289600
H	1.35567500	-4.75446500	1.26753900
O	-2.71159000	-3.67493200	-0.25926900
O	2.58122400	-4.05807600	-0.88570400

**TS1**

C	-0.00967300	-1.71936700	-3.30227500
C	-0.97315200	-0.74922500	-3.00419300
C	-0.72440700	0.66970000	-3.35883100
C	0.63361100	0.99349300	-3.76803700
C	1.60224500	0.03781500	-3.81260500
C	1.29550600	-1.33799000	-3.53985200
H	-2.01340800	-1.04685000	-2.89790400

O	2.23350500	-2.26077700	-3.36504900
H	-0.22810500	-2.77529800	-3.16897900
O	-1.62493500	1.52315500	-3.29263400
H	2.63592700	0.28477500	-4.04700100
H	0.83827200	2.03578500	-4.00823500
C	0.71128300	-4.50785300	0.34655600
C	0.81354500	-3.60823700	-0.71849400
C	1.60315200	-2.44372200	-0.66429300
C	2.29673900	-2.26201100	0.54905500
C	2.20328200	-3.14419000	1.61849900
C	1.40441500	-4.28950800	1.53634000
H	0.08454200	-5.39827300	0.25027700
H	0.26933200	-3.85867100	-1.63246700
H	2.97754400	-1.41300000	0.64558000
H	2.76974400	-2.95089000	2.53476800
B	3.09632400	-2.18178600	-2.21965700
O	3.67593800	-0.94550200	-1.98315500
H	4.37900800	-1.03462400	-1.32824200
O	3.86295800	-3.30430400	-1.95332600
H	3.33599000	-4.10428000	-2.06020800
Pd	-0.03738400	-0.64580500	-0.89985200
P	1.39668800	1.12057800	0.49562100
P	-2.18237300	-0.07815200	0.01800600
C	1.09263700	2.82672800	-0.11974700
C	1.86854700	3.92878200	0.26987100
C	0.08385900	3.01983700	-1.06057100
C	1.61219400	5.18902700	-0.25533200
H	2.68945600	3.79703500	0.97545500
C	-0.16477800	4.27779400	-1.60158100
H	-0.51418900	2.17705400	-1.39435100
C	0.59611800	5.36596700	-1.19499700
H	2.21933900	6.03748000	0.05749200
H	-0.94882000	4.37905500	-2.35140800
H	0.41232100	6.35352300	-1.61608600
C	3.23839200	1.14219900	0.55126800
C	3.96898200	0.73662000	1.67186100
C	3.92797800	1.53980900	-0.59923000
C	5.36068900	0.72761100	1.64104000
H	3.44914400	0.42165600	2.57723700
C	5.31667100	1.54827100	-0.62295400
H	3.36903700	1.82741100	-1.48970500
C	6.03729900	1.13617600	0.49623500
H	5.91722400	0.40715900	2.52041500
H	5.83847100	1.85974700	-1.52632100

H	7.12580200	1.13285300	0.47404100
C	0.99212700	1.18118100	2.29315200
C	0.89370300	2.36389700	3.03245500
C	0.77900300	-0.03875800	2.94387300
C	0.57059500	2.32609600	4.38489000
H	1.03705200	3.32720000	2.54473000
C	0.46737500	-0.07680300	4.29974400
H	0.85712200	-0.97156600	2.38381400
C	0.35328400	1.10660000	5.02168900
H	0.48655500	3.25717400	4.94432300
H	0.30800800	-1.03859600	4.78568900
H	0.09728900	1.08076100	6.07976700
C	-2.57186900	1.66722400	0.43971400
C	-2.11044400	2.20581900	1.64720200
C	-3.21312900	2.51540100	-0.47023100
C	-2.30089000	3.55106800	1.94256600
H	-1.60304400	1.57063300	2.37178900
C	-3.39903000	3.85989100	-0.17188700
H	-3.56418300	2.13887500	-1.42635000
C	-2.94508100	4.38353200	1.03405400
H	-1.93901300	3.94517900	2.89153900
H	-3.90040500	4.50223700	-0.89402900
H	-3.09140300	5.43765200	1.26380500
C	-2.28807000	-0.97299500	1.61324400
C	-1.55474400	-2.15426400	1.74984800
C	-3.16790900	-0.59551900	2.63476900
C	-1.68775700	-2.94094600	2.89046300
H	-0.87559900	-2.47369200	0.95568200
C	-3.29083000	-1.37645400	3.77782700
H	-3.76881200	0.30757700	2.53195100
C	-2.55233500	-2.55101900	3.90761800
H	-1.11100700	-3.86166700	2.97091800
H	-3.97615000	-1.07194200	4.56725700
H	-2.65772400	-3.16431500	4.80136900
C	-3.69510900	-0.69891200	-0.84459600
C	-4.48054400	-1.70833300	-0.27332000
C	-4.06961200	-0.19036900	-2.09885700
C	-5.61837900	-2.17592100	-0.92348600
H	-4.21343600	-2.13873000	0.68959600
C	-5.21387400	-0.65576000	-2.73719400
H	-3.44664700	0.55091200	-2.60241100
C	-5.99476700	-1.64698400	-2.15227200
H	-6.21375700	-2.96000100	-0.45836500
H	-5.48763900	-0.24243400	-3.70654300



H	-6.88764800	-2.01240200	-2.65687600
C	1.33769200	-5.26398800	2.67497200
H	0.47737100	-5.94023300	2.58075000
H	2.23871300	-5.89289000	2.71929600
H	1.26406200	-4.75083900	3.64449700

**IM1**

C	-0.00967300	-1.71936700	-3.30227500
C	-0.97315200	-0.74922500	-3.00419300
C	-0.72440700	0.66970000	-3.35883100
C	0.63361100	0.99349300	-3.76803700
C	1.60224500	0.03781500	-3.81260500
C	1.29550600	-1.33799000	-3.53985200
H	-2.01340800	-1.04685000	-2.89790400
O	2.23350500	-2.26077700	-3.36504900
H	-0.22810500	-2.77529800	-3.16897900
O	-1.62493500	1.52315500	-3.29263400
H	2.63592700	0.28477500	-4.04700100
H	0.83827200	2.03578500	-4.00823500
C	0.71128300	-4.50785300	0.34655600
C	0.81354500	-3.60823700	-0.71849400
C	1.60315200	-2.44372200	-0.66429300
C	2.29673900	-2.26201100	0.54905500
C	2.20328200	-3.14419000	1.61849900
C	1.40441500	-4.28950800	1.53634000
H	0.08454200	-5.39827300	0.25027700
H	0.26933200	-3.85867100	-1.63246700
H	2.97754400	-1.41300000	0.64558000
H	2.76974400	-2.95089000	2.53476800
B	3.09632400	-2.18178600	-2.21965700
O	3.67593800	-0.94550200	-1.98315500
H	4.37900800	-1.03462400	-1.32824200
O	3.86295800	-3.30430400	-1.95332600
H	3.33599000	-4.10428000	-2.06020800
Pd	-0.03738400	-0.64580500	-0.89985200
P	1.39668800	1.12057800	0.49562100
P	-2.18237300	-0.07815200	0.01800600
C	1.09263700	2.82672800	-0.11974700
C	1.86854700	3.92878200	0.26987100
C	0.08385900	3.01983700	-1.06057100
C	1.61219400	5.18902700	-0.25533200
H	2.68945600	3.79703500	0.97545500
C	-0.16477800	4.27779400	-1.60158100
H	-0.51418900	2.17705400	-1.39435100

C	0.59611800	5.36596700	-1.19499700
H	2.21933900	6.03748000	0.05749200
H	-0.94882000	4.37905500	-2.35140800
H	0.41232100	6.35352300	-1.61608600
C	3.23839200	1.14219900	0.55126800
C	3.96898200	0.73662000	1.67186100
C	3.92797800	1.53980900	-0.59923000
C	5.36068900	0.72761100	1.64104000
H	3.44914400	0.42165600	2.57723700
C	5.31667100	1.54827100	-0.62295400
H	3.36903700	1.82741100	-1.48970500
C	6.03729900	1.13617600	0.49623500
H	5.91722400	0.40715900	2.52041500
H	5.83847100	1.85974700	-1.52632100
H	7.12580200	1.13285300	0.47404100
C	0.99212700	1.18118100	2.29315200
C	0.89370300	2.36389700	3.03245500
C	0.77900300	-0.03875800	2.94387300
C	0.57059500	2.32609600	4.38489000
H	1.03705200	3.32720000	2.54473000
C	0.46737500	-0.07680300	4.29974400
H	0.85712200	-0.97156600	2.38381400
C	0.35328400	1.10660000	5.02168900
H	0.48655500	3.25717400	4.94432300
H	0.30800800	-1.03859600	4.78568900
H	0.09728900	1.08076100	6.07976700
C	-2.57186900	1.66722400	0.43971400
C	-2.11044400	2.20581900	1.64720200
C	-3.21312900	2.51540100	-0.47023100
C	-2.30089000	3.55106800	1.94256600
H	-1.60304400	1.57063300	2.37178900
C	-3.39903000	3.85989100	-0.17188700
H	-3.56418300	2.13887500	-1.42635000
C	-2.94508100	4.38353200	1.03405400
H	-1.93901300	3.94517900	2.89153900
H	-3.90040500	4.50223700	-0.89402900
H	-3.09140300	5.43765200	1.26380500
C	-2.28807000	-0.97299500	1.61324400
C	-1.55474400	-2.15426400	1.74984800
C	-3.16790900	-0.59551900	2.63476900
C	-1.68775700	-2.94094600	2.89046300
H	-0.87559900	-2.47369200	0.95568200
C	-3.29083000	-1.37645400	3.77782700
H	-3.76881200	0.30757700	2.53195100

C	-2.55233500	-2.55101900	3.90761800
H	-1.11100700	-3.86166700	2.97091800
H	-3.97615000	-1.07194200	4.56725700
H	-2.65772400	-3.16431500	4.80136900
C	-3.69510900	-0.69891200	-0.84459600
C	-4.48054400	-1.70833300	-0.27332000
C	-4.06961200	-0.19036900	-2.09885700
C	-5.61837900	-2.17592100	-0.92348600
H	-4.21343600	-2.13873000	0.68959600
C	-5.21387400	-0.65576000	-2.73719400
H	-3.44664700	0.55091200	-2.60241100
C	-5.99476700	-1.64698400	-2.15227200
H	-6.21375700	-2.96000100	-0.45836500
H	-5.48763900	-0.24243400	-3.70654300
H	-6.88764800	-2.01240200	-2.65687600
C	1.33769200	-5.26398800	2.67497200
H	0.47737100	-5.94023300	2.58075000
H	2.23871300	-5.89289000	2.71929600
H	1.26406200	-4.75083900	3.64449700

## IM2

C	2.51259100	-2.74100800	1.30724600
C	1.26996700	-3.23655100	1.23323800
C	0.45417000	-3.11915500	-0.00039500
C	1.02555900	-2.32038700	-1.10386900
C	2.34158500	-1.82406400	-1.02268300
C	3.15422700	-2.05523600	0.16102800
H	0.79746000	-3.77232600	2.05644800
O	4.34298400	-1.72424500	0.25164700
H	3.13472500	-2.84422400	2.19572100
O	-0.63520900	-3.67617100	-0.07451600
H	2.87223400	-1.48593500	-1.91318700
H	0.52979400	-2.43450000	-2.06910300
C	3.24333700	1.19983400	2.05847600
C	4.02688000	1.03790700	0.91191200
C	3.52812800	1.32321300	-0.35771500
C	2.20581400	1.80466400	-0.44745300
C	1.41883000	1.96795400	0.69923400
C	1.93577200	1.66074500	1.97374600
H	3.66607100	0.97532400	3.03895000
H	5.04607500	0.66852400	1.01834400
H	1.82438800	2.13149500	-1.41711000
H	0.44156600	2.44519900	0.62871600
B	4.34980600	1.04431200	-1.66428700

O	4.19654700	1.90506600	-2.71594300
H	4.71071800	1.58530000	-3.46973500
O	5.16000700	-0.03566600	-1.80018900
H	5.04546000	-0.67735100	-1.06493800
Pd	0.81317500	-0.28660100	-0.43539400
P	-1.51780700	0.17501000	-0.22425300
C	-2.69722800	-0.42574800	-1.49486900
C	-3.66512100	0.39141000	-2.08574500
C	-2.63641500	-1.78057000	-1.84462500
C	-4.55117100	-0.13426500	-3.02196200
H	-3.73289400	1.44395000	-1.81342500
C	-3.53029700	-2.30039100	-2.77326400
H	-1.90911300	-2.44350900	-1.36971100
C	-4.48473500	-1.47917300	-3.36812000
H	-5.29942600	0.51290400	-3.47708600
H	-3.48009800	-3.35680300	-3.03173600
H	-5.18027500	-1.88943200	-4.09870200
C	-1.88642800	1.96636500	-0.09873000
C	-2.35583000	2.56093700	1.07381500
C	-1.52080200	2.78435000	-1.17681500
C	-2.45628900	3.94780900	1.16730600
H	-2.63474500	1.93994000	1.92512200
C	-1.63649100	4.16515200	-1.08712500
H	-1.13099400	2.33085400	-2.09093900
C	-2.09925200	4.75073300	0.09041300
H	-2.81818100	4.39963500	2.08961000
H	-1.35223800	4.78823600	-1.93339100
H	-2.17579300	5.83386800	0.16730500
C	-2.19253400	-0.52190200	1.32804900
C	-3.56363000	-0.69822900	1.53630200
C	-1.29697000	-0.85265100	2.34783100
C	-4.02696300	-1.19186600	2.75059400
H	-4.26912300	-0.44977000	0.74227100
C	-1.76141600	-1.34167800	3.56472100
H	-0.22439100	-0.73121200	2.17218400
C	-3.12757500	-1.51196700	3.76508100
H	-5.09559600	-1.33148300	2.90561800
H	-1.05447100	-1.59747300	4.35247200
H	-3.49507000	-1.90165700	4.71309200
C	1.09027600	1.89755200	3.18816700
H	0.87606100	2.96830200	3.31821700
H	0.11573100	1.39327200	3.10589200
H	1.58159500	1.54121900	4.10170800

**TS2**

C	1.28047400	-3.14497700	1.15879000
C	-0.03575600	-3.41482500	1.27035000
C	-0.92940100	-3.36820800	0.09245300
C	-0.27604300	-3.07955800	-1.19047700
C	1.12670600	-3.00243400	-1.31462400
C	1.88354400	-2.80036100	-0.12744900
H	-0.50767900	-3.64208200	2.22515300
O	3.17461000	-2.49912600	-0.09947100
H	1.94944200	-3.13317000	2.01894900
O	-2.14396300	-3.53673900	0.20401800
H	1.62690300	-2.93244500	-2.27755700
H	-0.89867700	-3.16869900	-2.07927000
C	2.80282300	1.76668200	1.45659500
C	2.52885000	0.47359400	1.02153500
C	2.40210800	0.13925600	-0.34596200
C	2.55490400	1.21552300	-1.24902400
C	2.84110500	2.50365300	-0.83111100
C	2.95015300	2.80446100	0.53333500
H	2.89367600	1.98712900	2.52284200
H	2.42464600	-0.31893900	1.77029100
H	2.46888400	1.00677600	-2.31879400
H	2.96431700	3.30883000	-1.55987300
B	3.63917900	-1.39334100	-0.94272000
O	3.42611300	-1.53806100	-2.31787700
H	4.12860500	-1.06093800	-2.77523800
O	4.89932600	-0.92012100	-0.58618900
H	5.00775000	-0.91238300	0.37053500
Pd	0.53124800	-1.01197000	-0.60095000
P	-1.19885500	0.51025500	-0.11594200
C	-2.79013300	0.42378200	-1.02403900
C	-3.54338200	1.56841600	-1.30327400
C	-3.26732200	-0.82638800	-1.43732900
C	-4.75024300	1.46469100	-1.98758300
H	-3.18883500	2.54858100	-0.98683000
C	-4.48138600	-0.92473600	-2.10739200
H	-2.71433600	-1.73654500	-1.19981000
C	-5.22060000	0.21997500	-2.39141800
H	-5.32500600	2.36373200	-2.20441300
H	-4.84745400	-1.90378100	-2.41129000
H	-6.16623900	0.14076400	-2.92541800
C	-0.87600500	2.30649800	-0.03144600
C	-1.19158400	3.09447700	1.07868700
C	-0.34012800	2.91497000	-1.16996600

C	-0.96414900	4.46689800	1.05144700
H	-1.62178700	2.63393900	1.96760300
C	-0.13045100	4.28865400	-1.20287600
H	-0.08828000	2.30398600	-2.03808200
C	-0.43763700	5.06625600	-0.08930000
H	-1.21189100	5.07173600	1.92227400
H	0.28317400	4.75155400	-2.09778600
H	-0.26947100	6.14210700	-0.11232300
C	-1.58810900	-0.01462300	1.59703600
C	-2.68119000	-0.83488400	1.88499700
C	-0.65426300	0.25719000	2.60812200
C	-2.83905300	-1.36964000	3.16090500
H	-3.40641700	-1.08014400	1.11158000
C	-0.82429400	-0.26621400	3.88248200
H	0.21894900	0.87217200	2.38568000
C	-1.91655800	-1.08644700	4.16127500
H	-3.69007400	-2.01618000	3.36689100
H	-0.09614200	-0.04111000	4.66045400
H	-2.04414900	-1.50637900	5.15783300
C	3.18333900	4.21626400	0.97178800
H	4.06075100	4.65400700	0.47642600
H	2.31918800	4.84635200	0.70796800
H	3.33308100	4.28934700	2.05565300

### IM3

C	1.45779600	-2.81778400	1.21988300
C	0.17123100	-3.21544100	1.38295300
C	-0.75534400	-3.29783600	0.24705600
C	-0.16359900	-2.97770200	-1.05307000
C	1.21885300	-2.77148400	-1.22937100
C	1.99891600	-2.49821800	-0.08497300
H	-0.23479400	-3.45424400	2.36451600
O	3.33514800	-2.23968000	-0.08434500
H	2.13977500	-2.71249600	2.06336400
O	-1.95233400	-3.57597100	0.39191600
H	1.66149800	-2.69314600	-2.21887800
H	-0.79730600	-3.12732600	-1.92569800
C	3.45527300	1.68103000	1.49589400
C	2.37464800	0.82675000	1.26805000
C	1.85289900	0.65472900	-0.01653100
C	2.45526100	1.36180400	-1.06481200
C	3.52974100	2.21623700	-0.83180400
C	4.04915700	2.39081900	0.45340900
H	3.84527400	1.79938800	2.50935700

H	1.94409200	0.28356200	2.11260700
H	2.08816900	1.24003700	-2.08643200
H	3.98404800	2.75477200	-1.66682900
B	4.08034600	-1.63616700	-1.07406100
O	3.68544800	-1.64755800	-2.37749200
H	4.30344200	-1.13216500	-2.91062800
O	5.27238000	-1.07663200	-0.72778600
H	5.36233200	-1.02193800	0.23134900
Pd	0.46603600	-0.79466300	-0.42036800
P	-1.42187000	0.51592700	-0.07808900
C	-2.85705800	0.18306800	-1.16778600
C	-3.53735000	1.21917100	-1.81493700
C	-3.24759900	-1.14413200	-1.39937800
C	-4.59202200	0.93541200	-2.67758900
H	-3.24521100	2.25565900	-1.65168800
C	-4.31214400	-1.41632600	-2.25040600
H	-2.74529900	-1.97609400	-0.89821500
C	-4.98193100	-0.38051600	-2.89644400
H	-5.11004700	1.75139700	-3.17915400
H	-4.61409800	-2.44987000	-2.41111400
H	-5.80841800	-0.60073300	-3.57034800
C	-1.33380700	2.33633200	-0.03838900
C	-2.14407000	3.09248300	0.81416300
C	-0.51768200	2.98679300	-0.96591900
C	-2.12657000	4.48088300	0.74312900
H	-2.79461000	2.59216400	1.53150600
C	-0.50438000	4.37520700	-1.03798800
H	0.11410200	2.39786700	-1.62897700
C	-1.30702500	5.12270000	-0.18190600
H	-2.75832900	5.06505600	1.41027000
H	0.13957700	4.87320100	-1.76061600
H	-1.29457700	6.21013200	-0.23478200
C	-1.91452400	0.03523000	1.61694200
C	-2.97680200	-0.82653300	1.89008500
C	-1.07964600	0.45162700	2.66424500
C	-3.20191400	-1.26437200	3.19317000
H	-3.62836600	-1.17273000	1.09076700
C	-1.31507100	0.02088700	3.96180600
H	-0.24058000	1.11758100	2.45462500
C	-2.37586600	-0.84458800	4.22792900
H	-4.02755200	-1.94485700	3.39242300
H	-0.66627800	0.35658600	4.76940200
H	-2.55480300	-1.19130600	5.24448500
C	5.20584500	3.31613600	0.69321000

H	6.07715300	3.04254600	0.08199700
H	4.95312200	4.35515500	0.43880900
H	5.51992800	3.30277700	1.74437600
<b>TS3</b>			
C	0.52191700	3.75184200	1.26021300
C	1.21997300	3.01518100	2.14755800
C	2.33744300	2.15044500	1.70804600
C	2.59321100	2.11684100	0.24481500
C	2.01673300	3.08123300	-0.60794900
C	0.83362200	3.73280900	-0.17238000
H	1.00931100	3.02740200	3.21531400
O	0.03913100	4.36799700	-1.00612600
H	-0.32177300	4.37589200	1.55289400
O	3.00345500	1.50135600	2.50007400
H	2.33613400	3.21326600	-1.64122800
H	3.47507000	1.55061900	-0.05753000
Pd	0.60042700	1.39598800	-0.45365600
P	0.76753800	-0.92910600	-0.25993600
C	1.87881900	-1.65014500	-1.52227000
C	2.01244100	-3.03667100	-1.65620800
C	2.61347900	-0.80734400	-2.35820700
C	2.87520300	-3.56715300	-2.60628100
H	1.43321100	-3.70022700	-1.01292300
C	3.47665400	-1.34018500	-3.31150700
H	2.49166100	0.27343500	-2.26385800
C	3.60830900	-2.71895600	-3.43411200
H	2.97446900	-4.64674000	-2.70566400
H	4.04358100	-0.67643800	-3.96199000
H	4.28206800	-3.13693900	-4.18029600
C	-0.72039000	-1.98075400	-0.35252500
C	-0.93738400	-3.07868400	0.48397400
C	-1.66925600	-1.65474500	-1.32587300
C	-2.09382500	-3.84059800	0.34541100
H	-0.20737300	-3.33157100	1.25304400
C	-2.81740400	-2.42316600	-1.46764100
H	-1.50702200	-0.78345100	-1.96237900
C	-3.03279100	-3.51295900	-0.62833000
H	-2.26181500	-4.69296500	1.00231000
H	-3.55700400	-2.15651500	-2.22016500
H	-3.94200000	-4.10436100	-0.72837300
C	1.54287000	-1.33407100	1.34106500
C	2.87247400	-1.74494300	1.44139800
C	0.81456000	-1.07971600	2.51035100



C	3.45845200	-1.91726100	2.69221900
H	3.45711800	-1.92933500	0.54028500
C	1.39850900	-1.26716600	3.75523300
H	-0.21908600	-0.73378700	2.43994600
C	2.72395900	-1.68510900	3.84781400
H	4.49814800	-2.23271900	2.75959300
H	0.82198200	-1.07281600	4.65805400
H	3.18603700	-1.81810200	4.82440000
C	-3.20529300	-0.21150900	1.61223400
C	-2.58976700	0.71053600	0.77635500
C	-3.19196100	1.14495500	-0.41112200
C	-4.46267500	0.63621700	-0.70413800
C	-5.07663100	-0.30156700	0.11923700
C	-4.45090700	-0.75186700	1.28246800
H	-2.71572900	-0.53308100	2.53493400
H	-1.60495100	1.10585100	1.04876500
H	-4.97184500	0.97755700	-1.60555500
H	-6.05911500	-0.69909000	-0.14226800
C	-5.07789800	-1.80462100	2.14571800
H	-6.14602400	-1.92636900	1.92660200
H	-4.59486800	-2.78131300	1.98664400
H	-4.97598500	-1.56911100	3.21344100
B	-2.47410700	2.14125300	-1.39265100
O	-1.13264800	2.29550500	-1.45467600
H	-0.60045600	3.57358900	-1.39214700
O	-3.30335300	2.86769500	-2.22101600
H	-2.77326500	3.39653100	-2.83083700

#### IM4

C	0.74378600	3.70749700	1.22290900
C	1.33936100	2.94213000	2.16207600
C	2.40558700	1.98682200	1.79712500
C	2.72528200	1.90193500	0.34832700
C	2.28746300	2.90186700	-0.54613900
C	1.13290500	3.63390400	-0.18489700
H	1.07667300	2.99863300	3.21652700
O	0.46853100	4.37695300	-1.07481800
H	-0.06420200	4.39907700	1.45867400
O	2.98191300	1.30193600	2.62882900
H	2.67689700	2.99480800	-1.55943100
H	3.56566200	1.25383900	0.09736300
Pd	0.68935500	1.38619400	-0.43310300
P	0.67389200	-0.95117100	-0.26368000
C	1.76492900	-1.72413200	-1.51202900

C	1.82120200	-3.11566600	-1.64908700
C	2.56025700	-0.92223200	-2.33239600
C	2.66929800	-3.69180000	-2.58547000
H	1.19424400	-3.74727000	-1.01838400
C	3.40839500	-1.50105000	-3.27245600
H	2.49683500	0.16346300	-2.23776000
C	3.46422200	-2.88467400	-3.39715400
H	2.70890000	-4.77497900	-2.68691300
H	4.02229500	-0.86848200	-3.91136000
H	4.12610600	-3.33806000	-4.13316900
C	-0.86819200	-1.91780800	-0.39669600
C	-1.17632300	-2.97956600	0.45796500
C	-1.75797400	-1.57027900	-1.41708700
C	-2.37033800	-3.67631400	0.29872400
H	-0.48875900	-3.25411500	1.25792000
C	-2.94565200	-2.27261700	-1.57619400
H	-1.52437100	-0.72974800	-2.07267000
C	-3.25592000	-3.32072800	-0.71407900
H	-2.60924400	-4.50012100	0.96996100
H	-3.64342400	-1.98155300	-2.35920400
H	-4.19646400	-3.85780500	-0.82890500
C	1.39032300	-1.41714500	1.34839100
C	2.69186100	-1.90630800	1.46582700
C	0.65248800	-1.14701500	2.50850200
C	3.24038700	-2.14017100	2.72340800
H	3.28371200	-2.10441100	0.57227300
C	1.19952900	-1.39452600	3.75995600
H	-0.35811000	-0.74109600	2.42597300
C	2.49546600	-1.89233400	3.86909600
H	4.25804500	-2.51809400	2.80456600
H	0.61642000	-1.18606300	4.65531400
H	2.92861600	-2.07315300	4.85118500
C	-3.19927400	0.07256300	1.66461900
C	-2.51802100	0.92581400	0.80548800
C	-3.05792700	1.31116100	-0.42767100
C	-4.33986200	0.84034400	-0.73595600
C	-5.02047300	-0.02579100	0.11236900
C	-4.45185200	-0.44048900	1.31721200
H	-2.75558800	-0.21696700	2.62077200
H	-1.53071500	1.30127500	1.09636600
H	-4.80063700	1.15106100	-1.67375500
H	-6.00806000	-0.39978400	-0.16480500
C	-5.14027900	-1.43813000	2.19828100
H	-6.21645200	-1.48989400	1.99088200

H	-4.72561600	-2.44562000	2.03882600
H	-5.01014100	-1.20276200	3.26279400
B	-2.26369200	2.18724600	-1.46772700
O	-0.92408000	2.27542700	-1.53024300
H	-0.21052200	3.73751500	-1.48539700
O	-3.04890300	2.87266100	-2.37730800
H	-2.47594800	3.30927900	-3.02051300

**IM5**

C	4.55078900	-0.15727200	2.12104000
C	3.71505900	-1.26695800	2.03151100
C	3.09704600	-1.64138900	0.83210700
C	3.43652600	-0.88178800	-0.29442800
C	4.26230600	0.23743800	-0.21803000
C	4.81796200	0.63272300	0.99941900
H	5.00137600	0.11162700	3.07973200
H	3.52982100	-1.85802600	2.93171900
H	3.05893200	-1.19118400	-1.26957700
H	4.48670900	0.81427900	-1.11859000
Pd	0.34685600	-0.48788000	-1.04100000
P	-0.40158400	1.42597100	0.07947100
C	-2.13752900	1.91499300	-0.16119100
C	-2.54866900	3.24736600	-0.01721500
C	-3.08157300	0.92973800	-0.45777800
C	-3.88672600	3.58362400	-0.17231800
H	-1.81560900	4.02085500	0.21494400
C	-4.42032000	1.27339900	-0.61998400
H	-2.77258600	-0.11291200	-0.55122800
C	-4.82198200	2.59600400	-0.47851700
H	-4.20176400	4.61945000	-0.05859700
H	-5.14688900	0.49918800	-0.86177100
H	-5.86898900	2.86384200	-0.61179200
C	0.58505100	2.83193300	-0.55450000
C	1.79099600	3.19714500	0.04968000
C	0.19801200	3.46135500	-1.74533500
C	2.59558600	4.17512100	-0.52643300
H	2.10719400	2.71920100	0.97632900
C	1.00184800	4.44329900	-2.31231000
H	-0.74321700	3.18706500	-2.22552800
C	2.20440400	4.79920900	-1.70613400
H	3.53167800	4.45142500	-0.04307400
H	0.68647200	4.93311900	-3.23207100
H	2.83491500	5.56549000	-2.15375500
C	-0.11981100	1.40413600	1.87983800

C	1.06101000	0.81581000	2.34432100
C	-1.05476800	1.89493600	2.79451700
C	1.30716200	0.72894100	3.70915400
H	1.78090800	0.39692800	1.63929400
C	-0.80789800	1.79547900	4.16022300
H	-1.98732500	2.33375400	2.44207500
C	0.37042900	1.21306800	4.61834500
H	2.23270800	0.27035200	4.05468400
H	-1.54296700	2.17236000	4.86978100
H	0.55632700	1.13222400	5.68812300
C	5.68808000	1.85106500	1.10152100
H	5.35878000	2.51426900	1.91424500
H	6.73513300	1.59006400	1.31103400
H	5.67365200	2.43157100	0.16981000
O	1.90005300	-3.64201600	1.93721000
B	1.97650100	-2.81131900	0.77209400
O	0.62725300	-2.13874500	0.52705600
O	2.16479300	-3.75135900	-0.39524500
H	2.88302100	-4.35714900	-0.16861200
H	1.75424000	-3.10158900	2.72092900
C	-1.49665000	-1.73370000	-3.07131900
C	-1.33668500	-0.27322100	-3.21653500
C	0.05665400	0.23546900	-3.07064200
C	1.15372600	-0.64617900	-3.16208600
C	0.93715800	-2.00117200	-2.86731700
C	-0.42585400	-2.53640100	-2.88193800
H	-2.51078700	-2.12380300	-3.12995300
H	0.19296300	1.30118700	-3.25299800
H	2.17487600	-0.28769100	-3.27933300
H	-0.53405200	-3.60989200	-2.73182900
O	-2.27893400	0.48172200	-3.41112200
O	1.98541100	-2.81781100	-2.81052100
H	2.03805600	-3.30257500	-1.92440300
B	-0.51003000	-2.92537800	0.43497300
O	-0.48347300	-4.18249900	-0.08405100
H	0.45198800	-4.41684000	-0.25522700
C	-1.89452900	-2.36047200	0.90318500
C	-3.09334100	-2.82223100	0.34556300
C	-1.98498800	-1.41438500	1.93245200
C	-4.32482800	-2.33816100	0.77477600
H	-3.05384500	-3.58703100	-0.43125300
C	-3.21365700	-0.94068600	2.37521700
H	-1.06901600	-1.05663800	2.40557800
C	-4.40387200	-1.38647700	1.79442600

H	-5.24633300	-2.70957200	0.32246300
H	-3.25292900	-0.20490700	3.18196100
C	-5.72357000	-0.83379100	2.24151000
H	-6.56178900	-1.44348400	1.88191700
H	-5.79001700	-0.77933200	3.33611500
H	-5.87174600	0.18860400	1.86205800

**TS4**

C	-3.25356700	-1.37536300	2.16379200
C	-2.13734600	-1.47679600	1.34665200
C	-2.19911500	-1.31343300	-0.05513100
C	-3.48417600	-1.04204400	-0.57169400
C	-4.61057900	-0.92655700	0.24207700
C	-4.51233400	-1.07892300	1.62485700
H	-3.15359100	-1.52247500	3.24146800
H	-1.18422500	-1.73712300	1.80833200
H	-3.62214000	-0.95837300	-1.65123800
H	-5.58673400	-0.72356900	-0.20331600
Pd	-0.72981000	-0.02236700	-1.08259900
P	0.37652200	1.00691800	0.76001300
C	-0.52149500	2.57136200	1.06698100
C	0.11724000	3.71366300	1.55552600
C	-1.90575200	2.58876600	0.86657000
C	-0.61852200	4.86231600	1.82725400
H	1.19466000	3.70538800	1.71865000
C	-2.63902800	3.73641300	1.14749300
H	-2.40736100	1.69190300	0.49444600
C	-1.99474400	4.87547000	1.62248900
H	-0.11291700	5.75219700	2.19845400
H	-3.71622900	3.74179000	0.98960500
H	-2.56736000	5.77709600	1.83429900
C	2.12404000	1.52814500	0.52121800
C	3.16921300	1.09843300	1.34293200
C	2.40806400	2.41360900	-0.52808300
C	4.47093400	1.53648000	1.11595400
H	2.98150000	0.41923300	2.17080100
C	3.70821600	2.85259500	-0.74527700
H	1.61353000	2.79424200	-1.17108300
C	4.74545400	2.41438100	0.07432600
H	5.27294000	1.18472200	1.76412200
H	3.90482400	3.55064700	-1.55741900
H	5.76355700	2.76469900	-0.09333400
C	0.37737100	0.19395300	2.40067300
C	1.06118700	-1.01875700	2.54658600

C	-0.37216700	0.68262000	3.47299900
C	1.00207200	-1.72915600	3.73840800
H	1.63454600	-1.42720700	1.71435700
C	-0.42963400	-0.03059600	4.66758200
H	-0.92268600	1.61779300	3.37897700
C	0.25095800	-1.23650800	4.80288100
H	1.52720600	-2.67971800	3.81698600
H	-1.01684400	0.36013500	5.49736700
H	0.19410600	-1.79370100	5.73664500
C	-5.70964900	-0.93633700	2.51420100
H	-6.64202900	-0.91072300	1.93716200
H	-5.77831600	-1.76300600	3.23398100
H	-5.66021200	-0.00903500	3.10274600
O	-1.91338500	-3.02208700	-2.30354700
B	-1.28916500	-2.97914000	-1.01898600
O	0.09032800	-2.77706600	-1.09322500
O	-1.73390400	-3.98664600	-0.11261700
H	-2.55955800	-3.74671200	0.32307700
H	-2.67526800	-3.61145400	-2.23644100
C	-1.88151400	2.42901300	-3.08533100
C	-0.43541300	2.39097800	-2.79384300
C	0.19623500	1.05870300	-2.78752300
C	-0.50931900	-0.06941900	-3.28949300
C	-1.90045800	0.01783700	-3.42944100
C	-2.56673800	1.30695600	-3.36954100
H	-2.35061100	3.41053300	-3.06146100
H	1.28634600	1.04803700	-2.76650600
H	-0.00298700	-1.00649400	-3.52348600
H	-3.63618300	1.30799600	-3.57700800
O	0.18005900	3.43218800	-2.57263500
O	-2.67854700	-1.00188200	-3.77039700
H	-2.28036800	-1.84661700	-3.41586000
B	1.04458000	-3.10911800	-0.17028500
O	0.78585800	-3.89168600	0.91546400
H	-0.14627900	-4.18096200	0.87292900
C	2.48624300	-2.52586600	-0.34661500
C	3.54529700	-2.92195400	0.47932200
C	2.75290900	-1.54473700	-1.31140800
C	4.81426700	-2.37032200	0.33951400
H	3.36226400	-3.67409500	1.24845800
C	4.01643300	-0.98950300	-1.45320000
H	1.93367600	-1.21111600	-1.95015100
C	5.07076600	-1.40167400	-0.63282000
H	5.62671900	-2.69471600	0.99211400

H	4.19452500	-0.21239900	-2.19967900
C	6.43705700	-0.80659900	-0.79640500
H	6.92010400	-1.15378900	-1.72072300
H	6.38397800	0.29018200	-0.85270200
H	7.09606700	-1.07236000	0.03988000

**IM6**

C	-3.98084300	-0.52901100	1.48816700
C	-2.67007700	-0.40199500	1.01478500
C	-2.38213500	0.23020100	-0.19809800
C	-3.47929300	0.74499700	-0.91029500
C	-4.78473700	0.61615000	-0.44373400
C	-5.06359900	-0.02207900	0.76875100
H	-4.15543000	-1.00432600	2.45950500
H	-1.86807300	-0.82591300	1.62265800
H	-3.32456200	1.24588800	-1.86746900
H	-5.60916700	1.02534800	-1.03198700
Pd	-0.52472100	0.19351200	-1.11147400
P	0.59665300	1.30270100	0.60621700
C	0.42028600	3.11066700	0.39721600
C	1.24224400	4.00230900	1.09485900
C	-0.56192800	3.60878900	-0.46196600
C	1.07798900	5.37253600	0.93708900
H	2.01756200	3.61827200	1.75910100
C	-0.72439800	4.98232000	-0.61758400
H	-1.19642900	2.90954200	-1.01030400
C	0.09474000	5.86297200	0.08040100
H	1.72283000	6.06140000	1.48019500
H	-1.48908400	5.36388900	-1.29199200
H	-0.02836500	6.93744100	-0.04630100
C	2.40969400	1.05954900	0.73933300
C	3.07504800	0.91969400	1.96141400
C	3.15249400	1.08924300	-0.44566400
C	4.46131100	0.79730900	1.99433900
H	2.51241400	0.90450300	2.89393700
C	4.53705000	0.97657300	-0.40508100
H	2.67037800	1.22680600	-1.41508900
C	5.19438100	0.82571500	0.81283600
H	4.96778600	0.68539000	2.95229000
H	5.09783800	1.01016400	-1.33823400
H	6.27971200	0.73332100	0.84105800
C	-0.02498400	0.95798200	2.28606200
C	0.21745300	-0.30790000	2.83183500
C	-0.85330500	1.84886100	2.97002900

C	-0.34729000	-0.67308000	4.04733700
H	0.83888400	-1.02565000	2.29322300
C	-1.42356000	1.47884000	4.18493300
H	-1.06544700	2.83086000	2.54791000
C	-1.17320400	0.22112700	4.72504900
H	-0.15441600	-1.66787100	4.44680500
H	-2.07177900	2.17869900	4.70982200
H	-1.62479300	-0.06406100	5.67405300
C	-6.46696000	-0.10941100	1.29189000
H	-7.18960600	-0.30893100	0.48943600
H	-6.57264700	-0.89967300	2.04644000
H	-6.77526500	0.83225000	1.76839400
O	-2.93516700	-2.88254300	-1.27758200
B	-2.25174200	-3.24809800	-0.13957500
O	-0.91423400	-3.46393700	-0.24287800
O	-2.88644300	-3.44623700	1.06804500
H	-3.69110500	-2.91872000	1.17546300
H	-3.84501300	-2.60857100	-1.10136000
C	-0.06749900	1.40089600	-3.98876600
C	1.16064300	0.82338900	-3.41926900
C	0.98711400	-0.45607300	-2.73022400
C	-0.21561800	-1.19294500	-2.83488200
C	-1.37496300	-0.53557400	-3.27843900
C	-1.25830600	0.76265200	-3.90561400
H	0.03430400	2.36443800	-4.48512800
H	1.88939900	-0.94962300	-2.37163600
H	-0.28469700	-2.22154000	-2.47641300
H	-2.17360500	1.18572700	-4.32036000
O	2.24604300	1.40780900	-3.50254900
O	-2.57743400	-1.12642100	-3.39013300
H	-2.60229300	-1.89797300	-2.78621900
B	0.00696300	-3.38278100	0.79833200
O	-0.37566600	-3.43375000	2.10159700
H	-1.34199300	-3.51543600	2.17869100
C	1.51276100	-3.16227800	0.47603700
C	2.42706900	-2.92607100	1.51236500
C	2.01041800	-3.14560200	-0.83344800
C	3.76666400	-2.66308500	1.25335600
H	2.07399000	-2.95004900	2.54461400
C	3.34928600	-2.89241000	-1.09619900
H	1.33249500	-3.34621300	-1.66391100
C	4.24971200	-2.64388700	-0.05577000
H	4.45603300	-2.47327700	2.07747700
H	3.71078800	-2.88577000	-2.12645300



C	5.69913300	-2.40477700	-0.34974300
H	6.18594800	-3.32237900	-0.70993300
H	5.82950400	-1.64486600	-1.13210600
H	6.24161400	-2.06968100	0.54275800

**IM7**

C	-2.64230400	-1.09260600	-0.75490400
C	-1.35821400	-0.82363100	-0.30436400
C	-0.94301600	-1.15007600	1.00293800
C	-1.90132100	-1.75895800	1.83824300
C	-3.19051000	-2.03023500	1.38824000
C	-3.56715600	-1.70433200	0.08719800
H	-0.63753900	-0.35849000	-0.97751100
O	-4.82550400	-1.94051900	-0.40981800
H	-2.95041200	-0.82023900	-1.76478500
O	0.26436700	-0.89734900	1.47542200
H	-3.91428500	-2.50108700	2.05909800
H	-1.60769300	-2.00936500	2.85854800
C	4.98799800	1.13345400	-2.37519400
C	3.81797100	0.62669000	-1.80998000
C	3.53114300	0.80634900	-0.45537100
C	4.46603700	1.50179500	0.31898500
C	5.63921400	1.99568200	-0.24400800
C	5.91830800	1.82605800	-1.60303900
H	5.18872900	0.96989300	-3.43601900
H	3.13885300	0.05451700	-2.44722500
H	4.28098100	1.66545100	1.38259200
H	6.35043700	2.53745900	0.38395500
B	-4.46950600	0.79728400	1.87229600
O	-3.53552100	1.55881100	1.22416600
H	-2.74433900	1.68720900	1.77025000
O	-4.30412100	0.51292000	3.20048400
H	-5.03054500	-0.04080500	3.50976100
Pd	1.86761800	0.04622400	0.41163500
P	2.64143500	-2.17621400	0.15304900
C	2.86618700	-3.18329500	1.66302000
C	3.74901300	-4.26862700	1.66426000
C	2.12751100	-2.88763800	2.81479500
C	3.89743700	-5.04673900	2.80677700
H	4.32556700	-4.50468000	0.77004300
C	2.28186400	-3.67369100	3.95268700
H	1.41364500	-2.06248100	2.78664000
C	3.16600300	-4.74827000	3.95250900
H	4.58677100	-5.88956900	2.80070800

H	1.70521300	-3.44171900	4.84689500
H	3.28436200	-5.35740500	4.84749400
C	4.19416100	-2.45218300	-0.76937400
C	4.27412600	-3.20343500	-1.94230600
C	5.34926200	-1.83997600	-0.26849900
C	5.48711200	-3.31915900	-2.61808400
H	3.38599200	-3.69900600	-2.33255700
C	6.55699000	-1.96150100	-0.93971300
H	5.29495100	-1.24219700	0.64199700
C	6.62585500	-2.69517600	-2.12251700
H	5.53814300	-3.90370100	-3.53544100
H	7.44445100	-1.46720100	-0.54769400
H	7.57110100	-2.78121200	-2.65629600
C	1.31381500	-2.98768800	-0.79877400
C	0.44314400	-3.89978800	-0.20123300
C	1.04726700	-2.53983900	-2.09959300
C	-0.67011300	-4.36250900	-0.89641200
H	0.61941400	-4.23035900	0.82220000
C	-0.05222600	-3.01907500	-2.79748200
H	1.69859000	-1.79605700	-2.56307900
C	-0.91837400	-3.92714200	-2.19243900
H	-1.35767800	-5.05322500	-0.41155500
H	-0.25008500	-2.66165000	-3.80690600
H	-1.79758300	-4.28113200	-2.72782400
C	-9.48815100	-0.90618000	-0.15561500
C	-8.24523400	-0.45961900	0.27796000
C	-7.29955400	0.05098100	-0.61797500
C	-7.65057600	0.09296100	-1.97288900
C	-8.89041900	-0.35205600	-2.41025600
C	-9.83131200	-0.85590100	-1.50742500
H	-10.20908500	-1.30193800	0.56218600
H	-7.99742100	-0.50339100	1.33940900
H	-6.92639100	0.47679900	-2.69128800
H	-9.14073900	-0.31579700	-3.47211800
C	-11.18068100	-1.30973600	-1.97947400
H	-11.88027300	-0.46563400	-2.06542000
H	-11.12419000	-1.78072000	-2.96938200
H	-11.62912200	-2.03201300	-1.28566000
B	-5.89562900	0.52856500	-0.13393900
O	-5.59745400	0.38282600	1.21625200
H	-5.41496100	-2.17721300	0.32075200
O	-5.04693900	1.12514100	-1.01063300
H	-4.19670800	1.32295500	-0.57949700
P	0.89706200	2.22448900	0.31781800

C	-0.19945200	2.72024300	1.69541600
C	-0.57617500	1.77255500	2.65392700
C	-0.68773300	4.03035900	1.78628400
C	-1.45161000	2.13335400	3.67913700
H	-0.20160400	0.74916400	2.56982100
C	-1.55965600	4.38189500	2.80985500
H	-0.38468300	4.77407800	1.04806500
C	-1.94678100	3.43220900	3.75352100
H	-1.77487100	1.38204600	4.39714800
H	-1.94490400	5.39840500	2.86786000
H	-2.64210700	3.70414600	4.54570600
C	2.04640200	3.64322300	0.19245200
C	2.43834200	4.18159400	-1.03378500
C	2.65072000	4.10776800	1.36599700
C	3.41939400	5.16687400	-1.08529400
H	1.98005100	3.82955400	-1.95711600
C	3.62480400	5.09667100	1.31266400
H	2.35611000	3.69006200	2.33013400
C	4.01489300	5.62488700	0.08471000
H	3.71711900	5.57932700	-2.04799500
H	4.08290100	5.45423400	2.23354800
H	4.78197700	6.39637500	0.04079700
C	-0.14772400	2.27752200	-1.18684600
C	0.41398100	1.80758700	-2.38195500
C	-1.49860000	2.63259300	-1.16550900
C	-0.35869700	1.70434100	-3.53173500
H	1.46115400	1.50264700	-2.40342300
C	-2.27280800	2.51776900	-2.31768200
H	-1.96953600	2.96927700	-0.24309900
C	-1.70671300	2.05215400	-3.49944500
H	0.09072200	1.33808600	-4.45368500
H	-3.33045100	2.77490900	-2.28407500
H	-2.31875700	1.95483100	-4.39432100
C	7.17552100	2.38261500	-2.20370000
H	7.34270500	1.99436400	-3.21624700
H	7.14044800	3.47950000	-2.27472100
H	8.05857800	2.13193100	-1.59984200

**TS5**

C	-2.33600500	-1.28079700	1.69141700
C	-1.22453200	-1.17539400	0.86910600
C	-1.28500700	-0.51185300	-0.37745900
C	-2.54539100	-0.00760000	-0.77020800
C	-3.66080400	-0.12061700	0.05086200

C	-3.55074000	-0.74014500	1.28942300
H	-0.26774700	-1.58809500	1.19334500
O	-4.64296800	-0.79194200	2.14886200
H	-2.26987900	-1.76757800	2.66515900
O	-0.24117400	-0.38751900	-1.17179800
H	-4.62088500	0.29424500	-0.26705000
H	-2.62428300	0.48565900	-1.73893900
C	5.47335000	1.38288800	1.30997200
C	4.16510000	0.93021600	1.12830800
C	3.63564000	0.76727800	-0.15063500
C	4.45683800	1.06263400	-1.24428000
C	5.76266300	1.50139300	-1.06001900
C	6.29304900	1.67232500	0.22205000
H	5.86557900	1.50632200	2.32138400
H	3.56605900	0.69502700	2.01100900
H	4.07913700	0.93007600	-2.26082600
H	6.38914700	1.71276700	-1.92972800
B	-5.49399000	-2.12705000	2.24491600
O	-5.06532800	-3.19325200	1.43875200
H	-4.69749700	-3.88540000	2.00013300
O	-5.76777600	-2.45053800	3.56826100
H	-5.78958000	-1.66224300	4.12081200
Pd	1.74577000	0.14193900	-0.52959900
P	0.96305000	2.31096400	0.06266800
C	-0.10136700	3.17343500	-1.14552600
C	-0.42061900	4.52584300	-0.97236600
C	-0.60199700	2.47600300	-2.24728400
C	-1.23671900	5.17101800	-1.89267800
H	-0.02642800	5.07334400	-0.11527200
C	-1.41646000	3.13145700	-3.16800100
H	-0.38029100	1.41125700	-2.34511700
C	-1.73224200	4.47412200	-2.99300300
H	-1.48396800	6.22229200	-1.75379100
H	-1.80760700	2.58428800	-4.02452000
H	-2.36873400	4.98316000	-3.71535500
C	2.19032400	3.59685000	0.49788400
C	2.26116900	4.20587000	1.75131000
C	3.10695100	3.96549500	-0.49278300
C	3.24791700	5.15276500	2.01553900
H	1.54489700	3.94247600	2.52853900
C	4.08937400	4.90867700	-0.22718600
H	3.05817200	3.49790500	-1.47672600
C	4.16665700	5.49940400	1.03224200
H	3.29599200	5.62011900	2.99795800

H	4.80658400	5.17249700	-1.00296900
H	4.94229000	6.23391700	1.24318600
C	-0.05653900	2.08459700	1.56173500
C	-1.43709500	2.28708100	1.55348600
C	0.55271000	1.57347300	2.71630200
C	-2.19610900	1.98455100	2.68089800
H	-1.93012300	2.65435300	0.65470000
C	-0.20591200	1.28637200	3.84378800
H	1.63202600	1.40717200	2.73363500
C	-1.58406100	1.48872600	3.82570700
H	-3.27594900	2.12156100	2.65360800
H	0.27950600	0.90086400	4.73977700
H	-2.18265700	1.24625300	4.70227000
C	-8.88815000	1.74132500	-0.64663600
C	-8.20693900	0.75326000	0.05480800
C	-8.05621100	-0.53678300	-0.46595400
C	-8.62190000	-0.79903400	-1.72215300
C	-9.30409100	0.18380600	-2.42320100
C	-9.44474000	1.47215700	-1.89756100
H	-8.99724700	2.73899000	-0.21856500
H	-7.79455400	0.98794300	1.03720500
H	-8.51757800	-1.79718900	-2.14721600
H	-9.73871800	-0.04177800	-3.39862000
C	-10.16559200	2.53422000	-2.67233800
H	-9.57153400	2.87276400	-3.53312900
H	-11.11891800	2.16265600	-3.07123500
H	-10.37869600	3.41385400	-2.05290300
B	-7.27624100	-1.65098800	0.28811200
O	-6.62987800	-1.32413000	1.48871700
H	-5.75456300	-0.55370100	1.59496100
O	-7.21056700	-2.90489800	-0.20084700
H	-6.52946000	-3.40582700	0.29121700
P	2.71116500	-2.05869100	-0.59602300
C	1.91216400	-3.40821800	-1.54126200
C	0.54280700	-3.31050200	-1.80397400
C	2.61388700	-4.55361700	-1.94115200
C	-0.11692300	-4.35732200	-2.44293700
H	0.01379500	-2.39417300	-1.53718300
C	1.94839100	-5.59183900	-2.58040300
H	3.68798300	-4.62822700	-1.76959400
C	0.58027900	-5.49691600	-2.82649600
H	-1.18329300	-4.27293900	-2.64494000
H	2.50073300	-6.47802200	-2.88968300
H	0.06086500	-6.31270300	-3.32744800

C	4.45035600	-2.12584700	-1.15514500
C	5.52009200	-2.07716500	-0.26058700
C	4.70710900	-2.07407800	-2.53025800
C	6.82476600	-1.97665400	-0.73344800
H	5.33513700	-2.10176000	0.81269200
C	6.01159300	-1.98930100	-3.00001400
H	3.87710700	-2.09908100	-3.23850600
C	7.07429600	-1.93753200	-2.10088100
H	7.65024800	-1.92715100	-0.02469700
H	6.19924900	-1.95857300	-4.07215900
H	8.09658500	-1.86264900	-2.46828300
C	2.74209900	-2.69285200	1.12633100
C	2.21714300	-1.90100600	2.15003700
C	3.24978600	-3.95758700	1.44154400
C	2.19579300	-2.35894900	3.46378100
H	1.80832500	-0.91883700	1.90461900
C	3.23642400	-4.41302000	2.75411700
H	3.65765000	-4.59380200	0.65614500
C	2.70866300	-3.61493200	3.76722900
H	1.77175400	-1.73046200	4.24600000
H	3.63484300	-5.39896300	2.98765300
H	2.69430500	-3.97793300	4.79365100
C	7.70712300	2.13790900	0.40532700
H	7.96678500	2.22974700	1.46728600
H	8.42263300	1.43917900	-0.05258100
H	7.87663000	3.11798600	-0.06302500

**B**

C	-5.03333000	0.99158900	-1.53099700
C	-3.94651400	0.96381900	-2.40713400
C	-2.66096300	0.67210100	-1.95581000
C	-2.41963200	0.40749600	-0.60680200
C	-3.50951900	0.41454700	0.27069400
C	-4.79507300	0.69987200	-0.18660600
H	-4.11152600	1.17727200	-3.46531600
H	-1.83978800	0.64512100	-2.67488800
H	-3.36155000	0.18837300	1.33004500
H	-5.63129600	0.70093400	0.51629800
Pd	-0.58678600	0.02854400	0.14199200
P	-1.02504800	-2.31433100	0.11015500
C	0.49962700	-3.31217900	0.09573200
C	0.77218500	-4.27793800	1.06617900
C	1.41816100	-3.09647500	-0.93602400
C	1.95026800	-5.01570600	1.00284200

H	0.06366500	-4.45506500	1.87435000
C	2.59172400	-3.83684500	-0.99840100
H	1.21797600	-2.33360200	-1.68907200
C	2.85925900	-4.79656900	-0.02713600
H	2.15733200	-5.76502100	1.76537700
H	3.31152400	-3.64301500	-1.79142700
H	3.78609100	-5.36637200	-0.06708100
C	-1.79979500	-2.65761400	1.72995700
C	-1.20509900	-2.06986300	2.85615400
C	-2.94287800	-3.44299300	1.88083600
C	-1.75843600	-2.27260300	4.11431200
H	-0.29757400	-1.47330800	2.72929500
C	-3.49597300	-3.63381400	3.14487600
H	-3.40581100	-3.90581800	1.00975600
C	-2.90716900	-3.04857600	4.25996300
H	-1.29247000	-1.81786800	4.98720200
H	-4.39034900	-4.24508000	3.25502900
H	-3.34265200	-3.19735300	5.24705800
C	-2.09782500	-3.14022800	-1.12807500
C	-1.66094100	-4.26567300	-1.83491900
C	-3.38293000	-2.64114900	-1.38012500
C	-2.48683400	-4.87105100	-2.77759100
H	-0.66950400	-4.67647700	-1.65176700
C	-4.20484200	-3.25097900	-2.31940600
H	-3.74698300	-1.77243200	-0.83481900
C	-3.75806600	-4.36506600	-3.02422800
H	-2.13105000	-5.74580700	-3.31967500
H	-5.19822700	-2.84325900	-2.50183200
H	-4.40143200	-4.83884500	-3.76416100
C	2.73723600	-0.26430900	-0.55199500
C	4.02099500	-0.45400100	-1.04798800
C	4.99480000	-1.03987000	-0.24884800
C	4.66746300	-1.44671900	1.04205000
C	3.38552200	-1.25657200	1.53645300
C	2.37846500	-0.64939100	0.75538400
H	1.97058500	0.18565900	-1.18494200
H	4.26732700	-0.14690400	-2.06417400
H	5.43655300	-1.92422200	1.64857500
H	3.12033500	-1.59249600	2.53912400
O	1.17057000	-0.48439200	1.25544500
O	6.26632200	-1.29836100	-0.72008300
B	7.11844200	-0.35642300	-1.19473200
O	8.32915300	-0.83219400	-1.63461800
H	8.92269800	-0.15681500	-1.97350900

O	6.75825600	0.96961400	-1.21490600
H	7.44876800	1.55553300	-1.53764400
C	-6.40301500	1.37388300	-2.00888100
H	-6.55916800	2.46106100	-1.93784500
H	-6.56026900	1.09591400	-3.05909600
H	-7.19096200	0.89639500	-1.41196400
P	-0.15390700	2.38016600	0.21999500
C	0.30606300	3.03903100	1.86106800
C	0.88710100	2.18286000	2.80222000
C	0.14171100	4.39648900	2.16059800
C	1.29345800	2.69030200	4.03428900
H	1.03448000	1.12885000	2.54923800
C	0.54737500	4.89189500	3.39379200
H	-0.30440000	5.06820000	1.42685700
C	1.12186700	4.03787100	4.33222800
H	1.74832000	2.02292600	4.76456400
H	0.41477800	5.94823900	3.62273600
H	1.44024600	4.42761400	5.29817300
C	-1.50006200	3.49952700	-0.31901300
C	-1.42573700	4.31665700	-1.44786800
C	-2.68617200	3.47476400	0.42392600
C	-2.52487000	5.07803300	-1.83790500
H	-0.50724200	4.36333600	-2.03074900
C	-3.77971500	4.23522000	0.03482700
H	-2.75628700	2.84140700	1.30868300
C	-3.70406400	5.03401100	-1.10409800
H	-2.45481800	5.70919300	-2.72251000
H	-4.69971400	4.19343300	0.61639700
H	-4.56475300	5.62436300	-1.41500000
C	1.26704800	2.78496600	-0.85610500
C	1.18473500	2.47076200	-2.21897400
C	2.46216000	3.28941800	-0.34293400
C	2.27272400	2.68136800	-3.05553000
H	0.26239700	2.04726900	-2.62179200
C	3.55671000	3.48350400	-1.18059100
H	2.54711300	3.51099500	0.72005900
C	3.46347400	3.18452800	-2.53436900
H	2.19765400	2.43774100	-4.11410600
H	4.49289500	3.85287300	-0.76605200
H	4.32289000	3.33130900	-3.18648200
<b>C<sub>a</sub></b>			
C	-4.33370200	0.85771000	2.86084400
C	-3.18317700	0.22785200	3.33388300



C	-2.07433200	0.03557500	2.50745600
C	-2.08405200	0.47378900	1.18062900
C	-3.23818700	1.10395900	0.70392800
C	-4.34062600	1.29218800	1.53198600
H	-3.14985100	-0.11430200	4.37018300
H	-1.18278000	-0.44148100	2.92356000
H	-3.27883300	1.46916100	-0.32460000
H	-5.23003800	1.79092700	1.14089800
Pd	-0.44791300	0.15714600	0.03107300
P	0.08378300	2.44787300	-0.19213800
C	-2.48831000	-1.56682400	-1.62018900
C	-1.59502400	-1.62058900	-0.64867300
C	-0.77937200	-2.19258300	0.26798100
C	-3.26204300	-2.82040000	-1.93124900
O	-3.51413600	-3.09340200	-3.09213200
C	1.86723100	2.80616000	-0.33322600
C	2.46152600	3.33795000	-1.47876500
C	2.66069000	2.51512200	0.78003400
C	3.83427800	3.56058400	-1.51045900
H	1.85632600	3.57527000	-2.35284700
C	4.03020500	2.74479500	0.74740300
H	2.20569800	2.08924300	1.67542800
C	4.61975500	3.25865300	-0.40272500
H	4.29164900	3.96797500	-2.41074500
H	4.64115700	2.48857300	1.61089200
H	5.69572600	3.42011800	-0.43679900
C	-0.65943100	2.78639900	-1.82565500
C	-0.15068600	2.11639200	-2.94929800
C	-1.80489200	3.57731400	-1.95621300
C	-0.75747400	2.28293700	-4.18854600
H	0.69156100	1.43257900	-2.82605400
C	-2.41987400	3.71790000	-3.19731500
H	-2.22259500	4.08353500	-1.08609200
C	-1.89138300	3.08219300	-4.31583600
H	-0.35264400	1.76677600	-5.05749400
H	-3.31328600	4.33350200	-3.28808600
H	-2.36887700	3.20099800	-5.28715100
C	-0.50037200	3.79766000	0.89860200
C	-0.21672500	5.12395300	0.54472400
C	-1.16263400	3.53584900	2.09837100
C	-0.61142200	6.16875200	1.36843900
H	0.31916800	5.33645900	-0.38148300
C	-1.55379500	4.58713300	2.92449200
H	-1.37787400	2.50871900	2.38631100

C	-1.28348600	5.90023000	2.55996900
H	-0.38874500	7.19612900	1.08522600
H	-2.07356400	4.37119400	3.85646800
H	-1.59085700	6.72082000	3.20643000
C	-3.72648000	-3.68739400	-0.81441600
C	-3.95918700	-3.19589900	0.47494900
C	-4.01581200	-5.02423300	-1.10487200
C	-4.45455600	-4.03960900	1.46210200
H	-3.77440700	-2.14533300	0.70032100
C	-4.49308700	-5.86860900	-0.11352800
H	-3.85495600	-5.37850800	-2.12136600
C	-4.71204100	-5.37641000	1.17196100
H	-4.64264300	-3.64751300	2.46037700
H	-4.70234500	-6.91254300	-0.34100100
H	-5.09316100	-6.03805800	1.94855700
C	2.61603700	-0.61627400	0.69141600
C	3.86453800	-0.94779800	1.20415800
C	4.95849100	-1.05451800	0.35625000
C	4.80081500	-0.80172800	-1.00362500
C	3.55497200	-0.47221500	-1.51433500
C	2.41510900	-0.38522200	-0.68616100
H	1.75263400	-0.55169900	1.36153500
H	3.99274300	-1.14385700	2.26918800
H	5.67277200	-0.86933000	-1.65342700
H	3.42254500	-0.27969200	-2.57926200
O	1.24384200	-0.10143700	-1.22059500
O	6.21786500	-1.35313900	0.83782300
B	6.54167700	-2.51900800	1.44920000
O	7.84084300	-2.61318800	1.88110800
H	8.06075800	-3.44362400	2.31181900
O	5.60565800	-3.51664300	1.60392500
H	5.95235500	-4.30692400	2.02869000
C	-2.74276900	-0.40243000	-2.52520000
H	-3.73093700	0.04057100	-2.33182400
H	-1.98030700	0.37481000	-2.40857400
H	-2.74448400	-0.75348500	-3.56428900
C	-5.53433700	1.05568800	3.73873800
H	-5.31201500	0.81193900	4.78504800
H	-5.89290300	2.09345500	3.70598400
H	-6.37455700	0.42012300	3.42479300
C	0.42501400	-2.96495600	-0.03360100
C	1.17980500	-3.47337900	1.02914700
C	0.86927900	-3.16227000	-1.34621300
C	2.37413900	-4.13775700	0.79192600

H	0.83767100	-3.30282500	2.05159000
C	2.06194100	-3.82824400	-1.58071500
H	0.29869700	-2.74410400	-2.17361100
C	2.82277400	-4.30431700	-0.51441700
H	2.98977900	-4.47288100	1.62453800
H	2.41785600	-3.95301100	-2.60180000
H	3.78004200	-4.78833300	-0.70009000
H	-1.08419200	-2.15315800	1.31949400

**TS6<sub>a</sub>**

C	-0.75156100	-4.81158600	-2.13269900
C	-0.40395400	-3.73322500	-2.94809900
C	-0.16901900	-2.46855000	-2.41237100
C	-0.28947300	-2.23722700	-1.04019000
C	-0.63175900	-3.31629200	-0.21935200
C	-0.85472300	-4.58288100	-0.75801300
H	-0.30079800	-3.89069200	-4.02379000
H	0.12350600	-1.65465300	-3.07946100
H	-0.69875700	-3.17715000	0.86291700
H	-1.10884400	-5.41502800	-0.09746500
Pd	0.06645300	-0.43919000	-0.21234800
P	2.39420100	-0.85798400	-0.11554800
C	-3.18169600	-0.49208800	-0.63881100
C	-2.03033200	-0.16985800	-0.01480000
C	-1.98307000	0.59739200	1.15112100
C	-4.34930900	0.04766300	0.10513100
O	-4.16265700	0.75775000	1.10214300
C	3.36614100	0.68067200	-0.21616500
C	4.37149800	0.98607400	0.70315200
C	3.08651400	1.57455200	-1.25441500
C	5.08815400	2.17271300	0.58128700
H	4.59314000	0.29799500	1.51869200
C	3.80591400	2.75710900	-1.37504100
H	2.28292000	1.35229500	-1.95802800
C	4.80596800	3.05733000	-0.45487600
H	5.86803200	2.40786300	1.30405900
H	3.56180800	3.46029500	-2.16906400
H	5.35839500	3.99177600	-0.53918200
C	2.71005100	-1.51211000	1.56552800
C	2.02659200	-0.91330200	2.63313900
C	3.60073700	-2.55817000	1.81487100
C	2.23537400	-1.36843100	3.92960800
H	1.35274200	-0.07554400	2.43609300
C	3.79869900	-3.01196100	3.11639100

H	4.14034000	-3.02343600	0.99061800
C	3.11570600	-2.41999200	4.17322800
H	1.70044600	-0.89718000	4.75366200
H	4.49283800	-3.83015300	3.30244000
H	3.27106300	-2.77810600	5.19008300
C	3.26298600	-2.01635800	-1.23441500
C	4.38868300	-1.62462500	-1.96482100
C	2.78576900	-3.32682600	-1.36891500
C	5.02270000	-2.52541900	-2.81592000
H	4.77635000	-0.61143100	-1.86755900
C	3.42307800	-4.22275500	-2.21761200
H	1.90866200	-3.64837100	-0.80714200
C	4.54129800	-3.82336700	-2.94506600
H	5.89925500	-2.20837800	-3.37877800
H	3.03221700	-5.23461700	-2.31689300
H	5.03658600	-4.52527100	-3.61434800
C	-5.75259900	-0.20201600	-0.31334000
C	-6.17273000	-1.42294400	-0.84880300
C	-6.69599200	0.80519300	-0.08086600
C	-7.51368900	-1.62891100	-1.15189700
H	-5.45560100	-2.22672600	-1.00135300
C	-8.02868300	0.60760400	-0.41089900
H	-6.36077100	1.74156900	0.36030900
C	-8.43990700	-0.61146300	-0.94504400
H	-7.83622600	-2.58818300	-1.55263500
H	-8.75368500	1.40200700	-0.24297800
H	-9.48751800	-0.77099200	-1.19533300
C	0.03092300	2.88161900	-0.81939400
C	0.13409500	4.16913400	-1.33626700
C	0.81853000	5.15124500	-0.63086300
C	1.40513100	4.83594200	0.59305000
C	1.30349000	3.55415000	1.10986900
C	0.61844100	2.53284000	0.41585500
H	-0.49189900	2.10475100	-1.38357900
H	-0.32272500	4.41746600	-2.29356100
H	1.95286600	5.61408700	1.12377200
H	1.78602300	3.28882900	2.05117700
O	0.55586500	1.32570100	0.93562900
O	0.99900600	6.42256200	-1.13368500
B	-0.00726000	7.23929000	-1.53836700
O	0.38915600	8.46036800	-2.02293000
H	-0.33317700	9.02415300	-2.31253100
O	-1.31288600	6.82694600	-1.44663200
H	-1.95878100	7.48102900	-1.72792100

C	-3.28999900	-1.19276200	-1.95842700
H	-4.15087300	-0.83572100	-2.53734700
H	-2.38306300	-1.01738700	-2.54482900
H	-3.38556300	-2.28413000	-1.85417800
C	-1.01748100	-6.17107300	-2.71104900
H	-2.09325200	-6.34970300	-2.85450600
H	-0.53818900	-6.29301100	-3.69090200
H	-0.64740600	-6.96953500	-2.05418000
C	-1.76359000	0.09591100	2.49739600
C	-1.29268200	0.97301600	3.48014300
C	-2.00890300	-1.24544100	2.81982000
C	-1.07284100	0.51500200	4.77272000
H	-1.07591000	2.00561900	3.20807900
C	-1.79032300	-1.69869600	4.11089500
H	-2.37126600	-1.92088900	2.04396800
C	-1.32306100	-0.81855400	5.08757000
H	-0.70347200	1.19817500	5.53536000
H	-1.98313700	-2.73993100	4.36208100
H	-1.15136000	-1.17819200	6.10122100
H	-1.86091900	1.67627900	1.01578900

**D<sub>a</sub>**

C	1.10523000	-4.65507300	-2.48891000
C	1.14753000	-3.43690100	-3.16819500
C	0.89821100	-2.23503700	-2.50896500
C	0.58099200	-2.20669000	-1.14733300
C	0.52996200	-3.43011400	-0.46821000
C	0.79770600	-4.62983800	-1.12613600
H	1.40294300	-3.42789800	-4.23002000
H	0.97230300	-1.29955300	-3.06939500
H	0.29887900	-3.45062000	0.59952900
H	0.77040900	-5.56999700	-0.56980800
Pd	0.26107300	-0.45359200	-0.19822200
P	2.58784200	0.09730700	-0.05896500
C	-2.68803700	-1.54754200	-0.72690700
C	-1.69814400	-0.89675400	0.00273400
C	-2.33724000	-0.38850000	1.23773300
C	-3.87358700	-1.48241500	0.03267900
O	-3.73741500	-0.83142300	1.16687000
C	2.86723900	1.89791500	-0.14588700
C	3.58646400	2.59272300	0.82764600
C	2.29528400	2.60163500	-1.21060500
C	3.73745900	3.97296700	0.73077200
H	4.02575200	2.05540300	1.66796400

C	2.45077600	3.97885100	-1.30704800
H	1.70862300	2.06513700	-1.95849800
C	3.17156300	4.66574800	-0.33430900
H	4.29548000	4.50916900	1.49703000
H	1.98188100	4.51988500	-2.12689000
H	3.27925400	5.74716200	-0.40119800
C	3.17218300	-0.38317600	1.60805700
C	2.27934000	-0.24733200	2.67876100
C	4.46831200	-0.84908000	1.84369900
C	2.68614500	-0.58269000	3.96523900
H	1.27851600	0.15225500	2.49901000
C	4.86674000	-1.18516200	3.13391200
H	5.16872500	-0.95187700	1.01495700
C	3.97566100	-1.05541400	4.19428700
H	1.98321600	-0.47725600	4.79094100
H	5.87762800	-1.55051500	3.30922600
H	4.28770200	-1.32198000	5.20326200
C	3.83312100	-0.62654300	-1.18594100
C	4.72096100	0.15517500	-1.92905400
C	3.87697300	-2.02066800	-1.31493600
C	5.63533800	-0.44698000	-2.78951700
H	4.69855400	1.24043700	-1.83458900
C	4.79336100	-2.61751700	-2.17076000
H	3.18242700	-2.64109900	-0.74667900
C	5.67218200	-1.83163400	-2.91254000
H	6.32159000	0.17233000	-3.36523200
H	4.80797900	-3.70228700	-2.26792100
H	6.38531200	-2.29979700	-3.58959100
C	-5.20889400	-1.99460800	-0.24239400
C	-5.40772100	-3.09137600	-1.09225200
C	-6.31320000	-1.40243700	0.38812800
C	-6.68929600	-3.57759800	-1.31186400
H	-4.55627900	-3.58508900	-1.55446000
C	-7.59146700	-1.88296900	0.15143100
H	-6.15211200	-0.56080700	1.05746100
C	-7.78135600	-2.97048400	-0.69863600
H	-6.83576300	-4.43674700	-1.96313100
H	-8.44452900	-1.41141000	0.63515500
H	-8.78534200	-3.35112600	-0.87809600
C	-1.03508500	2.54450700	-0.85968500
C	-1.46426100	3.76153600	-1.37916900
C	-1.30996300	4.92920100	-0.64290200
C	-0.71521300	4.87330800	0.61528600
C	-0.28812700	3.66201000	1.13575000

C	-0.43193200	2.45400800	0.41543500
H	-1.13452700	1.62977400	-1.45058500
H	-1.91968300	3.81039000	-2.36811300
H	-0.58560100	5.80060400	1.17276500
H	0.19388500	3.61298700	2.11262500
O	-0.01862100	1.32672300	0.95035900
O	-1.66794700	6.16146300	-1.15130100
B	-2.93085300	6.49670500	-1.51691100
O	-3.07814900	7.76504400	-2.02101700
H	-3.97767700	7.98944800	-2.27393000
O	-3.95799200	5.59727200	-1.37087900
H	-4.81763400	5.93265100	-1.64056500
C	-2.53662400	-2.12678700	-2.09585300
H	-3.45404100	-2.01967100	-2.68842000
H	-1.72580500	-1.61024900	-2.61907900
H	-2.25814700	-3.19090700	-2.07199800
C	1.37211700	-5.95246300	-3.19559300
H	0.44261700	-6.49740800	-3.41698000
H	1.88672900	-5.79031400	-4.15131300
H	1.99579000	-6.62273300	-2.58858400
C	-1.76120400	-0.82553900	2.55550700
C	-1.39386500	0.12130900	3.50823700
C	-1.59496900	-2.18377700	2.82592200
C	-0.87556400	-0.29079600	4.73214400
H	-1.48903600	1.18066600	3.27345800
C	-1.06824900	-2.59393000	4.04418200
H	-1.88151600	-2.92140200	2.07438900
C	-0.71164000	-1.64638600	5.00088400
H	-0.59412000	0.45290300	5.47657300
H	-0.93571800	-3.65491400	4.24873200
H	-0.30129200	-1.96784300	5.95732600
H	-2.36039000	0.71164200	1.18072000

**TS7<sub>a</sub>**

C	-3.46287200	-3.26276000	-2.08919300
C	-2.70526900	-2.34384500	-2.82586600
C	-1.96968600	-1.35208500	-2.19517900
C	-1.92791500	-1.25616100	-0.78986200
C	-2.68386400	-2.18373900	-0.05793800
C	-3.43973800	-3.16300700	-0.69931400
H	-2.68772700	-2.42081700	-3.91475500
H	-1.37671300	-0.66933700	-2.80320600
H	-2.66245600	-2.16764300	1.02979100
H	-4.01541600	-3.87264800	-0.10258000

Pd	-0.29825100	-0.27223300	0.06369000
P	1.62588600	-1.70543900	-0.20548800
C	-2.77751900	1.50135900	-0.78643400
C	-2.06678200	0.62066400	0.06416300
C	-2.57671400	0.92957500	1.44058300
C	-3.77255200	2.10108700	-0.02841600
O	-3.74957200	1.74776500	1.25959100
C	2.93292100	-0.78037300	-1.09407900
C	4.08370800	-0.31278400	-0.45967500
C	2.69737500	-0.43183400	-2.43017500
C	4.98554400	0.49341300	-1.14949600
H	4.26863600	-0.55553700	0.58655600
C	3.61146800	0.35051500	-3.12353800
H	1.79197400	-0.78544000	-2.92918100
C	4.75535100	0.82015000	-2.48069800
H	5.85937700	0.88887300	-0.63389200
H	3.42457800	0.60647500	-4.16577000
H	5.46075800	1.45551700	-3.01408600
C	2.43015300	-2.26371000	1.34255400
C	2.29008000	-1.44898900	2.47202800
C	3.19199800	-3.43239800	1.42408100
C	2.91904400	-1.79936500	3.66312500
H	1.69862500	-0.53175400	2.39606400
C	3.80711000	-3.78326600	2.62102400
H	3.30074200	-4.07481000	0.55045900
C	3.67317900	-2.96643700	3.74061300
H	2.81780700	-1.15419200	4.53532100
H	4.39610700	-4.69758900	2.67818200
H	4.15983200	-3.24145400	4.67550000
C	1.46318400	-3.24379500	-1.19110900
C	2.49465100	-3.74067000	-1.99558400
C	0.26822600	-3.96225100	-1.09953500
C	2.33103200	-4.93391500	-2.69107400
H	3.43011100	-3.18655000	-2.07886100
C	0.10663200	-5.15712400	-1.79323800
H	-0.54729500	-3.57312100	-0.48914100
C	1.13719500	-5.64372000	-2.59124100
H	3.14018300	-5.31085100	-3.31502800
H	-0.83250500	-5.70382700	-1.71322800
H	1.01081300	-6.57664100	-3.13887400
C	-4.80428200	3.06274700	-0.39189900
C	-5.30172100	3.13690200	-1.69999400
C	-5.33529600	3.91027100	0.59105900
C	-6.29633000	4.05095700	-2.01881900



H	-4.93071100	2.45335200	-2.46033900
C	-6.32286500	4.82744000	0.26430400
H	-4.95558400	3.84308100	1.60789900
C	-6.80370600	4.90185500	-1.04086900
H	-6.68250900	4.09527200	-3.03533700
H	-6.72093600	5.48918300	1.03115900
H	-7.58068200	5.62084800	-1.29454700
C	1.80328200	2.40583900	-0.19777700
C	2.90302900	3.16592400	-0.56388400
C	3.93303500	3.38562400	0.34592700
C	3.84326000	2.85641700	1.62744100
C	2.74173000	2.09280600	1.99372200
C	1.69278500	1.83041100	1.08622900
H	1.00509100	2.20543700	-0.91730000
H	2.98714900	3.57265700	-1.57170700
H	4.65872600	3.03497800	2.32772100
H	2.67010600	1.67452500	2.99848800
O	0.66921500	1.07782700	1.44206800
O	5.09063700	4.04064400	-0.02479000
B	5.13263200	5.33370000	-0.43499700
O	6.37332200	5.79178700	-0.80415600
H	6.38743900	6.71133500	-1.08285300
O	3.98771700	6.08935300	-0.45888800
H	4.11584900	6.99867200	-0.74310100
C	-4.25556300	-4.32561000	-2.78742500
H	-4.78612600	-4.96830200	-2.07462300
H	-5.00313500	-3.89219100	-3.46627200
H	-3.60777900	-4.96807600	-3.40069700
H	-1.77655800	1.61349800	1.79990000
C	-2.46399600	1.77363600	-2.21943500
H	-3.01193500	1.10998600	-2.90510000
H	-2.69943200	2.81044400	-2.48995700
H	-1.39249600	1.62075600	-2.39854000
C	-2.78275600	-0.13774500	2.46825800
C	-1.65491300	-0.62239800	3.13408600
C	-4.03658100	-0.68682000	2.72499300
C	-1.77888100	-1.68910200	4.01703700
H	-0.68514900	-0.15630900	2.94400400
C	-4.15723600	-1.74211800	3.62471900
H	-4.91336100	-0.29546600	2.21173700
C	-3.02907300	-2.25352400	4.26004300
H	-0.89334000	-2.07521200	4.51966400
H	-5.13776000	-2.17251900	3.82289300
H	-3.12592300	-3.08608400	4.95515500

**E<sub>a</sub>**

C	-3.80152200	-1.88570500	4.15338800
C	-2.88684200	-0.83489300	4.08797100
C	-2.09791100	-0.62851200	2.96062800
C	-2.20888400	-1.47974700	1.85863900
C	-3.12001300	-2.54299900	1.92240400
C	-3.90069900	-2.74054900	3.05311500
H	-2.78730900	-0.16160900	4.94079500
H	-1.39074600	0.20253000	2.91236500
H	-3.21411800	-3.22312000	1.07398000
H	-4.60066300	-3.57681700	3.08580600
Pd	0.48795300	-0.19088600	0.74654700
P	2.73030800	0.61137900	0.44451200
C	-0.28736100	-2.18263300	0.29564200
C	-1.36319200	-1.30205900	0.65050800
C	-1.93058100	-0.75841500	-0.65445500
C	0.02661500	-1.86172200	-1.04161900
O	-0.91553400	-1.09594100	-1.62658600
C	4.01449400	-0.69212600	0.32111300
C	4.94986100	-0.78124100	-0.71067000
C	4.03649300	-1.64866300	1.34406300
C	5.88804300	-1.81138500	-0.72152400
H	4.94396000	-0.04252400	-1.51229700
C	4.97243700	-2.67549300	1.33358900
H	3.31058300	-1.57664900	2.15748600
C	5.89952900	-2.76018400	0.29556600
H	6.61403100	-1.87108000	-1.53128800
H	4.98241600	-3.41020300	2.13726600
H	6.63387100	-3.56420700	0.28454800
C	2.83695900	1.53058000	-1.13621500
C	2.47347700	0.86950200	-2.31726700
C	3.11943600	2.89727700	-1.18268400
C	2.39944400	1.56158500	-3.51833200
H	2.24847900	-0.19818700	-2.29931900
C	3.03174700	3.59122400	-2.38751200
H	3.39378400	3.42837600	-0.27139700
C	2.67020300	2.92809300	-3.55444100
H	2.11769100	1.03160100	-4.42759100
H	3.24469800	4.65870700	-2.40932400
H	2.59697500	3.47474500	-4.49321500
C	3.45233200	1.76365700	1.66678200
C	4.83564500	1.90271100	1.82492400
C	2.57983100	2.56983900	2.40544700

C	5.34352800	2.83787100	2.71833200
H	5.51594700	1.27780300	1.24502800
C	3.09883300	3.50794200	3.29471900
H	1.49992900	2.45288400	2.27279900
C	4.47426600	3.64143200	3.45318400
H	6.42067500	2.94174600	2.84120600
H	2.41991000	4.13502200	3.87050000
H	4.87404600	4.37365900	4.15359800
C	1.02699900	-2.40172900	-1.95473500
C	0.81894500	-2.27610200	-3.33762300
C	2.19665300	-3.02317800	-1.49616500
C	1.76148100	-2.75868400	-4.23451500
H	-0.08517200	-1.78919500	-3.69526100
C	3.13375200	-3.50415300	-2.39975800
H	2.39839500	-3.09264300	-0.42950100
C	2.92191500	-3.37229100	-3.76991700
H	1.58910400	-2.65467600	-5.30444200
H	4.04179900	-3.97361200	-2.02601800
H	3.66188000	-3.74653300	-4.47534200
C	-0.86105400	2.59458400	-0.42738200
C	-1.81421900	3.17723000	-1.25285100
C	-3.11356500	3.36958000	-0.79487800
C	-3.44967600	2.98837300	0.50102200
C	-2.49935200	2.39933700	1.32629200
C	-1.17164200	2.18203400	0.89092500
H	0.15672700	2.43838900	-0.79331400
H	-1.56051100	3.49191000	-2.26458100
H	-4.46716200	3.15199800	0.85612200
H	-2.76464600	2.09426600	2.33827100
O	-0.27878200	1.61901600	1.68226000
O	-4.02619000	3.98423500	-1.62349200
B	-5.14677500	3.37532100	-2.09080100
O	-5.90240700	4.11787800	-2.96015900
H	-6.72232000	3.69615600	-3.23157800
O	-5.45329000	2.09934000	-1.68568000
H	-6.18700600	1.68946300	-2.15293500
C	0.25369200	-3.29742200	1.13678100
H	0.12677700	-4.26723200	0.63385800
H	1.31716500	-3.18496800	1.37823900
H	-0.29405600	-3.33155800	2.08566400
C	-4.67005800	-2.08374200	5.36007000
H	-5.65357100	-1.61032200	5.22712100
H	-4.85141800	-3.14813600	5.55817400
H	-4.21876000	-1.64416200	6.25828800

C	-3.25357700	-1.35082900	-1.05232700
C	-4.41685200	-0.69967700	-0.64833900
C	-3.33712700	-2.57215400	-1.72049700
C	-5.65757600	-1.27880300	-0.89197100
H	-4.34092000	0.26449500	-0.14278700
C	-4.57956900	-3.14534700	-1.97016000
H	-2.42503600	-3.07151700	-2.05065800
C	-5.74166400	-2.50341300	-1.54842800
H	-6.56254100	-0.76852700	-0.56276400
H	-4.64196600	-4.09769400	-2.49488000
H	-6.71351600	-2.95777800	-1.73664800
H	-2.00642400	0.34243200	-0.63660600

**TS8<sub>a</sub>**

C	-2.48887200	-3.33083400	2.84449800
C	-1.28109000	-2.70847500	3.15734300
C	-0.58760300	-1.95799200	2.20953800
C	-1.07930700	-1.80865700	0.90517500
C	-2.28334100	-2.45672000	0.58536500
C	-2.97597100	-3.18704200	1.54082300
H	-0.87733600	-2.80156100	4.16697800
H	0.33646600	-1.46547000	2.51416700
H	-2.71572900	-2.35262400	-0.40857000
H	-3.92874200	-3.64784400	1.27145100
Pd	-0.41296400	-0.14201500	-0.16162800
P	-2.57050400	0.99826700	-0.22533900
C	0.43689100	-3.05120400	-1.25681400
C	0.55971700	-2.01811700	-0.40669500
C	1.54860700	-1.14556200	0.03813900
C	1.67800600	-3.82044800	-1.58130800
O	1.78908000	-4.36197000	-2.67093500
C	-2.57247400	2.64626300	-1.00654000
C	-3.45467000	2.99975600	-2.02977700
C	-1.66052600	3.59053700	-0.52449100
C	-3.42034500	4.28352000	-2.56801100
H	-4.17202600	2.27310100	-2.41115700
C	-1.62986900	4.86932500	-1.06359500
H	-0.95601600	3.32145900	0.26262500
C	-2.50724800	5.21601600	-2.08851900
H	-4.10933400	4.55184300	-3.36736200
H	-0.90507100	5.59096200	-0.69095800
H	-2.47522700	6.21660000	-2.51700400
C	-3.68384400	-0.01070900	-1.26445500
C	-3.22293600	-0.36021100	-2.54095100

C	-4.89605300	-0.52998900	-0.80775600
C	-3.96782100	-1.21153200	-3.34716800
H	-2.26859100	0.03689200	-2.89665300
C	-5.63539300	-1.39129900	-1.61538000
H	-5.25712400	-0.27234000	0.18811900
C	-5.17339700	-1.73410100	-2.88147300
H	-3.60188900	-1.47726600	-4.33755300
H	-6.57799300	-1.79593200	-1.24990400
H	-5.75242800	-2.40963800	-3.50885700
C	-3.50147400	1.26294500	1.32735300
C	-4.54383700	2.19556600	1.38926100
C	-3.19735500	0.49908900	2.45624200
C	-5.27362300	2.35069400	2.56152400
H	-4.78222400	2.80253400	0.51514300
C	-3.93398300	0.65305500	3.62676800
H	-2.37948700	-0.21903100	2.41834100
C	-4.97103500	1.57803400	3.68069900
H	-6.08086500	3.08009900	2.60364300
H	-3.68730500	0.04838300	4.49865400
H	-5.54363800	1.70305900	4.59843800
C	2.79046200	-3.88194100	-0.59092400
C	2.56552600	-4.00982100	0.78186300
C	4.09983200	-3.83742300	-1.07527900
C	3.64055100	-4.07393300	1.66044800
H	1.54379300	-4.05574100	1.16003500
C	5.17229800	-3.87808600	-0.19507800
H	4.25391600	-3.74379000	-2.14906300
C	4.94292100	-3.99617600	1.17381000
H	3.46252100	-4.18442100	2.72911500
H	6.19035400	-3.81696900	-0.57564800
H	5.78393000	-4.03196200	1.86491800
C	1.48915500	2.23953500	0.88482200
C	2.55264700	2.91649100	1.47297700
C	3.46115300	3.60207600	0.67899400
C	3.27947500	3.64067900	-0.70113300
C	2.22034400	2.96757600	-1.28852400
C	1.31119900	2.21377500	-0.51634500
H	0.78124200	1.68269100	1.50877200
H	2.69058900	2.90648200	2.55411700
H	3.99336700	4.19723700	-1.30748600
H	2.09069400	2.96493100	-2.36983700
O	0.34324900	1.54928400	-1.11330300
O	4.52064300	4.28992800	1.23517900
B	5.52895600	3.67914500	1.90605500

O	6.48401900	4.51411900	2.42552900
H	7.20188600	4.06760700	2.88232100
O	5.55021900	2.30784000	2.02661900
H	6.30264000	1.96790000	2.51982200
C	-0.79728600	-3.43130600	-2.00465100
H	-1.43898400	-4.09216300	-1.40134900
H	-1.39488600	-2.55660000	-2.28894800
H	-0.50554100	-3.97596800	-2.90906500
C	-3.24342100	-4.13344800	3.86079800
H	-2.82119700	-4.01033200	4.86556800
H	-4.30080200	-3.83855300	3.90076600
H	-3.22172800	-5.20645700	3.62365600
C	2.64110400	-0.63611400	-0.79315100
C	3.73476100	-0.04330800	-0.15172400
C	2.64953300	-0.73872400	-2.19112800
C	4.82761700	0.40391400	-0.88257000
H	3.72228300	0.08806900	0.93060400
C	3.74452200	-0.29678000	-2.91782300
H	1.78763700	-1.16249000	-2.70599500
C	4.84034900	0.26843200	-2.26649400
H	5.65421800	0.88411700	-0.36161000
H	3.74049100	-0.38628000	-4.00290500
H	5.69488200	0.61927800	-2.84329000
H	1.71129000	-1.03442200	1.11385200
<b>G<sub>a</sub></b>			
C	0.60074600	-5.22105400	2.01818100
C	-0.30350700	-4.28996200	1.50713400
C	-0.00057600	-2.93301400	1.48209300
C	1.22212000	-2.47227700	1.96973900
C	2.13516700	-3.40039300	2.47723300
C	1.82562500	-4.75296400	2.50048000
H	-1.26212100	-4.63381400	1.11661900
H	-0.71460800	-2.22151500	1.06293100
H	3.10225800	-3.05112300	2.84021700
H	2.55121700	-5.46546500	2.89525200
Pd	0.57042800	0.31748700	0.62161200
P	0.48137500	0.87826300	-1.69306100
C	1.02465100	-0.05680400	2.78019400
C	1.62989500	-1.04123800	1.94701000
C	2.54761100	-0.57782600	0.95229500
C	1.85909500	1.13016800	3.22948000
O	3.06581300	0.99521100	3.37457400
C	-1.05228100	0.35939400	-2.52824000

C	-1.65991000	1.13395400	-3.51872600
C	-1.59610200	-0.88357500	-2.19374900
C	-2.79908000	0.66663000	-4.16606700
H	-1.24344200	2.10709500	-3.78067200
C	-2.73378700	-1.34853200	-2.84196700
H	-1.13054700	-1.48139300	-1.40799800
C	-3.33796000	-0.57088500	-3.82572600
H	-3.27326200	1.27602500	-4.93381400
H	-3.17149900	-2.30256700	-2.55311800
H	-4.24113800	-0.92663400	-4.31860600
C	0.55177800	2.69909100	-1.87552500
C	-0.06188100	3.48794400	-0.89374300
C	1.19148500	3.31361700	-2.95684400
C	-0.02710800	4.87439900	-0.99909200
H	-0.57563300	3.00137200	-0.06003800
C	1.22118500	4.70098700	-3.05376500
H	1.67276600	2.70563500	-3.72312100
C	0.61567300	5.48203300	-2.07378800
H	-0.49968400	5.48190000	-0.22877300
H	1.72335400	5.17325600	-3.89679900
H	0.64698400	6.56801000	-2.14839800
C	1.79527000	0.27248300	-2.81013200
C	1.52094900	-0.47633500	-3.95637600
C	3.12565100	0.54934600	-2.47634900
C	2.56287200	-0.93653500	-4.75741600
H	0.48972200	-0.69918700	-4.22793800
C	4.16148700	0.09996700	-3.28260900
H	3.34779800	1.12543500	-1.57582100
C	3.88119700	-0.65013100	-4.42277500
H	2.33823000	-1.51967300	-5.64925400
H	5.19263900	0.31994500	-3.01092800
H	4.69488200	-1.01180500	-5.04966300
C	1.21345000	2.41992800	3.60076900
C	-0.04576200	2.81705700	3.13963000
C	1.95841400	3.28961700	4.40884200
C	-0.54276500	4.07088400	3.48464200
H	-0.63542700	2.17443900	2.48255900
C	1.44932400	4.52795400	4.76544800
H	2.94221400	2.96760900	4.74366700
C	0.19538300	4.92212500	4.29982200
H	-1.51905300	4.37873400	3.11269900
H	2.03093400	5.19265300	5.40230500
H	-0.20452000	5.89750200	4.57455700
C	-2.93207400	-0.56277000	1.08398200

C	-4.14279800	-1.13303600	0.70939300
C	-4.96177100	-0.48255200	-0.20742000
C	-4.56501600	0.74160700	-0.73801500
C	-3.35046000	1.30201700	-0.37301900
C	-2.49151600	0.66214100	0.54346400
H	-2.30629800	-1.05408100	1.83015300
H	-4.46454300	-2.08294400	1.13549200
H	-5.21554800	1.23194000	-1.46159700
H	-3.02618400	2.25004500	-0.80403200
O	-1.34790800	1.22857700	0.89784200
O	-6.13183600	-1.04883100	-0.66143300
B	-7.18823300	-1.36105700	0.13583500
O	-8.24880300	-1.94816200	-0.50520900
H	-8.99123600	-2.16041300	0.06697800
O	-7.14125900	-1.08377300	1.47727700
H	-7.93780200	-1.31380500	1.96385300
C	0.26692700	-6.68213000	2.06665500
H	-0.56458700	-6.92842500	1.39525500
H	1.12708500	-7.30177800	1.78177800
H	-0.02834600	-6.99073000	3.07957000
H	3.10318600	0.32634000	1.20847400
C	3.27605500	-1.44900700	0.01162600
C	4.67228300	-1.34163300	-0.01900200
C	2.66215000	-2.37119100	-0.84449800
C	5.43492100	-2.14253100	-0.86115100
H	5.16024700	-0.62519400	0.64323200
C	3.42147900	-3.15804200	-1.69957600
H	1.57524200	-2.45352100	-0.85282000
C	4.81021900	-3.05094200	-1.70907900
H	6.52020400	-2.05038100	-0.85923800
H	2.92327600	-3.85348800	-2.37336400
H	5.40231300	-3.67145900	-2.38024000
C	-0.12153400	-0.38643600	3.70262700
H	0.12962800	-0.14525600	4.74544900
H	-1.01878100	0.19024800	3.44247500
H	-0.38019100	-1.45007400	3.65438500

**TS9<sub>a</sub>**

C	-2.58775300	-4.35966400	3.26015000
C	-2.64900000	-2.96527600	3.24738400
C	-2.04131000	-2.22148900	2.24309500
C	-1.34813400	-2.86454400	1.21175000
C	-1.27394900	-4.26208200	1.22636500
C	-1.88380300	-4.99588200	2.23484100



H	-3.17785300	-2.44935700	4.05006600
H	-2.05260900	-1.12869100	2.26726300
H	-0.74344400	-4.77961000	0.42526700
H	-1.81567900	-6.08496500	2.22835000
Pd	0.47773100	-0.37074600	0.66608700
P	2.32408200	1.08668100	0.68804900
C	0.62314200	-2.28065500	-0.36238900
C	-0.72989500	-2.06557800	0.11979700
C	-1.57704000	-1.34523300	-0.81852700
C	0.64324600	-2.10901900	-1.81133100
O	-0.43304200	-1.85092500	-2.40650900
C	3.96764000	0.30165900	0.47070900
C	4.90688700	0.71142300	-0.47840100
C	4.26410500	-0.78971200	1.29661400
C	6.11961600	0.03604000	-0.60186400
H	4.68730500	1.55906100	-1.12757600
C	5.47369900	-1.46218100	1.17255400
H	3.52878100	-1.11669500	2.03530200
C	6.40298600	-1.05167800	0.21806700
H	6.84668700	0.36557900	-1.34323600
H	5.69243900	-2.31075200	1.81872400
H	7.34996100	-1.57949500	0.11654000
C	2.19425300	2.26923200	-0.70506300
C	1.94044000	1.75520200	-1.98427000
C	2.20762300	3.65252700	-0.51822500
C	1.71373400	2.61014700	-3.05457400
H	1.90580500	0.67414500	-2.13918800
C	1.96444300	4.50722900	-1.59067600
H	2.38580400	4.06723700	0.47350800
C	1.71720400	3.98985300	-2.85683900
H	1.51803000	2.19736500	-4.04280100
H	1.96158600	5.58407000	-1.43048500
H	1.51955800	4.66059000	-3.69137900
C	2.57236500	2.14799000	2.15387000
C	3.82221200	2.68670100	2.48003300
C	1.44923900	2.47169700	2.92248100
C	3.94776400	3.54666200	3.56415200
H	4.69919500	2.43577100	1.88190200
C	1.58471600	3.33875100	4.00399300
H	0.47926700	2.02923700	2.67217000
C	2.82749900	3.87463700	4.32494800
H	4.92195700	3.96316300	3.81633500
H	0.71017400	3.59174500	4.60122600
H	2.92711200	4.55007400	5.17360600

C	1.85359800	-2.27330000	-2.64703200
C	1.68614100	-2.73236200	-3.95954800
C	3.13724500	-1.95130200	-2.19386800
C	2.78429700	-2.89401200	-4.79183700
H	0.68139200	-2.96138500	-4.30848600
C	4.23195600	-2.09032800	-3.03842700
H	3.27872600	-1.55013400	-1.19176800
C	4.05949400	-2.57167800	-4.33278400
H	2.64608200	-3.26605500	-5.80553000
H	5.22118600	-1.81427600	-2.67609400
H	4.91990600	-2.68908300	-4.98972500
C	-1.45340900	2.20444800	-0.10308600
C	-2.36115000	2.98504300	-0.81043100
C	-3.66801300	3.13111800	-0.35828100
C	-4.05945600	2.48902800	0.81589400
C	-3.15589900	1.70379800	1.51881800
C	-1.81364100	1.54056700	1.09495400
H	-0.42893200	2.10873000	-0.46680300
H	-2.05570300	3.50693800	-1.71711500
H	-5.08008000	2.60664000	1.17799100
H	-3.46181200	1.20442200	2.43850700
O	-0.97704900	0.81846300	1.80378100
O	-4.49693200	3.98963200	-1.04972100
B	-5.78104600	3.76683000	-1.41215000
O	-6.41418100	4.82516500	-2.01200400
H	-7.31581800	4.64858300	-2.29356900
O	-6.37882000	2.54501200	-1.18804300
H	-7.29864900	2.50706900	-1.46740100
C	1.58909100	-3.21819900	0.32354400
H	1.59832200	-4.21938000	-0.13587100
H	2.61941400	-2.84433800	0.29796300
H	1.31438800	-3.33571300	1.37777800
C	-3.27138900	-5.15705300	4.33055500
H	-4.23959800	-5.54576400	3.98313900
H	-2.67064300	-6.02344100	4.63684700
H	-3.46734100	-4.54936400	5.22245500
C	-2.99563500	-1.57584700	-1.00610700
C	-3.82987000	-0.46520600	-1.20103600
C	-3.54671100	-2.86750500	-1.01322500
C	-5.19938100	-0.63940100	-1.35040400
H	-3.40376200	0.53979800	-1.20042100
C	-4.90586300	-3.03894900	-1.20935500
H	-2.89521100	-3.72862800	-0.87707900
C	-5.73309900	-1.92420300	-1.36331300

H	-5.83273700	0.23969400	-1.45080300
H	-5.33020100	-4.04101200	-1.23195200
H	-6.80536300	-2.06519000	-1.49516000
H	-1.27051300	-0.34389500	-1.13453900

**TS10<sub>a</sub>**

C	4.29187200	-2.98919000	-1.13890700
C	3.65415100	-1.93697300	-1.79840800
C	2.30006300	-1.70093200	-1.62651800
C	1.53464200	-2.48680600	-0.75387800
C	2.16740800	-3.55833500	-0.11007800
C	3.52165900	-3.80027800	-0.30508400
H	4.23404500	-1.26131900	-2.42947000
H	1.83439800	-0.84628200	-2.11119200
H	1.60185900	-4.21777200	0.54612300
H	3.99403200	-4.63869300	0.20897300
Pd	-0.26034800	-0.10960200	0.17869400
P	-1.47562700	1.81978700	0.65197600
C	-0.88785900	-2.04626300	-1.61543200
C	0.09673300	-2.19444700	-0.55400300
C	-0.70014900	-2.49870700	0.62064800
C	-2.10517300	-2.36300600	-1.07997800
O	-1.98652100	-2.76972900	0.22429000
C	-2.51798500	2.04505500	-0.84324100
C	-3.90662400	2.18030300	-0.79741700
C	-1.85917700	2.05789400	-2.08189700
C	-4.63307400	2.32819000	-1.97731200
H	-4.42787500	2.16864100	0.15982800
C	-2.59177900	2.21284400	-3.25303600
H	-0.77241100	1.93446600	-2.10877600
C	-3.97864500	2.34856400	-3.20420800
H	-5.71665300	2.42889800	-1.93281400
H	-2.07506700	2.22684700	-4.21198600
H	-4.54841200	2.46949600	-4.12503600
C	-2.68649900	1.79632300	2.02143100
C	-3.39699500	0.61173800	2.24699800
C	-2.95231100	2.91454600	2.81395900
C	-4.36727600	0.55263400	3.23888800
H	-3.18694400	-0.26796600	1.63256400
C	-3.91452500	2.84774200	3.81817500
H	-2.40255600	3.84081900	2.64867900
C	-4.62416400	1.67090000	4.02948600
H	-4.91708300	-0.37254100	3.40292400
H	-4.11041700	3.72221400	4.43659100

H	-5.37643300	1.62059900	4.81503300
C	-0.57361300	3.39711900	0.78344000
C	-1.15914500	4.61079500	0.40460700
C	0.75156900	3.37860000	1.21864300
C	-0.42419800	5.78795900	0.47103800
H	-2.18965100	4.62920700	0.04629400
C	1.49308800	4.55428100	1.26255600
H	1.22196600	2.43171400	1.47949200
C	0.90396300	5.75861200	0.89262900
H	-0.88256600	6.73022600	0.17468300
H	2.53880900	4.51739900	1.56391500
H	1.48489500	6.67927300	0.91879400
C	-3.46100800	-2.30275700	-1.60688400
C	-4.41068200	-3.26585200	-1.24110600
C	-3.84106000	-1.25802200	-2.45893800
C	-5.70316400	-3.20038800	-1.74178500
H	-4.12086800	-4.06985800	-0.56648400
C	-5.13716200	-1.19818600	-2.95635400
H	-3.12835800	-0.46781700	-2.69986800
C	-6.06885800	-2.16989500	-2.60557300
H	-6.43141200	-3.95832100	-1.45764400
H	-5.42047500	-0.37125300	-3.60621300
H	-7.08422200	-2.11990300	-2.99550900
C	2.82219200	0.88182100	0.22997000
C	4.16291300	1.15238600	0.47320000
C	4.91296200	1.85054000	-0.46528700
C	4.30596600	2.28946600	-1.63769900
C	2.96629600	2.01985200	-1.87951700
C	2.17688300	1.30104700	-0.95488100
H	2.24239300	0.29871800	0.95317400
H	4.63893500	0.80854000	1.39118100
H	4.90282200	2.84803600	-2.35816800
H	2.49135500	2.35553400	-2.80109800
O	0.92188200	1.02525000	-1.23615800
O	6.23658900	2.17176300	-0.23798800
B	7.21404700	1.24937600	-0.05750800
O	8.45482500	1.75472600	0.23752400
H	9.14532400	1.09205700	0.32347700
O	6.93629900	-0.09278000	-0.17564100
H	7.68599300	-0.66531900	0.01229300
C	-0.59927000	-1.66459400	-3.02534600
H	-1.45343200	-1.88179900	-3.67706600
H	-0.36166500	-0.59274900	-3.10312500
H	0.27188200	-2.21614300	-3.40328800

C	5.75650400	-3.23391300	-1.33929300
H	6.31260600	-2.28864800	-1.29149000
H	6.15994400	-3.91762200	-0.58153900
H	5.95741500	-3.67987300	-2.32409900
C	-0.26657200	-3.18072000	1.86022000
C	0.68816200	-2.59060700	2.69181700
C	-0.77523100	-4.44083300	2.17882600
C	1.15129500	-3.26737700	3.81113200
H	1.06564900	-1.59651100	2.44506800
C	-0.31577700	-5.11067900	3.30790000
H	-1.52139800	-4.89759200	1.53191500
C	0.65148800	-4.53030600	4.12166700
H	1.90003400	-2.80316800	4.45024400
H	-0.71505000	-6.09429900	3.54948300
H	1.01097400	-5.05769800	5.00355200
H	-1.02776900	-1.09625600	1.21129600

**IM8**

Pd	-0.67086600	0.74919500	-0.14527400
P	-2.52565400	-0.67810100	-0.17392900
C	-2.07438300	-2.44126500	-0.07995800
C	-2.51380700	-3.27932600	0.94668900
C	-1.22070100	-2.94836200	-1.06383500
C	-2.09783900	-4.60639300	0.98746700
H	-3.17542600	-2.89264300	1.72126700
C	-0.81222600	-4.27538100	-1.02392800
H	-0.85831000	-2.29196200	-1.85620900
C	-1.24358500	-5.10314600	0.00822900
H	-2.43700500	-5.25257500	1.79566800
H	-0.12007300	-4.65048100	-1.77573000
H	-0.90553500	-6.13703200	0.05262600
C	-3.48099900	-0.34661200	1.34897100
C	-2.77279500	-0.28034500	2.55767100
C	-4.86225500	-0.14438700	1.34042700
C	-3.45454800	-0.02350200	3.74078800
H	-1.69187000	-0.44573400	2.54892200
C	-5.53442600	0.12231600	2.53040500
H	-5.41773300	-0.19238700	0.40383800
C	-4.83280900	0.18148700	3.72925000
H	-2.90450000	0.02221300	4.67949400
H	-6.61149900	0.28200600	2.51759600
H	-5.36036300	0.38889600	4.65922000
C	-3.76788400	-0.60537800	-1.51370800
C	-4.55362900	-1.72072200	-1.82298800

C	-3.98898400	0.59584600	-2.19053300
C	-5.54483900	-1.63110900	-2.79404900
H	-4.38802300	-2.66244200	-1.29899600
C	-4.98654500	0.68564800	-3.15548900
H	-3.36568700	1.46025300	-1.95772100
C	-5.76349800	-0.42799700	-3.45942400
H	-6.14835500	-2.50529000	-3.03307800
H	-5.15086100	1.62692500	-3.67748000
H	-6.53895900	-0.35941600	-4.22084100
C	1.56522700	-1.64969700	-0.31052500
C	2.44979300	-2.66758800	-0.64475900
C	2.75558500	-3.65537300	0.28250200
C	2.15572000	-3.62497200	1.53889900
C	1.27653300	-2.60543200	1.87303800
C	0.96002100	-1.57548700	0.96070800
H	1.32514600	-0.88185700	-1.04925700
H	2.91594300	-2.68714800	-1.62985300
H	2.39048000	-4.41724200	2.24912400
H	0.80232700	-2.58019000	2.85424400
O	0.13128100	-0.61183100	1.31849000
O	3.59185900	-4.71176900	-0.01934600
B	4.84594700	-4.59289000	-0.51852200
O	5.49186500	-5.77910600	-0.76563700
H	6.37486400	-5.68290800	-1.13228400
O	5.40199700	-3.35487600	-0.74702900
H	6.31297800	-3.39252400	-1.05264100
P	1.09426500	2.30664300	-0.10371600
C	1.65682600	2.79038000	1.56893100
C	1.53034900	1.85834000	2.60554500
C	2.23660600	4.03782500	1.82053000
C	1.99448500	2.17807800	3.87839500
H	1.07314800	0.88559500	2.39940600
C	2.68895300	4.35047100	3.09731500
H	2.32963200	4.77151900	1.02030300
C	2.57014700	3.42049400	4.12611800
H	1.89934300	1.44941400	4.68190700
H	3.13549300	5.32516300	3.28835500
H	2.92541200	3.66742900	5.12566100
C	0.86010400	3.90724400	-0.95712300
C	1.90437000	4.56827500	-1.61010100
C	-0.39105800	4.52342300	-0.86998000
C	1.69554500	5.82360300	-2.17354300
H	2.88558800	4.09801800	-1.67985100
C	-0.59454500	5.78218800	-1.42339600

H	-1.20859900	4.00336600	-0.36902200
C	0.44769000	6.43187900	-2.07856500
H	2.51249900	6.32851200	-2.68668700
H	-1.57256300	6.25469700	-1.34814500
H	0.28647000	7.41447400	-2.51939900
C	2.55619000	1.55046300	-0.89607300
C	2.53394800	1.33782000	-2.28013600
C	3.59008900	1.00530400	-0.13432000
C	3.53804700	0.59580500	-2.88880800
H	1.71610700	1.74306700	-2.87904800
C	4.58401500	0.24715000	-0.74522200
H	3.60065200	1.14116500	0.94658800
C	4.55921300	0.04123400	-2.11905800
H	3.51437000	0.43478000	-3.96552900
H	5.36334500	-0.21038800	-0.13911600
H	5.32819100	-0.56786200	-2.59136200
H	-1.38031500	1.70979600	-1.17202500

## F

P	1.53600100	1.76724200	-0.13684400
Pd	-0.31252100	0.49501200	-0.51168400
P	0.58678500	-1.75011100	0.05544900
C	2.37946600	-2.02544100	0.36886600
C	2.95164100	-1.61382200	1.58048100
C	3.21181100	-2.56890100	-0.61392800
C	4.31532800	-1.75762300	1.80690200
H	2.32706400	-1.18635200	2.36516300
C	4.57748800	-2.71103300	-0.38569100
H	2.79032000	-2.88934900	-1.56660500
C	5.13307500	-2.31112800	0.82474100
H	4.73685300	-1.43589100	2.75864300
H	5.20955000	-3.13850000	-1.16308600
H	6.20109900	-2.42958200	1.00323600
C	0.24223900	-2.91250400	-1.31410000
C	0.23334800	-4.29688300	-1.12523900
C	0.04113300	-2.39159900	-2.59380100
C	0.03553000	-5.14851900	-2.20513100
H	0.37655700	-4.71220000	-0.12718600
C	-0.15148100	-3.24596100	-3.67517100
H	0.01319300	-1.30995300	-2.73247600
C	-0.15370100	-4.62321700	-3.48114200
H	0.02525600	-6.22634500	-2.05074500
H	-0.31308700	-2.83191600	-4.66902500
H	-0.31131100	-5.29216000	-4.32587200

C	-0.21964900	-2.49490800	1.52524100
C	-1.50672200	-2.05302500	1.85179900
C	0.37905500	-3.49046700	2.30666900
C	-2.17978500	-2.59693700	2.94103500
H	-1.98795400	-1.29320900	1.23693000
C	-0.29807100	-4.03093200	3.39463400
H	1.38385000	-3.84175200	2.07091200
C	-1.57719800	-3.58371700	3.71433500
H	-3.18173400	-2.24400200	3.17881300
H	0.17728500	-4.80542300	3.99489500
H	-2.10435800	-4.00788700	4.56767600
C	2.00661900	1.77557300	1.63176900
C	3.13917000	2.44513300	2.10866500
C	1.16715800	1.12496100	2.54058000
C	3.45809400	2.40615600	3.46083100
H	3.77128000	3.00985700	1.42228300
C	1.47809100	1.10028600	3.89722300
H	0.26461700	0.62971200	2.17372700
C	2.63244000	1.72652800	4.35463000
H	4.34823700	2.91867200	3.82189500
H	0.81657400	0.58676600	4.59277800
H	2.88275100	1.70271100	5.41400200
C	2.94800400	1.14345900	-1.11599200
C	2.68163500	0.91337100	-2.47251600
C	4.22446900	0.88340400	-0.61838600
C	3.68050400	0.44756300	-3.31715400
H	1.67807500	1.09939900	-2.86109000
C	5.22205000	0.40992700	-1.46679800
H	4.44237900	1.02338100	0.43897600
C	4.95506200	0.19635300	-2.81398600
H	3.46276700	0.27509900	-4.36983400
H	6.21137500	0.19840400	-1.06334600
H	5.73787100	-0.17425300	-3.47395400
C	1.50768300	3.55842100	-0.52852400
C	0.39332100	4.30224000	-0.12990300
C	2.58242200	4.20610000	-1.14089100
C	0.35875300	5.67537800	-0.33249500
H	-0.45546400	3.79444300	0.33108400
C	2.54019700	5.58178700	-1.35223900
H	3.45405300	3.63445800	-1.46060700
C	1.43184200	6.31674300	-0.94693400
H	-0.51447400	6.24591700	-0.02111100
H	3.37757100	6.07879000	-1.83961000
H	1.39951200	7.39192600	-1.11529900



C	-3.49172500	0.82812300	0.39966400
C	-4.78599700	1.16767900	0.77988500
C	-5.87786000	0.54745200	0.18846700
C	-5.66655900	-0.42747800	-0.78397100
C	-4.37707000	-0.76337800	-1.16617600
C	-3.24713100	-0.14277400	-0.59127800
H	-2.63318800	1.31973500	0.86500900
H	-4.96429900	1.91810500	1.54942400
H	-6.52179700	-0.91742800	-1.24715600
H	-4.20420700	-1.52397100	-1.92656400
O	-2.04393200	-0.53678900	-0.96917700
O	-7.13816500	0.87430100	0.64380500
B	-8.18999400	1.21527300	-0.14174700
O	-9.35579000	1.49015700	0.53030700
H	-10.09507000	1.71814800	-0.03970200
O	-8.05277000	1.27111100	-1.50631200
H	-8.84290200	1.55394900	-1.97509200
H	-0.99691900	1.86824500	-0.90873400

### TS11

P	-2.02980900	1.44433800	-0.21834600
Pd	-0.29014500	0.35075500	-1.22204100
P	0.04048400	-1.82092400	-0.04945200
C	-1.14671800	-2.50822300	1.16755500
C	-2.45946700	-2.75178200	0.74286400
C	-0.81427700	-2.74307600	2.50223500
C	-3.41031500	-3.24644200	1.62560100
H	-2.73384800	-2.56125900	-0.29681700
C	-1.77112900	-3.23042700	3.38971000
H	0.19948700	-2.54571400	2.85069200
C	-3.06613500	-3.48944300	2.95447300
H	-4.42362400	-3.44009200	1.27615800
H	-1.49735900	-3.41477100	4.42792500
H	-3.80901100	-3.87864900	3.64943700
C	1.64279200	-1.84086800	0.83558300
C	2.45324800	-2.97521000	0.93675800
C	2.07388000	-0.64007500	1.40650700
C	3.67701800	-2.90153400	1.59448200
H	2.13320700	-3.91540000	0.48642800
C	3.29424200	-0.56903300	2.06763500
H	1.46342200	0.25554100	1.28595600
C	4.09958200	-1.69999000	2.15740200
H	4.30974800	-3.78590300	1.65701400
H	3.64128300	0.37997100	2.47387900

H	5.07011100	-1.63538900	2.64697000
C	0.20197100	-3.16280500	-1.28946000
C	0.65951100	-2.79311500	-2.56046200
C	-0.08164500	-4.50644900	-1.02598100
C	0.83862500	-3.75938900	-3.54561400
H	0.88020600	-1.74283200	-2.77879900
C	0.09305100	-5.46753100	-2.01676300
H	-0.44348600	-4.80200000	-0.04039200
C	0.55380800	-5.09482500	-3.27637000
H	1.19553300	-3.46309100	-4.53071300
H	-0.13197400	-6.51172200	-1.80364500
H	0.68850400	-5.84849400	-4.05103300
C	-3.69573400	0.86856000	-0.71958900
C	-4.87011200	1.48846000	-0.28021200
C	-3.78480600	-0.23451400	-1.57162300
C	-6.11041800	1.00029600	-0.67353300
H	-4.81357200	2.36170800	0.37087200
C	-5.02695800	-0.72421400	-1.96504500
H	-2.86268700	-0.69599600	-1.93430900
C	-6.18948600	-0.10820000	-1.51375300
H	-7.01987100	1.48902100	-0.32758900
H	-5.08413000	-1.58262200	-2.63240900
H	-7.16211700	-0.48604500	-1.82526200
C	-1.95142500	1.14962700	1.58708100
C	-0.79056800	1.57375100	2.24717700
C	-2.91567800	0.43540600	2.29865400
C	-0.59729300	1.28528200	3.59132100
H	-0.02699600	2.12613500	1.69291300
C	-2.71955700	0.14686300	3.64779100
H	-3.82161500	0.09459600	1.79796300
C	-1.56320300	0.56687600	4.29399900
H	0.31356400	1.61357500	4.09001100
H	-3.47454500	-0.42017900	4.19032700
H	-1.40864600	0.33083700	5.34576100
C	-2.15395400	3.27332200	-0.33153800
C	-1.74061700	3.89118700	-1.51391700
C	-2.67323900	4.06074500	0.70195400
C	-1.86211300	5.26725600	-1.67249800
H	-1.31083000	3.27975400	-2.30917800
C	-2.78646500	5.43848000	0.54598200
H	-2.97952500	3.59587700	1.63980400
C	-2.38486800	6.04256300	-0.64180700
H	-1.53579700	5.73584200	-2.59945900
H	-3.18631300	6.04319700	1.35854900

H	-2.47091800	7.12151400	-0.76045000
C	3.46035300	-0.19895800	-1.83820700
C	4.57570400	-0.02727600	-1.03045300
C	4.71236500	1.12227400	-0.26073300
C	3.73519700	2.11008000	-0.31401100
C	2.62098600	1.94419200	-1.12813800
C	2.45463600	0.78112100	-1.90164100
H	3.33945800	-1.10759300	-2.42744000
H	5.33882800	-0.80127100	-0.95709400
H	3.85038100	3.00976600	0.28965500
H	1.84978700	2.71629900	-1.17062900
O	1.39399600	0.58088400	-2.70053400
O	5.77472900	1.20907700	0.61398100
B	6.72007200	2.18534100	0.55989700
O	7.69118300	2.11016500	1.52533300
H	8.35257600	2.80581700	1.47741900
O	6.65432600	3.14958500	-0.41132100
H	7.37831900	3.78197000	-0.40180400
H	0.18001200	1.44950000	-2.28951700

### IM9

P	-0.99610200	2.15364600	-0.06566400
Pd	0.11060200	0.11377500	-0.66590000
P	-1.59162700	-1.55176200	-0.11253700
C	-3.33178800	-1.21280000	0.40354200
C	-4.20251000	-0.72109100	-0.57663900
C	-3.81069500	-1.37614000	1.70481400
C	-5.51130100	-0.38110400	-0.26141800
H	-3.84831700	-0.60238000	-1.60148300
C	-5.12706800	-1.04468000	2.01970600
H	-3.15205400	-1.75939000	2.48382000
C	-5.97694300	-0.53848100	1.04298100
H	-6.17218800	0.00442100	-1.03609100
H	-5.48735300	-1.18461200	3.03852400
H	-7.00341400	-0.27403400	1.29265100
C	-0.87236400	-2.33790400	1.37826200
C	-0.54873100	-3.69092400	1.47322500
C	-0.57953300	-1.49063100	2.45728100
C	0.04314000	-4.19082300	2.63067500
H	-0.74071400	-4.36044700	0.63602400
C	-0.00847200	-1.99671700	3.61774300
H	-0.80469600	-0.42365300	2.39168600
C	0.30433200	-3.35144300	3.70718400
H	0.30855600	-5.24594800	2.68190700

H	0.19737500	-1.32332400	4.44925500
H	0.76117000	-3.74929000	4.61234000
C	-1.88091000	-2.91430200	-1.30722400
C	-1.27832800	-2.83786900	-2.56347300
C	-2.72618000	-3.99305400	-1.02140200
C	-1.49552400	-3.83134100	-3.51523600
H	-0.63569600	-1.98412500	-2.78698200
C	-2.93677300	-4.98912900	-1.96659200
H	-3.22358300	-4.04836800	-0.05181800
C	-2.31986300	-4.90929300	-3.21406600
H	-1.02098100	-3.75964400	-4.49278500
H	-3.58997000	-5.82871000	-1.73369800
H	-2.49011900	-5.68829500	-3.95578400
C	-2.54375400	2.45936400	-1.00792700
C	-3.50185600	3.40340200	-0.62368200
C	-2.70726800	1.78064600	-2.21777800
C	-4.61906900	3.63359800	-1.41715400
H	-3.37358400	3.96312900	0.30367000
C	-3.81592200	2.02594300	-3.02376900
H	-1.95476600	1.04685700	-2.52055500
C	-4.77755200	2.94502200	-2.61840600
H	-5.36504100	4.36208600	-1.10310100
H	-3.92926400	1.49427400	-3.96755300
H	-5.64879100	3.13576800	-3.24326700
C	-1.47252700	2.11629000	1.70302000
C	-0.44430000	2.22033600	2.65273500
C	-2.75995100	1.79323900	2.13936400
C	-0.70381800	2.03273000	4.00384400
H	0.57301400	2.44441500	2.32672800
C	-3.01539200	1.59669100	3.49535400
H	-3.57090600	1.68199300	1.41889100
C	-1.99372400	1.71756200	4.42948900
H	0.10400000	2.12709400	4.72815600
H	-4.02464600	1.34084800	3.81515700
H	-2.19773100	1.56270400	5.48777600
C	-0.18514400	3.79086500	-0.28893700
C	0.49631700	3.98009800	-1.49616800
C	-0.23678300	4.83649300	0.63447400
C	1.11152900	5.19323500	-1.77711100
H	0.56805800	3.15070200	-2.20402900
C	0.39534100	6.04626900	0.35939200
H	-0.76451500	4.70671300	1.57930300
C	1.06687400	6.22725600	-0.84513700
H	1.64096200	5.32697500	-2.71913600

H	0.35823200	6.85247000	1.09070600
H	1.56071500	7.17442400	-1.05660800
C	3.24196900	0.96259900	-0.81573800
C	2.15543800	0.21813100	-1.03752700
C	1.78106800	-1.06560200	-1.42798100
C	4.53984300	0.37754000	-1.28984600
O	4.62286000	-0.24823100	-2.33371100
C	5.77180000	0.56364000	-0.45755600
C	5.73577700	0.63196800	0.93713900
C	7.00857400	0.56591300	-1.10814900
C	6.91612200	0.71084300	1.66819800
H	4.77739200	0.59138100	1.45475300
C	8.18609200	0.66991500	-0.38144500
H	7.01943300	0.47538000	-2.19269100
C	8.14158300	0.74186700	1.00919100
H	6.87934000	0.74666000	2.75586200
H	9.14498200	0.68492400	-0.89739600
H	9.06560800	0.81339000	1.58128700
C	3.23532700	2.33659000	-0.20926200
H	3.66608900	3.08247200	-0.89479000
H	2.20796600	2.64558500	0.01039100
H	3.81765400	2.39801500	0.71903600
C	2.12931500	-2.29084000	-0.68918000
C	1.99368400	-3.53638400	-1.31589600
C	2.63313500	-2.26083000	0.61932100
C	2.36032800	-4.70981800	-0.66675900
H	1.61108000	-3.57623400	-2.33686000
C	2.99996800	-3.43160700	1.26598800
H	2.72317800	-1.30045200	1.12808200
C	2.86898800	-4.66383000	0.62716700
H	2.25447800	-5.66509600	-1.17995200
H	3.38500200	-3.38390500	2.28420900
H	3.16000800	-5.58107800	1.13777400
H	1.56440700	-1.21820300	-2.49111700

**TS12**

P	1.39142100	-2.07367200	-0.44781900
Pd	-0.05670500	-0.18444500	-0.38861900
P	1.23211700	1.69324600	0.37873900
C	2.91994800	1.51007500	1.09095400
C	3.98588000	1.23258600	0.22446600
C	3.17034800	1.56255200	2.46391200
C	5.27175700	1.05036800	0.71599000
H	3.80877400	1.17010400	-0.85082800

C	4.45687400	1.36053600	2.95733200
H	2.35445400	1.76788800	3.15702300
C	5.51254200	1.11718000	2.08648900
H	6.08938900	0.85038300	0.02434700
H	4.63251700	1.40160600	4.03171200
H	6.51983600	0.97055000	2.47430400
C	0.32242800	2.53591400	1.74316300
C	0.36211900	3.91198000	1.97915200
C	-0.48465100	1.73332100	2.55690000
C	-0.40015800	4.47461600	2.99927200
H	0.97832000	4.55448700	1.34998600
C	-1.23742700	2.29236700	3.58407400
H	-0.53530800	0.66077600	2.34970400
C	-1.20175700	3.66772600	3.80182000
H	-0.36863400	5.55057500	3.16671200
H	-1.86337500	1.65532100	4.20786600
H	-1.80052400	4.11099200	4.59620600
C	1.49695100	3.04231100	-0.84580700
C	0.64031000	3.07430800	-1.94915700
C	2.47921700	4.03276800	-0.72435000
C	0.74653500	4.08120000	-2.90356900
H	-0.12212500	2.29900300	-2.04847200
C	2.59180100	5.03440400	-1.68264600
H	3.16526600	4.01539500	0.12343200
C	1.72424300	5.06141600	-2.77239600
H	0.06200500	4.09389400	-3.75097300
H	3.36078300	5.79877700	-1.57775100
H	1.81648200	5.84653100	-3.52174200
C	2.66192400	-2.15436300	-1.77686200
C	3.40505800	-3.30257200	-2.06929300
C	2.89346500	-0.99305300	-2.52060600
C	4.37343800	-3.28144800	-3.06693400
H	3.22136800	-4.22312900	-1.51378300
C	3.86564100	-0.96898700	-3.51635400
H	2.29118100	-0.10434000	-2.31310800
C	4.60880200	-2.11320400	-3.78806100
H	4.94589200	-4.18187000	-3.28576700
H	4.03580200	-0.05650600	-4.08606800
H	5.36702300	-2.09895300	-4.56972800
C	2.37845000	-2.15194200	1.10075400
C	1.66447900	-2.14516200	2.30714800
C	3.77296100	-2.16088100	1.14605200
C	2.32885600	-2.17770000	3.52584100
H	0.57270700	-2.11736300	2.28214300

C	4.43895400	-2.18229100	2.36988400
H	4.34948900	-2.14010900	0.22117800
C	3.72173400	-2.19798500	3.55959900
H	1.75846900	-2.18311300	4.45385500
H	5.52819900	-2.17826500	2.38846700
H	4.24540400	-2.21684700	4.51450100
C	0.65680100	-3.76392200	-0.49722400
C	-0.52580300	-3.92061500	-1.22615300
C	1.20525000	-4.87647200	0.14982500
C	-1.13368200	-5.16685100	-1.33313100
H	-0.97731600	-3.04094300	-1.69022100
C	0.59196100	-6.12174600	0.05072500
H	2.11373500	-4.76582400	0.74363900
C	-0.57416900	-6.26997100	-0.69473200
H	-2.05438200	-5.27429400	-1.90486000
H	1.02683800	-6.98069100	0.56038400
H	-1.05301200	-7.24534500	-0.76949100
C	-3.07412900	-0.88971000	0.24353600
C	-2.11573500	-0.23823600	-0.50656200
C	-2.64914600	0.54497100	-1.55481800
C	-4.38466600	-0.63246700	-0.29639000
O	-4.47843900	0.09771700	-1.32971500
C	-5.64778100	-1.18737300	0.23360200
C	-5.84935100	-1.41978700	1.59836900
C	-6.69770500	-1.43274100	-0.66003700
C	-7.07111300	-1.90023200	2.05521600
H	-5.05716100	-1.19647300	2.30991200
C	-7.90872800	-1.93204500	-0.20429300
H	-6.54126600	-1.22261900	-1.71586500
C	-8.09851800	-2.16677700	1.15585600
H	-7.22146400	-2.06521200	3.12080100
H	-8.71290200	-2.13058000	-0.91080400
H	-9.05158200	-2.55109200	1.51605400
C	-2.75899900	-1.82933800	1.36676800
H	-3.47819800	-2.65511400	1.44352500
H	-1.76597900	-2.26538400	1.19223000
H	-2.72507800	-1.32923700	2.34824800
C	-2.72650100	2.01421600	-1.50808400
C	-2.89902100	2.73199100	-2.69409000
C	-2.66065900	2.70697600	-0.29305600
C	-2.98944200	4.11937600	-2.67389800
H	-2.96156500	2.19071800	-3.63899800
C	-2.75173900	4.09076600	-0.27394900
H	-2.51009200	2.15523700	0.63554100

C	-2.91102700	4.80100000	-1.46355800
H	-3.11808700	4.66840300	-3.60558600
H	-2.68095200	4.61723300	0.67689900
H	-2.97035200	5.88801300	-1.44526600
H	-2.57263000	0.12420000	-2.56309400

**IM10**

P	-1.80073200	1.80449600	-0.49471800
Pd	0.06629000	0.34125700	-0.35381200
P	-0.87931900	-1.67172400	0.55770300
C	-2.49170100	-1.78471900	1.44648500
C	-3.68028300	-1.81360700	0.70395700
C	-2.57659000	-1.76081800	2.84042200
C	-4.91429000	-1.86407700	1.34073400
H	-3.64026900	-1.81004000	-0.38688700
C	-3.81405300	-1.79534500	3.47736400
H	-1.66694200	-1.73384700	3.44006100
C	-4.98519300	-1.85951000	2.73160300
H	-5.82597600	-1.90196800	0.74543900
H	-3.85881200	-1.78109100	4.56565500
H	-5.95241200	-1.89832700	3.23111900
C	0.30708400	-2.30867200	1.81589500
C	0.72262500	-3.63849800	1.90057300
C	0.87611400	-1.36680800	2.68241300
C	1.69478500	-4.01639000	2.82506300
H	0.30088400	-4.38360300	1.22599800
C	1.83067000	-1.74691800	3.61785000
H	0.57209800	-0.31988400	2.59763700
C	2.24987200	-3.07444900	3.68415600
H	2.01934000	-5.05546000	2.87145400
H	2.25966800	-1.00400400	4.28955300
H	3.01121700	-3.37212300	4.40357400
C	-1.02911300	-3.06566000	-0.63339300
C	-0.35386900	-2.95167100	-1.85137800
C	-1.77026500	-4.22632300	-0.37617000
C	-0.42030200	-3.97107000	-2.79719100
H	0.23937700	-2.05496500	-2.04665400
C	-1.83366200	-5.24560100	-1.31945200
H	-2.30551500	-4.32850500	0.56864700
C	-1.16120400	-5.11747700	-2.53317200
H	0.11742700	-3.86581100	-3.73872300
H	-2.41320400	-6.14313000	-1.10718500
H	-1.21842700	-5.91449000	-3.27342700
C	-3.08745100	1.45410900	-1.76357700



C	-4.06896900	2.37083300	-2.15415500
C	-3.06774500	0.19215800	-2.36502500
C	-5.01972300	2.02413500	-3.10802300
H	-4.08657100	3.36821800	-1.71338400
C	-4.02086700	-0.15830900	-3.31667200
H	-2.28176300	-0.51342500	-2.08620000
C	-4.99972100	0.75769200	-3.68774700
H	-5.77816200	2.74765500	-3.40394400
H	-3.98876500	-1.14567300	-3.77529100
H	-5.74382200	0.48951800	-4.43640800
C	-2.73889500	1.86148600	1.08506300
C	-2.00997600	2.16960100	2.24222500
C	-4.09880300	1.57596400	1.20462900
C	-2.63190000	2.21613200	3.48263100
H	-0.94175100	2.38201500	2.16016500
C	-4.71986800	1.61158200	2.45160500
H	-4.68101600	1.31377800	0.32095000
C	-3.99281200	1.93653100	3.58995100
H	-2.05314200	2.46923300	4.37010900
H	-5.78097700	1.37691700	2.52923500
H	-4.48225100	1.96561600	4.56247400
C	-1.45508000	3.59690100	-0.76119200
C	-0.32991700	3.93074500	-1.51940100
C	-2.25734900	4.62324900	-0.25019900
C	-0.02852100	5.26154300	-1.78997200
H	0.31797100	3.12789400	-1.87806300
C	-1.95145400	5.95444800	-0.51397700
H	-3.12106400	4.37723600	0.36972500
C	-0.84006100	6.27501400	-1.28883900
H	0.85017800	5.50918900	-2.38408900
H	-2.58174400	6.74534300	-0.10930100
H	-0.60053200	7.31774400	-1.49307900
C	2.96046300	1.23900600	0.31803600
C	2.06527900	0.58794300	-0.57079100
C	2.94536100	0.06128600	-1.65189300
C	4.25367400	1.12189000	-0.17306600
O	4.32674300	0.46295000	-1.32969600
C	5.52531600	1.62475200	0.33400400
C	5.71967700	1.89798700	1.69494100
C	6.59182800	1.82083200	-0.55596500
C	6.94334000	2.37356400	2.14737700
H	4.91806800	1.70845600	2.40529200
C	7.80853700	2.30542600	-0.10035600
H	6.44626600	1.59117200	-1.60886200

C	7.98797200	2.58560800	1.25229800
H	7.08449700	2.57363100	3.20813300
H	8.62423400	2.46215700	-0.80406900
H	8.94477900	2.96214900	1.61037000
C	2.52703100	2.00171700	1.52756800
H	3.15017100	2.88639200	1.71473100
H	1.49262200	2.33773200	1.37208700
H	2.53621700	1.38657500	2.44106800
C	2.95639800	-1.43000800	-1.85014000
C	3.01222000	-1.96085500	-3.13673900
C	2.96711900	-2.29439400	-0.75208300
C	3.07669400	-3.33804700	-3.33251300
H	3.01117400	-1.28630000	-3.99379900
C	3.03115800	-3.66811000	-0.94673800
H	2.90938800	-1.88548500	0.25838200
C	3.08549600	-4.19325800	-2.23642100
H	3.12159500	-3.74162000	-4.34340700
H	3.02755100	-4.33206500	-0.08302300
H	3.12973600	-5.27125300	-2.38484300
H	2.72168900	0.56220200	-2.60669800

### TS13

C	-2.73721700	3.75462900	2.48219800
C	-2.34197500	4.02225400	1.16906600
C	-1.72444400	3.04791800	0.39068500
C	-1.48341400	1.76054100	0.88877300
C	-1.87472900	1.49684500	2.20461000
C	-2.49299700	2.47686200	2.98335500
H	-2.53003600	5.01160200	0.74582900
H	-1.45871400	3.28868400	-0.64025700
H	-1.74961900	0.50065500	2.63558100
H	-2.80141100	2.23615700	4.00293400
Pd	-0.67182600	0.40861300	-0.38633100
P	-2.83136500	-0.57662000	-0.57660900
C	1.83755200	2.30029900	-0.80885100
C	1.20776500	1.23954300	-0.03802500
C	2.25656900	0.76004300	0.78407700
C	3.13340300	2.39814300	-0.39091800
O	3.40534200	1.46327400	0.57182700
C	-3.10282300	-1.97615700	-1.72957600
C	-4.25570900	-2.76486300	-1.62097000
C	-2.18708100	-2.22335900	-2.75477700
C	-4.49268400	-3.78475800	-2.53181000
H	-4.97370500	-2.57561600	-0.82183000

C	-2.43240000	-3.25118700	-3.66485900
H	-1.26983300	-1.63281600	-2.80622600
C	-3.57955900	-4.02729500	-3.55743000
H	-5.39101300	-4.39394100	-2.44351100
H	-1.71283500	-3.44537400	-4.45862200
H	-3.76505500	-4.82877600	-4.27133100
C	-3.26452500	-1.32476600	1.04179000
C	-2.25326400	-2.04086000	1.69249100
C	-4.52116100	-1.22757500	1.64122000
C	-2.49600900	-2.64721000	2.91937600
H	-1.25809400	-2.10151700	1.24391300
C	-4.75835200	-1.82387700	2.87711100
H	-5.31838400	-0.67234900	1.14720900
C	-3.74829200	-2.53253500	3.51800900
H	-1.70126700	-3.20745400	3.41047100
H	-5.73985800	-1.73203200	3.33992800
H	-3.93564900	-2.99709100	4.48491500
C	-4.21270400	0.55725900	-0.98658000
C	-4.80656700	0.52317100	-2.25272700
C	-4.61692600	1.54274300	-0.07624300
C	-5.79065600	1.44511100	-2.59563600
H	-4.50024700	-0.23044300	-2.97749800
C	-5.60524400	2.45692900	-0.42099200
H	-4.15665800	1.60313800	0.90933600
C	-6.19548200	2.41113000	-1.68061200
H	-6.24449900	1.40282700	-3.58456700
H	-5.90535500	3.21483200	0.30192800
H	-6.96774900	3.13003800	-1.95009300
C	4.25751200	3.22513800	-0.80628300
C	4.04045900	4.51490600	-1.30622200
C	5.56905900	2.74339600	-0.70776600
C	5.11202300	5.29903500	-1.71329000
H	3.02865600	4.91485300	-1.34564400
C	6.63575300	3.53243800	-1.11453200
H	5.74031200	1.74172200	-0.31766700
C	6.41145000	4.81003700	-1.62174700
H	4.93131500	6.30214400	-2.09541700
H	7.65088700	3.14654300	-1.03820600
H	7.25094600	5.42614400	-1.93903400
C	2.65823100	-1.22786400	-1.86422800
C	3.73487100	-2.01513500	-1.45310600
C	3.51127400	-3.12956800	-0.65556900
C	2.20704400	-3.46371900	-0.28492600
C	1.13869600	-2.68457600	-0.69206300

C	1.32278400	-1.54013000	-1.50819400
H	2.81922200	-0.36600500	-2.51546400
H	4.74906600	-1.75998600	-1.75680200
H	2.05634300	-4.34717400	0.33464100
H	0.11724500	-2.94845900	-0.41105100
O	0.32622100	-0.78365800	-1.89952000
O	4.51989800	-3.97804400	-0.25979100
B	5.73001100	-3.63844200	0.24545800
O	6.58386700	-4.68545500	0.47322300
H	7.43955600	-4.43977900	0.83532000
O	6.03998400	-2.32262900	0.51545200
H	6.92073300	-2.19388600	0.88043900
C	1.16886100	3.02181200	-1.92583400
H	1.89037600	3.37387800	-2.67394600
H	0.45916100	2.34400400	-2.41847800
H	0.60087300	3.89432500	-1.57146200
C	-3.38697700	4.81280900	3.32479600
H	-2.64971100	5.52480200	3.72343500
H	-4.11537500	5.39938400	2.74852100
H	-3.91208100	4.37578200	4.18369100
C	2.29839800	-0.28068100	1.81659100
C	3.45805700	-1.03966800	1.99025700
C	1.16188600	-0.54827800	2.58130600
C	3.47314700	-2.06524300	2.92581400
H	4.33188200	-0.85705300	1.36770800
C	1.18625200	-1.57445100	3.51737900
H	0.27496100	0.06740500	2.44467400
C	2.33940500	-2.33632000	3.68781800
H	4.37397400	-2.66428100	3.04851600
H	0.30351600	-1.76804100	4.12553100
H	2.35580900	-3.14317200	4.41900400
H	1.92867100	0.16622000	-0.35060300

**3<sub>a</sub>**

C	-4.36122300	-2.06686500	0.17415100
C	-3.91499700	-1.12151700	1.10290400
C	-2.62764000	-0.60968000	1.04407500
C	-1.73893900	-1.01747800	0.04075800
C	-2.18322700	-1.96408700	-0.88661300
C	-3.47357200	-2.47821600	-0.81936700
H	-4.59272900	-0.78733300	1.89000500
H	-2.29421300	0.12282400	1.77916300
H	-1.50949600	-2.28710800	-1.68083300
H	-3.80262800	-3.20989400	-1.55831300

C	0.82689000	-1.27718000	-0.01634200
C	-0.36959800	-0.48543900	-0.02552700
C	0.03221600	0.83015200	-0.04429600
C	1.87277400	-0.38907300	-0.02366300
O	1.39021900	0.88555900	-0.03407000
C	-0.65547400	2.11074000	-0.11605500
C	-1.97688600	2.20457800	-0.57582800
C	0.01309200	3.28713900	0.25067600
C	-2.61247300	3.43635200	-0.64519900
H	-2.50192500	1.30508000	-0.89204100
C	-0.62653200	4.51676700	0.17363200
H	1.04249500	3.22528900	0.59806600
C	-1.94345300	4.59817500	-0.26942000
H	-3.63793100	3.48978600	-1.00752800
H	-0.09099300	5.41937300	0.46426800
H	-2.44377900	5.56334600	-0.32810300
C	0.88226700	-2.76406900	0.08111300
H	1.02375900	-3.24552900	-0.89833800
H	1.70464400	-3.09472600	0.72856600
H	-0.05395900	-3.15667300	0.49661000
C	3.31762800	-0.53033300	0.00482700
C	3.93777700	-1.73327900	-0.36267200
C	4.12684400	0.54740800	0.39431500
C	5.32026300	-1.85876700	-0.31859400
H	3.33388800	-2.56893400	-0.71039400
C	5.50760700	0.41815600	0.42938700
H	3.65628100	1.48817100	0.67283000
C	6.11246400	-0.78640700	0.07916000
H	5.78256700	-2.80060300	-0.61036000
H	6.11818200	1.26620900	0.73588100
H	7.19598000	-0.88630000	0.11027800
C	-5.74795800	-2.63035000	0.26304100
H	-5.84445600	-3.32632400	1.10839500
H	-6.49597300	-1.84076100	0.41388500
H	-6.01856500	-3.18073400	-0.64625000
<b>3<sub>a</sub>'</b>			
C	0.67936200	1.89205300	-0.06197200
C	-0.74225200	1.92088600	-0.06980000
C	-1.17943200	0.62614500	-0.02465800
C	1.02626700	0.56198900	-0.00889300
O	-0.10487300	-0.20325200	0.00864200
C	2.28816800	-0.15480300	0.00282500
C	3.48981900	0.49348100	0.32382500

C	2.32866900	-1.52364000	-0.30283800
C	4.69143400	-0.20262200	0.32245500
H	3.48212600	1.54513500	0.60184700
C	3.53153400	-2.21457200	-0.29687900
H	1.40257700	-2.03791400	-0.55071400
C	4.72061300	-1.55836500	0.01131600
H	5.61258500	0.31908600	0.57783400
H	3.54148500	-3.27608000	-0.53974200
H	5.66357500	-2.10225500	0.01336300
C	1.56721700	3.08831800	-0.13497800
H	2.40128400	2.93663600	-0.83277300
H	1.00228200	3.96372000	-0.47744200
H	2.00110900	3.34706200	0.84181400
C	-2.49754400	0.02240600	0.00491700
C	-2.65762900	-1.36490600	0.11218400
C	-3.64104100	0.82974400	-0.06597500
C	-3.92807000	-1.92425400	0.15082700
H	-1.77526700	-1.99885600	0.16849700
C	-4.90727800	0.26597200	-0.02649100
H	-3.53188700	1.91030500	-0.15341400
C	-5.05803900	-1.11468600	0.08339100
H	-4.03606900	-3.00443000	0.23655700
H	-5.78466000	0.90852800	-0.08053400
H	-6.05227900	-1.55668800	0.11642900
H	-1.35865300	2.81289400	-0.10640100

**1b**

C	2.23375900	0.52628000	-0.27086700
C	2.49870100	-0.68180400	0.16852700
C	2.77804300	-1.86923900	0.62366700
H	2.77157100	-2.74558700	-0.02426300
C	0.91623600	1.21489700	-0.20192200
O	0.89793700	2.43442400	-0.19488800
C	-0.34500000	0.42767800	-0.11556100
C	-0.47209000	-0.87186000	-0.61274400
C	-1.45968900	1.05868700	0.44638200
C	-1.69126600	-1.53515500	-0.53183900
H	0.37766600	-1.35573500	-1.08964100
C	-2.67093000	0.38991700	0.54266100
H	-1.34745900	2.07963500	0.80590400
C	-2.78753800	-0.90965400	0.05370400
H	-1.78762000	-2.54283100	-0.93245800
H	-3.53012600	0.88252300	0.99470300
H	-3.73979300	-1.43343400	0.12268900

H	3.02248600	-2.03135600	1.67300000
H	3.04842600	1.17291600	-0.60287500
<b>C<sub>b</sub></b>			
C	3.71289700	-2.19977100	2.95093700
C	2.80342800	-1.30497200	3.51262100
C	1.86702700	-0.63529100	2.72259500
C	1.81054200	-0.85370900	1.34445600
C	2.72838700	-1.74225200	0.77591900
C	3.66222300	-2.40274000	1.56893400
H	2.82417000	-1.12956000	4.59007200
H	1.15604600	0.04146200	3.20280000
H	2.70720700	-1.94464700	-0.29822400
H	4.36558700	-3.09921200	1.10768800
Pd	0.43550600	0.13150300	0.23239100
P	-0.68993400	-1.84082800	-0.37471400
C	2.87168900	1.30037200	-1.27709600
C	2.07132900	1.60268900	-0.28034800
C	1.36949900	2.15026600	0.72030500
C	3.91628100	2.22874500	-1.80378700
O	4.18306300	2.19883600	-2.99147600
C	-2.43973400	-1.58251600	-0.80929900
C	-2.93175500	-1.70619100	-2.10867000
C	-3.30949000	-1.22980400	0.22797900
C	-4.28133400	-1.48106800	-2.36488400
H	-2.26334500	-1.97536400	-2.92562300
C	-4.65540900	-1.00781100	-0.03168100
H	-2.92884300	-1.11532900	1.24407400
C	-5.14109200	-1.12969200	-1.33021700
H	-4.65936100	-1.57694200	-3.38150600
H	-5.32020300	-0.70894000	0.77666300
H	-6.19315300	-0.93897000	-1.53568900
C	0.18299400	-2.23638500	-1.92952100
C	0.26654200	-1.22444500	-2.89919400
C	0.85115300	-3.44556000	-2.13082600
C	0.99512000	-1.44072100	-4.06228000
H	-0.23050800	-0.26680000	-2.71911200
C	1.58542700	-3.64959700	-3.29701700
H	0.80585300	-4.22789500	-1.37391200
C	1.65632700	-2.65173400	-4.26206600
H	1.05888500	-0.65325300	-4.81117200
H	2.10518100	-4.59448600	-3.44727100
H	2.23348100	-2.81324400	-5.17096500
C	-0.74866800	-3.39511800	0.58653800

C	-1.48770100	-4.47047400	0.07340000
C	-0.11569800	-3.52769300	1.82322200
C	-1.57192000	-5.66278700	0.77885800
H	-2.00361700	-4.36625800	-0.88215900
C	-0.20942800	-4.72351400	2.53120800
H	0.44918700	-2.69499900	2.23756300
C	-0.93154100	-5.79031900	2.01023900
H	-2.14607300	-6.49318000	0.37145600
H	0.28645100	-4.81510500	3.49607800
H	-1.00272800	-6.72442900	2.56529700
C	4.60207800	3.16302000	-0.87174200
C	4.75312500	2.89730000	0.49288500
C	5.16663800	4.32125000	-1.41539400
C	5.44356000	3.79104700	1.30343700
H	4.36017500	1.97194200	0.91410800
C	5.83884900	5.22041800	-0.60155200
H	5.05935700	4.49490100	-2.48435200
C	5.97638300	4.95617100	0.75997700
H	5.57124500	3.57433700	2.36256800
H	6.26217300	6.12893900	-1.02638800
H	6.51036700	5.65814800	1.39863000
C	-2.30907600	1.79376800	0.79436500
C	-3.54241800	2.25212000	1.24663200
C	-4.54907400	2.54855800	0.33757700
C	-4.31405500	2.38349400	-1.02594100
C	-3.08847000	1.92277300	-1.47652200
C	-2.04465600	1.60768900	-0.58004900
H	-1.52382800	1.54569400	1.51532900
H	-3.72909500	2.37969200	2.31261700
H	-5.11850500	2.60914400	-1.72553300
H	-2.90120200	1.78349800	-2.54087000
O	-0.89519700	1.16232700	-1.04615100
O	-5.80595900	2.93957900	0.74924300
B	-6.05737700	4.07593800	1.44964000
O	-7.37472600	4.28510200	1.77070400
H	-7.53863800	5.09003700	2.26951800
O	-5.02954300	4.91924100	1.78647900
H	-5.30172300	5.71405800	2.25379500
C	4.72368300	-2.92058000	3.79378000
H	5.75013800	-2.62092200	3.53986300
H	4.57556700	-2.71651600	4.86140000
H	4.66695400	-4.00851800	3.65142200
H	1.70583700	2.04796000	1.75369500
H	0.55933800	2.84813600	0.50378300



H	2.72714500	0.38991200	-1.86019500
<b>TS6<sub>b</sub></b>			
C	0.01590700	-4.94340300	-1.77567100
C	0.07986900	-3.73338900	-2.47215500
C	0.00568100	-2.51524500	-1.80554500
C	-0.13371300	-2.46888400	-0.41526500
C	-0.23417300	-3.67374500	0.27968200
C	-0.15272700	-4.89377000	-0.39328400
H	0.21114100	-3.74922800	-3.55640700
H	0.09269500	-1.58993800	-2.38003600
H	-0.35273600	-3.67377700	1.36563100
H	-0.21559200	-5.82715000	0.17024900
Pd	-0.13754000	-0.69829500	0.55818800
P	2.22094300	-0.48639200	0.22505200
C	-3.32652700	-0.91948200	0.07834900
C	-2.17842400	-0.93650300	0.77397900
C	-2.18041900	-1.05589700	2.14914000
C	-4.47493100	-1.02256700	0.98242500
O	-4.26431300	-1.09917600	2.20884400
C	2.68042300	1.10756700	-0.52974100
C	3.83531800	1.79727700	-0.15361900
C	1.83837800	1.65117800	-1.50515000
C	4.13951800	3.01853900	-0.74559500
H	4.49088500	1.38501600	0.61367700
C	2.14515900	2.87164100	-2.09443800
H	0.92544600	1.12327200	-1.78646900
C	3.29338300	3.55811400	-1.70966200
H	5.03624300	3.55722700	-0.44318100
H	1.46859500	3.30579600	-2.82859800
H	3.51859100	4.52601400	-2.15462800
C	3.13821800	-0.52652900	1.80415500
C	2.55951400	0.12972200	2.89778400
C	4.40047700	-1.11325800	1.93112300
C	3.24767200	0.19244600	4.10498900
H	1.57527500	0.59503200	2.77787600
C	5.07811200	-1.04940200	3.14483400
H	4.85642500	-1.61840500	1.07945900
C	4.50232300	-0.39743200	4.23138700
H	2.79736500	0.70476400	4.95392000
H	6.06083100	-1.50883400	3.24053900
H	5.03510500	-0.34823800	5.18004100
C	3.00876500	-1.75221400	-0.82912700
C	3.49571300	-1.44792800	-2.10114300

C	2.99801100	-3.08530000	-0.40112600
C	3.95584500	-2.46320000	-2.93631400
H	3.50918000	-0.41402100	-2.44515100
C	3.45956600	-4.09436600	-1.23403100
H	2.60067500	-3.33638200	0.58279800
C	3.93412000	-3.78514000	-2.50724500
H	4.33167200	-2.21589000	-3.92794200
H	3.43218000	-5.12889500	-0.89431500
H	4.28728200	-4.57818200	-3.16499200
C	-5.86298800	-1.03468300	0.48086100
C	-6.15686300	-1.09476900	-0.88562600
C	-6.91227200	-0.98781300	1.40701200
C	-7.47658500	-1.10485200	-1.31715600
H	-5.35705600	-1.14716600	-1.62073700
C	-8.22911400	-0.99267600	0.97363600
H	-6.66672800	-0.94439400	2.46580000
C	-8.51268500	-1.05057600	-0.38948700
H	-7.69754600	-1.15538700	-2.38152800
H	-9.03958100	-0.95052300	1.69881000
H	-9.54691100	-1.05474600	-0.72973100
C	-1.05519300	2.50196400	-0.06222500
C	-1.01598500	3.69087300	-0.78001500
C	-0.10242300	4.68058400	-0.43592700
C	0.75687600	4.48201900	0.64012800
C	0.71986300	3.29415500	1.35467800
C	-0.17704600	2.25911000	1.01595000
H	-1.76762900	1.71996100	-0.33202000
H	-1.69082800	3.85497300	-1.62001100
H	1.47621300	5.26310700	0.88512900
H	1.41289600	3.12170500	2.17919300
O	-0.17674100	1.12492600	1.69529700
O	0.03771300	5.82765700	-1.19085000
B	-0.94975200	6.74327100	-1.37015700
O	-0.62070100	7.81025700	-2.16809000
H	-1.32891000	8.44907700	-2.28551700
O	-2.17074800	6.56497400	-0.77233000
H	-2.80035200	7.27503800	-0.92511500
C	0.15176700	-6.24951700	-2.50162500
H	-0.56257100	-6.33142600	-3.33249400
H	1.15626900	-6.36554200	-2.93599700
H	-0.01793600	-7.10205500	-1.83211800
H	-2.00569800	-0.16701400	2.75973400
H	-2.04664900	-2.02847900	2.62572000
H	-3.40891900	-0.82921300	-0.99981700

**D<sub>b</sub>**

C	-3.22486600	-3.85362200	-1.50102000
C	-2.42748700	-3.01783800	-2.28422400
C	-1.70393900	-1.97135800	-1.71686500
C	-1.73463800	-1.73370100	-0.33945700
C	-2.57060600	-2.54301300	0.43788600
C	-3.29936200	-3.58514600	-0.13349800
H	-2.36643800	-3.19479200	-3.36031200
H	-1.09270500	-1.33972000	-2.36530900
H	-2.64698600	-2.37014900	1.51386800
H	-3.93232500	-4.21234400	0.49904800
Pd	-0.58366000	-0.33098900	0.53707000
P	1.39162300	-1.68434200	0.25919100
C	-3.53494400	0.80167000	0.31581700
C	-2.18555100	0.89027100	0.61683800
C	-1.97476500	2.27515900	1.06840500
C	-4.12819700	2.04393400	0.56603000
O	-3.26833000	2.93775300	1.00844700
C	2.51737000	-0.84950100	-0.91556200
C	3.69334700	-0.23255100	-0.48484400
C	2.11545300	-0.69620300	-2.24921700
C	4.45939500	0.51576400	-1.37394100
H	3.99985900	-0.30701100	0.55772500
C	2.89416600	0.03265600	-3.13936400
H	1.18425600	-1.15060600	-2.59240400
C	4.06664100	0.64348900	-2.70110200
H	5.36032200	1.01443200	-1.02043300
H	2.57647200	0.13591700	-4.17595000
H	4.66743800	1.23388800	-3.39103300
C	2.40945400	-1.95393100	1.75509100
C	2.28000100	-1.07374700	2.83360400
C	3.34682100	-2.99145300	1.81096100
C	3.08558200	-1.23832500	3.95790800
H	1.56501500	-0.24937500	2.76653000
C	4.14296400	-3.15110400	2.93830800
H	3.45137000	-3.67696700	0.96938100
C	4.01146500	-2.27431400	4.01318000
H	2.98651000	-0.54822200	4.79470700
H	4.86913300	-3.96158900	2.97920900
H	4.63702300	-2.40032500	4.89585700
C	1.15589400	-3.38024200	-0.39134400
C	1.75747200	-3.86351000	-1.55381300
C	0.28772400	-4.21336100	0.32285400

C	1.47449900	-5.14901400	-2.00911900
H	2.44822500	-3.23407400	-2.11322100
C	0.01378400	-5.49780500	-0.12729100
H	-0.18976400	-3.84385900	1.23102000
C	0.59834800	-5.96420100	-1.30242000
H	1.94426700	-5.51245200	-2.92195300
H	-0.67296300	-6.13055400	0.43319300
H	0.37345000	-6.96688700	-1.66320000
C	-5.50622800	2.46784300	0.40311100
C	-6.46796500	1.56377200	-0.06730000
C	-5.88052900	3.78522300	0.70148100
C	-7.78186800	1.97259100	-0.23777000
H	-6.18333300	0.53981400	-0.30181200
C	-7.19596400	4.18788100	0.52861400
H	-5.12970700	4.48221900	1.06639100
C	-8.14645100	3.28406500	0.05883000
H	-8.52453100	1.26780000	-0.60569000
H	-7.48305400	5.21158800	0.76012000
H	-9.17806100	3.60387100	-0.07712800
C	1.26729300	2.32807700	-0.33555800
C	2.20002500	3.16238600	-0.94029200
C	3.26469700	3.66828300	-0.20538500
C	3.39071400	3.33419500	1.14027900
C	2.46224600	2.50099300	1.74645500
C	1.37043200	1.96229200	1.02693800
H	0.46674100	1.88453000	-0.93344100
H	2.11822500	3.40362200	-1.99989300
H	4.23911700	3.72851400	1.69888700
H	2.55987600	2.23440100	2.79938200
O	0.50655200	1.17527500	1.63014600
O	4.26149600	4.41924400	-0.79419000
B	4.05680200	5.60076900	-1.42949300
O	5.17890500	6.17469300	-1.97351600
H	5.02032700	7.01376900	-2.41437500
O	2.79810300	6.14346300	-1.49541900
H	2.75514200	6.99539600	-1.93880000
C	-3.94279400	-5.02485700	-2.10403800
H	-3.30021800	-5.91813600	-2.12475000
H	-4.84254100	-5.28902400	-1.53289300
H	-4.24745600	-4.82616900	-3.14001200
H	-1.27504700	2.84763800	0.44011900
H	-1.59363400	2.32943100	2.09676000
H	-4.04558400	-0.08173000	-0.05394600

**TS7<sub>b</sub>**

C	-2.76584500	-4.22808500	-1.41239000
C	-2.37946800	-3.09309100	-2.13594300
C	-1.90939300	-1.95978700	-1.48974900
C	-1.77032400	-1.92886100	-0.09279900
C	-2.20081900	-3.04723400	0.62886900
C	-2.68426600	-4.18008300	-0.02112000
H	-2.44745400	-3.10961200	-3.22529100
H	-1.62229900	-1.08511500	-2.07810700
H	-2.12162800	-3.05407800	1.71833200
H	-2.99549600	-5.04910600	0.56154900
Pd	-0.45633200	-0.53865500	0.72585600
P	1.74836700	-1.39585900	0.17432900
C	-3.26076900	0.59134700	0.01542000
C	-2.38149200	-0.13920900	0.83159500
C	-3.07601000	-0.22453600	2.14099300
C	-4.40992900	0.86618500	0.73209000
O	-4.38503800	0.36423300	1.96698900
C	2.51410400	-0.26610000	-1.04495300
C	3.56838800	0.58481600	-0.71183100
C	1.92840500	-0.16809900	-2.31364700
C	4.02909100	1.52253200	-1.63230500
H	4.01828600	0.53116300	0.27911200
C	2.40443200	0.75324700	-3.23700700
H	1.09653600	-0.82503300	-2.57750200
C	3.45339200	1.60473100	-2.89476900
H	4.83014100	2.20478500	-1.35219100
H	1.94916700	0.81615600	-4.22471200
H	3.81499900	2.34252100	-3.60951800
C	2.98429800	-1.51750600	1.51895400
C	2.77019000	-0.76217700	2.67634800
C	4.14180700	-2.29369700	1.40006800
C	3.71360000	-0.78529700	3.70041400
H	1.87198400	-0.14125500	2.74554100
C	5.07531800	-2.31635900	2.42894300
H	4.31339400	-2.88468000	0.49980200
C	4.86129000	-1.56168700	3.58058400
H	3.54676700	-0.19025800	4.59748200
H	5.97365100	-2.92454300	2.33324900
H	5.59488100	-1.57994500	4.38555700
C	1.83496900	-3.03466300	-0.64639400
C	2.71961500	-3.32970100	-1.68862800
C	0.97548800	-4.03529600	-0.18482900
C	2.73762400	-4.59926300	-2.25803800

H	3.39340100	-2.55808300	-2.06202300
C	0.99063100	-5.30281100	-0.75619700
H	0.27005800	-3.80896300	0.61477400
C	1.87141400	-5.58599900	-1.79546700
H	3.43029200	-4.81700500	-3.06975000
H	0.30281600	-6.06598400	-0.39293500
H	1.88271200	-6.57645400	-2.24833100
C	-5.60113200	1.60259700	0.34860500
C	-5.71941000	2.13867100	-0.94063100
C	-6.64305500	1.78470900	1.26754100
C	-6.85757000	2.84230300	-1.30175600
H	-4.91613500	2.00457800	-1.66274700
C	-7.78011900	2.48946600	0.90045600
H	-6.54538300	1.37037000	2.26814400
C	-7.88967600	3.01961300	-0.38227500
H	-6.94208900	3.25723700	-2.30413800
H	-8.58410700	2.62934700	1.62036400
H	-8.78134000	3.57534500	-0.66707900
C	0.63770200	2.48369600	-0.02910900
C	1.33764100	3.49905100	-0.66347700
C	2.40529800	4.11665500	-0.01936800
C	2.75422800	3.72055800	1.26662500
C	2.05701000	2.70042800	1.90033500
C	0.98443800	2.03557400	1.26499300
H	-0.18335900	1.97744600	-0.54458400
H	1.07247300	3.80818000	-1.67407400
H	3.59539400	4.21212200	1.75487500
H	2.33369800	2.38293600	2.90620200
O	0.36267500	1.04968800	1.87872700
O	3.19729100	5.05222700	-0.65547900
B	2.73642000	6.18460100	-1.24235300
O	3.69521200	6.96951000	-1.83518400
H	3.35266100	7.76856100	-2.24474300
O	1.39701500	6.48559500	-1.22240300
H	1.17393100	7.32981100	-1.62461100
C	-3.23314800	-5.46201700	-2.12285900
H	-3.68660700	-6.18066600	-1.42935000
H	-3.97339200	-5.22947500	-2.89997300
H	-2.39533000	-5.96984600	-2.62281500
H	-2.52885800	0.39737200	2.86760200
H	-3.20412400	-1.22921600	2.55537200
H	-3.07092700	0.88663200	-1.01096200

**E<sub>b</sub>**

C	-4.42813700	0.73649600	3.32144000
C	-4.75386500	0.02069900	2.17354600
C	-3.78184200	-0.65014700	1.43943500
C	-2.44247700	-0.63447600	1.84333900
C	-2.11063400	0.10045100	2.99460700
C	-3.08346100	0.76719300	3.71618100
H	-5.78310800	0.00712000	1.81255500
H	-4.08698700	-1.16658900	0.52795900
H	-1.06896600	0.15923800	3.31287400
H	-2.80210500	1.33518200	4.60438700
Pd	0.05953000	-0.02246300	0.16905400
P	2.19444800	1.01142300	-0.25198000
C	-0.10674400	-1.71148900	1.50478900
C	-1.42035800	-1.32241700	1.06345600
C	-1.77985200	-2.29169500	-0.02894200
C	0.38649900	-2.59680600	0.54061800
O	-0.54798800	-2.97287700	-0.34211100
C	3.36047100	0.60421100	1.11049900
C	4.66586400	0.15137000	0.90986000
C	2.88642200	0.74619600	2.42106500
C	5.48152700	-0.15187500	1.99836500
H	5.04969300	0.03080300	-0.10374900
C	3.69913500	0.44202200	3.50620300
H	1.86385500	1.09722300	2.58133300
C	5.00060200	-0.01280000	3.29577800
H	6.49902200	-0.50214200	1.82806700
H	3.31817500	0.55986500	4.51964900
H	5.63775700	-0.25469300	4.14502100
C	3.10731100	0.44321700	-1.73554500
C	3.00467200	-0.91178300	-2.06781900
C	3.92155200	1.27360900	-2.50879000
C	3.72068000	-1.43443900	-3.13723000
H	2.35400400	-1.55983000	-1.47873200
C	4.62584500	0.75211300	-3.59074600
H	4.00383300	2.33285900	-2.26549000
C	4.53191900	-0.60076000	-3.90281500
H	3.63517600	-2.49417900	-3.37508700
H	5.25287200	1.40789000	-4.19305700
H	5.08686700	-1.00463300	-4.74824600
C	2.29576100	2.83621000	-0.32730700
C	3.43536900	3.54459600	0.07165300
C	1.18914300	3.52633600	-0.83355700
C	3.47233700	4.92920800	-0.04401700
H	4.29717100	3.01038800	0.47432600

C	1.23635700	4.91324200	-0.94857200
H	0.28860700	2.97125900	-1.10682300
C	2.37245500	5.61353800	-0.55672200
H	4.36075500	5.47660600	0.26800100
H	0.37233100	5.44859000	-1.33894900
H	2.40175900	6.69880700	-0.64447600
C	1.69285400	-3.21851600	0.40771800
C	1.91490500	-4.16167300	-0.60557800
C	2.74972000	-2.85482200	1.25342500
C	3.17469700	-4.71973300	-0.77318600
H	1.09247100	-4.44157700	-1.25961600
C	4.00435100	-3.41895700	1.08076200
H	2.59709800	-2.10429300	2.02928100
C	4.22232100	-4.34838500	0.06533300
H	3.33960800	-5.45069400	-1.56294800
H	4.81999300	-3.11819400	1.73584500
H	5.21086500	-4.78326500	-0.07175600
C	-2.48759500	0.22615200	-2.24974000
C	-3.75169300	-0.13184400	-2.70576900
C	-4.88367700	0.42173800	-2.11842900
C	-4.74881100	1.35324500	-1.09278100
C	-3.49117400	1.69799300	-0.62448900
C	-2.31621100	1.14627100	-1.18614000
H	-1.58928600	-0.19074300	-2.71026900
H	-3.87647900	-0.84261500	-3.52225400
H	-5.64670600	1.77879500	-0.64318900
H	-3.37560300	2.39378800	0.20714400
O	-1.13215500	1.49522300	-0.74444000
O	-6.13268600	0.05757600	-2.57915900
B	-6.98675800	-0.69150400	-1.83709600
O	-8.20472300	-0.94711200	-2.40957300
H	-8.80080100	-1.47371100	-1.87041800
O	-6.60126400	-1.14914100	-0.59586500
H	-7.25733400	-1.69913300	-0.15748800
C	-5.47206300	1.46188900	4.11580500
H	-5.62422700	0.99970100	5.10186100
H	-5.18704000	2.50730700	4.29646800
H	-6.43947000	1.46395600	3.59905100
H	-2.15107500	-1.80736000	-0.94607600
H	-2.50657700	-3.05786900	0.28723800
H	0.37798600	-1.49001700	2.45121700
<b>TS8<sub>b</sub></b>			
C	-2.51540300	2.37941900	3.64042100



C	-1.61650400	1.40640100	4.06997100
C	-1.10457700	0.45676000	3.18410100
C	-1.46824500	0.47488600	1.83604000
C	-2.38408600	1.44536700	1.40398700
C	-2.89461200	2.37802700	2.29028600
H	-1.31145000	1.38550300	5.11713600
H	-0.39801000	-0.28546000	3.55789500
H	-2.68336300	1.48157300	0.35383000
H	-3.59293500	3.13693900	1.93288700
Pd	-0.13122700	-0.45227200	0.53177100
P	0.52665100	1.49232200	-0.71613500
C	-3.10029200	-1.49974500	0.54267900
C	-1.89027800	-1.47008100	1.10909900
C	-0.82673300	-2.26191000	1.48620500
C	-3.90811400	-2.73365100	0.62548800
O	-3.57178200	-3.68572600	1.31468700
C	2.08458600	1.39398600	-1.65702500
C	2.13239300	1.32131000	-3.04919400
C	3.27489700	1.38756100	-0.92242700
C	3.36139100	1.24544500	-3.69896300
H	1.21130800	1.32478200	-3.63089400
C	4.49875500	1.31411800	-1.57468600
H	3.24351800	1.42929100	0.16729800
C	4.54184700	1.24074900	-2.96435500
H	3.39329600	1.18814600	-4.78583400
H	5.41933000	1.29376100	-0.99457300
H	5.50127600	1.17176000	-3.47444900
C	-0.82402200	1.48845500	-1.95059800
C	-1.05968000	0.27998500	-2.62593700
C	-1.70033700	2.56016800	-2.13130000
C	-2.14583000	0.16533000	-3.48404600
H	-0.38901200	-0.56668900	-2.45853700
C	-2.79565300	2.43234500	-2.98308700
H	-1.53586900	3.49583500	-1.59684500
C	-3.01837900	1.23890700	-3.66056800
H	-2.31924100	-0.77272700	-4.00908600
H	-3.47693400	3.27138100	-3.11537600
H	-3.87374100	1.14235400	-4.32759800
C	0.58518400	3.18101300	-0.02220800
C	0.89839200	4.27410300	-0.84021200
C	0.35374700	3.38693400	1.33839400
C	0.94565500	5.55535700	-0.30703000
H	1.11189400	4.11360500	-1.89828500
C	0.40313000	4.67232300	1.87138900

H	0.13376400	2.53623000	1.98219200
C	0.69310600	5.75529200	1.04967900
H	1.18835800	6.40144700	-0.94776100
H	0.21412000	4.82038800	2.93406400
H	0.73336200	6.76057100	1.46634300
C	-5.17708100	-2.78079000	-0.16372000
C	-5.46826400	-1.89759200	-1.20735900
C	-6.09627300	-3.78581800	0.15450800
C	-6.66175700	-2.01202900	-1.91141500
H	-4.75321300	-1.12994600	-1.49861300
C	-7.29250600	-3.89171000	-0.53928300
H	-5.84332300	-4.47373300	0.95861900
C	-7.57783700	-3.00321200	-1.57402700
H	-6.87612500	-1.32505900	-2.72846500
H	-8.00611100	-4.67118900	-0.27753300
H	-8.51545700	-3.08697000	-2.12155200
C	2.88417500	-1.49507500	0.80369200
C	4.23250100	-1.69141600	1.08596500
C	5.09981500	-2.09487200	0.07879900
C	4.61057700	-2.28999100	-1.21119500
C	3.26961700	-2.08872900	-1.49384100
C	2.36372800	-1.67994200	-0.49278700
H	2.19991900	-1.17602300	1.59723500
H	4.61516700	-1.53900400	2.09404400
H	5.30771400	-2.59193400	-1.99211200
H	2.88450700	-2.22210300	-2.50423600
O	1.09620900	-1.48308500	-0.80445400
O	6.45317400	-2.24578800	0.29132700
B	7.00503600	-3.03310900	1.25056100
O	8.37670700	-3.04195900	1.27889200
H	8.75513800	-3.58793900	1.97336500
O	6.20526200	-3.74714600	2.10629300
H	6.68140800	-4.31481600	2.71887100
C	-3.07390100	3.40168900	4.58354700
H	-2.61851700	3.32497400	5.57812700
H	-2.90518300	4.42239200	4.21265100
H	-4.15962900	3.28474300	4.70639000
H	-0.45506800	-2.28068000	2.51072400
H	-0.53886800	-3.09043300	0.83790000
H	-3.50590300	-0.61232300	0.06202900
<b>G<sub>b</sub></b>			
C	2.45414100	0.19583900	4.80605800
C	1.36861700	0.91112800	4.29479700

C	0.41024600	0.29552400	3.50260600
C	0.51209300	-1.06375700	3.18490200
C	1.59405700	-1.78318600	3.70133900
C	2.54368200	-1.16360200	4.50268500
H	1.27679000	1.97390200	4.52121500
H	-0.41833900	0.88568600	3.10833400
H	1.67660900	-2.84922700	3.49149100
H	3.37307000	-1.74722200	4.90380600
Pd	-0.80375400	-0.83087900	0.37035200
P	-1.87872500	1.13983300	-0.31760100
C	-0.04492800	-2.68208400	1.35861800
C	-0.48963800	-1.74669200	2.33239300
C	-1.81920900	-1.26711700	2.22499400
C	-0.88696200	-3.73411600	0.73753500
O	-2.01497800	-4.00054200	1.13768000
C	-0.69800300	2.42995400	-0.82188800
C	-0.92687900	3.25378600	-1.92664000
C	0.47697200	2.58122100	-0.07816300
C	0.01244100	4.21695600	-2.28111400
H	-1.83457900	3.13549400	-2.51800000
C	1.41197800	3.54564200	-0.43476200
H	0.67042200	1.92332500	0.77032200
C	1.18133400	4.35973900	-1.53975000
H	-0.16694600	4.85177300	-3.14728300
H	2.33967100	3.63562600	0.12778400
H	1.92481100	5.09939500	-1.83193200
C	-2.95006100	0.88599100	-1.77262200
C	-2.47330300	0.04179000	-2.78344100
C	-4.17938300	1.53337800	-1.92484800
C	-3.23126900	-0.14888400	-3.93336000
H	-1.50468900	-0.44928500	-2.65474400
C	-4.93189300	1.33203200	-3.07761600
H	-4.55061200	2.19650200	-1.14339400
C	-4.45958200	0.49027200	-4.08001000
H	-2.86167600	-0.80838200	-4.71675500
H	-5.89126100	1.83432600	-3.19184000
H	-5.05202200	0.33103500	-4.97971700
C	-2.95521000	1.94527300	0.92162700
C	-2.73692800	3.25028400	1.36672400
C	-4.01837800	1.20776900	1.45831000
C	-3.57007800	3.80818800	2.33422400
H	-1.91563200	3.83530900	0.95400500
C	-4.85458100	1.77109900	2.41264800
H	-4.19384400	0.18650000	1.11457300

C	-4.62805000	3.07356100	2.85573700
H	-3.39084300	4.82627200	2.67612200
H	-5.68282500	1.19169700	2.81686700
H	-5.27960700	3.51299800	3.60912800
C	-0.27868100	-4.50159200	-0.38558000
C	0.78045100	-4.00672800	-1.15378300
C	-0.82411800	-5.75418100	-0.68673400
C	1.29021800	-4.76606300	-2.20147500
H	1.16670000	-3.00373000	-0.97721100
C	-0.30217800	-6.51496800	-1.72178300
H	-1.66161900	-6.10873300	-0.08872900
C	0.75850000	-6.02115900	-2.47997500
H	2.10273900	-4.36867300	-2.80708900
H	-0.72313100	-7.49454300	-1.94336900
H	1.16614000	-6.61571600	-3.29658200
C	2.32785200	-0.12627800	-0.42780000
C	3.50863900	0.60064500	-0.52084900
C	3.79722500	1.31567400	-1.67759800
C	2.89817000	1.29804200	-2.74082600
C	1.71780700	0.57814000	-2.64615800
C	1.39479300	-0.15502200	-1.48552400
H	2.09201300	-0.66179600	0.49532900
H	4.21072700	0.62179800	0.31207300
H	3.13132200	1.88087700	-3.63130200
H	0.99690200	0.58125400	-3.46408700
O	0.26235100	-0.83893100	-1.43772300
O	4.91345700	2.11707000	-1.77411300
B	6.19024500	1.66698700	-1.65089300
O	7.16130000	2.62848900	-1.76709400
H	8.05889200	2.29770000	-1.67436100
O	6.43100600	0.33599200	-1.42799900
H	7.36118000	0.09578000	-1.39228900
C	3.50275600	0.86906000	5.63885700
H	3.13395100	1.80753000	6.07033200
H	3.83821700	0.22609300	6.46259400
H	4.39143800	1.11305400	5.03954100
H	-2.14298100	-0.45135700	2.87147800
H	-2.59237600	-1.95285100	1.88242300
H	1.03267200	-2.81434200	1.25704400

**TS9<sub>b</sub>**

C	-4.25296600	3.75552400	-2.37203700
C	-4.68698200	2.53551500	-1.85134600
C	-3.88144300	1.78125800	-1.01034100

C	-2.60352900	2.22711900	-0.64001900
C	-2.16742700	3.44875800	-1.16960600
C	-2.97512200	4.19239700	-2.01743400
H	-5.67421300	2.15993400	-2.12485100
H	-4.24052900	0.81509500	-0.65414200
H	-1.18118200	3.83376100	-0.91242700
H	-2.60677500	5.14004700	-2.41341800
Pd	-0.09445700	0.12862300	-0.58421800
P	2.13736200	-0.52615800	-0.77212000
C	-0.41790300	1.79352700	0.68064500
C	-1.75275300	1.41128600	0.24356100
C	-2.32947400	0.44600600	1.11442900
C	-0.26997200	1.53316000	2.10122900
O	-1.22742700	1.00641900	2.72025000
C	3.31867600	0.86231400	-0.56479000
C	4.51683500	0.76421700	0.14658600
C	2.99902700	2.06861600	-1.19755700
C	5.38130400	1.85338000	0.21991400
H	4.77573700	-0.16851700	0.64842000
C	3.86188100	3.15614600	-1.12357900
H	2.05816000	2.14776700	-1.74681400
C	5.05546500	3.04967100	-0.41211500
H	6.31432000	1.76578500	0.77502000
H	3.60477900	4.08854300	-1.62383000
H	5.73327300	3.90003400	-0.35453400
C	2.57929600	-1.71023600	0.55050400
C	2.50195700	-1.27847900	1.88021800
C	2.89138100	-3.04499400	0.28474400
C	2.74607600	-2.15992700	2.92378700
H	2.25688300	-0.23868100	2.09742700
C	3.12275100	-3.93063000	1.33491100
H	2.94864700	-3.39640900	-0.74527900
C	3.05288200	-3.49185900	2.65241400
H	2.68870700	-1.80407100	3.95182400
H	3.36055300	-4.97075300	1.11770000
H	3.23473500	-4.18855900	3.46914000
C	2.73048600	-1.33846800	-2.30074700
C	4.08360700	-1.31611500	-2.65904700
C	1.81587000	-2.05766400	-3.07744600
C	4.51864200	-2.00645700	-3.78317200
H	4.80108700	-0.75640300	-2.05894400
C	2.26341000	-2.74975200	-4.20053700
H	0.76041100	-2.06326900	-2.79326700
C	3.60786100	-2.72529900	-4.55443200

H	5.57199400	-1.98395700	-4.05870500
H	1.55003300	-3.30842300	-4.80425100
H	3.95004900	-3.26637900	-5.43566200
C	0.97315700	1.82833900	2.84221600
C	1.09653700	1.34657900	4.15146300
C	2.04020900	2.52500200	2.26410700
C	2.27413200	1.53769200	4.85975900
H	0.25772800	0.80785800	4.58676100
C	3.21467800	2.72245000	2.97931200
H	1.96981100	2.89994200	1.24447000
C	3.33643200	2.22255900	4.27265500
H	2.36726600	1.15053300	5.87303400
H	4.03955600	3.25958600	2.51467900
H	4.26210600	2.36973600	4.82680500
C	-1.70439900	-2.71550300	-0.06679600
C	-2.78022400	-3.13139800	0.71002100
C	-4.07339500	-2.75836500	0.36089300
C	-4.29448300	-2.02376300	-0.80341000
C	-3.22371700	-1.60321000	-1.57576100
C	-1.89133000	-1.89547000	-1.20447900
H	-0.68137600	-2.97881400	0.21048600
H	-2.63043600	-3.73621100	1.60366500
H	-5.31852700	-1.77100000	-1.08175200
H	-3.37907800	-0.99585100	-2.46730100
O	-0.87824700	-1.39053000	-1.87883000
O	-5.12938800	-3.15337000	1.15390700
B	-5.87083800	-2.26480400	1.86445200
O	-6.91411700	-2.79555600	2.57424000
H	-7.42638700	-2.15789100	3.07863300
O	-5.54739000	-0.92557700	1.84253300
H	-6.11787600	-0.37390100	2.38607500
C	-5.13407700	4.57610400	-3.26538400
H	-5.80376400	5.22615700	-2.68348700
H	-4.54545200	5.22641100	-3.92466700
H	-5.77026300	3.94321500	-3.89724000
H	-1.85300700	-0.50761200	1.33605000
H	-3.40915000	0.43600800	1.29811400
H	0.08337000	2.66476500	0.25906500
<b>TS10<sub>b</sub></b>			
C	3.49841700	-3.64245600	1.16770300
C	2.82908700	-3.68472000	-0.05862200
C	1.47438500	-3.41988000	-0.14719100
C	0.73305800	-3.09992600	0.99755600

C	1.39019500	-3.09774600	2.23345100
C	2.75085000	-3.36446200	2.31222700
H	3.39628500	-3.89231100	-0.96643400
H	0.99748900	-3.39460800	-1.12460900
H	0.84111500	-2.86153300	3.14576600
H	3.24807300	-3.34054900	3.28262200
Pd	-0.53838300	-0.47463100	0.76112500
P	-0.94436400	1.77544500	0.37033200
C	-1.55225300	-2.89713800	-0.25078000
C	-0.67287700	-2.70084100	0.87398500
C	-1.55575900	-2.30934000	1.93279200
C	-2.83083800	-2.71055500	0.17704200
O	-2.85321700	-2.45537200	1.52333700
C	-2.24688000	1.72059200	-0.91441500
C	-3.46978200	2.37922700	-0.77770100
C	-2.00923100	0.91565000	-2.03926400
C	-4.45492200	2.22911900	-1.75121200
H	-3.66195700	3.00514100	0.09382400
C	-2.99433600	0.78306600	-3.00977500
H	-1.04991400	0.39525600	-2.12558200
C	-4.22001600	1.43050400	-2.86413100
H	-5.41104000	2.73714600	-1.63425000
H	-2.80944700	0.15573400	-3.88114500
H	-4.99475300	1.30622100	-3.61958400
C	-1.63231900	2.87299000	1.66123900
C	-2.35849400	2.31511700	2.71502800
C	-1.50696700	4.26317800	1.57590100
C	-2.95910100	3.13202100	3.66664500
H	-2.44763900	1.22952800	2.78208100
C	-2.10113000	5.07896900	2.53268200
H	-0.94332800	4.70624000	0.75459400
C	-2.82815500	4.51483800	3.57730200
H	-3.52333100	2.68726700	4.48474400
H	-1.99601700	6.16032300	2.46135300
H	-3.29097300	5.15571500	4.32611600
C	0.42492600	2.72773300	-0.35639300
C	0.29361500	3.45695300	-1.54037700
C	1.65670200	2.69978500	0.30478100
C	1.38507400	4.15270200	-2.05204300
H	-0.66108100	3.47553200	-2.06645900
C	2.74465700	3.39407400	-0.20987600
H	1.76967300	2.10695600	1.21266100
C	2.60863200	4.11904500	-1.38977300
H	1.28009900	4.71554200	-2.97835400

H	3.70934900	3.33612900	0.29155900
H	3.46620500	4.64710600	-1.80354800
C	-4.10396300	-2.70400300	-0.51817200
C	-5.31115600	-2.64441100	0.18825800
C	-4.13573900	-2.75720700	-1.91773200
C	-6.52072000	-2.64326900	-0.49411000
H	-5.29202300	-2.59997400	1.27487200
C	-5.34631800	-2.75586800	-2.59350900
H	-3.20157300	-2.77919300	-2.47792100
C	-6.54418900	-2.70047500	-1.88427700
H	-7.45333900	-2.59799700	0.06584300
H	-5.35612700	-2.79324900	-3.68149100
H	-7.49430000	-2.69817200	-2.41569400
C	2.71842500	-0.31350200	0.12934400
C	4.06831000	0.01556600	0.12211900
C	4.66287900	0.48427900	-1.04409700
C	3.89333300	0.62731700	-2.19542300
C	2.54583400	0.29867600	-2.18648500
C	1.91013700	-0.18327600	-1.02136300
H	2.26029900	-0.68922200	1.04745800
H	4.66670800	-0.09522400	1.02657700
H	4.36907200	1.01638000	-3.09545300
H	1.93653800	0.42754600	-3.08163200
O	0.63099900	-0.49494700	-1.04782600
O	5.98111300	0.89383300	-1.08775600
B	7.04902000	0.17178300	-0.67337900
O	8.26474600	0.79448100	-0.80812100
H	9.01593100	0.27644800	-0.50677200
O	6.88931700	-1.09486700	-0.15850200
H	7.71513500	-1.53072800	0.07237200
C	4.98209600	-3.83678700	1.22566800
H	5.33951500	-3.92225300	2.25948200
H	5.29292900	-4.74034300	0.68348400
H	5.49651100	-2.98364300	0.75678400
H	-1.47294200	-0.70193000	2.07517400
H	-1.40919700	-2.47924000	2.99598900
H	-1.24242300	-3.11583600	-1.26530600
<b>3<sub>b</sub></b>			
C	-4.87435700	-0.38965900	-0.03936400
C	-3.94048100	-1.37398600	0.29269400
C	-2.58192600	-1.09451800	0.32322500
C	-2.10451100	0.18406200	0.01414200
C	-3.03813400	1.16680900	-0.33141500



C	-4.39662200	0.88413000	-0.35189800
H	-4.28930500	-2.37855100	0.53672100
H	-1.87624900	-1.87546700	0.60609100
H	-2.68971800	2.16093700	-0.61177400
H	-5.10544400	1.66559700	-0.62858800
C	0.42144600	-0.43066900	-0.05981600
C	-0.67342300	0.48506100	0.05457600
C	-0.09306700	1.71027400	0.21997800
C	1.57055900	0.30027600	0.03587300
O	1.25556700	1.61456300	0.21054200
C	2.98194300	-0.03875800	-0.01246600
C	3.96080600	0.95721500	0.08681000
C	3.38660300	-1.37223700	-0.15503500
C	5.30833400	0.62469800	0.04647400
H	3.65313000	1.99476100	0.19726000
C	4.73430900	-1.69894700	-0.19566400
H	2.63536400	-2.15771700	-0.23283600
C	5.70233200	-0.70252400	-0.09424000
H	6.05806400	1.41025900	0.12738900
H	5.03207000	-2.74043700	-0.30617800
H	6.75932700	-0.96104000	-0.12459000
C	-6.34246200	-0.69488600	-0.04633600
H	-6.91130600	0.07648000	-0.57973200
H	-6.55149600	-1.66010800	-0.52608300
H	-6.74650000	-0.75180000	0.97453500
H	-0.49313900	2.70260200	0.38354400
H	0.35257800	-1.50007000	-0.22532300