

*Electronic Supplementary Information*  
*for*

**Mechanism and Origin of Regioselectivity in Rh-Catalyzed Desymmetric  
[2+2+2] Cycloaddition: Charge versus  $\pi$ - $\pi$  Stacking Interaction**

Boming Shen,<sup>a</sup> Yu Chen,<sup>a</sup> and Peiyuan Yu<sup>\*,a</sup>

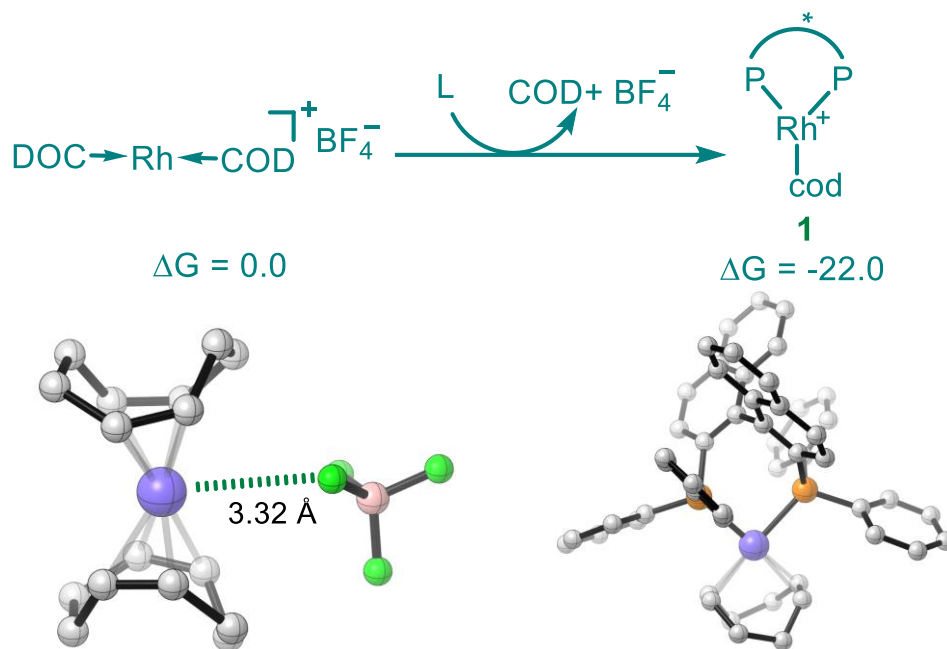
*<sup>a</sup> Department of Chemistry and Shenzhen Grubbs Institute, Guangdong Provincial Key  
Laboratory of Catalysis, Southern University of Science and Technology, Shenzhen  
518055, China*

**Table of Content**

<b>1. Calculated the thermodynamic stability of cationic Rh(I) species relative to the neutral Rh(I) species.....</b>	<b>S2</b>
<b>2. Comparison of different configurations of 3-ts, 3'-ts, 9-ts and 14-ts.....</b>	<b>S3</b>
<b>3. Calculated energies barrier differences of key transition states with various density functionals.....</b>	<b>S4</b>
<b>4. B3LYP-D3(BJ) and M06-D3 calculated absolute energies of all structures.....</b>	<b>S5</b>
<b>5. Cartesian coordinates for DFT-optimized structures for all the optimized compounds and transition state.....</b>	<b>S6</b>

## 1. Calculated the thermodynamic stability of cationic Rh(I) species, relative to the neutral Rh(I) species.

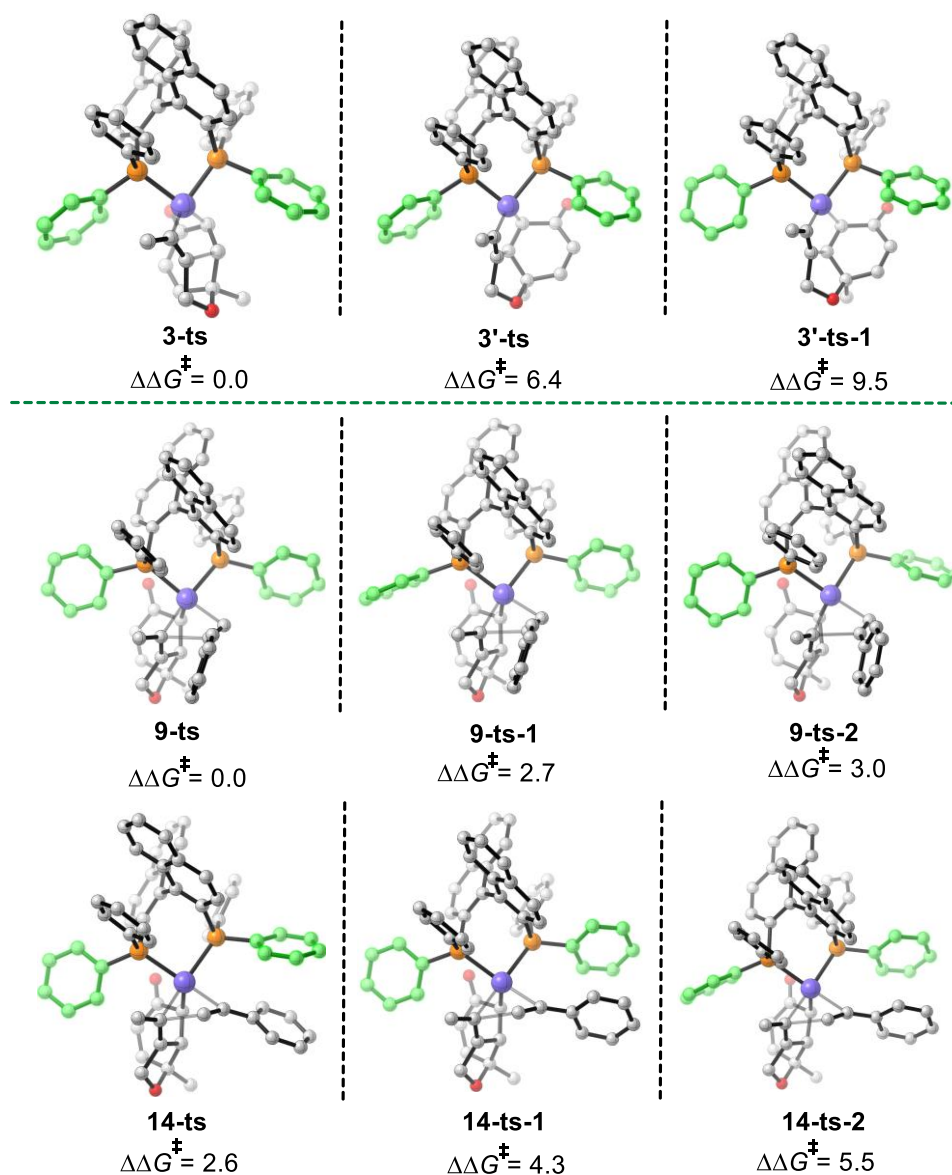
we have calculated the thermodynamic stability of cationic Rh(I) species relative to the precursor Rh(cod)2BF<sub>4</sub>. As shown in Fig. S1, Neutral Rh(cod)2BF<sub>4</sub> species can undergo ligand exchange with the (S)-BINAP ligand to afford a cationic Rh(I) species 1 with dissociation of the anionic BF<sub>4</sub>, which is exergonic by 22.0 kcal/mol. DFT calculation indicates that cationic Rh(I) species 1 is thermodynamically more favored than neutral Rh(cod)2BF<sub>4</sub> species. Therefore, the cationic Rh(I) species 1 was used as starting point for catalytic cycle.



**Fig. S1:** The values given by kcal/mol are the relative free energies calculated by M06-D3/6-311+G(d,p)/SMD(dichloroethane)//B3LYP-D3(bj)/6-31G(d)/SMD(dichloroethane) (LANL08(f) for Rh) method.

## 2. Comparison of different configurations of 3-ts, 3'-ts, 9-ts and 14-ts

The exploration of conformers and isomers are indeed important, especially for the investigation of selectivity-related problems. We have considered various conformations for the key transition states to ensure that they represent the corresponding lowest energy conformations. For example, by rotating the dihedral angle of the phenyl substituents on the catalyst, initial conformational structures were searched and optimized for the enantio- and regioselectivity-controlling transition states **3-ts**, **3'-ts**, **9-ts** and **14-ts**.



**Fig. S2:** Different configurations of the transition states transition states **3-ts**, **3'-ts**, **9-ts** and **14-ts**. Values are given in kcal/mol.

### 3. Calculated energies barrier differences of key transition states with various density functionals

we tried using various density functionals to calculate the energy barrier differences ( $\Delta\Delta G$ ) for key enantio- and regioselectivity-controlling transition states. As shown in Table S1, based on the optimized geometrical structures in the solution phase, the calculated solvation single-point energy barrier differences ( $\Delta\Delta G$ ) showed small differences between each other. Therefore, the reported energy data is reliable.

**Table S1.** The calculated energy barrier differences ( $\Delta\Delta G$ ) in key transition states determined enantio- and regioselectivity by using various density functionals in dichloroethane. Values are given in kcal/mol.

Energy Functionals	$\Delta\Delta G$ ( $\Delta G_{3'-ts} - \Delta G_{3-ts}$ )	$\Delta\Delta G$ ( $\Delta G_{14-ts} - \Delta G_{9-ts}$ )	$\Delta\Delta G$ ( $\Delta G_{TS2-CN} - \Delta G_{TS1-CN}$ )
<b>M06-D3</b>	6.4	2.6	-0.8
<b>M06</b>	6.4	2.9	-0.5
<b>M06L</b>	5.8	2.3	-1.1
<b><math>\omega</math>B97XD</b>	6.2	3.5	-0.9
<b>M11L</b>	6.0	3.1	-0.6

**4.SMD(dichloroethane)/M06-D3/6-311+G(d,p)//SMD(dichloroethane)/B3LYP-D3(BJ)/6-31G(d) (LANL08(f) basis set for Rh atom) calculated absolute energies of all structures.**

**Table S2.** SMD(dichloroethane)/M06-D3/6-311+G(d,p)//SMD(dichloroethane)/B3LYP-D3(BJ)/6-31G(d) (LANL08(f) basis set for Rh atom) calculated absolute energies of all structures. Values are given in Hartree.

Geometry	E <sub>(elec-B3-LYP-D3BJ)</sub> <sup>1</sup>	H <sub>(corr-B3-LYP-D3BJ)</sub> <sup>2</sup>	G <sub>(corr-B3-LYP-D3BJ)</sub> <sup>3</sup>	E <sub>(solv-M06-D3)</sub> <sup>4</sup>	IF <sup>5</sup>
<b>Rh(cod)<sub>2</sub>BF<sub>4</sub></b>	-1158.243075	0.407571	0.332553	-1157.815142	-
<b>(S)-BINAP</b>	-2378.924863	0.661812	0.552146	-2377.810506	-
<b>BF<sub>4</sub><sup>-</sup></b>	-424.585560	0.019724	-0.013174	-424.615059	-
<b>1</b>	-2800.535645	0.859011	0.733899	-2799.1666	-
<b>1a</b>	-576.782914	0.215908	0.162156	-576.50943	-
<b>COD</b>	-312.067812	0.189477	0.149693	-311.864837	-
<b>2</b>	-3065.241549	0.886230	0.749717	-3063.78866	-
<b>3-ts</b>	-3065.232588	0.885178	0.752063	-3063.77858	199.79i
<b>4</b>	-3065.277191	0.886288	0.757764	-3063.812443	-
<b>3'-ts</b>	-3065.223126	0.885405	0.754129	-3063.770514	174.23i
<b>3'-ts-1</b>	-3065.219448	0.885230	0.753669	-3063.765144	147.16i
<b>4'</b>	-3065.265146	0.885937	0.757444	-3063.801523	-
<b>5-ts</b>	-3065.176806	0.883831	0.750461	-3063.715065	268.29i
<b>1b</b>	-308.421894	0.117083	0.07925	-308.233925	-
<b>6</b>	-3373.685909	1.006913	0.854227	-3372.048248	-
<b>7-ts</b>	-3373.659126	1.004422	0.851103	-3372.006726	294.68i
<b>8</b>	-3373.709748	1.006809	0.858972	-3372.051655	-
<b>9-ts</b>	-3373.702155	1.006212	0.861339	-3372.041721	254.33i
<b>9-ts-1</b>	-3373.696173	1.005943	0.859562	-3372.035699	223.42i
<b>9-ts-2</b>	-3373.695088	1.005840	0.859726	-3372.035264	242.25i
<b>10</b>	-3373.780081	1.010642	0.864422	-3372.119567	-
<b>11-ts</b>	-3373.754666	1.008206	0.864260	-3372.105262	295.83i
<b>12</b>	-3373.821621	1.011786	0.867006	-3372.176721	-
<b>13</b>	-885.359844	0.340982	0.277294	-884.881369	-
<b>14-ts</b>	-3373.693627	1.006206	0.860961	-3372.037195	331.75i
<b>14-ts-1</b>	-3373.694534	1.006614	0.863731	-3372.037227	105.49i
<b>14-ts-2</b>	-3373.689506	1.006824	0.862348	-3372.033940	131.12i
<b>15</b>	-3373.776533	1.010249	0.865796	-3372.115042	-
<b>16-ts</b>	-3373.745912	1.007547	0.862116	-3372.097353	286.53i
<b>17</b>	-3373.813782	1.010899	0.865008	-3372.170522	-
<b>18</b>	-885.363543	0.341028	0.277403	-884.884846	-
<b>1c</b>	-387.237259	0.192624	0.141120	-387.027541	-
<b>1d</b>	-155.994927	0.091227	0.056469	-155.897719	-
<b>6-a</b>	-2952.884660	0.879454	0.740089	-2951.428937	-

<b>7-a-ts</b>	-2952.854762	0.879211	0.746291	-2951.384067	292.75 <i>i</i>
<b>1e</b>	-157.241845	0.114899	0.080695	-157.133205	-
<b>2-a</b>	-2875.685060	0.862626	0.731958	-2874.308481	-
<b>3-a-ts</b>	-2875.671341	0.860755	0.731191	-2874.294256	222.43 <i>i</i>
<b>2-b</b>	-2801.691438	0.877720	0.743760	-2800.324656	-
<b>3-b-ts</b>	-2801.656782	0.876415	0.745305	-2800.280211	261.81 <i>i</i>
<b>TS1-OMe</b>	-3488.233952	1.041068	0.889194	-3486.538856	259.08 <i>i</i>
<b>TS2-OMe</b>	-3488.223533	1.041122	0.889353	-3486.534780	377.61 <i>i</i>
<b>TS1- Nap</b>	-3527.366733	1.054906	0.902529	-3525.607536	231.64 <i>i</i>
<b>TS2- Nap</b>	-3527.357207	1.055900	0.905518	-3525.602288	374.16 <i>i</i>
<b>TS1-Me</b>	-3413.026385	1.034714	0.884529	-3411.338696	233.66 <i>i</i>
<b>TS2-Me</b>	-3413.017548	1.036186	0.887867	-3411.333970	341.13 <i>i</i>
<b>TS1-Br</b>	-5944.510477	0.996747	0.845527	-5945.461959	218.87 <i>i</i>
<b>TS2-Br</b>	-5944.503975	0.997662	0.847741	-5945.459616	361.20 <i>i</i>
<b>TS1-Cl</b>	-3833.298059	0.996927	0.847695	-3831.636169	219.89 <i>i</i>
<b>TS2-Cl</b>	-3833.291137	0.997295	0.847667	-3831.633960	374.64 <i>i</i>
<b>TS1-F</b>	-3472.934157	0.998348	0.850907	-3471.282637	223.27 <i>i</i>
<b>TS2-F</b>	-3472.925642	0.998228	0.849754	-3471.279749	377.69 <i>i</i>
<b>TS1-CN</b>	-3465.947689	1.005594	0.859395	-3464.253079	222.84 <i>i</i>
<b>TS2-CN</b>	-3465.942394	1.006389	0.857122	-3464.252140	359.49 <i>i</i>
<b>TS1-COOMe</b>	-3601.589705	1.053088	0.896554	-3599.868874	217.76 <i>i</i>
<b>TS2-COOMe</b>	-3601.584000	1.052929	0.894837	-3599.867995	394.92 <i>i</i>
<b>TS1-CF<sub>3</sub></b>	-3710.740203	1.013966	0.859302	-3709.075779	203.61 <i>i</i>
<b>TS2-CF<sub>3</sub></b>	-3710.734246	1.013646	0.857977	-3709.074731	363.56 <i>i</i>

<sup>1</sup>The electronic energy calculated by B3LYP-D3(BJ) in solution phase. <sup>2</sup>The thermal correction to enthalpy calculated by B3LYP-D3(BJ) in solution phase. <sup>3</sup>The thermal correction to Gibbs free energy calculated by B3LYP-D3(BJ) in solution phase. <sup>4</sup>The electronic energy calculated by M06-D3 in dichloroethane solvent. <sup>5</sup>The B3LYP-D3(BJ) calculated imaginary frequencies for the transition states.

## 5. Cartesian coordinates for DFT-optimized structures for all the optimized compounds and transition states

### Rh(cod)<sub>2</sub>BF<sub>4</sub>

C	7.07514400	1.99653900	-1.45535900
C	8.46871000	2.48592600	-1.13916800
C	8.72323600	3.95537600	-1.53073000
C	7.53950200	4.86771400	-1.25791500
C	6.54103900	5.19608500	-2.16591500
C	6.39849800	4.66743700	-3.57514000
C	6.76140900	3.17516200	-3.73302400
C	6.31407500	2.32825900	-2.55862700
H	7.64379700	5.50065900	-0.38127100
H	5.96123400	6.09494600	-1.95886300
H	7.00597000	5.27237700	-4.26474900
H	5.35613400	4.79510100	-3.87481300
H	6.25141600	2.80053400	-4.62319300
H	7.83466900	3.04827900	-3.89298400
H	5.38407500	1.78448000	-2.70595500
H	6.75328400	1.13536400	-0.87491100
H	9.21082500	1.83441900	-1.62452800
H	8.62094600	2.37242800	-0.06004900
H	9.57857400	4.32334200	-0.95488700
H	9.00547900	4.02712600	-2.58374000
Rh	5.65137000	3.65478700	-0.82266700
C	5.18842300	5.26607800	0.70458300
C	5.55782100	4.70004500	2.05557700
C	5.10064200	3.24508300	2.27507100
C	5.27268500	2.37169000	1.04553500
C	4.29363600	2.12706800	0.09547400
C	2.90304200	2.72031400	0.07156700
C	2.83684800	4.21493500	0.45825000
C	4.03171600	5.02229100	-0.01171400
H	6.13238400	1.70824700	1.06687000
H	4.42251100	1.25691500	-0.54585900
H	2.24002100	2.14081600	0.73097200
H	2.52752100	2.59977300	-0.94444400
H	1.93978900	4.64616500	0.00370600
H	2.72570000	4.32952700	1.53975500
H	3.86148600	5.63948500	-0.89081100
H	5.78662300	6.11886400	0.39331000
H	5.15457800	5.34523500	2.85058100
H	6.64885700	4.74854100	2.14489600
H	5.69209800	2.81427200	3.08946900
H	4.05788900	3.21732100	2.60049600
B	2.91273300	2.97531800	-3.78290300
F	3.16107300	1.77783200	-3.07094900
F	1.60118800	2.97510500	-4.26390500
F	3.82225300	3.07712800	-4.84957900
F	3.09573800	4.07267000	-2.90736700

### (S)-BINAP

P	-3.59749800	-3.28081300	0.21753000
P	-3.59607100	0.37242100	-0.98395100
C	-4.67477000	1.43691600	-2.03518200
C	-4.66134300	1.21667500	-3.41909900
C	-6.51854800	-0.67078000	2.53354500
C	-4.75941200	0.00330700	0.41405000
C	-8.27550400	-0.81283600	-4.20272100
C	-6.52208400	-2.23397400	-3.29715900
C	-6.35600600	2.91293000	-3.73109900
C	-2.43728600	-4.47781700	-0.56704500
C	-2.34823600	2.92484700	-0.53609100
C	-2.35487200	-5.83574300	-0.23040200
C	-2.43264100	1.56686000	-0.20016000
C	-0.50591700	-6.13437000	-1.76805100
C	-4.67653800	-4.34269300	1.27101400
C	-1.52490200	-3.95641800	-1.50271800
C	-4.76209400	-2.91052200	-1.17913700
C	-5.65043100	-1.05631600	0.25341300
C	-4.74826000	0.73027300	1.63466000
C	-8.31949100	-2.80983800	2.22116900
C	-6.55788100	-1.40325000	1.30300300
C	-0.56896600	1.86406700	1.33752000
C	-7.48676800	-2.47338000	1.17848900
C	-6.37767600	-6.04728700	1.59163700
C	-1.38380300	3.74373800	0.05838300
C	-5.59858000	0.40054600	2.66418200
C	-8.31940900	-0.09206600	-2.98345900
C	-7.39775600	-1.86232700	-4.35274600
C	-5.54274700	2.40746000	-1.50917000
C	-5.49916600	1.94842400	-4.26371500
C	-6.37416600	3.14395700	-2.35209800
C	-4.75316700	-3.63764400	-2.39966900
C	-5.60389700	-3.30674300	-3.42847300
C	-6.55931300	-1.50141700	-2.06660100
C	-6.35781900	-5.81470100	2.97035100
C	-1.39262300	-6.65669700	-0.82556900
C	-5.54624300	-5.31276300	0.74700400
C	-7.39399100	-1.04107200	3.58979800
C	-5.65150200	-1.84965200	-1.01774900
C	-0.49685400	3.21927200	0.99944800
C	-1.52002600	1.04329100	0.73406500
C	-4.66142800	-4.12086500	2.65466900
C	-8.27352700	-2.08915700	3.44040600
C	-7.48645200	-0.42984900	-1.94139200
C	-0.57604700	-4.77924000	-2.10685200
C	-5.49928200	-4.85060900	3.50098700
H	-4.00794200	0.45359700	-3.83343700
H	-8.93740300	-0.53305400	-5.01741600
H	-3.03608500	3.34874400	-1.25995300
H	-3.04257700	-6.25798600	0.49456700

H	-1.56687800	-2.90107300	-1.76334600	C	0.98283200	4.42098400	0.33989500
H	-4.05297000	1.55298000	1.75715300	C	0.98575900	-4.43985200	-0.14557700
H	-9.01333100	-3.63822100	2.11274200	C	0.96080600	3.19842900	1.02563200
H	0.12079500	1.44575400	2.06557500	C	1.98931300	-5.64727400	-1.99065200
H	-7.51975500	-3.03509600	0.25242800	C	-0.27308500	-2.12955800	1.45541200
H	-7.04771300	-6.79449900	1.17496200	C	1.48206800	-3.29325500	-2.21132100
H	-1.33144800	4.79477400	-0.21312900	C	-1.09963500	-1.17735800	-1.19660200
H	-5.57616900	0.96179800	3.59501700	C	-2.03203700	0.22502300	0.70287600
H	-9.01185300	0.73741600	-2.87452200	C	-1.28142500	1.62490400	2.54110700
H	-7.35766200	-2.42355200	-5.28286100	C	-4.95249400	-1.79349800	1.93492300
H	-5.57355800	2.57955500	-0.43744700	C	-3.06790200	-0.29891600	1.54622100
H	-5.48841400	1.75824300	-5.33321400	C	2.00415000	4.29181000	2.93550900
H	-7.04286200	3.89150600	-1.93387700	C	-3.99929400	-1.27239900	1.08871900
H	-4.05920200	-4.46138600	-2.52271700	C	-1.81154300	-3.36235300	2.86341400
H	-5.58314300	-3.86812100	-4.35927200	C	1.50362600	5.56593000	0.94806300
H	-1.34179600	-7.70765900	-0.55348400	C	-2.25738000	1.12423000	3.36602400
H	-5.57834800	-5.48606200	-0.32449200	C	-4.89397400	1.78730600	-2.03201900
H	-7.35228000	-0.47995100	4.51990500	C	-4.04029500	0.42025600	-3.83251600
H	-1.56356100	-0.01213100	0.99413500	C	-1.32107400	3.07849200	-1.53177400
H	-4.00663800	-3.35813800	3.06745400	C	-0.13930000	1.97956600	-3.81577600
H	-8.93525200	-2.36791000	4.25559300	C	-1.77894300	3.44059200	-2.79738100
H	-7.51788800	0.13191700	-1.01530800	C	-1.21502500	-1.63833400	-2.53680200
H	0.11356100	-4.36258300	-2.83599900	C	-2.16408600	-1.13237000	-3.38942200
H	-5.48723200	-4.65919100	4.57025000	C	-3.01990000	0.29301300	-1.59323800
H	-7.01247800	3.47930000	-4.38589800	C	-1.22039700	-2.80351400	3.99965600
H	0.24919500	3.85854200	1.46327000	C	1.49831800	-5.62171100	-0.68542900
H	-7.01432300	-6.37951300	3.62646300	C	-1.34552300	-3.02301300	1.59484800
H	0.23842400	-6.77524300	-2.23240500	C	-4.14764800	-0.42526200	3.75714300

#### BF<sub>4</sub>

B	0.00000300	-0.00004100	0.00003700
F	-1.23617800	-0.41857200	0.52499900
F	1.03049400	-0.34678700	0.89257800
F	-0.01492700	1.39499700	-0.17903900
F	0.22058400	-0.62958500	-1.23853300

#### 1

Rh	2.04260500	0.00157600	-0.02731300	C	2.00752800	5.50773600	2.24716900
P	0.37440400	-1.66589900	-0.18854500	C	1.49886700	3.14495700	2.32553600
P	0.36436600	1.64890800	0.23240600	C	0.32457000	-1.58198500	2.59830900
C	-0.26162800	2.16878800	-1.40232900	C	-5.02738600	-1.37206600	3.28409000
C	0.32947700	1.62505500	-2.55104300	C	-3.96253700	1.26735900	-1.16123800
C	-3.15893000	0.13488300	2.90603600	C	1.98050700	-4.47706800	-2.75295900
C	-1.13026900	1.16052200	1.20593700	C	-0.15230000	-1.91347900	3.86669100
C	-4.93326400	1.36599600	-3.38265200	H	1.13859600	0.90761600	-2.43728500
C	-3.07496300	-0.14013500	-2.95508500	H	-5.66944900	1.78971800	-4.05946700
C	-1.19389900	2.88736400	-3.93931500	H	0.59740500	4.48856100	-0.67005200
C	0.95667100	-3.26098400	-0.90578100	H	0.61193400	-4.44457000	0.87060500
				H	1.50982400	-2.38859500	-2.81002700



H	-0.62418200	2.39227200	2.92309300	H	3.18749700	-1.92476100	-1.58769400
H	-5.64910700	-2.54074200	1.56607000	H	3.03291100	-2.44394000	0.70426500
H	2.40485500	4.23123000	3.94305300	H	5.34065900	-1.62256800	1.69303600
H	-3.94557700	-1.61884400	0.06398900	H	3.87035500	-1.07610500	2.48373200
H	-2.64875400	-4.04595500	2.96419600	H	5.13432700	0.90606500	2.30372100
H	1.51188400	6.50358800	0.39998300	H	5.74617400	0.53318800	0.70652200
H	-2.34828900	1.48771900	4.38600200				
H	-5.59999100	2.53452200	-1.68151100	<b>1a</b>			
H	-4.06000200	0.08256700	-4.86514400	C	1.18081800	0.41131600	-1.25663800
H	-1.79384000	3.49087700	-0.64589100	C	0.58469000	0.99414100	0.00012900
H	0.31204300	1.54218200	-4.70162900	C	1.18073700	0.41097900	1.25677700
H	-2.60633100	4.13703700	-2.89160100	C	2.22427400	-0.43013600	1.25803900
H	-0.55517000	-2.41101500	-2.90142700	C	2.84310200	-0.89771200	-0.00005200
H	-2.22759300	-1.49603800	-4.41140800	C	2.22435600	-0.42979700	-1.25805800
H	1.51009500	-6.52292100	-0.07928300	H	0.72175000	0.74228200	-2.18602700
H	-1.81978000	-3.44275900	0.71332800	H	0.72161000	0.74169500	2.18622600
H	-4.19499100	-0.08762500	4.78890500	H	2.65625400	-0.81120200	2.17940800
H	1.53074600	2.20225300	2.86366300	H	2.65639700	-0.81061600	-2.17950000
H	1.14709700	-0.88079000	2.48148100	C	0.80357600	2.51757400	0.00034000
H	-5.78066800	-1.79654700	3.94133700	H	0.34011500	2.95546800	-0.88949300
H	-3.93534300	1.61477100	-0.13586100	H	0.34006300	2.95522600	0.89026400
H	2.37096700	-4.47968500	-3.76630500	H	1.87198300	2.75113400	0.00040200
H	0.30496000	-1.47264300	4.74777400	O	-0.84646700	0.83825900	0.00006400
H	-1.56388600	3.15977700	-4.92344000	C	-1.28967900	-0.52490700	-0.00014100
H	2.40786400	6.40022600	2.71904000	H	-0.90383100	-1.05455700	0.88295800
H	-1.59576800	-3.05835500	4.98645800	H	-0.90383000	-1.05428800	-0.88340200
H	2.38351100	-6.56857200	-2.40923400	C	-2.74870300	-0.54166700	-0.00015100
C	3.59864200	-1.55254500	0.43852300	C	-3.95866700	-0.57059500	-0.00010400
C	4.44671600	-0.99566100	1.55471200	C	-5.41820700	-0.60522800	0.00036200
C	4.85657400	0.47303300	1.33704000	H	-5.82785000	-0.10581800	-0.88591600
C	3.73492500	1.31026100	0.74953300	H	-5.78390000	-1.63930200	-0.00020700
C	3.52357400	1.59892900	-0.58954100	H	-5.82729500	-0.10697500	0.88754800
C	4.30906900	1.06407800	-1.76097500	O	3.81681400	-1.65252500	-0.00012200
C	4.76689600	-0.39533500	-1.57650000				
C	3.71068100	-1.26062500	-0.91232900	<b>1b</b>			
H	3.24012900	1.95843600	1.46121900	C	1.51229700	-1.20984200	-0.00002100
H	2.91548300	2.47336300	-0.81565700	C	0.11931000	-1.21510800	0.00003600
H	5.17689700	1.71203400	-1.95620000	C	-0.59198100	0.00002600	0.00006400
H	3.67038700	1.13233200	-2.64913900	C	0.11933800	1.21514300	0.00003200
H	4.98508300	-0.82056800	-2.56172100				
H	5.70044400	-0.43594500	-1.01127500				

C 1.51232500 1.20984400 -0.00002500  
C 2.21206300 -0.00000700 -0.00005300  
H 2.05300400 -2.15185300 -0.00004100  
H -0.42852300 -2.15213300 0.00006300  
H -0.42847200 2.15218100 0.00005500  
H 2.05305400 2.15184300 -0.00004900  
H 3.29828300 -0.00002000 -0.00009900  
C -2.02183000 0.00004300 0.00013900  
C -3.23301600 0.00004400 0.00013700  
H -4.30209000 -0.00016000 -0.00022900

## COD

C -1.21008800 -1.22153600 -0.50892500  
C -1.92279600 0.00797000 -0.00419100  
C -1.07449400 1.10598500 0.66977100  
C -0.01558000 1.68911400 -0.23779500  
C 1.21008700 1.22153600 -0.50892500  
C 1.92279500 -0.00797000 -0.00419200  
C 1.07449400 -1.10598500 0.66977100  
C 0.01558000 -1.68911400 -0.23779500  
H -0.31336400 2.60072800 -0.75721800  
H 1.81027700 1.80998300 -1.20512300  
H 2.71701200 0.30235900 0.69323300  
H 2.45266700 -0.45498200 -0.85782100  
H 1.75823400 -1.91120900 0.96450400  
H 0.64195000 -0.72799800 1.59828100  
H 0.31336400 -2.60072800 -0.75721800  
H -1.81027800 -1.80998300 -1.20512300  
H -2.71701300 -0.30235900 0.69323300  
H -2.45266800 0.45498200 -0.85782100  
H -1.75823400 1.91120900 0.96450400  
H -0.64195000 0.72799800 1.59828100

## 2

C 3.65122900 -1.21608800 -0.14323500  
C 5.05036400 -0.67547900 0.01822000  
C 5.24210000 0.09219700 1.30170800  
C 4.35358800 0.09068500 2.30528600  
C 3.09868100 -0.67821000 2.22652500

C 2.78741600 -1.32349900 0.92980000  
H 3.50017400 -1.84117900 -1.01715700  
H 6.18565200 0.62612900 1.39077500  
H 4.54054600 0.61486000 3.23817400  
C 6.00199600 -1.89070300 0.01917900  
H 5.91194100 -2.42531400 -0.93180600  
H 7.03337300 -1.54344500 0.13353400  
H 5.75783500 -2.57058300 0.83963900  
O 5.45794400 0.10086200 -1.11058100  
C 4.83850000 1.37316300 -1.16389100  
H 5.19924500 2.00929500 -0.34119000  
O 2.36031100 -0.79429000 3.21024300  
H 2.06948200 -2.12958000 0.96136800  
C 3.35730400 1.37187100 -1.13185600  
C 2.34078200 2.09566300 -1.35393300  
H 5.16764600 1.82354000 -2.10556400  
C 1.90853200 3.44009400 -1.80364000  
H 2.79719300 4.02638100 -2.06662200  
H 1.25430700 3.38982300 -2.67690600  
H 1.36707000 3.97629500 -1.02053100  
Rh 1.67566900 0.31735100 -0.34771500  
P -0.07781500 1.56426400 0.43056900  
P 0.15023100 -1.36261000 -0.72171400  
C -0.41375700 -2.59108700 0.51904300  
C -0.13883800 -2.46010400 1.88458000  
C -3.83999700 0.11838400 -2.61691200  
C -1.45392400 -0.83581900 -1.44597100  
C -4.74326900 -2.57698800 3.36884500  
C -3.00294200 -0.90053800 3.11370200  
C -1.45914700 -4.43535400 2.34758200  
C 0.62830500 2.86858200 1.51142300  
C 1.45195700 -3.63388100 -1.80165700  
C 1.54927700 2.47718600 2.49828100  
C 1.05820300 -2.30371000 -1.99944100  
C 1.90081300 4.78825400 3.11889800  
C -1.15661000 2.42341000 -0.77254500  
C 0.35560500 4.23280500 1.33753400  
C -1.30712600 0.65192200 1.46329800  
C -2.42366900 -0.26303800 -0.62300300  
C -1.68194400 -0.96706800 -2.84024500  
C -5.77864700 1.38031800 -1.02323000

C	-3.63192600	0.24312800	-1.20537000	H	-0.45473200	-3.25974600	3.85178800
C	2.38399200	-2.23015000	-4.03430500	H	-2.36906900	-5.37956300	0.63235300
C	-4.63387800	0.89457200	-0.43318700	H	-0.49610100	1.38730200	3.33867700
C	-3.08321200	3.82893100	-1.21099200	H	-1.97649300	0.05551500	4.76037000
C	2.30406500	-4.25630300	-2.71723700	H	2.87203000	3.10868900	4.06846000
C	-2.84627700	-0.50955600	-3.40716500	H	-2.40163000	3.30472400	0.76009000
C	-4.83419500	-2.68771900	1.96093500	H	-5.17028700	0.52903200	-4.26922900
C	-3.84222600	-1.70204300	3.93103300	H	1.27392800	-0.55997600	-3.26578800
C	-1.22868700	-3.64591000	0.07385400	H	-0.17803600	1.61661300	-2.50736700
C	-0.66229500	-3.38098800	2.79286400	H	-6.88994400	1.63873900	-2.86935900
C	-1.73958300	-4.56775800	0.98464200	H	-4.10851700	-2.03028000	0.06805600
C	-1.21889800	0.72605400	2.87897100	H	0.77631400	6.23848600	1.98606400
C	-2.04896000	-0.01946800	3.67888900	H	-1.70434000	2.71897200	-4.11811500
C	-3.10436000	-0.99321600	1.68835500	H	-1.87173400	-5.14516200	3.05844300
C	-2.89319300	3.66352400	-2.58466700	H	3.43340500	-4.04593100	-4.54128500
C	2.17225900	3.42954400	3.30236000	H	-3.57200100	4.13686200	-3.28773400
C	-2.22745200	3.20177700	-0.30657200	H	2.39375500	5.53179800	3.73839400
C	-5.03022300	0.63188200	-3.19659600				
C	-2.25391200	-0.18087000	0.86459400				
C	2.76971900	-3.55922400	-3.83275700	<b>3-ts</b>			
C	1.54348800	-1.60116900	-3.11918100	C	3.72102100	-0.89388900	-0.30166200
C	-0.97673700	2.25582200	-2.14970100	C	5.16871000	-0.57541600	0.07478600
C	-5.98269200	1.24830700	-2.41767700	C	5.25308200	0.17079500	1.38441800
C	-4.03692100	-1.91926800	1.14267800	C	4.28269400	0.13545900	2.30611900
C	0.99293000	5.18491700	2.13686800	C	3.07762900	-0.70229800	2.12886500
C	-1.84213700	2.87137400	-3.05180600	C	2.80978300	-1.23475300	0.77191800
H	0.45912400	-1.63713200	2.25523900	H	3.65313700	-1.52073100	-1.18698400
H	-5.37963900	-3.18947000	4.00091400	H	6.17944600	0.71475500	1.55628800
H	1.10857800	-4.18377200	-0.93349700	H	4.38138400	0.63816700	3.26411300
H	1.76368700	1.42718600	2.65213100	C	5.95934100	-1.88740600	0.15814700
H	-0.34345300	4.56193300	0.57877400	H	5.93735700	-2.39300800	-0.81254100
H	-0.93731500	-1.44318200	-3.46532900	H	6.99985100	-1.67389300	0.42154800
H	-6.52813000	1.87863100	-0.41535600	H	5.52939200	-2.54545400	0.91768400
H	2.74558900	-1.68071800	-4.89843600	O	5.76126500	0.18489100	-0.96977900
H	-4.48389700	1.02052600	0.63176600	C	4.96320600	1.32884400	-1.19593300
H	-3.91046400	4.42751500	-0.84200400	H	5.16907600	2.10349600	-0.44050100
H	2.60462000	-5.28681900	-2.55260600	O	2.36565400	-0.95912300	3.10754300
H	-3.01573800	-0.62126500	-4.47457400	H	2.33242900	-2.20770900	0.73578400
H	-5.53355300	-3.39317500	1.52182700	C	3.50548700	0.98927900	-1.15543600
H	-3.75000800	-1.61416000	5.01021200	C	2.43111700	1.64905900	-1.46176900
H	-1.47000000	-3.74077700	-0.98057400				

H	5.22494100	1.72757000	-2.18037900	C	2.31217600	3.52517900	3.05684600
C	2.17877900	2.96562100	-2.11114200	C	-2.17800400	3.30060200	-0.47246600
H	3.12724400	3.45575600	-2.36311300	C	-5.01522300	0.63647700	-3.20617700
H	1.59769900	2.84949900	-3.03076900	C	-2.27241000	-0.07856700	0.89621300
H	1.61008400	3.62903500	-1.45311100	C	2.57306600	-3.85920100	-3.66713000
Rh	1.58442100	0.23263800	-0.26195600	C	1.44801000	-1.82127500	-3.01230800
P	-0.09445100	1.61832300	0.34505600	C	-0.95508600	2.21791200	-2.26120100
P	0.07562800	-1.44307500	-0.60890600	C	-5.94922000	1.31718700	-2.45911400
C	-0.51606000	-2.61987800	0.65684600	C	-4.08699300	-1.76225300	1.27519900
C	-0.13412600	-2.50859800	1.99648700	C	1.26973300	5.26218500	1.74007600
C	-3.84511000	0.10905300	-2.59880900	C	-1.79223300	2.82172800	-3.19757800
C	-1.50000700	-0.88150800	-1.37167000	H	0.56624000	-1.74473100	2.31185800
C	-4.75251100	-2.32668800	3.53889300	H	-5.38614200	-2.90332100	4.20644500
C	-2.98562700	-0.69652200	3.18521100	H	0.94544700	-4.28928000	-0.71359500
C	-1.56376300	-4.38082700	2.55773300	H	1.74202000	1.51126100	2.58311900
C	0.70736300	2.93844900	1.32943200	H	-0.12457600	4.61244500	0.24205700
C	1.29861700	-3.79004900	-1.60830900	H	-1.00323600	-1.60270700	-3.35885200
C	1.60498800	2.55934800	2.34416700	H	-6.48255500	2.04881400	-0.48829600
C	0.95794600	-2.45279200	-1.85443700	H	2.60639100	-2.02695700	-4.81052600
C	2.14929400	4.88001500	2.75340700	H	-4.47065600	1.16956700	0.60591600
C	-1.13800000	2.45778600	-0.89524100	H	-3.81479200	4.55538100	-1.07850400
C	0.54993600	4.29870900	1.02948800	H	2.36256700	-5.52193600	-2.31023900
C	-1.31466200	0.77753900	1.44136600	H	-3.04020400	-0.74313700	-4.41622900
C	-2.44957800	-0.23030900	-0.58427300	H	-5.60948100	-3.18380900	1.74056700
C	-1.72891600	-1.06797600	-2.75982600	H	-3.70120100	-1.32981600	5.12257100
C	-5.74643100	1.50219000	-1.07040700	H	-1.74185900	-3.69576700	-0.76833200
C	-3.63748200	0.29020500	-1.19347300	H	-0.37306000	-3.28706400	3.98506100
C	2.24084000	-2.52404200	-3.91676800	H	-2.64660200	-5.26490700	0.91176200
C	-4.62007600	1.00590500	-0.45421400	H	-0.46874100	1.59175400	3.26863400
C	-3.00803500	3.90977500	-1.41198400	H	-1.91677300	0.31313000	4.77160700
C	2.10349600	-4.48690400	-2.51278900	H	2.99332000	3.21840600	3.84504800
C	-2.87162100	-0.58987600	-3.35384800	H	-2.34767500	3.46824400	0.58680700
C	-4.88233600	-2.48178800	2.13813900	H	-5.15528100	0.49123600	-4.27390100
C	-3.81969200	-1.45344000	4.04955000	H	1.22118900	-0.77624800	-3.19875700
C	-1.42803600	-3.61605100	0.26832200	H	-0.18147300	1.53146100	-2.58289800
C	-0.66309200	-3.38814600	2.94324400	H	-6.84158700	1.71714000	-2.93164300
C	-1.94073600	-4.49784700	1.21621500	H	-4.18793700	-1.90679200	0.20689100
C	-1.19903500	0.91155000	2.85054400	H	1.14013400	6.31265100	1.49651300
C	-2.01241900	0.19737200	3.69551800	H	-1.65382300	2.61573600	-4.25478400
C	-3.12033200	-0.84112600	1.76675300	H	-1.97883800	-5.05835400	3.29823500
C	-2.81784100	3.66998100	-2.77513300	H	3.19851700	-4.40412700	-4.36807700

H	-3.47661200	4.13215400	-3.50424300	C	-2.10292900	-3.40239900	1.43595100
H	2.70632800	5.63249100	3.30395200	C	-0.85155600	3.23341100	-2.09359500
<b>4</b>				C	-1.51544900	-2.17126700	1.75909400
				C	-0.79769300	5.61692000	-2.49027200
				C	1.84852300	2.36476400	1.05313900
C	-4.04140200	-0.49002800	0.34367400	C	0.71817700	4.62434300	-0.88104800
C	-5.50987800	-0.11997700	0.04969100	C	1.65816700	0.77733600	-1.36293300
C	-5.58622800	0.90963200	-1.05344200	C	2.32445100	-0.63872400	0.62937000
C	-4.63562900	1.06485800	-1.98839500	C	1.36099400	-1.34943700	2.76000400
C	-3.43627700	0.19995000	-2.03790400	C	5.93145300	0.20998600	1.26311700
C	-3.08024200	-0.58743800	-0.83423300	C	3.58234300	-0.43846900	1.29187600
H	-4.03937000	-1.42960700	0.90919400	C	-2.84717100	-2.08229100	3.78440400
H	-6.48919500	1.51766000	-1.07098100	C	4.73735600	0.02847700	0.60323100
H	-4.74350700	1.78384000	-2.79733700	C	4.01293600	3.26908900	1.66349700
C	-6.41121500	-1.30878000	-0.25849300	C	-3.05681200	-3.96772900	2.28513900
H	-6.39032000	-2.01161700	0.58132700	C	2.55868400	-1.15766300	3.40305100
H	-7.44511400	-0.98555900	-0.42083000	C	4.20884600	-3.30617000	-2.16294800
H	-6.06320900	-1.82189500	-1.16126800	C	3.56862000	-1.91441000	-4.03248700
O	-5.97318700	0.47010700	1.28734800	C	0.58174600	-3.71873000	-0.49511300
C	-4.87684700	1.11063300	1.96352200	C	-0.02312400	-3.02779200	-3.13654300
H	-4.99005600	2.20312300	1.92974000	C	0.90646600	-4.58659000	-1.53550200
O	-2.74080000	0.17246000	-3.07063700	C	1.66108300	1.02609100	-2.76145500
H	-2.82654600	-1.61135100	-1.11163000	C	2.27185100	0.15240000	-3.62783200
C	-3.63731200	0.63914500	1.24296600	C	2.92139800	-1.28223300	-1.73972400
C	-2.39970500	1.15588900	1.22851000	C	3.71195600	3.07830600	3.01461800
H	-4.90343900	0.79883100	3.01644800	C	-1.33596400	4.35607600	-2.76224500
C	-1.94298700	2.24379500	2.15482600	C	3.09006400	2.90759700	0.68399900
H	-2.81373500	2.77342500	2.56625500	C	4.93813000	-0.49193800	3.35088500
H	-1.38926300	1.82954900	3.00671600	C	2.26764200	-0.36994100	-0.84786900
H	-1.30079200	2.98291700	1.66746600	C	-3.43128600	-3.31007700	3.45695800
Rh	-1.30603200	0.50520300	-0.30382900	C	-1.90181200	-1.50958200	2.93765800
P	0.67040200	1.84464900	-0.23702900	C	1.55270600	2.17594700	2.40796000
P	-0.41462700	-1.33196400	0.57289900	C	6.03693600	-0.05139300	2.65016600
C	-0.06595000	-2.50603100	-0.77471500	C	3.57833700	-2.45788400	-1.28122200
C	-0.36796500	-2.16267100	-2.09837200	C	0.22433600	5.74730300	-1.54834500
C	3.69526600	-0.69808800	2.69581700	C	2.48230100	2.53119900	3.38466200
C	1.22504300	-1.08774000	1.37019100	H	-0.86558900	-1.22460800	-2.32380600
C	4.20543800	-3.03586300	-3.55223700	H	4.70343100	-3.71740600	-4.23559900
C	2.91962000	-1.01346100	-3.14755800	H	-1.83079800	-3.91662600	0.52181400
C	0.61107100	-4.23930000	-2.85670000	H	-1.28701800	2.25814300	-2.30549900
C	0.19154700	3.35460200	-1.15435100	H	1.50551100	4.74346600	-0.14573500

H	0.51555800	-1.72458600	3.32106100	C	-1.69139100	-1.64403200	2.81994400
H	6.79907400	0.56767900	0.71658100	C	-0.39424700	4.40053600	-1.00043300
H	-3.13740800	-1.56399500	4.69341200	C	-1.08302200	-2.36195300	1.77311600
H	4.67159000	0.25077100	-0.45432900	C	-1.97728400	5.06334600	-2.71040100
H	4.97434700	3.68056900	1.37139800	C	1.20294700	2.45542400	0.91470400
H	-3.50866900	-4.91980600	2.02336800	C	-1.50734200	2.72016700	-2.34444600
H	2.64729300	-1.36688500	4.46552000	C	1.37205700	0.83899100	-1.44847900
H	4.70430500	-4.19805900	-1.79063000	C	2.41680600	-0.27117800	0.57451700
H	3.55351700	-1.69610300	-5.09685000	C	1.61470800	-1.12902800	2.71242300
H	0.83709000	-3.97822300	0.52799700	C	5.75579200	1.34137100	1.18005400
H	-0.24483800	-2.74977600	-4.16247600	C	3.60695000	0.19542600	1.22312600
H	1.40864900	-5.52423700	-1.31711700	C	-2.07092700	-4.40033600	2.63143400
H	1.18467100	1.92049100	-3.14649500	C	4.62696900	0.90181500	0.52614200
H	2.27729600	0.35430200	-4.69549500	C	3.11667700	3.82710700	1.48447300
H	-2.13565800	4.24543700	-3.48882600	C	-2.46928100	-2.30422000	3.76835400
H	3.33983800	3.03101500	-0.36551500	C	2.76007100	-0.70787400	3.34351900
H	5.00050900	-0.69167900	4.41710400	C	4.84466700	-2.51562900	-2.15640300
H	-1.47579700	-0.54435400	3.18786200	C	3.90440100	-1.35620800	-4.05727200
H	0.61529700	1.72156400	2.69713000	C	1.25477600	-3.63259600	-0.39419200
H	6.98486900	0.10126900	3.15770000	C	0.70041600	-3.16706300	-3.09050800
H	3.57559700	-2.68736100	-0.22280900	C	1.77266600	-4.48357300	-1.36904900
H	0.64077400	6.72596000	-1.32796600	C	1.31235500	1.03681500	-2.85385600
H	2.25109800	2.36513900	4.43268200	C	2.13933700	0.33837200	-3.69874700
H	0.88443100	-4.90884200	-3.66672400	C	3.13439900	-0.82313600	-1.77748100
H	-4.17703500	-3.74872700	4.11333200	C	2.90388300	3.56024400	2.83926000
H	4.43935100	3.34545800	3.77536900	C	-1.08556600	5.39904600	-1.69184400
H	-1.17833600	6.49385100	-3.00566900	C	2.27711800	3.26945500	0.52169900
				C	4.95047000	0.43947800	3.27358900
<b>3'-ts</b>				C	2.28329300	-0.06726000	-0.90414400
				C	-2.65990100	-3.68596500	3.67582900
Rh	-1.58321400	0.33555800	0.08258300	C	-1.28682700	-3.74418300	1.67994700
P	0.15157200	1.68595000	-0.36224100	C	1.00050200	2.18362000	2.27132800
P	-0.15528400	-1.40187100	0.52259800	C	5.92301400	1.10859100	2.56623800
C	0.43233000	-2.55697200	-0.76464600	C	4.04334000	-1.80414200	-1.29216900
C	0.16483500	-2.32634800	-2.11665500	C	-2.18538300	3.71957800	-3.03795400
C	3.77667200	-0.02982900	2.62717700	C	1.84779200	2.73470400	3.23049800
C	1.42778600	-0.90842800	1.32306200	H	-0.42625700	-1.46948400	-2.40958000
C	4.78083300	-2.28912700	-3.55196100	H	5.42003400	-2.85847700	-4.22040700
C	3.06240500	-0.60966500	-3.19199300	H	-1.55464500	-0.56872400	2.88571200
C	1.49757500	-4.25073100	-2.71882200	H	0.28833800	4.67773000	-0.20619500
C	-0.59411600	3.05331800	-1.32623900	H	-1.69193900	1.67736000	-2.58435200

H	0.84941500	-1.64118700	3.28207400	C	-2.09537300	2.90556200	2.19204100
H	6.52158500	1.88044300	0.63002500	H	-1.67763000	2.48912400	3.11271800
H	-2.22518900	-5.47217500	2.54854700	H	-1.36558000	3.61625500	1.79135400
H	4.50707100	1.10087900	-0.53158900	H	-3.01088500	3.45633800	2.44274800
H	3.94865100	4.45257600	1.17553600	O	-2.64916300	-3.23846900	-1.16053300
H	-2.93022300	-1.74041100	4.57406900	H	-3.83349800	0.97269400	-1.71685700
H	2.89653500	-0.88801600	4.40638900	H	-2.37785100	-0.84150700	-2.19356400
H	5.52630100	-3.26484400	-1.76452100	C	-6.11144800	-0.44567100	-1.59030600
H	3.83668800	-1.17803200	-5.12702700	H	-5.73108900	-1.28429800	-2.18094500
H	1.50053900	-3.79850300	0.65037900	H	-7.11006800	-0.69903100	-1.22108000
H	0.50303900	-2.96836100	-4.13966300	H	-6.18827200	0.44062500	-2.22901900
H	2.40595100	-5.31560000	-1.07574100				
H	0.61902600	1.75912900	-3.26577900	<b>3'-ts-1</b>			
H	2.09434400	0.50794800	-4.77107100				
H	-0.92443500	6.44029500	-1.42843900	Rh	-1.64978400	0.29741500	-0.00555300
H	2.46304500	3.45730500	-0.53150300	P	0.07377600	1.68798200	-0.44787700
H	5.06179300	0.26044200	4.33957200	P	-0.13765600	-1.40449000	0.46109200
H	-0.85730200	-4.30712300	0.86168600	C	0.45597000	-2.57745400	-0.80865400
H	0.20464100	1.51262400	2.56766000	C	0.08952100	-2.44662900	-2.15053900
H	6.81806300	1.46368700	3.06862100	C	3.77716700	0.06680800	2.54359700
H	4.09276900	-2.00128300	-0.22865800	C	1.45504300	-0.89231400	1.24454800
H	-2.88000300	3.45038600	-3.82825100	C	4.72752200	-2.27729900	-3.63871900
H	1.69352100	2.50475600	4.28045200	C	2.90119000	-0.71803500	-3.26993500
H	1.91756100	-4.90321400	-3.47867000	C	1.52650900	-4.30004300	-2.73678700
H	-3.27038500	-4.20108400	4.41178700	C	-0.36664100	3.15607300	-1.46769400
H	3.57022800	3.98164900	3.58596000	C	-1.64154800	-1.62444900	2.77953800
H	-2.51179600	5.84288100	-3.24526300	C	-1.66863400	3.67362000	-1.46682200
C	-3.79809600	0.21216200	-0.93954700	C	-1.01020700	-2.35591700	1.75710700
C	-5.18247900	-0.14821000	-0.39878500	C	-0.98631300	5.47617300	-2.93063600
C	-5.11476000	-1.34247900	0.51756100	C	1.03000400	2.39842900	0.95378100
C	-4.19278700	-2.30225100	0.36764700	C	0.62153500	3.81004500	-2.22746600
C	-3.18787400	-2.22123900	-0.71774500	C	1.26302500	0.77499600	-1.51261300
C	-2.88918700	-0.87085800	-1.23701600	C	2.41764500	-0.21180000	0.49940200
H	-5.90036600	-1.41119300	1.26616400	C	1.67326500	-1.14135400	2.62450400
H	-4.18534100	-3.20026900	0.97696500	C	5.64958900	1.59277800	1.10579000
O	-5.75405000	0.95355800	0.32358900	C	3.58487100	0.30431100	1.14485600
C	-4.85992700	2.05215500	0.40895800	C	-1.83154300	-4.40661600	2.74819000
H	-4.96183600	2.70923000	-0.46933300	C	4.55235500	1.08186200	0.45018500
H	-5.11955100	2.62753500	1.30291100	C	2.75920000	3.86292100	1.81903600
C	-3.46694200	1.54818800	0.51681700	C	-2.34776300	-2.28315900	3.78368900
C	-2.40661500	1.84562200	1.19613300	C	2.80831000	-0.68582900	3.25128700

C	4.91246900	-2.38371800	-2.24037200	H	5.05232300	0.41748200	4.25275300
C	3.73666700	-1.46398900	-4.14066600	H	-0.66323200	-4.32701700	0.94615700
C	1.37576300	-3.57118200	-0.43638000	H	-0.00225100	1.22210500	2.42765500
C	0.62580200	-3.30245000	-3.11117200	H	6.70882300	1.76351000	2.99207900
C	1.89902400	-4.43468200	-1.39676900	H	4.26184100	-1.77804000	-0.30297000
C	1.04399100	0.80289100	-2.91943300	H	1.08767600	5.45203200	-3.52995700
C	1.84666100	0.08709300	-3.77055100	H	1.26694400	2.13491000	4.34074500
C	3.09696600	-0.80622500	-1.85427600	H	1.94940300	-4.96169800	-3.48701900
C	2.48484400	3.43094100	3.11788700	H	-2.99707700	-4.19273300	4.54920500
C	-1.97479700	4.82758900	-2.19116800	H	3.05374800	3.82518200	3.95468600
C	2.03611600	3.35248100	0.74151900	H	-1.22549400	6.37252000	-3.49537200
C	4.92135200	0.60412200	3.19034100	C	-3.89665100	0.01366900	-0.96614100
C	2.25346000	-0.04290700	-0.97738200	C	-5.25387500	-0.34452700	-0.36183800
C	-2.44329300	-3.67768000	3.76963700	C	-5.12811100	-1.46917900	0.63442600
C	-1.11715100	-3.75161900	1.74277900	C	-4.18577500	-2.41478100	0.52534100
C	0.76009900	1.97252100	2.25999200	C	-3.20669800	-2.37627600	-0.58436600
C	5.83896000	1.35214700	2.48839100	C	-2.96016400	-1.05423600	-1.19509700
C	4.11551600	-1.67288900	-1.37050300	H	-5.89352300	-1.50591100	1.40586900
C	0.31241900	4.96121600	-2.94906100	H	-4.13818700	-3.26906900	1.19331700
C	1.48115700	2.48516500	3.33547800	O	-5.84757000	0.78808800	0.29084200
H	-0.58159400	-1.65554100	-2.45159500	C	-4.97660200	1.90770500	0.32136800
H	5.36264300	-2.84554400	-4.31196900	H	-5.10503000	2.52475300	-0.58224300
H	-1.57611500	-0.54027700	2.78262900	H	-5.24024200	2.51471700	1.19323300
H	-2.44770600	3.17943200	-0.90289700	C	-3.57095800	1.44686800	0.43714800
H	1.62930200	3.41389800	-2.27593200	C	-2.51270900	1.78372600	1.10078700
H	0.93722400	-1.69485900	3.19353700	C	-2.21829800	2.88062900	2.06142200
H	6.37372600	2.19156200	0.56111400	H	-1.75006100	2.51117400	2.97648800
H	-1.91191200	-5.48949900	2.72740200	H	-1.53596800	3.61398400	1.61960800
H	4.41050700	1.28299500	-0.60525200	H	-3.15218400	3.39185600	2.32730700
H	3.54377700	4.59195300	1.63986900	O	-2.64323300	-3.40121400	-0.97462300
H	-2.82694200	-1.70925300	4.57145600	H	-3.96720300	0.72694300	-1.78447300
H	2.96623100	-0.88488600	4.30775700	H	-2.45809900	-1.07055600	-2.15644100
H	5.68423400	-3.03985700	-1.84876300	C	-6.20104500	-0.75633400	-1.50449100
H	3.57167800	-1.38401500	-5.21173800	H	-5.80909500	-1.62557600	-2.04081800
H	1.69647100	-3.65897400	0.59716600	H	-7.18174100	-1.01072800	-1.09053800
H	0.34928300	-3.17908100	-4.15407800	H	-6.32162800	0.07715100	-2.20435200
H	2.61125100	-5.19933200	-1.10143300				
H	0.23791600	1.40282600	-3.32502100	<b>4'</b>			
H	1.67703000	0.12381300	-4.84314000				
H	-2.98974900	5.21409800	-2.17631500	Rh	-1.32494600	0.61944700	-0.45653800
H	2.26960000	3.69440400	-0.25904200	P	0.75937600	1.82305700	-0.35271800



P	-0.55578000	-1.30894300	0.37426200	C	5.53265200	0.03304100	3.34046000
C	-0.04038300	-2.34818800	-1.02756600	C	3.73878400	-2.51654600	-0.81395500
C	-0.37473400	-1.95406300	-2.32885200	C	-1.01272400	3.99838700	-3.34642000
C	3.21810600	-0.64303100	3.04856300	C	2.77787500	2.87953800	3.09364000
C	0.97129200	-1.06752900	1.37718700	H	-0.97607100	-1.06514800	-2.48128100
C	4.64432400	-3.22208500	-2.95045600	H	5.22342800	-3.93871800	-3.52539300
C	3.31910200	-1.18734100	-2.82862000	H	-2.24236700	-0.68342300	2.70415500
C	0.80094200	-3.86843200	-3.21502800	H	1.09711300	4.79327100	-0.18662900
C	0.28208500	3.22501600	-1.43227500	H	-0.70652300	1.92817100	-2.85858300
C	-2.36528400	-1.73399800	2.48434500	H	-0.03415500	-1.61585500	3.22240600
C	0.51467500	4.56015400	-1.07048100	H	6.55815800	0.65839400	1.53490500
C	-1.68939400	-2.31657500	1.40016400	H	-2.93187900	-5.47581700	1.66560900
C	-0.76367500	5.32426200	-2.98306800	H	4.63831000	0.27563500	0.06305800
C	1.95408400	2.52773000	0.84389600	H	4.96328000	4.12839700	0.80370400
C	-0.50119200	2.95723700	-2.57340600	H	-3.71684000	-2.03318800	4.12555900
C	1.82406800	0.68091100	-1.32923900	H	1.91015600	-1.25076000	4.66043300
C	2.17413900	-0.64829800	0.79700300	H	4.93419500	-4.26604600	-1.07172600
C	0.89292200	-1.27349900	2.78217000	H	4.19130900	-1.97894600	-4.63995700
C	5.62756200	0.28331800	1.95033400	H	0.99492100	-3.81196100	0.17964600
C	3.31443700	-0.41424800	1.63809600	H	-0.19253300	-2.38439100	-4.42784900
C	-2.76722900	-4.42988200	1.90694200	H	1.70478100	-5.17537800	-1.75685300
C	4.55067400	0.06586200	1.12150100	H	1.65511500	1.76171700	-3.20290300
C	4.07557100	3.64800300	1.20456900	H	2.92147200	0.11069700	-4.51185900
C	-3.20802900	-2.49984500	3.28739200	H	0.18741200	6.62862400	-1.55364500
C	1.98396400	-1.07436600	3.59092000	H	3.24789200	3.24379000	-0.73700900
C	4.48062300	-3.40661100	-1.55673500	H	4.25498100	-0.60446500	4.94302900
C	4.07108100	-2.13608600	-3.57152300	H	-1.43829500	-4.13209000	0.25229000
C	0.71379800	-3.51197800	-0.82481100	H	0.94244700	1.87044400	2.62670600
C	0.05609300	-2.70411300	-3.42027400	H	6.39319500	0.20680800	3.97974700
C	1.11867800	-4.27636400	-1.91819500	H	3.60530700	-2.68446700	0.24758500
C	2.04638100	0.87634700	-2.71646600	H	-1.60375800	3.77300900	-4.22924600
C	2.76012900	-0.04212700	-3.44817900	H	2.65599300	2.75067300	4.16482500
C	3.13453200	-1.38062600	-1.42106300	H	1.13649400	-4.45498200	-4.06506300
C	3.91283300	3.51088000	2.58649300	H	-4.06993300	-4.44820500	3.62547500
C	-0.00451800	5.59985100	-1.84418700	H	4.67577400	3.88463600	3.26305000
C	3.10723000	3.15152100	0.33567000	H	-1.16247400	6.13734700	-3.58229000
C	4.34913900	-0.41843400	3.87659400	C	-4.14338100	1.08647400	-0.49045800
C	2.34777200	-0.43935800	-0.68053000	C	-5.57216200	0.72147300	-0.02694800
C	-3.40848700	-3.85213300	3.00358600	C	-5.57821600	-0.65565100	0.59062800
C	-1.91317200	-3.66957400	1.10685900	C	-4.71603300	-1.61759000	0.23269300
C	1.80021500	2.38935000	2.22589200	C	-3.70939800	-1.40887700	-0.83522200

C	-3.27778200	-0.02264100	-1.11697900
H	-6.36517300	-0.84867500	1.31811500
H	-4.78117800	-2.62300700	0.63774400
O	-5.87619800	1.71208100	0.98173800
C	-4.67210300	2.12483100	1.64769600
H	-4.68142700	3.22088600	1.70442400
H	-4.64192800	1.73290800	2.67470700
C	-3.54624500	1.56948200	0.81049100
C	-2.26684800	1.34076200	1.13139300
C	-1.61352000	1.70307500	2.42714600
H	-0.89758900	0.94124300	2.75109600
H	-1.06743900	2.64960100	2.34153800
H	-2.36489700	1.82168800	3.22013900
O	-3.28104400	-2.38244800	-1.46637300
H	-4.22800000	1.92197300	-1.19845500
H	-3.14362700	0.09652300	-2.19850700
C	-6.63717700	0.83585700	-1.11110500
H	-6.41550300	0.14485300	-1.93118500
H	-7.62798500	0.59174200	-0.71285700
H	-6.66001400	1.85893200	-1.50221900

**5-ts**

Rh	-1.32494600	0.61944700	-0.45653800
P	0.46900200	1.67893200	-0.32163700
P	-0.15888900	-1.43331400	0.19650800
C	0.40897100	-2.33436400	-1.28714300
C	0.03119400	-1.87870600	-2.55839300
C	3.47180800	-0.69040100	3.00113800
C	1.33373400	-1.26448800	1.24496800
C	5.18200700	-2.43945900	-3.18502500
C	3.60249900	-0.61565900	-2.89400600
C	1.32967100	-3.64298000	-3.57869800
C	0.11476400	3.28642900	-1.12180400
C	-1.75844500	-3.73493000	0.45706800
C	-0.50624900	3.28489500	-2.38373900
C	-1.32461500	-2.54013800	1.05316300
C	-0.59126700	5.70115100	-2.36445300
C	1.17746100	2.06613100	1.31483500
C	0.34942900	4.51051500	-0.47767700
C	1.83333200	0.86536900	-1.25267100

C	2.44357800	-0.57708800	0.75430500
C	1.31045900	-1.71242400	2.59184000
C	5.68272600	0.77951500	2.08212100
C	3.53335500	-0.27314800	1.63253200
C	-2.88069300	-2.90825900	2.88097300
C	4.67123300	0.46457500	1.20288100
C	2.92848500	3.11413700	2.62220500
C	-2.74321500	-4.50845400	1.07267200
C	2.35119700	-1.43514500	3.44365100
C	5.05035400	-2.76532500	-1.81409000
C	4.46991500	-1.38625000	-3.71213800
C	1.23950500	-3.45784700	-1.16858800
C	0.49513000	-2.52945500	-3.70117000
C	1.69294000	-4.11130000	-2.31318100
C	2.01417500	1.19704200	-2.62304700
C	2.86934100	0.47692600	-3.41888300
C	3.46211400	-0.94319400	-1.50728500
C	2.32134900	2.66330700	3.79608500
C	-0.84518100	4.48557800	-3.00410800
C	2.36572100	2.80992700	1.38379600
C	4.52929200	-0.34702500	3.88413300
C	2.55883300	-0.18608500	-0.68837700
C	-3.30480800	-4.09793700	2.28458200
C	-1.90658300	-2.12377800	2.26448500
C	0.57312100	1.61436800	2.49441400
C	5.61245200	0.37480100	3.43687300
C	4.21183900	-2.04035000	-0.99773300
C	-0.00033800	5.70940100	-1.09986400
C	1.14599600	1.91117700	3.72971300
H	-0.61065300	-1.00377600	-2.64226100
H	5.84372300	-3.02401100	-3.81738900
H	-1.32997200	-4.06218400	-0.48326200
H	-0.74169600	2.34700000	-2.87175400
H	0.79467000	4.53590200	0.50895600
H	0.46433100	-2.28150300	2.95440700
H	6.53929700	1.35063800	1.73623400
H	-3.31780200	-2.58152500	3.81973100
H	4.73200800	0.79424100	0.17276700
H	3.85014800	3.68578100	2.66737700
H	-3.06992000	-5.43215000	0.60416500
H	2.32154100	-1.77943800	4.47370400

H	5.60964600	-3.60130100	-1.40437700	C	-2.33936000	2.72704300	1.24831300
H	4.55900500	-1.12477200	-4.76297100	H	-3.14755800	3.12164100	1.87891700
H	1.54267200	-3.80877300	-0.18681100	H	-1.38794400	3.00107900	1.70826200
H	0.21311300	-2.16265000	-4.68367600	H	-2.39313200	3.22711300	0.27628900
H	2.34543300	-4.97381500	-2.21802100				
H	1.47558600	2.03370000	-3.04783600	<b>6</b>			
H	2.99533300	0.74120500	-4.46521400				
H	-1.31719900	4.46921300	-3.98197500	P	-0.71009400	-0.05461700	-1.39382700
H	2.85546600	3.14092300	0.47334600	P	0.71049900	0.77129400	1.51237100
H	4.46292800	-0.66572300	4.92082900	C	1.70769300	2.13569700	0.79569900
H	-1.59847600	-1.19275500	2.72353500	C	2.41693500	1.95660500	-0.39503900
H	-0.32953900	1.01623800	2.43990800	C	-3.80346000	1.85542700	1.91180600
H	6.41578800	0.63554200	4.11959100	C	-1.02307900	1.35171800	1.69338100
H	4.11054900	-2.31496300	0.04468700	C	0.07195400	6.75362600	-0.69707900
H	0.18777800	6.65002500	-0.59063000	C	0.01879000	4.55099500	-1.72238500
H	0.67945100	1.54463100	4.63915100	C	3.32379400	4.19049500	-0.20484900
H	1.69962200	-4.14456100	-4.46806000	C	-0.22881600	-0.70963100	-3.03416000
H	-4.07190700	-4.70127900	2.76113000	C	2.78653200	0.22712100	3.23532900
H	2.76866200	2.88937100	4.75942400	C	1.12950800	-0.64185200	-3.39082600
H	-0.86132300	6.63645900	-2.84606700	C	1.48010700	0.74218200	3.18172000
C	-4.33098600	-1.11920500	-0.16153000	C	0.67025800	-1.82190400	-5.44812900
C	-5.65730900	-0.54942300	0.27760100	C	-2.51846000	-0.25634000	-1.22890500
C	-5.94046100	0.79485300	-0.35810600	C	-1.12867600	-1.34984200	-3.89363000
C	-5.11927600	1.36812900	-1.25542400	C	-0.54406400	1.78070200	-1.54850000
C	-3.86009600	0.71233700	-1.61528200	C	-1.65328900	2.09889800	0.70189400
C	-3.70565400	-0.67864200	-1.31091100	C	-1.79044500	0.80499100	2.76270600
H	-4.06366700	-2.07187500	0.28231700	C	-5.10582900	3.38845000	-0.04533900
H	-6.85550100	1.28725700	-0.03755100	C	-3.06022100	2.37306500	0.80303000
H	-5.30669600	2.36033400	-1.65716600	C	1.64643400	1.30555000	5.53557500
C	-6.76777500	-1.54596800	-0.10188500	C	-3.75765000	3.13610600	-0.17352100
H	-6.58327500	-2.50826700	0.38582700	C	-4.77504700	0.24096900	-1.95241400
H	-7.73435400	-1.15874500	0.23553300	C	3.50566300	0.23477900	4.42786600
H	-6.79909000	-1.69165500	-1.18529100	C	-3.13474000	1.05492400	2.87217100
O	-5.69361400	-0.47731300	1.70412500	C	-0.57906600	6.23259400	0.44731700
C	-4.68520000	0.39254700	2.23510600	C	0.36020900	5.92856700	-1.76039200
H	-5.09236800	1.41931200	2.28148600	C	1.82550500	3.34686900	1.49525600
O	-2.83523100	1.39014700	-1.95143500	C	3.21957900	2.98262800	-0.89621600
H	-2.83604900	-1.20741700	-1.71283900	C	2.62654000	4.36957500	0.99325200
C	-3.43729000	0.42127500	1.44307200	C	0.04901500	2.33755600	-2.71233500
C	-2.53204200	1.24432700	1.09890700	C	0.31713800	3.68166900	-2.79900300
H	-4.50762600	0.04818300	3.25923000	C	-0.63129200	4.01812400	-0.56386100

C	-5.28248300	-0.46001800	-0.85405200	H	3.48823300	0.76804800	6.51897200
C	1.57507300	-1.18269100	-4.59472900	H	-6.35601300	-0.52986000	-0.70517500
C	-3.39792200	0.35204600	-2.13731300	H	1.01606200	-2.25258700	-6.38327200
C	-5.19216600	2.12735700	2.01379100	Rh	0.38743400	-1.24174900	0.32549600
C	-0.92057400	2.61780800	-0.49742800	C	0.40667100	-2.71982700	2.07059600
C	2.93107600	0.76470900	5.58673800	C	1.55526900	-2.30578500	1.86380400
C	0.92457500	1.30290700	4.33874600	C	4.33489300	-1.12572200	-0.76982200
C	-3.03254300	-0.95388100	-0.13060000	C	4.54602700	-2.61115700	-0.62276200
C	-5.83281900	2.88315400	1.05782900	C	5.18082300	-3.24262700	-1.83628000
C	-0.92480600	4.90144700	0.51158100	C	5.48166200	-2.56337100	-2.95178800
C	-0.67656400	-1.90698200	-5.09343600	C	5.20979500	-1.11655500	-3.06987300
C	-4.40949900	-1.05630300	0.05742300	C	4.65038800	-0.44354000	-1.87896000
H	2.32429900	1.02280800	-0.93629700	H	3.88961100	-0.62597700	0.08776500
H	0.34190100	7.80505200	-0.73144500	H	5.36055400	-4.31312900	-1.76423200
H	3.25269100	-0.15344000	2.33097400	H	5.91879800	-3.04704200	-3.82089800
H	1.84249600	-0.16795000	-2.72368800	H	4.49345100	0.62690400	-1.96188900
H	-2.17825400	-1.42199300	-3.63215100	C	5.38738400	-2.89237600	0.62640600
H	-1.30760000	0.17634300	3.50068300	H	4.89731800	-2.46646300	1.50829300
H	-5.61772200	3.97374300	-0.80365000	H	5.49257900	-3.97242200	0.76833800
H	1.20166000	1.74191600	6.42527400	H	6.38169800	-2.44734100	0.52490000
H	-3.21916600	3.51867800	-1.03174200	O	3.27428500	-3.25393300	-0.36470400
H	-5.45281600	0.71607300	-2.65541200	C	2.33117700	-3.15658900	-1.43398600
H	4.51443500	-0.16721400	4.45134900	H	2.33979100	-4.08491900	-2.02197600
H	-3.70317100	0.63575800	3.69782800	H	2.58990600	-2.33696300	-2.10860500
H	-0.80221600	6.88885100	1.28351200	C	0.96713900	-2.94371200	-0.92997500
H	0.85968900	6.31502000	-2.64468300	C	-0.25754100	-3.10089600	-0.80423500
H	1.28735800	3.49259600	2.42614400	C	-1.58974100	-3.68902000	-1.00552600
H	3.75133700	2.84099000	-1.83271800	H	-2.18299400	-3.69146000	-0.08955400
H	2.69939500	5.30930000	1.53228200	H	-2.14266400	-3.12841800	-1.76604800
H	0.30304300	1.69570200	-3.54536300	H	-1.48040900	-4.72393000	-1.35149500
H	0.78024600	4.08995400	-3.69309500	O	5.41797000	-0.50052500	-4.11678400
H	2.62653800	-1.11168900	-4.85815100	C	-0.78168700	-3.47170900	2.33538400
H	-3.00762200	0.92083500	-2.97586900	C	-0.76508400	-4.86503100	2.12693000
H	-5.73831500	1.72338700	2.86198200	C	-1.97294100	-2.84799800	2.74753700
H	-0.05837600	1.75707400	4.31637400	C	-1.92372300	-5.61217500	2.32230600
H	-2.34479900	-1.39919200	0.57863800	H	0.15327200	-5.34152900	1.80022500
H	-6.89593900	3.08816800	1.14349500	C	-3.12766600	-3.60272200	2.93578700
H	-1.41021200	4.51268600	1.39888600	H	-1.98745600	-1.77680200	2.90134900
H	-1.38304900	-2.40524300	-5.75102000	C	-3.10768700	-4.98418500	2.72059300
H	-4.79605500	-1.59206200	0.91948800	H	-1.90534300	-6.68507400	2.15569400
H	3.94389600	4.99084800	-0.59774800	H	-4.04382100	-3.11224500	3.25133800

H -4.01114400 -5.56934600 2.86450200  
H 2.60126300 -2.17756100 2.04527400

**7-ts**

P -1.34278700 -0.15752600 -1.29227200  
P 0.72926000 0.61169200 1.33410200  
C 1.81360400 1.72818000 0.36536500  
C 2.07233700 1.45428400 -0.98216900  
C -3.46113000 2.41650800 2.25846400  
C -0.85051300 1.48107400 1.68874400  
C 0.66036200 6.41636500 -1.37511400  
C 0.02829600 4.20966200 -2.17394700  
C 3.44720000 3.43241300 -1.14493600  
C -1.31001000 -1.04587100 -2.88565500  
C 2.41249800 -0.67061400 3.13295500  
C -0.06387300 -1.26015900 -3.50030000  
C 1.59901600 0.45563800 2.93491000  
C -1.11749300 -2.61982200 -5.19952900  
C -3.08878500 -0.10563600 -0.75254700  
C -2.45497900 -1.63828100 -3.43518100  
C -0.95250200 1.60570000 -1.65601300  
C -1.51880600 2.23702700 0.72754700  
C -1.50352800 1.14208900 2.91014200  
C -4.81431300 4.01808200 0.39146800  
C -2.83377300 2.74177100 1.01298600  
C 2.26833200 1.29908000 5.10874100  
C -3.55477100 3.54923200 0.09023300  
C -5.36208800 0.69147000 -1.01770800  
C 3.15565500 -0.80268800 4.30700100  
C -2.76883100 1.59475900 3.18419900  
C 0.20327500 6.07511700 -0.07902500  
C 0.57138800 5.50197600 -2.40007700  
C 2.39143500 2.86133100 0.95743100  
C 2.88326500 2.29995400 -1.73498400  
C 3.20141600 3.70932100 0.20216000  
C -0.52898900 1.98233500 -2.95779600  
C -0.06151200 3.24904600 -3.21103300  
C -0.43128000 3.85965900 -0.86381700  
C -5.72756300 0.05243400 0.17078600  
C 0.02908200 -2.03229900 -4.65578100

C -4.04784400 0.61982700 -1.47556700  
C -4.76472800 2.90452400 2.53510300  
C -0.94050500 2.54422600 -0.62195200  
C 3.08264100 0.17941800 5.29720300  
C 1.53177600 1.44102100 3.93239200  
C -3.46281100 -0.74654600 0.43707900  
C -5.42892600 3.69411000 1.62370800  
C -0.33117800 4.83104400 0.17021700  
C -2.35588200 -2.42230300 -4.58736900  
C -4.77735500 -0.66689000 0.89717100  
H 1.61171000 0.59309700 -1.44694400  
H 1.08209500 7.40084800 -1.55542200  
H 2.46668000 -1.43561000 2.36573200  
H 0.83379100 -0.82626400 -3.07129700  
H -3.42194100 -1.49394300 -2.96623200  
H -0.99151900 0.51482200 3.63144700  
H -5.34489500 4.63483200 -0.32810100  
H 2.20575700 2.06421900 5.87708100  
H -3.10601700 3.79441700 -0.86437100  
H -6.09759600 1.26085800 -1.57807400  
H 3.78559000 -1.67627800 4.44797600  
H -3.25477300 1.33076900 4.11946000  
H 0.28096400 6.80048100 0.72567500  
H 0.92025800 5.75037900 -3.39880200  
H 2.20960000 3.08966600 2.00150100  
H 3.06882800 2.07743100 -2.78117800  
H 3.63399300 4.59078600 0.66595300  
H -0.56862600 1.25862400 -3.76294600  
H 0.26022500 3.52369200 -4.21199200  
H 0.99648100 -2.18447100 -5.12563700  
H -3.76225000 1.13900300 -2.38555400  
H -5.22597400 2.64148800 3.48322100  
H 0.89971900 2.31293000 3.79779700  
H -2.72412300 -1.29137100 1.01902000  
H -6.42515300 4.06585900 1.84473200  
H -0.66755900 4.57607300 1.16865400  
H -3.24970400 -2.87716500 -5.00436800  
H -5.05289500 -1.15644500 1.82657300  
H 4.07606100 4.09591200 -1.73094300  
H 3.65481200 0.07220400 6.21416700  
H -6.74902900 0.12351000 0.53261900

H	-1.04351400	-3.23061500	-6.09449300				
Rh	-0.16280700	-1.35630000	0.44670900	<b>8</b>			
C	-0.65337000	-3.36489300	1.14526000				
C	0.01892600	-2.64209200	1.99318900	P	0.83766900	-0.90986000	1.54468000
C	4.78311000	-0.48322200	0.46421400	P	-0.09791100	0.17553900	-1.59528100
C	4.77295600	-1.97357000	0.23618600	C	0.10949200	2.01135000	-1.61094900
C	5.48223400	-2.38062600	-1.02970100	C	-0.37449800	2.77531400	-0.54081300
C	6.09936600	-1.51073000	-1.84116500	C	4.22940900	-1.59036800	-1.82215900
C	6.10813700	-0.05848500	-1.56162400	C	1.63153100	-0.46945400	-1.65178800
C	5.41292500	0.38526600	-0.33769200	C	3.93115300	5.01164900	-0.16233500
H	4.25385300	-0.14066100	1.34851100	C	2.62597300	3.37537700	1.07198800
H	5.47164300	-3.44601700	-1.25085600	C	0.40143300	4.80488200	-1.59159300
H	6.61292600	-1.83151000	-2.74347000	C	0.77794900	-1.30153800	3.34383000
H	5.41037400	1.45233000	-0.13921000	C	0.02320200	-0.06924100	-4.42230300
C	5.41682400	-2.67407800	1.44147700	C	1.54832500	-0.67764800	4.33321600
H	4.88000200	-2.40360100	2.35614400	C	-0.77880900	-0.16120100	-3.27091200
H	5.36921100	-3.75938000	1.30852100	C	0.71054400	-2.23086400	5.99507100
H	6.46311000	-2.37131100	1.54250900	C	2.07982800	-2.19274000	1.10507600
O	3.40866800	-2.46311400	0.21744800	C	-0.00219800	-2.41770600	3.69345400
C	2.64888300	-2.05957700	-0.92964400	C	1.63757000	0.73773800	1.36521900
H	2.92181000	-2.66631400	-1.80569700	C	2.64134500	0.02640000	-0.82222900
H	2.84869200	-1.01193300	-1.16498700	C	1.90903800	-1.55794800	-2.52378800
C	1.21783500	-2.28809900	-0.63129100	C	6.28273800	-0.63715000	-0.16189100
C	0.29463100	-3.19053900	-0.74429900	C	3.96533300	-0.52178000	-0.90820900
C	-0.18968400	-4.24067900	-1.66695700	C	-2.70123300	-0.59982400	-4.69049900
H	-0.36570000	-5.19388000	-1.16214800	C	5.02926700	-0.07338700	-0.07675300
H	-1.12247300	-3.93307400	-2.15120800	C	4.23671600	-3.22051600	1.51129100
H	0.56331900	-4.38563300	-2.45038600	C	-0.53490500	-0.23953000	-5.68850300
O	6.65680200	0.74089800	-2.32180300	C	3.16772800	-2.09376400	-2.61237100
C	-1.62722700	-4.43395500	1.00452100	C	4.18960800	4.04478600	-1.16256900
C	-1.42288500	-5.65134400	1.67799100	C	3.15780400	4.68294300	0.92829600
C	-2.78065400	-4.26530500	0.21989900	C	0.74316000	2.66775000	-2.67573400
C	-2.36734200	-6.67181300	1.57916500	C	-0.23344400	4.16070500	-0.52964600
H	-0.52324900	-5.78662000	2.27093700	C	0.88758400	4.05423600	-2.66429700
C	-3.72002900	-5.28919300	0.12553500	C	1.31361600	1.75312000	2.31093900
H	-2.93083800	-3.32996300	-0.30854400	C	1.80161100	3.02864400	2.17255700
C	-3.51679100	-6.49456000	0.80378900	C	2.89711000	2.38917600	0.06996900
H	-2.20288500	-7.60863500	2.10385500	C	3.89122500	-4.27995700	0.66477800
H	-4.61118600	-5.14693600	-0.47908700	C	1.50669100	-1.13747800	5.65208500
H	-4.24857300	-7.29337800	0.72566900	C	3.33391900	-2.18670500	1.73853700
H	0.28489300	-2.63632400	3.04169100	C	5.53019100	-2.15529000	-1.88394500

C	2.37429900	1.06300300	0.22494900	C	-4.66227700	-2.77781700	-0.21791200
C	-1.89911000	-0.50498700	-5.82769600	C	-4.23959500	-3.27455000	-1.57314400
C	-2.14526000	-0.42767100	-3.42239100	C	-2.97703100	-3.23086000	-2.02232300
C	1.73592200	-3.25132500	0.26079600	C	-1.85163500	-2.70281000	-1.23006900
C	6.54003200	-1.68787300	-1.07401800	C	-2.13361100	-2.07039000	0.10748100
C	3.67803800	2.77070300	-1.05512900	H	-3.78122100	-1.77610300	1.46406500
C	-0.03902300	-2.87742600	5.00860100	H	-5.03106700	-3.69723400	-2.18976200
C	2.64243800	-4.29408100	0.04568800	H	-2.70641300	-3.62045700	-2.99994300
H	-0.86434800	2.29230700	0.29721100	C	-5.03786200	-3.94317000	0.68905600
H	4.33729000	6.01390200	-0.26294500	H	-5.40916500	-3.55966900	1.64539700
H	1.08759400	0.11590800	-4.34133900	H	-5.81980400	-4.55835100	0.23123400
H	2.19387800	0.15650100	4.08489700	H	-4.16360200	-4.57613300	0.87443800
H	-0.57247000	-2.93835700	2.92669400	O	-5.83500600	-1.94667800	-0.36716200
H	1.10756400	-1.98830600	-3.10664400	C	-5.42695200	-0.61338700	-0.72149600
H	7.07934200	-0.27815200	0.48330900	H	-5.52153400	-0.45786800	-1.80712000
H	-3.76217900	-0.81387900	-4.78243100	O	-0.70568000	-2.83711500	-1.66560100
H	4.84777600	0.71842700	0.63905300	C	-3.99047500	-0.50169500	-0.25920100
H	5.21149900	-3.19881300	1.98943700	C	-3.06036900	0.44368600	-0.43871600
H	0.10146100	-0.16894600	-6.56582200	H	-6.11418500	0.07968300	-0.22173200
H	3.35914000	-2.92985700	-3.27925200	C	-3.33679600	1.74998700	-1.12547700
H	4.78740900	4.31409800	-2.02841100	H	-3.09308300	2.60728700	-0.49090600
H	2.93948300	5.41888500	1.69751100	H	-2.74263600	1.86172800	-2.03966100
H	1.13500600	2.10591000	-3.51447500	H	-4.39618100	1.83578700	-1.40340800
H	-0.61444200	4.73029700	0.31184200	Rh	-1.25808100	-0.19635300	0.40830100
H	1.39028000	4.54687400	-3.49135700	C	-4.95248800	3.66128400	1.83964600
H	0.67370900	1.51609700	3.15284300	C	-4.45505200	2.36884600	1.96261300
H	1.56067100	3.78972000	2.90983800	C	-3.09217800	2.16997900	2.26249400
H	2.10721300	-0.64163400	6.40940800	C	-2.24214800	3.27982300	2.44420400
H	3.60610800	-1.37145500	2.40101100	C	-2.75137000	4.56793300	2.31585300
H	5.70815500	-2.96987600	-2.58072700	C	-4.10291800	4.75943200	2.01097100
H	-2.77615000	-0.50794900	-2.54815900	H	-6.00115400	3.81552200	1.60536100
H	0.78249000	-3.24115100	-0.25355100	H	-5.09787100	1.50780300	1.81924500
H	7.53208000	-2.12682300	-1.12623800	H	-1.19407000	3.11728400	2.67091400
H	3.87012900	2.04424000	-1.83555400	H	-2.09649300	5.42285300	2.45252100
H	-0.64877200	-3.74002800	5.26124800	H	-4.49561300	5.76668600	1.90877700
H	2.37145600	-5.10906600	-0.61980300	C	-2.57499900	0.85518000	2.38522600
H	0.52247400	5.88401400	-1.58202900	C	-2.10706300	-0.27980300	2.51466300
H	-2.33033400	-0.64062100	-6.81536500	H	-1.91971700	-1.15419100	3.10524800
H	4.59708500	-5.08707400	0.49026800	H	-1.66244900	-2.69585700	0.87296400
H	0.68156800	-2.58450900	7.02145800				
C	-3.61405000	-1.81339300	0.38031700				

**9-ts**

P	0.82857800	-0.89597100	1.53498700	C	-1.93140500	-0.42612900	-3.47566000
P	0.03717400	0.26197600	-1.60163700	C	1.79915100	-3.19595100	0.23136900
C	0.20486000	2.10090000	-1.55121400	C	6.63625300	-1.64537800	-0.82059200
C	-0.41406600	2.82323500	-0.52128300	C	3.79893500	2.83839000	-0.84530100
C	4.37488600	-1.49612700	-1.70051400	C	-0.30576600	-2.68990800	5.03057100
C	1.77998300	-0.35227000	-1.64058700	C	2.72028900	-4.22805100	0.03010000
C	3.94778400	5.07880100	0.07088700	H	-0.96742700	2.30780500	0.25476500
C	2.57898800	3.41696700	1.19834300	H	4.34423200	6.08776200	0.00457000
C	0.40691200	4.90219300	-1.43699100	H	1.24241100	0.43678600	-4.34762600
C	0.67960000	-1.25551800	3.33275200	H	2.20821100	0.09593700	4.05205200
C	0.19852000	0.16236800	-4.44559200	H	-0.83237000	-2.74861000	2.94710900
C	1.49252300	-0.67424600	4.31600200	H	1.33614300	-1.79307600	-3.19819700
C	-0.59578500	-0.03960800	-3.30417700	H	7.09676600	-0.29355500	0.81171900
C	0.49285100	-2.09077600	6.00768800	H	-3.50242400	-0.90935900	-4.86110100
C	2.08784000	-2.17051200	1.13512900	H	4.86749200	0.72112500	0.87148800
C	-0.21159100	-2.27568500	3.70236700	H	5.16551100	-3.20468600	2.16310000
C	1.61563200	0.76299900	1.40601700	H	0.29508700	0.14171100	-6.59173700
C	2.74466800	0.09749800	-0.73605000	H	3.58367200	-2.75933000	-3.26693100
C	2.10255000	-1.40186500	-2.54396700	H	4.96023700	4.40079600	-1.72300900
C	6.33573500	-0.62280700	0.11015600	H	2.81095800	5.46341600	1.85028100
C	4.06681800	-0.45919000	-0.76419900	H	1.44713400	2.27213000	-3.31427300
C	-2.46572900	-0.60385400	-4.75235900	H	-0.80541700	4.75086400	0.34239400
C	5.08410100	-0.04919700	0.14170500	H	1.61411100	4.71977400	-3.21584600
C	4.22089000	-3.20978400	1.62752000	H	0.53725700	1.50622400	3.14330000
C	-0.33545900	-0.01526000	-5.72136000	H	1.38653900	3.80076400	2.96355000
C	3.35888100	-1.95118700	-2.57624600	H	2.02595300	-0.62466600	6.39825400
C	4.29926000	4.11985400	-0.90833000	H	3.53503700	-1.39728500	2.54773300
C	3.09835400	4.73374800	1.09810700	H	5.88394900	-2.86540800	-2.41785600
C	0.93574400	2.80350300	-2.52049000	H	-2.55729900	-0.59421600	-2.61012800
C	-0.31851900	4.21261900	-0.46537700	H	0.87906600	-3.16633700	-0.33854300
C	1.03456600	4.19258400	-2.46371400	H	7.62542000	-2.09382400	-0.82944100
C	1.21872100	1.76359800	2.34053000	H	4.06285500	2.11834300	-1.61032500
C	1.68899800	3.04903600	2.23961500	H	-1.00177600	-3.47879600	5.30049600
C	2.93804900	2.44108600	0.21419200	H	2.49195900	-5.01670100	-0.68144100
C	3.93000700	-4.23660000	0.72271900	H	0.49076400	5.98402500	-1.39173200
C	1.39303900	-1.08692300	5.64614800	H	-2.08248200	-0.53819000	-6.87426700
C	3.30275900	-2.18650300	1.84078600	H	4.64770500	-5.03565700	0.56006000
C	5.67184600	-2.07347700	-1.70461600	H	0.41804100	-2.40901300	7.04339400
C	2.41888200	1.10850200	0.31883200	C	-3.50221000	-1.94973000	0.29508900
C	-1.66971000	-0.39771800	-5.87940400	C	-4.50804200	-2.96802700	-0.30176200
				C	-4.02448100	-3.52602700	-1.61256900



C	-2.77097700	-3.39583800	-2.06776800	C	0.25229500	2.13133000	-1.47600100
C	-1.68776900	-2.75066200	-1.30120400	C	-0.37140900	2.83366200	-0.43948500
C	-2.01154700	-2.15811000	0.04767200	C	4.42037600	-1.31048300	-1.94050300
H	-3.67653500	-1.88870200	1.37689200	C	1.78827800	-0.26248700	-1.74990800
H	-4.77555500	-4.04577400	-2.20482500	C	4.02060400	4.96647900	0.36817400
H	-2.46964000	-3.80506100	-3.02845100	C	2.60535900	3.26535700	1.37396000
C	-4.91154000	-4.08033700	0.65530900	C	0.57924800	4.90461700	-1.23721100
H	-5.32879900	-3.64678000	1.57027100	C	0.67791800	-1.48644200	3.26056300
H	-5.66482600	-4.73090400	0.19880200	C	-1.21472900	1.26998800	-3.98605000
H	-4.03921800	-4.68873700	0.91593700	C	1.48602900	-0.94515300	4.27123000
O	-5.68165200	-2.16416800	-0.56300800	C	-0.72147400	0.14020800	-3.30959200
C	-5.23872900	-0.89222500	-1.05172000	C	0.46973800	-2.41713700	5.90415400
H	-5.13408600	-0.90748500	-2.14808200	C	2.13508500	-2.25656400	1.01308200
O	-0.54597300	-2.77690200	-1.76236300	C	-0.22361600	-2.51196000	3.58936200
C	-3.91537400	-0.66146200	-0.36617800	C	1.60640600	0.61945200	1.42476600
C	-3.08485900	0.40014200	-0.39327900	C	2.73343700	0.08236800	-0.77535500
H	-5.99827700	-0.14598000	-0.79507900	C	2.16921300	-1.11375700	-2.82000300
C	-3.38282800	1.65266300	-1.16446500	C	6.33768500	-0.65123300	0.00083600
H	-3.09796300	2.55874600	-0.62601000	C	4.06867600	-0.43614500	-0.86398800
H	-2.82374300	1.65920400	-2.10681200	C	-1.55158200	-1.24396300	-5.13379100
H	-4.44965400	1.73101900	-1.40901700	C	5.06749100	-0.13065500	0.10274800
Rh	-1.18951800	-0.27193100	0.40386600	C	4.30396600	-3.24774900	1.44241800
C	-5.64488300	3.31706400	1.70783200	C	-1.86615700	1.14172300	-5.21356700
C	-4.97868300	2.09990900	1.61263700	C	3.44046000	-1.62452600	-2.91187700
C	-3.59368600	2.03890100	1.84513400	C	4.36098800	4.06382500	-0.66601200
C	-2.88428600	3.21429400	2.15760500	C	3.15180600	4.57491800	1.36190300
C	-3.55795500	4.43104900	2.24133700	C	1.05507500	2.83130600	-2.38977000
C	-4.93596900	4.48371700	2.01553800	C	-0.21205000	4.21333600	-0.31931700
H	-6.71566100	3.36127000	1.53357900	C	1.21198000	4.21050700	-2.27269000
H	-5.51293400	1.19277100	1.35058200	C	1.21240800	1.57215500	2.40942900
H	-1.81366200	3.16011500	2.32799400	C	1.69932900	2.85430300	2.38485700
H	-3.00883600	5.33654400	2.48144300	C	2.95358200	2.34389800	0.33445700
H	-5.45870400	5.43359300	2.07704200	C	4.09941000	-4.15315500	0.39699600
C	-2.87595300	0.79441700	1.77234200	C	1.37728400	-1.40575300	5.58452300
C	-2.13781100	-0.12653200	2.24510900	C	3.32714000	-2.30586800	1.75369200
H	-1.90505800	-0.55870500	3.20575300	C	5.73482500	-1.84372600	-2.01199300
H	-1.55069500	-2.79789000	0.80591900	C	2.41243200	1.01291900	0.35676800
<b>9-ts-1</b>				C	-2.03569900	-0.11480400	-5.79526600
P	0.83300000	-1.04631600	1.48046800	C	-0.90987600	-1.12144700	-3.90083700
P	0.02753000	0.31452700	-1.62731100	C	1.92704800	-3.16912500	-0.02390200
				C	6.67794900	-1.51924600	-1.06418500

C	3.83164200	2.79265900	-0.69029200	H	-3.80176400	-1.85828000	1.40392800
C	-0.32760100	-2.97346000	4.90144400	H	-4.98350000	-3.73447500	-2.30958400
C	2.90948700	-4.11385600	-0.32942500	H	-2.64736400	-3.61718400	-3.07905100
H	-0.97370200	2.29736200	0.28418800	C	-5.07513600	-4.01435400	0.56995500
H	4.43982500	5.96838800	0.37082100	H	-5.47641100	-3.63279900	1.51480200
H	-1.09761100	2.25837800	-3.56149200	H	-5.84544000	-4.61813900	0.07888900
H	2.20624700	-0.16834800	4.04094600	H	-4.21400100	-4.65614200	0.78285000
H	-0.84911500	-2.95243300	2.81897700	O	-5.80401400	-1.99393200	-0.49950400
H	1.45235600	-1.36000200	-3.59060900	C	-5.32100300	-0.72121800	-0.94925200
H	7.08253200	-0.40455100	0.75187000	H	-5.27017000	-0.68601300	-2.04824200
H	-1.67559500	-2.23025600	-5.57196500	O	-0.67177200	-3.06568500	-1.59623900
H	4.81905100	0.51458900	0.93623900	C	-3.95791900	-0.58746300	-0.31644100
H	5.23024400	-3.26756600	2.00894600	C	-3.06867600	0.42414600	-0.36542700
H	-2.23820100	2.03158600	-5.71328700	H	-6.02679000	0.04779800	-0.61617700
H	3.70783300	-2.27609100	-3.73935500	C	-3.34856000	1.69581900	-1.11047700
H	5.03557600	4.38061200	-1.45603900	H	-2.84667800	1.67702000	-2.08278000
H	2.87159000	5.26034500	2.15722900	H	-4.42231000	1.82395600	-1.29570800
H	1.55873800	2.29738200	-3.18987800	H	-2.99549900	2.58432200	-0.58368100
H	-0.70031500	4.74164600	0.49406300	Rh	-1.19239400	-0.31710000	0.38983700
H	1.84078100	4.74236000	-2.98039500	C	-5.45869500	3.41411800	1.84867500
H	0.52355600	1.27688400	3.19245000	C	-4.85528100	2.17013000	1.69793700
H	1.40299200	3.56802900	3.14867000	C	-3.47634200	2.02734100	1.93123200
H	2.00830700	-0.97440500	6.35629500	C	-2.70955600	3.14878400	2.30194400
H	3.50048600	-1.60546100	2.56313900	C	-3.32043900	4.39314000	2.44115200
H	5.97851100	-2.51193200	-2.83356400	C	-4.69277800	4.52692800	2.21412000
H	-0.56594000	-2.01600300	-3.40081400	H	-6.52491900	3.52161700	1.67409900
H	1.01025100	-3.12448400	-0.59646200	H	-5.43389600	1.30446300	1.39314600
H	7.68187000	-1.92886700	-1.12746300	H	-1.64398200	3.03205800	2.47175800
H	4.08737400	2.12159100	-1.50041300	H	-2.72723600	5.25687800	2.72615100
H	-1.03140300	-3.76604900	5.13839100	H	-5.16671700	5.49824800	2.32031200
H	2.74388700	-4.81210000	-1.14530000	C	-2.82146000	0.75306800	1.81274500
H	0.71264600	5.97821500	-1.14247400	C	-2.09646600	-0.19865000	2.24419800
H	-2.54019600	-0.21321200	-6.75211200	H	-1.86464800	-0.67859900	3.18212000
H	4.86601700	-4.88314300	0.15335100	H	-1.69047600	-2.80841300	0.86734500
H	0.38730500	-2.77304100	6.92693500				
C	-3.60866000	-1.90080700	0.32461700				
C	-4.65519100	-2.85047400	-0.31494900				
C	-4.20428400	-3.32283900	-1.67064400				
C	-2.93678000	-3.24986700	-2.09849700				
C	-1.82399300	-2.81225600	-1.23481700				
C	-2.12890700	-2.17893800	0.09039800				
				<b>9-ts-2</b>			
				C	-3.54818200	-1.81898500	0.73076200
				C	-4.49506500	-3.00517900	0.40963300
				C	-3.89142500	-3.94176500	-0.60015500
				C	-2.59616400	-3.93768200	-0.94085400

C	-1.58905000	-3.06181200	-0.31103600	C	3.13559200	2.21788600	-0.66133800
C	-2.03793200	-2.04460700	0.70623400	C	-0.62487500	1.71309700	5.28923900
H	-3.82861900	-1.41435200	1.71184600	C	3.91481400	2.08988100	-1.84501000
H	-4.58415800	-4.64120400	-1.06448000	C	1.15338600	3.08827100	-3.68197200
H	-2.19938800	-4.63063600	-1.67793700	C	0.40381700	-0.36075800	5.95368400
C	-4.98505400	-3.76058200	1.63664400	C	2.23105000	3.65670700	1.09790700
H	-5.49810500	-3.07069800	2.31475700	C	6.32559700	-0.73724500	0.49139600
H	-5.68100600	-4.55600400	1.35051900	C	5.60944400	-2.73706800	-0.65804400
H	-4.13823200	-4.21293600	2.16297400	C	3.20946200	-1.21100600	2.69194300
O	-5.63870800	-2.36244200	-0.19943300	C	2.63236700	-3.81190000	1.85893800
C	-5.14866400	-1.30673200	-1.03391200	C	4.12611800	-2.23311000	2.91879400
H	-4.93333000	-1.67440800	-2.05017300	C	2.08284100	-2.29211800	-1.77750800
O	-0.40324200	-3.24180500	-0.58963300	C	3.31074700	-2.86303100	-1.56570800
C	-3.90170000	-0.82521500	-0.34063700	C	4.06045100	-0.83883300	-0.40448100
C	-3.08446500	0.21627600	-0.61573400	C	0.58695900	4.11100500	-2.91920500
H	-5.92714900	-0.54017000	-1.11047200	C	-0.11732100	-1.99660500	-5.34418200
C	-3.30974200	1.15732600	-1.76316200	C	1.00995300	1.75717000	-3.29154200
H	-4.36413900	1.18051100	-2.06620700	C	3.59462500	4.63844100	-0.72117000
H	-3.00625700	2.18004600	-1.53136000	C	2.75916600	-0.26480700	-0.61698900
H	-2.72052200	0.84136700	-2.63137200	C	-0.26750700	0.81324900	6.29458800
Rh	-1.24077500	-0.11843800	0.44228200	C	-0.30630500	1.44297200	3.95862900
P	0.08432200	-0.31820000	-1.56220400	C	-0.27750500	2.46338400	-1.37873800
P	0.76386100	-0.14882200	1.83757500	C	4.34718000	4.47676100	-1.86189300
C	1.99337800	-1.48632300	2.04434000	C	5.09300500	-0.15439600	0.29490000
C	1.70680800	-2.79004800	1.63198800	C	-2.30460600	-2.19904600	-4.34548600
C	2.98169900	3.52158800	-0.09411000	C	-0.13434200	3.79396700	-1.76676800
C	1.74585200	1.26477300	1.12382200	H	0.79092200	-2.99346200	1.09217100
C	6.58987400	-2.04199700	0.01343400	H	7.56367300	-2.49281000	0.18163900
C	4.33439500	-2.15697000	-0.88648900	H	1.26326700	-1.54199500	4.39143100
C	3.84003000	-3.53669200	2.50021000	H	1.40748700	-1.11913800	-4.12556100
C	-0.49241600	-1.17999000	-3.08440500	H	-2.49481700	-1.45124900	-2.34527200
C	0.73858000	-0.62428700	4.62407600	H	1.11655500	2.70908100	2.61926700
C	0.36078300	-1.39510600	-4.18106600	H	5.09739400	3.06716900	-3.32953700
C	0.40673700	0.28185300	3.60248600	H	-1.16496500	2.62319300	5.53367100
C	-1.45257900	-2.39896800	-5.43142100	H	4.03204100	1.11298500	-2.29781300
C	0.29665000	1.42695500	-2.13131700	H	1.72168700	3.32597700	-4.57631500
C	-1.82642700	-1.59385400	-3.18203400	H	0.67603200	-1.07824000	6.72237500
C	1.79298500	-0.97386600	-1.32464500	H	2.13879500	4.63817900	1.55536200
C	2.50316600	1.09040000	-0.03885000	H	7.09851000	-0.19396300	1.02742800
C	1.64234000	2.56525500	1.68834600	H	5.79356900	-3.74289200	-1.02602300
C	4.50876400	3.18799900	-2.42480500	H	3.43728000	-0.19934600	3.01327800

H	2.41083100	-4.81991200	1.51974500	H	-4.56253800	-1.48633700	1.01669600
H	5.06971400	-2.01147600	3.40815300	H	-3.33692400	-4.36224100	-1.96777500
H	1.31409700	-2.86354600	-2.27624700	H	-1.21703900	-4.69001500	-0.69506000
H	3.51003700	-3.87310000	-1.91335100	C	-5.25940100	-3.87150500	0.26338300
H	0.55774100	-2.15626500	-6.18000900	H	-6.12906000	-3.27488400	0.55847700
H	1.46947600	0.98064200	-3.89051100	H	-5.59945300	-4.70837500	-0.35562900
H	3.46065600	5.62102900	-0.27672300	H	-4.78142000	-4.27587200	1.16117800
H	-0.64534800	2.13513200	3.19876400	O	-4.98229400	-2.40561200	-1.60475600
H	-0.83980800	2.24829600	-0.47596400	C	-4.21841900	-1.27696200	-2.03107000
H	4.81711200	5.33453400	-2.33415800	H	-3.42716400	-1.58126500	-2.72947000
H	4.90471400	0.83780800	0.68521500	O	-1.06272400	-3.85204600	1.79836600
H	-3.34162300	-2.51826000	-4.39569600	H	-2.62237200	-1.80429600	2.19432500
H	-0.58409000	4.57941800	-1.16640200	C	-3.65781200	-0.68665300	-0.75431200
H	4.56135600	-4.33094000	2.66976300	C	-3.43402700	0.64390100	-0.57402100
H	-0.51938200	1.02059700	7.33048100	H	-4.89403000	-0.59879200	-2.55822200
H	0.70817400	5.14742000	-3.22020000	C	-3.62613600	1.63126400	-1.70358500
H	-1.82186000	-2.87091000	-6.33734400	H	-4.67052700	1.96595100	-1.74658900
C	-5.73773700	3.67040200	0.32873200	H	-3.00480800	2.51809100	-1.55693200
C	-5.10928100	2.46323300	0.61808700	H	-3.37468800	1.19539800	-2.67206600
C	-3.74139900	2.44416000	0.93816500	Rh	-1.12601500	-0.75368100	0.15850900
C	-3.00689100	3.64413900	0.93927700	P	0.15303800	0.52423200	-1.55683300
C	-3.64003500	4.84743200	0.63433400	P	0.70296800	-0.84150900	1.50805500
C	-5.00399800	4.86177400	0.33053400	C	1.76919100	-2.20980000	0.94065100
H	-6.79744800	3.68460700	0.09259100	C	1.39814900	-2.90820300	-0.21665200
H	-5.66217700	1.52959000	0.59729600	C	2.66407200	3.39164700	1.19845000
H	-1.94651100	3.62039600	1.17122800	C	1.56191500	0.78380500	1.34789200
H	-3.07044200	5.77193500	0.63328400	C	6.51160300	-1.97505700	-0.81074000
H	-5.49595000	5.80021900	0.09231100	C	4.38206400	-1.43608700	-1.85026000
C	-3.06695700	1.21078900	1.26163400	C	3.31094200	-4.35877200	0.03144200
C	-2.38126200	0.49198700	2.06160200	C	-0.65396900	0.10888600	-3.14882400
H	-2.26355100	0.35045400	3.12299600	C	-0.38969200	-1.73656400	3.96921000
H	-1.64288100	-2.34493900	1.68170700	C	-0.95121600	-1.24123500	-3.40263200

## 10

C	-3.76268700	-1.78127000	0.32772400	C	-1.02022200	1.07574300	-4.09436900
C	-4.27614700	-2.99342500	-0.50450300	C	1.87607400	-0.11958400	-1.75554800
C	-3.13719800	-3.83269400	-1.03792600	C	2.48268500	1.07269100	0.34756600
C	-1.98886700	-3.99862700	-0.36714200	C	1.14947300	1.81299000	2.24633700
C	-1.79993900	-3.33971500	0.94728400	C	4.59574900	3.98320100	-0.75021700
C	-2.48880800	-2.04305600	1.14322400	C	3.07786100	2.37922900	0.27646400

C	1.72703500	-0.72626900	5.48591600	H	4.57005200	-3.96762300	1.73843200
C	4.05258100	2.71799800	-0.70139000	H	1.52041100	-1.09478400	-3.66323800
C	1.35789700	4.35622800	-2.41020800	H	3.69242800	-2.22366100	-3.74245900
C	-0.37222100	-1.91042700	5.35445700	H	-1.78785800	-2.66874200	-4.77677400
C	1.67592500	3.07594200	2.16542900	H	1.82772900	2.37736000	-3.11246900
C	6.20714800	-1.10369700	0.26361000	H	2.89947400	5.44647400	1.82015200
C	5.61819400	-2.13466800	-1.84585700	H	2.52621600	-0.00557900	3.63368900
C	2.90907700	-2.60689100	1.65198100	H	-1.09486800	2.61890000	0.03335500
C	2.16504700	-3.97713400	-0.67127200	H	4.61426600	5.97578200	0.10768200
C	3.67914100	-3.67448100	1.19161900	H	4.78536600	0.24384500	1.11939900
C	2.22323100	-0.95079100	-2.85272200	H	-1.94786600	1.45544200	-5.99695300
C	3.44166400	-1.58587700	-2.89913500	H	-0.87176800	5.08195200	0.06164400
C	4.06854000	-0.56185400	-0.76095000	H	3.91500000	-5.18814300	-0.32425100
C	0.60392300	5.12070000	-1.51424900	H	0.69056100	-1.54006300	7.19378300
C	-1.57436700	-1.62016300	-4.59082900	H	0.71658800	6.20077000	-1.49653800
C	1.22694500	2.96940500	-2.42899200	H	-2.43335300	-0.94081200	-6.44932400
C	3.23204300	4.68903000	1.11572800	C	-5.75638700	3.66398200	1.64588300
C	2.80330200	0.09879600	-0.73775700	C	-5.10041400	2.55413400	1.11376100
C	0.68003500	-1.40282400	6.11639300	C	-3.72257000	2.36859400	1.31832000
C	1.70975600	-0.54076600	4.10505900	C	-3.01938100	3.33068800	2.06659100
C	-0.41934400	3.10637600	-0.65490700	C	-3.67750500	4.43589400	2.60317500
C	4.18316600	4.98056300	0.16365400	C	-5.04864300	4.60877800	2.39325600
C	5.01672800	-0.41270800	0.28795100	H	-5.66020500	1.81726400	0.54460500
C	-1.66368200	0.69580800	-5.27463000	H	-1.94874400	3.21535400	2.20853600
C	-0.28635400	4.49541600	-0.64041700	H	-3.11702900	5.17032400	3.17525100
H	0.51252900	-2.60431200	-0.76948300	H	-5.55953000	5.47476700	2.80431900
H	7.45261900	-2.51724400	-0.81323900	C	-3.02255400	1.19479100	0.75055300
H	-1.17334600	-2.19267300	3.38563800	C	-1.93806300	0.62338700	1.29789100
H	-0.68623700	-2.00361800	-2.67383400	H	-1.54783400	0.87490900	2.27981100
H	-0.81069800	2.12355800	-3.91232200	H	-6.82265900	3.78941900	1.47892200
H	0.41852500	1.59607200	3.01512600				
H	5.34163700	4.21950400	-1.50341300	<b>11-ts</b>			
H	2.55811900	-0.33806800	6.06731800	C	4.27281500	-0.45937000	-0.08857000
H	4.37035900	1.97121000	-1.41813300	C	4.82563800	-1.42283100	-1.17047600
H	2.05921600	4.83962100	-3.08360200	C	3.86916800	-1.60463900	-2.32009900
H	-1.18258200	-2.45191200	5.83382600	C	2.93445300	-0.70447100	-2.64756000
H	1.34559600	3.84953900	2.85296200	C	2.77956000	0.57472400	-1.92315300
H	6.91754500	-0.98611200	1.07669300	C	3.36756400	0.67264800	-0.54179000
H	5.84166900	-2.80086600	-2.67478300	H	5.12278800	-0.04201600	0.46386100
H	3.20009400	-2.08697800	2.55771500	H	4.01480900	-2.50400800	-2.91350700
H	1.87429000	-4.50551600	-1.57424600				

H	2.31798400	-0.82013600	-3.53441400	C	-2.47523400	-3.49502600	3.16192100
C	6.20259000	-1.02138600	-1.68852000	C	1.46560900	5.08982300	-0.46056900
H	6.91132600	-0.97403500	-0.85500200	C	-2.35434400	1.28408900	3.13352200
H	6.56730200	-1.75002700	-2.41977100	C	-5.65322800	0.98177100	-2.30373600
H	6.15289800	-0.04040900	-2.17163900	C	-4.95106200	-0.85559500	-3.71278400
O	4.97591100	-2.67045800	-0.46772300	C	-1.89863900	2.25017500	-2.47710400
C	3.86452000	-2.81701300	0.42230600	C	-1.01487200	0.30911800	-4.27914000
H	3.02728200	-3.31368900	-0.07743900	C	-2.40833500	2.21929200	-3.77418600
O	2.32210400	1.56310400	-2.51003600	C	-2.01247900	-2.52383100	-2.13212700
H	3.81996900	1.65664400	-0.43708000	C	-3.04355800	-2.26885000	-3.00377600
C	3.52302300	-1.40854700	0.83920800	C	-3.77830100	-0.39974300	-1.59720600
C	2.99929200	-1.00497200	2.04167500	C	-2.00930400	-2.76325600	4.25947900
H	4.18730200	-3.44398500	1.25915000	C	1.73192500	-4.65937500	-2.22667000
C	2.66583800	-2.02800800	3.10201100	C	-1.95911400	-3.25381000	1.89068200
H	2.09049700	-1.59863900	3.92182500	C	-4.35485200	0.07736800	3.94585400
H	2.09340700	-2.85483900	2.67308800	C	-2.71603000	-0.69580200	-0.68752300
H	3.58927300	-2.45031900	3.51829300	C	0.47414400	5.92408500	0.05848200
Rh	1.34116600	-0.15821800	0.20388900	C	-0.97230700	4.00530200	0.34935500
P	-0.29388800	-1.91997500	0.04957100	C	-0.50729400	-1.54811500	2.81069200
P	-0.26811200	1.35145400	-0.37137400	C	-5.37071900	-0.82779600	3.73284100
C	-0.95097200	1.29961700	-2.07044900	C	-4.67285900	0.68504800	-1.38395200
C	-0.50661500	0.33551000	-2.98199400	C	1.34809000	-5.70776500	-0.08398500
C	-3.43233900	0.38813200	2.91450800	C	-1.02516700	-1.79015000	4.08275300
C	-1.61115600	0.99428800	0.83326000	H	0.21990100	-0.40253000	-2.66526400
C	-5.79466300	0.20711900	-3.48083600	H	-6.57090800	0.45579100	-4.19856200
C	-3.92897900	-1.18559800	-2.78415600	H	1.99584500	3.08365700	-1.02913100
C	-1.96831500	1.24901000	-4.67710400	H	0.96146100	-2.66631300	-2.44938200
C	0.48736000	-3.47823900	-0.50542400	H	0.23525600	-4.55837700	1.35042300
C	1.24587400	3.71601800	-0.56992900	H	-0.64028200	2.24314600	2.32639700
C	1.05026500	-3.52420800	-1.79218000	H	-6.29058400	-2.18624300	2.31583400
C	0.03092500	3.15582400	-0.14764400	H	-1.53519000	6.01990700	0.84056700
C	1.88545700	-5.75411000	-1.37111300	H	-4.71355900	-1.69210100	0.50569500
C	-0.96327500	-2.28093700	1.71114000	H	-3.25148700	-4.24255800	3.29561900
C	0.64884900	-4.57853900	0.34906800	H	2.41321500	5.50698000	-0.78956100
C	-1.81469700	-1.72046600	-0.97894700	H	-2.23345800	1.73227900	4.11590900
C	-2.61790400	0.06642200	0.59617400	H	-6.32118400	1.82032700	-2.12960500
C	-1.46675600	1.56991400	2.13005900	H	-5.04904200	-1.45692100	-4.61256900
C	-5.49521500	-1.46424400	2.47635800	H	-2.24581200	3.00883200	-1.78430400
C	-3.56024600	-0.24443600	1.63717800	H	-0.67156000	-0.45037900	-4.97556800
C	-0.74902700	5.37858700	0.45259300	H	-3.15359000	2.94900300	-4.07603300
C	-4.61098900	-1.18486900	1.45693200	H	-1.34188900	-3.34895700	-2.33448400

H	-3.18002200	-2.88952900	-3.88518200	H	-6.54073900	-2.83495800	0.50227000
H	2.15318300	-4.68357400	-3.22736000	H	-6.07139000	-3.24409700	2.16879800
H	-2.33521400	-3.81079800	1.03756600	H	-6.36279200	-1.54875800	1.72548400
H	-4.23768100	0.56504200	4.90993700	O	-4.03988800	-3.62744000	0.46845600
H	-1.93047000	3.60375000	0.65732500	C	-3.18867000	-3.46034700	-0.66982900
H	0.23450800	-0.77369100	2.65452300	H	-2.21065700	-3.90451200	-0.48404800
H	-6.07213200	-1.06071400	4.52864400	O	-3.33313800	1.53602800	1.94300200
H	-4.56500300	1.29214900	-0.49245300	H	-4.98069400	0.65863800	0.07697300
H	1.46942500	-6.55160500	0.58895900	C	-3.13101000	-1.99046900	-0.94807700
H	-0.67216600	-1.20682700	4.92818800	C	-2.52257700	-1.37957800	-2.02591000
H	-2.36799600	1.22496900	-5.68670700	H	-3.63939900	-3.98870200	-1.52436100
H	0.64845800	6.99273200	0.14519800	C	-1.88041200	-2.23430400	-3.09006200
H	-2.42285800	-2.94585100	5.24696400	H	-1.23587800	-1.67061700	-3.75943400
H	2.42700500	-6.63423500	-1.70497600	H	-1.28683700	-3.02953700	-2.63012400
C	2.86034100	0.45052900	2.29283200	H	-2.66143300	-2.71470300	-3.69420300
C	2.47281200	1.18560400	1.20144100	Rh	-1.19735000	-0.34326500	-0.48840400
H	2.39201400	2.26506800	1.19870700	P	0.69146600	-1.81135700	-0.17956700
C	2.98599500	1.02509500	3.64749100	P	0.15730300	1.45749100	0.08539200
C	3.91679800	0.51053000	4.56737800	C	0.55275000	1.51621300	1.87601200
C	2.18005800	2.11020100	4.03940200	C	0.02505400	0.54120600	2.72852700
C	4.04090500	1.06847400	5.83883200	C	3.92348400	0.88323000	-2.60895500
H	4.55733500	-0.31664000	4.27773700	C	1.71438100	1.26798500	-0.87572200
C	2.30761400	2.66739600	5.30971500	C	5.18444900	1.20245600	4.07767500
H	1.44218300	2.50337200	3.34636500	C	3.67261400	-0.46550400	3.16199100
C	3.23711700	2.14746800	6.21509600	C	1.03999200	1.63457100	4.62848200
H	4.76944700	0.66262800	6.53493000	C	0.11277900	-3.46068200	0.36668400
H	1.67451700	3.50211800	5.59700100	C	-1.59380000	3.62613300	0.27557200
H	3.33246600	2.57840700	7.20751500	C	-0.68825500	-3.51419200	1.52153200

## 12

C	-4.26798700	-1.36388500	-0.18255900	C	0.35674800	-4.64041900	-0.34848800
C	-4.49264600	-2.35138500	0.97612600	C	1.98853700	-1.35707800	1.06391700
C	-3.67852200	-1.99492100	2.18919100	C	2.78325000	0.49166500	-0.44321400
C	-3.24893900	-0.75257400	2.45759000	C	1.71516900	1.79527600	-2.20035800
C	-3.50898300	0.38146700	1.56242300	C	6.10925900	-0.66444600	-1.76878000
C	-4.03026100	0.11181700	0.14412600	C	3.91806700	0.29551900	-1.30438600
H	-5.14306000	-1.43369100	-0.84388000	C	0.16724000	5.52351800	-0.76341300
H	-3.50164200	-2.80727100	2.89002500	C	5.03881300	-0.48998700	-0.91879600
H	-2.73170500	-0.51579200	3.38296600	C	3.53339800	-3.08710300	-2.86730300
C	-5.96116000	-2.50332200	1.37018000	C	-1.98357300	4.96117700	0.17281100

C	2.78815500	1.61874600	-3.03405200	H	3.10431400	-3.40173000	-0.78263300
C	5.14119100	1.91018900	2.85179100	H	5.02039200	1.13391100	-4.45221500
C	4.46687100	0.03727000	4.22622800	H	1.56570300	3.91415700	-0.96498600
C	1.31436200	2.56456700	2.41237600	H	0.45115400	-0.74106600	-2.86345300
C	0.26791600	0.59775500	4.10025000	H	6.96210900	-0.22143900	-3.71425000
C	1.56176700	2.61708800	3.78271000	H	4.34584100	2.00302700	0.87235000
C	2.09902200	-2.08638600	2.27725400	H	0.01173200	-6.76038700	-0.47177900
C	2.91908400	-1.65718100	3.29240500	H	1.75187400	-1.06753300	-4.95230500
C	3.61987900	0.25141600	1.92443600	H	1.23551700	1.67769500	5.69600200
C	3.15391100	-2.43375900	-4.04400300	H	-1.41742500	6.95096300	-0.44304900
C	-1.20629100	-4.72681200	1.96892600	H	3.73863900	-2.56553300	-4.94968400
C	2.79354500	-2.91068000	-1.69985800	H	-1.36684500	-6.84565000	1.59523800
C	5.03784100	0.68315200	-3.46353500	C	-2.62088900	0.08659800	-2.05888100
C	2.77438500	-0.22079300	0.87178100	C	-3.05805000	0.71987400	-0.86383500
C	-1.11013300	5.91257300	-0.35844700	C	-2.29910100	0.87157300	-3.27925400
C	0.56315800	4.18844200	-0.66147500	C	-2.65973900	0.38856000	-4.54774700
C	1.29395300	-1.42110800	-2.88118700	C	-1.69969400	2.13843400	-3.19518200
C	6.11356000	-0.07223100	-3.05292700	C	-2.39583000	1.13593400	-5.69709400
C	4.38176300	1.44595700	1.80137000	H	-3.16775500	-0.56468100	-4.64119000
C	-0.17937700	-5.85321000	0.09417200	C	-1.43164000	2.88179000	-4.34147000
C	2.03608700	-1.59845100	-4.04841400	H	-1.43082200	2.54090600	-2.22829000
H	-0.56161400	-0.26743800	2.30595300	C	-1.77142200	2.38025200	-5.60117600
H	5.78528400	1.58320900	4.89842800	H	-2.68446600	0.74264100	-6.66759400
H	-2.27444800	2.90927500	0.72076200	H	-0.95512500	3.85352200	-4.24636100
H	-0.91804300	-2.60217000	2.06301000	H	-1.56000500	2.95756200	-6.49653800
H	0.95434500	-4.61949700	-1.25215600	H	-3.05395800	1.80207500	-0.87297600
H	0.84915300	2.33501000	-2.56074000				
H	6.95451700	-1.26883400	-1.45252700	<b>13</b>			
H	0.86502300	6.25801100	-1.15536900				
H	5.04717000	-0.96232900	0.05560300	O	3.24335000	-1.74955800	-0.05497600
H	4.41487000	-3.72123300	-2.85579300	O	0.90095900	2.91440600	-0.84681200
H	-2.97165700	5.25661400	0.51438800	C	2.86221200	1.62156900	-0.99715700
H	2.77225500	2.02970100	-4.03981100	H	3.21336100	2.27370200	-1.79338500
H	5.70779700	2.83042100	2.74303700	C	1.07867200	1.15779700	0.79845000
H	4.49138700	-0.51543600	5.16150500	H	1.42794200	1.71430600	1.67889300
H	1.71743000	3.33382700	1.76191600	C	1.66201200	-0.25659800	0.83553700
H	-0.13771200	-0.17009800	4.75277200	H	1.49786900	-0.67790000	1.83844100
H	2.16650900	3.42199200	4.18947800	C	1.55823400	1.97597700	-0.41037400
H	1.52644800	-2.99439800	2.41305000	C	-0.43149500	1.07143300	0.81534400
H	2.98584700	-2.22391300	4.21720200	H	-0.98938700	1.86361900	1.30372300
H	-1.82149300	-4.75263300	2.86296900	C	0.99010400	-1.13182400	-0.19524400



C	3.15209200	-0.40869200	0.47989100	H	6.55902700	2.03041100	2.48763700
C	-1.08207600	0.05969400	0.20242000	H	5.45164500	0.65394000	2.68237400
C	-0.30915700	-0.99949500	-0.50676400	O	5.42850500	2.93582400	0.22331900
C	2.04158300	-2.03469600	-0.78555300	C	4.42688800	3.28800300	-0.73824300
H	1.82933100	-3.10298000	-0.66331000	H	3.90935200	4.21644300	-0.44744300
H	2.18463900	-1.84018300	-1.86024800	O	0.94762000	1.33053300	2.67553000
C	3.57795400	0.55990000	-0.59623600	C	3.48938000	2.10966500	-0.75270300
H	4.53514400	0.33558700	-1.06429300	C	2.42969800	1.82633500	-1.54091000
C	4.09469300	-0.32940700	1.67441300	H	4.92239300	3.46347100	-1.69899600
H	3.82623200	-1.09801700	2.40669900	C	1.96661000	2.71306700	-2.65962900
H	4.02430200	0.65451600	2.14992000	H	2.75278900	3.42047700	-2.95338400
H	5.13211600	-0.48947600	1.36219400	H	1.68185500	2.13861600	-3.54689600
C	-2.56804700	0.02591600	0.19650100	H	1.08697900	3.29388000	-2.36283800
C	-0.97147900	-1.82866900	-1.57818400	Rh	1.27356100	0.26800000	-0.59328700
H	-0.22491500	-2.32948600	-2.20256900	P	-0.62122400	1.71482700	-0.11701400
H	-1.59552000	-1.20487000	-2.22870800	P	-0.11082000	-1.70584300	0.04100700
H	-1.62676300	-2.60230000	-1.16040500	C	-0.71168800	-2.15080900	1.70664700
C	-3.30385800	1.17262200	-0.14439800	C	-0.14338000	-1.55416300	2.83633900
H	-2.77070700	2.07009800	-0.44452100	C	-3.87938200	-1.03149800	-2.70540900
C	-3.26944800	-1.13719400	0.55676900	C	-1.66025700	-1.48562800	-0.97961000
H	-2.71673900	-2.02878400	0.83810500	C	-5.28417000	-1.56120900	3.79664800
C	-4.69903300	1.16028700	-0.11940300	C	-3.55777900	0.00284500	3.10214100
H	-5.25044400	2.05636000	-0.39125900	C	-1.56438300	-2.89480400	4.26509700
C	-4.66377000	-1.14999800	0.58263100	C	-0.43991200	3.46999200	0.41160500
H	-5.18853500	-2.05652700	0.87197400	C	1.11077300	-3.37415000	-1.88464200
C	-5.38431500	-0.00145800	0.24344700	C	-1.54586400	4.21408500	0.86117200
H	-6.47061900	-0.01340200	0.25926300	C	0.58027100	-3.30044300	-0.58517200

#### 14-ts

C	3.84704600	1.20980300	0.39131500	C	-1.84806100	1.05318800	1.09511600
C	4.79903700	2.10671400	1.22569300	C	-2.69379200	-0.64245800	-0.56617000
C	4.03231700	2.99928800	2.16253400	C	-1.76154400	-2.12228000	-2.24767000
C	2.75467300	2.79071100	2.50488100	C	-5.94959200	0.68110200	-1.89458300
C	1.99239100	1.59979400	2.08296700	C	-3.82053000	-0.40505800	-1.42167800
C	2.56863300	0.68940900	1.03405300	C	1.26778300	-5.60579500	-0.23102100
H	4.42925400	0.36102100	0.01126700	C	-4.88772800	0.45842100	-1.04717400
H	4.58283600	3.85009700	2.55933300	C	-3.28483800	2.78575600	-3.11211300
H	2.23457700	3.44677200	3.19718200	C	1.69335800	-4.54915100	-2.35461500
C	5.89398100	1.34255500	1.95524800	C	-2.82863700	-1.90072800	-3.08260900
H	6.48473800	0.76725400	1.23474400	C	-5.32163300	-2.09256900	2.48614800

C	-4.41459400	-0.53694300	4.09691700	H	0.30404200	-4.40461600	1.25343600
C	-1.71113500	-3.12565600	1.86320500	H	-0.08725700	0.63056800	-2.77450300
C	-0.57466400	-1.92363600	4.11244200	H	-6.84013600	0.25269000	-3.82706600
C	-2.12978600	-3.49797700	3.13742600	H	-4.51618500	-2.03504900	0.51474300
C	-1.84285400	1.57721700	2.41928100	H	1.91183700	5.93416200	0.54629400
C	-2.66229100	1.06267400	3.38997800	H	-1.20378500	0.82542600	-4.95568000
C	-3.58506000	-0.53586100	1.77809800	H	-1.90269600	-3.17778300	5.25775100
C	-2.76791400	2.12138900	-4.22610100	H	2.24507100	-6.58183600	-1.88816400
C	-1.40778300	5.56194300	1.18616300	H	-3.26213300	2.20668100	-5.18937100
C	-2.65906800	2.66970600	-1.87184100	H	-0.05896000	7.24076000	1.32801700
C	-4.98127400	-0.77495600	-3.56320000	C	4.31846100	-3.76510100	0.72464600
C	-2.69090500	-0.00855300	0.78447700	C	3.50633700	-2.69507300	0.35691900
C	1.77749500	-5.67036500	-1.52748200	C	3.66726500	-2.07466100	-0.89285100
C	0.67446900	-4.43251100	0.23715100	C	4.67982100	-2.54223500	-1.75726400
C	-0.98766600	1.23223200	-2.85524600	C	5.49180300	-3.60755200	-1.38277900
C	-5.99917500	0.06208200	-3.16670200	C	5.31242300	-4.22649500	-0.14118200
C	-4.48834600	-1.60050600	1.50604800	H	4.17188000	-4.24102700	1.68985400
C	0.93823600	5.46019500	0.63116300	H	2.73337900	-2.34723500	1.03136400
C	-1.61405900	1.34652500	-4.09544200	H	4.81735400	-2.05931300	-2.72022600
H	0.58588900	-0.76320400	2.71859300	H	6.26579100	-3.95741400	-2.06002700
H	-5.93956300	-1.96561600	4.56263000	C	2.87355400	-0.94016400	-1.30701500
H	1.10098400	-2.50302400	-2.52861100	C	2.74577500	-0.02797300	-2.19989800
H	-2.51375900	3.74076200	0.97933100	H	2.83292200	0.24441900	-3.24170800
H	1.66094100	3.55174600	-0.03096800	H	2.68984900	-0.29929800	1.48003400
H	-0.99842000	-2.81635600	-2.56605100	H	5.94507700	-5.06017100	0.14911300
H	-6.75233600	1.34590200	-1.58917800				
H	1.33590000	-6.46723000	0.42712200				
H	-4.85655700	0.95360200	-0.08445900				
H	-4.18621600	3.38423600	-3.20342300	C	-3.88500700	-1.04196000	0.32142100
H	2.09971700	-4.57899100	-3.36123900	C	-4.97452200	-1.77728200	1.13817100
H	-2.87929900	-2.40338200	-4.04472600	C	-4.37413500	-2.66018300	2.19685100
H	-6.00452400	-2.90473800	2.25415000	C	-3.09229700	-2.59929900	2.58356500
H	-4.37088400	-0.12056100	5.09977200	C	-2.12067100	-1.63261000	2.04143500
H	-2.16286300	-3.58592100	0.99018700	C	-2.59176100	-0.63464100	1.01091500
H	-0.14313200	-1.44054600	4.98448800	H	-4.34346400	-0.15972800	-0.13928600
H	-2.91047500	-4.24379100	3.25067200	H	-5.05073600	-3.38800100	2.64082800
H	-1.16274700	2.37554700	2.67418600	H	-2.69474400	-3.26640200	3.34376500
H	-2.63297000	1.46695900	4.39816100	C	-6.03644400	-0.85889200	1.72721200
H	-2.27242600	6.11970600	1.53409900	H	-6.80236600	-1.43756000	2.25397700
H	-3.08471300	3.18073500	-1.01702600	H	-5.58090100	-0.15998700	2.43647200
H	-5.00335500	-1.25619900	-4.53722300	H	-6.51723700	-0.29041000	0.92431100

**14-ts-1**

O	-5.61596600	-2.61847000	0.15301700	C	0.90272500	1.32107300	4.42050300
C	-4.60827400	-3.11028600	-0.74220600	C	2.28388800	3.05646300	3.46403900
H	-4.20941900	-4.07429000	-0.38955900	C	2.05645600	-1.69092300	2.30716100
O	-0.97159600	-1.64168100	2.48366000	C	3.01496200	-1.22432800	3.16935400
C	-3.54672500	-2.03735400	-0.74902500	C	3.73765900	0.41430300	1.49478200
C	-2.40296100	-1.91995700	-1.44109100	C	2.64588500	-2.34744600	-4.22462900
H	-5.07843600	-3.27362400	-1.71760500	C	1.26966600	-5.66810000	1.24619500
C	-1.97081400	-2.88976200	-2.49945200	C	2.55765400	-2.81746300	-1.85210200
H	-2.77680100	-3.59858900	-2.72872400	C	4.17669200	1.05670000	-4.04411700
H	-1.69080500	-2.38791900	-3.43234600	C	2.72638400	-0.08212900	0.60620100
H	-1.09711400	-3.46942200	-2.18510800	C	-1.55301300	5.86530900	0.57402600
Rh	-1.26108900	-0.30382700	-0.56348000	C	-1.78579700	3.49947200	1.00932200
P	0.56992500	-1.80515300	-0.08458100	C	0.88978200	-1.40024800	-2.86227200
P	0.03736700	1.52732900	0.38937700	C	5.34007500	0.34288900	-3.86308300
C	0.83166500	1.73856100	2.03744000	C	4.57278100	1.51570700	1.15815500
C	0.39598200	1.02028300	3.15217600	C	-1.09990000	-5.46320100	0.85153100
C	3.21860900	1.15785100	-3.00251800	C	1.50225400	-1.55846400	-4.10444100
C	1.36007800	1.39664700	-0.88264000	H	-0.30907200	0.21033600	3.02517900
C	5.65636000	1.40390600	3.32529700	H	6.39467500	1.79540600	4.01901400
C	3.88386600	-0.17151400	2.79165600	H	1.01693600	4.13632600	-0.82005500
C	1.84605800	2.33421900	4.57958900	H	2.44343400	-3.91144600	0.92728400
C	0.35161100	-3.54612100	0.48778600	H	-1.78167000	-3.54187100	0.19669300
C	0.09272700	4.31009000	-0.28130100	H	0.17013400	2.51466900	-2.31688500
C	1.44783300	-4.33487200	0.87913600	H	6.49454500	-0.88866400	-2.50183100
C	-0.61137800	3.24078700	0.28786000	H	-3.16533300	4.99061300	1.70976100
C	-0.00488100	-6.23858700	1.23250100	H	4.85397300	-0.76573700	-0.67894400
C	1.40498100	-2.02878900	-1.72075200	H	4.06910500	-3.58146700	-3.17268100
C	-0.92153600	-4.12934700	0.48283500	H	0.16793700	6.43595900	-0.59426900
C	1.91388800	-1.14672900	1.00134700	H	1.79767600	2.32345300	-4.14614200
C	2.50488300	0.62239100	-0.69381400	H	6.13492600	2.83694300	1.76923300
C	1.09619500	1.97461300	-2.15792600	H	4.94710500	-0.10985500	4.67097500
C	5.58216100	-0.31455200	-2.63385700	H	2.11329400	3.34056400	1.34574800
C	3.46613900	0.50665300	-1.75170400	H	0.56225300	0.75055300	5.28016300
C	-2.25136200	4.80393400	1.15467000	H	3.02581300	3.84126300	3.57703400
C	4.66465200	-0.24446400	-1.60936500	H	1.37987200	-2.46608400	2.63682000
C	3.17085600	-2.97621300	-3.09339200	H	3.10330000	-1.64542800	4.16703500
C	-0.38325400	5.61514400	-0.14427400	H	2.13040500	-6.25736400	1.54898900
C	2.00233400	1.86539100	-3.18225500	H	2.99606000	-3.29934700	-0.98745200
C	5.50948000	1.99363100	2.04740100	H	3.97131800	1.55474000	-4.98790700
C	4.85569500	0.34469300	3.68826300	H	-2.33224300	2.67836500	1.46431300
C	1.77461700	2.76824200	2.20252100	H	0.01219400	-0.77092600	-2.78912800

H	6.07012500	0.27455500	-4.66432700	C	1.63095600	3.56219300	-1.18467100
H	4.46227000	1.99120100	0.19157500	C	-1.35223600	1.34864900	0.83945500
H	-2.09886200	-5.88961100	0.84587100	C	-2.76014400	-0.22661100	-0.55340400
H	1.09103000	-1.05273800	-4.97326800	C	-2.33674300	-2.03145000	-2.13445200
H	2.24227400	2.56339700	5.56473600	C	-5.76661000	1.66611700	-1.77968000
H	-1.92067300	6.88168900	0.68101100	C	-3.88830200	0.17588900	-1.34261400
H	3.13082500	-2.46525400	-5.18913200	C	0.91179200	-4.86278000	-2.39295300
H	-0.14202100	-7.27629600	1.52258900	C	-4.69667300	1.29493100	-0.99733800
C	-5.01507500	3.86608000	-0.75600700	C	-2.77034900	2.99526200	-3.26951500
C	-4.39007300	2.62083500	-0.73411200	C	0.38821800	-5.87379800	-0.26842000
C	-3.24284300	2.38951300	-1.51113900	C	-3.41404400	-1.65678500	-2.89913000
C	-2.72048500	3.43923000	-2.28702100	C	-5.40127300	-0.52000700	2.82694000
C	-3.33964300	4.68654400	-2.29004000	C	-4.00471500	0.95549100	4.13372200
C	-4.49193700	4.90352200	-1.52995700	C	-2.40517000	-3.05735300	1.72944600
H	-5.90919300	4.02668000	-0.16044200	C	-1.50706700	-1.73041400	4.01848000
H	-4.79582500	1.82456900	-0.12003300	C	-3.02974600	-3.27932700	2.95480800
H	-1.83577600	3.26561800	-2.89049400	C	-1.05100900	1.94921800	2.09693500
H	-2.92169700	5.48998500	-2.88941200	C	-1.90569700	1.82724000	3.16176600
C	-2.64787000	1.06725300	-1.58613100	C	-3.37218400	0.38108500	1.82166100
C	-2.50488200	0.04186900	-2.31604900	C	-2.60988900	2.16300700	-4.38024700
H	-2.59606600	-0.42943600	-3.27986800	C	0.24467700	5.62649900	0.07791200
H	-2.65596000	0.34669300	1.49275900	C	-2.02349600	2.77477700	-2.11570500
H	-4.97490900	5.87617200	-1.53786500	C	-5.31405600	-0.13224800	-3.32901800

#### 14-ts-2

P	-0.11065000	1.53494700	-0.50255100	C	0.87905000	-5.98924300	-1.56911800
P	-0.50902700	-1.84591900	0.03107900	C	0.47082500	-3.62848600	-1.91692600
C	-1.30940600	-2.18456900	1.64613400	C	-0.94477100	0.88568500	-3.16877400
C	-0.87448600	-1.51684400	2.79462700	C	-6.08059500	0.94888800	-2.95896700
C	-4.21108400	-0.54543100	-2.53546700	C	-4.53678400	-0.43268700	1.75832200
C	-1.98568600	-1.31906300	-0.95815500	C	2.07098200	4.87820100	-1.31382400
C	-5.13951100	0.18347800	4.02556800	C	-1.69510500	1.11243100	-4.32481600
C	-3.09972500	1.07024500	3.04740200	H	-0.05015500	-0.81674900	2.72211800
C	-2.58212100	-2.61576200	4.10119800	H	-5.82937100	0.10339800	4.86060900
C	0.49161200	3.26634800	-0.42310800	H	-0.45570500	-4.58388500	1.21617200
C	-0.06748900	-4.64317200	0.20726400	H	-1.09879800	4.10909700	0.77849900
C	-0.20300200	4.31116300	0.20296400	H	2.17048700	2.76368400	-1.68535600
C	-0.02824900	-3.50158700	-0.60908500	H	-1.75690200	-2.89350600	-2.43438600
C	1.38068300	5.91339200	-0.68038500	H	-6.36797700	2.52535100	-1.49721900
C	-1.10499900	1.71253100	-2.05471200	H	1.28635100	-4.93885600	-3.40959900
				H	-4.45736400	1.86850700	-0.11049600
				H	-3.48598300	3.81171700	-3.29569300

H	0.35263400	-6.74259900	0.38252400	H	5.03652800	-3.22152000	1.79742400
H	-3.66657300	-2.21514000	-3.79643400	C	1.98208300	-2.81998000	2.46369700
H	-6.28617000	-1.14527500	2.75283000	H	1.12061700	-3.41047700	2.15060800
H	-3.77907500	1.48731000	5.05421300	H	2.79842500	-3.51939800	2.68344800
H	-2.77085900	-3.55749900	0.83768100	H	1.70172200	-2.33206100	3.40403900
H	-1.16950200	-1.19513100	4.90091800	Rh	1.27201200	-0.21791700	0.51788400
H	-3.87709300	-3.95617700	3.01249500	C	2.44878100	0.11662400	2.30642500
H	-0.13973800	2.52403100	2.20313800	C	2.55754700	1.15219200	1.57812800
H	-1.67716400	2.31155400	4.10727800	H	2.93356600	0.73117700	-1.19409600
H	-0.30035900	6.42676300	0.57038100	C	3.12226500	2.48574200	1.47354900
H	-2.16619100	3.42743200	-1.26238800	C	2.61668100	3.52579700	2.27259800
H	-5.53822600	-0.68956200	-4.23453700	C	4.22105900	2.74323100	0.63571600
H	0.51432700	-2.76707900	-2.57026600	C	3.20473100	4.78822300	2.23981900
H	-0.23860900	0.07289200	-3.12938300	H	1.77195700	3.33351000	2.92545400
H	-6.92360700	1.25750900	-3.57030500	C	4.81653700	4.00272900	0.62278200
H	-4.74443600	-0.99225600	0.85535700	H	4.61102300	1.95715200	0.00001200
H	2.95879000	5.09320500	-1.90039900	C	4.31056000	5.03000600	1.42115400
H	-1.56543000	0.45501300	-5.18004100	H	2.79992700	5.58309200	2.85943300
H	-3.08139900	-2.77800100	5.05186500	H	5.67289300	4.18301300	-0.02069700
H	1.23056700	-6.94809200	-1.93874600	H	4.76988200	6.01390400	1.40228600
H	-3.19567700	2.33412500	-5.27878700	H	2.54093600	-0.33539900	3.28021600
H	1.72852200	6.93784800	-0.77585600				
C	4.03158400	-0.86300100	-0.17405300	<b>15</b>			
C	5.14609300	-1.58154500	-0.97063100				
C	4.57328900	-2.38590800	-2.10380600	C	4.28740700	0.32734200	0.27338000
C	3.34710500	-2.18268400	-2.60349600	C	5.46573800	-0.15645100	-0.62846400
C	2.46119400	-1.09515100	-2.14682900	C	5.03640500	-0.40218800	-2.05392600
C	2.82340700	-0.31953200	-0.91582100	C	3.98250400	0.19262700	-2.62495300
H	4.50432600	-0.05756100	0.39939300	C	3.21808500	1.22420300	-1.89856100
H	5.22365200	-3.15369000	-2.51867200	C	3.22435600	1.20087300	-0.40814600
H	2.97637700	-2.75623600	-3.44790100	H	4.70771600	0.89553900	1.10947600
C	6.25924300	-0.66234700	-1.45470700	H	5.67164400	-1.08494400	-2.61567600
H	6.70572100	-0.14361200	-0.59984500	H	3.73495600	0.05049100	-3.67386600
H	7.04092400	-1.23388000	-1.96588900	C	6.67937200	0.76251000	-0.58039100
H	5.85936000	0.07937800	-2.15386000	H	7.04571200	0.83429900	0.44918800
O	5.71156000	-2.48542100	0.00259700	H	7.48480800	0.37819000	-1.21518800
C	4.63929300	-3.00856600	0.79911900	H	6.40736000	1.76286000	-0.93219700
H	4.25773300	-3.94849500	0.37288600	O	5.84295900	-1.42711500	-0.07176500
O	1.48729600	-0.80072600	-2.84085100	C	4.61268400	-2.09919200	0.21521700
C	3.58664900	-1.92549300	0.78284200	H	4.16911900	-2.49527600	-0.70682300
C	2.41309400	-1.83059600	1.42270300	O	2.61582900	2.08498800	-2.55041900

H	3.21629600	2.21921100	-0.02321900	C	-2.15466300	-2.77701000	-3.06137200
C	3.77148700	-1.01547000	0.85056600	C	-3.24290600	-0.77460600	-2.15989700
C	3.05502200	-1.16618800	2.00252400	C	-2.62325400	-2.38118200	4.29607200
H	4.83782100	-2.93655800	0.87632100	C	2.43197700	-4.51236600	-1.18402900
C	2.86740100	-2.48036600	2.71346200	C	-2.19925900	-2.97189400	1.98818300
H	1.80972200	-2.64486300	2.94213500	C	-4.92850000	0.34091200	3.08026800
H	3.22969300	-3.33903700	2.14844600	C	-2.39478900	-0.86249800	-1.01450400
H	3.39763900	-2.43982800	3.67543400	C	-0.31345200	6.13999700	-0.90632700
Rh	1.48034400	0.13511700	0.13712300	C	-1.44426500	4.04463900	-0.47328500
P	-0.16731100	-1.79099100	0.42726500	C	-0.81607800	-1.31875100	3.09413900
P	-0.22089700	1.49961600	-0.61297800	C	-5.84395100	-0.64709200	2.79606900
C	-0.50458400	1.05877400	-2.36659500	C	-4.20045100	0.26539300	-2.31065300
C	0.21589100	0.00278800	-2.94007100	C	1.42079200	-5.60543000	0.71958100
C	-3.84915400	0.60499300	2.19735100	C	-1.56022200	-1.47745100	4.26344700
C	-1.71069700	1.11484300	0.40424700	H	0.89945200	-0.58252800	-2.33016000
C	-4.81540300	-0.58638700	-4.49677300	H	-5.42254200	-0.49762800	-5.39289000
C	-3.10211400	-1.73482200	-3.21161000	H	1.81574300	3.51393100	-1.26687700
C	-0.84405300	0.41499000	-5.06931700	H	1.80134100	-2.49034300	-1.55195500
C	0.78870200	-3.33175900	0.16280700	H	-0.02527100	-4.45467000	1.81782400
C	0.90608700	4.05236200	-1.03790800	H	-1.19247900	2.68657000	1.81194900
C	1.68926300	-3.36403500	-0.91436300	H	-6.42930100	-2.19945900	1.39997600
C	-0.24599200	3.34002800	-0.67775500	H	-2.40779200	5.96319300	-0.41544800
C	2.30340800	-5.63506400	-0.36159600	H	-4.56393900	-1.80561800	-0.13795900
C	-1.13261200	-2.06066100	1.95055000	H	-3.76874900	-3.82988700	3.17991900
C	0.66084800	-4.46274100	0.97866300	H	1.77653500	5.97849900	-1.41804800
C	-1.42509400	-1.85907600	-0.93038500	H	-2.99938200	2.20996400	3.37706700
C	-2.59340900	0.07610200	0.12805300	H	-5.68469600	1.16457600	-3.55647000
C	-1.87669500	1.88039800	1.59538700	H	-3.78363500	-2.34344000	-5.17075100
C	-5.70771800	-1.41741600	1.61742800	H	-1.93945400	2.63211600	-2.73794000
C	-3.70305600	-0.17465200	1.00677200	H	0.60440800	-1.14703000	-4.71403800
C	-1.47360900	5.43517800	-0.58303000	H	-2.25580000	2.04532200	-5.11303600
C	-4.66106700	-1.19437700	0.75036500	H	-0.61321500	-3.63614100	-1.87960000
C	-2.93661600	-3.13270500	3.15949000	H	-2.07109400	-3.52801700	-3.84229900
C	0.87216900	5.44196200	-1.14525500	H	3.11678200	-4.52687500	-2.02686400
C	-2.90138500	1.62295200	2.46839800	H	-2.46258500	-3.53745100	1.09985500
C	-4.96465500	0.35816700	-3.45191300	H	-5.01669500	0.93829000	3.98367200
C	-3.90553300	-1.61246700	-4.37595800	H	-2.35968000	3.52051400	-0.22932400
C	-1.38570400	1.80275100	-3.16317800	H	0.00499800	-0.61669100	3.06096800
C	0.04761400	-0.32001100	-4.28383100	H	-6.66890300	-0.84071900	3.47545900
C	-1.55864900	1.47462500	-4.50724900	H	-4.31208400	0.99879400	-1.51988000
C	-1.33737900	-2.83578000	-1.95771700	H	1.31830500	-6.47416000	1.36338500

H	-1.31548100	-0.88755600	5.14218800	C	2.94443800	-1.08363600	2.05716600
H	-0.98163000	0.16174100	-6.11637000	H	4.10457700	-3.50463300	1.22422400
H	-0.33650900	7.22319900	-0.98393000	C	2.62524700	-2.11654700	3.10870900
H	-3.21045200	-2.49897500	5.20208800	H	2.10317000	-1.68173900	3.96225100
H	2.88823700	-6.52740100	-0.56446200	H	2.01134100	-2.92396600	2.70169100
C	2.49646400	0.01194100	2.68219300	H	3.56182900	-2.56429200	3.46763500
C	1.75248900	0.88652400	1.98593500	Rh	1.42922100	-0.04831100	0.25475800
H	2.68270400	0.12717000	3.75169700	P	-0.21578100	-1.79722200	0.07983100
C	1.21320600	2.11645400	2.58694400	P	-0.21908500	1.44125300	-0.40603400
C	1.43071500	3.37787600	2.01332200	C	-0.90329700	1.23944000	-2.10041400
C	0.50269500	2.04782900	3.80126600	C	-0.33751400	0.32880400	-2.99515900
C	0.91796800	4.53163500	2.60393500	C	-3.29739300	0.52458600	2.97627300
H	2.00209800	3.45288200	1.09948100	C	-1.51727800	1.07191000	0.84342800
C	-0.00160900	3.20180800	4.39761500	C	-5.81679600	0.20409100	-3.38097100
H	0.33476000	1.08443600	4.26904300	C	-3.91981400	-1.15152200	-2.69661100
C	0.18952000	4.44755300	3.79288500	C	-1.83103800	1.08575400	-4.73905500
H	1.08401000	5.49387300	2.12859600	C	0.54068600	-3.35678100	-0.50905000
H	-0.55471500	3.12632200	5.32967100	C	0.57167100	3.85952200	-1.53150400
H	-0.21860500	5.34483000	4.24905700	C	1.12286700	-3.37662700	-1.78833200

### 16-ts

C	4.32944700	-0.49830400	0.03347700	C	1.85741400	-5.65460700	-1.44284500
C	4.87714500	-1.41016600	-1.09047900	C	-0.90663400	-2.19546500	1.72777100
C	3.95160100	-1.46169900	-2.27740600	C	0.64307600	-4.49453700	0.30365900
C	3.09306500	-0.47826700	-2.57417800	C	-1.75467300	-1.61463700	-0.93310200
C	3.00378600	0.76158100	-1.77113100	C	-2.55356700	0.16891200	0.63846900
C	3.54183400	0.72820600	-0.36999600	C	-1.30048500	1.61817700	2.14375500
H	5.17403100	-0.19515900	0.66424200	C	-5.42675700	-1.26469900	2.60176600
H	4.06131800	-2.32696000	-2.92668800	C	-3.47518400	-0.11230000	1.70698600
H	2.51084100	-0.48870600	-3.49076900	C	-0.79514400	5.52712100	0.22733500
C	6.28725100	-1.03885100	-1.53790600	C	-4.55509300	-1.02530300	1.56147200
H	6.96904600	-1.08151600	-0.68192700	C	-2.46762000	-3.43878400	3.10335600
H	6.64315800	-1.73252100	-2.30655200	C	0.57552100	5.23651800	-1.73172100
H	6.29755200	-0.02601200	-1.95298600	C	-2.17398700	1.36920600	3.16952100
O	4.94895200	-2.70287900	-0.46433400	C	-5.67054500	0.99319700	-2.21403000
C	3.81097300	-2.85616400	0.39211000	C	-4.96069500	-0.84852800	-3.61326900
H	2.98852100	-3.33393000	-0.14188300	C	-1.93599500	2.08433200	-2.53950200
O	2.65522200	1.82014200	-2.30633400	C	-0.79833500	0.25110500	-4.31017600
H	4.09017000	1.64692800	-0.19514300	C	-2.40103400	2.00079300	-3.84912400
C	3.46912500	-1.45845200	0.83949800	C	-1.95638600	-2.43309400	-2.07484100
				C	-3.01259300	-2.21420600	-2.92519000
				C	-3.76621300	-0.35337500	-1.51850100

C	-2.02350400	-2.74632600	4.23458800	H	-0.10412000	7.15428100	-1.00706800
C	1.76429600	-4.52174100	-2.25664700	H	-2.46427300	-2.95395500	5.20518800
C	-1.91771200	-3.16229700	1.85415900	H	2.36786400	-6.54302400	-1.80263100
C	-4.20744000	0.25471900	4.02983500	C	2.87175500	0.33433000	2.38096200
C	-2.67856700	-0.61429000	-0.62871400	C	2.60196800	1.24487700	1.39038500
C	-0.10468600	6.07947000	-0.84958000	H	2.92630500	0.62298200	3.42966400
C	-0.80707200	4.14414800	0.42851000	C	2.49934300	2.69668500	1.62324300
C	-0.47184000	-1.50399100	2.86105400	C	2.82417500	3.66107400	0.65576500
C	-5.25750600	-0.61762100	3.84737400	C	2.04264200	3.14563400	2.88090100
C	-4.67432800	0.71969800	-1.30387000	C	2.74811100	5.02111400	0.95253400
C	1.30169200	-5.63502800	-0.16310300	H	3.10925100	3.35471300	-0.34332100
C	-1.02597100	-1.77959100	4.11138400	C	1.94799500	4.50483900	3.16615300
H	0.45619400	-0.32377200	-2.65622400	H	1.74559000	2.42261400	3.63312100
H	-6.60590800	0.43412900	-4.09083800	C	2.31248700	5.45146700	2.20525300
H	1.10247900	3.21983200	-2.22251100	H	3.00675900	5.74539300	0.18698600
H	1.08236900	-2.49182100	-2.41260900	H	1.58654300	4.82374000	4.13971200
H	0.21663700	-4.49555800	1.29956200	H	2.24119500	6.51242400	2.42611400
H	-0.42310900	2.22745400	2.32832300				
H	-6.24656800	-1.96411000	2.46606300				
H	-1.34257600	6.16667700	0.91380200				
H	-4.69268800	-1.54096900	0.61941400	C	-4.17509300	-1.58252500	-0.29198900
H	-3.25412800	-4.18216100	3.19314300	C	-4.38641600	-2.55926500	0.87368900
H	1.11059500	5.65044900	-2.58178600	C	-3.65842900	-2.11538000	2.11028100
H	-2.00330300	1.80143700	4.15173400	C	-3.32410500	-0.83877500	2.34886000
H	-6.34771000	1.82432200	-2.03997400	C	-3.64029100	0.25648200	1.42111900
H	-5.06088400	-1.45996200	-4.50596800	C	-4.13577700	-0.08303000	0.00293000
H	-2.37634000	2.80468900	-1.85871400	H	-4.98459500	-1.76257900	-1.01421300
H	-0.35249300	-0.46470600	-4.99487400	H	-3.45694900	-2.89159800	2.84442400
H	-3.21111800	2.64681900	-4.17356300	H	-2.86258600	-0.53611500	3.28429600
H	-1.26830900	-3.24047600	-2.28728800	C	-5.85629300	-2.81998000	1.19807900
H	-3.14955800	-2.84454800	-3.79964600	H	-6.36481300	-3.20962300	0.30993000
H	2.20257100	-4.52436900	-3.25024500	H	-5.94823900	-3.55485200	2.00441700
H	-2.28087300	-3.68733300	0.97585200	H	-6.34925600	-1.89509900	1.51560500
H	-4.05335200	0.74651400	4.98659600	O	-3.80618900	-3.80327600	0.41905500
H	-1.38928000	3.75233000	1.25013700	C	-2.92539300	-3.58884800	-0.69113900
H	0.28352200	-0.73566200	2.75504100	H	-1.94406300	-4.00708500	-0.47827500
H	-5.95034500	-0.81825900	4.65932800	O	-3.56772900	1.42140800	1.80005000
H	-4.56267000	1.33897200	-0.42131300	H	-5.16709500	0.28802800	-0.03211500
H	1.37785500	-6.50800000	0.47855700	C	-2.92341000	-2.11306900	-0.95246800
H	-0.68983100	-1.22607800	4.98338900	C	-2.41020200	-1.47002800	-2.06560100
H	-2.19247700	1.02447900	-5.76148500	H	-3.33282000	-4.11760600	-1.56772900

**17**



C	-1.80457400	-2.21462200	-3.22086400	C	2.84264800	-2.76813500	-1.61898900
H	-1.31510500	-1.54461500	-3.92936800	C	4.79781400	0.99498000	-3.60252200
H	-1.08191300	-2.96365700	-2.88756600	C	2.75261300	-0.05542900	0.81734400
H	-2.60726500	-2.74278500	-3.75411000	C	-1.18772400	5.95440400	0.19428300
Rh	-1.24659000	-0.39763600	-0.48806200	C	0.34498800	4.24095600	-0.56823400
P	0.68186600	-1.73796800	-0.14315300	C	1.28556400	-1.39449900	-2.86156400
P	0.03469100	1.47753600	0.13684400	C	5.94098200	0.32118300	-3.23328100
C	0.45985900	1.48773800	1.92575100	C	4.32456500	1.68046100	1.67887000
C	-0.08242400	0.51015200	2.76459000	C	0.09785800	-5.82038500	0.25626400
C	3.70416800	1.11286800	-2.70716400	C	2.05522300	-1.56217400	-4.01251500
C	1.55094100	1.35363900	-0.88756500	H	-0.67197200	-0.28895300	2.32838900
C	5.19734100	1.49887700	3.93550700	H	5.80323900	1.91456800	4.73529600
C	3.72873800	-0.23831900	3.08153900	H	-2.24339600	2.87779700	1.16909700
C	0.91306300	1.58259400	4.68681900	H	-0.83816500	-2.57285400	2.14538300
C	0.22212400	-3.40617200	0.45659300	H	1.12137900	-4.55062600	-1.14171400
C	-1.61819700	3.62933200	0.70409800	H	0.53254400	2.34382300	-2.53556300
C	-0.55733500	-3.48197700	1.62419500	H	6.92531900	-0.81295100	-1.66962200
C	-0.45759700	3.24945800	0.01215200	H	0.60623100	6.34252900	-0.93875500
C	-0.66013500	-5.88831800	1.42573100	H	5.05467200	-0.64917800	-0.09169000
C	1.66431500	-2.00478900	-1.66307100	H	4.52124200	-3.52418900	-2.72831300
C	0.54156900	-4.58640800	-0.22728300	H	-2.88310900	5.24594000	1.32765400
C	1.99666800	-1.20368400	1.05602400	H	2.41918200	2.16490200	-4.09627000
C	2.68212300	0.64922200	-0.49883700	H	5.61372900	3.13175300	2.56963800
C	1.45248700	1.86614500	-2.21494000	H	4.60323000	-0.23169400	5.05754100
C	6.02719300	-0.27154900	-1.95242300	H	1.63133100	3.30232600	1.84266600
C	3.79171100	0.52659600	-1.40462300	H	-0.28058500	-0.21318500	4.78220000
C	-0.02585900	5.58548600	-0.48303000	H	2.05820200	3.36517800	4.27389600
C	4.97815600	-0.17768100	-1.06367200	H	1.62461800	-2.82975200	2.44664500
C	3.60831500	-2.93770900	-2.77027200	H	3.12735100	-1.99897200	4.18330000
C	-1.97763500	4.97101500	0.79531400	H	-1.58624900	-4.75698600	3.01412500
C	2.50161600	1.76191100	-3.09054900	H	3.16681200	-3.21545400	-0.68436500
C	5.09058100	2.18941400	2.70371700	H	4.71091300	1.44331900	-4.58866600
C	4.53252200	0.30729600	4.11661800	H	1.26849000	3.98429400	-1.07154500
C	1.22107000	2.52742100	2.48116200	H	0.40752400	-0.76211100	-2.87470000
C	0.14167500	0.55534500	4.14093500	H	6.77396100	0.23658600	-3.92512300
C	1.45351600	2.56703900	3.85394300	H	4.23978600	2.22551000	0.74600400
C	2.16928800	-1.91130600	2.27518800	H	0.34556200	-6.72769500	-0.28709100
C	3.01469100	-1.44841000	3.25328200	H	1.75914400	-1.07055000	-4.93464300
C	3.61599700	0.45737100	1.83616000	H	1.09305600	1.61822400	5.75741100
C	3.21494800	-2.33621400	-3.96976300	H	-1.47231100	7.00070300	0.26076200
C	-0.98560300	-4.71417300	2.11066500	H	3.82116500	-2.45914700	-4.86238900

H	-1.00427100	-6.84879400	1.79766600	C	1.24151400	3.54062200	0.13150800
C	-2.67371900	-0.05129800	-2.11375500	H	2.32209500	3.71102400	0.15240200
C	-3.31914700	0.65039600	-1.07854300	H	0.83269600	3.82694800	1.10967000
H	-2.35482900	0.48541100	-2.99891900	H	0.80408000	4.22593100	-0.60691300
C	-3.54608300	2.10331100	-1.29646600	H	-1.23610700	2.54094400	-0.39877100
C	-4.64584400	2.77301000	-0.73280300	C	-2.37147100	0.09042000	-0.26463500
C	-2.71011000	2.84150500	-2.16021000	C	-2.81536200	-1.09509300	-0.87850200
C	-4.91921900	4.10396400	-1.04819000	C	-3.33906000	0.93355600	0.31567400
H	-5.29929900	2.26381800	-0.03685100	C	-4.17180300	-1.41770300	-0.92308000
C	-2.98436900	4.16618900	-2.47930400	H	-2.09938700	-1.76209300	-1.34915800
H	-1.81434900	2.38466100	-2.56628000	C	-4.69343400	0.61170200	0.27080400
C	-4.09677900	4.80703500	-1.92829100	H	-3.01709400	1.83308900	0.83105900
H	-5.78062400	4.59038000	-0.59916200	C	-5.11854500	-0.56643800	-0.35008700
H	-2.31227600	4.70719700	-3.13891300	H	-4.48848300	-2.33564700	-1.41092200
H	-4.30802900	5.84496200	-2.16850300	H	-5.41840900	1.27536800	0.73439400
				H	-6.17430200	-0.82068500	-0.37966500

## 18

O	3.74491700	-0.14708000	-0.69086000
O	-0.56960000	-0.74869500	2.27187000
C	1.66236000	-1.37242300	1.86794100
H	1.75784500	-1.64511500	2.91626700
C	0.11041600	-0.63755200	-0.04534400
H	-0.24758100	-1.59358800	-0.44525000
C	1.40060500	-0.25368000	-0.76957000
H	1.22535100	-0.31734500	-1.85431200
C	0.33080400	-0.89440000	1.45392100
C	-0.94070700	0.45195000	-0.23694500
C	1.81949800	1.15226300	-0.41556900
C	2.66020400	-1.06930200	-0.43160100
C	-0.51317800	1.73476400	-0.29611300
C	0.90378200	2.11119000	-0.19817300
C	3.32191900	1.17764000	-0.33137100
H	3.79712500	1.87474700	-1.03146800
H	3.66640700	1.43182700	0.68310600
C	2.70327100	-1.45700100	1.02589300
H	3.66969000	-1.81049400	1.38158300
C	2.87762100	-2.28936700	-1.31794500
H	2.92849200	-1.97852500	-2.36668500
H	2.05259000	-2.99926800	-1.19715400
H	3.81184000	-2.79781300	-1.05709600

## 1c

C	9.04785900	-0.42778300	-3.04773500
C	10.54271700	-0.39507000	-3.19100700
C	8.85466900	0.01043000	-0.53972700
C	8.34078000	-0.26804200	-1.92222100
H	8.51304000	-0.61867500	-3.97759600
O	11.00039200	0.47958100	-4.22993500
C	10.85950000	1.86528900	-3.92692900
H	11.09047700	2.04901500	-2.86639300
H	7.25547500	-0.34678400	-1.99811800
C	9.53981300	2.42206900	-4.25540100
C	8.45889400	2.88773000	-4.54031400
H	11.62732800	2.37787700	-4.51862800
C	7.15523200	3.44598800	-4.88622900
H	7.00793600	4.42426400	-4.41253700
H	7.05187100	3.58023500	-5.96975000
H	6.34349000	2.78906700	-4.55009300
H	11.03694300	-0.13541000	-2.24569800
H	10.90796200	-1.38388600	-3.49525600
H	9.93682700	0.16202300	-0.50479200
H	8.37131300	0.90584500	-0.12641100
H	8.60934400	-0.81710700	0.14033000

**1d**

C	-1.38322800	-0.08696700	3.05464400
H	-1.54932100	0.09452500	4.12369200
H	-2.18409900	0.42143700	2.50372500
C	-0.06613500	0.38743900	2.63420000
C	1.02514300	0.78057600	2.28600900
C	2.34219700	1.25553500	1.86637300
H	3.04260000	0.42186200	1.73283900
H	2.28563700	1.79689700	0.91395000
H	2.77521200	1.93648900	2.60947300
H	-1.49291100	-1.16442200	2.88012600

**6-a**

P	-0.79870300	-0.02509100	-1.39360200
P	0.55527200	0.71767400	1.54388000
C	1.66949000	1.99157000	0.83737500
C	2.42702700	1.68568900	-0.29939400
C	-3.92820400	1.97196200	1.73533100
C	-1.16072600	1.36636400	1.63306300
C	0.37096900	6.71617300	-0.66086500
C	0.19755800	4.52771600	-1.70263600
C	3.48954200	3.85407100	-0.18264900
C	-0.50068600	-0.68466500	-3.07844300
C	2.46017000	0.16602800	3.48584200
C	0.82296000	-0.71199700	-3.54964400
C	1.18891300	0.72458200	3.27424600
C	0.10404300	-1.82145800	-5.57247500
C	-2.58779100	-0.23126900	-1.09116200
C	-1.51471700	-1.24152300	-3.86600100
C	-0.56850300	1.80287200	-1.56572200
C	-1.71252700	2.17385700	0.64471500
C	-2.00018400	0.82065500	2.64757500
C	-5.06631600	3.64431400	-0.21049300
C	-3.10795800	2.51275200	0.69483500
C	1.15601500	1.42180200	5.60127600
C	-3.72163600	3.35126300	-0.27569700
C	-4.89783400	0.28256600	-1.60614800
C	3.05989500	0.21417500	4.74268000
C	-3.33880300	1.11268000	2.69663800

C	-0.35631300	6.23833900	0.45635200
C	0.63739500	5.87745000	-1.71928000
C	1.84325700	3.22879100	1.47458400
C	3.33338200	2.61621100	-0.80966500
C	2.74501100	4.15797800	0.96096200
C	0.09977500	2.32203400	-2.70679900
C	0.46846500	3.64323400	-2.77427900
C	-0.52903100	4.03834100	-0.57103000
C	-5.31729500	-0.57554300	-0.58499200
C	1.12265700	-1.26608300	-4.79131200
C	-3.53858200	0.45977700	-1.85763200
C	-5.31218100	2.28252000	1.77014800
C	-0.91388600	2.66165100	-0.52236200
C	2.40284500	0.83225200	5.80943500
C	0.55407400	1.37582100	4.34157800
C	-3.01380700	-1.08783600	-0.07003700
C	-5.87265900	3.10543700	0.81905900
C	-0.79824800	4.93499600	0.49942200
C	-1.21037100	-1.80939700	-5.10664400
C	-4.37395100	-1.26172900	0.18195100
H	2.28986200	0.72126000	-0.78363600
H	0.71640400	7.74566400	-0.67837000
H	3.00168300	-0.27554900	2.65830400
H	1.62007000	-0.29559300	-2.94076100
H	-2.54047200	-1.24267800	-3.51627900
H	-1.57669200	0.15958300	3.39341500
H	-5.51353500	4.28865500	-0.96182100
H	0.64798300	1.92919700	6.41630400
H	-3.12256300	3.76042400	-1.07972600
H	-5.62966100	0.82679200	-2.19528600
H	4.04305000	-0.22488600	4.88552100
H	-3.96447300	0.68298300	3.47395400
H	-0.56213800	6.90584400	1.28805900
H	1.19344300	6.23134700	-2.58324800
H	1.27050700	3.46566300	2.36536400
H	3.91017900	2.37656000	-1.69839600
H	2.86289200	5.12081000	1.44870300
H	0.32936500	1.66988700	-3.53871800
H	0.98797700	4.02105500	-3.65066900
H	2.14968000	-1.27431600	-5.14455700
H	-3.21641500	1.14266100	-2.63753800

H	-5.91901800	1.85610900	2.56432200	C	2.17342900	1.86966400	0.95056200
H	-0.40059500	1.86679800	4.19995600	C	1.95201200	1.49765200	2.28083300
H	-2.27251400	-1.60487000	0.52783800	C	1.43218300	-1.41828700	-3.58351600
H	-6.93264500	3.33944200	0.85355000	C	1.21920100	0.54148300	-1.55432000
H	-1.34255700	4.57711000	1.36562500	C	6.40848000	-0.96248800	1.04847600
H	-2.00617400	-2.24206400	-5.70610100	C	4.11957400	-1.44232400	1.71110100
H	-4.69182800	-1.92406600	0.98203900	C	4.24229000	2.03829800	2.83010100
H	4.19093700	4.58082800	-0.58220700	C	-1.28678200	-1.85318900	2.37100600
H	2.86724300	0.86735200	6.79060000	C	0.09700500	4.44920800	-0.55927100
H	-6.37746900	-0.70201300	-0.38560400	C	-1.19274100	-1.13556100	3.57591400
H	0.33722000	-2.26354700	-6.53679200	C	0.90633300	3.42465000	-1.07222400
Rh	0.50512200	-1.20755500	0.23230100	C	-2.70674400	-2.69409700	4.63811200
C	0.66632500	-2.70366200	1.86667000	C	-0.84616100	-2.32604600	-0.47835100
C	1.80789300	-2.29412400	1.58927300	C	-2.10611200	-2.98839900	2.31125800
C	2.64711900	-2.78896400	-1.53721900	C	1.34596500	-1.40736700	1.14234600
H	2.82845200	-3.43537700	-2.40479400	C	1.79144300	-0.68972300	-1.24195400
H	2.97903900	-1.77761200	-1.79086300	C	0.69698100	0.77653400	-2.86040700
C	1.22499100	-2.81861100	-1.18141600	C	2.69984300	-3.86415000	-3.04127700
C	0.03485900	-3.10548600	-1.03202100	C	1.93868500	-1.68200100	-2.27013100
C	-1.29075300	-3.72283500	-1.15243200	C	1.88680700	5.00627400	-2.62765800
H	-1.74877600	-3.90047900	-0.17656600	C	2.56777800	-2.93520500	-2.03303900
H	-1.96504200	-3.08792400	-1.73488400	C	-0.57171900	-4.44622300	-1.61501700
H	-1.19560500	-4.68524200	-1.67005300	C	0.18746000	5.74309800	-1.07292700
C	-0.46444600	-3.48889100	2.26830000	C	0.79576000	-0.17698400	-3.84124900
C	-0.39544600	-4.89151900	2.15915000	C	5.95196700	-0.56889700	-0.23284700
C	-1.65421100	-2.89048700	2.71842700	C	5.50944100	-1.39262900	1.99781500
C	-1.49976800	-5.67211100	2.49305300	C	3.43993700	2.33677200	0.56739200
H	0.51948000	-5.35217900	1.80099800	C	2.98103500	1.58259800	3.21784200
C	-2.75396200	-3.67806900	3.04841700	C	4.46904200	2.41491700	1.50385900
H	-1.71156900	-1.81273200	2.79003700	C	1.82972000	-1.84555400	2.40323700
C	-2.68182300	-5.06954700	2.93380700	C	3.17578500	-1.86928300	2.67696200
H	-1.43990800	-6.75266900	2.40255100	C	3.65354100	-1.03936700	0.41878200
H	-3.66815900	-3.20462600	3.39438000	C	-1.37324500	-3.98937200	-2.66580800
H	-3.54258000	-5.68161000	3.18653500	C	-1.89118300	-1.55994400	4.70409500
H	2.87299200	-2.21707500	1.69354700	C	-0.30205800	-3.61784700	-0.52704500
H	3.26240100	-3.14743800	-0.70401600	C	1.56714300	-2.40268000	-4.59672700
				C	2.24928900	-1.03928600	0.14248400
				C	1.08008600	6.02265000	-2.11007200
				C	1.80608400	3.71311000	-2.10973300
P	-0.46636900	-1.17525300	0.88870400	C	-1.65728200	-1.87854900	-1.52876300
P	0.80772900	1.78483500	-0.26696300	C	2.19329400	-3.60062300	-4.33554800

**7-a-ts**

C	4.61080900	-0.60894600	-0.54122800
C	-2.81212300	-3.40541500	3.44227300
C	-1.91948100	-2.70551200	-2.62108700
H	0.98422500	1.11111000	2.57251800
H	7.46926400	-0.92227200	1.27808900
H	-0.60621300	4.22931100	0.23776900
H	-0.57258100	-0.24648300	3.63036400
H	-2.19777700	-3.54581800	1.38579700
H	0.21158500	1.72164100	-3.07749200
H	3.18947500	-4.81225600	-2.83866800
H	2.58195900	5.21915600	-3.43455700
H	2.94804300	-3.15863700	-1.04394600
H	-0.14065700	-5.44209900	-1.65345000
H	-0.44294100	6.52911900	-0.66718300
H	0.39403800	0.01237900	-4.83288800
H	6.66661700	-0.22616700	-0.97547500
H	5.84653900	-1.69652800	2.98525500
H	3.62773100	2.63252200	-0.45878800
H	2.79984100	1.27915200	4.24468100
H	5.45022700	2.76317100	1.19543300
H	1.12691500	-2.16098700	3.16454500
H	3.53131500	-2.20383000	3.64777700
H	-1.80602300	-1.00199700	5.63206500
H	0.34250800	-3.96646300	0.27402500
H	1.16986800	-2.18667500	-5.58482400
H	2.43850400	2.93147100	-2.51775200
H	-2.07120500	-0.87650600	-1.48804000
H	2.29818000	-4.34555700	-5.11890400
H	4.27158800	-0.29269400	-1.52093300
H	-3.44360200	-4.28733900	3.38522700
H	-2.54058100	-2.34423300	-3.43547100
H	5.04730300	2.09718900	3.55676400
H	1.14609500	7.02847400	-2.51465300
H	-1.56620800	-4.63285100	-3.51915500
H	-3.25775500	-3.01921500	5.51579400
Rh	-1.32837900	0.97917500	0.21446800
C	-3.37054200	1.46171800	-0.43538100
C	-2.46312700	2.32018200	-0.79067900
C	-1.46412700	2.52957100	3.02664300
H	-2.16576500	2.57491600	3.86950900
H	-0.48336900	2.22526900	3.39878700

C	-1.98657300	1.61749400	1.99113400
C	-3.04956500	0.97566100	1.62676800
C	-4.18733600	0.21977000	2.19929800
H	-5.15318200	0.53569300	1.79745800
H	-4.07629200	-0.85428400	2.01687500
H	-4.18880100	0.37367600	3.28503600
C	-4.66905200	0.90108800	-0.76747300
C	-5.72022200	1.77254600	-1.10730000
C	-4.89481800	-0.48564200	-0.78721400
C	-6.96268400	1.26127300	-1.47759700
H	-5.55156500	2.84485200	-1.07781700
C	-6.13887200	-0.99003400	-1.15838000
H	-4.09312100	-1.15954100	-0.50750700
C	-7.17614500	-0.11986200	-1.50505700
H	-7.76706400	1.94238800	-1.74019700
H	-6.29981500	-2.06419200	-1.17388100
H	-8.14658700	-0.51522600	-1.79066000
H	-2.33152300	3.15252100	-1.46864600
H	-1.36080800	3.54287600	2.61590100

## 1e

C	0.36608500	-3.73884300	5.25387400
H	-0.22891400	-3.77902300	6.17688300
H	-0.32756400	-3.95286100	4.42890500
C	0.99341900	-2.38508500	5.08368800
C	2.29658600	-2.09288700	4.98366500
C	3.45649500	-3.04605900	5.01703900
H	3.14924200	-4.08790400	5.14370500
H	4.04345000	-2.97811900	4.09051600
H	4.14294800	-2.79526700	5.83763800
H	1.10051100	-4.54824500	5.29281500
H	0.28716300	-1.55487500	5.03845400
H	2.56872100	-1.04339000	4.86294600

## 2-a

C	3.66920000	-1.31380900	-0.10235300
C	5.07274700	-0.77884500	-0.07685500
C	3.18345000	-0.89831200	2.37161200
C	2.86431600	-1.42632000	0.99986600

H	3.41723800	-1.89297600	-0.98619900	C	-1.21368900	-3.66162800	0.08116000
O	5.39998200	0.05585000	-1.17953300	C	-0.66115600	-3.34034800	2.79918100
C	4.85753900	1.34983100	-1.01348200	C	-1.70954400	-4.57757200	1.00683200
H	5.22618000	1.79228700	-0.07290600	C	-1.19529500	0.79414400	2.84440100
H	2.08448300	-2.17654800	0.95956400	C	-2.01146600	0.05802900	3.66731200
C	3.37601900	1.42612000	-1.03421000	C	-3.08822700	-0.95241600	1.70621900
C	2.37846300	2.16050600	-1.28110600	C	-2.85535600	3.63040900	-2.72835800
H	5.24160700	1.94933000	-1.84548600	C	2.23518800	3.48397200	3.17448600
C	1.92374900	3.49724000	-1.72837400	C	-2.26284300	3.18470700	-0.42697800
H	2.80406600	4.12111400	-1.92539300	C	-5.04584100	0.63158600	-3.20033100
H	1.32779300	3.44043700	-2.64249000	C	-2.25508500	-0.14708000	0.85852200
H	1.31455900	3.99868000	-0.97193000	C	2.70049100	-3.53279800	-3.90430300
Rh	1.65484900	0.34024700	-0.35856200	C	1.52674700	-1.56769600	-3.12568200
P	-0.08142300	1.59782300	0.37831100	C	-0.92797900	2.26210600	-2.22020400
P	0.14339300	-1.34996800	-0.72642500	C	-5.99777800	1.25013500	-2.42251300
C	-0.41794700	-2.58645400	0.50912200	C	-4.01793700	-1.89580200	1.18648300
C	-0.15499300	-2.42827700	1.87351800	C	0.77939900	5.18980000	2.27727200
C	-3.85746700	0.11459000	-2.61966100	C	-1.77308900	2.85725100	-3.15474900
C	-1.47007000	-0.83670400	-1.44715800	H	0.40232000	-1.56732200	2.21843600
C	-4.69498300	-2.52005100	3.43120600	H	-5.32000100	-3.12629600	4.08038700
C	-2.97060300	-0.83501900	3.12856900	H	1.05624700	-4.19583600	-1.00394100
C	-1.43395600	-4.41872600	2.36782400	H	1.99695800	1.51706100	2.33886600
C	0.60540200	2.91129400	1.46356400	H	-0.60630800	4.56156000	0.76504900
C	1.40197200	-3.63112100	-1.86155700	H	-0.96029700	-1.45906700	-3.46281100
C	1.64778300	2.54317500	2.33080800	H	-6.54593500	1.87560600	-0.41943800
C	1.03681500	-2.28768700	-2.01905500	H	2.71005000	-1.62589200	-4.91854800
C	1.80283700	4.81275400	3.14742200	H	-4.50409200	1.01516300	0.62860200
C	-1.15705000	2.43065700	-0.84966800	H	-3.95236900	4.37161500	-1.02497500
C	0.17931500	4.24592200	1.44012800	H	2.50898400	-5.28927000	-2.66821100
C	-1.30643400	0.70132300	1.43065500	H	-3.03622000	-0.63356200	-4.47515600
C	-2.43655800	-0.25572100	-0.62663800	H	-5.49693800	-3.37638100	1.60741800
C	-1.70348400	-0.97841600	-2.83932100	H	-3.69325600	-1.52045900	5.04520500
C	-5.79555800	1.37879500	-1.02751000	H	-1.45289000	-3.77640600	-0.97172100
C	-3.64810800	0.24235300	-1.20851800	H	-0.46583600	-3.19498300	3.85729300
C	2.34393300	-2.19032400	-4.06600900	H	-2.32416100	-5.40610300	0.66736800
C	-4.65162200	0.89125400	-0.43697900	H	-0.46477600	1.46398700	3.28103200
C	-3.09824800	3.79290700	-1.36305000	H	-1.92529700	0.14956900	4.74665900
C	2.23020600	-4.24821000	-2.80248600	H	3.03380300	3.18107000	3.84554900
C	-2.86633900	-0.51922300	-3.40804600	H	-2.48774600	3.27611500	0.63080000
C	-4.79926800	-2.65721600	2.02657000	H	-5.18506200	0.52903400	-4.27314200
C	-3.79548000	-1.62780700	3.96867600	H	1.27740900	-0.51738400	-3.24076300

H	-0.10311000	1.63910500	-2.54690600	C	3.18036600	-0.49059900	-2.89834600
H	-6.90325900	1.64359000	-2.87513400	C	1.81420200	-4.09438800	-2.75815000
H	-4.10005000	-2.02467500	0.11451100	C	-0.93303200	2.84766100	-1.58125800
H	0.44439700	6.22235500	2.24332000	C	-1.31196600	-4.05731400	1.28965200
H	-1.59423800	2.70461200	-4.21499800	C	-1.74801800	2.40019400	-2.63560000
H	-1.83500800	-5.12458400	3.08906200	C	-1.22083100	-2.68250500	1.54373600
H	3.34566400	-4.01547300	-4.63250200	C	-2.17795200	4.68394800	-3.30129900
H	-3.51726100	4.08962100	-3.45652200	C	0.58107800	2.47686900	0.90743900
H	2.26532700	5.54987200	3.79733700	C	-0.75936400	4.22469700	-1.39123900
H	5.29507400	-0.25751400	0.86293400	C	1.18562800	0.83019200	-1.38403800
H	5.74857500	-1.63959500	-0.15075100	C	2.09593800	-0.14128500	0.76463200
H	3.76744500	0.02494100	2.34158700	C	1.13110400	-1.04864300	2.81065800
H	2.27168900	-0.70763300	2.94431300	C	5.15902400	1.81217300	1.72500100
H	3.76555300	-1.64436100	2.93191500	C	3.14314200	0.45662800	1.54017900

### 3-a-ts

C	-3.90445500	-1.19750500	-0.08149100	C	-2.09685500	-4.87401700	2.10798700
C	-5.36625800	-1.09964500	-0.49942000	C	2.13116700	-0.48736100	3.56663700
C	-3.18895000	-1.14881500	-2.53568000	C	5.04300900	-2.15558300	-1.61673200
C	-2.90151200	-1.49329500	-1.08912700	C	4.17807700	-1.16932100	-3.64645700
H	-3.79521600	-1.75362500	0.84641900	C	1.42099500	-3.53884800	-0.43697700
O	-6.09632800	-0.36880200	0.46344500	C	0.89221200	-3.12213300	-3.14919800
C	-5.47077300	0.89175900	0.54935700	C	2.07588400	-4.30277000	-1.40102000
H	-5.73996500	1.51180000	-0.32260100	C	1.25282800	0.98048100	-2.79496300
H	-2.40733600	-2.45191600	-0.95010200	C	2.22300600	0.34222600	-3.52835000
C	-3.97613800	0.74398300	0.59908300	C	3.12900100	-0.65454300	-1.47684300
C	-3.00154200	1.54735100	0.88239700	C	1.87910200	3.77963000	3.01714400
H	-5.82475900	1.39026900	1.45647500	C	-2.35809300	3.31128300	-3.49534800
C	-2.92531400	2.95003400	1.37865900	C	1.64265400	3.35747700	0.64791700
H	-3.92860200	3.33950800	1.59170700	C	4.17930300	0.89049200	3.73323800
H	-2.32537700	3.02361700	2.28987300	C	2.11694400	0.02861000	-0.72373800
H	-2.45550500	3.60046100	0.63367100	C	-2.79534000	-4.32973400	3.18586700
Rh	-1.88893200	0.08194100	-0.03092700	C	-1.94577300	-2.13800100	2.62022500
P	-0.22796800	1.57758000	-0.46119900	C	0.18840100	2.24109800	2.23025800
P	-0.33197000	-1.52572400	0.43054400	C	5.16481900	1.63764300	3.12965500
C	0.48334100	-2.56991300	-0.82724600	C	4.08451400	-1.51351300	-0.86548200
C	0.22784000	-2.36351400	-2.18610100	C	-1.38193200	5.13583800	-2.24842200
C	3.15325200	0.28389300	2.96153400	C	0.83534300	2.89004000	3.28082000
C	1.09446900	-0.87363700	1.40219600	H	-0.45666400	-1.58128500	-2.48486100
C	5.09460900	-1.98297100	-3.02050400	H	5.85544500	-2.49803500	-3.59970300

H	-0.78092300	-4.49619500	0.45339500	C	3.18598600	-1.23596900	0.68800800
H	-1.89991100	1.33620700	-2.78110800	H	3.52539300	-1.63362400	-1.35679500
H	-0.15358800	4.59465300	-0.57318300	C	2.59748200	1.26628800	-3.07910600
H	0.36696300	-1.63868400	3.29952500	H	2.85112300	2.08092000	-3.76887200
H	5.93403000	2.41037400	1.25477300	H	2.61660900	-2.15693500	0.78378400
H	-3.26460400	-2.52280000	4.27273500	C	2.68463200	1.74683100	-1.68979000
H	4.17306200	1.40017100	-0.11981400	C	3.05488700	2.36189200	-0.69288600
H	3.10436700	4.68903600	1.49154900	H	1.60371700	0.89602000	-3.33942500
H	-2.16051200	-5.93759500	1.89728600	C	3.67074200	3.21132400	0.32567200
H	2.14794500	-0.63219200	4.64338900	H	4.53888900	3.72169900	-0.11123000
H	5.76029000	-2.80932700	-1.12912000	H	2.97814700	3.97299200	0.69201300
H	4.19976400	-1.03290700	-4.72423000	H	4.01821400	2.62921300	1.18364800
H	1.64643400	-3.68719600	0.61492100	Rh	1.67736700	0.21966600	-0.25518700
H	0.70105700	-2.94187700	-4.20292200	P	-0.10686600	1.57089800	0.34346100
H	2.80380000	-5.04772500	-1.09393900	P	0.27024000	-1.53001600	-0.49786200
H	0.53709000	1.61530100	-3.30195500	C	-0.34572800	-2.45478500	0.95478900
H	2.26774500	0.47308200	-4.60616000	C	0.12492000	-2.12976300	2.23219100
H	-2.97708600	2.95010300	-4.31159300	C	-3.43031000	-0.01757200	-2.94022500
H	1.98150900	3.51578900	-0.37134600	C	-1.26035900	-1.03228800	-1.41712700
H	4.16801300	0.75101600	4.81078500	C	-5.00288000	-2.42058400	3.11968100
H	-1.91476600	-1.06857900	2.80551200	C	-3.25330900	-0.74460400	2.92441400
H	-0.60070300	1.52554600	2.43139300	C	-1.26876700	-3.85345500	3.19641700
H	5.94645000	2.09769800	3.72714600	C	0.57510600	2.81860900	1.50131100
H	4.04825200	-1.67087900	0.20526300	C	1.22835500	-4.14190900	-1.12031200
H	-1.24329100	6.20089700	-2.08683900	C	1.39579300	2.35633400	2.54492000
H	0.53461100	2.68892500	4.30475700	C	1.08156100	-2.81303400	-1.54137500
H	2.33848300	-4.67977400	-3.50768300	C	1.73804600	4.62304300	3.31008300
H	-3.40337500	-4.96788900	3.82034400	C	-1.08638300	2.51013000	-0.88168400
H	2.38825700	4.27904800	3.83601300	C	0.35873500	4.19524100	1.36357400
H	-2.65881300	5.39578900	-3.96583300	C	-1.42261700	0.72501400	1.33596800
H	-5.78122900	-2.11165900	-0.52894400	C	-2.29396100	-0.35833000	-0.76625000
H	-5.47244700	-0.64079000	-1.49045900	C	-1.32259200	-1.21502200	-2.82553100
H	-3.61029000	-0.14460700	-2.64080800	C	-5.51621600	1.35826300	-1.66138100
H	-2.28780200	-1.20211400	-3.15043900	C	-3.39805300	0.16220400	-1.52065700
H	-3.91303400	-1.85857200	-2.96360700	C	2.35923000	-3.34215600	-3.54567200
				C	-4.47038600	0.87085000	-0.91031700
				C	-2.96823300	3.93741100	-1.42534400
				C	1.92762400	-5.06103300	-1.90723600
				C	-2.37061900	-0.72122900	-3.56288000
				C	-4.98671600	-2.59375500	1.71482900
				C	-4.15155900	-1.51444900	3.70980200
<b>2-b</b>							
C	3.75912400	-0.96125800	-0.53722500				
C	4.98854800	-0.11779000	-0.73275700				
C	3.64547100	-0.63816800	1.99172300				



C	-1.28778400	-3.48413200	0.80658500	H	0.06759300	1.81820500	-2.55493900
C	-0.33618500	-2.82549800	3.34957400	H	-6.37388300	1.56873400	-3.64396600
C	-1.74112500	-4.18356200	1.92335800	H	-4.11015700	-2.02320600	-0.14323700
C	-1.48645300	0.90897600	2.74304000	H	0.76805200	6.15712300	2.14514800
C	-2.37252700	0.19512000	3.51264100	H	-1.30305000	3.00234900	-4.24392800
C	-3.22884600	-0.92013700	1.50410500	H	-1.63354800	-4.39130300	4.06656000
C	-2.64772700	3.84620100	-2.78276000	H	3.02672800	-5.38619000	-3.73352800
C	1.96357800	3.25066500	3.44973000	H	-3.26106700	4.35517700	-3.52049600
C	-2.19822400	3.26579900	-0.47797800	H	2.18544900	5.32290400	4.00980200
C	-4.51777200	0.50384300	-3.68953300	H	3.97629500	0.39837100	1.88494400
C	-2.29605000	-0.16770100	0.71791700	H	2.85374600	-0.67077500	2.74577500
C	2.48700400	-4.66834000	-3.12279000	H	4.49476600	-1.21692300	2.38576300
C	1.67661100	-2.42072600	-2.75464400	H	5.00760600	0.36887100	-1.71130800
C	-0.76861300	2.42661500	-2.24084300	H	5.10831800	0.65045300	0.03373000
C	-5.54376300	1.17523900	-3.06457500	H	5.86986500	-0.77469800	-0.68281500
C	-4.12180800	-1.86642200	0.92834800	H	3.30699400	0.44717300	-3.23887000
C	0.94123100	5.09139300	2.26401100				
C	-1.54817100	3.08875300	-3.18934800				
H	0.82864700	-1.31347000	2.34702200				
H	-5.68683200	-3.00555500	3.72767600				
H	0.80548300	-4.46848100	-0.17840300				
H	1.58676100	1.29260600	2.64586900				
H	-0.25466700	4.57521000	0.55524500				
H	-0.54273900	-1.76680800	-3.33177000				
H	-6.32295900	1.89803200	-1.17407900				
H	2.80259800	-3.02096700	-4.48376800				
H	-4.45537700	1.03573700	0.15980200				
H	-3.83123000	4.51455800	-1.10685200				
H	2.03276900	-6.08589500	-1.56317700				
H	-2.40143700	-0.87681800	-4.63794900				
H	-5.65703000	-3.31398600	1.25477600				
H	-4.15129500	-1.37098500	4.78700000				
H	-1.67300300	-3.72948400	-0.17846000				
H	0.02334800	-2.55624100	4.33850800				
H	-2.47687000	-4.97275500	1.80227300				
H	-0.83150700	1.62377600	3.22280800				
H	-2.40597600	0.34599800	4.58829400				
H	2.58891300	2.87809800	4.25597100				
H	-2.46938800	3.31548200	0.57209700				
H	-4.52184800	0.35819100	-4.76644600				
H	1.61995600	-1.38559300	-3.07187200				
				<b>3-b-ts</b>			
				C	-3.89707100	-1.21754900	-0.46169900
				C	-5.32397300	-0.95140000	-0.93197200
				C	-3.14056100	-0.41686300	-2.79725000
				C	-2.86009800	-1.11857700	-1.49470200
				H	-3.80834100	-2.09707000	0.16960500
				C	-4.94078200	-0.24311100	1.95889600
				H	-4.92004600	-1.33236500	2.04561000
				H	-2.31456600	-2.05104200	-1.63602000
				C	-3.97268500	0.27118800	0.94080700
				C	-3.42583200	1.39772300	0.58554900
				H	-5.96941100	0.06673900	1.74429400
				C	-3.58466000	2.84624500	0.87186000
				H	-2.69727200	3.24726000	1.37403400
				H	-3.69618500	3.41302400	-0.06089500
				H	-4.46278200	3.04427400	1.50082100
				Rh	-1.98010100	0.05545600	-0.02491600
				P	-0.31304900	1.60821900	-0.50733600
				P	-0.41931200	-1.64802300	0.23665500
				C	0.51550500	-2.43448500	-1.12465900
				C	0.29049000	-2.04291400	-2.44989300
				C	2.68047300	0.15322900	3.22469700
				C	0.88866000	-1.02263500	1.37413700

C	5.38051600	-1.67533900	-2.59688400	H	6.21815800	-2.13844900	-3.11022700
C	3.44276600	-0.20787500	-2.60915700	H	-0.56341000	-4.63727800	-0.16090100
C	2.00089700	-3.57431800	-3.20743000	H	-1.47988100	1.66912300	-3.16920000
C	-0.89285000	2.99134400	-1.56646700	H	-0.49076100	4.57538500	-0.15074100
C	-1.20003600	-4.36273000	0.67147600	H	0.01670700	-1.95924600	3.12801600
C	-1.45347800	2.69396300	-2.82004800	H	5.52868600	2.49289600	1.97025400
C	-1.26843900	-3.03107300	1.10180600	H	-3.53388100	-3.42637000	3.62681200
C	-1.97781900	5.02842200	-3.17133900	H	3.98297700	1.49813400	0.34985000
C	0.26260900	2.40834600	1.03486600	H	2.63740200	4.53962100	2.22375600
C	-0.89741500	4.32060000	-1.12163900	H	-1.89868400	-6.37692300	0.95499600
C	1.23887400	0.96930400	-1.27230000	H	1.55655300	-0.92441700	4.72598100
C	1.89436000	-0.17931200	0.89798200	H	5.81255800	-2.63813500	-0.70228600
C	0.78403200	-1.28670800	2.76614500	H	4.69970100	-0.59639400	-4.32287200
C	4.73384100	1.83799900	2.31529900	H	1.70296200	-3.68451200	0.17858300
C	2.81769200	0.41383200	1.82361500	H	0.86070000	-2.28565100	-4.50916800
C	-2.87903300	-3.69444300	2.80277600	H	2.99908400	-4.70364800	-1.66389900
C	3.86884100	1.27614100	1.40349400	H	0.86470800	1.93613100	-3.17871200
C	1.78805700	3.86336100	2.22939700	H	2.76464200	0.90976300	-4.33219800
C	-1.96071600	-5.35020600	1.30405700	H	-2.40342400	3.45705700	-4.59046900
C	1.64900000	-0.71225900	3.66417200	H	1.86172100	3.52486600	0.10547500
C	5.15120300	-1.95615600	-1.22886500	H	3.45297000	0.55314700	5.20221200
C	4.53948000	-0.82013100	-3.27153700	H	-2.23754100	-1.67106500	2.47556300
C	1.49984300	-3.39594900	-0.84831300	H	-1.20568500	1.40055000	2.24156300
C	1.03087200	-2.60961100	-3.48662800	H	5.27465000	2.03769800	4.40798700
C	2.23287900	-3.96742500	-1.88706500	H	3.91887200	-1.62542200	0.47858000
C	1.50656700	1.25197500	-2.63851900	H	-1.43742800	6.35503800	-1.55957400
C	2.57350100	0.68106200	-3.28718500	H	-0.41827500	2.40352800	4.37366200
C	3.20357300	-0.49046000	-1.22630100	H	2.58343900	-4.00996600	-4.01375700
C	1.15494600	3.54315400	3.43308100	H	-3.38213500	-5.79284400	2.86348900
C	-1.98169300	3.70476000	-3.62057900	H	1.51012400	3.97502400	4.36405000
C	1.34982900	3.29404200	1.03474900	H	-2.39732800	5.81610900	-3.79041600
C	3.57881200	0.75919000	4.14262200	H	-3.56507800	0.57954400	-2.65228200
C	2.08226400	0.11176300	-0.56233500	H	-2.22832500	-0.32490400	-3.39317800
C	-2.79431300	-5.02242600	2.37302500	H	-3.85669900	-1.00700600	-3.39019600
C	-2.13431600	-2.70585700	2.16362800	H	-6.05527000	-1.09622500	-0.13664600
C	-0.37367800	2.09856000	2.24378500	H	-5.44710400	0.05168900	-1.34586700
C	4.58873600	1.58232100	3.69965300	H	-5.55050600	-1.67539000	-1.72603800
C	4.09016600	-1.38455000	-0.56325100	H	-4.66542900	0.17872600	2.93308000
C	-1.43841800	5.33069700	-1.92097800				
C	0.07197500	2.66123600	3.43934900				
H	-0.43157300	-1.26604300	-2.66487500				

**TS1-OMe**

P	1.18963000	-0.39930800	1.66346800	C	2.93201300	-2.45877000	0.85285300
P	0.30405300	-0.17263900	-1.64648700	C	7.09493600	0.35436300	-0.46492300
C	-0.13840800	1.59659900	-1.94510500	C	2.96525400	3.56939300	-1.41749000
C	-0.97646100	2.25707000	-1.03549100	C	0.36315600	-1.82538600	5.40567000
C	4.97097000	-0.40739800	-1.36950600	C	4.14531900	-3.15290300	0.86565300
C	2.14963600	-0.17930300	-1.55438600	H	-1.34089900	1.75052800	-0.14891700
C	2.36290500	5.87197400	-0.95254400	H	2.42382700	6.92289600	-1.21991700
C	1.54238700	4.10668000	0.50253000	H	1.59095500	-0.12892500	-4.36580800
C	-0.87263600	4.28019600	-2.35255600	H	2.02204000	1.38014800	3.98792300
C	1.01533300	-0.47066000	3.49433600	H	0.03068000	-2.38867600	3.35822300
C	0.69123800	-0.73167400	-4.41701200	H	2.29755300	-1.94800200	-2.79887500
C	1.54348400	0.48663400	4.37235900	H	6.98618400	2.06039100	0.86960900
C	-0.07892700	-0.96183200	-3.26445600	H	-2.45725600	-2.98097600	-4.64165400
C	0.87526000	-0.85786500	6.27337600	H	4.55034200	2.28487200	0.71555600
C	2.81419800	-1.24750000	1.53888800	H	5.98063000	-1.01444000	2.77202500
C	0.43306100	-1.63280500	4.02631000	H	0.93514800	-1.11167800	-6.51773300
C	1.44025000	1.37065900	1.22505700	H	4.73452400	-2.12622100	-2.66025000
C	2.85439100	0.71669500	-0.74807700	H	3.60467200	5.22305100	-2.60787000
C	2.85208300	-1.21496600	-2.23004700	H	1.09381800	6.20616900	0.74562500
C	6.42029200	1.37714000	0.24286600	H	0.99365400	1.82639900	-3.77287700
C	4.28396300	0.62640500	-0.65806100	H	-1.99554000	4.07690400	-0.52100200
C	-1.57734000	-2.34638500	-4.58734200	H	0.35183000	4.17067600	-4.12556200
C	5.05197600	1.50656800	0.15370200	H	0.09568000	2.04530300	2.79624300
C	5.12676600	-1.42606000	2.24212500	H	0.21158600	4.41796000	2.18055700
C	0.32657700	-1.29878900	-5.63769900	H	1.87681300	1.04657000	6.42141200
C	4.21659200	-1.32213700	-2.14457100	H	3.83790100	0.20258900	2.77854900
C	3.03599400	4.90675500	-1.73829300	H	6.88335400	-1.31782800	-1.79355500
C	1.62589300	5.47638400	0.14115900	H	-1.81173000	-1.97714700	-2.48742000
C	0.33182700	2.30427500	-3.06078700	H	2.09391000	-2.83444000	0.27951900
C	-1.34557300	3.58580600	-1.23905100	H	8.17348200	0.25913800	-0.37914800
C	-0.03128100	3.63495200	-3.26194000	H	3.47178100	2.83829700	-2.03608200
C	0.70650200	2.35084700	1.95424900	H	-0.09255200	-2.72873500	5.80073800
C	0.76423200	3.67781200	1.60808500	H	4.23095800	-4.08909000	0.32094900
C	2.23177200	3.12789700	-0.28237700	H	-1.15073900	5.31837000	-2.50866900
C	5.24261500	-2.63949800	1.55546400	H	-1.08957000	-2.54991900	-6.67879500
C	1.46694600	0.29459900	5.75318700	H	6.18674500	-3.17676000	1.55820000
C	3.91823900	-0.73653300	2.24170800	H	0.81785300	-1.00415400	7.34803500
C	6.38107200	-0.52068200	-1.25207400	C	-2.48033500	-3.02079300	0.61435700
C	2.15551500	1.74453100	0.08672700	C	-3.06839600	-4.39777100	0.21029000
C	-0.80972100	-2.10648900	-5.72751500	C	-2.34032600	-4.99128500	-0.96528300
C	-1.21313100	-1.77812000	-3.36611300	C	-1.16057300	-4.54789200	-1.42037800

C -0.39371500 -3.46367300 -0.77718100  
C -0.98456400 -2.77615400 0.42797000  
H -2.74177200 -2.82795600 1.66287000  
H -2.84532900 -5.82026100 -1.45787500  
H -0.67698200 -5.00135000 -2.28165800  
C -3.16799300 -5.39407900 1.35632700  
H -3.77473500 -4.96896400 2.16274200  
H -3.63246100 -6.32731400 1.02104200  
H -2.17006100 -5.62289600 1.74451200  
O -4.41387100 -4.07629000 -0.21333100  
C -4.35821600 -2.83691900 -0.92980800  
H -4.17075000 -3.00966400 -2.00172200  
O 0.72959500 -3.20298400 -1.21071900  
C -3.23359900 -2.07272700 -0.28074000  
C -2.78966700 -0.81353300 -0.48688200  
H -5.33059900 -2.34221800 -0.83285900  
C -3.41012700 0.11545400 -1.48965100  
H -3.43278000 1.14994700 -1.14134400  
H -2.82956400 0.10790300 -2.41916400  
H -4.43848900 -0.17802300 -1.73610800  
Rh -0.82961400 -0.69521500 0.41165300  
C -6.36270500 1.37787700 0.93426500  
C -5.33872900 0.46611100 1.09874200  
C -4.02389800 0.90676200 1.36211100  
C -3.77076300 2.28982600 1.43209000  
C -4.79442200 3.21524000 1.26035600  
C -6.09944300 2.76121700 1.00760000  
H -7.37930300 1.05320900 0.73783400  
H -5.53561500 -0.59799600 1.01941800  
H -2.75828500 2.63408000 1.61699800  
H -4.57412400 4.27380600 1.32034200  
C -2.94096400 -0.00797400 1.53013600  
C -1.93230100 -0.49689200 2.14456600  
H -1.65261300 -0.58141600 3.18501700  
H -0.40242300 -3.08669300 1.30114200  
O -7.16324100 3.56818100 0.81713500  
C -6.96185000 4.98377300 0.85180400  
H -7.94141300 5.42486700 0.66258800  
H -6.59771000 5.30694600 1.83349000  
H -6.25963500 5.30091000 0.07270400

## TS2-OMe

C 2.98368900 2.63185200 0.33404200  
C 3.48431400 3.85677500 1.14504800  
C 2.39085500 4.41792300 2.01448600  
C 1.30615700 3.72122500 2.37613500  
C 1.14499200 2.28858200 2.05660400  
C 1.99520200 1.67173200 0.98630300  
H 3.86191200 2.06750300 -0.00555000  
H 2.53436800 5.44272100 2.35188500  
H 0.54990400 4.14026000 3.03375400  
C 4.75512700 3.60066100 1.94183600  
H 5.55350300 3.27338300 1.26754500  
H 5.07998600 4.50993600 2.45828300  
H 4.57888400 2.82040800 2.68926500  
O 3.79385800 4.82373000 0.11659000  
C 2.77471700 4.73080100 -0.88559500  
H 1.94109100 5.41715400 -0.66662500  
O 0.39728100 1.60806500 2.76009100  
C 2.33833600 3.29119800 -0.84628700  
C 1.47305000 2.59867700 -1.62095500  
H 3.20987400 5.02540600 -1.84696600  
C 0.72209100 3.19252800 -2.77724500  
H 1.21643500 4.09936700 -3.14938000  
H 0.63484600 2.48773000 -3.61056500  
H -0.29780800 3.46281000 -2.48258600  
Rh 0.90329100 0.80132200 -0.62530700  
P -1.38795200 1.51693300 -0.14006400  
P 0.20969200 -1.57828400 -0.08117200  
C -0.03414200 -2.27256700 1.58781900  
C 0.32893700 -1.51407300 2.70572600  
C -3.79306700 -2.22839100 -2.46893500  
C -1.40496300 -1.91906900 -0.95152200  
C -4.37930400 -3.07060300 4.08286200  
C -3.33452900 -1.03040400 3.27380700  
C -0.42172300 -3.29625000 4.16085700  
C -1.81945700 3.23312300 0.36028700  
C 1.71811500 -2.51477300 -2.25007900  
C -3.08727800 3.54935100 0.88185500  
C 1.35504300 -2.75373300 -0.91321500  
C -2.48696300 5.89221000 0.98120200

C	-2.31295800	1.31869200	-1.72152600	H	-5.27744800	1.99595500	-3.25640200
C	-0.89629600	4.26587900	0.16153200	H	2.89477300	-3.14491800	-3.93363700
C	-2.23880800	0.49986600	1.14719800	H	-2.55011300	-3.33283900	-3.85136500
C	-2.60669600	-1.41503500	-0.45553700	H	-4.71303500	-4.60704000	2.58936700
C	-1.41646900	-2.62989700	-2.18359300	H	-3.91711100	-1.38170900	5.32436600
C	-6.19221300	-1.11458000	-1.52572400	H	-0.89678700	-4.13162500	0.89781400
C	-3.81694100	-1.54917000	-1.21129100	H	0.39501900	-1.42385800	4.85388100
C	2.85406900	-4.66315800	-0.89123400	H	-1.22569300	-5.03997200	3.17446600
C	-5.05080800	-1.00002600	-0.76438900	H	-1.93843000	2.00960300	2.67944200
C	-4.26127000	1.63341900	-3.13260100	H	-2.87503600	0.68899700	4.50361900
C	2.62757000	-3.34525800	-2.90004200	H	-4.39842700	5.09552900	1.59229100
C	-2.56921600	-2.78217800	-2.91467600	H	-4.14072300	2.29190700	-1.09706300
C	-4.32850200	-3.60837800	2.77535600	H	-4.94756400	-2.84621400	-4.18837500
C	-3.88733500	-1.80785400	4.32510600	H	1.69245800	-4.02994300	0.79585200
C	-0.59597200	-3.54769100	1.76211200	H	-0.66622900	0.28088600	-2.65853700
C	0.13085200	-2.02657800	3.98954800	H	-7.07046600	-1.86440800	-3.36307100
C	-0.78169800	-4.05764500	3.04455800	H	-3.73445100	-3.31859500	0.74950000
C	-2.31588100	1.02014000	2.47128900	H	-0.49177200	6.37266500	0.31674500
C	-2.83654100	0.27690000	3.49889600	H	-1.79332400	0.02396300	-4.83448900
C	-3.27256600	-1.57212500	1.95207300	H	-0.58227900	-3.69089200	5.16001200
C	-3.60885200	0.99945700	-4.19167200	H	3.92323800	-5.06163200	-2.72072600
C	-3.41635100	4.86830200	1.18785000	H	-4.11494500	0.86914100	-5.14366800
C	-3.61747900	1.79665400	-1.90598700	H	-2.74498200	6.91897400	1.22406100
C	-4.98549000	-2.33038400	-3.23271700	C	4.85877200	-2.10508200	0.93909600
C	-2.69177400	-0.78975300	0.89569100	C	3.81320600	-1.31694600	0.48739100
C	3.20354700	-4.42103500	-2.21932600	C	3.86935800	-0.68685000	-0.77126500
C	1.93510900	-3.83653500	-0.24174900	C	5.02466400	-0.87921700	-1.55381500
C	-1.66480300	0.68739800	-2.79359900	C	6.07907700	-1.67142100	-1.11247000
C	-6.16246800	-1.78501700	-2.77240500	C	5.99931900	-2.29521900	0.14280300
C	-3.78200500	-2.88319700	1.73976900	H	4.80809200	-2.59678600	1.90532900
C	-1.22642000	5.58733000	0.46953300	H	2.93423600	-1.19994200	1.11060800
C	-2.30528500	0.52839200	-4.02034100	H	5.09146500	-0.39655800	-2.52436000
H	0.70275300	-0.50526700	2.57901700	H	6.94976600	-1.79861600	-1.74445600
H	-4.80471500	-3.65697100	4.89218300	C	2.82354600	0.17442600	-1.26106400
H	1.29681600	-1.67036000	-2.78387300	C	2.46454400	0.98957500	-2.18616000
H	-3.81430200	2.76589200	1.06539600	H	2.51440400	1.24626200	-3.23457400
H	0.08709900	4.03445400	-0.21805100	H	2.48153500	0.79487600	1.41285100
H	-0.50675500	-3.07648600	-2.55730200	O	6.96395500	-3.09045700	0.66814000
H	-7.12287300	-0.68133500	-1.17100800	C	8.13634700	-3.33107600	-0.10895200
H	3.30248800	-5.49152800	-0.35050700	H	8.67854000	-2.39963200	-0.31126700
H	-5.08364200	-0.47289600	0.18169900	H	8.76164100	-3.99157600	0.49411700

**TS1- Nap**

C	-1.967869	-3.4087190	0.76166500	C	-0.220880	-2.7699980	-5.5404050
C	-2.327832	-4.8822500	0.44215700	C	-0.220930	1.29822900	-2.1254440
C	-1.471386	-5.4390610	-0.6624720	C	-0.763238	-2.2940890	-3.2326670
C	-0.347101	-4.8602600	-1.1059550	C	2.2695760	-0.0634330	-1.4761030
C	0.2216570	-3.6298810	-0.5232970	C	1.8970990	1.93916400	0.01780000
C	-0.520518	-2.9541030	0.60204500	C	0.2739950	2.38359800	1.78634100
H	-2.294772	-3.1897930	1.78637800	C	2.2996110	5.10050200	-1.9698890
H	-1.828382	-6.3652480	-1.1091640	C	1.7457500	3.29001000	-0.4383870
H	0.2365990	-5.2966780	-1.9121360	C	1.2678610	0.77318200	5.74152200
C	-2.321767	-5.8000200	1.65670200	C	2.4485860	3.79191900	-1.5677270
H	-3.018686	-5.4184950	2.41025000	C	-0.310897	3.19754100	-3.6339430
H	-2.624303	-6.8152450	1.37947200	C	0.6035510	-1.5396920	5.53413000
H	-1.317342	-5.8436240	2.09057200	C	0.1055220	3.67375900	1.34895600
O	-3.688203	-4.7970200	-0.0409950	C	6.1594810	2.30890200	0.29290100
C	-3.793145	-3.6129010	-0.8408990	C	6.4854180	0.32705200	-1.0507680
H	-3.542437	-3.8253000	-1.8924890	C	3.9857040	-0.0770930	2.35349500
O	1.3133600	-3.2341170	-0.9343740	C	4.6460270	-2.5232230	1.18436100
C	-2.817646	-2.6461390	-0.2185960	C	5.2894890	-0.5560450	2.43210200
C	-2.553876	-1.3546610	-0.5071490	C	3.1549100	-1.0160260	-2.0502910
H	-4.831959	-3.2680810	-0.8042570	C	4.5147930	-0.8878770	-1.9249240
C	-3.271567	-0.5983110	-1.5853740	C	4.2091510	1.15027100	-0.5968480
H	-4.231072	-1.0684690	-1.8351020	C	-1.309210	3.78487600	-2.8522670
H	-3.469691	0.43929000	-1.3115490	C	0.7953380	-1.8129370	-5.4897590
H	-2.663849	-0.5733270	-2.4971360	C	0.2292400	1.96393900	-3.2748210
Rh	-0.670033	-0.8759610	0.44192900	C	0.7096710	5.51101600	-0.1954400
P	0.4497280	-0.3489560	-1.6244250	C	2.7890690	0.99434000	-0.7261090
P	1.2595400	-0.2414930	1.71166700	C	0.8899280	-0.4319250	6.33580300
C	3.0025250	-0.8165600	1.67413300	C	1.3533700	0.87763100	4.35182500
C	3.3367580	-2.0417290	1.09243900	C	-1.216150	1.90139500	-1.3458290
C	0.8522210	4.17160400	0.25062200	C	1.4240840	5.97111500	-1.2787890
C	1.2112380	1.51260700	1.15629900	C	4.7926310	2.20227300	0.16244900
C	7.0174000	1.36370700	-0.3179340	C	-0.998818	-3.0093380	-4.4072980
C	5.0809120	0.19538100	-1.2092590	C	-1.761892	3.13230500	-1.7057260
C	5.6227120	-1.7838010	1.84950000	H	2.5876920	-2.5939490	0.53925300
C	0.2514290	-1.3301330	-3.1699690	H	8.0931780	1.45602000	-0.2003970
C	0.6826590	-1.4364680	4.14570200	H	0.4600820	-2.3043350	3.53111200
C	1.0308810	-1.0979870	-4.3157630	H	1.8379620	-0.3751420	-4.2966030
C	1.0484390	-0.2233810	3.53931400	H	-1.369372	-2.4923020	-2.3596080
				H	-0.311409	2.02266800	2.62442400
				H	2.8497040	5.46497900	-2.8325090
				H	1.5037830	1.63589200	6.35797600

H	3.1096400	3.13093100	-2.1150890	C	-5.239622	-0.2540100	0.93707000
H	0.0558150	3.70548600	-4.5212000	C	-3.972454	0.34420400	1.19790200
H	0.3176710	-2.4840340	5.98822600	H	-7.297475	0.08125200	0.47028200
H	-0.601784	4.33250500	1.84571200	H	-5.321282	-1.3355800	0.95261200
H	6.5832590	3.12071200	0.87697800				
H	7.1305830	-0.4128430	-1.5168450				
H	3.7365770	0.87544800	2.80901300				
H	4.8998680	-3.4722850	0.72038000				
H	6.0480640	0.03061300	2.94160800	C	1.79524100	3.63485900	0.23690700
H	2.7488050	-1.8724500	-2.5699380	C	1.87450900	4.93541900	1.08104700
H	5.1757390	-1.6314600	-2.3617680	C	0.67487800	5.06959800	1.98232100
H	1.4105130	-1.6219460	-6.3643350	C	-0.07922300	4.03067700	2.36335600
H	1.0106580	1.53144200	-3.8879200	C	0.28615500	2.63962800	2.02857700
H	0.0237630	6.16503000	0.33632500	C	1.21801700	2.38087900	0.88496500
H	1.6654000	1.81678600	3.90938300	H	2.80153300	3.41167900	-0.14245600
H	-1.564873	1.41585100	-0.4429130	H	0.45684600	6.07705800	2.33145400
H	1.3121670	6.99890800	-1.6115180	H	-0.91033100	4.14893200	3.05260800
H	4.1502130	2.92562700	0.64958300	C	3.17463700	5.10046900	1.85416400
H	-1.786883	-3.7565500	-4.4307570	H	4.02164300	5.07847200	1.16051000
H	-2.534898	3.57942300	-1.0880580	H	3.18627100	6.05238600	2.39512900
H	6.6412440	-2.1559150	1.91360500	H	3.28691800	4.28802200	2.57915800
H	0.8242950	-0.5098790	7.41706300	O	1.81875800	5.97618400	0.08105300
H	-1.725332	4.74785600	-3.1333810	C	0.86498500	5.57395500	-0.90854500
H	-0.400709	-3.3269390	-6.4554800	H	-0.14260600	5.94310300	-0.65887600
C	-2.805407	-0.4518150	1.46530300	O	-0.08472000	1.73128600	2.77368900
C	-1.804817	-0.7871250	2.17676900	C	0.92638700	4.07003700	-0.90292900
H	-1.533929	-0.8251880	3.22022200	C	0.30500900	3.14883700	-1.67353200
H	0.0619640	-3.1077680	1.51520600	H	1.15719400	6.01527900	-1.86795300
C	-5.907546	4.75526400	0.50010000	C	-0.64883400	3.48368000	-2.78377400
C	-4.818102	3.97223600	0.81065500	H	-0.49962300	4.51079600	-3.14140300
C	-4.942172	2.55757700	0.87197500	H	-0.53563200	2.80758900	-3.63800400
C	-6.215320	1.95242600	0.61073000	H	-1.68653500	3.39407000	-2.44394200
C	-7.317692	2.78840600	0.29863500	Rh	0.36380600	1.24842000	-0.70799000
C	-7.166640	4.15782100	0.24312300	P	-1.98975700	1.18473300	-0.10505100
H	-2.867259	2.17707700	1.35547500	P	0.49022000	-1.25671100	-0.26060300
H	-5.806868	5.83542500	0.45149800	C	0.70722400	-2.06538800	1.35769800
H	-3.848568	4.42073200	1.01111400	C	0.81693000	-1.27406100	2.50637200
C	-3.836445	1.72520400	1.16708700	C	-3.29936600	-3.17056300	-2.27483600
C	-6.328716	0.53364900	0.66344100	C	-0.99814000	-2.11589400	-0.98013800
H	-8.282835	2.32977100	0.10120300	C	-2.96154200	-4.07299200	4.27800900
H	-8.017399	4.78774100	0.00015700	C	-2.74924500	-1.81272900	3.40992000
				C	0.92885900	-3.27143100	3.86884100

**TS2- Nap**

C	-2.94978300	2.65894800	0.42426800	H	-1.43663700	4.04822100	-0.20154700
C	1.85796000	-1.47425400	-2.68141600	H	0.06973000	-2.99278500	-2.65857700
C	-4.23106400	2.53320900	0.99151100	H	-6.81674800	-2.65782900	-0.68345000
C	1.83841800	-1.88776600	-1.33683600	H	4.74660200	-3.65812600	-1.31378500
C	-4.44070800	4.94174300	1.10157700	H	-4.82368000	-1.84364200	0.49921000
C	-2.85229500	0.67104000	-1.65026400	H	-5.92831700	0.29231200	-3.06428400
C	-2.42814200	3.93952500	0.21111700	H	2.89437600	-1.53006500	-4.56317200
C	-2.38151000	-0.04047100	1.22036300	H	-1.90433300	-3.89050000	-3.76276200
C	-2.24395100	-1.99920300	-0.36928300	H	-2.82104600	-5.65886500	2.80499200
C	-0.89713000	-2.83542200	-2.20320000	H	-3.04738800	-2.30528400	5.49260700
C	-5.83267400	-2.80053000	-1.12043100	H	0.58831200	-4.08117500	0.58212800
C	-3.41784700	-2.50950100	-1.01253400	H	0.98844200	-1.26191800	4.65041300
C	3.93237400	-3.05505500	-1.70451200	H	0.80596000	-5.14588100	2.80490500
C	-4.71603400	-2.34700700	-0.45444000	H	-2.51956000	1.50990800	2.73644700
C	-4.84552200	0.29788600	-2.98278200	H	-2.83999000	-0.01542200	4.61108600
C	2.89547400	-1.85621500	-3.52710700	H	-5.95673000	3.55359000	1.76325700
C	-2.00815900	-3.34762100	-2.82710400	H	-4.87530100	0.96632400	-0.94693200
C	-2.80431000	-4.58518400	2.96838700	H	-4.35981300	-4.12415200	-3.89856200
C	-2.93174700	-2.71344600	4.49206600	H	2.90016500	-2.99945400	0.17720700
C	0.69985300	-3.46500400	1.46904500	H	-0.98611300	0.25519600	-2.66768500
C	0.92477600	-1.88030300	3.75957600	H	-6.60141200	-3.79541700	-2.88951900
C	0.81851100	-4.06316200	2.72136500	H	-2.48403600	-4.14484800	0.90715200
C	-2.54408300	0.44684200	2.54953500	H	-2.74275700	6.06074000	0.38239100
C	-2.72107300	-0.40966400	3.60551400	H	-2.04575000	-0.38424200	-4.79270700
C	-2.58804100	-2.32498100	2.08457700	H	1.00469200	-3.74119000	4.84524700
C	-4.05829000	-0.08173200	-4.07141500	H	4.76475000	-2.92291500	-3.68814800
C	-4.96950500	3.66667900	1.32476300	H	-4.52667300	-0.38004200	-5.00474400
C	-4.24767100	0.67614200	-1.78066200	H	-5.01694900	5.82373900	1.36591500
C	-4.46819800	-3.62929300	-2.93716800	C	2.35723700	1.25760700	-1.43697100
C	-2.39502200	-1.41127200	0.99265600	C	1.74153800	1.96306400	-2.31352900
C	3.94311600	-2.64096000	-3.03622500	H	1.67286400	2.24686200	-3.35408400
C	2.88375300	-2.68494200	-0.85940100	H	1.99263700	1.70485500	1.24211900
C	-2.06990100	0.29193600	-2.75214900	C	4.71948800	0.78783000	-1.86941500
C	-5.71111600	-3.44607500	-2.37471600	C	5.98920600	0.29302100	-1.48901700
C	-2.61796200	-3.73524900	1.90081100	C	3.62282100	0.69937900	-1.01986700
C	-3.16845900	5.07504700	0.54696900	C	7.11286900	0.36247800	-2.35813600
C	-2.66647400	-0.08120200	-3.95463400	C	6.14761000	-0.30446400	-0.19512500
H	0.75906400	-0.19382600	2.43106300	C	3.79322600	0.09487900	0.26098400
H	-3.10258600	-4.75565900	5.11102300	C	8.33458600	-0.13688600	-1.96608400
H	1.05825700	-0.84962300	-3.06616200	H	6.98715800	0.81494100	-3.33837300
H	-4.64739600	1.55149600	1.19004200	C	7.42093300	-0.80692900	0.17938600



C	5.01630800	-0.38182700	0.66029400	C	-1.50080900	1.06336000	-1.36406700
H	2.93834500	-0.00785800	0.91769000	C	-6.97744500	-0.60918700	0.45150200
C	8.49035500	-0.72682700	-0.68612400	C	-4.77210100	-0.92816600	1.42340300
H	9.18659500	-0.08157900	-2.63762000	C	-4.65636800	-3.48517300	-1.22098100
H	7.53597100	-1.25909200	1.16110500	C	0.29322700	-0.50394200	3.32267600
H	5.12793500	-0.84441500	1.63730300	C	-0.05716600	-2.02405700	-3.86159400
H	9.46010700	-1.11689200	-0.39057400	C	-0.50318700	-0.26545900	4.45528100
H	4.60454700	1.24252400	-2.84934400	C	-0.80195200	-0.91327200	-3.43257100

### TS1-Me

C	3.01970600	-2.56424300	-0.34665100	C	-2.01983700	-0.25843400	1.55525900
C	3.80298400	-3.79514900	0.17921500	C	-2.29644100	1.44903700	-0.28513900
C	3.16879800	-4.37286100	1.41508600	C	-0.88073400	2.05458700	-2.17961500
C	1.93692300	-4.06425000	1.84244300	C	-3.70342800	4.62931800	1.13625600
C	1.02243100	-3.16484700	1.11359500	C	-2.58468600	2.83862800	-0.07773700
C	1.50559600	-2.52549100	-0.16441800	C	-1.36581000	-0.44078600	-5.74560400
H	3.25238900	-2.43770600	-1.41174400	C	-3.43065700	3.28962100	0.97219500
H	3.78908800	-5.06902700	1.97673200	C	-0.61808300	3.99679800	2.83332200
H	1.52451500	-4.49844700	2.74941300	C	0.03632000	-2.33518800	-5.21781800
C	4.04783300	-4.87241900	-0.86761500	C	-1.12489300	3.38953900	-1.97549400
H	4.58780700	-4.44375000	-1.71841500	C	-6.45768600	0.41148900	-0.37955500
H	4.64191500	-5.69234500	-0.45070700	C	-6.14778400	-1.26615600	1.33168300
H	3.09413300	-5.27894900	-1.21991400	C	-3.62286800	-1.49809900	-2.13183000
O	5.08541500	-3.24044100	0.55227200	C	-3.50119800	-3.74775800	-0.48613600
C	4.84666100	-1.96087000	1.15162600	C	-4.71543000	-2.35510300	-2.04360200
H	4.68611600	-2.05943100	2.23698500	C	-2.56332100	-1.30254700	2.35254300
O	-0.12314300	-3.01867200	1.54215500	C	-3.89590600	-1.62169100	2.29373900
C	3.61970000	-1.43540200	0.44931300	C	-4.24260000	0.10714300	0.58981100
C	2.98799900	-0.24823200	0.55314800	C	0.21926100	4.67542800	1.94406800
H	5.73629300	-1.34135800	0.99610300	C	-0.05668900	-0.63029100	5.72499500
C	3.46500800	0.85009100	1.45791100	C	-0.75996700	2.61279200	2.74993100
H	4.50716300	0.69533100	1.76497900	C	-2.28619600	5.19210200	-0.73941000
H	3.39915300	1.83658900	0.99452500	C	-2.84545900	0.42501800	0.65922700
H	2.85109500	0.88679900	2.36482800	C	-0.61424000	-1.54013700	-6.16434700
Rh	1.04157000	-0.50038900	-0.36429700	C	-1.46548200	-0.13057000	-4.38800000
P	-0.19986200	0.04696500	1.63541200	C	0.77185500	2.57638800	0.88820200
P	-0.98744900	-0.68482300	-1.61611800	C	-3.12721600	5.59224400	0.27459700
C	-2.46192800	-1.75500000	-1.38295100	C	-5.12599600	0.75682800	-0.31639700
C	-2.40460800	-2.88431200	-0.56244800	C	1.98660600	-1.48442100	4.76613000
C	-1.99947300	3.81726400	-0.94389000	C	0.91659300	3.96018200	0.97036000

H	-1.52514500	-3.06455100	0.04241300	H	3.93086400	4.86570400	-1.79565100
H	-8.02842700	-0.87544400	0.38667200	C	2.97991700	0.37817100	-1.56422700
H	0.45309400	-2.64790700	-3.13348100	C	2.09328400	-0.33066500	-2.14008300
H	-1.48415900	0.18366400	4.35395700	H	1.83206700	-0.60037000	-3.15183100
H	2.16207500	-1.32069000	2.63469300	H	0.97546400	-3.00925700	-0.99014900
H	-0.20766900	1.74861400	-2.97271000	C	6.62351000	4.82939500	-1.31180600
H	-4.35717400	4.95147200	1.94150000	H	6.09241200	5.78508100	-1.34772400
H	-1.88240700	0.17674900	-6.47477300	H	7.22522000	4.80202200	-0.39585100
H	-3.86455900	2.56457000	1.64994300	H	7.32411800	4.79977400	-2.15634500
H	-1.17467500	4.54799700	3.58552800				
H	0.61741500	-3.19696400	-5.53316300	<b>TS2-Me</b>			
H	-0.65352600	4.13578000	-2.60930700	C	3.48908200	1.96883700	0.45867300
H	-7.11367000	0.92043200	-1.07987800	C	4.19614100	3.04623200	1.32384200
H	-6.52933500	-2.05979900	1.96843100	C	3.21016300	3.77520800	2.19666000
H	-3.67730500	-0.62496400	-2.77358500	C	2.00273400	3.28814800	2.50869400
H	-3.45192700	-4.61772000	0.16287800	C	1.58088100	1.92318000	2.13554600
H	-5.61603100	-2.13797100	-2.61017700	C	2.32820900	1.18713200	1.06157400
H	-1.90941700	-1.87242300	2.99773000	H	4.25313200	1.26393000	0.10686900
H	-4.29187800	-2.42781400	2.90529400	H	3.53865300	4.74057000	2.57699200
H	-0.68747900	-0.44077300	6.58873300	H	1.32324900	3.82127200	3.16747100
H	-1.43329200	2.11095300	3.43444300	C	5.37773100	2.52424200	2.12796500
H	-1.82911400	5.92148500	-1.40272400	H	6.11274000	2.07315300	1.45320400
H	-2.06658900	0.71793600	-4.08084600	H	5.85935400	3.33649100	2.68228000
H	1.31012500	2.03169200	0.12243600	H	5.04025100	1.76755700	2.84333900
H	-3.34546400	6.64616800	0.42037900	O	4.70420500	3.97165000	0.33743500
H	-4.74164000	1.52866500	-0.97194200	C	3.70161600	4.11410800	-0.67541900
H	2.95445900	-1.96510300	4.87630100	H	3.00734500	4.93413200	-0.43161500
H	1.56844900	4.47387300	0.26977700	O	0.69957400	1.37842500	2.80156300
H	-5.51047800	-4.15306700	-1.15432400	C	3.00238500	2.78113400	-0.70233000
H	-0.53934300	-1.77890600	-7.22122900	C	2.04340200	2.29577100	-1.52168500
H	0.32117000	5.75481000	2.00778200	H	4.19954300	4.36209000	-1.61906800
H	1.53509500	-1.52381800	6.87525500	C	1.45248900	3.06873200	-2.66504800
C	6.13378500	2.35465300	-1.16218900	H	1.31460100	2.44127000	-3.55183400
C	5.26806800	1.27174800	-1.21009800	H	0.46659000	3.46597100	-2.40093600
C	3.90324800	1.47233400	-1.48756000	H	2.09234600	3.91537300	-2.94538200
C	3.42859700	2.78034100	-1.69571500	Rh	1.13492400	0.57967400	-0.59760300
C	4.30669900	3.85897100	-1.63543100	P	-0.99272100	1.66317300	-0.11965700
C	5.66931200	3.66629900	-1.36885200	P	0.06945200	-1.63695600	-0.14869600
H	7.18765000	2.19059600	-0.95357800	C	-0.32856900	-2.33135600	1.48911700
H	5.63028500	0.26517400	-1.02839000	C	0.12961800	-1.67940900	2.63891900
H	2.37403300	2.93871600	-1.89781000				

C	-3.92463800	-1.51458700	-2.63280900	C	-1.94401300	1.17372100	-4.08739300
C	-1.55244000	-1.65755500	-1.06803000	H	0.66149800	-0.73976200	2.55414500
C	-4.77309100	-2.50183900	3.90343700	H	-5.29933600	-3.03803700	4.68788800
C	-3.40721200	-0.62784100	3.17443300	H	1.20440300	-1.84459900	-2.83511800
C	-0.92121600	-3.36859500	4.01700600	H	-3.19629200	3.28130400	1.06912400
C	-1.13013100	3.41426500	0.42960300	H	0.89982600	3.89369500	-0.08628700
C	1.45737500	-2.76172800	-2.31564500	H	-0.80130400	-2.83889700	-2.73089700
C	-2.34053700	3.93139300	0.92602900	H	-7.04114900	0.37373600	-1.26061100
C	1.01867000	-2.96886900	-0.99603000	H	2.46475700	-6.00790100	-0.46570700
C	-1.35280300	6.13363200	1.10672100	H	-5.01975300	0.21590300	0.12015800
C	-1.91606800	1.68897000	-1.71278600	H	-4.84538300	2.67773800	-3.14198900
C	-0.03955600	4.27830100	0.28070200	H	2.56297900	-3.53716800	-3.98634900
C	-2.03542700	0.76761100	1.11553800	H	-2.82246400	-2.69115500	-4.07400400
C	-2.67537500	-1.00634700	-0.55796700	H	-5.31393000	-3.92304000	2.35705100
C	-1.64024000	-2.27975700	-2.34416000	H	-4.07635900	-0.94323000	5.20436300
C	-6.16952300	-0.15345200	-1.63748600	H	-1.46488000	-4.00262600	0.71947100
C	-3.87939200	-0.92451200	-1.33132300	H	0.16897800	-1.67489300	4.78939100
C	2.17781400	-5.10301300	-0.99350400	H	-1.97421000	-4.92602100	2.95610300
C	-5.03718900	-0.24508000	-0.85987500	H	-1.53770000	2.16902700	2.69765000
C	-3.84661400	2.25866700	-3.06611800	H	-2.71240000	0.96478000	4.46324000
C	2.23473200	-3.71653000	-2.96662100	H	-3.38946400	5.66145500	1.64680600
C	-2.78342800	-2.20791100	-3.10146600	H	-3.69954400	2.65524900	-0.96481600
C	-4.78205100	-3.00264100	2.58023900	H	-5.11622900	-1.84613400	-4.40505500
C	-4.09483100	-1.33932300	4.19258000	H	1.09232500	-4.32610400	0.68257400
C	-1.09044400	-3.50471700	1.60849800	H	-0.29277200	0.74316300	-2.78124400
C	-0.17116100	-2.19785600	3.90005500	H	-7.10404900	-0.64630300	-3.53334400
C	-1.37747100	-4.02318000	2.86869100	H	-4.10997900	-2.75160800	0.57368300
C	-2.06086000	1.25723800	2.45287900	H	0.71243400	6.28123400	0.50220200
C	-2.71621900	0.57843200	3.44768600	H	-1.45276000	0.75331500	-4.96018000
C	-3.40412600	-1.13470100	1.83740600	H	-1.16036700	-3.76750600	4.99857600
C	-3.22492300	1.71916900	-4.19444200	H	3.21945800	-5.62999000	-2.80670400
C	-2.44871900	5.27927800	1.26131900	H	-3.73726400	1.72351800	-5.15200300
C	-3.19738800	2.24464700	-1.83265700	H	-1.43915200	7.18353400	1.37145400
C	-5.10338000	-1.39732500	-3.41551600	C	4.55143600	-2.96720600	0.94362500
C	-2.68528200	-0.42486200	0.81555500	C	3.63783200	-2.01954500	0.49025300
C	2.60231500	-4.89053900	-2.30472800	C	3.83168000	-1.36872700	-0.73859200
C	1.39146500	-4.15011700	-0.34313000	C	4.97961100	-1.69527000	-1.49267700
C	-1.29387600	1.16222300	-2.85407200	C	5.88446600	-2.64141900	-1.03117700
C	-6.20529200	-0.73116300	-2.92950500	C	5.68612900	-3.29999200	0.19412800
C	-4.10906000	-2.34239600	1.57624100	H	2.76150400	-1.79375100	1.08685400
C	-0.14879500	5.62938900	0.61735800	H	5.15030300	-1.19230200	-2.44010900

H	6.76158000	-2.87812400	-1.62851600	C	-3.59394300	1.92843600	0.93291100
C	2.94265500	-0.34379100	-1.22841800	C	-0.81733600	-4.20174400	0.60349200
C	2.74191500	0.54257800	-2.13369300	C	-1.30904200	-1.50216700	1.29454000
H	2.84731600	0.81874400	-3.17313800	C	-7.12560400	-1.75618100	-0.11806500
H	2.63798300	0.22501800	1.46917000	C	-5.25648000	-0.58093700	-1.13552300
H	4.37589400	-3.46251300	1.89505800	C	-5.86132500	1.64661200	1.73512100
C	6.65519800	-4.35147100	0.66814300	C	-0.53211100	1.02327600	-3.26973600
H	6.50074900	-5.29581600	0.12868300	C	-0.86700800	1.68661100	4.02552200
H	7.69350400	-4.04769200	0.49306100	C	-1.29375200	0.63350500	-4.38414900
H	6.53111100	-4.55719400	1.73597600	C	-1.21192200	0.42294600	3.51963400

### TS1-Br

C	1.58989200	3.51642100	0.53175800	C	0.08711000	-1.48073300	-2.00314300
C	1.86659800	4.99229900	0.14407200	C	0.40384100	2.05421900	-3.42246800
C	0.98484600	5.44723700	-0.98713200	C	-2.46293300	-0.20365200	-1.45088300
C	-0.09626200	4.78009300	-1.41339800	C	-1.98215000	-2.05440400	0.20386100
C	-0.59144100	3.54200300	-0.78319400	C	-0.32011500	-2.26637000	1.98064700
C	0.17139100	2.97591800	0.38947200	C	-2.26091900	-5.39580000	-1.48958900
H	1.92594600	3.36335500	1.56523500	C	-1.77024800	-3.43091800	-0.13711800
H	1.28786400	6.37328100	-1.47237900	C	-1.39210700	-0.40282600	5.79421100
H	-0.69747300	5.14268000	-2.24303700	C	-2.47064800	-4.06629800	-1.19876000
C	1.80476900	5.96504600	1.31294700	C	0.19481800	-3.53272200	-3.29682700
H	2.51666600	5.65846200	2.08635900	C	-0.78042200	1.90076800	5.40076600
H	2.05396600	6.98057800	0.98787200	C	-0.08372600	-3.57587200	1.64397700
H	0.79703000	5.97546100	1.74120800	C	-6.21686100	-2.59529500	0.56938200
O	3.23047200	4.96103300	-0.33522400	C	-6.65153600	-0.76785900	-0.95061100
C	3.39990500	3.75226400	-1.08602500	C	-4.14732700	0.07018300	2.38585200
H	3.13660400	3.90726300	-2.14428800	C	-4.92240500	2.35955400	0.99127200
O	-1.64305200	3.05138100	-1.19608400	C	-5.47073200	0.49703900	2.43053400
C	2.47901100	2.75979800	-0.41994100	C	-3.39983500	0.64682300	-2.09892400
C	2.27962000	1.44941500	-0.65977700	C	-4.75069500	0.45990700	-1.95193000
H	4.45648900	3.46829500	-1.03861200	C	-4.33330000	-1.43054100	-0.44782200
C	3.03604000	0.68559000	-1.70666600	C	1.27370900	-3.97494500	-2.52725700
H	3.92690600	1.23478000	-2.03685700	C	-1.11649600	1.25974800	-5.61730500
H	3.36219300	-0.29734900	-1.36108800	C	-0.39512400	-2.29732500	-3.03656100
H	2.40409700	0.51561000	-2.58533000	C	-0.60952800	-5.56476100	0.26796700
Rh	0.44237300	0.90761100	0.35871000	C	-2.92343300	-1.21793700	-0.60662200
P	-0.66259600	0.16942400	-1.64396900	C	-1.03781500	0.85359500	6.28890000
P	-1.43712200	0.28675700	1.69943800	C	-1.48513200	-0.61828300	4.41787700
C	-3.20221900	0.78228400	1.62826700	C	1.16589600	-1.93748300	-1.23435300
				C	-1.32167100	-6.15463700	-0.75214200
				C	-4.85812800	-2.43389800	0.41345900

C	0.58215200	2.67996800	-4.65671300
C	1.75821800	-3.17249300	-1.49450300
H	-2.87359700	2.45465200	0.31985500
H	-8.19452200	-1.89073300	0.01962800
H	-0.66121300	2.50494700	3.34166200
H	-2.04444400	-0.14240600	-4.29175700
H	0.99338400	2.37400300	-2.57433000
H	0.25129800	-1.80679900	2.77905400
H	-2.81162700	-5.86374700	-2.30029400
H	-1.60255700	-1.21941700	6.47884600
H	-3.18017300	-3.49186300	-1.78188300
H	-0.19887300	-4.15749700	-4.09307100
H	-0.51023800	2.88332100	5.77671800
H	0.66614900	-4.15224100	2.17916000
H	-6.59476600	-3.36777200	1.23292200
H	-7.33650200	-0.10805100	-1.47630400
H	-3.85316500	-0.82086700	2.93036100
H	-5.22074700	3.24672000	0.43962400
H	-6.19944600	-0.06973700	3.00230600
H	-3.04119000	1.47240600	-2.69756500
H	-5.45110700	1.12590000	-2.44830300
H	-1.71751000	0.94838200	-6.46682800
H	-1.24629600	-1.98559700	-3.62965500
H	0.12280100	-6.13276600	0.83542800
H	-1.77577600	-1.59672700	4.05211900
H	1.55174000	-1.33406300	-0.42226000
H	-1.16048900	-7.20017800	-0.99800500
H	-4.17732000	-3.07525200	0.95958800
H	1.31026800	3.48055300	-4.75114600
H	2.59290500	-3.50561300	-0.88462600
H	-6.89487100	1.97868000	1.77324500
H	-0.96651200	1.01773500	7.36012500
H	1.72716200	-4.94115000	-2.72790300
H	-0.04248600	2.77189800	-6.71943100
C	6.22170700	-0.00577900	0.61238200
C	5.02522900	0.66367200	0.83903500
C	3.85207200	-0.05504700	1.12398500
C	3.89229200	-1.45997700	1.17102000
C	5.08520900	-2.13844200	0.93703400
C	6.23606400	-1.40198100	0.65702800
H	7.12791500	0.54828700	0.39599800

H	4.98902800	1.74644800	0.78697100
H	2.98514400	-2.01549400	1.38466500
H	5.11487500	-3.22149700	0.97075800
C	2.60473100	0.61514500	1.37456600
C	1.59849500	0.91251700	2.08887600
H	1.32860500	0.98182600	3.13070700
H	-0.43109500	3.15529500	1.28495700
Br	7.87208000	-2.32573500	0.32027800

### TS2-Br

C	1.87976000	3.4566700	0.2117520
C	2.04906000	4.7660070	1.0281020
C	0.88732500	4.9797240	1.9604350
C	0.06784200	3.9967750	2.3543860
C	0.30463900	2.5822390	2.0052000
C	1.24508300	2.2456880	0.8851850
H	2.86521200	3.1753070	-0.181577
H	0.74881100	5.9986340	2.3168630
H	-0.7415690	4.1736660	3.0568070
C	3.37905500	4.8793430	1.7583350
H	4.20199600	4.7987170	1.0404480
H	3.45606300	5.8409130	2.2763910
H	3.47214300	4.0778030	2.4980710
O	2.01516700	5.7904290	0.0098820
C	1.01550900	5.4184000	-0.945594
H	0.03216900	5.8321790	-0.670320
O	-0.1866880	1.7075080	2.7191990
C	1.01280200	3.9135370	-0.920756
C	0.34272200	3.0107980	-1.671882
H	1.29701300	5.8361840	-1.918441
C	-0.6000040	3.3819860	-2.779312
H	-0.5100550	2.7067110	-3.636598
H	-1.6400540	3.3259590	-2.440372
H	-0.4155600	4.4049100	-3.132038
Rh	0.36981400	1.1054130	-0.694354
P	-1.9832900	1.1174170	-0.070846
P	0.44733600	-1.3668060	-0.162005
C	0.47864500	-2.1080420	1.5034610
C	0.66002600	-1.2824340	2.6183330
C	-3.2941040	-3.1034550	-2.424089

C	-1.0381090	-2.1301180	-0.990590	H	0.71678100	-0.2079450	2.4947260
C	-3.2962990	-4.2044080	4.1437700	H	-3.4891660	-4.9009980	4.9545400
C	-2.9399470	-1.9362690	3.3459170	H	1.44843800	-1.1070690	-2.890440
C	0.52735300	-3.2130260	4.0717930	H	-4.6014550	1.5949640	1.2848980
C	-2.8708780	2.6286740	0.4872500	H	-1.3222360	3.9570430	-0.182659
C	2.10497900	-1.8040000	-2.382167	H	0.08326400	-2.8910860	-2.689888
C	-4.1484860	2.5567100	1.0720770	H	-6.8592140	-2.7506870	-0.898319
C	1.85554200	-2.1575630	-1.045034	H	4.53475000	-4.2076370	-0.567974
C	-4.2680870	4.9728740	1.1612740	H	-4.9165130	-1.9539050	0.3720690
C	-2.9012100	0.6840440	-1.610211	H	-6.0399740	0.3077680	-2.879763
C	-2.3082810	3.8877450	0.2508590	H	3.38062800	-2.0329760	-4.095827
C	-2.4408920	-0.1231610	1.2190130	H	-1.8511920	-3.7038520	-3.918982
C	-2.3080650	-2.0333720	-0.422192	H	-3.2351710	-5.7511810	2.6248700
C	-0.8980510	-2.7590190	-2.258132	H	-3.2919520	-2.4706290	5.4092690
C	-5.8621140	-2.8493320	-1.317516	H	0.15924500	-4.1347040	0.8187450
C	-3.4568000	-2.515196	-1.131113	H	0.79859900	-1.1874030	4.7625210
C	3.85087200	-3.5409230	-1.085164	H	0.21606500	-5.1097020	3.0895620
C	-4.7729560	-2.4049710	-0.602301	H	-2.5297090	1.3879320	2.7762200
C	-4.9548760	0.3410880	-2.856442	H	-2.9512630	-0.1741000	4.6010130
C	3.20500500	-2.3199370	-3.063138	H	-5.8235500	3.6471130	1.8578970
C	-1.9868220	-3.2271990	-2.951879	H	-4.8883560	0.8673440	-0.780130
C	-3.1536590	-4.6860100	2.8212390	H	-4.2933820	-3.9871990	-4.124494
C	-3.1870010	-2.8560290	4.3986260	H	2.59239300	-3.3020720	0.6327270
C	0.31919300	-3.4921990	1.6788210	H	-1.0852080	0.4327090	-2.758170
C	0.68025900	-1.8368420	3.8998400	H	-6.5653120	-3.7664430	-3.154489
C	0.35073400	-4.0403740	2.9584760	H	-2.7699390	-4.2075210	0.7804660
C	-2.6077590	0.3338670	2.5577120	H	-2.5420720	6.020478	0.4017960
C	-2.8392220	-0.5435040	3.5852940	H	-2.2435700	-0.1269050	-4.858148
C	-2.7853660	-2.4181610	2.0086330	H	0.53512800	-3.6421290	5.0695720
C	-4.2193010	0.0561760	-4.008604	H	4.95361400	-3.5781460	-2.937825
C	-4.8391400	3.7201360	1.4048280	H	-4.7309300	-0.1950380	-4.933054
C	-4.3014460	0.6548600	-1.665509	H	-4.8081550	5.8778740	1.4242180
C	-4.4362470	-3.5479650	-3.140872	C	5.07829300	-0.5099150	0.6421520
C	-2.5093120	-1.4859170	0.9506530	C	3.82165300	-0.0674860	0.2394000
C	4.08658300	-3.1871890	-2.413489	C	3.64416400	0.5794920	-0.995068
C	2.74319000	-3.0317630	-0.404926	C	4.77337600	0.7849990	-1.815420
C	-2.1716210	0.4078880	-2.776297	C	6.03281700	0.3495460	-1.421903
C	-5.6959780	-3.4247390	-2.600313	C	6.17224000	-0.2994800	-0.193771
C	-2.8963080	-3.8183290	1.7830750	H	5.19802100	-1.0174670	1.5924410
C	-3.0009650	5.0532340	0.5855760	H	2.97101600	-0.2405410	0.8878720
C	-2.8241630	0.0947340	-3.967385	H	4.65303700	1.2911480	-2.768082

H	6.89228900	0.5103590	-2.062803	C	-5.25793700	-0.57895200	-1.13602300
C	2.36529100	1.0851240	-1.428600	C	-5.86047400	1.64833300	1.73553000
C	1.73705400	1.7666990	-2.314438	C	-0.53214300	1.02138500	-3.27022000
H	1.65094800	2.0251250	-3.360407	C	-0.86459200	1.68415600	4.02493100
H	1.98512700	1.5450620	1.2716860	C	-1.29369700	0.63175000	-4.38473000
Br	7.89981500	-0.9132280	0.3500280	C	-1.21158400	0.42101000	3.51918300

**TS1-CI**

C	1.58948800	3.51429900	0.53180900	C	-2.46402800	-0.20399800	-1.45139400
C	1.86651200	4.99021500	0.14461800	C	-1.98494100	-2.05536100	0.20334000
C	0.98532000	5.44544400	-0.98689300	C	-0.32341000	-2.26942700	1.98028600
C	-0.09564500	4.77841300	-1.41369400	C	-2.26736300	-5.39633700	-1.49041600
C	-0.59126000	3.54030900	-0.78379900	C	-1.77452000	-3.43207200	-0.13779900
C	0.17097300	2.97387200	0.38908300	C	-1.39212000	-0.40446200	5.79385300
H	1.92539200	3.36094200	1.56527100	C	-2.47569800	-4.06665300	-1.19941400
H	1.28861600	6.37152600	-1.47189600	C	0.19089000	-3.53569300	-3.29489900
H	-0.69648700	5.14112900	-2.24354600	C	-0.77717400	1.89821900	5.40014500
C	1.80428500	5.96271500	1.31367200	C	-0.08822100	-3.57905700	1.64330000
H	2.51587700	5.65593100	2.08728700	C	-6.21998100	-2.59232900	0.56910300
H	2.05364400	6.97831700	0.98893300	C	-6.65315000	-0.76463800	-0.95101000
H	0.79638700	5.97307400	1.74156300	C	-4.14758700	0.07037200	2.38543700
O	3.23062600	4.95889100	-0.33409500	C	-4.92108000	2.36085100	0.99186200
C	3.40018700	3.75028500	-1.08518100	C	-5.47067300	0.49819600	2.43044000
H	3.13767800	3.90575700	-2.14357500	C	-3.40026200	0.64712200	-2.09957700
O	-1.64282900	3.05000700	-1.19719000	C	-4.75127600	0.46135100	-1.95257800
C	2.47867300	2.75786600	-0.41999000	C	-4.33545300	-1.42929100	-0.44831200
C	2.27914000	1.44754300	-0.66013300	C	1.27004400	-3.97794100	-2.52573300
H	4.45662500	3.46581900	-1.03710300	C	-1.11598700	1.25778100	-5.61793000
C	3.03622000	0.68363100	-1.70644300	C	-0.39818100	-2.29979600	-3.03507500
H	3.92648600	1.23335700	-2.03736900	C	-0.61587600	-5.56714700	0.26684900
H	3.36349100	-0.29850700	-1.35952300	C	-2.92538400	-1.21789900	-0.60712000
H	2.40436800	0.51184300	-2.58482400	C	-1.03576400	0.85144100	6.28839100
Rh	0.44201900	0.90555000	0.35808000	C	-1.48599600	-0.61979100	4.41756100
P	-0.66342300	0.16807700	-1.64421300	C	1.16455500	-1.93930000	-1.23438000
P	-1.43729300	0.28507400	1.69901200	C	-1.32872600	-6.15619300	-0.75324300
C	-3.20199000	0.78209300	1.62816100	C	-4.86112100	-2.43211600	0.41308400
C	-3.59293800	1.92878500	0.93325800	C	0.58302500	2.67746900	-4.65719400
C	-0.82236100	-4.20398300	0.60263700	C	1.75582200	-3.17495500	-1.49397300
C	-1.31144800	-1.50400700	1.29425300	H	-2.87230800	2.45464200	0.32024400
C	-7.12803600	-1.75247500	-0.11835200	H	-8.19706300	-1.88606800	0.01943500

H	-0.65780200	2.50214200	3.34095200	C	1.59967400	0.90891900	2.08710900
H	-2.04470900	-0.14385300	-4.29239600	H	1.32948900	0.97604900	3.12906200
H	0.99372900	2.37159800	-2.57467200	H	-0.43180800	3.15334200	1.28436500
H	0.24843900	-1.81066200	2.77884400	Cl	7.75801700	-2.22712400	0.35482500
H	-2.81869000	-5.86363700	-2.30107600				
H	-1.60348300	-1.22074300	6.47857800	<b>TS2-CI</b>			
H	-3.18472500	-3.49145300	-1.78238100	C	1.87724900	3.47045100	0.25394400
H	-0.20378900	-4.16088400	-4.09032400	C	2.01314900	4.78095800	1.07473500
H	-0.50535500	2.88036900	5.77597400	C	0.82585600	4.98031000	1.97893400
H	0.66109200	-4.15625100	2.17837500	C	0.02019800	3.98396300	2.36808400
H	-6.59851200	-3.36440500	1.23275600	C	0.30381000	2.57259200	2.04105500
H	-7.33756800	-0.10426600	-1.47671000	C	1.24418500	2.25233200	0.91766600
H	-3.85405300	-0.82115600	2.92950600	H	2.87347700	3.19854300	-0.11943500
H	-5.21881600	3.24842600	0.44054400	H	0.65944300	5.99964600	2.32193600
H	-6.19975800	-0.06829100	3.00202700	H	-0.80403600	4.14986900	3.05578700
H	-3.04093600	1.47232300	-2.69833500	C	3.32328200	4.90652800	1.83828400
H	-5.45112800	1.12785500	-2.44905900	H	4.16462800	4.83795600	1.14080100
H	-1.71697500	0.94655100	-6.46752300	H	3.37654900	5.86676200	2.36179100
H	-1.24982500	-1.98815400	-3.62756200	H	3.40666200	4.10318300	2.57722500
H	0.11595800	-6.13594400	0.83415400	O	1.99430100	5.80602000	0.05695400
H	-1.77818200	-1.59782400	4.05192200	C	1.02331500	5.42486300	-0.92419300
H	1.55157400	-1.33528300	-0.42319900	H	0.03050500	5.83397200	-0.67756600
H	-1.16858900	-7.20185400	-0.99928200	O	-0.14340800	1.69206500	2.77735200
H	-4.18083800	-3.07398300	0.95926100	C	1.02957700	3.92042800	-0.89590800
H	1.31145800	3.47777200	-4.75158500	C	0.37998900	3.01013900	-1.65645500
H	2.59071300	-3.50829500	-0.88450200	H	1.32848800	5.84125800	-1.89061800
H	-6.89377100	1.98115200	1.77387000	C	-0.55316800	3.36125500	-2.77835400
H	-0.96376800	1.01547600	7.35958700	H	-0.35650800	4.37222900	-3.15833700
H	1.72273400	-4.94460500	-2.72588100	H	-0.46672800	2.66064500	-3.61559700
H	-0.04124100	2.76942900	-6.72003000	H	-1.59509100	3.32578200	-2.44190700
C	6.22892000	0.01142500	0.61959700	Rh	0.38038100	1.11802100	-0.67072700
C	5.02876600	0.67431200	0.84439500	P	-1.97865000	1.13514000	-0.08395100
C	3.85794900	-0.05066800	1.12373900	P	0.42934200	-1.37996200	-0.17861900
C	3.90353500	-1.45570300	1.16518600	C	0.53067700	-2.14500600	1.47247500
C	5.09943600	-2.12883000	0.93248600	C	0.65978700	-1.32395200	2.59803300
C	6.24749600	-1.38500200	0.65988200	C	-3.34636100	-3.15789200	-2.33748400
H	7.13614800	0.56636400	0.40834500	C	-1.06118500	-2.18172300	-0.95548200
H	4.98750900	1.75704400	0.79621600	C	-3.27059400	-4.12193800	4.21680700
H	2.99768300	-2.01498600	1.37421000	C	-2.92957100	-1.86523300	3.38096600
H	5.13812400	-3.21197400	0.96129700	C	0.60124800	-3.27579600	4.02782000
C	2.60811400	0.61396900	1.37488900				



C	-2.88065400	2.64596500	0.44367900	H	-1.31852900	3.97295500	-0.19620300
C	1.95494900	-1.72836400	-2.49650400	H	0.03686400	-3.05954300	-2.61349500
C	-4.16705100	2.57279500	1.00852900	H	-6.89846300	-2.58727400	-0.84636700
C	1.80963100	-2.10658300	-1.14963600	H	4.59590800	-4.04561600	-0.86966900
C	-4.28899300	4.98866400	1.09380400	H	-4.92605000	-1.81958600	0.39951500
C	-2.85084600	0.66906600	-1.63748800	H	-5.92776000	0.43499200	-3.07917800
C	-2.31321800	3.90467700	0.21731800	H	3.12587300	-1.88959600	-4.29091400
C	-2.43800000	-0.08684500	1.22228100	H	-1.92357900	-3.88911500	-3.79326000
C	-2.32409000	-2.03329000	-0.38553200	H	-3.18258200	-5.69537700	2.72673100
C	-0.93993100	-2.88288600	-2.18715500	H	-3.29140400	-2.36609500	5.45124700
C	-5.90492400	-2.74643400	-1.25529300	H	0.30811300	-4.17569000	0.76043000
C	-3.48894100	-2.50577500	-1.07299300	H	0.76958500	-1.24815800	4.74463400
C	3.85304500	-3.40317400	-1.33330700	H	0.38761300	-5.17366800	3.02183200
C	-4.79996700	-2.31919700	-0.55371400	H	-2.53508100	1.45089000	2.75370400
C	-4.84662700	0.39059500	-2.98772800	H	-2.95757200	-0.08055900	4.60388300
C	3.03021800	-2.18998100	-3.25145600	H	-5.85585400	3.66328500	1.76535500
C	-2.04341200	-3.35672400	-2.85352400	H	-4.86373300	1.05815700	-0.95067800
C	-3.11393300	-4.62598900	2.90414800	H	-4.37678800	-4.07645000	-4.00016300
C	-3.17642300	-2.76819400	4.44820800	H	2.69142400	-3.23909700	0.46283100
C	0.43141300	-3.53683100	1.62942200	H	-0.99873500	0.16289500	-2.63236600
C	0.69201800	-1.89203400	3.87319200	H	-6.64036100	-3.71411600	-3.05329800
C	0.47396800	-4.09768200	2.90359900	H	-2.72762600	-4.17952400	0.85614300
C	-2.60600800	0.39241600	2.55349600	H	-2.55052200	6.03745900	0.36504000
C	-2.83896800	-0.46763900	3.59551900	H	-2.06537500	-0.41891100	-4.77376600
C	-2.76568800	-2.36944100	2.05293500	H	0.61671400	-3.71553000	5.02087400
C	-4.06802500	-0.02362200	-4.07000000	H	4.83642300	-3.37089500	-3.25148300
C	-4.86399900	3.73599300	1.32882400	H	-4.54157100	-0.29930900	-5.00765000
C	-4.24310500	0.73950300	-1.77951500	H	-4.83357700	5.89361500	1.34743800
C	-4.50394300	-3.58756600	-3.03798700	C	5.02995700	-0.57050400	0.73706900
C	-2.50255400	-1.45355400	0.97727200	C	3.79176200	-0.09615500	0.31482600
C	3.98863100	-3.02345100	-2.66832900	C	3.64213900	0.53034600	-0.93378600
C	2.76909600	-2.95008400	-0.57834800	C	4.77970400	0.67049800	-1.75573400
C	-2.07723900	0.25644300	-2.73270100	C	6.02129500	0.19884600	-1.34694100
C	-5.75900500	-3.38561400	-2.51019600	C	6.13252800	-0.42003300	-0.10048500
C	-2.86170900	-3.77438400	1.85151800	H	5.13037500	-1.05836600	1.70022800
C	-3.01207500	5.06982900	0.53990400	H	2.93180200	-0.23001000	0.95957700
C	-2.67872100	-0.08743400	-3.94111800	H	4.68044700	1.15438300	-2.72216300
H	0.66920400	-0.24573800	2.48753800	H	6.88963000	0.30661000	-1.98746900
H	-3.46248400	-4.80584700	5.03854000	C	2.38248200	1.07429200	-1.37911600
H	1.22855400	-1.06870600	-2.95832800	C	1.78524300	1.77395900	-2.27260700
H	-4.62103200	1.60929200	1.21327000	H	1.72260300	2.03492600	-3.31965500

H	1.98648600	1.55325200	1.30076200	C	0.5028610	-0.5143100	-4.419307
Cl	7.70114200	-1.02691700	0.42034400	C	0.7793950	-0.7458930	3.4875480
<b>TS1-F</b>				C	-1.181224	-1.5564880	-5.811194
C	-3.058893	-2.5071110	0.4631630	C	0.0467910	1.79114100	-1.860082
C	-3.852753	-3.7532970	-0.006799	C	-1.559161	-1.2940020	-3.437318
C	-3.213105	-4.4038770	-1.203043	C	1.9945770	-0.3481940	-1.526210
C	-1.972359	-4.1341210	-1.631256	C	2.2807420	1.45618700	0.2206080
C	-1.054829	-3.2066750	-0.942235	C	0.8944360	2.16594800	2.1007790
C	-1.542814	-2.4946340	0.2949110	C	3.6868280	4.55034900	-1.379523
H	-3.299868	-2.3240910	1.5181180	C	2.5762450	2.83133600	-0.059065
H	-3.8361110	-5.1214600	-1.733915	C	1.3538480	-0.1791080	5.7769720
H	-1.555429	-4.6214130	-2.508714	C	3.4031100	3.22294800	-1.147418
C	-4.122260	-4.7704000	1.0930980	C	0.5723800	3.83540100	-3.059445
H	-4.663011	-4.2897610	1.9151960	C	-0.074281	-2.0760160	5.3353070
H	-4.724854	-5.6025830	0.7144860	C	1.1553240	3.48680200	1.8344020
H	-3.177690	-5.1714100	1.4750610	C	6.4399990	0.42186600	0.3535690
O	-5.124301	-3.2029040	-0.421802	C	6.1198600	-1.3537530	-1.253242
C	-4.866352	-1.9556800	-1.078520	C	3.6068160	-1.3860380	2.2091990
H	-4.700630	-2.1064590	-2.157076	C	3.4691560	-3.7337120	0.7080380
O	0.0965400	-3.0959780	-1.365460	C	4.6963780	-2.2502780	2.1687680
C	-3.637089	-1.4124170	-0.394184	C	2.5329770	-1.4404940	-2.260035
C	-2.986399	-0.2422130	-0.552082	C	3.8642160	-1.7605610	-2.183926
H	-5.749584	-1.3191100	-0.958102	C	4.2201640	0.06610200	-0.587426
C	-3.438033	0.82353600	-1.506726	C	-0.198221	4.57560600	-2.159479
H	-4.487498	0.68659700	-1.797066	C	0.0691050	-0.9494560	-5.671096
H	-3.334706	1.82921000	-1.094302	C	0.6951390	2.45477600	-2.911634
H	-2.833247	0.79542400	-2.420045	C	2.3191010	5.21593000	0.4994570
Rh	-1.057576	-0.4663160	0.3989240	C	2.8229330	0.38242300	-0.671217
P	0.1760590	-0.0382760	-1.628495	C	0.5880900	-1.2483960	6.2449250
P	0.9695080	-0.6013720	1.6626910	C	1.4555360	0.06872100	4.4068440
C	2.4409170	-1.6857230	1.4843310	C	-0.721446	2.54520000	-0.962798
C	2.3752330	-2.8638500	0.7364220	C	3.1425040	5.55860200	-0.549446
C	2.0190880	3.85589800	0.7715750	C	5.1087840	0.76621900	0.2750770
C	1.4930820	1.13048600	1.3254750	C	-1.993425	-1.7289870	-4.689937
C	6.9545150	-0.6478460	-0.416661	C	-0.846975	3.92533900	-1.109664
C	4.7447100	-1.0181580	-1.359574	H	1.4916410	-3.0779710	0.1488020
C	4.6290470	-3.4295920	1.4191800	H	8.0051400	-0.9123180	-0.339893
C	-0.309837	-0.6789510	-3.284964	H	-0.498771	-2.4769770	3.2682920
C	0.0209020	-1.8268900	3.9663630	H	1.4865990	-0.0684580	-4.330329
				H	-2.193707	-1.4395270	-2.573953
				H	0.2268480	1.90565400	2.9144970

H	4.3247020	4.82720900	-2.213795				
H	1.8801330	0.46315700	6.4772550	<b>TS2-F</b>			
H	3.8127040	2.46182000	-1.800511				
H	1.0908560	4.33545600	-3.872240	C	1.87694200	3.47101700	0.25797600
H	-0.666087	-2.9151510	5.6893630	C	2.00714100	4.78100900	1.08054200
H	0.7034690	4.26746900	2.4404800	C	0.81688300	4.97613700	1.98196800
H	7.0997310	0.97073600	1.0194050	C	0.01437100	3.97665700	2.36943100
H	6.4968530	-2.1850360	-1.842910	C	0.30648700	2.56641300	2.04433800
H	3.6676850	-0.4736560	2.7932050	C	1.24661300	2.25040200	0.92008800
H	3.4140110	-4.6423620	0.1149680	H	2.87454400	3.20249300	-0.11390400
H	5.6008220	-2.0010990	2.7156690	H	0.64562000	5.99497000	2.32409900
H	1.8759960	-2.0463190	-2.868040	H	-0.81205300	4.13928100	3.05529700
H	4.2559580	-2.6039170	-2.745951	C	3.31505300	4.90935400	1.84743600
H	0.7126950	-0.8171450	-6.535991	H	4.15826700	4.84433400	1.15185800
H	1.3121610	1.90426700	-3.611383	H	3.36429400	5.86890700	2.37260900
H	1.8844530	5.98064400	1.1376030	H	3.39902800	4.10507600	2.58530300
H	2.0683530	0.89383800	4.0614630	O	1.98789500	5.80722500	0.06395500
H	-1.219376	2.05779700	-0.133381	C	1.01931300	5.42474000	-0.91912400
H	3.3701190	6.60191800	-0.747646	H	0.02532500	5.83166400	-0.67364900
H	4.7299230	1.57753400	0.884296	O	-0.13352300	1.68458500	2.78360500
H	-2.963845	-2.2078130	-4.784204	C	1.02978600	3.92017200	-0.89302900
H	-1.444527	4.48888700	-0.399147	C	0.38501400	3.00956700	-1.65704900
H	5.4808370	-4.1031160	1.3896590	H	1.32510100	5.84296800	-1.88459200
H	0.5117670	-1.4392350	7.3113980	C	-0.54713100	3.36034000	-2.78004300
H	-0.285588	5.65208200	-2.273504	H	-0.35474300	4.37373100	-3.15578100
H	-1.516008	-1.8968760	-6.786865	H	-0.45486700	2.66336300	-3.61970100
C	-6.134240	2.42255000	1.0147950	H	-1.58977000	3.31832100	-2.44656200
C	-5.259036	1.35021900	1.1265760	Rh	0.38448400	1.11755800	-0.67071200
C	-3.896857	1.57021100	1.4011220	P	-1.97688900	1.13585100	-0.08796200
C	-3.418575	2.88699700	1.5455020	P	0.42967800	-1.37966500	-0.18182100
C	-4.286482	3.96777600	1.4259350	C	0.53593500	-2.14984100	1.46682700
C	-5.628082	3.71214000	1.1616100	C	0.66369700	-1.33168100	2.59460500
H	-7.189492	2.27788800	0.8103990	C	-3.35259400	-3.15924500	-2.32945900
H	-5.619133	0.33547900	0.9968780	C	-1.06323600	-2.18201000	-0.95465500
H	-2.365945	3.05334200	1.7483990	C	-3.26491500	-4.11158400	4.22628300
H	-3.940813	4.99022700	1.5324040	C	-2.92505200	-1.85667300	3.38508200
C	-2.976546	0.47741200	1.5400880	C	0.61042400	-3.28758100	4.01906200
C	-2.115542	-0.2184540	2.1647360	C	-2.88111500	2.64637400	0.43739200
H	-1.865577	-0.4530560	3.1877240	C	1.94236800	-1.72563200	-2.50818800
H	-1.025071	-2.9381730	1.1505540	C	-4.16794100	2.57277600	1.00121900
F	-6.473336	4.75420600	1.0406090	C	1.80513600	-2.10499500	-1.16080000

C	-4.29087900	4.98860100	1.08627400	H	-4.92443600	-1.81618200	0.40970900
C	-2.84913800	0.66629300	-1.64068900	H	-5.92510400	0.42597200	-3.08347400
C	-2.31389000	3.90527300	0.21171400	H	3.10042000	-1.88799800	-4.31079000
C	-2.43556500	-0.08313900	1.22163100	H	-1.93377700	-3.89383700	-3.78740200
C	-2.32459100	-2.03271300	-0.38172400	H	-3.17622400	-5.68854500	2.73993300
C	-0.94562300	-2.88558600	-2.18532800	H	-3.28635500	-2.35288100	5.45662600
C	-5.90821100	-2.74352200	-1.24188600	H	0.31704700	-4.17898300	0.74928900
C	-3.49151500	-2.50544500	-1.06547800	H	0.77433800	-1.26154600	4.74136700
C	3.84331800	-3.40735100	-1.36004400	H	0.40051300	-5.18312600	3.00789700
C	-4.80111500	-2.31692100	-0.54328900	H	-2.53226500	1.45814100	2.74958700
C	-4.84393300	0.38337400	-2.99153400	H	-2.95333300	-0.06897800	4.60357800
C	3.01111200	-2.18924400	-3.27100300	H	-5.85779200	3.66267300	1.75666300
C	-2.05100500	-3.35994900	-2.84817900	H	-4.86297300	1.05263100	-0.95506200
C	-3.10818100	-4.61869600	2.91479300	H	-4.38792300	-4.07855300	-3.98868500
C	-3.17136400	-2.75724400	4.45448900	H	2.69458500	-3.24170700	0.44433500
C	0.43965400	-3.54230100	1.61999500	H	-0.99569700	0.16332200	-2.63401600
C	0.69781200	-1.90320300	3.86819000	H	-6.64889800	-3.71224100	-3.03719800
C	0.48433200	-4.10659900	2.89260800	H	-2.72259900	-4.17670700	0.86559900
C	-2.60259400	0.39913200	2.55191300	H	-2.55207000	6.03801800	0.35922600
C	-2.83498800	-0.45848700	3.59611000	H	-2.06061100	-0.42303500	-4.77579600
C	-2.76136200	-2.36395600	2.05823000	H	0.62741900	-3.73005700	5.01087900
C	-4.06421700	-0.03048700	-4.07315600	H	4.81267300	-3.37709900	-3.28548300
C	-4.86562700	3.73570600	1.32087000	H	-4.53695100	-0.30760900	-5.01080400
C	-4.24146700	0.73429700	-1.78335800	H	-4.83600500	5.89336100	1.33945500
C	-4.51228700	-3.58841300	-3.02678300	C	5.03151000	-0.56648100	0.74636800
C	-2.49988100	-1.45041700	0.98022700	C	3.79231800	-0.09780800	0.32051800
C	3.97065400	-3.02685300	-2.69563400	C	3.64436600	0.52680200	-0.93038200
C	2.76619800	-2.95149400	-0.59693300	C	4.78289400	0.66790600	-1.75256200
C	-2.07445600	0.25392600	-2.73524800	C	6.02550900	0.20233000	-1.33947400
C	-5.76591700	-3.38425800	-2.49642100	C	6.12640200	-0.40880200	-0.09305600
C	-2.85668000	-3.76941500	1.86011100	H	5.15094600	-1.05461900	1.70763300
C	-3.01346900	5.07021400	0.53357900	H	2.93018900	-0.23211000	0.96211500
C	-2.67487200	-0.09198100	-3.94363800	H	4.68167300	1.14985100	-2.71973300
H	0.67120900	-0.25310300	2.48713800	H	6.90613500	0.30452100	-1.96467400
H	-3.45638100	-4.79364500	5.04965700	C	2.38513300	1.07218500	-1.37730300
H	1.21458900	-1.06347200	-2.96412500	C	1.79175900	1.77487700	-2.27156300
H	-4.62148800	1.60907300	1.20606400	H	1.73729700	2.04520900	-3.31654200
H	-1.31870500	3.97364200	-0.20047800	H	1.99052600	1.55191300	1.30085900
H	0.02991100	-3.06337100	-2.61400800	F	7.33318600	-0.86275600	0.31354600
H	-6.90062000	-2.58272400	-0.83085000				
H	4.58672300	-4.05357000	-0.90250900				

**TS1-CN**

C	-2.75765600	-2.80718500	0.45426000	C	-1.35164300	-1.46839800	-3.45254900
C	-3.43182700	-4.12540700	-0.00783900	C	2.09522100	-0.22393500	-1.52289700
C	-2.73708700	-4.71789400	-1.20323000	C	2.22009600	1.60013000	0.21827100
C	-1.52934500	-4.33260400	-1.63741700	C	0.74553400	2.19713500	2.06974200
C	-0.70179800	-3.32019400	-0.95499000	C	3.39228900	4.79406000	-1.37271500
C	-1.25112900	-2.65092200	0.28061000	C	2.40462600	2.99371000	-0.06385600
H	-3.01375900	-2.64254400	1.50868400	C	1.37029400	-0.06309600	5.77049300
H	-3.29105000	-5.49353400	-1.72883500	C	3.21687800	3.44854100	-1.13843600
H	-1.07041400	-4.78163100	-2.51425600	C	0.35139300	3.83514800	-3.05444700
C	-3.60376500	-5.15751900	1.09730900	C	0.16486800	-2.10912200	5.33126400
H	-4.18908600	-4.72612300	1.91610000	C	0.89691300	3.53418000	1.79855900
H	-4.12366500	-6.04544900	0.72290700	C	6.44560300	0.89104800	0.40509100
H	-2.62563800	-5.46438700	1.48200400	C	6.28292900	-0.90608500	-1.20230200
O	-4.74967300	-3.69773900	-0.42205000	C	3.75141700	-1.14498200	2.23825900
C	-4.60791900	-2.43948200	-1.09224200	C	3.81336800	-3.48102700	0.71288900
H	-4.42562600	-2.58560000	-2.16864000	C	4.90195000	-1.92658300	2.20964100
O	0.43365900	-3.10454500	-1.38066800	C	2.72534400	-1.26795400	-2.25398000
C	-3.43482700	-1.77878800	-0.41187300	C	4.07688200	-1.48290400	-2.16359200
C	-2.89232200	-0.55792200	-0.58283200	C	4.27252200	0.36465100	-0.56363600
H	-5.54660000	-1.88664800	-0.98048500	C	-0.51546300	4.49927500	-2.18283600
C	-3.43134900	0.45948500	-1.54463100	C	0.24538100	-0.96504400	-5.67890100
H	-4.46399000	0.23127100	-1.83723900	C	0.59759200	2.47210300	-2.89933800
H	-3.41603100	1.47357300	-1.14079500	C	1.93490200	5.35004200	0.47449700
H	-2.82219800	0.47838300	-2.45520000	C	2.85629000	0.57085400	-0.66261500
Rh	-0.95627500	-0.58313600	0.37822900	C	0.72061000	-1.20559600	6.24030200
P	0.25850100	-0.06044300	-1.63573700	C	1.46047700	0.18362400	4.39912000
P	1.07442200	-0.55515000	1.65571100	C	-0.88415200	2.42894300	-0.99703400
C	2.62450300	-1.52234900	1.48853200	C	2.74731700	5.75629100	-0.56030400
C	2.65880300	-2.69323500	0.72808900	C	5.09320200	1.13254200	0.30827100
C	1.74638100	3.97075900	0.74975900	C	-1.73963500	-1.93576400	-4.70865500
C	1.44452200	1.21361300	1.31143400	C	-1.13422500	3.79112900	-1.15252400
C	7.04972000	-0.13777800	-0.35583700	H	1.80351700	-2.96374700	0.12242600
C	4.88780700	-0.67645500	-1.32796600	H	8.11615200	-0.32208300	-0.26417200
C	4.93453700	-3.10018300	1.44848800	H	-0.18598100	-2.57269900	3.26380400
C	-0.16491200	-0.74153900	-3.29312900	H	1.57101100	0.03659800	-4.32885200
C	0.24902900	-1.86268900	3.96135600	H	-1.97435500	-1.67671400	-2.59337600
C	0.63316900	-0.49789400	-4.42364900	H	0.08849600	1.88586900	2.87407900
C	0.88841700	-0.70779500	3.48058800	H	4.02178400	5.12025300	-2.19544600
C	-0.94349800	-1.68352300	-5.82629000	H	1.81473100	0.63880300	6.47021300
C	-0.02172100	1.75050500	-1.86858700	H	3.70292000	2.72176000	-1.77794300
				H	0.84848700	4.38207300	-3.85014700

H	-0.33532500	-3.00529200	5.68677200	C	3.22321500	2.33622900	0.32532900
H	0.36894000	4.27653200	2.39100500	C	3.87293900	3.47740600	1.15147700
H	7.05305400	1.48965200	1.07769700	C	2.87529300	4.11104900	2.08294800
H	6.73072500	-1.70644900	-1.78514800	C	1.73079300	3.52244200	2.45381700
H	3.73205000	-0.23924500	2.83502000	C	1.38252000	2.14103200	2.06966300
H	3.83486000	-4.38554700	0.11145100	C	2.16509900	1.45983000	0.98209100
H	5.77552800	-1.61871500	2.77647300	H	4.02876500	1.69893600	-0.06247300
H	2.12465400	-1.92160100	-2.87051000	H	3.14088200	5.09750000	2.45843900
H	4.53951200	-2.29189200	-2.72225300	H	1.04542300	3.99479900	3.15169500
H	0.87658700	-0.76935400	-6.54089100	C	5.14166900	3.07093400	1.88681200
H	1.28885100	1.98189700	-3.57406300	H	5.87593500	2.68709800	1.17080400
H	1.42455700	6.07837600	1.09898000	H	5.57622100	3.92714400	2.41298600
H	1.98376000	1.06807200	4.05384500	H	4.91697000	2.28945700	2.61977000
H	-1.36073600	1.89571600	-0.18386300	O	4.23638600	4.44334700	0.14021100
H	2.88994100	6.81415100	-0.76074100	C	3.17938000	4.48132900	-0.82566200
H	4.64421600	1.91382900	0.90911800	H	2.42119300	5.23303700	-0.55325900
H	-2.66176600	-2.50111000	-4.80818400	O	0.52950300	1.54082400	2.72384500
H	-1.80560700	4.29566600	-0.46398200	C	2.60737400	3.08947000	-0.81210700
H	5.83352900	-3.70965800	1.43001000	C	1.65050000	2.50954500	-1.57157400
H	0.65231500	-1.39443100	7.30764100	H	3.60738300	4.76742700	-1.79247100
H	-0.70035600	5.56261300	-2.30344400	C	0.92651800	3.20947000	-2.68393300
H	-1.24268600	-2.04828400	-6.80469500	H	1.49287200	4.08096700	-3.03696700
C	-6.21458300	1.84577100	0.96231600	H	0.75265700	2.54944600	-3.53951800
C	-5.25644800	0.84956400	1.07876300	H	-0.05600400	3.56056800	-2.35104200
C	-3.92134100	1.18422100	1.35896500	Rh	0.97923700	0.71342900	-0.61757800
C	-3.55197000	2.53266500	1.51263600	P	-1.23804000	1.57946400	-0.08020900
C	-4.50405200	3.53668300	1.38727800	P	0.14614100	-1.62470600	-0.06657300
C	-5.83747000	3.19284000	1.10989100	C	-0.19897500	-2.28379600	1.59798700
H	-7.24832600	1.59521900	0.75154500	C	0.22195000	-1.56751400	2.72353400
H	-5.52843800	-0.19143200	0.94540200	C	-3.81292100	-1.91404700	-2.59210700
H	-2.51767900	2.78258300	1.72251200	C	-1.45745200	-1.80965900	-0.99922300
H	-4.22534200	4.57856600	1.50002300	C	-4.63100700	-2.91405300	3.93157600
C	-2.90820700	0.16722600	1.50371100	C	-3.42666400	-0.93009600	3.20938000
C	-2.01888000	-0.44291400	2.17027700	C	-0.69018000	-3.28751600	4.16105200
H	-1.74613600	-0.67322100	3.18701800	C	-1.53022200	3.30576500	0.48534700
H	-0.69017200	-3.03636700	1.13693300	C	1.67407100	-2.70990500	-2.16026800
C	-6.82117500	4.22349400	0.97325300	C	-2.77321300	3.70244000	1.01201400
N	-7.61955600	5.06182100	0.86236900	C	1.22676300	-2.89849400	-0.84097700
				C	-1.99334400	5.98633300	1.19787600
				C	-2.17385900	1.51563600	-1.66649700
				C	-0.52831200	4.27005000	0.32784100

**TS2-CN**

C	-2.17700600	0.58195200	1.15816000	H	-5.14982700	2.35192700	-3.09752300
C	-2.64038300	-1.24839500	-0.51659200	H	2.88857500	-3.44939000	-3.77087100
C	-1.47195500	-2.46261100	-2.26270600	H	-2.59194400	-3.01945700	-3.99337400
C	-6.18179000	-0.73502300	-1.65304200	H	-5.05239900	-4.36943300	2.38016200
C	-3.83543900	-1.28801700	-1.30688100	H	-4.06632400	-1.30688900	5.23785200
C	2.58329600	-4.90960200	-0.71605900	H	-1.21202700	-4.05830700	0.88977400
C	-5.05375900	-0.70143400	-0.86456100	H	0.28328600	-1.49897400	4.87267500
C	-4.13826000	1.96527300	-3.01797000	H	-1.63700900	-4.94746000	3.15736400
C	2.55398700	-3.61437100	-2.75089200	H	-1.78333700	2.00815300	2.74764300
C	-2.60790800	-2.51132000	-3.03297500	H	-2.85797400	0.70393500	4.50804000
C	-4.59823500	-3.40916400	2.60682600	H	-3.96537400	5.31965200	1.77079100
C	-4.05213300	-1.69988800	4.22480000	H	-3.97572500	2.46706900	-0.94200200
C	-0.87002000	-3.50693100	1.75989500	H	-4.95197100	-2.40388400	-4.36220000
C	-0.02751900	-2.07000200	4.00240500	H	1.38669400	-4.16979900	0.89945600
C	-1.10840600	-4.00683900	3.03730500	H	-0.54594400	0.55483600	-2.71897200
C	-2.23659300	1.06080200	2.49848700	H	-7.04944400	-1.36607200	-3.53953300
C	-2.83350000	0.32588900	3.48966600	H	-3.95029200	-3.09615500	0.60133800
C	-3.38179400	-1.42995500	1.87045200	H	0.03808300	6.33150000	0.55957900
C	-3.51561000	1.39595200	-4.13030100	H	-1.72482900	0.44798300	-4.87521000
C	-3.00073700	5.03141800	1.36335600	H	-0.89016900	-3.67377700	5.15632000
C	-3.47253500	2.02694200	-1.79421500	H	3.71375100	-5.41381700	-2.48202900
C	-4.98987000	-1.92776100	-3.38616900	H	-4.03996000	1.34155700	-5.07972000
C	-2.72124100	-0.66036200	0.85221800	H	-2.17236900	7.02105600	1.47540200
C	3.01641800	-4.71607800	-2.02784200	C	4.88450800	-2.43358000	0.70470000
C	1.69453400	-4.00928600	-0.12610000	C	3.84420000	-1.60205300	0.31698800
C	-1.55238400	0.95722600	-2.79361800	C	3.88990200	-0.91674000	-0.91071900
C	-6.15255400	-1.35168000	-2.92714900	C	5.02768000	-1.07162600	-1.73481900
C	-3.98268600	-2.69166200	1.60512100	C	6.07346700	-1.89541000	-1.35282800
C	-0.75675100	5.60138700	0.68206600	C	6.00565400	-2.58663500	-0.12814700
C	-2.21706400	0.89528900	-4.01659300	H	4.83474500	-2.96801200	1.64705000
H	0.68471600	-0.59543100	2.60511600	H	2.98368600	-1.49008300	0.96425100
H	-5.11089300	-3.49487400	4.71393600	H	5.07548800	-0.53592400	-2.67722000
H	1.35059900	-1.84360500	-2.72549600	H	6.94160000	-2.01343800	-1.99235600
H	-3.56130200	2.97413100	1.16683600	C	2.84588700	-0.02277200	-1.33554000
H	0.43672500	3.98006600	-0.05900700	C	2.46561900	0.82689000	-2.21789800
H	-0.58011800	-2.95043100	-2.62807100	H	2.43629300	1.07827500	-3.26902000
H	-7.10073800	-0.27693400	-1.29909400	H	2.57487400	0.53738900	1.39513100
H	2.94151100	-5.75941300	-0.14235500	C	7.07415800	-3.44870300	0.26667500
H	-5.08630900	-0.21308500	0.10194500	N	7.94262700	-4.15404500	0.58776400
<b>TS1-COOMe</b>				C	1.5243190	3.56229900	0.6171070
				C	1.7653140	5.05155100	0.2567480

C	0.8898960	5.49853100	-0.882553	C	-0.246225	-2.3065980	1.9494860
C	-0.166750	4.80965100	-1.334898	C	-2.024220	-5.4114790	-1.629705
C	-0.640191	3.55229100	-0.727097	C	-1.615547	-3.4635240	-0.226849
C	0.1231730	2.98646700	0.4453230	C	-1.441220	-0.5226130	5.7750800
H	1.8502310	3.40135200	1.6527180	C	-2.274670	-4.0939610	-1.317452
H	1.1766030	6.43844500	-1.350759	C	0.3930640	-3.4221790	-3.383475
H	-0.764342	5.16790400	-2.168981	C	-0.886958	1.80217600	5.4237630
C	1.6559150	6.00372400	1.4389970	C	0.0312250	-3.6027840	1.5922490
H	2.3634040	5.70570100	2.2197390	C	-6.089048	-2.7888690	0.4522560
H	1.8813370	7.03078300	1.1334240	C	-6.571153	-0.9432810	-1.030692
H	0.6412330	5.97866800	1.8497670	C	-4.143982	-0.0830600	2.3346660
O	3.1367000	5.06625400	-0.199936	C	-4.958271	2.21432900	0.9754170
C	3.3521210	3.87575300	-0.967826	C	-5.478132	0.30995800	2.3695700
H	3.1028410	4.04150100	-2.027810	C	-3.359445	0.60332000	-2.118295
O	-1.676447	3.04365600	-1.156820	C	-4.704405	0.36789900	-1.988298
C	2.4472600	2.84742900	-0.334540	C	-4.236397	-1.5414230	-0.523037
C	2.2845070	1.53821500	-0.603876	C	1.4610750	-3.8581610	-2.595264
H	4.4151540	3.62009200	-0.905947	C	-1.058940	1.36021900	-5.603488
C	3.0700790	0.81226000	-1.655891	C	-0.236210	-2.2096000	-3.107725
H	3.9575550	1.38306600	-1.957340	C	-0.410990	-5.5752130	0.1637290
H	3.4052680	-0.1742250	-1.330028	C	-2.832978	-1.2785930	-0.664374
H	2.4542970	0.65535100	-2.548456	C	-1.133228	0.73663100	6.2929690
Rh	0.4501820	0.92706600	0.3811610	C	-1.498977	-0.7225380	4.3944550
P	-0.612406	0.20623500	-1.648618	C	1.2638290	-1.8600370	-1.253936
P	-1.429125	0.22083700	1.6902080	C	-1.083966	-6.1615890	-0.884615
C	-3.207253	0.66710100	1.6033180	C	-4.735078	-2.5803030	0.3113450
C	-3.618807	1.81727900	0.9262310	C	0.5962190	2.80294800	-4.600673
C	-0.660310	-4.2246890	0.5207320	C	1.8959180	-3.0716070	-1.528665
C	-1.237866	-1.5551740	1.2543320	H	-2.904224	2.37481100	0.3344060
C	-7.019332	-1.9647160	-0.22427	H	-8.084366	-2.1366830	-0.098601
C	-5.181611	-0.7072680	-1.199677	H	-0.742945	2.43735800	3.3760500
C	-5.888591	1.46328700	1.6918690	H	-1.964784	-0.0884570	-4.311840
C	-0.492876	1.09711600	-3.254511	H	0.9926220	2.47077700	-2.518894
C	-0.938441	1.60394500	4.0444530	H	0.2921540	-1.8495450	2.7719180
C	-1.234158	0.70876400	-4.383164	H	-2.543688	-5.8764970	-2.462413
C	-1.236073	0.33755200	3.5154220	H	-1.643607	-1.3534590	6.4448190
C	-0.142219	2.40825900	-5.716848	H	-2.984897	-3.5252680	-1.905488
C	0.1940520	-1.4106530	-2.038578	H	0.0389900	-4.0342650	-4.207763
C	0.4200310	2.15213400	-3.379200	H	-0.653472	2.78706400	5.8177260
C	-2.400304	-0.2300020	-1.480746	H	0.7813950	-4.1718290	2.1348730
C	-1.873797	-2.1017350	0.1390860	H	-6.446652	-3.5877960	1.0954010



				<b>TS2-COOMe</b>			
H	-7.273047	-0.2941240	-1.547221				
H	-3.834118	-0.9756810	2.8675460				
H	-5.271249	3.10517300	0.4379690	C	2.2656230	3.15816900	0.2660340
H	-6.199668	-0.2856860	2.9207460	C	2.6221170	4.40305100	1.1204770
H	-3.023456	1.45411400	-2.694342	C	1.5319770	4.71556500	2.1103850
H	-5.422647	1.02130200	-2.475853	C	0.6129310	3.82467000	2.5046410
H	-1.643074	1.04929700	-6.464852	C	0.6481880	2.41062800	2.0846280
H	-1.075265	-1.9009470	-3.718906	C	1.5105610	2.00990300	0.9229210
H	0.3213070	-6.1367650	0.7376220	H	3.1942770	2.77059500	-0.173850
H	-1.755619	-1.7034280	4.0104030	H	1.5348550	5.72742300	2.5109970
H	1.6081380	-1.2697900	-0.414013	H	-0.140029	4.07072700	3.2477760
H	-0.891420	-7.1978930	-1.146476	C	3.9820010	4.32416000	1.7995760
H	-4.038453	-3.2112100	0.8495000	H	4.7624090	4.17509300	1.0460630
H	1.3065290	3.62151600	-4.673874	H	4.1944560	5.24628600	2.3504540
H	2.7215040	-3.3983660	-0.903248	H	4.0020200	3.48615800	2.5037380
H	-6.930537	1.76879600	1.7228620	O	2.6760750	5.46513700	0.1424570
H	-1.089771	0.88887500	7.3674080	C	1.6139020	5.25125300	-0.794292
H	1.9445490	-4.8070350	-2.808210	H	0.6951450	5.77012400	-0.476175
H	-0.008828	2.91520200	-6.668191	O	0.0560030	1.57287300	2.7658590
C	6.2189270	0.09242100	0.7160580	C	1.4281390	3.75840500	-0.820927
C	5.0142690	0.74986000	0.9188970	C	0.6317530	2.96956600	-1.578639
C	3.8465070	0.00987800	1.1712990	H	1.9186970	5.66821100	-1.760489
C	3.9029110	-1.3952270	1.2082680	C	-0.303664	3.48240100	-2.633977
C	5.1115090	-2.0503740	0.9966710	H	0.0064210	4.47186900	-2.994286
C	6.2740840	-1.3088850	0.7476340	H	-0.354995	2.80890800	-3.495397
H	7.1288180	0.65014800	0.5245840	H	-1.321451	3.57186800	-2.239359
H	4.9598870	1.83216900	0.8768980	Rh	0.4589520	1.04648500	-0.657708
H	2.9970630	-1.9609330	1.3990010	P	-1.861164	1.30348300	0.0418360
H	5.1539360	-3.1327090	1.0237610	P	0.2637580	-1.4465960	-0.240123
C	2.5837060	0.66064400	1.4137090	C	0.2415120	-2.2693010	1.3860150
C	1.5760360	0.93255400	2.1349190	C	0.5359730	-1.5269550	2.5347530
H	1.2899730	0.98244500	3.1729860	C	-3.692525	-2.6187220	-2.498418
H	-0.496239	3.12984500	1.3354950	C	-1.312554	-1.9987410	-1.067032
C	7.5937890	-1.9607410	0.5088570	C	-3.723269	-4.0676930	3.9766140
O	8.6220570	-1.3504650	0.2754870	C	-3.106842	-1.8144970	3.3047470
O	7.5242650	-3.3001200	0.5806820	C	0.2123540	-3.5028010	3.8943820
C	8.7622910	-4.0037380	0.3640770	C	-2.529436	2.87968900	0.7108590
H	9.5037350	-3.7100950	1.1115410	C	1.8063690	-1.9642860	-2.526048
H	8.5166630	-5.0609500	0.4656380	C	-3.782105	2.93578300	1.3483420
H	9.1492690	-3.7956100	-0.636778	C	1.5568220	-2.3416550	-1.194993
				C	-3.587997	5.33844800	1.5678090

C	-2.863918	1.07059800	-1.486232	H	-6.026775	1.28406200	-2.731706
C	-1.819804	4.06973300	0.5131880	H	3.0088850	-2.2559830	-4.282554
C	-2.429255	0.05239100	1.2759770	H	-2.356558	-3.3497630	-4.033751
C	-2.553594	-1.7640790	-0.474501	H	-3.874076	-5.5153560	2.3689200
C	-1.269605	-2.5942260	-2.358167	H	-3.488275	-2.4270530	5.3407760
C	-6.192953	-2.0704210	-1.344584	H	-0.318388	-4.2084370	0.6095470
C	-3.763075	-2.0619330	-1.183523	H	0.7265620	-1.5596860	4.6772030
C	3.3977290	-3.9185100	-1.342565	H	-0.331484	-5.2997980	2.8287880
C	-5.047339	-1.7984550	-0.631108	H	-2.293059	1.46240500	2.9218420
C	-4.953476	1.11951000	-2.717332	H	-2.875383	-0.1456190	4.6616450
C	2.8313080	-2.5623410	-3.255795	H	-5.271743	4.18138300	2.2664720
C	-2.418100	-2.8933980	-3.049419	H	-4.781033	1.60298300	-0.636916
C	-3.660733	-4.4816520	2.6252850	H	-4.816847	-3.3025560	-4.212611
C	-3.447079	-2.7601720	4.3072220	H	2.2131380	-3.6202920	0.4179280
C	-0.071571	-3.6337100	1.4967670	H	-1.138514	0.48058900	-2.642747
C	0.5173990	-2.1454900	3.7866430	H	-7.029875	-2.8231780	-3.200207
C	-0.079022	-4.2469790	2.7468490	H	-3.256432	-3.9291680	0.6075550
C	-2.509792	0.44231000	2.6436200	H	-1.773792	6.20291300	0.7845230
C	-2.829589	-0.4619810	3.6231370	H	-2.385337	0.19032800	-4.747039
C	-3.034417	-2.2288480	1.9382050	H	0.1907230	-3.9809690	4.8693660
C	-4.289429	0.72309500	-3.879779	H	4.4446040	-3.9947990	-3.226371
C	-4.304702	4.15579400	1.7727480	H	-4.843945	0.58093300	-4.802635
C	-4.246565	1.29589400	-1.527957	H	-3.996480	6.28767500	1.9021610
C	-4.890597	-2.8847930	-3.212139	C	5.0052200	-1.1210300	0.4552260
C	-2.666437	-1.2731810	0.9298870	C	3.7887400	-0.5441020	0.1143920
C	3.6357280	-3.5385460	-2.663337	C	3.6444000	0.17238300	-1.087518
C	2.3657500	-3.3257990	-0.612930	C	4.7684360	0.30743300	-1.933600
C	-2.206026	0.67933700	-2.661127	C	5.9818760	-0.2663550	-1.589625
C	-6.117348	-2.6175000	-2.648218	C	6.1124070	-0.9891220	-0.393195
C	-3.317420	-3.5893530	1.6338100	H	5.0960270	-1.6796040	1.3793330
C	-2.344515	5.29177600	0.9389950	H	2.9403870	-0.6611960	0.7777410
C	-2.910277	0.50622000	-3.850346	H	4.6694880	0.86616700	-2.858922
H	0.7153910	-0.4608150	2.4610120	H	6.8430450	-0.1680370	-2.241601
H	-3.986632	-4.7838890	4.7495330	C	2.4124110	0.81581600	-1.461654
H	1.2084600	-1.1910160	-2.994525	C	1.8134620	1.57690700	-2.304367
H	-4.346173	2.02748700	1.5289690	H	1.6956260	1.83928800	-3.346874
H	-0.849296	4.03988700	0.0409230	H	2.1712080	1.21177900	1.2614750
H	-0.318759	-2.8353460	-2.810368	C	7.4301600	-1.5984760	-0.079859
H	-7.163935	-1.8563700	-0.907512	O	8.4154960	-1.5094470	-0.793335
H	4.0213240	-4.6716870	-0.869789	O	7.4222090	-2.2725690	1.0858470
H	-5.119191	-1.3661630	0.3598190	C	8.6636050	-2.9002960	1.4527200

H	8.4672790	-3.4021670	2.4006380	C	0.7923100	-1.6283100	4.0642610
H	8.9658050	-3.6259960	0.6929820	C	1.2463380	-0.8084220	-4.367469
H	9.4510570	-2.1516650	1.5744570	C	1.1668750	-0.3836060	3.5322300
<b>TS1-CF<sub>3</sub></b>				C	0.0211450	-2.4036110	-5.714528
				C	-0.029799	1.44629400	-2.054915
				C	-0.553274	-2.0825200	-3.387561
C	-1.792125	-3.4175960	0.5559200	C	2.4438330	0.05428100	-1.453923
C	-2.140073	-4.8776340	0.1664620	C	2.0487930	1.97112900	0.1492200
C	-1.278853	-5.3732230	-0.963193	C	0.4084810	2.31894600	1.9252300
C	-0.157943	-4.7654760	-1.375296	C	2.5021120	5.24822200	-1.629222
C	0.3993340	-3.5599180	-0.733703	C	1.9109600	3.34834700	-0.225133
C	-0.348176	-2.9466750	0.4243620	C	1.3755300	0.48133100	5.7896730
H	-2.128630	-3.2485680	1.5866050	C	2.6351140	3.91551100	-1.309261
H	-1.629112	-6.2782240	-1.456257	C	-0.053399	3.44712200	-3.429661
H	0.4302430	-5.1568080	-2.201081	C	0.7042440	-1.8129910	5.4435270
C	-2.127190	-5.8536260	1.3343940	C	0.2511330	3.63366900	1.5636420
H	-2.823619	-5.5128220	2.1075890	C	6.3045960	2.32329700	0.5046220
H	-2.426362	-6.8550760	1.0078060	C	6.6532140	0.43485400	-0.961737
H	-1.121503	-5.9147660	1.7631090	C	4.1135500	-0.1811900	2.3913350
O	-3.500411	-4.7788710	-0.313133	C	4.7827010	-2.5465060	1.0696040
C	-3.610881	-3.5625920	-1.062661	C	5.4159290	-0.6667390	2.4506700
H	-3.360730	-3.7299970	-2.122231	C	3.3398610	-0.8572480	-2.075973
O	1.4861170	-3.1330700	-1.125985	C	4.6977470	-0.7295940	-1.931480
C	-2.637304	-2.6193000	-0.400677	C	4.3682680	1.22021200	-0.481952
C	-2.367004	-1.3221910	-0.643192	C	-1.073873	3.98863500	-2.644008
H	-4.651185	-3.2240380	-1.010228	C	1.0306800	-1.4465340	-5.588413
C	-3.078342	-0.5146010	-1.688199	C	0.4661730	2.18741700	-3.137397
H	-4.015053	-0.9952790	-1.997585	C	0.8859750	5.55738500	0.1419730
H	-3.317888	0.49582400	-1.351889	C	2.9497790	1.06910800	-0.637096
H	-2.448558	-0.4061380	-2.578272	C	0.9904780	-0.7552820	6.3101830
Rh	-0.513609	-0.8630030	0.3735590	C	1.4696930	0.66740000	4.4089750
P	0.6278860	-0.2307540	-1.644837	C	-1.048467	2.00219000	-1.270868
P	1.3955580	-0.2967670	1.7093430	C	1.6207810	6.07971900	-0.898626
C	3.1370040	-0.8725600	1.6543650	C	4.9398120	2.22212100	0.3507300
C	3.4753950	-2.0570510	0.9960270	C	-0.768928	-2.7209320	-4.609379
C	1.0133100	4.19169400	0.5054260	C	-1.570465	3.26142100	-1.562441
C	1.3473730	1.48273900	1.2528660	H	2.7316640	-2.5689980	0.3988080
C	7.1731390	1.42280500	-0.156691	H	8.2471240	1.51024500	-0.020594
C	5.2509370	0.30915400	-1.143747	H	0.5672000	-2.4560500	3.3977850
C	5.7533350	-1.8541500	1.7918500	H	2.0498260	-0.0855800	-4.289484
C	0.4534050	-1.1180580	-3.249378	H	-1.169548	-2.3424570	-2.538288

H	-0.185002	1.91256600	2.7362260	C	-7.402480	2.55823500	0.5075330
H	3.0695270	5.66291600	-2.457203	F	-7.153119	3.83497700	0.1448110
H	1.6101590	1.30536000	6.4573070	F	-8.140047	2.60928700	1.6432960
H	3.3011090	3.28551100	-1.886328	F	-8.196184	2.01659200	-0.443926
H	0.3497770	4.01249400	-4.264686				
H	0.4111780	-2.7810340	5.8393680				
H	-0.457300	4.26576300	2.0921240				
H	6.7183310	3.09579400	1.1463760				
H	7.3060040	-0.2715870	-1.467387				
H	3.8603820	0.73919600	2.9069580				
H	5.0401510	-3.4631280	0.5461990				
H	6.1702250	-0.1165690	3.0052010				
H	2.9431970	-1.6822970	-2.650773				
H	5.3666460	-1.4413510	-2.407395				
H	1.6562690	-1.1958510	-6.440231				
H	1.2716140	1.79684800	-3.746993				
H	0.1970620	6.18197200	0.704317				
H	1.7869300	1.62990800	4.0239590				
H	-1.435814	1.46007400	-0.417864				
H	1.5214220	7.12760600	-1.166254				
H	4.2899970	2.91048800	0.8769320				
H	-1.551758	-3.4695040	-4.691483				
H	-2.357538	3.67403600	-0.938238				
H	6.7707360	-2.2315160	1.8414040				
H	0.9186390	-0.8965140	7.3846030				
H	-1.471591	4.97364200	-2.869670				
H	-0.143490	-2.9008090	-6.666132				
C	-6.207591	0.36503600	0.6692250				
C	-5.057739	-0.3841330	0.8802600				
C	-3.838148	0.26013700	1.1452400				
C	-3.782644	1.66372900	1.1837950				
C	-4.934355	2.41364900	0.9622980				
C	-6.142240	1.76304700	0.7031500				
H	-7.150726	-0.1313330	0.4670300				
H	-5.089404	-1.4669660	0.8332840				
H	-2.837075	2.15752800	1.3803650				
H	-4.890459	3.49654000	0.9863000				
C	-2.631639	-0.4921420	1.3896010				
C	-1.655851	-0.8430800	2.1190190				
H	-1.383853	-0.9415580	3.1572400				
H	0.2366980	-3.1418020	1.3278790				
				<b>TS2-CF<sub>3</sub></b>			
				C	1.86000600	3.51662900	0.36518000
				C	1.90279300	4.81889800	1.21033800
				C	0.64961800	4.96761200	2.03440500
				C	-0.12608300	3.93413800	2.38680600
				C	0.26348200	2.54032600	2.09347700
				C	1.23557000	2.27168600	0.98671300
				H	2.88411100	3.28372800	0.04304800
				H	0.41286300	5.98024600	2.35522500
				H	-0.99420600	4.06221900	3.02680200
				C	3.15287500	4.96973600	2.06487400
				H	4.04188700	4.94025400	1.42611200
				H	3.13976500	5.92098800	2.60688000
				H	3.21078500	4.15560600	2.79434600
				O	1.92586400	5.85668800	0.20671300
				C	1.03442600	5.46538900	-0.84316300
				H	0.02093100	5.86036400	-0.66976500
				O	-0.12099000	1.63927300	2.84011200
				C	1.05857800	3.96020800	-0.81966900
				C	0.44203400	3.04851600	-1.60406600
				H	1.40353500	5.88844200	-1.78416600
				C	-0.44792900	3.38956700	-2.76321900
				H	-0.29429400	4.42472300	-3.09417000
				H	-0.27057300	2.72979400	-3.61974600
				H	-1.50259200	3.27597300	-2.49097500
				Rh	0.40660400	1.15388400	-0.62923100
				P	-1.98900500	1.16743200	-0.14347800
				P	0.43450000	-1.35611900	-0.20189900
				C	0.61894000	-2.17419900	1.41627100
				C	0.73745500	-1.38951900	2.56871900
				C	-3.38815200	-3.17257300	-2.23938500
				C	-1.07054500	-2.17213300	-0.93283600
				C	-3.14850800	-3.94786400	4.35484100
				C	-2.89258400	-1.71575800	3.42780700
				C	0.81281600	-3.39386000	3.92340100

C	-2.93312200	2.67396500	0.31916500	H	-1.35345700	4.01724400	-0.23976200
C	1.82635800	-1.61913200	-2.61282600	H	-0.01146300	-3.09501300	-2.59209700
C	-4.24201900	2.58683700	0.82779100	H	-6.90453100	-2.53860500	-0.68942000
C	1.77551000	-2.02668800	-1.26730900	H	4.63862700	-3.87033600	-1.19530300
C	-4.38961500	5.00093800	0.91463500	H	-4.90024000	-1.77733700	0.50802700
C	-2.79740700	0.64147700	-1.71172200	H	-5.82544100	0.23572000	-3.21820800
C	-2.36663300	3.93809600	0.12387000	H	2.87412900	-1.73074100	-4.48557000
C	-2.44726000	-0.01305100	1.19934100	H	-2.00109300	-3.94602400	-3.70758100
C	-2.31786300	-2.01196800	-0.33583500	H	-2.98623800	-5.57735400	2.93260000
C	-0.97788500	-2.90695000	-2.14746900	H	-3.24863000	-2.14499200	5.51550200
C	-5.92095200	-2.71426200	-1.11540100	H	0.46614400	-4.18463800	0.63267900
C	-3.49955400	-2.49673600	-0.98432500	H	0.90289100	-1.38880700	4.71345500
C	3.83770100	-3.26232200	-1.60504500	H	0.66041600	-5.26170200	2.85164100
C	-4.79778800	-2.29039500	-0.44091000	H	-2.61101700	1.58349500	2.66396700
C	-4.74579600	0.25377000	-3.10428800	H	-3.00003000	0.11659800	4.57324500
C	2.85568900	-2.04796700	-3.44686200	H	-5.97151900	3.65945200	1.51551300
C	-2.09740900	-3.39259100	-2.77734500	H	-4.84361900	0.90552000	-1.06537600
C	-2.96361400	-4.49953700	3.06482800	H	-4.46087200	-4.10640900	-3.86646300
C	-3.11163700	-2.58305300	4.53037900	H	2.78950700	-3.15909900	0.26413200
C	0.58473200	-3.57386300	1.52243700	H	-0.89493300	0.26357600	-2.67592300
C	0.83093500	-2.00240900	3.81997400	H	-6.70156300	-3.69889100	-2.88489900
C	0.69072100	-4.17897200	2.77257400	H	-2.58847000	-4.12142900	0.99972100
C	-2.64061500	0.51531800	2.50834900	H	-2.63004900	6.06830500	0.26877700
C	-2.85762500	-0.30793400	3.58317500	H	-1.88553800	-0.38362200	-4.83517800
C	-2.70247100	-2.26839600	2.12247700	H	0.88004700	-3.86873700	4.89794300
C	-3.92155000	-0.10936900	-4.17129800	H	4.68603800	-3.18256200	-3.58507500
C	-4.96307500	3.74228000	1.12076600	H	-4.35843900	-0.40619200	-5.12024800
C	-4.18866600	0.63055600	-1.88286900	H	-4.95248200	5.90007700	1.14825900
C	-4.56367900	-3.60016600	-2.91044000	C	4.93761800	-0.78384100	0.82606800
C	-2.47323200	-1.38945500	1.01017300	C	3.76203400	-0.14909400	0.44473800
C	3.87019700	-2.86593300	-2.94177800	C	3.64520300	0.44730600	-0.82236900
C	2.79162500	-2.85305700	-0.77487600	C	4.75543500	0.41541100	-1.69032500
C	-1.97743000	0.27830300	-2.79117300	C	5.92805400	-0.22638100	-1.31475100
C	-5.80627800	-3.37332900	-2.36323900	C	6.01700200	-0.83388900	-0.05782200
C	-2.74316300	-3.68287100	1.97803800	H	5.00518900	-1.25764800	1.79933400
C	-3.09009900	5.09575800	0.41856700	H	2.91743200	-0.14920200	1.12195300
C	-2.53400700	-0.09453900	-4.01332100	H	4.67910100	0.87842600	-2.66861400
H	0.69963500	-0.30784100	2.49777800	H	6.76777500	-0.26562800	-2.00026200
H	-3.31673700	-4.60462400	5.20348500	C	2.42681000	1.08809300	-1.25789900
H	1.05892300	-0.96505900	-3.01302600	C	1.88026900	1.81031300	-2.16481600
H	-4.69256600	1.61813300	1.01539900	H	1.87415600	2.09850000	-3.20644600

H	1.98447100	1.58252500	1.37168900
C	7.22973100	-1.63877500	0.29644900
F	7.09301900	-2.93559400	-0.09117500
F	7.46362100	-1.66016800	1.62777000
F	8.35045500	-1.17639000	-0.30166600