

## Supporting Information

# A pyridine-boryl radical mediated cascade reaction towards the synthesis of indolizines: a computational mechanistic analysis

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# 1. The reaction mechanism for the B<sub>2</sub>pin<sub>2</sub>-mediated cyclization/aromatization to construct indolizine

## 1.1 The complete potential energy surface of a radical addition pathway (path a)

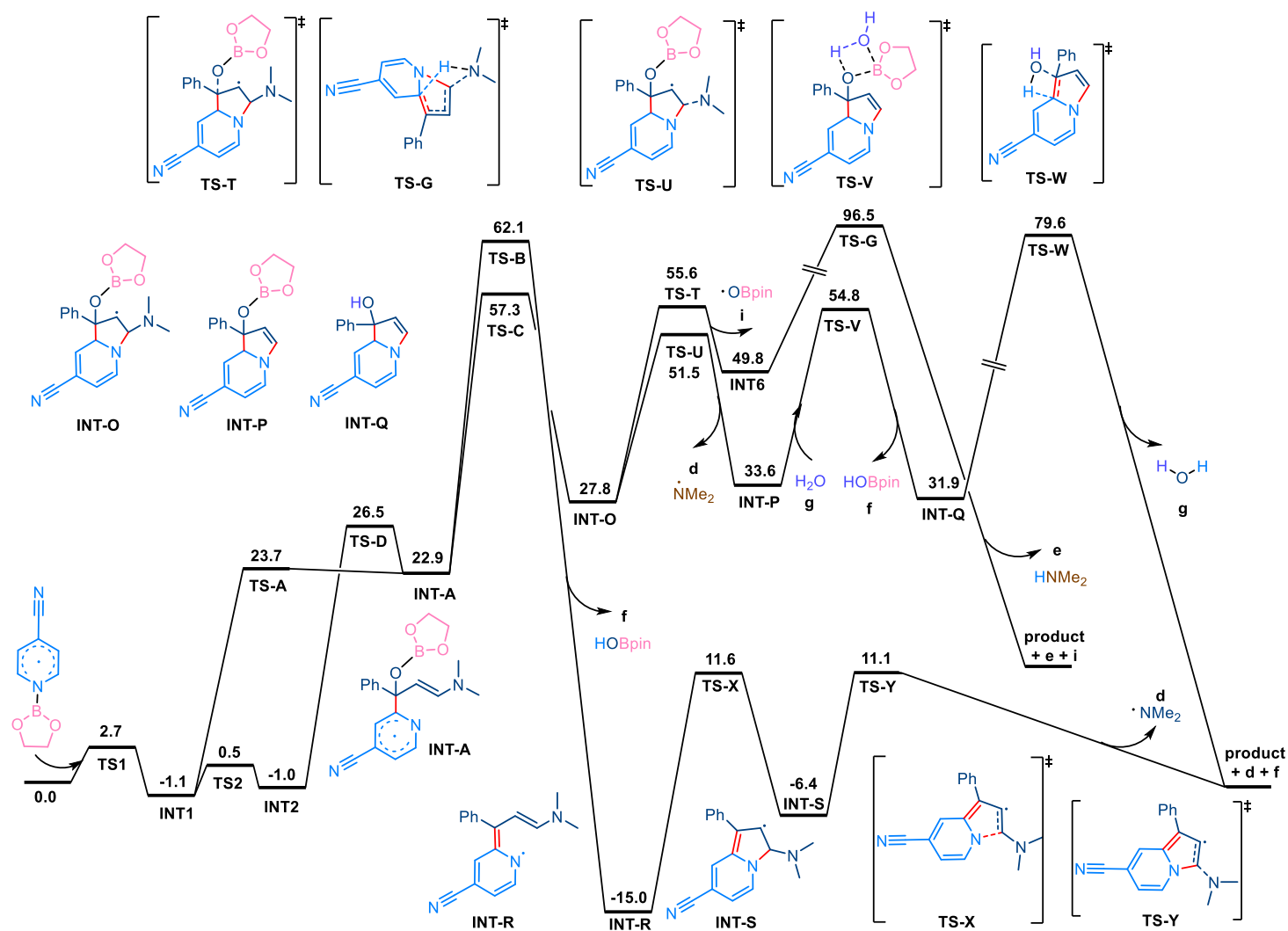


Figure S1 Radical addition pathway (path a). The repeated same structures with the manuscript were not shown.

We first performed theoretical calculations on the traditional Minisci-type radical addition route, however, it was ruled out due to the high barriers of TS-B and TS-C ( $\Delta G_{\text{INT1} \rightarrow \text{TS-B}^\ddagger} = 63.2$  kcal/mol,  $\Delta G_{\text{INT1} \rightarrow \text{TS-C}^\ddagger} = 58.4$  kcal/mol).

## 1.2 Transition states of Py-[B] $\cdot$ and ketyl radical cross-coupling

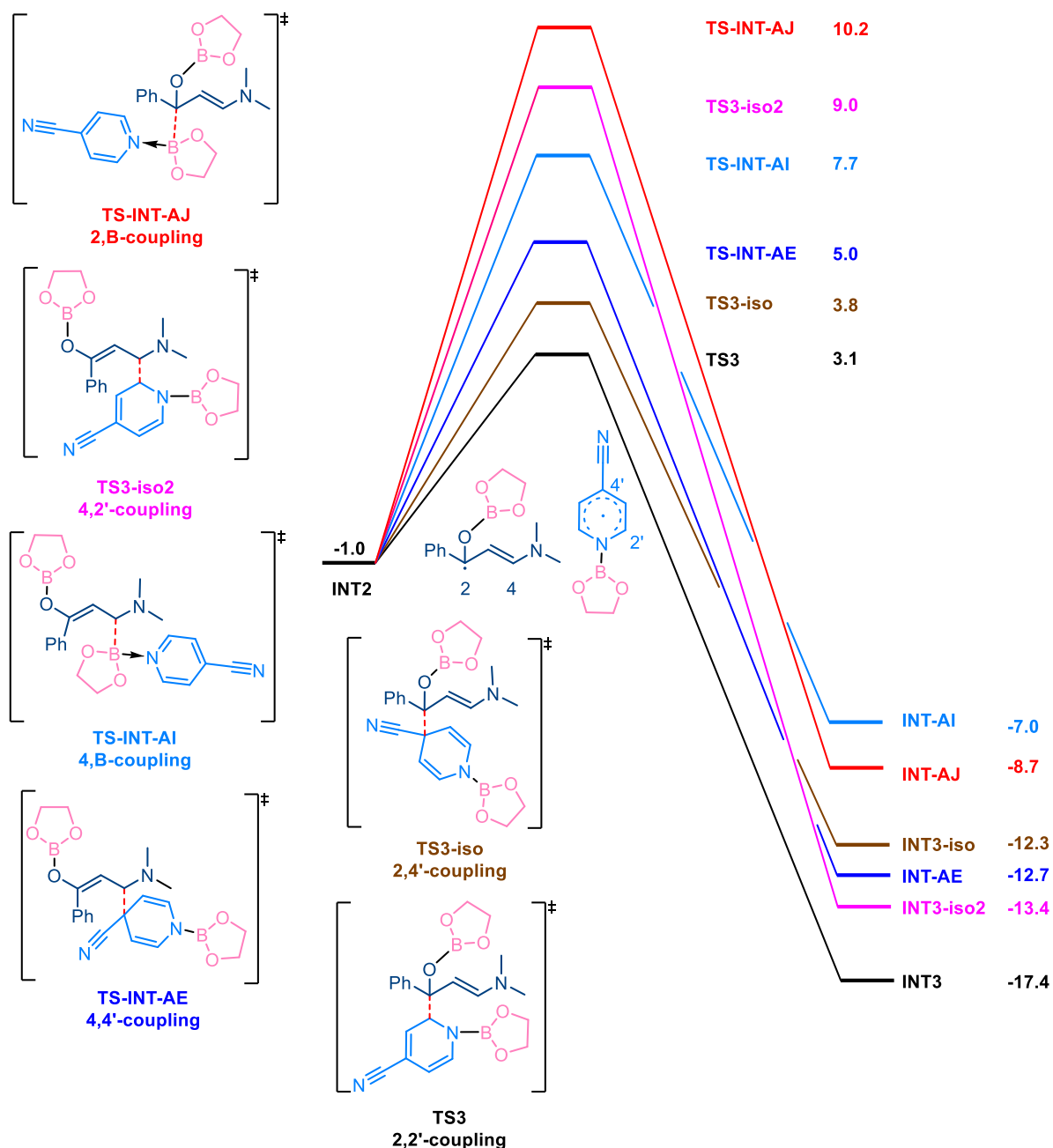


Figure S2 The possible pathways for radical-radical cross-coupling between Py-[B] $\cdot$  and ketyl radicals

These results suggested that 2,2'-coupling was the most favourable pathway for radical-radical cross-coupling, which was in consistency with experimental observations.

### 1.3 1,3-Amine elimination facilitated by H-shuttle

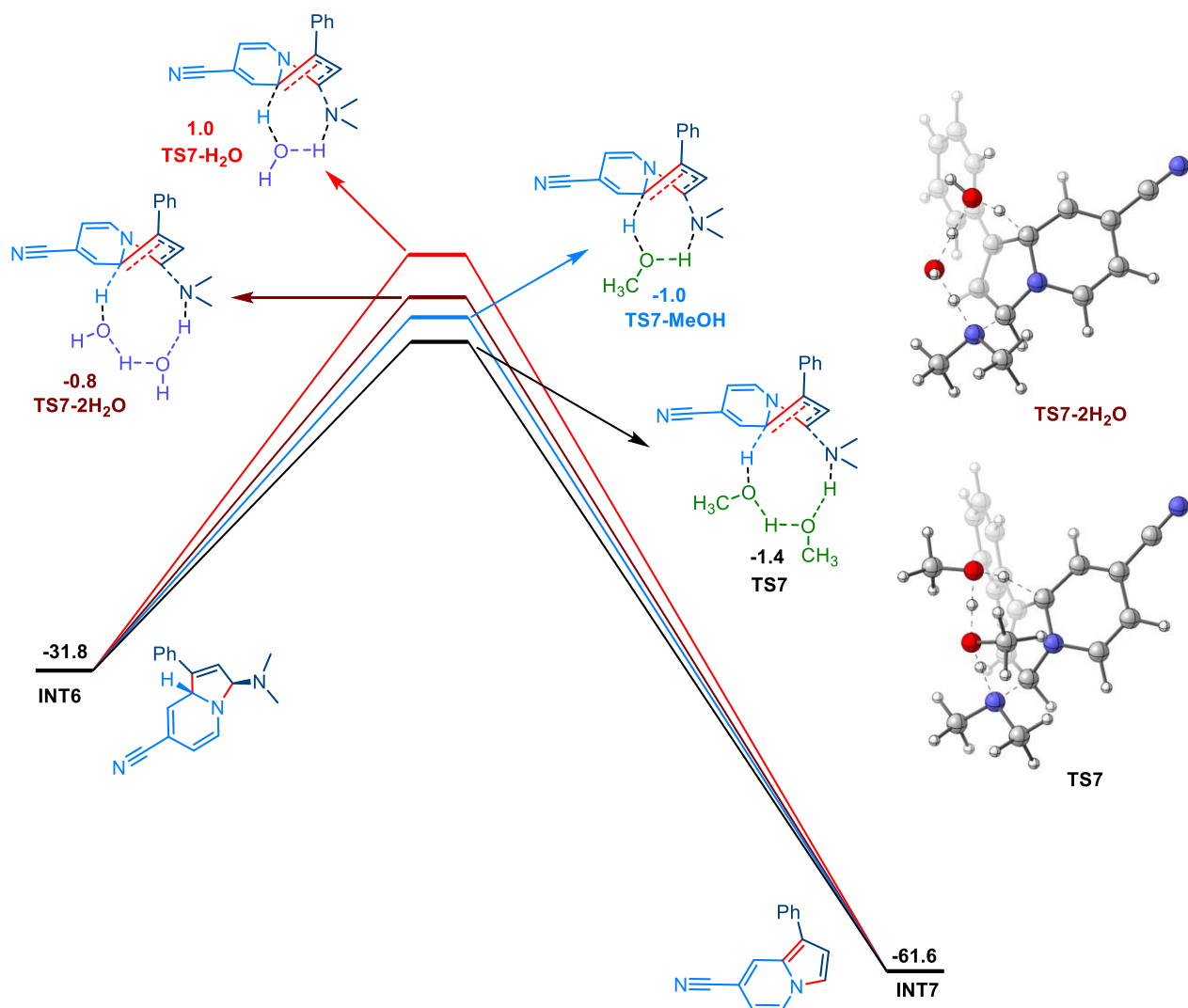
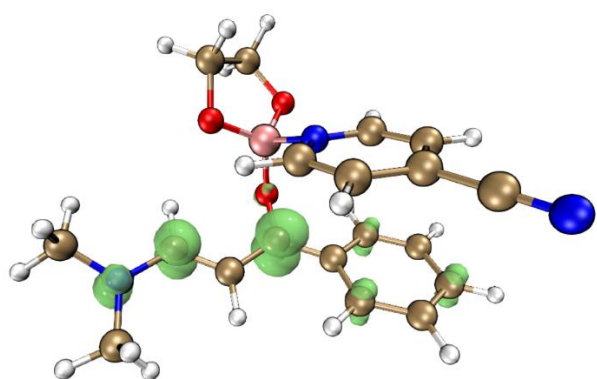


Figure S3 1,3-amine elimination pathways

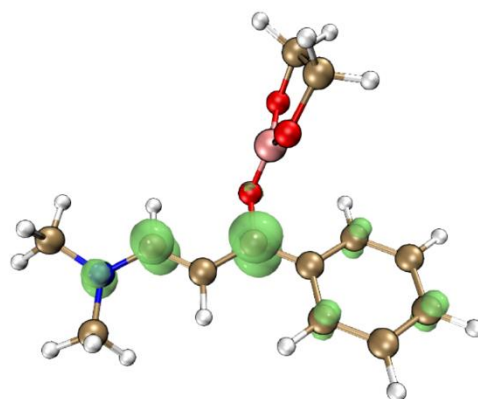
DFT calculations indicate that, compared to the direct 1,3-amine elimination without the assistance of hydrogen-shuttle, the H-shuttle assisted 1,3-amine elimination process can significantly lower the barrier of the elimination process ( $\Delta G_{\text{INT6} \rightarrow \text{TS-G}^\ddagger} = 46.7$  kcal/mol,  $\Delta G_{\text{INT6} \rightarrow \text{TS7}^\ddagger} = 30.4$  kcal/mol,  $\Delta G_{\text{INT6} \rightarrow \text{TS7-2H}_2\text{O}^\ddagger} = 31.0$  kcal/mol,  $\Delta G_{\text{INT6} \rightarrow \text{TS8}^\ddagger} = 25.4$  kcal/mol), with the amine-bridge assisted elimination having the lowest barrier, followed by the alcohol bridge and then the water bridge.

### 1.4 Spin density analysis

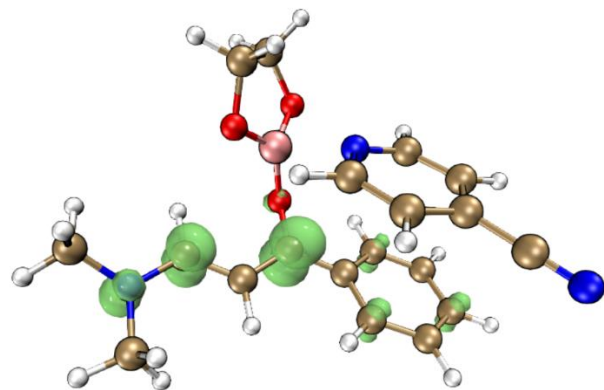
Table S1 Spin density analysis of selected intermediates and transition states



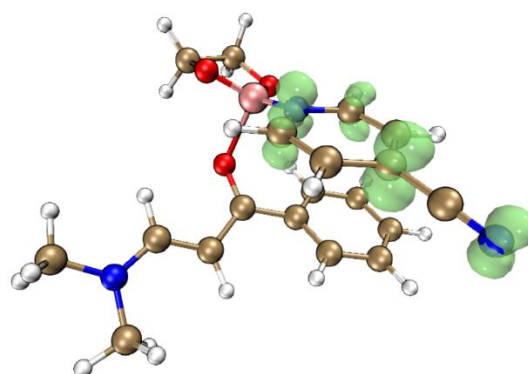
INT1



INT2



TS1



TS2

## 1.5 The other possible reaction pathways starting from INT3

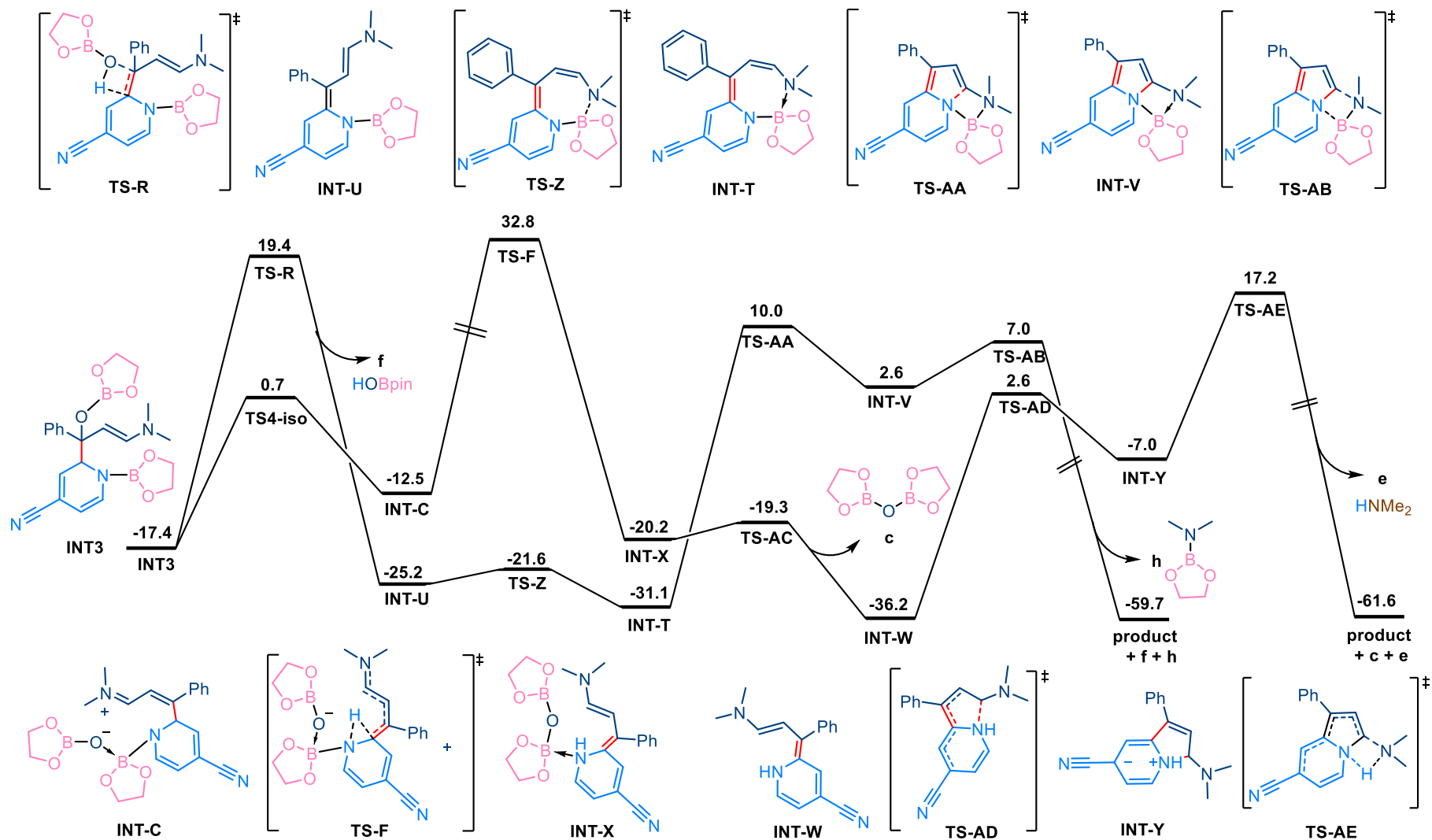


Figure S4 The other possible reaction pathways starting from INT3

Calculations identified additional possible pathways for the production of the final product from INT3. INT3 could generate INT-C via TS4-iso, with INT-C and INT4 being diastereoisomers. Due to the constraints of their spatial structures, INT-C could only undergo a 1,2-H shift process, followed by a cyclisation and 1,2-elimination of an amine to produce the final product. This pathway was excluded due to the high energy barrier at TS-F ( $\Delta G_{\text{INT3} \rightarrow \text{TS-F}}^{\ddagger} = 50.2$  kcal/mol).

Alternatively, INT3 could proceed by elimination of H[B], affording INT-U containing N-[B] motifs. The following coordination of the B atom by -NMe<sub>2</sub> would generate a cyclic structure, which might facilitate the formation of the cyclisation intermediate INT-V and the final elimination of [B]NMe<sub>2</sub> to afford the desired product. This pathway was also excluded due to the high energy barrier at TS-R ( $\Delta G_{\text{INT-3} \rightarrow \text{TS-R}}^\ddagger = 36.8$  kcal/mol) and TS-AA ( $\Delta G_{\text{INT-T} \rightarrow \text{TS-AA}}^\ddagger = 41.1$  kcal/mol).

### 1.6 The other possible reaction pathways starting from INT4

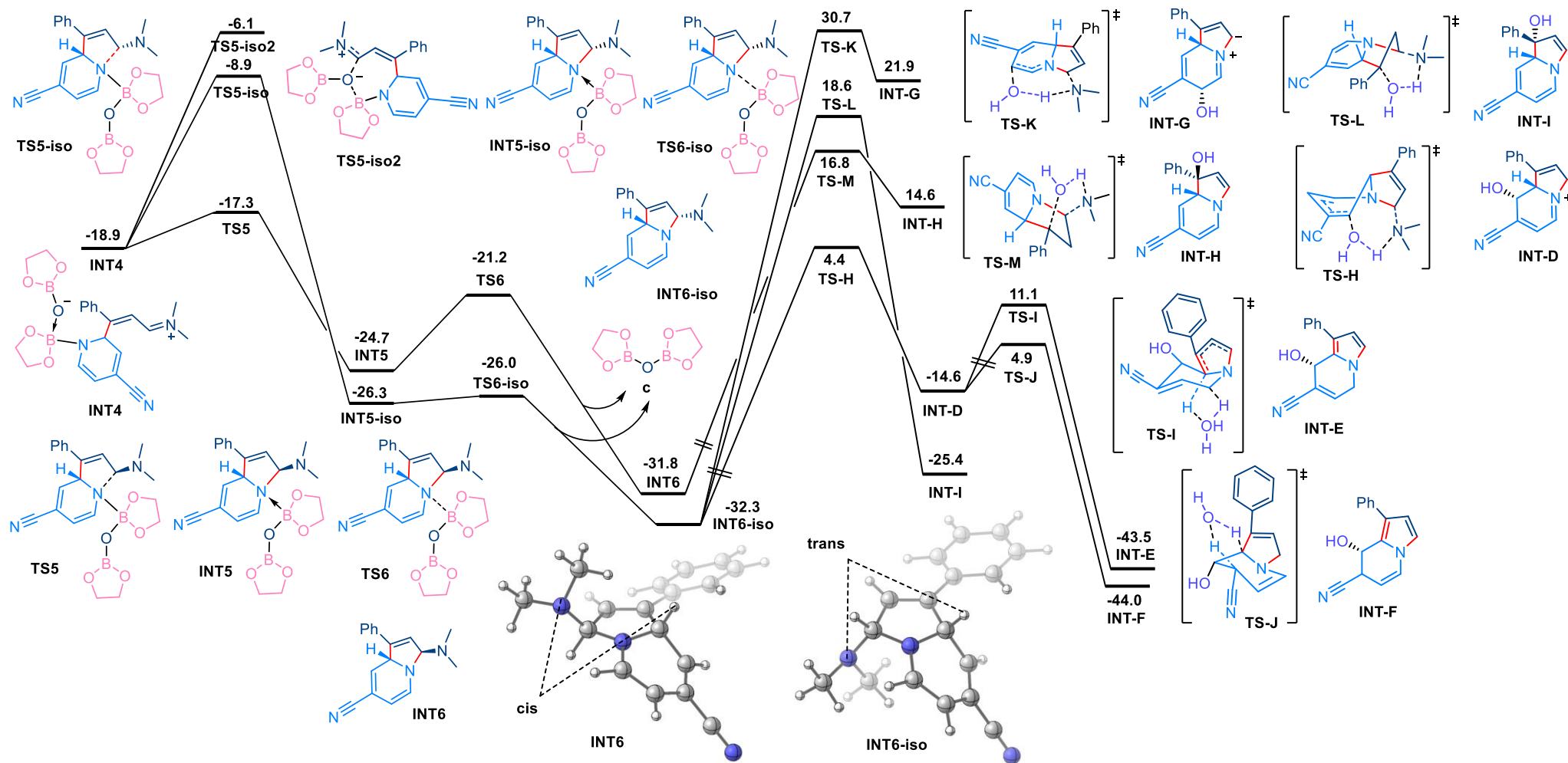


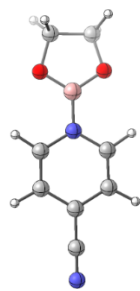
Figure S5 The other possible reaction pathways starting from INT4



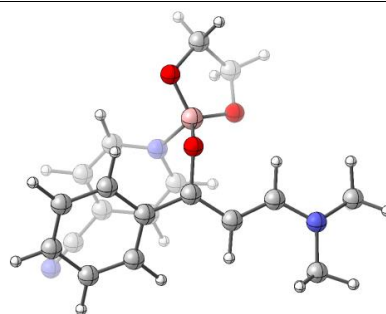
Structures corresponding to the molecular weights detected by HRMS-ESI, as reported in the experimental literature, were calculated. INT6-iso can be generated via TS5-iso and TS6-iso, with these isomers containing NMe<sub>2</sub> and H on the opposite sides of the cyclised ring, preventing the direct elimination of amines. Subsequently, the possible pathways for the formation of byproducts from INT6-iso were explored. The pathway with the lowest energy barrier involved passing through TS-H and TS-J to generate INT-F, which corresponded to the molecular weight detected by HRMS-ESI. The highest energy barrier encountered in forming INT-F is  $\Delta G_{\text{INT6} \rightarrow \text{TS-H}^\ddagger} = 36.7$  kcal/mol. At a reaction temperature of 110 °C, it was plausible for the formation of a trace amount of INT-F.

## 1.7 Structures of important intermediates and transition states

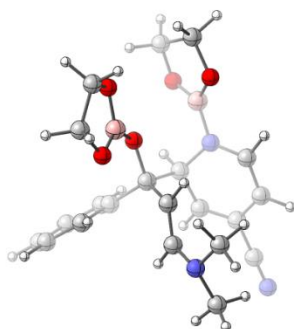
Table S2 Structures of important intermediates and transition states



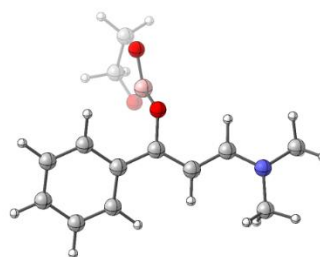
**a**



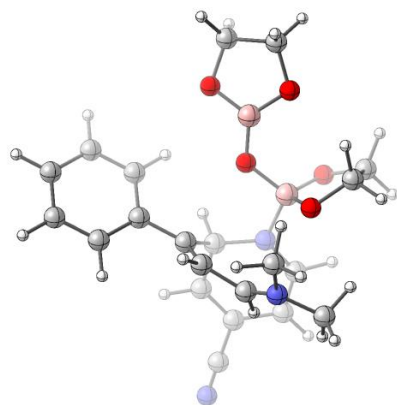
**INT1**



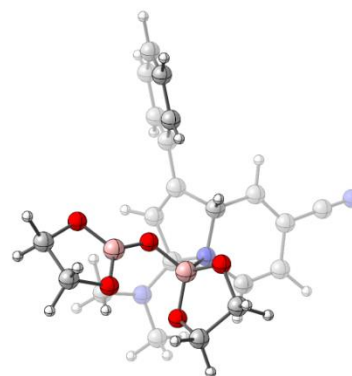
**INT2**



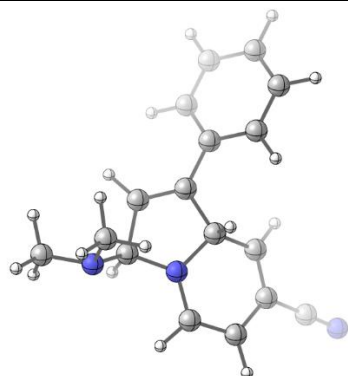
**INT3**



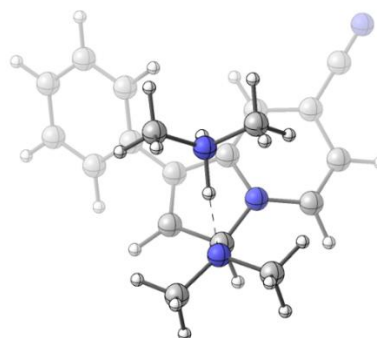
**INT4**



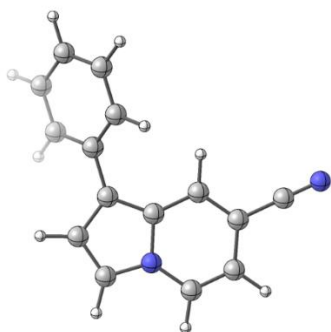
**INT5**



**INT6**

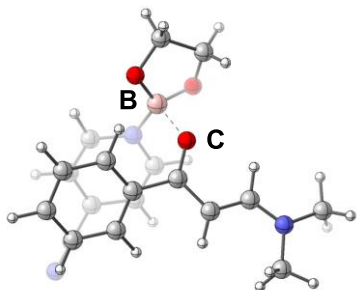


**INT7**



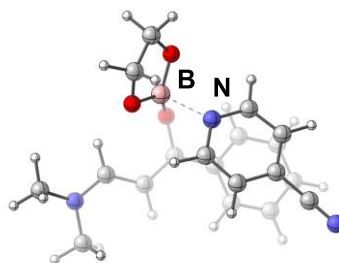
**INT8**

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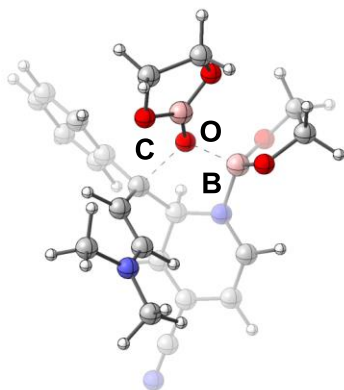
**TS1**  
B-O:1.91849

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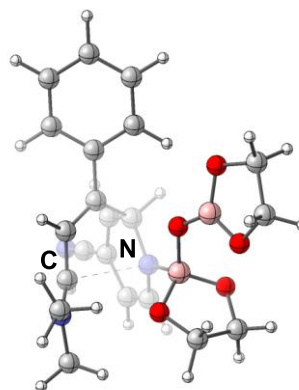
**TS2**  
B-N:2.20558

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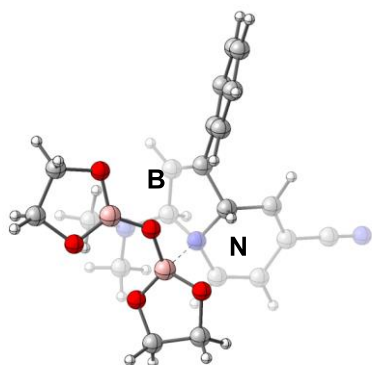
**TS3-1**  
C-O:1.86949  
B-O:1.60323

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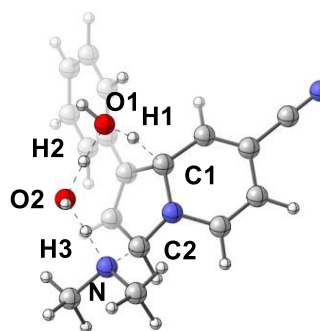
**TS4**  
C-N:2.53806

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**TS5**  
B-N:2.10453

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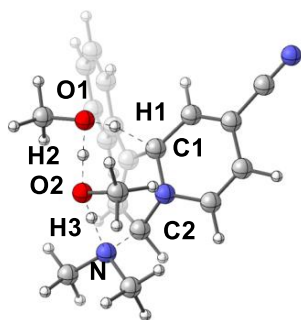


**TS6**  
C1-H1:1.50419  
H1-O1:1.14971  
O1-H2:1.21004  
H2-O2:1.18624  
O2-H2:1.18215

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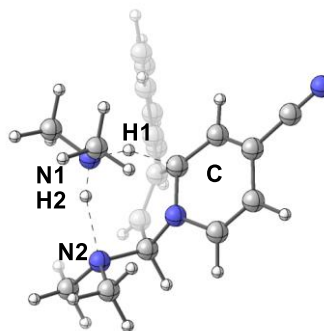
H3-N:1.30614  
N-C2:1.53513

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TS7

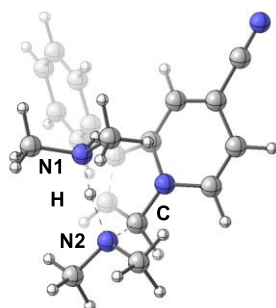
C1-H1:1.59599  
H1-O1:1.09818  
O1-H2:1.17219  
H2-O2:1.21604  
O2-H2:1.07935  
H3-N:1.47665  
N-C2:1.52552



TS8

C-H1:1.52276  
H1-N1:1.20316  
N1-H2:1.05014  
H2-N2:1.85691

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TS9

N1-H:1.16633  
H-N2:1.47041  
N2-C:1.56553

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## 2. The reaction mechanism for the B<sub>2</sub>pin<sub>2</sub>-mediated cyclization/aromatization to construct pyrrolo[2,1,5-cd]indolizines

### 2.1 B<sub>2</sub>pin<sub>2</sub>-mediated cyclization/aromatization to construct pyrrolo[2,1,5-cd]indolizine

In addition to the cyclization/aromatization reaction of enaminones with pyridines, Huang group has shown that cyclopropyl-containing enaminones can undergo cascade reactions with pyridines to construct pyrrolo[2,1,5-cd]indolizines. DFT calculation was also performed to explore the detailed reaction mechanism of this cascade reaction.

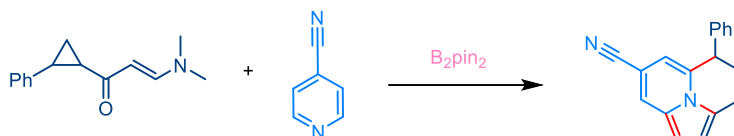


Figure S6 The construction of pyrrolo[2,1,5-cd]indolizines

### 2.2 Ring opening of cyclopropane and radical-radical cross-coupling

As shown in Figure S7, the ketyl radical intermediate **INT11** was obtained via stepwise boryl radical transfer processes, by virtue of the intermediation of four-coordinate boryl species **INT10**. The following ring opening of cyclopropane was realized via **TS12**, with an energy barrier of 11.5 kcal/mol relative to **INT11** ( $\Delta G_{\text{INT11} \rightarrow \text{TS-12}^\ddagger} = 11.5$  kcal/mol). The generated **INT12** was 2.3 kcal/mol more stabilized thermodynamically than **INT11**, probably due to the release of small-ring strain and the conjugated stabilization effect of benzylic radical species. Then, the radical-radical cross-coupling process could be realized via **TS-INT13** with an energy barrier of 3.1 kcal/mol ( $\Delta G_{\text{INT-12} \rightarrow \text{TS-INT13}^\ddagger} = 3.1$  kcal/mol), affording **INT13**, which was much more stabilized than **INT12** by 34.9 kcal/mol, making this process hardly reversible.

### 2.3 H-shuttle assisted removal of the O[B] moiety and 1,2-amine elimination processes

After the generation of intermediate **INT13** through radical-radical cross-coupling, as shown in Figure S8, the migration of the O[B] moiety to Py-[B] could be realized via **TS-AJ**. However, this transition state was calculated to be endothermic by 43.4 kcal/mol, relative to **INT13**. This high energy barrier made this transition state hard to reach, rendering us to find other pathways to remove the O[B] moiety.

Fortunately, H-shuttle was found to be capable of facilitating the removal. As depicted, **TS13**, containing H-shuttle consisting of three MeOH molecules, was more feasible than **TS-AJ** by 14.9 kcal/mol. Unlike the common H-shuttle that transfer an H atom along the molecular chain, **TS13** resembled a metathesis process. Via **TS13**, the boryl group on pyridines was connected to the methoxy of one MeOH, while the O[B] moiety was connected to the H atom at the other end of these three MeOH chain. By virtue of **TS13**, HO[B] and MeO[B] were generated simultaneously, with the latter MeO[B] still coordinated to pyridines. In the meanwhile, the zwitterionic intermediate **INT14**, containing iminium cation, borate inion and allene units, was obtained. This species was 27.0 kcal/mol more endothermic than **INT13**.

The following intramolecular nucleophilic attack of pyridyl N towards the internal C atom of the allene occurred via **TS15**, a facile transition state with a very low energy barrier of 3.6 kcal/mol. The IRC analysis showed MeO[B] would be released simultaneously during the cyclisation process, leading to **INT16**, which was 37.5 kcal/mol more exothermic than **INT14**. This implied the formation of **INT16** was irreversible.

Direct elimination of the amine via a metathesis process from **INT16** exhibited an extremely high energy barrier ( $\Delta G_{\text{INT16} \rightarrow \text{TS-AK}^\ddagger} = 94.6$  kcal/mol). Alternatively, **INT16** could undergo a H-shuttle assisted 1,4-H shift process to yield another zwitterionic species **INT17**. The rearomatization of pyridyl structure made **INT17** exothermic by 3.7 kcal/mol, relative to **INT16**.

Subsequently, the zwitterionic **INT17** underwent intramolecular nucleophilic attack to form **INT18** ( $\Delta G_{\text{INT17} \rightarrow \text{TS19}^\ddagger} = 25.0$  kcal/mol). Finally, the product was obtained via **TS20**, an H-shuttle assisted elimination of the amine transition state ( $\Delta G_{\text{INT18} \rightarrow \text{TS20}^\ddagger} = 24.4$  kcal/mol), because 1,2-elimination from **INT18** was found energetically unfeasible (**TS-AL**, 56.4 kcal/mol).

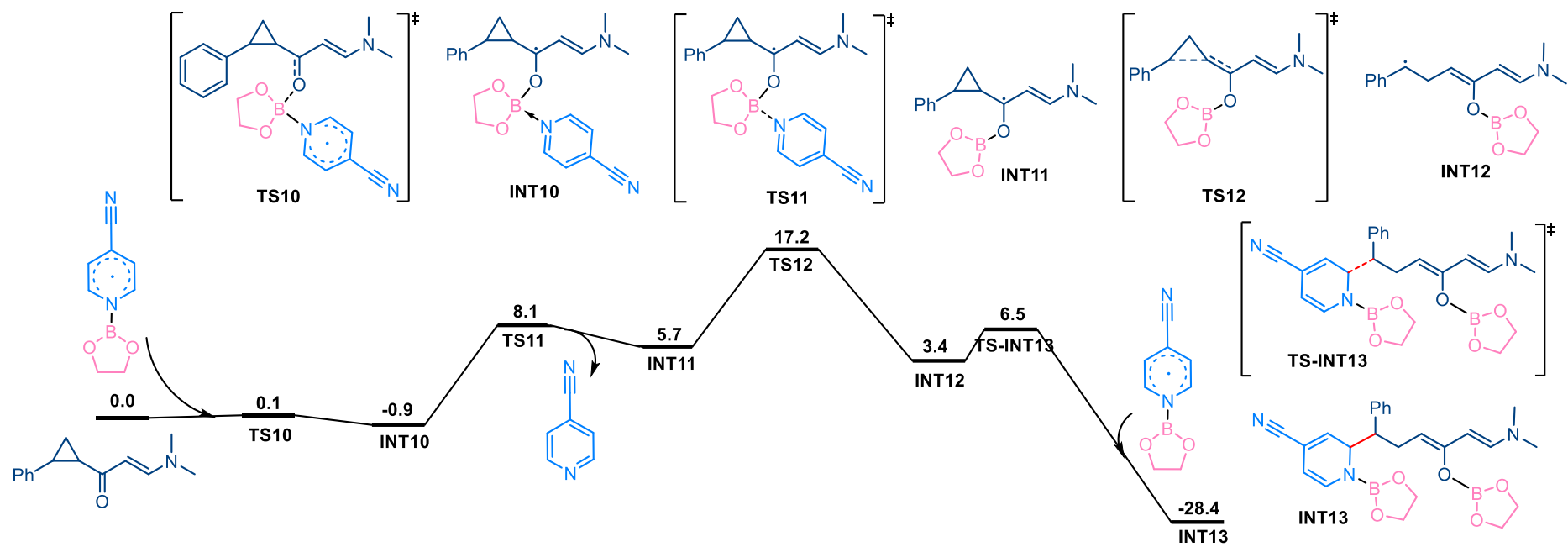


Figure S7 Ring opening of cyclopropane and radical-radical cross-coupling processes

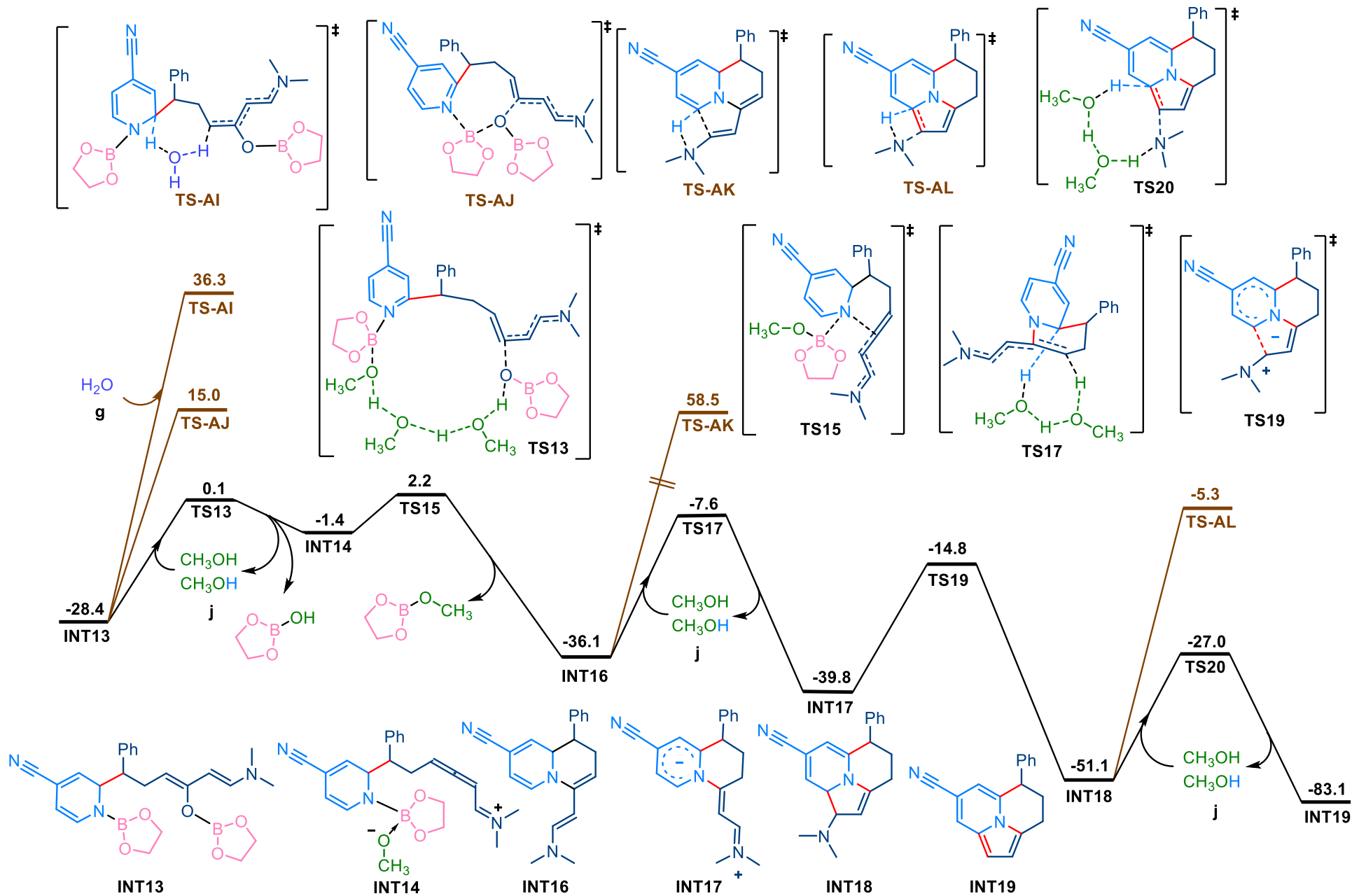


Figure S8 H-shuttle assisted removal of the O[B] moiety and 1,2-amine elimination processes  
S16



## 2.4 Other H-shuttle assisted removal of the O[B] moiety pathways

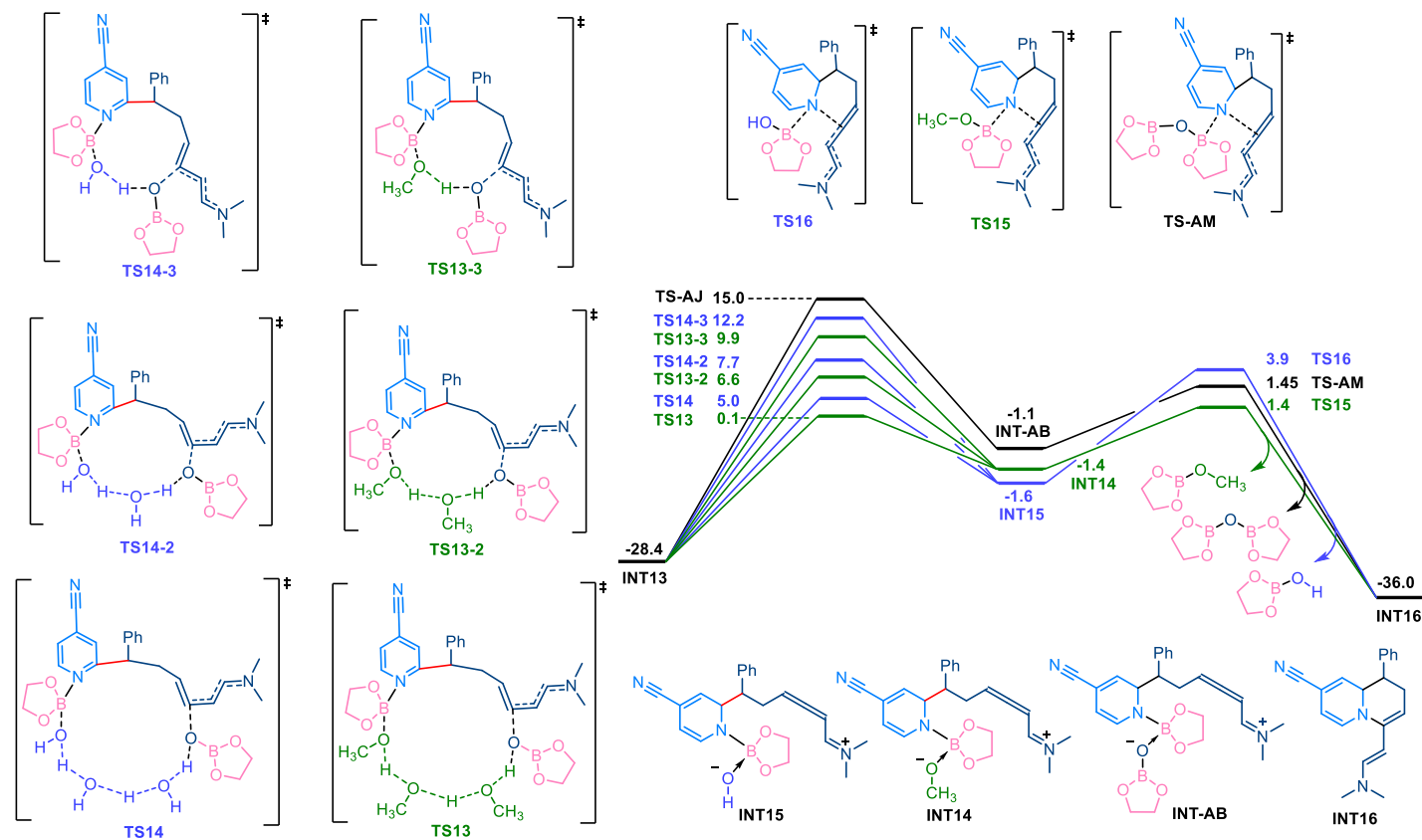


Figure S9 Other H-shuttle assisted removal of the O[B] moiety pathways

The water- and amine-assisted O[B] migration processes were calculated. In these steps, the migration can be facilitated by up to three assisting molecules, with the barrier decreasing as the number of bridging molecules increased. The barrier for alcohol bridges were lower than that of water bridges.

## 2.5 Other 1,4-H shift pathways facilitated by “water bridge” or “alcohol bridge”

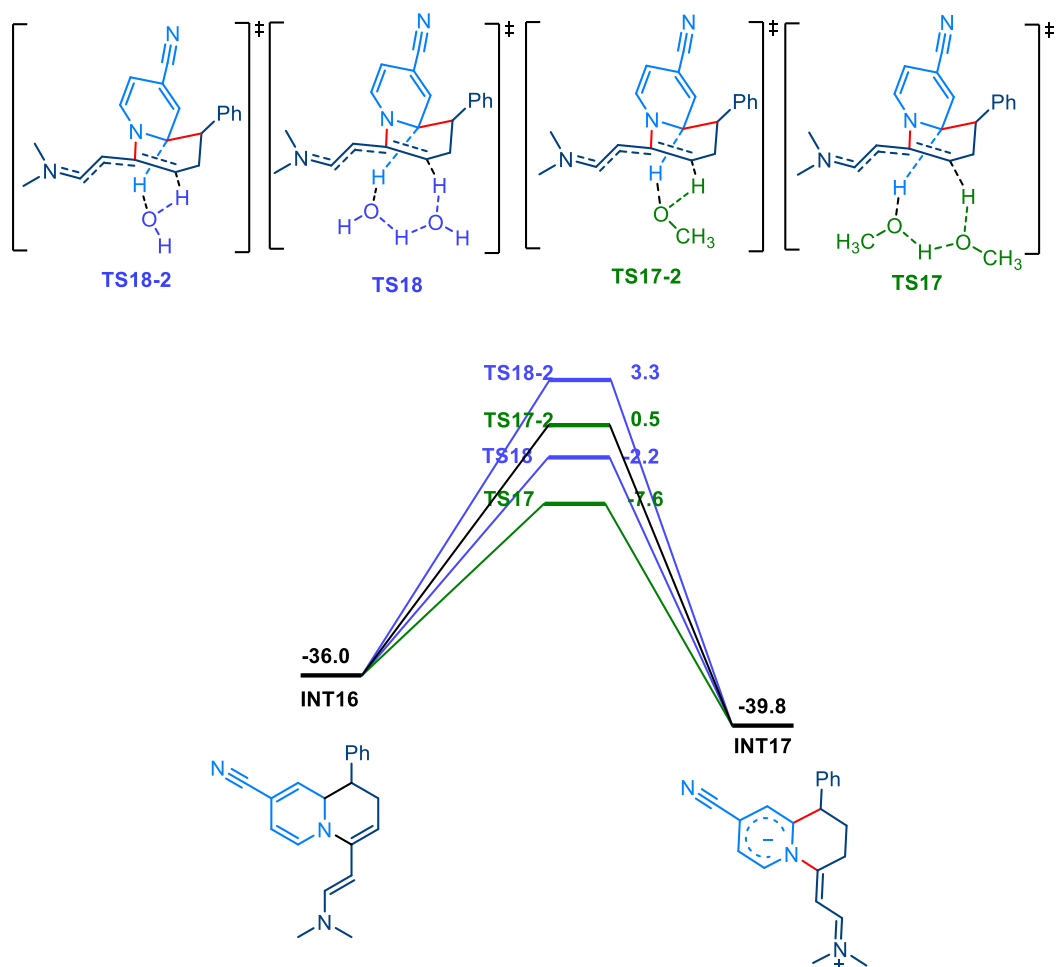


Figure S10 Other 1,4-H shift pathways

## 2.6 Other elimination pathways of amines facilitated by “water bridge” and “alcohol bridge”

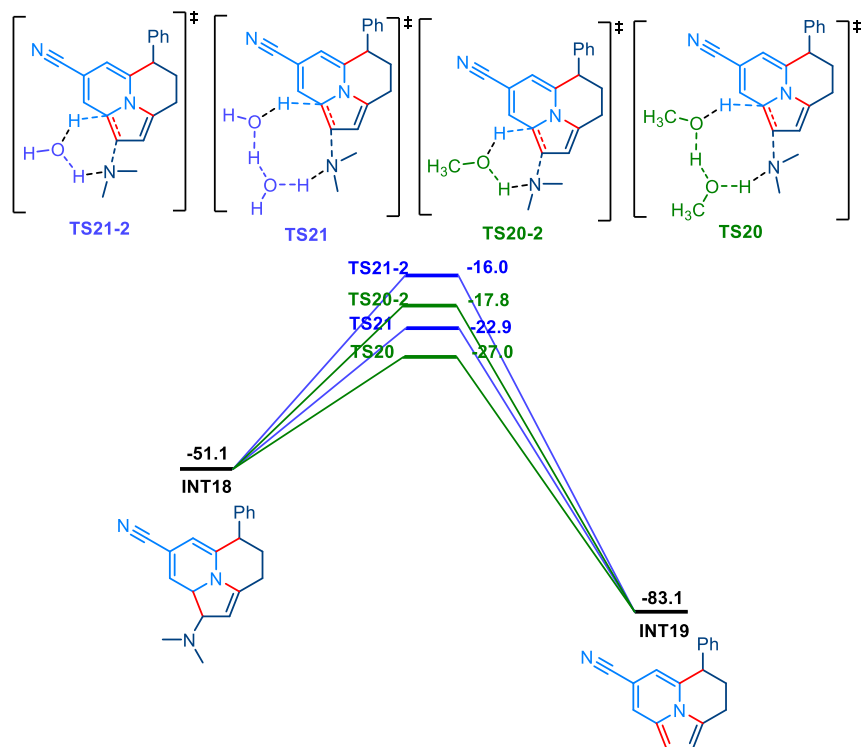
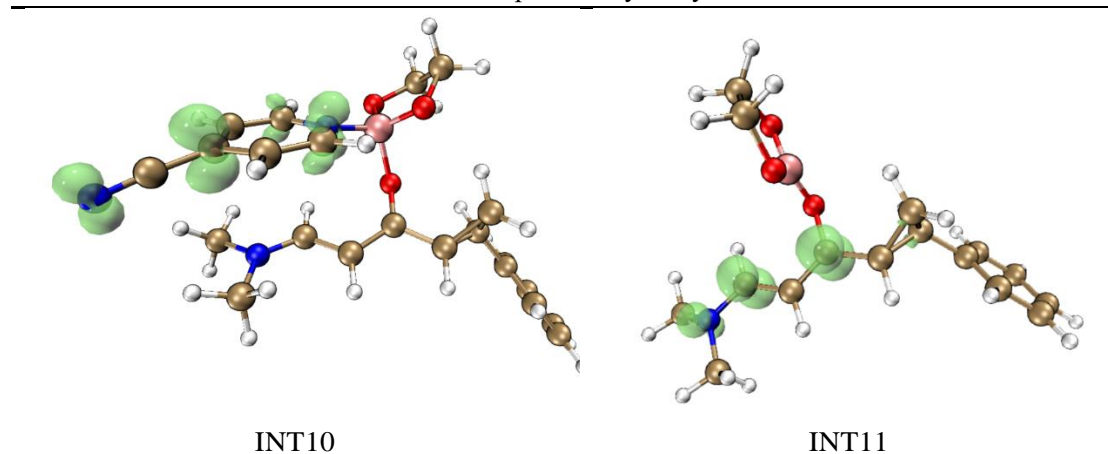
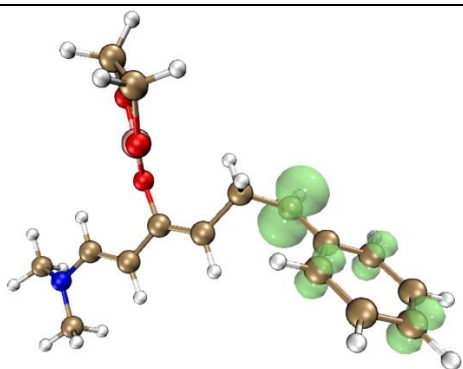


Figure S11 Other elimination pathways of amines

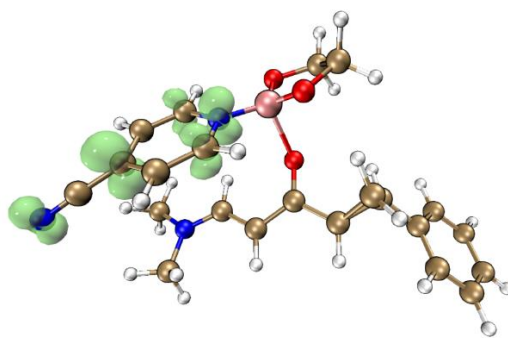
## 2.7 Spin density analysis

Table S3 Spin density analysis

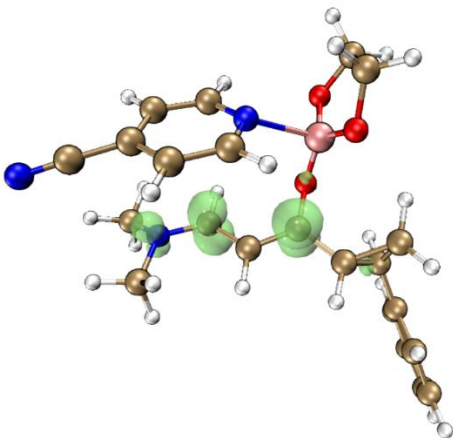




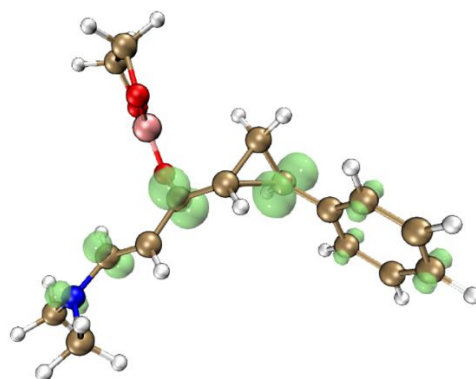
INT12



TS10



TS11

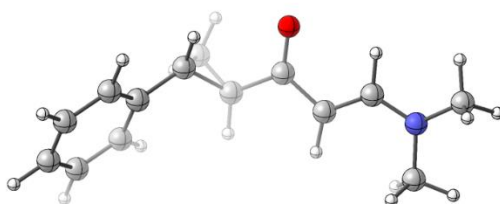


TS12

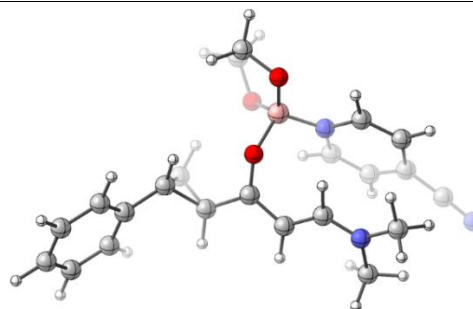
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## 2.8 Structures of important intermediates and transition states

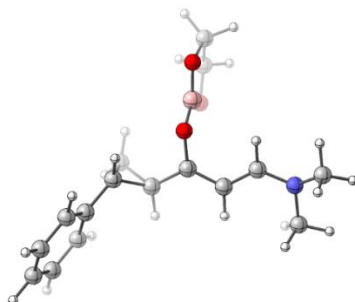
Table S4 Structures of important intermediates and transition states



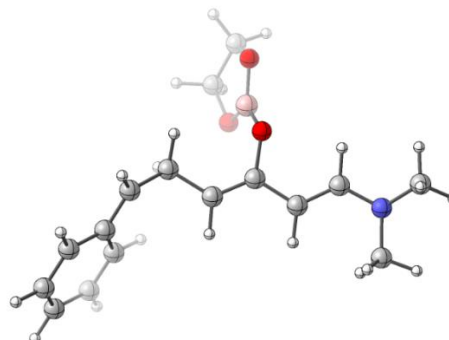
INT9



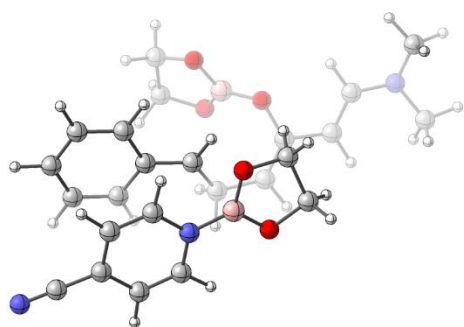
INT10



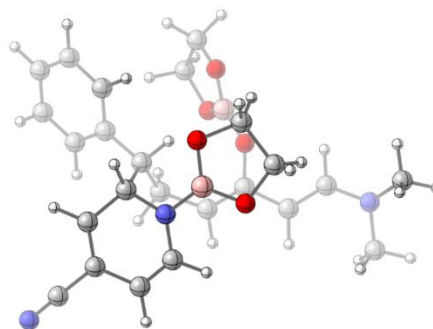
INT11



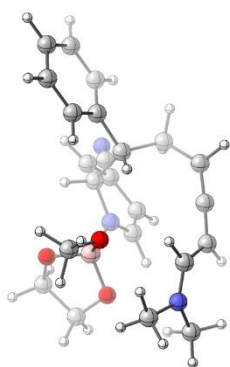
INT12



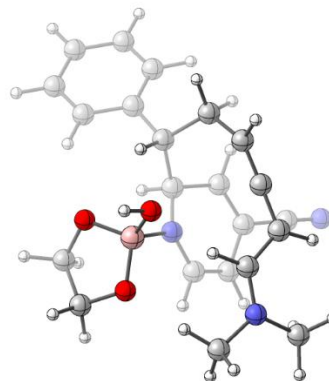
**INT12+a**



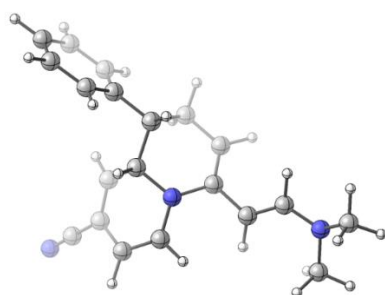
**INT13**



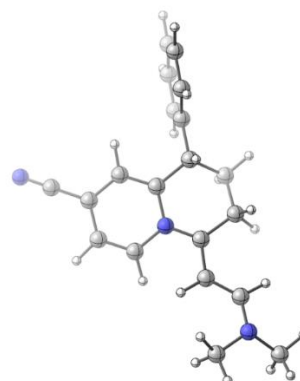
**INT14**



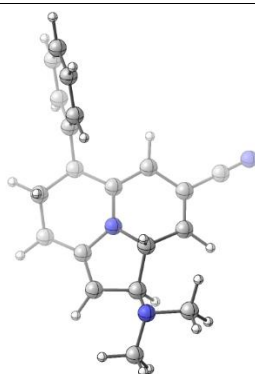
**INT15**



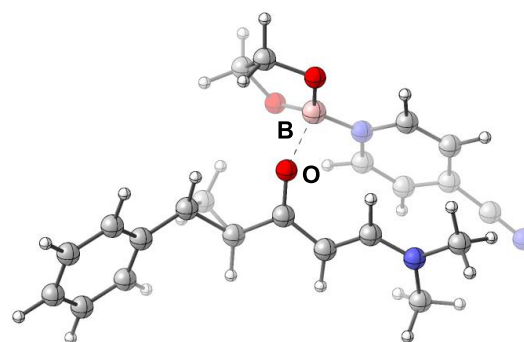
**INT16**



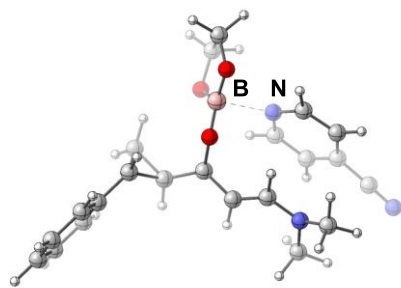
**INT17**



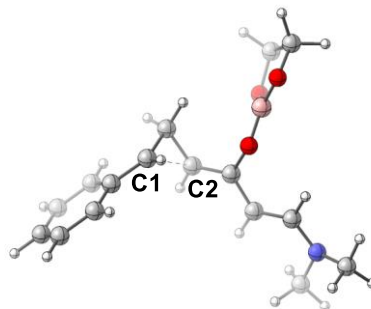
**INT18**



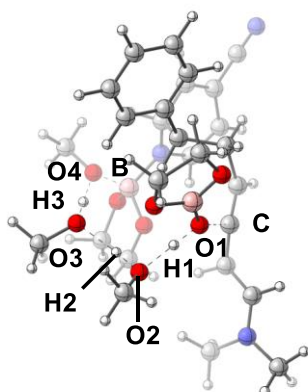
**TS10**  
**B-O:1.93221**



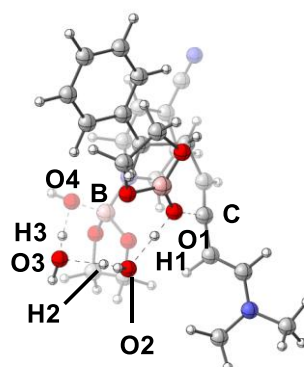
**TS11**  
B-N:2.12686



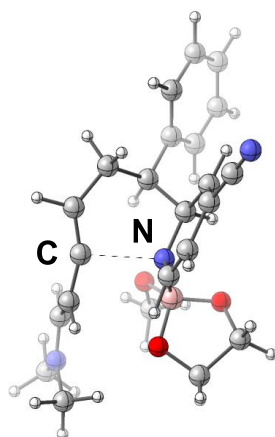
**TS12**  
C1-C2:1.94817



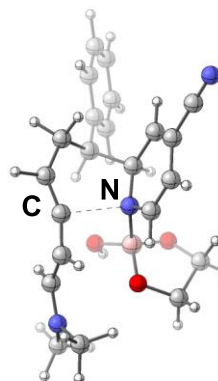
**TS13**  
C-O1:1.93054  
O1-H1:1.06020  
H1-O2:1.41009  
O2-H2:1.01533  
H2-O3:1.56102  
O3-H3:1.01072  
H3-O4:1.53324  
O4-B:1.48791



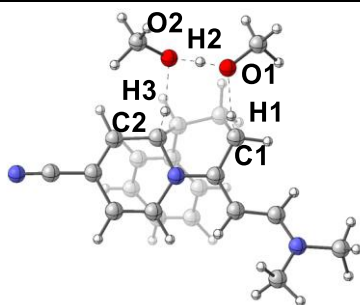
**TS14**  
C-O1:1.93557  
O1-H1:1.05550  
H1-O2:1.42548  
O2-H2:1.00971  
H2-O3:1.60233  
O3-H3:1.00193  
H3-O4:1.60786  
O4-B:1.48518



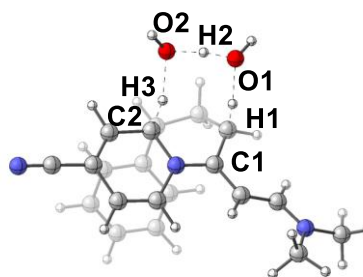
**TS15**  
C-N:2.36593



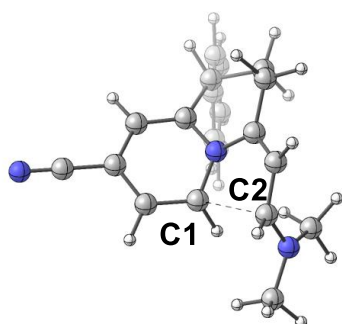
**TS16**  
C-N:2.38162



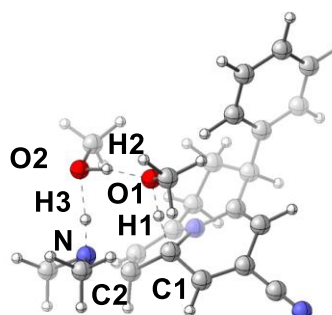
TS17  
C1-H1:1.12899  
H1-O1:1.79441  
O1-H2:1.10676  
H2-O2:1.30624  
O2-H3:1.76336  
H3-C2:1.12084



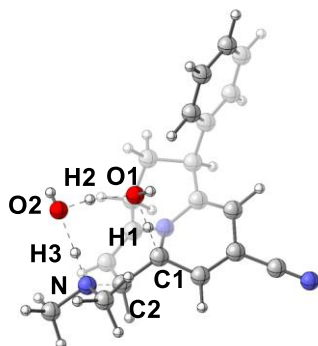
TS18  
C1-H1:1.15067  
H1-O1:1.68603  
O1-H2:1.12292  
H2-O2:1.30507  
O2-H3:1.66461  
H3-C2:1.14319



TS19  
C1-C2:2.38498



TS20  
C1-H1:1.36536  
H1-O1:1.24278  
O1-H2:1.43279  
H2-O2:1.04115  
O2-H3:1.53568  
H3-H:1.08699  
N-C2:1.55131

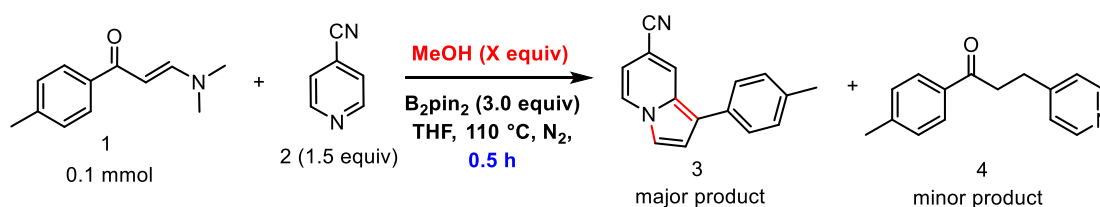


TS21  
C1-H1:1.37527  
H1-O1:1.24644  
O1-H2:1.41819  
H2-O2:1.05590  
O2-H3:1.50669  
H3-H:1.09528  
N-C2:1.54477

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### 3 Control experiments

Experimental procedure: To a 20 mL sealed tube with magnetic stirrer bar, enaminone (0.1 mmol), B<sub>2</sub>pin<sub>2</sub> (3.0 equiv), THF (1.0 mL), pyridine derivative (1.5 equiv) and MeOH (1.0 equiv) were successively added and vigorously stirred together in 110 °C oil bath under N<sub>2</sub> atmosphere. After the reaction was finished, the mixture was cooled to room temperature. The reaction was quenched with saturated NH<sub>4</sub>Cl aq. and extracted with EtOAc (3 × 15 mL). The combined ethyl acetate layer was washed with brine (10 mL) and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. The solvent was removed under vacuum. The crude product was purified by flash column chromatography (eluting with petroleum ether/ethyl acetate) on silica gel to afford **3** and **4**.



entry	MeOH (equiv)	major product yield (%)	minor product yield (%)
1	0	30.0	trace
2	1	46.3	20.9

If the alcohol-mediated amine elimination process was the rate-determining step, the reaction rate should increase as the concentration of alcohols increased. In the same time scale, adding additional alcohols should produce more products. However, when we performed the reactions containing additional MeOH at 110 °C for 24 hours. An inseparable mixture was obtained. Therefore, the reaction time was shortened herein.

As shown above, when 1.0 equiv of alcohols were added to the reaction system, the yield of the desired product **3** increased correspondingly, indicating the alcohols were involved in the rate-determining step. Furthermore, it was found that the added alcohols could induce and accelerate other side reactions, which also eliminated amino motifs and led to the minor product **4**.

### 4. NMR Spectra of 4

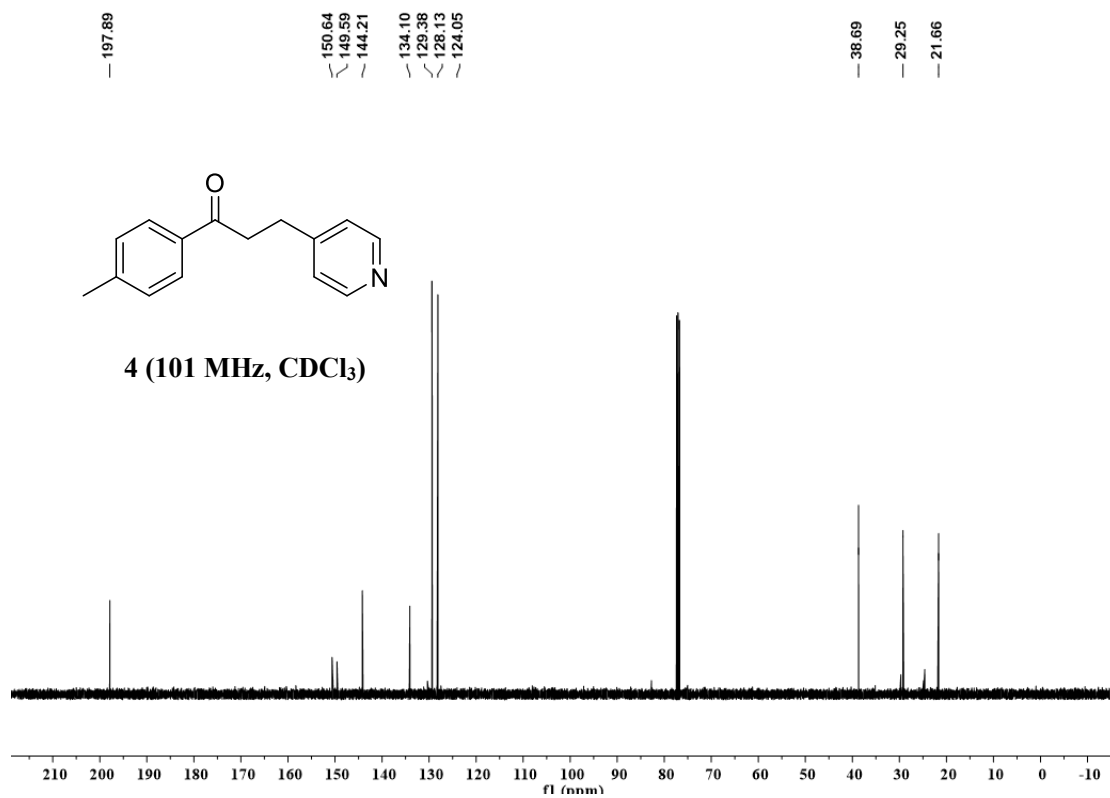
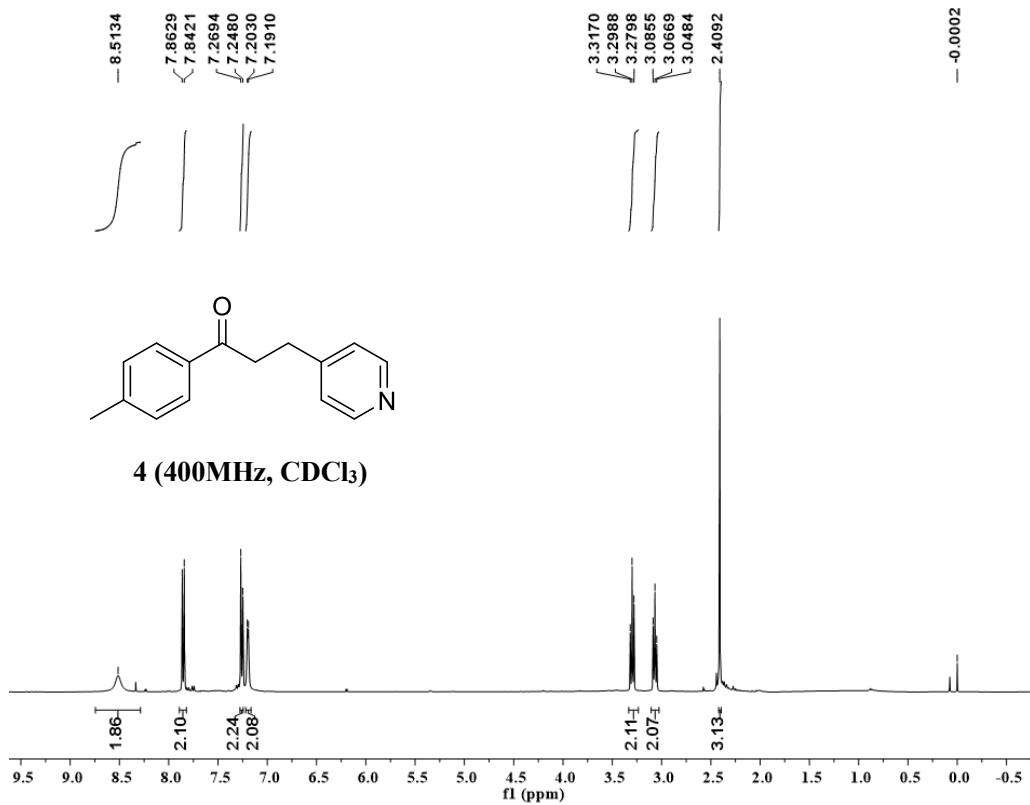
3-(pyridin-4-yl)-1-(p-tolyl)propan-1-one (**4**)

The compound was obtained as yellow oil. (PE/EtOAc =10:1) 4.7mg, 20.9% yield.

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.51 (s, 2H), 7.85 (d, *J* = 8.4 Hz, 2H), 7.26 (d, *J* = 8.4 Hz, 2H), 7.20 (d, *J* = 4.8 Hz, 2H), 3.30 (t, *J* = 7.2 Hz, 2H), 3.07 (t, *J* = 7.6 Hz, 2H), 2.41 (s, 2H).

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 197.9, 150.6, 149.6, 144.2, 134.1, 129.4, 128.1, 124.1, 38.7, 29.6, 21.7.





## 5. The calculated energies and imaginary frequencies.

Table S5 The computed data

Entry	$E_c^a$	$E_c^b$	$H^c$	$G^d$	Imaginary frequency
a	0.122217	-594.156113	-594.144144	-594.194808	/
b	0.058175	-340.300485	-340.293573	-340.330719	/
B <sub>2</sub> Pin <sub>2</sub>	0.104698	-507.666629	-507.656212	-507.704549	/
c	0.110573	-582.975773	-582.964783	-583.013852	/
d	0.051623	-134.356150	-134.350520	-134.382871	/
e	0.068000	-134.999184	-134.993853	-135.024644	/
f	0.057681	-329.671015	-329.664702	-329.699963	/
g	0.003416	-76.362206	-76.358426	-76.380504	/
h	0.122249	-388.302268	-388.292676	-388.335582	/
i	0.044383	-328.990260	-328.984150	-329.019702	/
INT-A	0.326584	-1150.648225	-1150.623224	-1150.703645	/
INT3-iso2	0.396340	-1404.563420	-1404.533936	-1404.625649	/
INT-C	0.395518	-1404.565682	-1404.536030	-1404.627233	/
INT-D	0.196356	-762.927647	-762.912390	-762.969571	/
INT-E	0.197055	-762.973472	-762.958021	-763.015691	/
INT-F	0.197086	-762.974363	-762.959023	-763.016410	/
INT-G	0.195441	-762.869353	-762.854154	-762.911312	/
INT-H	0.195187	-762.943791	-762.928385	-762.986316	/
INT-I	0.195215	-762.944440	-762.928991	-762.986835	/
INT-J	0.194211	-762.861263	-762.845460	-762.903955	/
INT-K	0.193976	-762.879101	-762.863128	-762.921177	/
INT-L	0.196790	-762.940438	-762.925034	-762.982198	/
INT-M	0.193596	-762.924311	-762.908014	-762.967299	/
INT-N	0.330412	-1150.676659	-1150.652376	-1150.731084	/
INT-O	0.327666	-1150.639960	-1150.615553	-1150.695839	/
INT-P	0.249495	-1016.253634	-1016.233680	-1016.303768	/
INT-Q	0.194982	-762.944427	-762.929066	-762.987034	/

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INT-R	0.245571	-821.015595	-820.996392	-821.064112	/
INT-S	0.248761	-821.004225	-820.986275	-821.050449	/
INT-T	0.320803	-1074.904195	-1074.882283	-1074.953916	/
INT-U	0.315623	-1074.892105	-1074.868555	-1074.944550	/
INT-V	0.318925	-1074.850289	-1074.828083	-1074.900144	/
INT-W	0.258948	-821.600528	-821.581131	-821.648071	/
INT-X	0.397006	-1404.575981	-1404.546324	-1404.636399	/
INT-Y	0.260642	-821.555046	-821.536497	-821.601630	/
enaminone	0.178590	-556.504515	-556.490765	-556.545357	/
INT1	0.325881	-1150.686708	-1150.661567	-1150.742745	/
INT2	0.242848	-810.362622	-810.344097	-810.411106	/
INT3	0.397288	-1404.571258	-1404.541699	-1404.632091	/
INT4	0.394882	-1404.572422	-1404.542663	-1404.634411	/
INT5	0.398195	-1404.583314	-1404.554645	-1404.643640	/
INT6	0.261190	-821.594852	-821.576568	-821.641048	/
INT7	0.348800	-956.574839	-956.551030	-956.627095	/
product(P)	0.171730	-686.624167	-686.610698	-686.663898	/
j	0.029406	-115.611223	-115.606996	-115.633926	/
TS-A	0.326147	-1150.647118	-1150.622810	-1150.702299	-112.32
TS-B	0.321972	-1150.583717	-1150.558398	-1150.641076	-155.88
TS-C	0.325795	-1150.594164	-1150.569732	-1150.648876	-2249.70
TS-D	0.325384	-1150.642374	-1150.617469	-1150.697854	-476.20
TS-E	0.326740	-1150.649486	-1150.624865	-1150.704285	-384.02
TS-F	0.389040	-1404.489870	-1404.459796	-1404.552004	-1825.69
TS-G	0.257479	-821.521722	-821.503743	-821.566652	-1522.05
TS-H	0.284837	-897.917760	-897.898664	-897.963898	-860.69
TS-I	0.213599	-839.265079	-839.248130	-839.308995	-1573.69
TS-J	0.213546	-839.275373	-839.258372	-839.318898	-1560.03
TS-K	0.286052	-897.875455	-897.856262	-897.921992	-415.66
TS-L	0.285231	-897.895240	-897.875768	-897.941194	-472.90

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TS-M	0.285548	-897.897955	-897.878573	-897.944120	-441.59
TS-N	0.190100	-762.842025	-762.826613	-762.884590	-1326.30
TS-O	0.193563	-762.867103	-762.851652	-762.908937	-235.93
TS-P	0.189365	-762.835243	-762.819694	-762.878098	-1496.83
TS-Q	0.194836	-762.895772	-762.880578	-762.937266	-474.88
TS-R	0.392062	-1404.512820	-1404.483202	-1404.573248	-177.17
TS-S	0.329239	-1150.612701	-1150.589070	-1150.666040	-941.90
TS-T	0.328636	-1150.597294	-1150.573200	-1150.651512	-161.53
TS-U	0.324751	-1150.602403	-1150.577913	-1150.658049	-669.59
TS-V	0.272858	-1092.601148	-1092.580279	-1092.650394	-1278.06
TS-W	0.188532	-762.868866	-762.853485	-762.910962	-1879.71
TS-X	0.246869	-820.975657	-820.957556	-821.021663	-518.43
TS-Y	0.245691	-820.976446	-820.958306	-821.022559	-570.70
TS-Z	0.317285	-1074.888097	-1074.865346	-1074.938792	-54.17
TS-AA	0.318068	-1074.838887	-1074.817092	-1074.888287	-501.36
TS-AB	0.316244	-1074.842835	-1074.820382	-1074.893105	-549.59
TS-AC	0.397595	-1404.575555	-1404.546362	-1404.634991	-117.16
TS-AD	0.258776	-821.539910	-821.521252	-821.586172	-385.98
TS-AE	0.256930	-821.517748	-821.499644	-821.562944	-1556.02
TS1	0.326099	-1150.680307	-1150.655292	-1150.735861	-162.54
TS2	0.324783	-1150.683333	-1150.658315	-1150.739314	-133.87
TS4	0.396641	-1404.547534	-1404.518410	-1404.607265	-256.27
TS4-iso	0.397159	-1404.543854	-1404.514790	-1404.603165	-242.50
TS5	0.397379	-1404.572467	-1404.543598	-1404.631860	-16.06
TS5-iso	0.398772	-1404.559908	-1404.531363	-1404.618379	-67.54
TS5-iso2	0.397072	-1404.553935	-1404.524886	-1404.613899	-263.43
TS6	0.399614	-1404.579526	-1404.551223	-1404.638011	-150.15
TS6-iso	0.394830	-1404.583573	-1404.554539	-1404.645696	-154.59
TS7-2H <sub>2</sub> O	0.298943	-974.302721	-974.280628	-974.352725	-1394.65
TS7-H <sub>2</sub> O	0.278258	-897.921910	-897.901985	-897.969296	-1521.56

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TS7	0.354943	-1052.806739	-1052.781574	-1052.860493	-878.76
TS7-MeOH	0.304577	-937.176261	-937.154650	-937.225974	-1532.63
TS8	0.345963	-956.572996	-956.549502	-956.625178	-871.71
TS9	0.348004	-956.576620	-956.553442	-956.627871	-205.03
INT-Z	0.457605	-1521.167366	-1521.135259	-1521.231774	/
INT-AA	0.465436	-1521.183920	-1521.153818	-1521.242972	/
INT-AB	0.457531	-1521.145925	-1521.113625	-1521.209075	/
INT-AC	0.231597	-803.193952	-803.177838	-803.237808	/
INT-AD	0.382334	-1267.242167	-1267.213721	-1267.305467	/
INT9	0.237147	-673.102944	-673.086273	-673.148502	/
INT10	0.386708	-1267.285388	-1267.257582	-1267.344744	/
INT11	0.300232	-926.949367	-926.927714	-927.003448	/
INT12	0.300311	-926.946882	-926.925096	-927.000424	/
INT12+a	0.450783	-1521.135705	-1521.101960	-1521.201930	/
INT13	0.459365	-1521.188918	-1521.156463	-1521.252732	/
INT14	0.426532	-1307.083924	-1307.054172	-1307.143636	/
INT15	0.398912	-1267.832197	-1267.803743	-1267.890576	/
INT16	0.320054	-938.200319	-938.178681	-938.251060	/
INT17	0.322088	-938.207805	-938.187001	-938.256990	/
INT18	0.324257	-938.226408	-938.205953	-938.275041	/
INT19	0.233190	-803.258133	-803.242259	-803.301326	/
TS10	0.386399	-1267.284185	-1267.256479	-1267.343176	-206.00
TS11	0.383503	-1267.270354	-1267.242486	-1267.330417	-145.73
TS12	0.300093	-926.932296	-926.910912	-926.985238	-575.37
TS13	0.602434	-1868.030561	-1867.986769	-1868.109008	-323.08
TS13-2	0.555944	-1752.393841	-1752.354817	-1752.464667	-373.27
TS13-3	0.501999	-1636.756027	-1636.720046	-1636.825538	-341.82
TS14	0.526325	-1750.271260	-1750.232619	-1750.340874	-307.12
TS14-2	0.504155	-1673.889787	-1673.854100	-1673.956057	-365.24
TS14-3	0.476360	-1597.501143	-1597.466839	-1597.568498	-341.27

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TS15	0.425793	-1307.078504	-1307.049311	-1307.137839	-232.56
TS16	0.400423	-1267.825077	-1267.797558	-1267.881793	-229.49
TS17	0.414056	-1169.412159	-1169.383049	-1169.473559	-72.85
TS17-2	0.362624	-1053.770589	-1053.745222	-1053.826713	-740.28
TS18	0.360407	-1090.901468	-1090.875643	-1090.958134	-278.52
TS18-2	0.335439	-1014.515735	-1014.492152	-1014.568751	-1592.92
TS19	0.321037	-938.168080	-938.147449	-938.217150	-377.29
TS20	0.416289	-1169.445437	-1169.417109	-1169.504347	-1200.04
TS20-2	0.367824	-1053.802463	-1053.778243	-1053.855781	-1297.89
TS21	0.364262	-1090.937408	-1090.912593	-1090.990975	-1219.36
TS21-2	0.342169	-1014.549190	-1014.526871	-1014.599513	-1381.57
TS-AF	0.462321	-1521.107006	-1521.077281	-1521.165425	-592.93
TS-AG	0.457397	-1521.091934	-1521.060732	-1521.153789	-597.91
TS-AH	0.381902	-1267.227188	-1267.198867	-1267.288916	-514.47
TS-AI	0.47218	-1597.462178	-1597.427576	-1597.530112	-669.11
TS-AJ	0.454610	-1521.119205	-1521.086903	-1521.183487	-297.67
TS-AK	0.321436	-938.051416	-938.030814	-938.100261	-269.37
TS-AL	0.317778	-938.153369	-938.132784	-938.202030	-1607.13
TS-AM	0.456088	-1521.141727	-1521.109741	-1521.205088	-245.88
TS-AN	0.343658	-1014.451892	-1014.428646	-1014.503264	-203.50
TS-AO	0.246853	-879.520032	-879.502298	-879.565391	-2181.95
TS-AP	0.271051	-955.906851	-955.887073	-955.954141	-1492.10
TS-AQ	0.410250	-1073.190693	-1073.165184	-1073.245111	-330.77
TS-AR	0.384371	-1267.203222	-1267.175653	-1267.262964	-707.48
INT-AF	0.454273	-1521.169832	-1521.136935	-1521.235686	/
INT-AG	0.455079	-1521.183802	-1521.150847	-1521.250565	/
INT-AH	0.396900	-1404.563288	-1404.533589	-1404.623819	/
INT-AI	0.394294	-1404.553373	-1404.523663	-1404.615374	/
INT-AJ	0.395197	-1404.556772	-1404.527265	-1404.618129	/
INT-AE	0.394502	-1404.560946	-1404.531157	-1404.624424	/

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TS-INT-Z	0.451995	-1521.130569	-1521.097763	-1521.195965	-509.22
TS-INT-AA	0.457408	-1521.133453	-1521.102219	-1521.195160	-517.75
TS-INT-AA	0.457408	-1521.133453	-1521.102219	-1521.195160	-517.75
TS-INT-AG	0.449745	-1521.123875	-1521.090407	-1521.190789	-187.08
TS-INT-AF	0.451611	-1521.131349	-1521.098321	-1521.196611	-470.26
TS-INT-AJ	0.392603	-1404.526722	-1404.496804	-1404.588042	-318.23
TS3-iso2	0.396102	-1404.530240	-1404.500758	-1404.589934	-121.52
TS-INT-AI	0.395762	-1404.531966	-1404.502680	-1404.591887	-191.73
TS-INT-AK	0.393309	-1404.534857	-1404.504932	-1404.596270	-379.28
TS3-iso	0.392667	-1404.535875	-1404.505730	-1404.598058	-336.61
TS3	0.395915	-1404.539966	-1404.510365	-1404.599288	-405.25
TS-INT13	0.452350	-1521.132427	-1521.099474	-1521.196986	-508.74
INT5-iso	0.396689	-1404.584829	-1404.555641	-1404.646189	/
INT6-iso	0.261904	-821.596270	-821.578075	-821.641931	/

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<sup>a</sup> Thermal correction to Gibbs Free Energy

<sup>b</sup> Sum of electronic and zero-point Energies

<sup>c</sup> Sum of electronic and thermal Enthalpies

<sup>d</sup> Sum of electronic and thermal Free Energies

## 6. Cartesian coordinates

**a**

C	3.74353900	-0.76489300	-0.10529900
C	3.74342700	0.76504300	0.10597100
B	1.63867500	-0.00001600	-0.00011100
O	2.37607800	-1.15080400	0.05697100
O	2.37600100	1.15082600	-0.05689500
C	-0.51495300	-1.20030200	0.01363300
C	-1.87015000	-1.21803900	0.01418300
C	-2.61334900	-0.00006000	-0.00009100
C	-1.87016100	1.21790200	-0.01465900
C	-0.51495200	1.20017800	-0.01441700
N	0.20166700	-0.00005400	-0.00040300
H	0.09153800	-2.09654700	0.02324900
H	-2.38779100	-2.16971200	0.02520500
H	-2.38779300	2.16958100	-0.02572200
H	0.09152100	2.09643500	-0.02424800
C	-4.02804600	-0.00008600	0.00031400
N	-5.19149700	0.00024000	0.00067400
H	4.07051700	-1.04059900	-1.11281900
H	4.35946600	1.29445500	-0.62361700
H	4.06992200	1.04079100	1.11363500
H	4.35929800	-1.29426200	0.62456300

**b**

C	-1.50272200	1.14059700	0.00002900
C	-0.11287900	1.20327700	0.00003100
C	0.59344700	0.00006700	0.00012300
C	-0.11285100	-1.20332900	0.00005300
C	-1.50250800	-1.14077400	0.00000900
N	-2.19421200	-0.00004200	-0.00008900
H	-2.08807000	2.05630700	0.00008700
H	0.40703800	2.15401200	-0.00017400
H	0.40720900	-2.15398000	0.00022500
H	-2.08789200	-2.05646100	-0.00033800
C	2.03469700	0.00070000	-0.00001500
N	3.19115500	-0.00040200	-0.00007900

**b<sub>2pin2</sub>**

C	-2.98557500	0.44921000	0.62702100
C	-2.98557200	-0.44924700	-0.62702400
B	-0.85146300	0.00002200	-0.00000200
O	-1.61004700	0.76950400	0.84331200
O	-1.61001900	-0.76947900	-0.84334700
C	2.98569900	0.62677600	-0.44967500
C	2.98566700	-0.62682400	0.44966200
B	0.85141300	0.00003800	0.00003300
O	1.60990100	0.84525900	-0.76738500
O	1.60987700	-0.84521500	0.76742000
H	-3.55389700	1.37205700	0.48761300
H	-3.37088800	0.06890000	-1.51091400
H	-3.55383300	-1.37212200	-0.48757700
H	-3.37085500	-0.06896900	1.51091200
H	3.37354800	-1.51047500	-0.06690600
H	3.55176800	-0.48578600	1.37364200
H	3.55174100	0.48563200	-1.37367400
H	3.37365800	1.51042200	0.06683300

**c**

C	3.42412900	-0.14183300	-0.32967000
C	2.85520400	1.05322100	0.47153300
B	1.21929600	-0.42744400	0.01840800
O	2.35113000	-1.07465500	-0.40172200
O	1.44684400	0.84410900	0.48043200
C	-3.42442500	-0.14146400	0.32854400
C	-2.85472600	1.05325000	-0.47244400
B	-1.21937400	-0.42734300	-0.01745600
O	-2.35183700	-1.07478400	0.40068900
O	-1.44624400	0.84463600	-0.47874700
H	3.71442000	0.14629100	-1.34542900
H	3.07955600	2.01719600	0.00849200
H	3.22039400	1.06714400	1.50381600
H	4.28293300	-0.60733700	0.15983700
H	-3.21812700	1.06615700	-1.50537800
H	-3.08027000	2.01747600	-0.01053100
H	-4.28339400	-0.60650300	-0.16110200
H	-3.71467200	0.14679700	1.34428600
O	-0.00008600	-1.02834600	0.00103100

**d**



N	0.00000000	-0.64390600	-0.00000100
C	-1.18535500	0.17331800	0.00000400
H	-2.08032100	-0.45126900	0.00016800
H	-1.21270500	0.83265400	0.88221400
H	-1.21285200	0.83238100	-0.88240900
C	1.18535300	0.17331800	-0.00000600
H	1.21293000	0.83226100	0.88249300
H	2.08032100	-0.45126900	-0.00031300
H	1.21263500	0.83276800	-0.88213100

**e**

H	-0.00002700	1.32718100	0.52664700
N	-0.00000900	0.57125000	-0.15067200
C	-1.20340700	-0.22388800	0.02051800
H	-1.26064900	-0.96499700	-0.78362600
H	-1.24829800	-0.77082700	0.97864900
H	-2.08583700	0.41615600	-0.05411100
C	1.20342500	-0.22389100	0.02052000
H	1.26109100	-0.96440000	-0.78412000
H	2.08581800	0.41629100	-0.05320200
H	1.24786100	-0.77147900	0.97824100

**f**

C	1.32004900	0.80181700	-0.09489100
C	1.37460500	-0.72927000	0.09722800
B	-0.76453400	-0.04776400	-0.00151400
O	-0.05448300	1.13187600	0.08320100
O	0.03119900	-1.16176800	-0.08648800
H	1.92813100	1.34348000	0.63358700
H	1.70475700	-1.00102200	1.10614500
H	2.02494300	-1.22382700	-0.62828600
H	1.63214900	1.09790400	-1.10258100
O	-2.11696400	-0.11663500	-0.00195700
H	-2.51325100	0.75922100	0.02663700

**g**

O	0.00000000	0.11780800	0.00000000
H	0.76025700	-0.47123300	0.00000000
H	-0.76025700	-0.47123000	0.00000000

**h**

C	2.15271200	0.75964500	0.12695400
C	2.15267600	-0.75966000	-0.12708400
B	0.03449900	0.00002800	0.00012500
O	0.80068200	1.15200200	-0.07482800
O	0.80066000	-1.15196100	0.07488400
H	2.44998300	-0.99672100	-1.15572800
H	2.80488700	-1.30571100	0.55954700
H	2.80483900	1.30573600	-0.55971600
H	2.45014400	0.99659600	1.15559500
N	-1.36680700	0.00002100	0.00037900
C	-2.13983200	1.22178100	-0.02537700
H	-1.46925500	2.08183100	-0.03531000
H	-2.77985500	1.26473100	-0.91688200
H	-2.79118900	1.29361200	0.85614700
C	-2.13975100	-1.22182300	0.02516500
H	-1.46910200	-2.08180200	0.03639800
H	-2.78116100	-1.26453600	0.91566000
H	-2.78970700	-1.29400900	-0.85737900

**i**

C	1.29174000	0.76261900	0.10858500
C	1.29164200	-0.76275300	-0.10855900
B	-0.80399800	0.00010100	-0.00001500
O	-0.07011800	1.15110700	-0.09597800
O	-0.07024400	-1.15100900	0.09593100
H	1.58779100	1.03049700	1.12818500
H	1.93035800	-1.29531400	0.59908500
H	1.58774000	-1.03067300	-1.12813900
H	1.93052100	1.29512900	-0.59902600
O	-2.17422700	-0.00001500	0.00002300

**j**

C	0.65848700	-0.01986200	0.00000200
H	1.08100800	0.98649100	-0.00067000
H	1.02961300	-0.54417600	-0.89059800
H	1.02971500	-0.54304200	0.89123000
O	-0.74459600	0.12215300	0.00000200

H -1.13449000 -0.75732500 0.00001000

**enaminone**

C -0.14486800 -0.79981800 -0.11132300  
O -0.00945100 -2.01229000 -0.23889200  
C -1.53539000 -0.22480000 -0.04359300  
C -1.81734800 1.12921500 -0.23860800  
C -2.58671300 -1.11165900 0.20371600  
C -3.12951100 1.58998300 -0.17718400  
H -1.01897400 1.82807300 -0.46584300  
C -3.89499100 -0.65146500 0.27552300  
H -2.34536800 -2.16129200 0.33391400  
C -4.16883400 0.70239500 0.08643100  
H -3.34046700 2.64229500 -0.33920100  
H -4.70422700 -1.34662700 0.47589300  
H -5.19104800 1.06406500 0.13922300  
C 0.99340500 0.11075300 0.00179400  
H 0.83791000 1.16089100 0.20792200  
C 2.23646700 -0.42768200 -0.09846400  
H 2.29886800 -1.50307400 -0.25494400  
N 3.41631800 0.22534100 -0.04374100  
C 3.43281200 1.65010500 0.20788700  
H 3.10297600 1.88482800 1.22877200  
H 4.44603000 2.02980000 0.06704900  
H 2.76759500 2.15933300 -0.49615800  
C 4.66820500 -0.49521400 0.06800000  
H 4.50597300 -1.54150900 -0.19430700  
H 5.41091000 -0.07558900 -0.61767600  
H 5.07179400 -0.45113300 1.08760400

**INT1**

C -1.70442200 3.83338200 -0.46202800  
C -2.24272900 3.08966800 0.76910600  
B -1.01084200 1.64973200 -0.47856500  
O -0.76041400 2.94194600 -1.02526100  
O -2.13310900 1.72489300 0.41452100  
C 0.18544900 0.41149600 1.51396200  
C 1.28069500 -0.14112200 2.15527700  
C 2.55708000 0.24440800 1.73217700  
C 2.70025800 1.18937400 0.71905000

C 1.54762300 1.68995000 0.12765500  
N 0.33446900 1.29327200 0.51747200  
H -0.84174100 0.15321700 1.75044200  
H 1.15177100 -0.87034700 2.94491600  
H 3.67832100 1.49560700 0.37097300  
H 1.55788500 2.40664300 -0.68678100  
C 1.51638900 -0.13438900 -2.28900200  
C 0.78497100 -0.97138100 -1.41496600  
C 1.48455300 -2.01303800 -0.76496600  
C 2.84666100 -2.18761600 -0.96137400  
C 3.55700100 -1.34336900 -1.81779600  
C 2.87545600 -0.32751100 -2.49017000  
H 0.98587400 0.66365300 -2.79892100  
H 0.96152900 -2.65475800 -0.06180100  
H 3.36608800 -2.97985500 -0.43014100  
H 3.41259100 0.32325300 -3.17452100  
C -0.60338800 -0.67820800 -1.13750000  
O -1.02440200 0.58277300 -1.44067300  
H 4.62248900 -1.48448100 -1.96589300  
C -1.51240700 -1.59440300 -0.57245400  
C -2.79950000 -1.24067800 -0.24033400  
C 3.72326600 -0.34978300 2.33497000  
N 4.65541900 -0.83105500 2.82112800  
H -1.22963600 4.78625300 -0.20497500  
H -2.50716700 4.02899200 -1.18495500  
H -3.28200700 3.33596100 1.00578700  
H -1.62361200 3.30822400 1.65383200  
H -1.17109400 -2.61517200 -0.43705300  
N -3.77174500 -2.08820800 0.21900500  
C -4.86901400 -1.51805200 0.97460500  
H -5.75771200 -2.14705400 0.87241000  
H -4.63229000 -1.41978600 2.04471500  
H -5.09674600 -0.52512900 0.58251500  
C -3.42648100 -3.45724900 0.52330200  
H -4.33493100 -4.01166100 0.76646700  
H -2.95935300 -3.92498100 -0.34765500  
H -2.72929700 -3.53296500 1.37304700  
H -3.10911700 -0.20807600 -0.36859900

**INT2**

C 2.09028700 2.65921400 1.28650100  
C 1.88641000 3.63466200 0.10857500

B 0.75278400 1.73165900 -0.25518000  
 O 1.13676700 1.62624500 1.05749400  
 O 1.22754200 2.85475400 -0.88597400  
 C -0.23735600 -0.42663800 -0.37928000  
 H 3.09441200 2.22029300 1.28285600  
 H 2.82664000 4.02196600 -0.29054900  
 H 1.24652500 4.48034500 0.38426700  
 H 1.91005200 3.12083500 2.25997400  
 O -0.02713300 0.83164200 -0.91358900  
 C 0.91785100 -1.27527100 -0.22190900  
 C 0.86047800 -2.49103700 0.49396800  
 C 2.15969500 -0.90774400 -0.78445100  
 C 1.98197600 -3.29312100 0.62785100  
 H -0.06508400 -2.79242900 0.97308500  
 C 3.27725400 -1.71604200 -0.64120600  
 H 2.23190200 0.00297500 -1.37144100  
 C 3.20145600 -2.91605200 0.06362300  
 H 1.90896600 -4.21997000 1.18893000  
 H 4.21616800 -1.41032600 -1.09317600  
 H 4.07710300 -3.54676200 0.17388600  
 C -1.56908200 -0.78348300 -0.12593200  
 H -1.75668900 -1.80115500 0.19484100  
 C -2.61957300 0.08641900 -0.29802900  
 H -2.41722700 1.10638700 -0.60888800  
 N -3.94960300 -0.22178600 -0.16977700  
 C -4.31803600 -1.52740400 0.32834000  
 H -4.00239100 -1.68018200 1.37212000  
 H -5.40218200 -1.64065200 0.26884600  
 H -3.85689000 -2.30311800 -0.28920400  
 C -4.87510500 0.85679200 0.11299500  
 H -4.55736700 1.75431100 -0.42191200  
 H -5.87535900 0.58540100 -0.23499000  
 H -4.93021100 1.09339100 1.18595600

**INT3**

C 3.04032800 1.97064300 2.40459000  
 C 4.09602700 0.98492600 1.86203600  
 B 2.18177500 0.79848300 0.68173700  
 O 1.83300700 1.60049600 1.74247700  
 O 3.52448500 0.47688800 0.66089300  
 C 3.62686000 -1.86700500 -1.62761000  
 C 3.65566000 -2.76494300 -0.37315800

B 1.54850800 -2.16005200 -0.86239100  
 O 2.24649200 -1.80007100 -1.98302400  
 O 2.31516300 -2.73087500 0.12324300  
 C -0.63707500 -2.79999000 0.07745000  
 C -1.98222500 -2.73263300 0.12271900  
 C -2.63338700 -1.79151200 -0.77817700  
 C -1.92822900 -0.89686400 -1.49898800  
 C -0.44494800 -0.76311800 -1.30226000  
 N 0.12211400 -1.99701500 -0.74515400  
 H -0.07175500 -3.53424600 0.64385900  
 H -2.56443300 -3.39757800 0.74472000  
 H -2.42530500 -0.23520800 -2.19989900  
 H 0.06458300 -0.59080200 -2.25515800  
 C -0.06149300 0.44736300 -0.35830300  
 C -4.06777000 -1.84095500 -0.90887300  
 N -5.22298400 -1.87885400 -0.97535000  
 H 2.90363800 1.89453000 3.48572600  
 H 4.27086000 0.15467200 2.55547100  
 H 5.05152700 1.46743400 1.64301000  
 H 3.28150800 3.00841700 2.15124700  
 H 3.92279700 -3.80086000 -0.60768200  
 H 4.33262300 -2.38175800 0.39364900  
 H 4.19828000 -2.28187500 -2.46134100  
 H 3.98257800 -0.85813200 -1.39844500  
 O 1.37190200 0.31821300 -0.28712600  
 C -0.38836000 1.80569000 -0.98322400  
 C -0.63343900 1.97294900 -2.34824400  
 C -0.35713200 2.94527300 -0.16868000  
 C -0.86086500 3.23927700 -2.88355300  
 H -0.64481600 1.12321400 -3.02175800  
 C -0.57416900 4.20956100 -0.70408300  
 H -0.15629700 2.82574300 0.89056700  
 C -0.83283400 4.36153700 -2.06419300  
 H -1.05610500 3.34382800 -3.94598100  
 H -0.54547400 5.07920900 -0.05512700  
 H -1.00855600 5.34765800 -2.48222100  
 C -0.67385900 0.22955400 0.99964500  
 H -0.12119800 -0.44115600 1.64940700  
 C -1.90918600 0.64316500 1.31542900  
 H -2.46736600 1.26237100 0.61461100  
 N -2.59765500 0.38088000 2.48668400  
 C -1.96574800 -0.53335500 3.41341300  
 H -0.98382600 -0.14390200 3.69714300  
 H -2.58004000 -0.61294400 4.31286000

H	-1.82959800	-1.53697600	2.97926500
C	-4.03412600	0.20559100	2.34298100
H	-4.42983400	0.97548700	1.67643000
H	-4.30303800	-0.77722200	1.92583400
H	-4.51506900	0.31474000	3.31861300

#### INT4

C	4.85706900	0.44866700	-0.92636000
C	4.90678100	-1.00189700	-0.40427200
B	2.75423100	-0.29875600	-0.52219100
O	3.50953800	0.84929800	-0.73391100
O	3.55302700	-1.42670300	-0.40297700
C	1.30616700	-3.60727900	-0.94461300
C	1.30105500	-3.34858600	0.57357000
B	0.55147200	-1.43637600	-0.51425000
O	0.96434500	-2.37872100	-1.53066900
O	0.46492000	-2.22066200	0.73387000
C	-1.83057200	-1.69464100	-1.23528600
C	-3.11718900	-1.35173100	-1.52066200
C	-3.42115600	0.06759500	-1.51658600
C	-2.47892800	0.99836300	-1.25833600
C	-1.05823100	0.61661700	-0.89903800
N	-0.86920100	-0.83644800	-0.83314700
H	-1.50136400	-2.73055600	-1.26700300
H	-3.84945300	-2.07748200	-1.84180500
H	-2.71442500	2.05730000	-1.28602300
H	-0.35722800	1.05163100	-1.62409200
C	-0.76224700	1.29498400	0.44472900
C	-4.76688100	0.49631200	-1.81031200
N	-5.85460000	0.82204900	-2.03472300
H	5.52872600	1.11725500	-0.38052600
H	5.30492700	-1.05103900	0.61664800
H	5.50435000	-1.65916900	-1.04156500
H	5.10364700	0.50197800	-1.99345400
H	0.90139900	-4.19927600	1.14322800
H	2.31587800	-3.13526400	0.93159200
H	0.56561100	-4.37804000	-1.21539500
H	2.28967300	-3.94357200	-1.29314200
O	1.42272000	-0.25612900	-0.42949900
C	-0.12913300	2.62644600	0.44182800
C	-0.65090500	3.64267600	1.25347400
C	0.99377200	2.88868300	-0.35453700

C	-0.06429000	4.90208600	1.26890300
H	-1.53695200	3.44218700	1.84926700
C	1.58764700	4.14483900	-0.31869700
H	1.43219700	2.09435200	-0.94856900
C	1.05895300	5.15321800	0.48399200
H	-0.48502100	5.68723300	1.88862100
H	2.47366300	4.33103200	-0.91661700
H	1.52176200	6.13502000	0.49915200
C	-1.11620400	0.70073600	1.60767000
H	-0.77375000	1.11423200	2.55037500
C	-1.81989500	-0.55401400	1.59035400
H	-2.58996600	-0.73557600	0.84425200
N	-1.65211200	-1.50373500	2.45901800
C	-0.57361400	-1.46040200	3.44623200
H	0.36651600	-1.58781100	2.90105200
H	-0.58943400	-0.51230000	3.98367400
H	-0.72264300	-2.27330900	4.15621800
C	-2.25879200	-2.81158500	2.22905800
H	-3.01990600	-2.72423800	1.45287000
H	-1.46532200	-3.47790700	1.87853000
H	-2.69685300	-3.18726500	3.15570300

#### INT5

C	3.79278300	3.10801500	-0.09608400
C	4.55177600	1.98459200	-0.83220100
B	2.42386100	1.34040400	-0.42014000
O	2.43729400	2.68452200	-0.09932700
O	3.67891200	0.86487200	-0.76349900
C	1.93155900	-2.26328400	-2.26040800
C	2.98839300	-2.22045000	-1.14657800
B	1.26606100	-0.80831300	-0.59974500
O	1.09011000	-1.16494400	-1.97760700
O	2.30728200	-1.62856600	-0.05218400
C	-0.33140800	-2.68081500	0.01718700
C	-1.48282300	-3.26729300	-0.30246200
C	-2.68005900	-2.45084400	-0.53769100
C	-2.58082800	-1.11592300	-0.60076700
C	-1.26575800	-0.41053500	-0.41752000
N	-0.18873500	-1.25877300	0.19774200
H	0.58643000	-3.22550700	0.20596800
H	-1.54400000	-4.34385300	-0.40263200
H	-3.44839200	-0.49104600	-0.79198400

H	-0.90941200	-0.05145300	-1.39110400	O	3.02559300	2.62049000	0.54604800
C	-1.45206600	0.72082400	0.57918800	O	3.99797900	0.83455800	-0.52970400
C	-3.94905200	-3.10559200	-0.71116400	C	2.86686800	-1.74505800	-1.87206800
N	-4.96071900	-3.65097700	-0.84591900	C	3.12389200	-2.42363100	-0.50860800
H	4.13538800	3.21601800	0.93991900	B	1.60623900	-0.69831300	-0.26586800
H	5.50797700	1.74034200	-0.36259200	O	1.72694600	-0.93423300	-1.66657200
H	4.73299800	2.23821700	-1.88306500	O	2.43117200	-1.63526900	0.44036500
H	3.88308400	4.07662700	-0.59426600	C	-0.18828300	-2.46536100	-0.23176500
H	3.35594400	-3.21334200	-0.86587700	C	-1.21571600	-2.92555700	-0.93899800
H	3.83732200	-1.58840300	-1.43262400	C	-2.28172600	-2.01170900	-1.36602900
H	1.36058000	-3.20401600	-2.23338600	C	-2.14544400	-0.69041700	-1.19366600
H	2.36574600	-2.15630700	-3.25941900	C	-0.91374300	-0.09771200	-0.57019000
O	1.30424700	0.60624100	-0.36762500	N	-0.01925400	-1.08019800	0.12847700
C	-2.19668900	1.93588400	0.21075800	H	0.61725700	-3.09433100	0.12525300
C	-3.13631600	2.49152800	1.08572000	H	-1.27941700	-3.97580500	-1.19514000
C	-1.95812400	2.55650600	-1.02114500	H	-2.92540000	0.00359600	-1.49252200
C	-3.82028800	3.65136400	0.73870600	H	-0.31072100	0.39171500	-1.34646900
H	-3.33529900	1.99729400	2.03204000	C	-1.30411600	0.88134500	0.52272100
C	-2.64241600	3.71721400	-1.36423800	C	-3.47481500	-2.55956100	-1.95381000
H	-1.20656100	2.14867800	-1.69060200	N	-4.42763000	-3.02088100	-2.42121100
C	-3.57591500	4.26511600	-0.48749700	H	4.81228300	3.57869900	0.94484700
H	-4.55030500	4.07207500	1.42247300	H	5.70793100	1.40425200	0.46946600
H	-2.44230700	4.19801100	-2.31608000	H	5.61713600	1.91151900	-1.23203700
H	-4.11261600	5.16807100	-0.75964200	H	4.19022100	3.76725600	-0.70885200
C	-0.91028500	0.41816300	1.75283100	H	2.73972500	-3.45533700	-0.49718800
H	-0.91033900	1.05120500	2.63238000	H	4.18903000	-2.45685800	-0.25824800
C	-0.23995400	-0.92546400	1.77852800	H	2.66951000	-2.47196900	-2.66722800
H	-0.92178800	-1.70178400	2.15327600	H	3.71947400	-1.12076600	-2.16122200
N	0.93798800	-1.00099600	2.52418500	O	1.69634000	0.66446300	0.18254700
C	1.94302400	0.05045900	2.49260600	C	-2.04844500	2.11338200	0.21444000
H	1.48692100	0.99940000	2.20542000	C	-2.91399900	2.67383600	1.16254500
H	2.36912300	0.15189500	3.49741100	C	-1.91393800	2.74200100	-1.02921700
H	2.75005900	-0.18059200	1.78621100	C	-3.60977100	3.84234600	0.88211300
C	1.46488100	-2.31324900	2.84426500	H	-3.05100800	2.17465500	2.11712000
H	0.63904500	-3.02165500	2.96287600	C	-2.61462900	3.91073200	-1.31014300
H	2.14864300	-2.67918100	2.06788000	H	-1.24109200	2.33085100	-1.77565000
H	2.00701500	-2.26021800	3.79452800	C	-3.46250500	4.46488400	-0.35616200
				H	-4.27754800	4.26311300	1.62670700
				H	-2.49378300	4.38994000	-2.27602400
				H	-4.01091300	5.37457000	-0.57710200
				C	-0.90529100	0.44862200	1.71609700
				H	-1.03594300	0.97294200	2.65544100
				C	-0.17171700	-0.85715100	1.68691600
				H	0.85724800	-0.74805500	2.03920600
<b>INT5-iso</b>							
C	4.30673800	3.06385300	0.12382600				
C	5.03870200	1.77765900	-0.31426800				
B	2.85364600	1.33697000	0.06989000				

N	-0.78469000	-1.88550600	2.43472700	H	-2.38089400	-3.43569000	-1.97361700
C	-2.20290600	-2.15427000	2.30129400	H	-1.62178400	-1.83516200	-1.99676700
H	-2.60840600	-2.46458300	3.27068000	C	-2.37023800	-3.70291500	0.67814200
H	-2.72677700	-1.25026400	1.98423200	H	-2.81010400	-3.46649400	1.65154600
H	-2.41414700	-2.95054800	1.57331400	H	-3.03186700	-4.40842100	0.16823500
C	0.01085700	-3.03102200	2.82979000	H	-1.40379200	-4.21033300	0.84694900
H	1.07275200	-2.78114100	2.76649200				
H	-0.22730200	-3.31670100	3.86093900				
H	-0.17284200	-3.90728500	2.18955600				

**INT6**

C	-2.80663900	0.56667100	-0.20218900
C	-2.75819600	1.91663100	-0.28691300
C	-1.47330700	2.55001400	-0.00540900
C	-0.32298300	1.84546500	0.01162300
C	-0.37881500	0.42062900	-0.48053100
N	-1.66160200	-0.17062500	-0.11978500
H	-3.73167400	-0.00279700	-0.17074600
H	-3.65387000	2.51160700	-0.39199300
H	0.61256300	2.27493100	0.35404800
H	-0.26218000	0.41384700	-1.58326900
C	0.60853600	-0.55037000	0.13791100
C	-1.46781200	3.93803600	0.38357100
N	-1.47562500	5.05606800	0.68268300
C	2.06147600	-0.33444600	0.04749500
C	2.94209400	-0.98747500	0.91950500
C	2.59151600	0.53738500	-0.91190500
C	4.31259700	-0.78934700	0.82195300
H	2.54370100	-1.63970800	1.69069600
C	3.96515600	0.73558700	-1.00906200
H	1.92732300	1.06270900	-1.59238300
C	4.82969000	0.07182800	-0.14485600
H	4.98039500	-1.29998600	1.50831400
H	4.35843700	1.41345700	-1.75949500
H	5.90070600	0.23026600	-0.21660300
C	-0.04428400	-1.56601400	0.71181700
H	0.41679800	-2.42199200	1.19200900
C	-1.54880200	-1.43369000	0.59191500
H	-2.01878200	-1.37347400	1.58557900
N	-2.25510800	-2.49440900	-0.11779900
C	-1.70192700	-2.76915300	-1.43503100
H	-0.70701200	-3.24299600	-1.39641300

**INT6-iso**

C	-2.55190400	0.16451100	-1.22136600
C	-2.68728300	1.47538900	-0.89919900
C	-1.63273100	2.06646500	-0.08289200
C	-0.42205900	1.47949800	0.03257800
C	-0.15236100	0.32012700	-0.89468600
N	-1.36306700	-0.48231100	-1.04296800
H	-3.37286500	-0.42928100	-1.61558100
H	-3.60617000	2.01261700	-1.08527500
H	0.32078200	1.81301200	0.74956000
H	0.13351300	0.71207200	-1.88916800
C	0.86365000	-0.70122500	-0.42958900
C	-1.95342200	3.22439200	0.71273000
N	-2.22122000	4.16074600	1.33810900
C	2.26785300	-0.33440700	-0.18661600
C	3.12221900	-1.18574400	0.52714700
C	2.77594700	0.88247800	-0.65772500
C	4.44805500	-0.83851700	0.74582000
H	2.73659900	-2.11876800	0.92623200
C	4.10475100	1.23120900	-0.43586400
H	2.13106700	1.56330700	-1.20573300
C	4.94536400	0.37162300	0.26348700
H	5.09489500	-1.50895700	1.30222500
H	4.48120000	2.17745800	-0.81019100
H	5.98069900	0.64410300	0.43940900
C	0.28602000	-1.90044400	-0.31079800
H	0.76791700	-2.82486200	-0.01647900
C	-1.19761400	-1.87371500	-0.58371000
H	-1.47408800	-2.56405200	-1.39344200
N	-1.95946200	-2.27951900	0.57943800
C	-1.83831500	-1.37516300	1.71343700
H	-2.28965400	-1.84620900	2.59063300
H	-0.78516900	-1.18385100	1.93022400
H	-2.33831300	-0.40768600	1.54091700
C	-3.34783100	-2.61693800	0.31604000

H	-3.41497700	-3.24617200	-0.57598900
H	-3.74500600	-3.18630400	1.16167000
H	-3.99622900	-1.73606800	0.17616700

**INT7**

C	2.34481000	0.83993800	-1.39801700
C	2.33910800	2.15351800	-1.12149900
C	1.22329700	2.74469100	-0.38174300
C	0.07180000	1.97713600	-0.21894900
C	0.07438000	0.62225600	-0.51729100
N	1.34783500	0.00054700	-0.85639800
H	3.09091800	0.35775700	-2.02181500
H	3.11825300	2.79422900	-1.51641400
H	-0.85397600	2.44683500	0.09950200
H	0.29917800	-0.22769400	1.28405200
C	-0.91488800	-0.38171100	-0.67923700
C	1.25131300	4.10638000	0.00974600
N	1.28546800	5.22033700	0.34602600
C	-2.35153600	-0.21260100	-0.39263100
C	-3.30960100	-0.81076700	-1.22025900
C	-2.79323700	0.51716500	0.71876100
C	-4.66632700	-0.67797100	-0.94849500
H	-2.97600000	-1.36511200	-2.09213200
C	-4.15101500	0.65312100	0.98867100
H	-2.06267700	0.97431800	1.38108200
C	-5.09350900	0.05540800	0.15635300
H	-5.39414400	-1.14274500	-1.60616400
H	-4.47272200	1.22449000	1.85366000
H	-6.15280700	0.16146500	0.36590400
C	-0.31928400	-1.54851900	-1.10854500
H	-0.84647400	-2.44880100	-1.39162000
C	1.16267200	-1.37583500	-1.21816700
H	1.61591900	-1.63045400	-2.20350800
N	1.92516300	-2.26273100	-0.21049700
C	1.59158300	-3.67241100	-0.40582300
H	1.82481200	-4.00354200	-1.43021400
H	2.16487700	-4.28771800	0.29220300
H	0.52741700	-3.82660500	-0.22082700
C	3.36857600	-2.05860000	-0.34228700
H	3.71780000	-2.29616000	-1.36006500
H	3.61624400	-1.01765200	-0.12366900
H	3.90058400	-2.70351600	0.36256400

N	0.94437000	-0.83067100	1.83355400
C	0.19032200	-1.59953900	2.83660100
H	0.86985400	-2.27277700	3.36258100
H	-0.28208800	-0.92549800	3.55380100
H	-0.57482300	-2.17681000	2.31527700
C	2.01049200	0.03998700	2.36989200
H	2.78966000	-0.57935700	2.81902900
H	2.41484200	0.62399800	1.54001500
H	1.59733900	0.71449000	3.12229300
H	1.37442400	-1.51539400	1.06318700

**product(P)**

C	2.89223300	-1.50929800	0.09859100
C	3.45742400	-0.28343500	0.00263200
C	2.62116100	0.87928400	-0.10374900
C	1.25489600	0.75053400	-0.08536600
C	0.66883700	-0.52699400	0.04495700
N	1.52177600	-1.64308700	0.10798300
H	3.45835700	-2.43002900	0.16627900
H	4.53459400	-0.18173000	-0.00331800
H	0.61020900	1.61668900	-0.18133700
C	-0.64646300	-1.00169200	0.07429200
C	3.22433300	2.17411500	-0.23936400
N	3.71992900	3.21509200	-0.34745700
C	-1.87028700	-0.18829200	0.04291300
C	-1.96143600	1.00999200	0.76255700
C	-2.98189200	-0.61143200	-0.69649700
C	-3.12418800	1.77265700	0.72773000
H	-1.12544400	1.32482300	1.38039000
C	-4.14766300	0.14560000	-0.72094900
H	-2.91725300	-1.53290800	-1.26807100
C	-4.22135000	1.34352400	-0.01393500
H	-3.17699600	2.69737700	1.29351000
H	-4.99863900	-0.19538200	-1.30217400
H	-5.12979700	1.93634600	-0.03721100
C	-0.56282500	-2.40943900	0.14035700
H	-1.40166800	-3.08878700	0.19664000
C	0.76718400	-2.77871000	0.16553400
H	1.23491700	-3.74892500	0.23338900

**INT-A**

C	-3.38191400	0.66274100	2.13910100	H	3.79980900	3.35362700	0.53921000
C	-3.00485100	1.84702200	1.22605700	H	3.31923200	4.85235800	-0.27195700
B	-1.37638600	0.27446000	1.18243800	H	2.45553600	4.31812800	1.18928800
O	-2.20489800	-0.13709800	2.19948300				
O	-1.83437700	1.40543900	0.53653000				
C	-1.15408100	-3.03374100	-0.57526700				
C	-2.42247100	-2.37719100	-0.51062000				
C	-2.53575400	-1.13332800	-1.16957000				
C	-1.42250100	-0.53966100	-1.70735700				
C	-0.08261800	-1.11605700	-1.41746600				
N	-0.06734500	-2.51371600	-1.04148400				
H	-1.09179900	-4.06699500	-0.23327600				
H	-3.27726900	-2.84636900	-0.04156800				
H	-1.50804000	0.39399300	-2.25077400				
H	0.59522600	-0.97691700	-2.26852700				
C	0.60823500	-0.28587800	-0.22025700				
C	-3.80749900	-0.45703100	-1.22380500				
N	-4.81881300	0.10629300	-1.21349900				
H	-3.66681000	0.97687800	3.14605900				
H	-2.75870600	2.74776600	1.79870900				
H	-3.78719600	2.08081700	0.50054400				
H	-4.19780900	0.07132900	1.70808600				
O	-0.25573900	-0.43780000	0.90339400				
C	1.92410500	-0.97410000	0.12125700				
C	2.95403400	-1.00692600	-0.82368700				
C	2.11784600	-1.59176700	1.35429200				
C	4.15562800	-1.64340500	-0.53932500				
H	2.81859600	-0.51564600	-1.78354500				
C	3.32579100	-2.22509500	1.64095400				
H	1.31732600	-1.57701400	2.08362400				
C	4.34660300	-2.25551500	0.69818800				
H	4.94483700	-1.66104800	-1.28446300				
H	3.46404600	-2.69955300	2.60754400				
H	5.28525300	-2.75230600	0.92194200				
C	0.78168600	1.15727100	-0.61688400				
H	-0.07677400	1.63157500	-1.07454900				
C	1.86088100	1.89203300	-0.29454700				
H	2.69858600	1.43415600	0.22618200				
N	2.05390200	3.22115800	-0.59406000				
C	0.92874500	3.95217700	-1.13536300				
H	0.06788000	3.95406500	-0.44891800				
H	1.23115300	4.98172700	-1.33545200				
H	0.61033600	3.49798400	-2.07841400				
C	2.94553600	3.97656100	0.26531500				
				<b>INT3-iso2</b>			
				C	5.26272100	0.48780500	1.44774300
				C	5.46953500	-1.03927100	1.54847700
				B	3.33537400	-0.58196200	1.03115800
				O	3.84891100	0.64858900	1.34419400
				O	4.25318000	-1.59856900	1.05603700
				C	0.74532000	-2.98675100	-1.38667800
				C	-0.05761500	-4.11025600	-0.69988100
				B	-1.15369700	-2.15206900	-0.51509800
				O	-0.15055700	-1.87186700	-1.41147600
				O	-1.10567900	-3.43014000	-0.01097400
				C	-3.35022500	-1.73595200	0.42945600
				C	-4.50947500	-1.06091100	0.44985300
				C	-4.55682200	0.24085900	-0.21627100
				C	-3.44557700	0.81242300	-0.71079300
				C	-2.09050700	0.18395700	-0.54958800
				N	-2.19521200	-1.23557300	-0.16345200
				H	-3.24896100	-2.73491300	0.83957000
				H	-5.39730800	-1.47827300	0.90342000
				H	-3.49116100	1.77512700	-1.20839400
				H	-1.56629700	0.19688800	-1.51323200
				C	1.17836200	0.20484400	0.36358000
				C	-5.82759900	0.90261000	-0.35834000
				N	-6.85804200	1.41939500	-0.46353300
				H	5.62975800	1.02555700	2.32457100
				H	5.61879900	-1.36502600	2.58335700
				H	6.30736800	-1.39373400	0.94392200
				H	5.73261700	0.90715500	0.55193600
				H	-0.49864800	-4.80272700	-1.42475600
				H	0.54064300	-4.67872300	0.01532700
				H	1.03682500	-3.24002100	-2.40903700
				H	1.63232900	-2.70931800	-0.80854200
				O	2.02742900	-0.82502400	0.72932000
				C	1.68976400	1.06943900	-0.73047000
				C	2.16498600	0.48206100	-1.90663900
				C	1.73253500	2.45861000	-0.58930300
				C	2.65571000	1.27814100	-2.93633400
				H	2.12444700	-0.59786100	-2.01182700



C	2.22158200	3.25263600	-1.62101800
H	1.39824300	2.90261500	0.34402400
C	2.68223700	2.66379900	-2.79643200
H	3.01271700	0.81767800	-3.85203700
H	2.25459300	4.33092400	-1.50290400
H	3.06473300	3.28403000	-3.60070200
C	-0.03604200	0.25487100	0.91105200
H	-0.25286300	-0.47682100	1.68601800
C	-1.18234600	1.07938100	0.38429000
H	-0.78551400	1.84101100	-0.29531100
N	-1.94293500	1.81558800	1.38918100
C	-1.20000000	2.96232100	1.87961900
H	-0.93371000	3.61815200	1.04449800
H	-1.82946100	3.53132400	2.56973100
H	-0.27239800	2.68195300	2.41201400
C	-2.42715000	1.00785700	2.49655500
H	-2.95004400	0.12464200	2.12522300
H	-1.62270800	0.68218400	3.17896200
H	-3.14169200	1.59770000	3.07842800

**INT-C**

C	-4.79387500	0.24467000	-0.74437600
C	-4.78836900	-0.16867800	0.73870500
B	-2.75023800	-0.57415100	-0.16394100
O	-3.42332300	0.20730000	-1.12242500
O	-3.57786100	-0.88578400	0.89853600
C	-0.71811500	-1.38581000	3.06295000
C	-1.52311000	-2.61302600	2.61375800
B	-0.67621100	-1.50124700	0.78007800
O	-0.66238100	-0.57361000	1.90844800
O	-1.20628900	-2.75849200	1.24889400
C	1.12102100	-2.75500700	-0.50153900
C	2.33239200	-2.96393100	-1.08819500
C	3.35666200	-1.98819400	-0.79609000
C	3.12966800	-0.90862500	-0.01542700
C	1.74999300	-0.62015200	0.53100200
N	0.79704500	-1.68608100	0.25495500
H	0.31000100	-3.47232100	-0.60119900
H	2.54862500	-3.84810900	-1.66777900
H	3.92244400	-0.20782900	0.22258900
H	1.80051300	-0.43723000	1.61501700
C	1.27651500	0.70419800	-0.08724800

C	4.68604900	-2.18487300	-1.32300000
N	5.74602000	-2.34341300	-1.76035000
H	-5.36153900	-0.46435900	-1.35904100
H	-5.63879600	-0.80241700	1.00265400
H	-4.78595600	0.70659800	1.39983900
H	-5.20212700	1.24766300	-0.90384700
H	-1.25204100	-3.51661500	3.17234500
H	-2.59899600	-2.42809800	2.73529100
H	0.29673600	-1.68535900	3.37530100
H	-1.18805500	-0.83909100	3.88818400
O	-1.47920400	-0.92776800	-0.34154400
C	1.53380000	1.95999500	0.62904200
C	2.15354400	3.03454200	-0.02481100
C	1.17437300	2.08098100	1.98034000
C	2.41674700	4.21418900	0.66358100
H	2.45805600	2.91930600	-1.06136000
C	1.42597800	3.27000900	2.65390500
H	0.64780600	1.25599800	2.45251900
C	2.05172500	4.33241700	2.00238400
H	2.91353300	5.03581100	0.15828100
H	1.13122100	3.36989300	3.69331400
H	2.25680800	5.25268100	2.53974300
C	0.64114300	0.62286700	-1.28705100
H	0.56151700	-0.35670300	-1.74246200
C	-0.24446400	1.64380600	-1.70165700
H	-0.24343100	2.59884500	-1.18123400
N	-1.15891200	1.48461000	-2.61686100
C	-1.31016500	0.21264900	-3.33522000
H	-1.41298200	-0.59186900	-2.60356800
H	-2.21219000	0.27054500	-3.94107700
H	-0.44229000	0.04661100	-3.97767200
C	-2.17227100	2.50212000	-2.86942500
H	-1.94504900	3.39725300	-2.29088900
H	-2.18615900	2.74741600	-3.93380000
H	-3.13746600	2.09450100	-2.56110000

**INT-D**

C	-2.83546700	-1.58811100	-0.34877800
C	-3.34876000	-0.28405400	-0.30823200
C	-2.57641600	0.82760500	-0.07287900
C	-1.10035700	0.68166200	0.20430400
C	-0.61340000	-0.57930500	-0.51762500

N	-1.49391000	-1.74549700	-0.25261100
H	-3.44567500	-2.47919700	-0.35903200
H	-4.42104900	-0.16506700	-0.42291600
H	-0.55707700	1.52265400	-0.24672500
H	-0.73004300	-0.38117900	-1.59442100
C	0.76017200	-1.10574500	-0.20860100
C	-3.16112900	2.11198700	0.09254600
N	-3.61401800	3.17557300	0.20716400
C	1.95420100	-0.27246000	-0.18239900
C	3.05655100	-0.62887600	0.61455100
C	2.03143700	0.91312100	-0.93201000
C	4.19292600	0.16555600	0.65043800
H	3.00096200	-1.52461000	1.22581800
C	3.16931200	1.71214400	-0.88562900
H	1.21118400	1.19287600	-1.58669100
C	4.25383700	1.34259500	-0.09648600
H	5.03132100	-0.12504600	1.27513100
H	3.20942200	2.62165600	-1.47591300
H	5.14045000	1.96645600	-0.06019500
C	0.63417700	-2.43429300	0.05940000
H	1.43853500	-3.12410300	0.27906300
C	-0.74081500	-2.80898200	0.02202600
H	-1.19049200	-3.77238500	0.21279400
O	-0.88027900	0.63906100	1.59589600
H	0.05258300	0.82786300	1.76029300

**INT-E**

C	2.85354800	1.72460600	-0.12408800
C	3.38547300	0.33496000	0.00440000
C	2.61770400	-0.75683400	-0.00344600
C	1.11516700	-0.74120300	-0.16988100
C	0.58201800	0.66510200	-0.18108400
N	1.40697900	1.75790700	-0.12434200
H	3.22573900	2.33219000	0.70941900
H	4.46240100	0.23839000	0.09993600
H	0.90462100	-1.22527400	-1.13699200
C	-0.72671900	1.11742700	-0.14565700
C	3.22314100	-2.05719400	0.12328100
N	3.71945400	-3.09908900	0.20353300
C	-1.94541100	0.29041300	-0.12373900
C	-3.02732300	0.65541700	0.68850000
C	-2.06068400	-0.87295300	-0.89830400

C	-4.17994600	-0.12004600	0.73150500
H	-2.94570800	1.54682400	1.30319200
C	-3.20899400	-1.65870800	-0.84218600
H	-1.25733200	-1.14502900	-1.57762900
C	-4.27346100	-1.28501900	-0.02739800
H	-5.00496400	0.17913200	1.37019000
H	-3.27573400	-2.55574800	-1.44948900
H	-5.17008900	-1.89431900	0.01394400
C	-0.66963500	2.53853000	-0.06330300
H	-1.51530300	3.21036700	-0.03662500
C	0.65274500	2.90020700	-0.06078200
H	1.12600400	3.87046900	-0.02877200
O	0.58378500	-1.52005700	0.87955900
H	-0.37071600	-1.59349700	0.74248000
H	3.24003600	2.17698200	-1.04737300

**INT-F**

C	2.71530000	1.64861900	-0.10039900
C	3.32905300	0.47730800	-0.25317100
C	2.51336600	-0.77481000	-0.51008800
C	1.14670900	-0.70481600	0.19949700
C	0.50668500	0.61600400	-0.10906100
N	1.31758200	1.73144200	-0.12939300
H	3.23460100	2.58663500	0.05474400
H	4.40855500	0.41121300	-0.22049300
H	0.51348200	-1.52605500	-0.15535400
C	-0.80540000	1.04348800	-0.15502700
C	3.24479900	-1.98705100	-0.11736700
N	3.83526100	-2.94060600	0.15797200
C	-2.01481800	0.20190000	-0.12734800
C	-3.10516200	0.56569400	0.67209900
C	-2.10967500	-0.96175100	-0.90062000
C	-4.25258200	-0.21909100	0.70745600
H	-3.03831400	1.46472500	1.27809100
C	-3.25324100	-1.75237300	-0.85683900
H	-1.29070500	-1.22658000	-1.56319900
C	-4.32814700	-1.38437000	-0.05185200
H	-5.08758200	0.07613700	1.33481900
H	-3.30996100	-2.65040600	-1.46358400
H	-5.22194000	-1.99870300	-0.02113800
C	-0.77232100	2.47330400	-0.20798200
H	-1.63061800	3.12464900	-0.28528400

C	0.54070700	2.86183200	-0.19325600
H	0.99603700	3.83926000	-0.25100000
O	1.41524200	-0.83673700	1.58141200
H	0.58408200	-0.71161400	2.05447900
H	2.31888200	-0.85453800	-1.58967400

**INT-G**

C	2.64582000	-1.13034500	1.24931500
C	3.22703700	-0.13886800	0.27783200
C	2.19553400	0.98542600	0.04140700
C	0.90427000	0.90599500	0.39106100
C	0.28669600	-0.37352100	0.94781000
N	1.34679300	-1.39485600	0.79920700
H	2.60286300	-0.70801300	2.25577200
H	4.11800500	0.32761100	0.72255900
H	0.22874500	1.74634800	0.25833500
H	-0.02504100	-0.25001500	1.99214700
C	-0.79323700	-0.84288600	0.01782900
C	2.68555000	2.20949600	-0.53185000
N	3.11405400	3.18616900	-0.98285200
C	-2.13866100	-0.27667100	-0.00313400
C	-3.09195700	-0.71706900	-0.93517000
C	-2.50228000	0.73856600	0.89393900
C	-4.36210300	-0.16181100	-0.96545700
H	-2.83188700	-1.49841000	-1.64200900
C	-3.77741900	1.29243800	0.86332400
H	-1.78708900	1.10040500	1.62691700
C	-4.71140200	0.84549200	-0.06564800
H	-5.08500400	-0.51425600	-1.69370700
H	-4.03928200	2.07586000	1.56660100
H	-5.70574200	1.27832700	-0.09130300
C	-0.26437400	-1.85659600	-0.72823700
H	-0.74844000	-2.40591100	-1.52360900
C	1.04260600	-2.14983000	-0.24027000
H	1.75839500	-2.87392200	-0.60121700
O	3.51465400	-0.67123600	-1.00320300
H	4.09483000	-1.42622700	-0.83586300

**INT-H**

C	-2.67457200	-1.10997400	0.84562600
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C	-3.16351200	0.09455100	0.48157100
C	-2.27299500	0.98894700	-0.25332000
C	-1.10434900	0.56487200	-0.77541500
C	-0.78692500	-0.90027400	-0.75089100
N	-1.45845700	-1.53550700	0.39009900
H	-3.18776700	-1.77882000	1.52973800
H	-4.13125100	0.43576300	0.81859400
H	-0.40892700	1.25043600	-1.24686100
H	-1.12821800	-1.38887900	-1.67976100
C	0.70928200	-1.33915300	-0.60612300
C	-2.63016600	2.38235500	-0.34138900
N	-2.93659300	3.49623200	-0.40895600
C	1.61904300	-0.22630900	-0.09029400
C	1.63082600	0.10802900	1.26610500
C	2.39942600	0.51636600	-0.97859500
C	2.41988600	1.15665500	1.72693400
H	1.02000000	-0.46020600	1.96120600
C	3.19311600	1.56338600	-0.51558100
H	2.37172600	0.27739300	-2.03668000
C	3.20714600	1.88482400	0.83799100
H	2.41970000	1.40616300	2.78308800
H	3.79762300	2.13041900	-1.21627200
H	3.82386100	2.70143300	1.19876300
C	0.58975000	-2.49189500	0.37733300
H	1.42042000	-3.12407200	0.65937600
C	-0.63477500	-2.52365700	0.91170100
H	-1.02583800	-3.18232600	1.67862500
O	1.09624200	-1.74644300	-1.90840700
H	2.01698800	-2.03317300	-1.86447700

**INT-I**

C	-2.68958700	-1.59583200	-0.63318300
C	-3.37552400	-0.44345600	-0.78778200
C	-2.74032700	0.79163500	-0.32999700
C	-1.43425100	0.84340700	-0.00219800
C	-0.57748800	-0.35118800	-0.28911500
N	-1.38440600	-1.57560100	-0.22722500
H	-3.12972200	-2.57641900	-0.78493200
H	-4.40300500	-0.44121700	-1.12090600
H	-0.98425500	1.72739800	0.43389000
H	-0.14174600	-0.28606900	-1.30232100
C	0.59459300	-0.62910300	0.69203600

C	-3.57173700	1.95365200	-0.14220200
N	-4.25153000	2.88047100	-0.00754900
C	1.89424500	-0.00906100	0.19964200
C	2.64776800	-0.63345900	-0.79789300
C	2.32789900	1.21382100	0.71306900
C	3.81477000	-0.04527200	-1.27317900
H	2.31441300	-1.58716600	-1.19814400
C	3.49780700	1.80212300	0.23748100
H	1.74192900	1.69890900	1.48653100
C	4.24390100	1.17505800	-0.75521500
H	4.39285000	-0.54211400	-2.04575100
H	3.82460100	2.75374900	0.64439000
H	5.15597500	1.63300100	-1.12383000
C	0.57795100	-2.15118100	0.72993700
H	1.35282400	-2.75070200	1.18751900
C	-0.59743400	-2.59957900	0.27038300
H	-0.97991900	-3.61363200	0.25613400
O	0.21993600	-0.08774000	1.95229600
H	0.87260800	-0.37730100	2.60177000

**INT-J**

C	2.57607800	1.68518900	0.52485700
C	3.16284200	0.45115100	0.61459700
C	2.64449400	-0.71533100	0.05732100
C	1.20396000	-0.80086700	-0.36979400
C	0.58479900	0.58067200	-0.37596800
N	1.49023100	1.73721300	-0.49880700
H	2.99032500	2.64409100	0.78329300
H	4.10841200	0.38906100	1.14723200
H	1.12748700	-1.22599100	-1.38518400
H	1.90974500	1.68121800	-1.44704200
C	-0.67020800	1.04082300	-0.21897200
C	3.36484100	-1.93225900	0.09273700
N	3.95579400	-2.93496000	0.08366200
C	-1.90723900	0.24988700	-0.08394700
C	-2.84844300	0.57582300	0.89542400
C	-2.16746700	-0.81471400	-0.95439300
C	-4.01713700	-0.16837500	1.02071700
H	-2.64984900	1.39799400	1.57699500
C	-3.33537700	-1.55889800	-0.82697300
H	-1.45870000	-1.04031300	-1.74804200
C	-4.26107300	-1.23823000	0.16370600

H	-4.73572600	0.08423600	1.79322900
H	-3.52724600	-2.38252700	-1.50666300
H	-5.17213000	-1.81849800	0.26383700
C	-0.62433500	2.50879300	-0.21603900
H	-1.48612800	3.15148600	-0.09431100
C	0.63566200	2.91116900	-0.38805300
H	1.09496600	3.88624100	-0.43898600
O	0.48873000	-1.62912500	0.53314700
H	-0.28155400	-1.99875800	0.08516400

**INT-K**

C	-2.81465300	-0.46283700	-0.96197900
C	-1.43521800	-0.88345000	-1.37644700
C	-0.55111800	-1.47467200	-0.55764200
C	-0.76761100	-1.61437500	0.95806300
C	-1.20815000	-0.25092900	1.46613600
N	-3.27544900	0.61398000	-0.47572300
H	-3.56018700	-1.25216600	-1.12080100
H	-1.20658400	-0.81440800	-2.43769100
H	-1.62596800	-2.29232500	1.09392100
H	-2.22268900	-0.20791000	1.85260900
C	-0.66434800	0.89662000	1.01497700
C	0.69582800	-1.94120700	-1.10550700
N	1.69269100	-2.29495600	-1.57518900
C	0.73090000	0.98367000	0.51924200
C	1.02116000	1.61310700	-0.69974600
C	1.77951000	0.41473800	1.24989700
C	2.31964900	1.63406400	-1.19132500
H	0.21207800	2.05448700	-1.27415600
C	3.08067100	0.44184200	0.75966100
H	1.56168500	-0.05051600	2.20381100
C	3.35248200	1.04420200	-0.46422500
H	2.52725500	2.10380900	-2.14724100
H	3.88154900	-0.01264100	1.33310700
H	4.36564400	1.05536300	-0.85227500
C	-1.55319700	2.01248400	0.66113300
H	-1.26526800	3.04073500	0.86111100
C	-2.62194000	1.80562000	-0.13492500
H	-3.17848800	2.67154300	-0.48874700
O	0.39064600	-2.20238700	1.50571900
H	0.28132200	-2.22330800	2.46309700

**INT-L**

C	2.81619500	1.56139400	0.06599700
C	3.33730200	0.30201000	-0.20186400
C	2.52296500	-0.81724300	-0.27010100
C	1.12856800	-0.77778400	0.27606300
C	0.62036500	0.61336100	0.10254000
N	1.45936100	1.65404300	0.13321200
H	3.38155800	2.47987100	0.10211500
H	4.39550800	0.21148100	-0.42142800
H	0.46997800	-1.47928900	-0.24301700
H	1.05597500	3.49023900	-0.80031500
C	-0.74846400	1.11140700	-0.00499800
C	3.03873300	-2.06221000	-0.73116500
N	3.44648400	-3.07967500	-1.11386700
C	-1.94954200	0.25744800	-0.05251200
C	-2.05935800	-0.87477700	0.76438100
C	-3.00740700	0.59640100	-0.90300000
C	-3.21465700	-1.64926700	0.72474600
H	-1.24803200	-1.13231300	1.43972700
C	-4.15952000	-0.18028600	-0.93661500
H	-2.90961400	1.46163400	-1.55218200
C	-4.26447700	-1.30621200	-0.12317000
H	-3.29395400	-2.52364800	1.36227200
H	-4.97151000	0.08728600	-1.60485300
H	-5.16118700	-1.91657800	-0.15332300
C	-0.71021100	2.46011400	-0.03022900
H	-1.55572200	3.13358300	-0.03353800
C	0.71126900	2.91953100	0.06692800
H	0.90801500	3.50570800	0.97119500
O	1.05360500	-1.18726700	1.65052300
H	1.78866600	-0.76373400	2.11173900

**INT-M**

C	2.82879300	1.59177600	0.17841600
C	3.31295800	0.32694200	-0.36345200
C	2.48781100	-0.73512300	-0.34698200
C	1.12566500	-0.62895900	0.31200200
C	0.65461400	0.81256200	0.30577100
N	1.59903600	1.82727100	0.47509500
H	3.54536900	2.39625200	0.33789700
H	4.32521200	0.25590200	-0.74684200

H	0.40746900	-1.25376600	-0.22229500
H	0.46916200	3.44452900	-0.98501600
C	-0.66151500	1.15392000	0.16571300
C	2.90501100	-2.02358400	-0.81878700
N	3.22209500	-3.06803700	-1.20500800
C	-1.74732400	0.14649000	0.05708100
C	-1.82749100	-0.96654900	0.90590900
C	-2.75752500	0.34095700	-0.89693400
C	-2.87838000	-1.87075300	0.78210400
H	-1.06963700	-1.11229300	1.66875000
C	-3.80053900	-0.56775300	-1.02202900
H	-2.70584300	1.20567800	-1.55226800
C	-3.86344700	-1.67766800	-0.18156100
H	-2.92788000	-2.72626800	1.44767800
H	-4.56540300	-0.41033600	-1.77549800
H	-4.68068100	-2.38546700	-0.27518800
C	-1.12030700	2.55183600	0.09398000
H	-2.10303600	2.72525300	0.52892100
C	-0.48452800	3.57129900	-0.48863600
H	-0.92253300	4.56421200	-0.48714400
O	1.20591300	-1.19236700	1.61638000
H	1.78981000	-0.63177000	2.14378600

**INT-N**

C	1.24119000	2.04181200	-2.51799600
C	1.78390700	2.84978200	-1.30905700
B	0.05758100	1.55812400	-0.66115700
O	0.18245200	1.23951200	-1.99219900
O	0.95150800	2.48321600	-0.21384000
C	-1.68979900	-0.01699500	-0.06894500
H	0.83946200	2.68528000	-3.30568400
H	1.71454300	3.92928100	-1.46739600
H	2.81878300	2.59180500	-1.06929800
H	2.00449300	1.39059700	-2.95365600
O	-0.91452500	1.08151500	0.17275300
C	-3.11634500	0.20634100	0.27226900
C	-3.96012400	-0.85645700	0.61388300
C	-3.63414600	1.50478900	0.26368800
C	-5.29852800	-0.62902900	0.90697200
H	-3.56155000	-1.86398400	0.67808200
C	-4.97413500	1.73078000	0.56004700
H	-2.97876100	2.33474100	0.02511100

C	-5.81176100	0.66587900	0.87766100	H	3.29883000	2.39881600	0.78331400
H	-5.93857600	-1.46333000	1.17489100	H	4.91340900	0.86586500	-0.40150900
H	-5.36351100	2.74358800	0.54424800	H	1.55064700	-1.64750900	-1.48027000
H	-6.85607700	0.84427200	1.11244800	H	0.76755200	0.97214600	-1.71167300
C	-1.21650400	-1.19068500	-0.50982900	C	-0.35052800	0.05127400	-0.14326700
H	-1.93946300	-1.97303400	-0.70802900	C	4.19284600	-1.58368600	-1.35979700
C	0.18778600	-1.57926400	-0.88983700	N	4.93351500	-2.41923700	-1.66409800
H	0.35294100	-1.28216100	-1.93357600	H	-5.08068400	-1.49525200	-1.48153500
N	0.31890200	-3.02422700	-0.83901800	H	-5.07101000	-0.72802400	0.78828200
C	0.18036800	-3.59445800	0.49343400	H	-5.02724800	0.97697400	0.28468400
H	-0.72790400	-3.21534100	0.97047100	H	-5.55122300	0.16437600	-1.90902800
H	0.09198200	-4.68083500	0.40583000	O	-1.29414700	0.01208500	-1.20914800
H	1.03873000	-3.37084600	1.14799300	C	-0.30335500	-1.28970600	0.58525400
C	1.52212900	-3.51413200	-1.48959800	C	0.39747100	-1.39459800	1.78925800
H	2.44618000	-3.25760400	-0.94499900	C	-0.88398200	-2.43381100	0.03738200
H	1.46552600	-4.60337200	-1.56716300	C	0.50326100	-2.61837100	2.44055400
H	1.58814000	-3.10520300	-2.50256400	H	0.87028000	-0.51478100	2.21718600
C	2.41795900	-0.52684300	-0.77686600	C	-0.78159000	-3.65833800	0.69350300
C	3.46729000	0.02337900	-0.11413300	H	-1.40305400	-2.37354300	-0.91428900
C	3.38510800	0.27921500	1.28691200	C	-0.09045900	-3.75447300	1.89648800
C	2.17369600	-0.10290800	1.94174500	H	1.05176100	-2.68414800	3.37462300
C	1.15143800	-0.65898300	1.24456700	H	-1.23924700	-4.54017300	0.25655600
N	1.22815300	-0.84796600	-0.13215900	H	-0.00858300	-4.70971800	2.40458200
H	2.44178300	-0.74290400	-1.83854000	C	-0.56449700	1.20383900	0.79724000
H	4.37202400	0.26333700	-0.66115700	H	-1.46921600	1.30345000	1.38078500
H	2.05812800	0.05609500	3.00690300	C	0.68646000	2.00569000	1.02255200
H	0.21005000	-0.93800000	1.70018200	H	0.99298700	1.97086500	2.08176600
C	4.45931500	0.87062500	1.98858800	N	0.63502200	3.43196300	0.68551500
N	5.34817900	1.36018900	2.55931300	C	0.27740800	3.66984600	-0.70588000

## INT-O

C	-4.80432100	-0.43965000	-1.38865700
C	-4.62131800	-0.02087600	0.08790300
B	-2.62721100	-0.06567400	-0.96480800
O	-3.52634400	-0.24058700	-1.98445100
O	-3.20818400	0.00625700	0.28049000
C	2.98742900	1.52516800	0.21837500
C	3.84716000	0.69496100	-0.40928800
C	3.28841600	-0.52620600	-0.98365800
C	1.95976100	-0.71315100	-1.11119000
C	1.02489600	0.41803200	-0.78914700
N	1.64143800	1.29025600	0.20190500

## INT-P

C	4.77750900	-0.58917600	-1.18666400
C	4.58899100	-0.49825900	0.34470200
B	2.59403700	-0.75753200	-0.67328300
O	3.49351500	-0.94046800	-1.69169700

O	3.17634800	-0.42816200	0.52892200	H	3.17173100	-1.79011400	-1.55261600
C	-2.95686800	-2.07781000	0.90819300	H	4.16821700	0.36214100	-0.73060800
C	-3.84904100	-1.48623500	0.08534100	H	0.42435500	1.21206300	1.28693200
C	-3.36125100	-0.41278100	-0.77638300	H	1.10238300	-1.45275100	1.62912500
C	-2.04521500	-0.17125700	-0.94427400	C	-0.75285600	-1.33261800	0.55436700
C	-1.05046200	-1.13403600	-0.36833400	C	2.70365400	2.31210000	0.46415600
N	-1.62377700	-1.79660600	0.80883900	N	3.04723100	3.41174100	0.57260400
H	-3.24107000	-2.76509400	1.69933600	O	-1.26742400	-1.77008300	1.79585600
H	-4.90388800	-1.71136100	0.14124500	C	-1.63383600	-0.18730700	0.07615900
H	-1.69144300	0.67840200	-1.51795100	C	-1.39782100	0.38489700	-1.17744400
H	-0.77795600	-1.90417600	-1.11041200	C	-2.64633400	0.32782800	0.88281300
C	0.32416500	-0.57747700	0.14372200	C	-2.16685300	1.45519000	-1.61833600
C	-4.33044800	0.45958100	-1.39015100	H	-0.60629600	-0.01257500	-1.80799900
N	-5.12265700	1.14637800	-1.87995100	C	-3.42005600	1.39793500	0.43597200
H	5.08033700	0.37101600	-1.61781000	H	-2.82600300	-0.11553500	1.85464400
H	5.05771200	0.38838400	0.77757200	C	-3.18334300	1.96377500	-0.81190600
H	4.97169100	-1.38616300	0.85897000	H	-1.97348600	1.89309600	-2.59236700
H	5.50753300	-1.34837400	-1.47736700	H	-4.21002100	1.78907000	1.06932400
O	1.25968800	-0.89039200	-0.88265200	H	-3.78547900	2.79845700	-1.15618500
C	0.29962200	0.92896600	0.39334800	C	-0.64818900	-2.44314600	-0.47784700
C	-0.34455900	1.43396700	1.52440200	H	-1.49790800	-3.03318300	-0.79054700
C	0.83867100	1.82166300	-0.53494500	C	0.57925300	-2.47683600	-1.00901000
C	-0.43274200	2.80622800	1.73290300	H	0.95759600	-3.10734400	-1.80550800
H	-0.77151300	0.74537600	2.24731300	H	-0.83459100	-2.60519600	2.00775100
C	0.75419900	3.19546100	-0.32268300				
H	1.31507600	1.44245900	-1.43378100				
C	0.12060200	3.69193200	0.81177400	<b>INT-R</b>			
H	-0.93404900	3.18420500	2.61820400				
H	1.18127200	3.87844700	-1.05015200	C	-2.21197600	-2.84319600	-0.20208700
H	0.05347100	4.76248400	0.97581200	C	-3.44432000	-2.21305500	-0.05643800
C	0.51685700	-1.38170100	1.41753900	C	-3.42378200	-0.82390400	0.11889000
H	1.42346500	-1.33945000	2.00208500	C	-2.21582300	-0.14256700	0.12794200
C	-0.61924800	-2.00618700	1.74350900	C	-1.01630300	-0.86998300	-0.05123400
H	-0.83689300	-2.60200000	2.62254600	N	-1.04272700	-2.21746300	-0.20380100
				H	-2.17237000	-3.92350000	-0.32835700
				H	-4.37384400	-2.76770700	-0.06988600
<b>INT-Q</b>				H	-2.19697800	0.92866900	0.28603500
				C	0.27901800	-0.21948300	-0.04311400
C	2.66505200	-1.13248600	-0.85271200	C	-4.65732800	-0.09947100	0.30046200
C	3.18288700	0.03944300	-0.42784900	N	-5.65011300	0.47692100	0.44344500
C	2.30463700	0.93472700	0.32246600	C	0.35997800	1.26026800	-0.05270600
C	1.11374100	0.52669600	0.80596800	C	1.04886100	1.94617600	0.95750100
C	0.75929900	-0.92677700	0.71700500	C	-0.24104000	2.01080700	-1.07308200
N	1.42326800	-1.53145400	-0.44140500	C	1.13344200	3.33467700	0.94863700

H	1.50756600	1.37459500	1.75962200
C	-0.15895900	3.39914500	-1.08140000
H	-0.77121700	1.49123300	-1.86660300
C	0.52959300	4.06639300	-0.07081300
H	1.66303300	3.84716300	1.74574900
H	-0.63092200	3.96054700	-1.88157700
H	0.59212800	5.14972200	-0.07639700
C	1.44214000	-1.01099600	-0.01047500
H	1.27855700	-2.07947600	0.07660600
C	2.72757500	-0.52385900	-0.12188800
H	2.90162600	0.54177200	-0.24074100
N	3.85531500	-1.28370300	-0.13637000
C	3.76496000	-2.71199000	0.08308500
H	3.06757200	-3.15739300	-0.63118600
H	4.74908400	-3.15841600	-0.06670600
H	3.41762700	-2.94639300	1.09882600
C	5.14591600	-0.66089000	0.07638200
H	5.10145500	0.38249600	-0.24060400
H	5.44837800	-0.69137300	1.13217900
H	5.90926100	-1.17064300	-0.51786200

**INT-S**

C	2.66949700	0.63095500	0.61244600
C	2.62516000	1.96262300	0.34974200
C	1.41357700	2.56398200	-0.12405800
C	0.24785800	1.76630000	-0.18937400
C	0.32293700	0.43370000	0.11279900
N	1.55808500	-0.15524700	0.39834200
H	3.54897900	0.13142700	0.99932800
H	3.50531800	2.57102700	0.51531600
H	-0.70828600	2.20429500	-0.45167200
C	-0.68673200	-0.60010800	0.27068500
C	1.36892200	3.94479900	-0.44830600
N	1.33622500	5.07621900	-0.71303000
C	-2.13743900	-0.38698800	0.11397900
C	-2.76558200	0.73166500	0.67357000
C	-2.91010100	-1.32459600	-0.57859400
C	-4.13815300	0.90913700	0.53670000
H	-2.17795600	1.44786500	1.23978800
C	-4.28254500	-1.14652800	-0.71209100
H	-2.41990100	-2.18267600	-1.02886400
C	-4.89917400	-0.02770100	-0.15743500

H	-4.61439500	1.77794400	0.97927100
H	-4.87016800	-1.87775600	-1.25774100
H	-5.96959600	0.11383700	-0.26616200
C	-0.07006100	-1.75102700	0.60890500
H	-0.57087900	-2.67686300	0.85629900
C	1.43196600	-1.59412100	0.60655500
H	1.89931400	-1.86129700	1.57900000
N	2.05236500	-2.37162000	-0.47595700
C	1.81384900	-3.79337300	-0.26398700
H	0.74708900	-4.01554900	-0.32349400
H	2.31463000	-4.35617200	-1.05436300
H	2.19660200	-4.15396500	0.70896200
C	3.48062600	-2.11765300	-0.58807700
H	3.90023100	-2.79646800	-1.33373500
H	3.66161700	-1.09802700	-0.93194800
H	4.02304800	-2.27947400	0.36378000

**INT-T**

C	2.80768000	-0.25911200	2.39664500
C	3.97466700	0.28144200	1.56270200
B	2.13656100	-0.13240900	0.23632300
O	1.96762000	-0.87487700	1.43984900
O	3.38469500	0.58163300	0.30810400
C	1.30573700	2.17596300	-0.22962600
C	0.40809200	3.18553200	-0.33698200
C	-0.97591600	2.82808700	-0.31574600
C	-1.34373300	1.52164100	-0.21231800
C	-0.37018000	0.45467000	-0.14436400
N	0.96883700	0.85057400	-0.10545300
H	2.37059500	2.36236400	-0.21156200
H	0.72800100	4.21421700	-0.42338100
H	-2.39141300	1.25617300	-0.23869600
C	-0.80579800	-0.87079700	-0.18092000
C	-1.98514400	3.84755300	-0.43608000
N	-2.78492000	4.67837400	-0.53330200
H	4.43157200	1.18037800	1.98782000
H	4.75822300	-0.48031700	1.43682100
H	2.27980400	0.56288300	2.90130900
H	3.11514200	-0.99076900	3.14938900
C	-2.24753000	-1.15647700	0.08155000
C	-2.86418900	-0.73042200	1.26632500
C	-3.01068800	-1.90334000	-0.82422700



C	-4.19852300	-1.02233900	1.52607800	H	-2.66423700	-2.05657000	2.85951700
H	-2.27728600	-0.16920800	1.98864000	H	-3.13303400	-1.21749600	1.35442000
C	-4.34338700	-2.20760800	-0.56166300	C	0.59109400	1.97410600	0.10000300
H	-2.55170700	-2.23634200	-1.75164700	C	0.25936500	3.03342800	-0.75655000
C	-4.94430100	-1.76439400	0.61288800	C	1.28397800	2.26616400	1.28205300
H	-4.65332000	-0.68028500	2.45060600	C	0.63280200	4.33684100	-0.45265000
H	-4.91605600	-2.78334900	-1.28225400	H	-0.28961700	2.81774100	-1.66824600
H	-5.98451500	-1.99658700	0.81702700	C	1.66206400	3.57094100	1.58420800
C	-0.03276400	-2.04930200	-0.48113700	H	1.50921700	1.45663500	1.97100400
H	-0.61274500	-2.96688100	-0.41244800	C	1.33918800	4.61086100	0.71729700
C	1.23787300	-2.27022400	-0.85226100	H	0.37746100	5.14275100	-1.13370700
H	1.60618400	-3.27511400	-1.01647400	H	2.19826200	3.77608700	2.50539600
N	2.23998900	-1.22613400	-1.01420600	H	1.62924600	5.62947700	0.95402300
C	2.09273400	-0.54479000	-2.32778600	C	-1.17628300	0.31740200	-0.66011000
H	1.06378200	-0.20383000	-2.43399200	H	-1.31133700	-0.56878000	-1.27797800
H	2.77468900	0.30940900	-2.35390200	C	-2.25436200	1.04952100	-0.31160500
H	2.33059100	-1.24910800	-3.12903500	H	-2.13142500	1.93625800	0.30793900
C	3.58777800	-1.84643800	-0.93427800	N	-3.57128300	0.75395900	-0.61674300
H	3.69335800	-2.28523600	0.05867600	C	-3.81220100	-0.36057100	-1.50698100
H	3.67153100	-2.62327900	-1.69861900	H	-3.34711400	-1.26676500	-1.10336700
H	4.34045400	-1.07468800	-1.08558600	H	-4.88818700	-0.52801300	-1.58906400

**INT-U**

C	-2.44841700	-1.95436400	1.79409300
C	-2.48009300	-3.29484500	1.03898600
B	-0.63319300	-2.13441500	0.50713700
O	-1.10901200	-1.49589200	1.61734200
O	-1.42672200	-3.17146000	0.07707600
C	1.42211900	-2.81811700	-0.62638200
C	2.74418100	-2.65158700	-0.79773400
C	3.31971800	-1.35783300	-0.46202500
C	2.52532700	-0.30780500	-0.12901400
C	1.08711700	-0.45085500	-0.13058900
N	0.60835400	-1.79406700	-0.15243300
H	0.91673300	-3.76267500	-0.79663600
H	3.37144400	-3.45727000	-1.15281800
H	2.95472000	0.67108000	0.04667800
C	0.19209800	0.58443400	-0.22535100
C	4.74401900	-1.18601600	-0.52889500
N	5.89453800	-1.06634000	-0.58655500
H	-2.26380400	-4.14305400	1.69707600
H	-3.42500000	-3.47601400	0.52178300

**INT-V**

C	1.68639700	0.35676300	2.42351800
C	3.15675100	0.35206700	1.97079300
B	1.83115400	-0.71814700	0.47631300
O	1.09613600	-0.69864200	1.66917400
O	3.11677600	-0.19327500	0.65333300
C	1.78368900	0.76267100	-1.72232500
C	1.69521300	2.08849600	-1.51485800
C	0.69412400	2.65772700	-0.65338700
C	-0.37602000	1.82119100	-0.29597100
C	-0.30397600	0.46934000	-0.50737900
N	1.01512400	-0.11942100	-0.84558400
H	2.46747400	0.27868800	-2.40608400
H	2.35002100	2.74820900	-2.07453000
H	-1.30774500	2.24414500	0.06737400

C	-1.24584000	-0.59494000	-0.54604600
C	0.65742000	4.05310800	-0.39997200
N	0.63844400	5.19444100	-0.17832000
H	3.59102100	1.35450500	1.94237900
H	3.77583800	-0.28837000	2.61076800
H	1.20134600	1.30736900	2.16468600
H	1.55896100	0.16237500	3.49107600
C	-2.65784200	-0.43823700	-0.14599100
C	-2.97477000	0.21569900	1.04941500
C	-3.68699900	-0.95612500	-0.93657500
C	-4.30161000	0.35358700	1.44204800
H	-2.16903000	0.59126500	1.67375300
C	-5.01328100	-0.81367600	-0.54339000
H	-3.43963700	-1.45245400	-1.87034700
C	-5.32325200	-0.15764000	0.64555000
H	-4.53786200	0.85936800	2.37265000
H	-5.80663000	-1.21009300	-1.16894400
H	-6.35866600	-0.04480700	0.95031900
C	-0.67920900	-1.74537100	-1.01684600
H	-1.19414500	-2.67246800	-1.22548300
C	0.76135900	-1.52846700	-1.29072900
H	1.11451000	-1.74004000	-2.31075100
N	1.74602600	-2.16119600	-0.29807200
C	3.03071300	-2.51652200	-0.93695400
H	3.41593100	-1.65159600	-1.47785800
H	3.74900400	-2.77653900	-0.15929200
H	2.88436500	-3.35940000	-1.61819200
C	1.22102200	-3.27843900	0.51110800
H	0.29630100	-2.96052000	0.98802900
H	1.04720800	-4.15125900	-0.12479400
H	1.96217700	-3.51646400	1.27540800

H	0.33079000	-2.66270800	0.52150100
C	-0.23748500	-0.20053400	0.00221200
C	4.66653600	0.02971200	-0.30846500
N	5.65492900	0.61084300	-0.47001300
C	-0.40319400	1.27347300	0.01755800
C	-1.20737800	1.91213600	-0.93824700
C	0.21579300	2.06610800	0.99331400
C	-1.36600700	3.29230500	-0.93149700
H	-1.70265400	1.30777300	-1.69255900
C	0.06354900	3.45004200	0.99689600
H	0.81322600	1.58212600	1.76122300
C	-0.72743100	4.06915800	0.03420900
H	-1.98380400	3.76632700	-1.68812900
H	0.55545900	4.04228100	1.76221900
H	-0.85105700	5.14725200	0.03824200
C	-1.42297600	-1.05208000	-0.09752400
H	-1.29673900	-2.02693300	-0.56543200
C	-2.65698400	-0.67125400	0.30335100
H	-2.79290300	0.31861100	0.73504700
N	-3.81114600	-1.42325200	0.26334700
C	-3.75000800	-2.71351400	-0.38232500
H	-2.98156700	-3.32869300	0.09526000
H	-4.71214400	-3.21718400	-0.27068300
H	-3.51124100	-2.63558600	-1.45548900
C	-5.06331500	-0.70600100	0.11140500
H	-5.03473000	0.20436700	0.71425400
H	-5.26495800	-0.42278600	-0.93286000
H	-5.88898000	-1.32806900	0.46725300

**INT-X**

**INT-W**

C	2.36037600	-2.80406500	0.25803600
C	3.52589600	-2.14921700	0.08483000
C	3.45245100	-0.71168800	-0.10286000
C	2.26043400	-0.05930500	-0.10332700
C	1.00920000	-0.76591100	0.06557400
N	1.15607900	-2.15494600	0.24407700
H	2.30877600	-3.87515300	0.41542100
H	4.47401900	-2.66647100	0.08327600
H	2.22272000	1.01013400	-0.26926600

C	-3.05986900	1.11483600	1.95870600
C	-3.92629600	0.02250900	1.29509300
B	-1.78482700	-0.70042500	1.49039300
O	-1.81943500	0.48069900	2.21997000
O	-3.00052000	-0.97006300	0.88221700
C	-0.46208800	-4.61856800	0.27636000
C	-0.92023700	-3.95612000	-1.03181700
B	-0.17508300	-2.35156700	0.45807000
O	0.30077300	-3.62162100	0.91887200
O	-0.94699400	-2.57399800	-0.73021500
C	2.24076400	-2.30469300	-0.74611000
C	3.51395600	-1.90447000	-0.79137300

C	3.89734600	-0.66888300	-0.10424700
C	2.92768600	0.23935900	0.21860400
C	1.55060600	-0.12022100	0.00859600
N	1.34056600	-1.57260700	0.13671900
H	1.82091700	-3.16107100	-1.25571400
H	4.25327300	-2.43696700	-1.37812500
H	3.18869800	1.24790800	0.52183600
H	1.69590300	-1.76442600	1.08479300
C	0.57368200	0.77223500	-0.34173600
C	5.28485800	-0.34653300	0.04428800
N	6.41137400	-0.09980700	0.15689100
H	-2.89669400	1.96630100	1.28369700
H	-4.47830000	0.39784000	0.42681300
H	-4.63941600	-0.41767000	2.00153400
H	-3.49192600	1.49006800	2.89036200
H	-0.21237200	-4.15456300	-1.85055900
H	-1.91221700	-4.28859500	-1.35370100
H	0.14639100	-5.51335500	0.10872700
H	-1.32638300	-4.89801800	0.89446000
O	-0.69380500	-1.47167700	1.45067600
C	0.84368900	2.22414700	-0.09947000
C	1.45215000	3.02399400	-1.06788300
C	0.43834000	2.78653600	1.11481200
C	1.66834500	4.37690000	-0.81919800
H	1.75938600	2.57955300	-2.01039100
C	0.65088900	4.14191900	1.35485400
H	-0.04497800	2.15119100	1.85406800
C	1.26752500	4.93676700	0.39144300
H	2.15224900	4.99272600	-1.57049200
H	0.33764500	4.57585300	2.29922500
H	1.43782400	5.99112100	0.58418600
C	-0.67190400	0.40575800	-0.93901800
H	-0.80311100	-0.62168900	-1.25166700
C	-1.67944400	1.30894000	-1.13287900
H	-1.53706000	2.35033900	-0.84952200
N	-2.89723400	1.02685600	-1.63930200
C	-3.19521900	-0.30486800	-2.14310500
H	-2.83178000	-1.06006200	-1.44230400
H	-4.27876200	-0.40479400	-2.24064400
H	-2.73484900	-0.46447300	-3.12722400
C	-3.79543200	2.09460500	-2.02868700
H	-3.50256400	3.02122300	-1.53115100
H	-3.78123900	2.26067400	-3.11364000
H	-4.82026100	1.84812400	-1.73260600

**INT-Y**

C	2.64273200	0.90273800	-0.36355900
C	2.40941000	2.23199600	-0.35655500
C	1.13063700	2.78689500	-0.04399900
C	0.04306500	1.89623100	0.03023900
C	0.23200300	0.54392600	0.04261200
N	1.61772500	0.02290700	0.21063600
H	3.56526300	0.40157200	-0.61702000
H	3.20929000	2.89482000	-0.67150300
H	-0.97397000	2.27445900	-0.00724300
H	1.79858000	-0.11200600	1.22031100
C	-0.60577400	-0.61995800	-0.08617300
C	0.93169300	4.19252000	-0.02867600
N	0.77341400	5.34357500	-0.00483700
C	-2.08130300	-0.56605300	-0.05674300
C	-2.82959400	-1.37023800	-0.92252700
C	-2.75053600	0.26628200	0.84671100
C	-4.21876700	-1.34491000	-0.88467100
H	-2.31188800	-1.99989100	-1.63990700
C	-4.14074900	0.28985800	0.88413600
H	-2.17452500	0.87950000	1.53322900
C	-4.87764300	-0.51442000	0.01855900
H	-4.78897000	-1.96807700	-1.56605500
H	-4.64884000	0.93592600	1.59266800
H	-5.96219900	-0.49176400	0.04587400
C	0.14459500	-1.73674500	-0.25347900
H	-0.23248100	-2.73861500	-0.41095200
C	1.60253600	-1.38377600	-0.37558300
H	1.89847300	-1.23316000	-1.42675300
N	2.61508700	-2.17411400	0.26889300
C	3.32030900	-3.07432700	-0.63149000
H	3.69040600	-2.52055000	-1.49747300
H	4.17981700	-3.50049300	-0.10788900
H	2.69061000	-3.90687900	-0.98664900
C	2.18060300	-2.85872700	1.47985700
H	1.63501200	-2.17530900	2.13548200
H	1.52126500	-3.71574300	1.27096600
H	3.06127000	-3.21811900	2.01812500

**TS1**

C	0.50459800	4.25395700	0.19929900	H	3.67484600	-3.15662000	1.66972400
C	1.72452100	3.71304700	-0.56733300	H	3.14106700	-3.76744000	0.08616800
B	0.14102900	2.15152700	-0.53418500	H	3.14907500	-0.00061700	-0.20202300
O	-0.36030100	3.12980200	0.32518500				
O	1.20551500	2.61933900	-1.30722000				
C	-0.28799000	0.10294400	-1.85779600	<b>TS2</b>			
C	-1.04245700	-0.98376700	-2.16585700				
C	-2.40416200	-1.05872700	-1.74667600	C	-1.88035200	3.80749900	-0.30399900
C	-2.93335400	0.07832000	-1.05748300	C	-2.29633500	2.93447100	0.89752900
C	-2.13418500	1.13526600	-0.76631100	B	-1.33690700	1.64879700	-0.66054100
N	-0.79565600	1.16776500	-1.12687900	O	-1.14412200	2.93175500	-1.14619900
H	0.75121100	0.20273800	-2.14862200	O	-2.24716400	1.60540300	0.39723700
H	-0.60068600	-1.79717000	-2.73002500	C	0.36128200	0.59794900	1.63066300
H	-3.97006900	0.09097800	-0.74298100	C	1.48366900	-0.02694600	2.15338500
H	-2.47764300	2.00383400	-0.21836900	C	2.72809400	0.30115700	1.60591700
C	-1.14290300	0.60275200	2.17517600	C	2.80912200	1.25334500	0.59322400
C	-0.48214000	-0.42653600	1.49441400	C	1.62120600	1.82419300	0.14507200
C	-1.12119900	-1.65222000	1.29110500	N	0.43306000	1.49864700	0.64684600
C	-2.41847800	-1.84531100	1.75402200	H	-0.64356100	0.35715900	1.96988900
C	-3.06574700	-0.82532300	2.44771500	H	1.39902900	-0.76931000	2.93776800
C	-2.42578000	0.39506500	2.66376400	H	3.75915700	1.50553300	0.13837900
H	-0.64639200	1.56182300	2.28622600	H	1.60793300	2.54558000	-0.66814000
H	-0.62627600	-2.43221100	0.71972100	C	1.49717900	-0.14114000	-2.24198100
H	-2.92826500	-2.78244500	1.55587200	C	0.78150700	-0.93320800	-1.31687300
H	-2.93578600	1.18954300	3.19895600	C	1.48835100	-1.95119500	-0.64027600
C	0.87747000	-0.15901300	0.95943300	C	2.84341000	-2.14870500	-0.86334500
O	1.18107900	1.00482100	0.59894100	C	3.53840600	-1.35014100	-1.77311900
H	-4.07637300	-0.97889700	2.81322800	C	2.84895600	-0.35601900	-2.46863400
C	1.82650400	-1.23160400	0.87736600	H	0.96532000	0.64094400	-2.77341400
C	3.00941800	-0.99029500	0.22990700	H	0.98107500	-2.55565300	0.10579200
C	-3.17387400	-2.22484700	-1.94907500	H	3.36949800	-2.92057800	-0.30937900
N	-3.80319800	-3.19457400	-2.09811800	H	3.37352300	0.26184100	-3.19193000
H	-0.00886800	5.04270400	-0.36345300	C	-0.61207600	-0.65345000	-1.04966900
H	0.76561600	4.64030200	1.18866300	O	-1.05117100	0.57494600	-1.48027300
H	2.49519600	3.35611900	0.12873000	H	4.59852900	-1.50780900	-1.94132600
H	2.16553900	4.44599200	-1.24781500	C	-1.51141000	-1.56291900	-0.47025400
H	1.58129600	-2.19273800	1.30914800	C	-2.84130900	-1.29219100	-0.24644500
N	4.02039400	-1.84993400	0.06850200	C	3.91690900	-0.37487000	2.06057800
C	5.16991100	-1.52979400	-0.75818000	N	4.86637300	-0.92566100	2.42505000
H	5.11879700	-0.48278200	-1.05812600	H	-1.25950900	4.65747400	-0.00695500
H	6.09712400	-1.69177300	-0.20017300	H	-2.75208000	4.18547100	-0.85125000
H	5.18924400	-2.15232300	-1.65933900	H	-3.30172900	3.15568400	1.26436800
C	3.91962800	-3.19530500	0.60414800	H	-1.58209700	3.03697400	1.72477400
H	4.87639300	-3.70281000	0.47981200	H	-1.11850900	-2.54671900	-0.23902300

N	-3.77183600	-2.18770700	0.21033100
C	-4.95658400	-1.66572000	0.86178000
H	-5.77970400	-2.37801100	0.75853600
H	-4.79360100	-1.47137100	1.93215800
H	-5.24638900	-0.72796800	0.38375600
C	-3.33992900	-3.50211500	0.62631900
H	-4.21605200	-4.11107500	0.85701100
H	-2.78775400	-3.98571700	-0.18411000
H	-2.69118700	-3.46642200	1.51560700
H	-3.23146600	-0.30374800	-0.46073800

**TS4**

C	3.53778500	-0.49051000	2.14772300
C	4.08192700	-1.46833600	1.09301000
B	2.20160800	-0.49735700	0.32566900
O	2.24062800	-0.14461700	1.66439200
O	3.34139600	-1.15388500	-0.07952900
C	2.11738400	-2.49433700	-2.61547800
C	1.76147100	-3.42352600	-1.43625000
B	0.56607400	-1.45638500	-1.30952200
O	1.08502100	-1.53137200	-2.62976200
O	0.90849100	-2.65635800	-0.60399500
C	-1.91487200	-1.94723000	-1.15494100
C	-3.22631000	-1.59998600	-1.02326000
C	-3.51469400	-0.17919200	-0.98121500
C	-2.54786700	0.76176400	-1.03972500
C	-1.09631600	0.37925800	-1.19556000
N	-0.90348100	-1.06355300	-1.21507500
H	-1.59146100	-2.98436700	-1.18015600
H	-4.01737800	-2.33358400	-0.99349000
H	-2.79551800	1.81572900	-0.97241200
H	-0.68527800	0.78662400	-2.13215800
C	-0.20816900	0.97027800	-0.06994100
C	-4.88419400	0.24544400	-0.81974100
N	-5.98579800	0.57039700	-0.67652400
H	3.45312400	-0.93497300	3.14188700
H	3.88749700	-2.51049800	1.37096700
H	5.14993000	-1.34222400	0.90322500
H	4.14879000	0.41710700	2.21474600
H	1.22950700	-4.32258400	-1.77551700
H	2.65215600	-3.73551300	-0.87911800
H	2.14349600	-3.02447800	-3.57323400

H	3.09045300	-2.01593600	-2.44879200
O	1.17749000	-0.19975700	-0.52376400
C	0.43579000	2.29225000	-0.35657900
C	-0.04916500	3.12580400	-1.36920900
C	1.50349100	2.74433000	0.43118100
C	0.51567100	4.38047400	-1.58586100
H	-0.88156100	2.81709100	-1.99176600
C	2.07707800	3.98729600	0.20033000
H	1.89222200	2.10302100	1.21609400
C	1.58295100	4.81280900	-0.80822800
H	0.11890900	5.01586200	-2.37059600
H	2.91273600	4.31473400	0.81041000
H	2.02846400	5.78623600	-0.98502300
C	-0.54331500	0.74230200	1.29566500
H	-0.04090200	1.34804500	2.03851400
C	-1.40852700	-0.24999100	1.69192200
H	-1.94570000	-0.84796000	0.96384700
N	-1.68441200	-0.57174800	2.95766600
C	-1.00242300	0.08781100	4.05594200
H	-1.34396900	1.12286900	4.17252200
H	-1.20502500	-0.45728800	4.97835700
H	0.07530800	0.08865100	3.86894800
C	-2.73494800	-1.52397500	3.27465300
H	-3.12445000	-1.94628900	2.34703300
H	-2.33981900	-2.33226000	3.89732800
H	-3.55480800	-1.03349100	3.80981200

**TS4-iso**

C	3.14240400	1.65266400	1.87011200
C	4.15698800	0.62068800	1.34787800
B	2.16858300	0.29917500	0.33954600
O	1.89090700	1.20289900	1.35605700
O	3.52018000	0.05973600	0.20866000
C	3.15032700	-2.66707600	-1.33615100
C	3.10362800	-2.99390300	0.16986000
B	1.21112000	-1.85699900	-0.48123000
O	1.81473400	-2.35275700	-1.66841200
O	1.95027200	-2.32724200	0.65539900
C	-0.88958800	-2.83043500	0.55173300
C	-2.23351200	-2.86967100	0.76743600
C	-3.04572200	-2.07698000	-0.12891600
C	-2.51137000	-1.24648700	-1.05186500

C	-1.01832500	-1.04262100	-1.12551800	C	4.74998400	0.90520300	-0.87074600
N	-0.29645500	-2.06218200	-0.38438400	C	4.95723100	-0.55880800	-0.42967100
H	-0.19155500	-3.43679800	1.12206600	B	2.74437200	-0.05967700	-0.43368100
H	-2.68036400	-3.53131600	1.49364700	O	3.37923700	1.16395200	-0.61238600
H	-3.15187200	-0.69412200	-1.73015600	O	3.64996800	-1.10988300	-0.39771000
H	-0.66321600	-1.05905000	-2.16505900	C	1.62763500	-3.42176500	-1.18814800
C	-0.62010600	0.34079700	-0.54461700	C	1.62810000	-3.34805500	0.35034900
C	-4.48232300	-2.19467500	-0.05673200	B	0.67374200	-1.40291700	-0.49356500
N	-5.63379300	-2.28289200	0.02199700	O	1.16516000	-2.16898600	-1.61844400
H	3.09839700	1.69674600	2.96098700	O	0.69514200	-2.32921400	0.65318500
H	4.34006100	-0.17069400	2.08413200	C	-1.69922700	-1.88292400	-1.10641600
H	5.11140100	1.06738100	1.05962900	C	-3.00404200	-1.65605700	-1.41119500
H	3.34984500	2.65777700	1.48354500	C	-3.42736000	-0.26654400	-1.45079600
H	3.00277300	-4.07336100	0.34489700	C	-2.56501000	0.74533800	-1.22442500
H	3.99585400	-2.63453000	0.69541700	C	-1.12010800	0.49480800	-0.84871100
H	3.49352500	-3.51466900	-1.93865900	N	-0.81681100	-0.93399800	-0.71163000
H	3.81010700	-1.80933900	-1.52329700	H	-1.28755700	-2.88922400	-1.09960300
O	1.22953100	-0.25317400	-0.47142300	H	-3.67302200	-2.45014000	-1.70808900
C	-0.50184900	1.48369200	-1.48899500	H	-2.88570000	1.77998900	-1.29057500
C	-1.22683200	1.48659700	-2.68555700	H	-0.45249100	0.95410100	-1.59065600
C	0.33000400	2.57485000	-1.20092400	C	-0.89545300	1.24498400	0.46868800
C	-1.14536800	2.56682900	-3.55878600	C	-4.80243000	0.03919600	-1.76030700
H	-1.86627300	0.64932100	-2.94238800	N	-5.91208300	0.26736300	-1.99722000
C	0.42025800	3.64549000	-2.08216900	H	5.37569400	1.60699700	-0.31260300
H	0.91927700	2.56093300	-0.28879200	H	5.40309700	-0.62089700	0.57038600
C	-0.32170900	3.64750100	-3.26121800	H	5.58383300	-1.12401100	-1.12462800
H	-1.72183700	2.55663400	-4.47771900	H	4.94923500	1.03604200	-1.94084400
H	1.07853800	4.47702600	-1.85187400	H	1.31840300	-4.29260000	0.81726000
H	-0.25062300	4.48366800	-3.94911200	H	2.62496800	-3.08237400	0.72246400
C	-0.99883700	0.54499200	0.80428800	H	0.95719000	-4.22061900	-1.54516900
H	-1.11812900	-0.35130200	1.40417300	H	2.63167100	-3.62040700	-1.58115300
C	-1.24513000	1.77683000	1.35605200	O	1.41827800	-0.15245400	-0.29674600
H	-1.24460600	2.66804800	0.73417700	C	-0.41661300	2.63871000	0.41783000
N	-1.52639000	1.98840600	2.64421800	C	-1.05515800	3.62699100	1.17775300
C	-1.49103100	0.88172800	3.58671900	C	0.68658500	2.98230800	-0.37444700
H	-0.53281700	0.36131400	3.50166300	C	-0.60219300	4.94080200	1.14481200
H	-1.59947300	1.27455200	4.59787400	H	-1.92362700	3.35962000	1.77309800
H	-2.29904400	0.16742700	3.39123300	C	1.14621200	4.29411100	-0.38744800
C	-1.98941400	3.27640400	3.12476600	H	1.21481200	2.21296500	-0.92700000
H	-1.89702700	4.01608200	2.32864700	C	0.50156500	5.27491900	0.36318700
H	-3.03863600	3.22528400	3.43564400	H	-1.11193600	5.70326500	1.72463600
H	-1.38630400	3.59979500	3.97829100	H	2.01791000	4.54573800	-0.98226000
				H	0.85912000	6.29942800	0.34050300
				C	-1.16923300	0.64094400	1.64318700

TS5

H	-0.89241000	1.11832000	2.57723900
C	-1.70697600	-0.70056400	1.65371200
H	-2.51823900	-0.96561400	0.97904600
N	-1.36443500	-1.62573400	2.49827400
C	-0.21914200	-1.48270700	3.39641800
H	0.67575800	-1.70561200	2.80739000
H	-0.17239400	-0.47197700	3.79713500
H	-0.33435100	-2.19091600	4.21718600
C	-1.84746700	-2.99180400	2.31629000
H	-2.66982500	-2.99125400	1.60005800
H	-1.01589100	-3.57373400	1.90905500
H	-2.17519000	-3.39936200	3.27468400

**TS5-iso**

C	-5.97854900	0.09287600	1.04045300
C	-5.43096500	1.36511900	0.36234600
B	-3.74541900	-0.10973000	0.72438400
O	-4.82337300	-0.63380500	1.41985300
O	-4.10240600	1.02541800	-0.00128600
C	-1.79833900	1.19703800	-1.89989800
C	-1.39663400	2.14802100	-0.74498000
B	-1.39307900	-0.06851300	0.04790000
O	-1.60330500	-0.10884300	-1.41801800
O	-1.11025300	1.32432800	0.35616500
C	-0.27995400	-2.22951900	0.77903000
C	0.70294700	-3.03114900	1.28099000
C	1.98370300	-2.40002300	1.52700400
C	2.19290300	-1.09044700	1.28048900
C	1.08014600	-0.19566700	0.77706200
N	-0.14057900	-0.92711900	0.45489700
H	-1.28391300	-2.61147500	0.61554700
H	0.52387000	-4.06207300	1.54736200
H	3.15493500	-0.62711100	1.47670400
H	0.85265600	0.54780800	1.55514600
C	1.61282400	0.64371900	-0.39098500
C	3.08658900	-3.20515900	1.99289500
N	3.96961900	-3.87009100	2.33696700
H	-6.58968000	0.31376000	1.91992200
H	-5.41282800	2.21602600	1.05409000
H	-6.00228000	1.65160100	-0.52521500
H	-6.57732900	-0.50834600	0.34495700
H	-0.50640500	2.74283100	-1.00340300

H	-2.21594600	2.83503400	-0.50569300
H	-1.16962100	1.36953800	-2.79309900
H	-2.84347600	1.34693600	-2.19127000
O	-2.52615900	-0.64872200	0.75724200
C	2.32516200	1.88692600	-0.00597300
C	3.60206300	2.15696500	-0.50983800
C	1.71427100	2.80656100	0.85765300
C	4.26673900	3.32489800	-0.15109500
H	4.07738500	1.43412200	-1.16723800
C	2.37865600	3.97944700	1.20013800
H	0.70658700	2.60734900	1.21362800
C	3.65468100	4.23795500	0.70389500
H	5.26289100	3.51929700	-0.53483700
H	1.89592100	4.69594500	1.85653700
H	4.17174200	5.15024600	0.98312900
C	1.48078600	0.37074400	-1.70672500
H	1.76906500	1.14305700	-2.41728800
C	0.71926700	-0.71652700	-2.30186300
H	-0.13242800	-0.45035200	-2.91699300
N	0.98281300	-1.98004700	-2.23868200
C	2.20913500	-2.55040000	-1.68032700
H	2.72120500	-3.07766300	-2.49013100
H	2.83714400	-1.75724700	-1.28385700
H	1.94499700	-3.24754900	-0.88558100
C	0.01193300	-2.95484400	-2.73908500
H	-0.90569600	-2.43675900	-3.01412800
H	0.43401800	-3.49984100	-3.58676500
H	-0.20350700	-3.64933500	-1.92397400

**TS5-iso2**

C	4.84681900	0.43988900	1.28627200
C	4.82783300	1.28661200	0.00072300
B	2.81784000	0.30357800	0.29400800
O	3.63229200	-0.30525100	1.23154400
O	3.45369900	1.33086500	-0.36623500
C	1.30442700	2.27610000	-2.30939900
C	2.11244700	1.20704100	-3.07343800
B	0.79870700	0.20962400	-1.49317700
O	0.33573200	1.54024200	-1.57808600
O	1.88285100	-0.00479800	-2.37504300
C	0.01517500	-2.11981000	-1.74680200
C	-0.80272300	-3.16891100	-1.50802400

C	-2.10352200	-2.86761700	-0.92443200				
C	-2.49165300	-1.60548900	-0.66604000				
C	-1.59381000	-0.41776700	-0.93370600	<b>TS6</b>			
N	-0.28801700	-0.82054700	-1.45952000				
H	1.00429900	-2.24879600	-2.17722600	C	3.78083500	2.71262000	-0.09378200
H	-0.52956200	-4.18113500	-1.76592500	C	4.64199000	1.43426200	-0.10495700
H	-3.46151200	-1.39591400	-0.22613600	B	2.50240200	0.92051400	-0.56686000
H	-2.08131200	0.24786400	-1.66290600	O	2.44245300	2.23231700	-0.14886800
C	-1.51418700	0.39155500	0.36921600	O	3.79092800	0.44179700	-0.66788200
C	-2.99604200	-3.95438600	-0.60663100	C	0.92349800	-2.95289000	-2.34920100
N	-3.69803600	-4.83859500	-0.35123600	C	2.07446700	-3.21486100	-1.34964400
H	5.69646000	-0.24430600	1.33587100	B	1.19397400	-1.14644400	-0.98762400
H	5.39951300	0.81414000	-0.80537800	O	0.59216200	-1.58729100	-2.16747500
H	5.20258100	2.30096900	0.15369900	O	2.03648200	-2.12078400	-0.44407200
H	4.84220900	1.06486400	2.18692000	C	-0.91099500	-2.58490600	0.19177600
H	1.76542800	1.10385700	-4.10943100	C	-2.17402100	-2.91736900	-0.08813000
H	3.18313400	1.43433900	-3.07997300	C	-3.17758400	-1.85640900	-0.24030100
H	0.79963800	2.97830400	-2.98028500	C	-2.79769700	-0.57175100	-0.31578300
H	1.94656100	2.83700700	-1.62222900	C	-1.33766700	-0.20233100	-0.29307600
O	1.52495400	-0.04917400	0.07265200	N	-0.45945800	-1.24218600	0.31084500
C	-2.58174400	1.40437000	0.55575100	H	-0.14329300	-3.33116200	0.37716500
C	-3.41310300	1.37613200	1.67887700	H	-2.47390600	-3.95425000	-0.17711800
C	-2.75459600	2.41111800	-0.40252700	H	-3.52369100	0.23092500	-0.41001400
C	-4.40599800	2.33832700	1.84302900	H	-1.00892100	-0.00269600	-1.32236600
H	-3.28529400	0.58432400	2.41163900	C	-1.11962400	0.99738700	0.60994200
C	-3.74134800	3.37482900	-0.23025900	C	-4.56985300	-2.21723000	-0.27900400
H	-2.07860400	2.44655000	-1.25246900	N	-5.68438200	-2.52796700	-0.30723700
C	-4.57176800	3.33794600	0.88883400	H	3.92293300	3.31374500	0.80755500
H	-5.05339500	2.30263900	2.71330900	H	4.92333900	1.12828300	0.91021000
H	-3.86125800	4.16054600	-0.96926700	H	5.54883000	1.53224400	-0.70626800
H	-5.34662800	4.08707900	1.01577500	H	3.97509100	3.34139500	-0.97012400
C	-0.59351000	0.20730800	1.32278700	H	1.94806200	-4.15615700	-0.80267700
H	-0.62798900	0.83784400	2.20567300	H	3.05020200	-3.23489700	-1.84785600
C	0.49924700	-0.79397300	1.23559400	H	0.04937400	-3.58076100	-2.14093900
H	0.25862800	-1.67230700	0.64573500	H	1.22864800	-3.11902800	-3.38641000
N	1.14588000	-1.13215200	2.37574700	O	1.38523500	0.22245400	-0.84059200
C	1.53378600	-0.15590800	3.37986400	C	-1.53851200	2.34664200	0.19390600
H	1.27636800	0.85344200	3.05748000	C	-2.29330100	3.16365200	1.04085000
H	1.04110500	-0.36260800	4.33595800	C	-1.16405800	2.82458000	-1.06716000
H	2.61845000	-0.19458100	3.51913000	C	-2.66784000	4.44027400	0.63360000
C	1.83318400	-2.40980400	2.46612400	H	-2.59536300	2.78385200	2.01258800
H	1.42114900	-3.09686600	1.72475200	C	-1.53650400	4.10193000	-1.46904300
H	2.90686500	-2.28911600	2.29130800	H	-0.54752500	2.20209500	-1.70951100
H	1.67192500	-2.83554600	3.46135300	C	-2.29206500	4.91018000	-0.62193400



H	-3.25998100	5.06556300	1.29409700
H	-1.23191800	4.46980000	-2.44346000
H	-2.58782400	5.90461300	-0.94031000
C	-0.56215100	0.62261800	1.75657100
H	-0.31123800	1.27396300	2.58573400
C	-0.25914500	-0.85015000	1.80160900
H	-1.04586100	-1.39360900	2.34922300
N	0.96589100	-1.17398200	2.43636300
C	2.16972000	-0.40865900	2.15781500
H	2.76555700	-0.83776600	1.34198400
H	1.90965400	0.62423800	1.91078500
H	2.78915500	-0.39368300	3.06260200
C	1.22847200	-2.57739800	2.68069500
H	0.29923000	-3.08216600	2.96422000
H	1.66230100	-3.08161100	1.80378800
H	1.93502200	-2.67344900	3.51234300

### TS6-iso

C	4.57224600	2.63170500	0.17119100
C	5.27322800	1.32399300	-0.25917800
B	3.05770900	0.97737600	-0.01928100
O	3.24376700	2.23865500	0.49312000
O	4.20674600	0.42804100	-0.54911400
C	1.93028200	-2.57761600	-2.02644200
C	2.66338100	-3.00155400	-0.73354600
B	1.71475200	-0.96163700	-0.44969200
O	1.58045300	-1.21890500	-1.81001000
O	2.28213900	-2.03793100	0.24008900
C	-0.59965600	-2.45997900	-0.07528100
C	-1.65729600	-2.81582800	-0.81445500
C	-2.63552200	-1.78993500	-1.18963600
C	-2.36575800	-0.48785200	-1.00546200
C	-1.00852900	-0.05954200	-0.51350400
N	-0.27592300	-1.12125000	0.22300600
H	0.10543900	-3.18301000	0.32371600
H	-1.83800600	-3.85210100	-1.06966800
H	-3.10530500	0.28017400	-1.21159300
H	-0.38826900	0.23202100	-1.37598500
C	-1.09360500	1.06994600	0.49524900
C	-3.91947500	-2.20959100	-1.68640700
N	-4.94437000	-2.56753800	-2.08757900
H	5.04186600	3.09620700	1.04163100

H	5.88523800	0.90480800	0.54709400
H	5.90098000	1.45208400	-1.14431000
H	4.54254900	3.36450900	-0.64264900
H	2.38044100	-4.00588200	-0.40087000
H	3.75130000	-2.96812400	-0.85839500
H	1.02460900	-3.17123600	-2.19541400
H	2.56855200	-2.65321800	-2.91079800
O	1.86292100	0.34878500	0.00159700
C	-1.63312800	2.38935600	0.12971100
C	-2.16610300	3.23723300	1.10978600
C	-1.63636600	2.82004500	-1.20254500
C	-2.66610200	4.48698100	0.77044700
H	-2.20109000	2.90115000	2.14161100
C	-2.14160600	4.07134400	-1.54238400
H	-1.22640800	2.18203300	-1.97972200
C	-2.65544600	4.90933300	-0.55805500
H	-3.07570600	5.13027200	1.54244200
H	-2.13097500	4.39080200	-2.57929000
H	-3.05178800	5.88384700	-0.82341900
C	-0.62907600	0.67401400	1.67949300
H	-0.54325200	1.28481500	2.57021800
C	-0.18625300	-0.76165200	1.70608100
H	0.87042700	-0.84943800	1.98136200
N	-0.93102500	-1.54767400	2.64034300
C	-2.37632600	-1.57681700	2.50552900
H	-2.81758800	-1.87066100	3.46323500
H	-2.74831500	-0.58272700	2.24918500
H	-2.72162800	-2.28664100	1.73860600
C	-0.36755500	-2.82207700	3.04249700
H	0.72375500	-2.77295500	3.00083800
H	-0.66634100	-3.04735200	4.07220400
H	-0.69979100	-3.66103100	2.41046100

### TS7-2H<sub>2</sub>O

C	2.20841800	1.60819100	-0.70105800
C	1.72598100	2.85063200	-0.58712600
C	0.34076900	3.05326700	-0.13996400
C	-0.43974800	1.96683600	0.09571500
C	0.08257300	0.62440100	0.13768800
N	1.50656500	0.46664400	-0.28058400
H	3.19605400	1.41597700	-1.10936200
H	2.32989200	3.70049000	-0.87703500

H	-1.49854900	2.10061600	0.29909800	N	1.63430100	0.17309900	-0.36205400
H	0.02695900	0.16766600	1.56977500	H	3.22826800	0.88923300	-1.52440600
C	-0.59213900	-0.52028400	-0.46352400	H	2.65119200	3.27669000	-1.20403400
C	-0.19778900	4.37269600	-0.05400300	H	-1.02698100	2.10239100	0.73313600
N	-0.62277800	5.45064200	0.01137700	H	0.52098200	-0.25196600	1.47918500
C	-2.03982800	-0.77289700	-0.33485400	C	-0.56844200	-0.57094200	-0.38444200
C	-2.71605500	-1.52379600	-1.30469900	C	0.45114200	4.20685100	0.12855300
C	-2.77193700	-0.27738100	0.75272100	N	0.19026800	5.32609400	0.28441400
C	-4.07560100	-1.78221300	-1.18473700	C	-2.02973500	-0.60489300	-0.21148800
H	-2.16809400	-1.88373700	-2.17001300	C	-2.85974900	-0.98607000	-1.27118100
C	-4.13406300	-0.53563600	0.87207200	C	-2.60980600	-0.25531400	1.01356200
H	-2.27394900	0.32189300	1.51030200	C	-4.24015200	-1.01537200	-1.11011600
C	-4.79044700	-1.29206100	-0.09380900	H	-2.41183700	-1.23660800	-2.22825600
H	-4.58238000	-2.36013800	-1.95105000	C	-3.99110100	-0.28708700	1.17242500
H	-4.68243000	-0.14141000	1.72174300	H	-1.96758800	0.01580400	1.84699000
H	-5.85317800	-1.49099100	-0.00260200	C	-4.81019700	-0.66543600	0.11172200
C	0.30113700	-1.33945800	-1.07032400	H	-4.87304300	-1.30479900	-1.94301100
H	0.06505400	-2.27025100	-1.56773500	H	-4.42862700	-0.01880400	2.12881000
C	1.68550000	-0.77577500	-0.98160500	H	-5.88798300	-0.68591500	0.23627300
H	2.20038100	-0.64927100	-1.95686000	C	0.18190100	-1.49468900	-1.03218900
N	2.63141800	-1.69300200	-0.19384300	H	-0.18770300	-2.37996200	-1.53169200
C	2.72911900	-3.01432100	-0.82617600	C	1.63392200	-1.16417400	-0.86576200
H	3.04238500	-2.92454500	-1.87460700	H	2.27869500	-1.29508300	-1.74962000
H	3.46196700	-3.61899900	-0.28806000	N	2.27279400	-2.05710800	0.23572500
H	1.76066800	-3.51194800	-0.77517200	C	2.05037100	-3.48969800	0.00307100
C	3.95806900	-1.07617700	-0.06201800	H	2.45931400	-3.78918700	-0.96953500
H	4.40475900	-0.88786600	-1.04739800	H	2.54445700	-4.06297500	0.78966100
H	3.85792700	-0.13492500	0.48021300	H	0.98039600	-3.69333500	0.03051400
H	4.61490600	-1.74594700	0.49887600	C	3.70032000	-1.74418300	0.38230300
O	1.77805900	-2.02080300	2.12010500	H	4.25008900	-2.02301100	-0.52446900
H	2.18173000	-1.84539900	1.02293900	H	3.80479000	-0.67277200	0.55978500
H	2.49098900	-1.94862700	2.76437600	H	4.11064600	-2.29438300	1.23200200
O	0.09473100	-0.38006100	2.57834400	O	0.99887900	-1.10483100	2.16861200
H	-0.75132900	-0.83135600	2.69498000	H	1.69470000	-1.67020800	1.24554000
H	0.94371300	-1.22045000	2.38555200	H	1.55568200	-0.66193500	2.82048400

### TS7-H<sub>2</sub>O

C	2.35948200	1.20367900	-0.95166000
C	2.03755900	2.49285800	-0.78175800
C	0.79407600	2.83174900	-0.07071300
C	-0.05464400	1.84916400	0.31966000
C	0.29371700	0.44370400	0.23420500

### TS7

C	1.99864700	1.44882500	-1.24603000
C	1.64829500	2.72406800	-1.03807500
C	0.38983300	3.02975500	-0.34631300
C	-0.45867500	2.00060800	-0.05478400
C	-0.06593600	0.63202000	-0.15510200

N	1.30007600	0.36296400	-0.68555000
H	2.86436100	1.18225500	-1.84435100
H	2.24649500	3.52763100	-1.44792100
H	-1.46454800	2.21577100	0.29339100
H	-0.00575500	0.15359600	1.36630300
C	-0.87328400	-0.47383900	-0.62758100
C	0.01077500	4.38204300	-0.10458600
N	-0.28512000	5.48817900	0.08927600
C	-2.32619900	-0.59318300	-0.39829100
C	-3.13053600	-1.27054800	-1.32313700
C	-2.93634400	-0.03776600	0.73456900
C	-4.49917100	-1.39691500	-1.11761000
H	-2.67393200	-1.67820800	-2.21955400
C	-4.30647100	-0.16308000	0.93938400
H	-2.33063600	0.48829400	1.46784600
C	-5.09310900	-0.84510400	0.01531100
H	-5.10623400	-1.92050200	-1.84921600
H	-4.75930800	0.27421700	1.82341000
H	-6.16224900	-0.94075800	0.17333500
C	-0.09389000	-1.39184400	-1.26025800
H	-0.44717000	-2.30837200	-1.71315800
C	1.32673700	-0.92532100	-1.34620600
H	1.70429700	-0.85511800	-2.38825100
N	2.32641700	-1.83335500	-0.63675300
C	2.04632400	-3.25606400	-0.84721000
H	2.04857100	-3.51554900	-1.91605800
H	2.81292400	-3.84890100	-0.34316800
H	1.07251000	-3.50314600	-0.42384500
C	3.69100500	-1.51988900	-1.07684400
H	3.82123400	-1.70883900	-2.15205200
H	3.90824500	-0.46921000	-0.87343500
H	4.40483500	-2.13446900	-0.52176500
O	2.45273000	-1.11564500	1.81170400
H	2.36424500	-1.43960900	0.78592800
O	0.25754400	-0.32782600	2.31757400
H	1.34757800	-0.70693200	2.11228700
C	-0.55951400	-1.47225600	2.58078800
H	-0.00153800	-2.13953800	3.24177700
H	-1.47920500	-1.15927600	3.07705700
H	-0.80660200	-1.99449700	1.65152300
C	3.36166100	-0.01740500	1.91245000
H	3.08757600	0.78311500	1.21668500
H	3.32517800	0.36133500	2.93539300
H	4.37643200	-0.36466900	1.70194900

### TS7-MeOH

C	2.25624200	1.08688100	-1.19966400
C	2.02126400	2.39191400	-0.99871200
C	0.79160900	2.79834200	-0.29994100
C	-0.10938500	1.86313300	0.09556800
C	0.16562100	0.44512200	0.01623800
N	1.44471200	0.10061300	-0.65909100
H	3.10493400	0.72692100	-1.77503900
H	2.69285700	3.14125400	-1.39423800
H	-1.06295100	2.16992000	0.51555200
H	0.48089300	-0.21756000	1.27909300
C	-0.76482500	-0.56676600	-0.48332300
C	0.52078100	4.18956600	-0.10626300
N	0.31775500	5.32150900	0.04523900
C	-2.20988800	-0.54810700	-0.20556900
C	-3.12157900	-0.99196800	-1.17012300
C	-2.69596000	-0.08597300	1.02365400
C	-4.48713700	-0.97402800	-0.91150500
H	-2.74883800	-1.32961800	-2.13245200
C	-4.06278100	-0.06960800	1.28028700
H	-1.99262500	0.23713300	1.78609700
C	-4.96241000	-0.51241700	0.31411000
H	-5.18343200	-1.31382000	-1.67153400
H	-4.42534600	0.28643500	2.23918100
H	-6.02877300	-0.49618600	0.51399000
C	-0.08788200	-1.53949600	-1.14494100
H	-0.51753100	-2.43378300	-1.57511100
C	1.38058800	-1.24947100	-1.10772800
H	1.95020000	-1.43317200	-2.03354500
N	2.08680400	-2.12629100	-0.02506500
C	1.77846000	-3.55418700	-0.16765400
H	2.07521200	-3.91564300	-1.16036900
H	2.32124600	-4.11910700	0.59251500
H	0.70847900	-3.70572800	-0.02937700
C	3.53619000	-1.88717100	-0.05340700
H	3.96084200	-2.21462500	-1.01109500
H	3.72342400	-0.82050700	0.08226300
H	4.01803200	-2.44024000	0.75591800
O	1.10811000	-0.95084900	1.95346600
H	1.61045100	-1.62638500	1.03270600
C	2.11127600	-0.15147700	2.56071800

H	3.01986400	-0.74488500	2.71150300
H	2.35514200	0.71694100	1.93239800
H	1.76705100	0.20290000	3.53575900

**TS8**

C	2.32355400	1.14381000	-1.18889600
C	2.12080900	2.45292700	-0.98719100
C	0.89025000	2.89849300	-0.31497500
C	-0.07553500	1.98036200	-0.02402300
C	0.15408600	0.57282500	-0.13494700
N	1.48685100	0.16139800	-0.65041200
H	3.17173600	0.76638700	-1.75341400
H	2.81800700	3.18293200	-1.37645100
H	-1.04982000	2.31118400	0.32480900
H	0.37930700	-0.11375100	1.20545700
C	-0.76506700	-0.43195300	-0.64494300
C	0.67076900	4.28594800	-0.06775100
N	0.50563300	5.41731700	0.13487300
C	-2.22140600	-0.40292400	-0.41510000
C	-3.10127100	-0.92944700	-1.36843600
C	-2.75532800	0.13860100	0.76134300
C	-4.47353000	-0.91993700	-1.14850200
H	-2.69754800	-1.32707100	-2.29458400
C	-4.12894400	0.14916900	0.98046100
H	-2.08208200	0.54524000	1.51178600
C	-4.99319900	-0.38145800	0.02669600
H	-5.14202700	-1.32618900	-1.90098500
H	-4.52453700	0.57201200	1.89855300
H	-6.06500600	-0.37116000	0.19557000
C	-0.07912400	-1.43041000	-1.25617600
H	-0.52237000	-2.31144900	-1.70044300
C	1.40262100	-1.16480800	-1.22976600
H	1.89160200	-1.20721600	-2.22728300
N	2.13962200	-2.14132100	-0.35097200
C	1.92499300	-3.51310400	-0.79989500
H	2.22585000	-3.65648600	-1.85205000
H	2.51619500	-4.19371000	-0.18219800
H	0.87193200	-3.78035600	-0.69755700
C	3.56696300	-1.83396800	-0.35080300
H	4.00572600	-1.90352800	-1.36176200
H	3.72612100	-0.82167400	0.02747500
H	4.09434500	-2.53678900	0.29996300

N	0.93659200	-0.88964600	1.93690900
C	-0.04193400	-1.64875200	2.71962200
H	0.45407200	-2.37031700	3.37575600
H	-0.63502100	-0.96173500	3.32846300
H	-0.70518500	-2.17211600	2.02784800
C	1.90453600	-0.11752400	2.72301000
H	2.53474000	-0.77382500	3.33019900
H	2.52046000	0.46070300	2.03106000
H	1.36704100	0.57270400	3.37763700
H	1.42612900	-1.50513700	1.24098400

**TS9**

C	2.32863700	0.87561700	-1.39999500
C	2.31655900	2.18428600	-1.09851500
C	1.19092200	2.76066200	-0.36331300
C	0.04706800	1.98250200	-0.20391900
C	0.05346100	0.63291300	-0.52550900
N	1.32072800	0.02699400	-0.90277200
H	3.08803400	0.40688500	-2.01795000
H	3.10287600	2.83210200	-1.46645200
H	-0.87830200	2.43937400	0.13387700
H	0.30539100	-0.28554500	1.30851500
C	-0.92726000	-0.37667800	-0.67872900
C	1.20904700	4.11908400	0.04104100
N	1.23493000	5.23077900	0.38500400
C	-2.36257500	-0.22244600	-0.37893900
C	-3.32154800	-0.82293100	-1.20397900
C	-2.80293500	0.49671800	0.73979700
C	-4.67735600	-0.70126600	-0.92344800
H	-2.99078100	-1.36966700	-2.08191000
C	-4.16001400	0.62250500	1.01776700
H	-2.07131300	0.95118300	1.40277400
C	-5.10333600	0.02323900	0.18760800
H	-5.40583300	-1.16671200	-1.58014500
H	-4.47975600	1.18668800	1.88832600
H	-6.16224900	0.12137100	0.40338100
C	-0.32566700	-1.53385200	-1.13592900
H	-0.84756100	-2.43514100	-1.42487700
C	1.14859800	-1.34612800	-1.25404200
H	1.61631100	-1.61461400	-2.22764600
N	1.93249600	-2.23168400	-0.22828100
C	1.59864900	-3.64437000	-0.40487000

H	1.82659600	-3.98120700	-1.42791300
H	2.17645400	-4.25352600	0.29501900
H	0.53501000	-3.79419700	-0.21350100
C	3.37525900	-2.02307900	-0.37103200
H	3.71146000	-2.25737500	-1.39318800
H	3.62230400	-0.98201700	-0.15205000
H	3.91747300	-2.66861300	0.32571400
N	0.99266500	-0.87164800	1.81375700
C	0.31559300	-1.67310400	2.84359700
H	1.03468200	-2.35632700	3.30067100
H	-0.11076200	-1.02800500	3.61549700
H	-0.48086300	-2.24426300	2.36365600
C	2.05560300	0.02184900	2.31353500
H	2.87788900	-0.58146500	2.70555300
H	2.40027600	0.63826500	1.47951300
H	1.66849400	0.66792000	3.10497900
H	1.42622000	-1.55933200	0.97743300

**TS-A**

C	1.49840800	4.24130000	0.17851400
C	1.95974700	3.60671600	-1.14904600
B	1.26971900	2.00090100	0.24228000
O	0.91599900	3.16375800	0.90140100
O	2.10919000	2.22879200	-0.83983900
C	-0.07610500	0.13435900	-1.11283400
C	-1.02077700	-0.82122900	-1.72491000
C	-2.34267100	-0.48776300	-1.84222200
C	-2.78847200	0.79627700	-1.44050300
C	-1.80895500	1.74075800	-1.03588600
N	-0.53992600	1.48341500	-0.94862500
H	0.87723100	0.16078800	-1.65691800
H	-0.65808200	-1.79439400	-2.03946500
H	-3.83623200	1.06214100	-1.48278400
H	-2.11853700	2.75684700	-0.79452600
C	-1.22454000	0.60246100	2.09135300
C	-0.83724300	-0.45213100	1.26143200
C	-1.64188800	-1.59494000	1.20951900
C	-2.80766400	-1.68078600	1.96360500
C	-3.18662800	-0.62394700	2.78698300
C	-2.38985000	0.51453700	2.84862600
H	-0.60725300	1.49291700	2.14319100
H	-1.37558800	-2.42832700	0.56571300

H	-3.41905800	-2.57572300	1.90659600
H	-2.67341000	1.34360200	3.48939900
C	0.40412900	-0.30499200	0.38174000
O	1.18492700	0.76322900	0.85266000
H	-4.09554500	-0.68973000	3.37652000
C	1.22894000	-1.55731600	0.29017400
C	2.57127500	-1.49966700	0.25806800
C	-3.28552900	-1.44241000	-2.36864000
N	-4.04350200	-2.20960100	-2.78672300
H	0.76189100	5.03602800	0.03127600
H	2.34101600	4.64584400	0.75153600
H	2.90544400	4.01323000	-1.51545400
H	1.19492700	3.72138700	-1.92767100
H	0.70136500	-2.50247600	0.24795900
N	3.44200600	-2.56409400	0.23521300
C	4.75544200	-2.34630600	-0.33851200
H	5.46038000	-3.07784700	0.06567000
H	4.75894200	-2.42977300	-1.43583900
H	5.10573600	-1.34762800	-0.06918900
C	2.88592600	-3.88579900	0.06498800
H	3.68326300	-4.62689000	0.14840500
H	2.15094100	-4.08061700	0.85128400
H	2.38895800	-4.00776400	-0.91125900
H	3.05277000	-0.52512100	0.29662600

**TS-B**

C	4.35796400	0.63782400	-0.56992200
C	4.40188700	0.91441800	-2.07958900
B	2.22163500	0.52430000	-1.45319800
O	3.07046100	0.10020600	-0.35365500
O	3.05715500	1.11290600	-2.43264500
C	-1.88350300	-3.06999900	-0.59945900
C	-3.27385600	-2.78755100	-0.66544400
C	-3.66513400	-1.42918600	-0.57357600
C	-2.72065400	-0.44670300	-0.48914100
C	-1.26092000	-0.78101400	-0.57302900
N	-0.93482000	-2.19020500	-0.52394900
H	-1.57189100	-4.11484800	-0.59326500
H	-4.00606900	-3.58071700	-0.73665100
H	-3.01900600	0.59257100	-0.41901400
H	-0.86511100	-0.40741500	-1.54443800
C	-0.42136400	0.07123300	0.39193600

C	-5.06600900	-1.08755200	-0.55263200	C	1.02170200	0.23675800	-1.30372700
N	-6.19226300	-0.82488200	-0.53434000	N	2.05985400	1.03176600	-0.62727700
H	5.13541700	-0.06634300	-0.24401800	H	3.56181300	0.91471000	0.79281600
H	4.81823800	0.05243800	-2.62282000	H	3.97231100	-1.49851900	0.56308400
H	5.00378900	1.79518900	-2.32796100	H	0.88962500	-1.66572300	-2.45936400
H	4.48136300	1.56848100	0.00501200	H	0.72202300	0.79183800	-2.20468400
O	0.93534000	0.38205800	-1.50479800	C	-0.29062800	0.27436500	-0.42658400
C	-0.89063100	1.47625200	0.54463900	C	2.80634900	-3.11313900	-1.30618300
C	-0.91665700	2.35811800	-0.54269700	N	3.08923900	-4.21370400	-1.52708400
C	-1.37694100	1.89325400	1.78843300	H	-5.20387200	-1.23318700	-0.67277900
C	-1.42357900	3.64173600	-0.37247100	H	-4.84462600	0.22239100	1.19393600
H	-0.47994600	2.02476900	-1.47932800	H	-4.79870900	1.66176200	0.15172800
C	-1.88885300	3.17823400	1.94630200	H	-5.64047000	0.23217500	-1.57889500
H	-1.37317800	1.20110000	2.62568400	O	-1.34051400	-0.02867800	-1.34203800
C	-1.91442700	4.05386900	0.86558600	C	-0.33656400	-0.71936100	0.73114800
H	-1.42649300	4.32828600	-1.21291300	C	-0.33898500	-0.32483700	2.06959800
H	-2.27064100	3.49097300	2.91278900	C	-0.45577100	-2.08422500	0.43949800
H	-2.31287200	5.05591600	0.98783400	C	-0.38777400	-1.27104200	3.09077200
C	0.51958800	-0.36252200	1.29706500	H	-0.34693300	0.72872900	2.32400100
H	0.90460100	0.39223600	1.97311300	C	-0.50022700	-3.02987200	1.45668000
C	1.29822800	-1.50820000	1.06559600	H	-0.52623000	-2.40656800	-0.59353300
H	1.00771600	-2.17894000	0.26445100	C	-0.45086100	-2.62652700	2.78881200
N	2.41944300	-1.78006200	1.69085300	H	-0.38946500	-0.94193500	4.12511700
C	2.99085000	-0.84234900	2.64923000	H	-0.57711400	-4.08309500	1.20683900
H	2.26447500	-0.61000300	3.42966000	H	-0.48261600	-3.36383000	3.58464500
H	3.86788700	-1.29821200	3.10818700	C	-0.30288500	1.74206700	-0.03826000
H	3.27500900	0.06936300	2.11237500	H	-0.90502300	2.37808800	-0.67800900
C	3.33640600	-2.76315700	1.13128400	C	0.84236600	2.23708100	0.58961000
H	2.79278600	-3.42262200	0.45545600	H	1.26161600	1.69065000	1.42865100
H	4.11344000	-2.23788100	0.56682500	N	1.24167000	3.55088500	0.53813000
H	3.78778200	-3.35138100	1.93318500	C	0.91262800	4.27997700	-0.67631600

### TS-C

C	-4.86337600	-0.23585400	-0.96993000
C	-4.46393600	0.62376000	0.25202500
B	-2.63567200	0.06012300	-0.93735500
O	-3.66780700	-0.36281800	-1.73366300
O	-3.03898400	0.59468200	0.26234400
C	2.93522600	0.31913500	0.12874400
C	3.17414000	-1.01958700	0.01159600
C	2.45090400	-1.74916400	-1.01510800
C	1.45023200	-1.14807500	-1.68795000

### TS-D

C	-3.53072100	0.43796000	2.10648000
C	-3.11169700	1.73882900	1.38564100

B	-1.47953000	0.18278100	1.20354300	H	2.97200200	4.37722000	1.11868200
O	-2.37206900	-0.39124100	2.07039500				
O	-1.88678700	1.40779300	0.72510600				
C	-1.12131800	-2.90653100	-0.91451200	<b>TS-E</b>			
C	-2.37134000	-2.26915800	-0.81275500				
C	-2.45935900	-0.95795700	-1.31860200	C	-3.31150400	1.60048100	-0.88615700
C	-1.33109200	-0.32642000	-1.80098600	C	-2.44796300	2.51836400	-1.77890300
C	-0.06019700	-0.97778400	-1.63133500	B	-1.23518900	0.75265600	-1.09893500
N	-0.02303400	-2.34138100	-1.35903700	O	-2.39246900	0.62451200	-0.38125600
H	-1.04249700	-3.95794800	-0.64167700	O	-1.24073600	1.78685000	-1.99513600
H	-3.23809100	-2.77609000	-0.40907100	C	0.18941300	-1.22046500	-0.44901800
H	-1.39096700	0.67749900	-2.20551400	H	-3.75899000	2.13914200	-0.04940000
H	0.75304800	-0.64031900	-2.27398200	H	-2.21204700	3.45883200	-1.27134200
C	0.66199100	-0.16403200	-0.01134200	H	-2.91747700	2.73630900	-2.74112600
C	-3.71618100	-0.25314700	-1.28958500	H	-4.09044200	1.08173100	-1.45411700
N	-4.71675700	0.32549900	-1.21904200	O	-0.11212500	-0.02420000	-1.01224600
H	-3.82534700	0.60902600	3.14484700	C	-0.86713200	-2.20025100	-0.09326500
H	-2.92089300	2.55747600	2.08741800	C	-0.81130700	-3.47926100	-0.65750000
H	-3.84637200	2.05794600	0.64364600	C	-1.86149800	-1.91022800	0.84743500
H	-4.34909200	-0.06544100	1.58229600	C	-1.74159200	-4.44983100	-0.30047800
O	-0.32170000	-0.47569000	0.91697300	H	-0.03824800	-3.69952900	-1.38747100
C	1.88558700	-0.98008200	0.24855500	C	-2.78892700	-2.88284000	1.20148800
C	2.95893700	-0.96873900	-0.65184700	H	-1.90219400	-0.92456400	1.29528300
C	1.95578300	-1.81208800	1.36886900	C	-2.73394600	-4.15170600	0.62841000
C	4.08315500	-1.75130700	-0.42300000	H	-1.69203700	-5.43607200	-0.75060600
H	2.90923300	-0.34562000	-1.54055900	H	-3.55497800	-2.65076800	1.93434600
C	3.08556800	-2.59097400	1.59825700	H	-3.46185400	-4.90656400	0.90872900
H	1.11953100	-1.84050200	2.05659000	C	1.50516000	-1.51030700	-0.30560800
C	4.15310100	-2.56402500	0.70713600	H	1.76183800	-2.44855200	0.16928800
H	4.90429800	-1.73249500	-1.13253800	C	2.52315600	-0.54356200	-0.64080300
H	3.12706100	-3.22577500	2.47781100	H	2.27912600	0.11808700	-1.46797500
H	5.03154100	-3.17570000	0.88625400	N	3.85752900	-0.85011000	-0.54478600
C	0.82173800	1.26880000	-0.32164100	C	4.29501900	-1.52595000	0.66600300
H	-0.08332000	1.79374500	-0.60055800	H	3.72447300	-2.43919700	0.83451100
C	1.98479700	1.94545900	-0.19787500	H	5.34610300	-1.80189000	0.55845100
H	2.87779600	1.44325500	0.16561700	H	4.18606200	-0.86385200	1.53851300
N	2.17998900	3.26415700	-0.51390300	C	4.75021800	0.23352600	-0.92076800
C	1.02740100	4.05520400	-0.88674000	H	4.76494900	1.01559500	-0.14718100
H	0.29615200	4.13323700	-0.06816600	H	5.76111300	-0.15719700	-1.05781700
H	1.35619100	5.05675700	-1.16929300	H	4.41620700	0.67120300	-1.86458900
H	0.52843800	3.59831600	-1.74638400	C	1.94653300	2.12313400	0.02002500
C	3.26393100	3.97305600	0.13865700	C	0.81650900	2.87115700	0.21888300
H	4.10580000	3.29275900	0.28357100	C	-0.12948400	2.44408400	1.18148400
H	3.59569900	4.80155400	-0.49287200	C	0.18736900	1.29187200	1.94029500

C	1.34557400	0.60974500	1.66993100
N	2.22970200	0.96058000	0.68812000
H	2.67720200	2.42331800	-0.72791700
H	0.64312200	3.76931400	-0.36305500
H	-0.47117000	0.95950300	2.73544800
H	1.59497500	-0.28839900	2.22830000
C	-1.35605500	3.13788100	1.36789700
N	-2.36929000	3.69637300	1.48914900

**TS-F**

C	5.42947200	0.06543700	1.22064200
C	5.30126100	0.05635800	-0.31434100
B	3.33237200	-0.54377900	0.62928300
O	4.09236500	-0.05669400	1.68349900
O	4.05069700	-0.56914500	-0.55868100
C	1.31402500	-0.97773500	-2.66396700
C	2.08677400	-2.25887300	-2.30927200
B	1.25187900	-1.31131500	-0.37477800
O	1.08241000	-0.33423100	-1.42636000
O	1.72714700	-2.53071900	-0.97269900
C	-0.38240700	-2.94305900	0.74207200
C	-1.55680300	-3.53316300	1.01114800
C	-2.78677700	-2.78315300	0.74769400
C	-2.74159900	-1.49255100	0.36635100
C	-1.46145900	-0.77476100	0.19887900
N	-0.23750400	-1.64881100	0.24479100
H	0.56681300	-3.45215200	0.86584200
H	-1.60390000	-4.54229900	1.39501500
H	-3.65452800	-0.92791600	0.21961100
H	-0.94572100	-1.21121300	-0.83065700
C	-1.37203600	0.63049200	0.27150700
C	-4.06163200	-3.42194800	0.92561100
N	-5.08291000	-3.94766400	1.07098600
H	6.01924900	-0.78565200	1.58120200
H	6.10348500	-0.49940200	-0.80630100
H	5.28164500	1.07517000	-0.72348700
H	5.87670600	0.98618900	1.60542100
H	1.81471000	-3.10161700	-2.95464300
H	3.16810400	-2.09105600	-2.38071300
H	0.35636500	-1.21613000	-3.15550700
H	1.87793900	-0.31600800	-3.32985400
O	2.04339400	-0.87176400	0.76534300

C	-2.59456100	1.40558400	-0.06806000
C	-3.10543600	2.34592700	0.83480700
C	-3.25228800	1.21336200	-1.28862500
C	-4.25343700	3.06897100	0.52620500
H	-2.60149600	2.49118400	1.78577700
C	-4.39975900	1.93678900	-1.59552800
H	-2.84952300	0.49675800	-1.99919100
C	-4.90398100	2.86588200	-0.68830000
H	-4.64524800	3.78639300	1.24006800
H	-4.89670600	1.77885200	-2.54717500
H	-5.79984700	3.42924500	-0.92754900
C	-0.16376200	1.29403400	0.56554700
H	0.66317500	0.68924300	0.91127000
C	0.03631100	2.63152200	0.31459400
H	-0.77842900	3.25671900	-0.04321900
N	1.21278700	3.25735100	0.46029700
C	2.41267300	2.47532500	0.72110400
H	2.55713000	1.74932600	-0.09012200
H	3.27058500	3.14700600	0.77386100
H	2.33749300	1.92845400	1.66531900
C	1.37349900	4.66065100	0.13895600
H	0.39646000	5.10596500	-0.05274500
H	1.84114800	5.19298000	0.97329100
H	1.99992900	4.78918400	-0.75151500

**TS-G**

C	-2.78502000	-0.13625800	0.99807800
C	-3.10032200	1.10594100	0.59151300
C	-2.04593400	1.97940100	0.06338100
C	-0.79030400	1.49685900	-0.14145300
C	-0.50071800	0.10714300	0.09393900
N	-1.47031700	-0.58168400	0.97377900
H	-3.50810200	-0.81100200	1.44769000
H	-4.10949100	1.48116600	0.69561600
H	-0.01308300	2.14646800	-0.53174200
H	-0.78524300	-1.00213500	-0.90136700
C	0.76298200	-0.53012000	0.48066300
C	-2.35551600	3.34215600	-0.24475900
N	-2.62218100	4.44288500	-0.49407400
C	2.10320600	0.00576700	0.20334700
C	3.14296800	-0.19707500	1.11838800
C	2.36856500	0.71015200	-0.97723700



C	4.41644500	0.29543600	0.85991600	H	2.05828300	1.88080900	-1.05975500
H	2.93422900	-0.72519200	2.04393400	C	4.93358300	0.68876400	0.28532300
C	3.64417700	1.20175700	-1.23361800	H	5.21383900	-1.31169400	1.03272900
H	1.57532800	0.84738100	-1.70656800	H	4.34743000	2.59794600	-0.51521400
C	4.67146500	0.99747100	-0.31607200	H	5.94306700	1.00646800	0.52411000
H	5.21064000	0.13844100	1.58283100	C	0.45888800	-1.80561100	-0.67691100
H	3.83682700	1.74230700	-2.15482500	H	1.01876400	-2.72492500	-0.55848700
H	5.66519800	1.38537200	-0.51495200	C	-1.04315100	-1.76100700	-0.84654700
C	0.46422700	-1.73508200	1.03875000	H	-1.47973100	-2.54888200	-1.47710900
H	1.15685300	-2.51382900	1.32550100	N	-1.67425300	-1.93562500	0.55047800
C	-1.01553900	-1.91974700	0.85175600	C	-1.15492400	-3.13015100	1.23807600
H	-1.56968800	-2.66366700	1.43140400	H	-0.09768900	-2.99699600	1.47032400
N	-1.20394800	-2.22076400	-0.69121700	H	-1.70502900	-3.27187400	2.16963800
C	-0.36695300	-3.28885300	-1.23284400	H	-1.28055600	-4.02261100	0.61295700
H	-0.68940800	-4.26594500	-0.84743400	C	-3.14875400	-1.98653900	0.50227500
H	-0.45044900	-3.29708600	-2.32247800	H	-3.52844700	-2.07674300	1.52173800
H	0.67324800	-3.11564000	-0.96527300	H	-3.52776900	-1.07152200	0.05216000
C	-2.60602100	-2.36890200	-1.07844200	H	-3.47624600	-2.85511900	-0.08201800
H	-3.10973700	-3.11123400	-0.44416300	O	-0.75031400	0.16020200	1.53277500
H	-3.12547700	-1.41233900	-0.99215200	H	0.14451900	-0.01888900	1.86160100
H	-2.66275900	-2.70240400	-2.11726900	H	-1.26096600	-0.88818500	1.12569300

### TS-H

C	-2.49162100	0.16403800	-1.62970400
C	-2.77487400	1.31502700	-0.98362300
C	-1.89719400	1.88777000	0.00796100
C	-0.64140800	1.27506800	0.26354000
C	-0.16661200	0.42151000	-0.92575100
N	-1.23187600	-0.45591400	-1.39221600
H	-3.11048700	-0.27046100	-2.40721100
H	-3.68488300	1.85179400	-1.23362100
H	0.12480300	1.91351500	0.70698800
H	0.10305300	1.11712800	-1.73299900
C	0.94860700	-0.55922400	-0.63810600
C	-2.27369800	3.03833800	0.74080400
N	-2.57407300	3.99025200	1.34068500
C	2.32239700	-0.13282300	-0.32859300
C	3.23047200	-1.01738000	0.27143500
C	2.74314000	1.17530100	-0.60022900
C	4.52452700	-0.61366400	0.56905900
H	2.91239100	-2.02618200	0.51795000
C	4.03888400	1.58122100	-0.29639300

### TS-I

C	2.74552700	-1.48563900	-0.01977500
C	3.23451800	-0.14786100	-0.12859000
C	2.43685400	0.95478000	-0.19310600
C	0.93368800	0.86526800	-0.28775500
C	0.49224300	-0.55012100	0.07729800
N	1.35962200	-1.60019800	-0.33235300
H	3.35023000	-2.32016000	-0.35481800
H	4.30960000	-0.00987100	-0.05953400
H	0.48589100	1.56064100	0.43531500
H	0.89365800	-0.70995200	1.44611900
C	-0.83804200	-1.06142700	-0.11835100
C	3.00861100	2.26223600	-0.22613500
N	3.45691800	3.33237900	-0.23584400
C	-2.06566500	-0.27599400	0.04733300
C	-3.17274500	-0.51140800	-0.77992900
C	-2.15216100	0.73357600	1.01666900
C	-4.33243500	0.24108800	-0.64031300
H	-3.10488400	-1.27360200	-1.55023800
C	-3.31143600	1.49041400	1.14936500

H	-1.31524700	0.90199100	1.68861200
C	-4.40464700	1.24641600	0.32214200
H	-5.17898900	0.05041600	-1.29183700
H	-3.36318500	2.26597300	1.90638200
H	-5.30896500	1.83657600	0.42659700
C	-0.72801300	-2.37982700	-0.53337200
H	-1.53679400	-3.07276200	-0.71748700
C	0.64266600	-2.67921200	-0.64039600
H	1.12692500	-3.61923200	-0.86800200
O	0.53995200	1.23550100	-1.59727300
H	-0.40132200	1.45075700	-1.57413200
O	1.66877700	-1.01697300	2.33065100
H	2.39560800	-1.34465900	1.57455200
H	1.32808300	-1.80333700	2.77831600

**TS-J**

C	2.65987400	-1.67839100	0.07995500
C	3.22225000	-0.44827800	0.02748400
C	2.45402900	0.77294000	-0.02254300
C	1.04269400	0.60930300	-0.56425800
C	0.44493900	-0.61500000	0.13945400
N	1.25982900	-1.77491500	0.06802300
H	3.20092700	-2.61219800	0.13086900
H	4.30477800	-0.38272500	0.07200800
H	0.43399400	1.48328700	-0.29490200
C	-0.90820400	-1.09398700	0.05224800
C	3.13441000	1.97705200	-0.38606800
N	3.67665400	2.97581400	-0.62590900
C	-2.09571700	-0.23368700	0.04962900
C	-3.24222400	-0.61414100	-0.66025700
C	-2.10336400	0.98105800	0.75000800
C	-4.36622400	0.20259300	-0.67441400
H	-3.23537900	-1.54504000	-1.21959700
C	-3.22910300	1.79714900	0.73019000
H	-1.23666900	1.26810100	1.33996100
C	-4.36184300	1.41210600	0.01759900
H	-5.24519700	-0.10101800	-1.23361900
H	-3.22307600	2.73257900	1.27981200
H	-5.23875100	2.05076500	0.00271000
C	-0.86288300	-2.48135100	0.02269700
H	-1.70492300	-3.15831200	0.04371500
C	0.48825400	-2.86354900	0.03389900

H	0.92554500	-3.85256800	0.05219000
O	1.07700600	0.44780500	-1.96778600
H	0.17636400	0.53426200	-2.30415200
H	1.65784100	0.05124100	2.97690500
O	1.21836600	0.56419000	2.28407800
H	0.65560700	-0.15982800	1.43217100
H	1.94924500	0.84629700	1.52304300

**TS-K**

C	-2.26967700	0.13443100	-1.78318100
C	-2.66372500	1.09125600	-0.81199900
C	-1.54409000	1.76062800	-0.03318400
C	-0.25211000	1.46733100	-0.24196900
C	0.13771700	0.35734100	-1.19520300
N	-0.99687000	-0.48583600	-1.54375800
H	-2.58009900	0.24111200	-2.81461400
H	-3.38151800	1.83377600	-1.16759500
H	0.53514000	2.01656600	0.27078400
H	0.57070900	0.80274300	-2.10563100
C	1.11034100	-0.61359300	-0.55104700
C	-1.89438500	2.77511500	0.92702900
N	-2.18333600	3.59793400	1.68918400
C	2.49723100	-0.25650700	-0.21416000
C	3.22768800	-1.01622700	0.71040100
C	3.11047500	0.86181700	-0.79234200
C	4.53639700	-0.68162300	1.02921000
H	2.75551100	-1.86536600	1.19527100
C	4.42130300	1.19941500	-0.46987900
H	2.56428100	1.46855600	-1.50769000
C	5.13912400	0.42820600	0.43843300
H	5.08581500	-1.28040600	1.74830900
H	4.88083600	2.06766400	-0.93048600
H	6.16027100	0.69298700	0.69196400
C	0.48871800	-1.78400100	-0.34734000
H	0.93147600	-2.68499500	0.06210500
C	-0.94448300	-1.67763400	-0.77059200
H	-1.33449800	-2.53653000	-1.32804700
N	-1.91003500	-1.63495300	0.48298700
C	-1.28239200	-1.32876200	1.78747300
H	-0.65218100	-0.44743200	1.68054900
H	-2.08140700	-1.10787400	2.49797300
H	-0.68618400	-2.17506800	2.13571800

C	-2.74196900	-2.84949200	0.55686100	C	-2.80229900	-1.96539900	0.86433800
H	-3.43684000	-2.75946400	1.39415500	H	-3.06798000	-2.39854200	1.83186400
H	-3.30316300	-2.93559400	-0.37479700	H	-2.95031100	-0.88623400	0.90220500
H	-2.11115700	-3.73177500	0.69616400	H	-3.44878700	-2.40013400	0.09330600
O	-3.47766500	0.43611800	0.45606000	O	0.30927700	-0.53628600	1.42528400
H	-2.61373100	-0.79809500	0.33903500	H	1.08640800	-0.91957100	1.85154800
H	-4.30723500	0.16402300	0.03839500	H	-0.71865200	-1.59568000	1.12924600

### TS-L

C	-2.57866500	0.05613000	-1.44214200
C	-2.94262800	1.30556400	-1.06857000
C	-2.09721400	1.97618300	-0.07864400
C	-0.84396800	1.54591100	0.18225100
C	-0.27845600	0.51455500	-0.75641900
N	-1.34824000	-0.42417800	-1.09438700
H	-3.23095800	-0.61584000	-1.99455800
H	-3.88964400	1.73241600	-1.36648700
H	-0.26113900	1.90681500	1.02051800
H	0.06542700	1.00219100	-1.68667700
C	0.82392000	-0.43449800	-0.29217800
C	-2.68531600	3.02617700	0.71339700
N	-3.17297000	3.87404400	1.33260500
C	2.21518600	0.08742500	-0.16064400
C	3.25781600	-0.79682600	0.13885600
C	2.51066200	1.44528800	-0.30485000
C	4.56209400	-0.33860500	0.27939100
H	3.03782100	-1.85369300	0.26180000
C	3.81780600	1.90515900	-0.16872700
H	1.71867500	2.15404200	-0.52805800
C	4.84733600	1.01638500	0.12383300
H	5.35824800	-1.03947200	0.50962400
H	4.02943500	2.96275600	-0.28883700
H	5.86511500	1.37627300	0.23315000
C	0.55335600	-1.65991600	-0.94235700
H	1.22371700	-2.50461300	-0.99798400
C	-0.89770100	-1.76732500	-0.96253300
H	-1.41202900	-2.47874300	-1.61965700
N	-1.39556100	-2.25268100	0.55546700
C	-1.05528300	-3.66375100	0.75574700
H	-0.00213300	-3.80358700	0.50962200
H	-1.22874500	-3.95238100	1.79473300
H	-1.67115700	-4.29073800	0.10209100

### TS-M

C	2.31344400	1.77751900	-0.05040300
C	1.65398600	2.94004400	0.08549500
C	0.19299900	2.88759600	0.17512400
C	-0.45835500	1.72596800	0.35935000
C	0.31763400	0.47229900	0.64941700
N	1.68966300	0.55169000	0.10671800
H	3.37364900	1.73631700	-0.28888400
H	2.16473500	3.89070500	0.02349900
H	-1.54217800	1.67288200	0.33080900
H	0.34874600	0.29922200	1.73327600
C	-0.22325100	-0.79475500	-0.05106700
C	-0.54630200	4.10562800	-0.03434300
N	-1.12084800	5.09745400	-0.19564900
C	-1.70621200	-0.99980700	-0.04415700
C	-2.42883500	-0.79285600	-1.22300000
C	-2.39764500	-1.31463400	1.13071400
C	-3.81460300	-0.92311800	-1.23325000
H	-1.88791900	-0.51570200	-2.12204300
C	-3.78369600	-1.43694700	1.11900100
H	-1.83094900	-1.47580400	2.04143100
C	-4.49596800	-1.24553500	-0.06264800
H	-4.36310500	-0.76402500	-2.15624600
H	-4.30925000	-1.68358100	2.03621800
H	-5.57698500	-1.34188500	-0.06958700
C	0.54314300	-0.95014300	-1.22088400
H	0.34898400	-1.69851000	-1.97767400
C	1.88574100	-0.51062700	-0.84977600
H	2.62284200	-0.26695800	-1.62455800
N	2.61687700	-1.68582900	0.01022300
C	2.89778700	-2.84624400	-0.84370000
H	3.63098100	-2.57222500	-1.60942600
H	3.29533400	-3.66610800	-0.24215000
H	1.96954400	-3.15802900	-1.32161700

C	3.81397500	-1.22772000	0.72755100
H	3.53347800	-0.41992400	1.40127000
H	4.24646000	-2.05141700	1.29961200
H	4.55582600	-0.86785900	0.00578700
O	0.35243000	-1.92324400	1.20911300
H	-0.05146900	-2.75874400	0.93711700
H	1.76894200	-1.91562000	0.68068100

**TS-N**

C	2.80344800	1.67638000	0.13369900
C	3.36488500	0.42426000	0.09297100
C	2.62402800	-0.74511000	-0.07503000
C	1.15455000	-0.77129000	0.22712900
C	0.54361000	0.55497700	-0.14294800
N	1.43563400	1.72247900	-0.23480400
H	3.31998500	2.62137000	0.10055800
H	4.44614000	0.35170700	0.15404800
H	0.66215300	-1.56113000	-0.35069700
H	1.28820300	1.11379900	-1.26500600
C	-0.75322300	1.03916000	-0.19634000
C	3.27480400	-2.00112600	-0.18878800
N	3.78632800	-3.03697900	-0.31948000
C	-1.97570100	0.22227100	-0.16320300
C	-3.07821500	0.65830500	0.58268600
C	-2.06306200	-0.99308200	-0.85362500
C	-4.23663300	-0.10677400	0.64238600
H	-3.01226200	1.59175900	1.13432000
C	-3.22064600	-1.76167200	-0.78330300
H	-1.23465300	-1.31821900	-1.47543700
C	-4.30948400	-1.32198300	-0.03567900
H	-5.08130800	0.24133700	1.22776600
H	-3.27453100	-2.70029900	-1.32479500
H	-5.21231800	-1.92117000	0.01578800
C	-0.68464300	2.45902500	-0.29050100
H	-1.53807200	3.11467600	-0.39931200
C	0.61749600	2.85816200	-0.31712200
H	1.07456900	3.83039800	-0.41152200
O	0.95101700	-1.00422300	1.61693200
H	0.03293900	-1.27794700	1.74482700

**TS-O**

C	-2.93324000	1.68243000	-0.19266800
C	-3.14604600	0.22755900	-0.40970300
C	-2.40962300	-0.84684200	-0.05197400
C	-1.06386900	-0.97990800	0.67342800
C	-0.56057100	0.37491300	1.05380200
N	-1.84556400	2.29875800	-0.16389700
H	-3.88019800	2.21574400	-0.00374700
H	-4.12068100	0.00519200	-0.84021600
H	-1.30336800	-1.56155600	1.58335000
H	-1.29157300	0.95679400	1.60217100
C	0.55977700	1.00780800	0.62914200
C	-3.00091200	-2.13565500	-0.32710100
N	-3.48254200	-3.16877200	-0.52844800
C	1.80766300	0.31242400	0.22753700
C	2.48597900	0.64844000	-0.94911200
C	2.35472600	-0.67313000	1.06181100
C	3.66252800	-0.00609100	-1.29749800
H	2.06619000	1.40793100	-1.60168000
C	3.52795500	-1.33423400	0.70825700
H	1.85999300	-0.89477500	2.00471700
C	4.18395600	-1.00214900	-0.47443300
H	4.16997300	0.25432000	-2.22080600
H	3.93741300	-2.09622900	1.36369500
H	5.10037400	-1.51300900	-0.75067500
C	0.47590000	2.43031400	0.36497900
H	1.36180800	3.05735700	0.38483400
C	-0.68306000	2.95664100	-0.13526800
H	-0.68307800	3.96925900	-0.54290300
O	-0.26085300	-1.72572300	-0.20323900
H	0.59973300	-1.88026800	0.20640400

**TS-P**

C	2.81304300	1.67122500	0.15704300
C	3.35182200	0.40194500	0.16467800
C	2.62564600	-0.76204300	-0.01516600
C	1.12601400	-0.78188400	-0.03491100
C	0.58995100	0.62417000	-0.18845800
N	1.45016300	1.74023800	-0.20552100
H	3.33706600	2.60879900	0.23460100
H	4.42287500	0.31952900	0.32225700
H	0.76601100	-1.40588400	-0.86463400
H	1.26348800	2.21637500	-1.29621500

C	-0.71117900	1.09006100	-0.16728700
C	3.27648000	-2.02279000	-0.04136900
N	3.79412600	-3.06252600	-0.09432200
C	-1.92870600	0.25588800	-0.13544200
C	-2.97831300	0.60376200	0.72126400
C	-2.05644200	-0.88193400	-0.94003800
C	-4.12836000	-0.17531300	0.77934500
H	-2.87654000	1.47673600	1.35940600
C	-3.20582700	-1.66400600	-0.87562100
H	-1.26529800	-1.13898100	-1.63766100
C	-4.24301100	-1.31347600	-0.01545000
H	-4.93234500	0.10109100	1.45339700
H	-3.29307000	-2.54315700	-1.50534800
H	-5.13817200	-1.92428600	0.03435200
C	-0.69853700	2.50682600	-0.18980800
H	-1.56474600	3.14775200	-0.26775800
C	0.60814400	2.93403800	-0.23029800
H	1.09342800	3.89359200	-0.13988200
O	0.63397700	-1.33744600	1.18301500
H	-0.23888500	-1.71478600	1.01137400

**TS-Q**

C	2.84773600	1.44806700	0.35288400
C	3.31804000	0.20711600	-0.18653000
C	2.45540800	-0.83819800	-0.30001100
C	1.08613500	-0.74517400	0.34436500
C	0.63952400	0.68668700	0.24332100
N	1.55993700	1.66706900	0.47864800
H	3.53185900	2.23494500	0.64944200
H	4.35734700	0.10615200	-0.48264900
H	0.37041300	-1.38127700	-0.18043900
H	1.08762800	2.87135900	-1.22376500
C	-0.66667600	1.12751600	-0.04660300
C	2.85389000	-2.07961200	-0.88684900
N	3.15621000	-3.09053900	-1.36664200
C	-1.85590000	0.25631200	-0.04670500
C	-1.98790400	-0.81860300	0.84425900
C	-2.90150300	0.53690800	-0.93584100
C	-3.13835100	-1.60018900	0.82812400
H	-1.19716600	-1.02384200	1.56026800
C	-4.04984500	-0.24532200	-0.94659000
H	-2.79245100	1.36529400	-1.62983600

C	-4.16866200	-1.31803500	-0.06551400
H	-3.23284500	-2.42807200	1.52305300
H	-4.84947700	-0.02258200	-1.64543800
H	-5.06386000	-1.93145600	-0.07422600
C	-0.74636400	2.52052200	-0.16773100
H	-1.62461200	3.05440100	0.18112700
C	0.48456500	3.14720400	-0.36625600
H	0.66355700	4.15448800	0.00470800
O	1.11608000	-1.24935000	1.67370900
H	1.78737400	-0.75151700	2.15809200

**TS-R**

C	3.24113800	1.39909600	-0.37147400
C	3.63891400	1.92561000	-1.76403000
B	1.49197500	1.08740100	-1.88076200
O	2.06052500	0.66861700	-0.59959300
O	2.44395800	1.92996100	-2.49718400
C	3.20162000	-1.96971000	-1.67470200
C	3.64693000	-2.35307600	-0.24834800
B	1.45873600	-1.82500800	-0.29117500
O	1.78104300	-1.95690100	-1.60698100
O	2.52174400	-2.03147000	0.57487200
C	-0.31953600	-2.37109600	1.31344600
C	-1.62398700	-2.69059000	1.42911600
C	-2.49348700	-2.38827400	0.29259700
C	-2.10798300	-1.50498400	-0.65092700
C	-0.84259900	-0.72705100	-0.37987100
N	0.13400300	-1.61399800	0.23903000
H	0.44041400	-2.73624600	2.00006400
H	-1.98705500	-3.28446800	2.25680900
H	-2.68130600	-1.34455300	-1.55653000
H	-0.35204400	-0.22973000	-1.34898400
C	-1.13877500	0.51840600	0.38932100
C	-3.71688400	-3.13363000	0.14927700
N	-4.70413500	-3.73197000	0.06333000
H	4.01290900	0.75861800	0.07904100
H	4.37807000	1.25983800	-2.23596400
H	4.07418300	2.92987500	-1.71997400
H	3.04435700	2.23456800	0.32336300
H	3.85859600	-3.42378100	-0.15627600
H	4.52162200	-1.79043700	0.08886900
H	3.52617200	-2.68887600	-2.42939200

H	3.55026800	-0.96966200	-1.95456600
O	0.33029700	0.72773900	-2.31013200
C	-2.34756600	1.25147300	-0.06601500
C	-2.52001200	1.55317400	-1.42437200
C	-3.31253800	1.64462500	0.86665700
C	-3.65758500	2.24453600	-1.82746700
H	-1.73506500	1.28826700	-2.13130100
C	-4.45443700	2.31886800	0.44792500
H	-3.17852000	1.38980100	1.91425600
C	-4.62694800	2.62082000	-0.90013300
H	-3.78443000	2.49345000	-2.87606400
H	-5.20995000	2.60366800	1.17307200
H	-5.51600300	3.15070900	-1.22708100
C	-0.39523200	1.13737700	1.36961300
H	-0.74756100	2.10809000	1.70307000
C	0.85402400	0.68307900	1.83763100
H	1.24216800	-0.27586700	1.53398100
N	1.64448300	1.36606300	2.63278700
C	1.30649300	2.70758300	3.10126200
H	0.36954200	2.69034400	3.66271800
H	2.10431400	3.06166600	3.75270100
H	1.20486800	3.38759600	2.25085300
C	2.94671100	0.82611500	3.01274100
H	3.08494200	-0.14106300	2.52588900
H	3.73497400	1.50973900	2.68523400
H	3.00041900	0.70815900	4.09854300

**TS-S**

C	-4.36466700	1.42921900	0.40884200
C	-4.57886400	1.03315400	-1.07099800
B	-2.38371100	0.98290200	-0.57438100
O	-2.97683400	1.21846800	0.64520900
O	-3.27145200	0.95913200	-1.62148200
C	-0.10712500	0.57959400	0.17942800
H	-4.60114700	2.48200100	0.59405100
H	-5.17106600	1.76885600	-1.62121600
H	-5.06486300	0.05526200	-1.16666300
H	-4.95189600	0.81372800	1.09727500
O	-1.04768400	0.89776200	-0.80545700
C	0.93629000	1.62067200	0.33467800
C	2.09303300	1.33922400	1.07497100
C	0.82801400	2.86217700	-0.29944300

C	3.09762700	2.28984700	1.20893400
H	2.21348000	0.35737000	1.52788500
C	1.83785600	3.81004300	-0.16755200
H	-0.05283700	3.07708700	-0.89369500
C	2.97285100	3.53124500	0.58915600
H	3.98780300	2.05342000	1.78295000
H	1.73645400	4.77252900	-0.65936000
H	3.76078900	4.27090300	0.68618800
C	-0.46708700	-0.23242900	1.29237800
H	0.07815100	-0.07953400	2.21918400
C	-0.78949200	-1.67798000	0.95058200
H	-0.79212400	-2.32370800	1.84719400
N	-2.04227600	-1.81398400	0.21221500
C	-3.14688000	-1.72343500	1.16269800
H	-3.04714600	-0.81534200	1.75941200
H	-4.09349800	-1.68090500	0.61539200
H	-3.17648300	-2.59934100	1.83558100
C	-2.12433300	-3.07192800	-0.52037900
H	-2.01833300	-3.94989000	0.14208100
H	-3.10054100	-3.12529500	-1.00821000
H	-1.34914700	-3.12132400	-1.28551300
C	1.41649100	-2.69196300	0.78056000
C	2.71415700	-2.49176700	0.45867900
C	3.02202800	-1.54255600	-0.58585500
C	2.01279400	-0.87789400	-1.22391100
C	0.65369300	-1.03532800	-0.81139900
N	0.37457600	-2.06544300	0.13092800
H	1.11888100	-3.38262700	1.56282900
H	3.50101800	-3.04183100	0.95609900
H	2.22851100	-0.16331800	-2.01035600
C	4.39013300	-1.30724200	-0.94795900
N	5.50003900	-1.12676600	-1.22564800
H	-0.12518100	-0.89802200	-1.55829400

**TS-T**

C	4.63268500	-0.48815800	-1.13047700
C	4.26128100	-0.83667700	0.32702900
B	2.38459700	-0.60143800	-0.92626400
O	3.41005800	-0.58050600	-1.84957500
O	2.84436700	-0.70848700	0.37998200
C	-3.10771000	-1.55380500	-0.56964200
C	-4.07206900	-0.63393800	-0.78826000

C	-3.77755500	0.74616900	-0.40566000	C	-4.64831200	-0.65251800	-1.31169300
C	-2.51678000	1.15763800	-0.16475100	C	-4.45607000	-0.60184500	0.21972500
C	-1.40420800	0.20246900	-0.52075700	B	-2.48329200	-0.28012400	-0.82453000
N	-1.81934600	-1.17939700	-0.27295500	O	-3.39713100	-0.23436800	-1.84729200
H	-3.28340300	-2.62600200	-0.58224200	O	-3.04162600	-0.56374400	0.40144500
H	-5.07400800	-0.91845200	-1.07728100	C	2.55821900	2.31037400	0.40078800
H	-2.30040200	2.13597500	0.25158200	C	3.62504300	1.79861400	-0.25337100
H	-1.13694900	0.31596200	-1.58361500	C	3.51453800	0.42373400	-0.73236700
C	-0.14691100	0.32428600	0.31901600	C	2.32759700	-0.21535000	-0.80504700
C	-4.88273900	1.63742000	-0.15920600	C	1.08091900	0.58814400	-0.56489100
N	-5.77874600	2.34559000	0.02814600	N	1.37901400	1.62134900	0.42973100
H	5.02498300	0.53131000	-1.21623300	H	2.57745800	3.24361400	0.95547300
H	4.71825500	-0.15723000	1.05165800	H	4.56610300	2.32652000	-0.30321700
H	4.53756800	-1.86482100	0.58590100	H	2.25636500	-1.26297600	-1.07544400
H	5.36423800	-1.18038400	-1.55488800	H	0.75431600	1.05853100	-1.50697400
O	1.08548200	-0.52717800	-1.29150300	C	-0.20037800	-0.12871300	0.00069900
C	0.58508000	1.59480400	0.43963300	C	4.72798800	-0.28756400	-1.04563400
C	1.44072300	1.83840500	1.51997700	N	5.71107600	-0.84285100	-1.29964400
C	0.43744600	2.57959700	-0.54514400	H	-4.86601500	-1.66728400	-1.66169000
C	2.13536100	3.03805300	1.61021100	H	-4.86720500	-1.47614600	0.72919900
H	1.56023800	1.08396900	2.29040100	H	-4.89484300	0.30112000	0.65800600
C	1.13094600	3.78039200	-0.45177000	H	-5.43972700	0.01494200	-1.66048500
H	-0.20949400	2.39601400	-1.39772700	O	-1.16531900	-0.05831100	-1.05739100
C	1.98159500	4.01241700	0.62567700	C	0.04558500	-1.58537700	0.37676700
H	2.79390400	3.21681500	2.45399600	C	0.74117100	-1.88002200	1.55170300
H	1.00892500	4.53362700	-1.22283500	C	-0.33608100	-2.62808000	-0.46739400
H	2.52108900	4.95102400	0.70059500	C	1.03420300	-3.19742000	1.88659900
C	0.03087700	-0.81667300	1.04505000	H	1.05233500	-1.06783600	2.20310200
H	0.85922900	-1.00582200	1.71648500	C	-0.04412200	-3.94784900	-0.12937800
C	-1.08607700	-1.80888500	0.82235100	H	-0.85098100	-2.40731000	-1.39672100
H	-1.69923200	-1.83947300	1.74089100	C	0.63861300	-4.23658900	1.04768000
N	-0.76466200	-3.19043000	0.52780600	H	1.57386300	-3.41263200	2.80316700
C	0.21448800	-3.36387500	-0.53548700	H	-0.34914800	-4.75131900	-0.79231100
H	1.23544200	-3.09839000	-0.21131500	H	0.86688400	-5.26504100	1.30798300
H	0.21061700	-4.41213100	-0.84739800	C	-0.55035200	0.72194500	1.19450500
H	-0.04750600	-2.73104800	-1.38326500	H	-1.37560200	0.48974000	1.85072400
C	-0.39977300	-3.93841500	1.71744000	C	0.33294900	1.76662900	1.34159800
H	-1.17875700	-3.83785000	2.47862000	H	0.53186900	2.29689100	2.26544500
H	-0.30976800	-4.99686600	1.45908100	N	-0.64773500	3.40902600	0.69219900
H	0.56211300	-3.61735000	2.15532100	C	-0.79066400	3.33804000	-0.74638600
				H	-1.42541000	2.50780500	-1.09057700
				H	-1.25183200	4.27327800	-1.09507500
				H	0.19491900	3.25899900	-1.21277600
				C	-1.94090900	3.43033500	1.34343400

TS-U

H	-1.82038900	3.27494600	2.42041800
H	-2.39088200	4.42193800	1.19650800
H	-2.64913100	2.68262400	0.95375200

H	-1.31453700	-2.64785700	2.54620100
O	2.55004800	-2.58742600	-1.10857200
H	2.89502500	-3.09189700	-0.36095700
H	1.38286300	-2.28325600	-1.03585800

**TS-V**

C	4.08420300	0.58540200	-0.84743200
C	3.71075400	0.32679000	0.62852900
B	2.53316200	-1.07976100	-0.73435200
O	3.17053700	-0.18920100	-1.60439900
O	2.95680700	-0.87784600	0.59884100
C	-3.36470100	-1.73633500	0.91003000
C	-4.17088100	-0.98387700	0.13207000
C	-3.54425400	0.04722100	-0.69135400
C	-2.21006700	0.09853300	-0.88122800
C	-1.36584700	-1.03198000	-0.37365300
N	-2.00552400	-1.64176500	0.79629300
H	-3.73473900	-2.41230100	1.67470800
H	-5.24656300	-1.05529100	0.19992400
H	-1.74077000	0.91148400	-1.42361900
H	-1.25324300	-1.80645600	-1.15435900
C	0.09405100	-0.72887300	0.11274900
C	-4.38668100	1.07859300	-1.24220100
N	-5.08228100	1.89155700	-1.68285700
H	3.98261400	1.64297700	-1.11374200
H	3.09494500	1.13763700	1.03673800
H	4.58871400	0.19373600	1.26761100
H	5.11097200	0.26753800	-1.06730100
O	0.96418700	-1.13486300	-0.94399600
C	0.34761800	0.74602300	0.40263200
C	0.04728700	1.28530000	1.65314200
C	0.83707200	1.58535100	-0.60421900
C	0.25551600	2.63900900	1.90548400
H	-0.33814300	0.63986200	2.43611500
C	1.04475000	2.93806000	-0.34812100
H	1.08773400	1.16832200	-1.57422800
C	0.75864600	3.46835200	0.90745100
H	0.02553900	3.04448500	2.88564500
H	1.43229500	3.57825000	-1.13456200
H	0.92405800	4.52238300	1.10577900
C	0.19023600	-1.61359100	1.34380600
H	1.10893700	-1.73158400	1.89929700
C	-1.02595500	-2.05616200	1.68486800

**TS-W**

C	2.97202000	-1.24340300	-0.43659400
C	3.41951300	0.01564000	-0.29680700
C	2.47611200	1.09400500	0.00425100
C	1.18276400	0.80714100	0.29948300
C	0.76054000	-0.56914500	0.42395300
N	1.62906900	-1.53134900	-0.23083500
H	3.59704800	-2.07517900	-0.74106200
H	4.46636000	0.24252700	-0.44874700
H	0.46453800	1.59255500	0.51644700
H	0.42495700	-0.97949200	1.69459500
C	-0.62944000	-1.12554500	0.26804700
C	2.93315800	2.45189600	-0.02881800
N	3.31780500	3.54428600	-0.05990300
O	-0.70231700	-1.48146700	2.00477900
C	-1.80759300	-0.23068500	0.05691000
C	-2.33534000	-0.13693000	-1.23417200
C	-2.32797500	0.58174300	1.06868800
C	-3.37728600	0.74361000	-1.50695600
H	-1.91504200	-0.75128000	-2.02475400
C	-3.36262700	1.46839100	0.78850400
H	-1.93520500	0.48964800	2.07447500
C	-3.89207500	1.55079500	-0.49689100
H	-3.78215000	0.80297700	-2.51210200
H	-3.76217200	2.09227600	1.58160300
H	-4.70163600	2.24138800	-0.70971200
C	-0.45208800	-2.35947800	-0.46871900
H	-1.25500000	-2.99588500	-0.80968700
C	0.88813000	-2.55827300	-0.69554000
H	1.37143100	-3.38954100	-1.19456000
H	-0.66957600	-2.44739100	2.09842200

**TS-X**

C	2.70925500	0.64848100	0.80895000
C	2.65289900	1.97377800	0.43879600



C	1.41524300	2.45382900	-0.07989000	H	3.55661100	-0.85453500	1.07041200
C	0.32170200	1.61322700	-0.14965500	H	4.17095700	1.45116100	0.28401700
C	0.44033300	0.27984800	0.29678300	H	-0.02860700	2.26125800	-0.36138900
N	1.66346400	-0.18296900	0.72670700	C	-0.73479300	-0.40655400	0.59271300
H	3.63358100	0.22175700	1.19217900	C	2.41776700	3.32861500	-0.56341300
H	3.51876600	2.61837800	0.50856600	N	2.69113200	4.38302100	-0.95799800
H	-0.61777400	1.96638600	-0.55937500	C	-2.08810700	0.07106200	0.27533100
C	-0.59596700	-0.70370500	0.36211900	C	-2.50698800	1.36098100	0.62430900
C	1.30544100	3.80892800	-0.54078600	C	-2.99034000	-0.77599400	-0.37956100
N	1.22680700	4.90360600	-0.91165900	C	-3.79047500	1.79600100	0.31127100
C	-2.02665700	-0.40159200	0.18053500	H	-1.83076400	2.01149600	1.17171200
C	-2.61217600	0.77266600	0.67722900	C	-4.27536700	-0.34321500	-0.68331500
C	-2.85322300	-1.33528300	-0.46001800	H	-2.66414600	-1.77186600	-0.66718500
C	-3.97129400	1.01416100	0.51279100	C	-4.67819100	0.94654700	-0.34350600
H	-2.00021000	1.48369900	1.22383600	H	-4.10125700	2.79756700	0.59078000
C	-4.21322600	-1.09593300	-0.61876100	H	-4.96151700	-1.01024600	-1.19552100
H	-2.40828600	-2.24846700	-0.84521500	H	-5.67968300	1.28643600	-0.58603100
C	-4.77731300	0.08350300	-0.13871100	C	-0.37514900	-1.67508300	1.04544900
H	-4.40459600	1.92760600	0.90782800	H	-1.05800800	-2.47953000	1.28166300
H	-4.83372700	-1.82911100	-1.12465900	C	1.03192500	-1.76131000	1.13545300
H	-5.83808600	0.27358400	-0.26598500	H	1.60863300	-2.42888200	1.76043500
C	-0.15716100	-1.95708900	0.76504900	N	1.78403300	-2.74842000	-0.51623700
H	-0.81153100	-2.64621700	1.28907000	C	1.35127000	-1.98109100	-1.66331800
C	1.26825500	-2.20163500	0.78018700	H	1.85222700	-1.00879600	-1.68539600
H	1.73699800	-2.54304100	1.70603300	H	1.62765800	-2.51910200	-2.58209100
N	1.96163600	-2.58348000	-0.31487700	H	0.25954400	-1.82135600	-1.69771500
C	1.46858300	-2.23289900	-1.63543000	C	1.10673900	-4.02793600	-0.48618600
H	0.39585800	-2.42125200	-1.68112200	H	1.52340900	-4.67516000	-1.27108100
H	1.65279800	-1.17153500	-1.85263900	H	1.27763700	-4.52347100	0.47539600
H	1.98416500	-2.84638100	-2.37712300	H	0.02014300	-3.96111900	-0.66183900
C	3.40661900	-2.66637200	-0.21103000				
H	3.86845800	-1.69249200	-0.42239500				
H	3.68520600	-2.97814800	0.79801500				
H	3.78714600	-3.39834600	-0.92714900				

**TS-Y**

C	2.82684100	-0.10636900	0.78806700
C	3.13713100	1.13739600	0.34403200
C	2.08874600	2.02394800	-0.07150200
C	0.77067300	1.61560300	-0.01606500
C	0.46009300	0.33983100	0.47071200
N	1.51290700	-0.49295100	0.87295200

**TS-Z**

C	2.91550000	-1.74057000	2.04845000
C	4.01106800	-0.72364300	1.68671800
B	2.00461200	-0.01484600	0.96353000
O	1.70120800	-1.02905800	1.82628100
O	3.35802900	0.17668700	0.79018400
C	1.46332500	2.19039600	0.14482600
C	0.60787500	3.21352400	-0.02035800
C	-0.81214900	2.92589400	0.05275500
C	-1.25052300	1.64420400	0.16163800
C	-0.32851900	0.53071900	0.17735000

N	1.03670600	0.88409200	0.37403100	C	1.75245600	1.53218900	-1.13312400
H	2.53973100	2.31996300	0.15226500	C	1.19115800	2.75386000	-1.02642300
H	0.96312600	4.22144200	-0.18400400	C	-0.10739100	2.93462100	-0.44891300
H	-2.31182500	1.43311700	0.13633900	C	-0.82018600	1.79400400	-0.12157700
C	-0.72493400	-0.76183000	-0.09642000	C	-0.27500100	0.52429000	-0.28985000
C	-1.75742800	4.00207400	-0.04300100	N	1.10650400	0.34786800	-0.66817700
N	-2.50607100	4.88242300	-0.12019900	H	2.76634200	1.39196800	-1.48380200
H	4.35743400	-0.16717000	2.56433600	H	1.75750400	3.61712300	-1.35753000
H	4.87202800	-1.17584600	1.18913300	H	-1.85232800	1.86258600	0.20654700
H	2.96171800	-2.07678300	3.08593800	C	-1.00959000	-0.66045700	-0.54560300
H	2.93786900	-2.61398700	1.38530200	C	-0.66763400	4.23469200	-0.29156700
C	-2.15500300	-1.14400100	0.04887600	N	-1.11789400	5.29669100	-0.16137400
C	-2.90090800	-0.79626700	1.18361800	H	3.59640100	1.15034600	2.47315400
C	-2.77265000	-1.92651400	-0.93535900	H	3.89782800	-0.60244500	2.58045000
C	-4.22854500	-1.18889200	1.31356800	H	1.20557300	0.85993400	2.60519000
H	-2.41992800	-0.22737000	1.97474000	H	1.67082800	-0.58064100	3.55205300
C	-4.09854600	-2.32436500	-0.80441700	C	-2.41922000	-0.82178100	-0.13284400
H	-2.19893300	-2.21262300	-1.81261900	C	-2.79419100	-0.52893100	1.18322200
C	-4.83358400	-1.95340900	0.31887200	C	-3.38938800	-1.28326100	-1.02823100
H	-4.78763000	-0.90990400	2.20118100	C	-4.11313100	-0.69280300	1.59358400
H	-4.56106400	-2.92201300	-1.58382900	H	-2.03304600	-0.18730200	1.87930200
H	-5.86812000	-2.26438800	0.42214500	C	-4.70690300	-1.44672400	-0.61656000
C	0.15563500	-1.85584800	-0.49779700	H	-3.11023300	-1.49296400	-2.05658700
H	-0.17247700	-2.84265700	-0.18316200	C	-5.07257400	-1.15242400	0.69531100
C	1.31074600	-1.84273100	-1.20726400	H	-4.39063000	-0.46417400	2.61763900
H	1.86372500	-2.77839500	-1.29228400	H	-5.45233500	-1.79780700	-1.32305200
N	1.92013100	-0.76705800	-1.81837000	H	-6.10188900	-1.27864200	1.01503900
C	1.15110200	0.21221100	-2.56073700	C	-0.34235800	-1.52677100	-1.38985800
H	0.08877400	0.08493600	-2.35801100	H	-0.86588100	-2.26655000	-1.98493400
H	1.43775400	1.23543500	-2.28824600	C	1.03608200	-1.19907000	-1.62634600
H	1.32141900	0.08134400	-3.63872300	H	1.41580300	-1.26530400	-2.65244100
C	3.29971400	-0.88632700	-2.23356400	N	2.09204300	-1.73331300	-0.68547900
H	3.79668500	-1.66180600	-1.64724800	C	3.41881700	-1.72911900	-1.34050000
H	3.39045700	-1.13087100	-3.30263300	H	3.62200600	-0.73506600	-1.73984800
H	3.82387800	0.05681800	-2.04474500	H	4.18110000	-1.96566700	-0.59912700
				H	3.42499200	-2.46385800	-2.15044600
				C	1.79517900	-3.07443500	-0.13623200
				H	0.82346300	-3.04315700	0.35098600
				H	1.79491800	-3.81058100	-0.94462000
				H	2.56588900	-3.31817300	0.59747800
<b>TS-AA</b>				<b>TS-AB</b>			
C	1.77168000	-0.08200500	2.58474400				
C	3.22920700	0.16592500	2.17062900				
B	1.97444100	-0.52980100	0.39585600				
O	1.26986800	-0.92049700	1.55364100				
O	3.20323600	0.07173000	0.75152400				

C	1.53438500	0.46471800	2.33614900	H	1.65718500	-3.62289200	1.52436600
C	2.94021100	0.69825800	1.71376300				
B	1.85811400	-0.93501900	0.61960900				
O	1.02738700	-0.70620900	1.69533500	<b>TS-AC</b>			
O	3.09191000	-0.32804200	0.73080700				
C	1.88717500	0.67323800	-1.68219200	C	-2.83753900	-1.07262000	-2.10383600
C	1.85424300	1.99778400	-1.47633900	C	-3.78786100	-0.01989400	-1.49266700
C	0.80918800	2.60805400	-0.67305100	B	-1.68237000	0.80054600	-1.59169700
C	-0.28986200	1.82803300	-0.33258300	O	-1.62055200	-0.37404200	-2.31956400
C	-0.28152900	0.46145300	-0.56572500	O	-2.92897000	1.01789000	-1.03864500
N	0.98519100	-0.16700200	-0.94804800	C	0.03783800	4.72350400	-0.01345900
H	2.61230800	0.16593600	-2.30629200	C	-0.61160200	3.98818200	1.17408200
H	2.58604100	2.63062200	-1.96505700	B	-0.19674000	2.50343900	-0.51113900
H	-1.19398300	2.28769300	0.05453800	O	0.46586100	3.69247500	-0.88239700
C	-1.25328400	-0.54288600	-0.60256200	O	-0.97426500	2.72485500	0.64504200
C	0.83426200	4.00303400	-0.40108900	C	2.43715800	2.17819400	0.67062200
N	0.87004500	5.14052200	-0.16584100	C	3.67074300	1.66754000	0.71850900
H	3.00708000	1.67779900	1.23039200	C	3.92898200	0.36753200	0.09615000
H	3.74612800	0.60377800	2.44653900	C	2.87848000	-0.45329400	-0.19161400
H	0.86556000	1.30709200	2.13071500	C	1.53806200	0.03231100	0.02720500
H	1.57174700	0.28835900	3.41414400	N	1.41881600	1.48693700	-0.09986700
C	-2.65417200	-0.36423800	-0.18489800	H	2.14448900	3.12098700	1.11573000
C	-2.95698700	0.31295000	1.00193000	H	4.47171000	2.17455800	1.24388600
C	-3.69823400	-0.88519300	-0.95591600	H	3.04543400	-1.48480000	-0.48427900
C	-4.27912300	0.47868700	1.39983400	H	1.67225100	1.65839600	-1.08173900
H	-2.14280800	0.68085700	1.61991100	C	0.49263500	-0.78086000	0.36202400
C	-5.01922700	-0.71785900	-0.55651500	C	5.27933600	-0.08476600	-0.05866300
H	-3.46533200	-1.40425100	-1.88102400	N	6.37688700	-0.43691300	-0.17704300
C	-5.31340400	-0.03338900	0.62073300	H	-2.65463300	-1.90622300	-1.41260000
H	-4.50173300	1.00293900	2.32364700	H	-4.36456100	-0.41383800	-0.65050600
H	-5.82184400	-1.11821100	-1.16772500	H	-4.47976400	0.38651800	-2.23897700
H	-6.34500200	0.09765600	0.93103200	H	-3.20721700	-1.47801100	-3.04924500
C	-0.70122500	-1.71613000	-1.12020500	H	0.09365200	3.85863700	2.00693300
H	-1.24117100	-2.62227700	-1.35312000	H	-1.50080600	4.49805000	1.55571800
C	0.70392500	-1.52789300	-1.33495300	H	0.88903500	5.34256300	0.28945100
H	1.21823000	-1.91103200	-2.22387000	H	-0.68800100	5.36445900	-0.52926800
N	1.74178700	-2.28965000	-0.10958400	O	-0.63241200	1.63718600	-1.51677600
C	3.00129100	-2.75435200	-0.70228400	C	0.65671700	-2.25441900	0.16272800
H	3.48103100	-1.92892000	-1.23195400	C	1.03925700	-3.08615100	1.21682000
H	3.68627900	-3.10268000	0.07499200	C	0.37428400	-2.80660000	-1.08982200
H	2.79505900	-3.57264500	-1.39926700	C	1.15288500	-4.45912500	1.01787400
C	1.05894000	-3.33920100	0.65479600	H	1.24904500	-2.64854400	2.18875700
H	0.09431000	-2.95471400	0.98726100	C	0.48366900	-4.18199700	-1.28253900
H	0.90735900	-4.21350500	0.01454700	H	0.06377200	-2.14605400	-1.89607300

C	0.87402400	-5.00837200	-0.23161100
H	1.46145300	-5.09951500	1.83796800
H	0.26698000	-4.60805900	-2.25714200
H	0.96340100	-6.07890600	-0.38617300
C	-0.74581700	-0.31264500	0.91509100
H	-0.81799900	0.73358700	1.18156300
C	-1.80486300	-1.14726100	1.12613000
H	-1.71318300	-2.20668200	0.89283300
N	-3.02175600	-0.78459800	1.59349500
C	-3.25318200	0.57484700	2.05131500
H	-2.85195400	1.28613200	1.32748200
H	-4.33029100	0.73251000	2.14277900
H	-2.78566700	0.74729400	3.03087200
C	-3.94502000	-1.79747500	2.06330400
H	-3.71700100	-2.75261200	1.58566900
H	-3.88824600	-1.92978000	3.15220600
H	-4.97038100	-1.51528000	1.80509600

**TS-AD**

C	2.36618400	1.46496900	-0.32300600
C	1.86317100	2.71051600	-0.39084600
C	0.49102100	2.95369200	0.00896300
C	-0.36465900	1.85395400	0.09724900
C	0.17395600	0.57329300	0.13054700
N	1.60688000	0.47640100	0.41295700
H	3.31420900	1.15132300	-0.74897800
H	2.42742000	3.51682700	-0.84990800
H	-1.43870800	1.99739100	0.02610700
H	1.74489600	0.62788300	1.42002700
C	-0.43224400	-0.69086600	-0.07393100
C	-0.02564600	4.28064500	0.00670600
N	-0.43785800	5.36666300	0.01453000
C	-1.90097600	-0.87797400	-0.05824100
C	-2.50454900	-1.73871300	-0.98148200
C	-2.70302800	-0.23468500	0.89166000
C	-3.87982500	-1.94355400	-0.96382400
H	-1.88342400	-2.22976700	-1.72446200
C	-4.07785600	-0.44241600	0.91076500
H	-2.23658700	0.41541200	1.62536400
C	-4.67007100	-1.29491800	-0.01812600
H	-4.33623300	-2.60607100	-1.69223200
H	-4.68749200	0.05924700	1.65523700

H	-5.74357000	-1.45318800	-0.00446600
C	0.42890200	-1.75541500	-0.21863300
H	0.11432800	-2.79005800	-0.17844000
C	1.81634300	-1.41428500	-0.44234300
H	2.07514800	-0.81288100	-1.32206200
N	2.83241100	-2.15531700	0.00129400
C	4.19274800	-1.88388100	-0.42936200
H	4.17747500	-1.30922800	-1.35614200
H	4.73340300	-1.31535200	0.33696200
H	4.72130300	-2.82503100	-0.60396300
C	2.71590800	-2.99683600	1.18105200
H	1.68032700	-3.01001000	1.51605100
H	3.04427300	-4.01489700	0.95304500
H	3.34693700	-2.59697200	1.98349900

**TS-AE**

C	2.61367400	0.76081300	-0.73808900
C	2.45685200	2.08627600	-0.58379100
C	1.27064800	2.64932900	0.01423400
C	0.18569900	1.79017500	0.19502500
C	0.31923200	0.42751500	0.03642200
N	1.66877500	-0.14704400	-0.12249000
H	3.45616500	0.29984000	-1.23865600
H	3.21985900	2.75144600	-0.97357400
H	-0.80421900	2.19520100	0.38178500
H	2.14463400	-0.98629100	0.85155800
C	-0.60864600	-0.60604000	-0.24891300
C	1.14784200	4.04974800	0.20523200
N	1.05545900	5.19755000	0.36715500
C	-2.07129300	-0.45406500	-0.12356500
C	-2.92448600	-0.99045200	-1.09388900
C	-2.62778100	0.20832100	0.97629300
C	-4.30301500	-0.86299000	-0.96961100
H	-2.49534600	-1.48813600	-1.95839000
C	-4.00733100	0.33540600	1.09920400
H	-1.96886300	0.60763000	1.74157800
C	-4.84844600	-0.19925700	0.12692700
H	-4.95404100	-1.27578900	-1.73366400
H	-4.42617000	0.84931000	1.95846000
H	-5.92474500	-0.09783100	0.22228300
C	0.03048300	-1.73252800	-0.71116000
H	-0.44627200	-2.61772700	-1.10773800

C	1.49055400	-1.54078200	-0.67455600
H	2.06106300	-1.75333600	-1.58926700
N	2.23797700	-2.21176300	0.50829700
C	3.61207100	-2.61465700	0.17482300
H	4.12553100	-1.78274400	-0.31141300
H	4.14513000	-2.87040900	1.09198000
H	3.61124800	-3.48146900	-0.49423200
C	1.51486000	-3.25488500	1.24701300
H	0.50131700	-2.90919600	1.44604000
H	1.47276800	-4.18327300	0.66754600
H	2.04095000	-3.43998600	2.18538300

**INT9**

C	-1.42588400	1.10197000	0.08509100
C	-1.05482400	1.85792900	-1.14774700
C	-0.23052300	0.66579600	-0.75170900
H	-0.57231600	2.81814400	-1.00265200
H	-1.70275900	1.76605100	-2.01289900
H	-0.34797200	-0.25466000	-1.31569600
C	1.11675100	0.94707500	-0.16466600
C	2.14711700	-0.06844100	-0.36033800
H	1.90443100	-0.97011600	-0.90955200
C	3.37267200	0.16031800	0.17773400
H	3.49970200	1.08655200	0.73591500
C	5.62945300	-0.38680000	0.91685800
H	6.54615500	-0.50052300	0.33000700
H	5.59152500	0.63142800	1.30651400
H	5.67089600	-1.08235000	1.76502100
C	4.37258400	-1.89863300	-0.59349700
H	3.74264700	-2.60616200	-0.03768700
H	5.37105700	-2.32444000	-0.70448800
H	3.93977000	-1.75854200	-1.58839300
N	4.46801300	-0.62342900	0.08389900
O	1.30290700	1.98931800	0.45644000
H	-1.14229900	1.57767000	1.01985700
C	-2.64320800	0.24925000	0.13899600
C	-3.32151000	0.09035100	1.35027300
C	-3.13911200	-0.41135000	-0.99044800
C	-4.46218600	-0.70251300	1.43375800
H	-2.94769600	0.59696900	2.23584000
C	-4.27718100	-1.20546700	-0.90926300
H	-2.63197100	-0.30576100	-1.94651000

C	-4.94549400	-1.35478900	0.30381300
H	-4.97285300	-0.81032000	2.38569300
H	-4.64488800	-1.70893700	-1.79811800
H	-5.83470000	-1.97371700	0.36520500

**INT10**

C	-3.04524800	0.22670600	-0.12692100
C	-2.45500100	0.64070900	-1.42761500
C	-1.86496300	-0.55295000	-0.70941200
H	-1.83255600	1.52948200	-1.44168400
H	-3.01756900	0.42359700	-2.32944200
H	-2.08865800	-1.54257300	-1.09469200
C	-0.56728300	-0.40048900	-0.03222700
C	0.33318800	-1.46903600	-0.01418400
H	0.13360900	-2.33839300	-0.62758500
C	1.42450800	-1.42479800	0.85138400
H	1.43737900	-0.64843600	1.61432800
C	3.42796900	-2.25508200	1.93553000
H	4.43439100	-2.20760000	1.51086900
H	3.26041800	-1.38840400	2.57529200
H	3.32835300	-3.17222100	2.52471500
C	2.65702500	-3.21434200	-0.21860200
H	2.12758000	-4.15166100	-0.01771800
H	3.72858800	-3.40616400	-0.30716600
H	2.30110000	-2.77982000	-1.15468600
N	2.44852000	-2.25210700	0.85660700
O	-0.33484000	0.71960000	0.56703600
H	-2.76925500	0.84324200	0.72337500
C	-4.37508800	-0.43386800	-0.02763600
C	-5.14112200	-0.24823500	1.12530000
C	-4.89087900	-1.23723700	-1.04958000
C	-6.39137400	-0.84496200	1.25612700
H	-4.75091400	0.37431600	1.92568900
C	-6.13861500	-1.83733000	-0.91948900
H	-4.31625900	-1.39752200	-1.95889800
C	-6.89504600	-1.64293800	0.23376800
H	-6.97129000	-0.68471000	2.15960600
H	-6.52255100	-2.45746200	-1.72342000
H	-7.86970800	-2.10927400	0.33329200
C	-0.25253800	3.91423500	-0.57787500
C	-0.26839300	3.84918000	0.95374500
B	0.62967900	1.93425100	0.15496400

O	0.02248000	2.58116700	-0.97361700
O	0.66020700	2.82645500	1.25717300
C	3.01162300	1.32160600	0.78952700
C	4.15413900	0.60448300	0.61725600
C	4.34408600	-0.16996000	-0.57452300
C	3.36347000	-0.00744000	-1.60907500
C	2.25149400	0.73860400	-1.37811400
N	2.01093100	1.34419300	-0.16201600
H	2.81035000	1.91980900	1.67083400
H	4.91633700	0.61506300	1.38896800
H	3.50637000	-0.47603400	-2.57623700
H	1.48185900	0.89500700	-2.12594900
C	5.36503400	-1.13321900	-0.66833600
N	6.16295200	-1.98708100	-0.69990200
H	0.54194800	4.58406800	-0.93407400
H	-1.20621400	4.24628800	-1.00198100
H	0.03619000	4.78620200	1.42929100
H	-1.26940500	3.57729900	1.32060700

## INT11

C	-1.89349900	0.70173400	0.23183600
C	-1.27351500	1.46164100	-0.90496800
C	-0.82880400	0.04936900	-0.65092100
H	-0.57774000	2.25552700	-0.65611600
H	-1.88519000	1.65346900	-1.78023800
H	-1.20429600	-0.70902900	-1.33240000
C	0.49877600	-0.24049900	-0.09951900
C	1.22932200	-1.39078300	-0.33762800
H	0.78895600	-2.09933100	-1.03242700
C	2.45289100	-1.66831300	0.25199000
H	2.85099700	-0.99538800	1.00514900
C	4.10745600	-3.24326900	1.01983100
H	4.92896500	-3.82984300	0.59959500
H	4.53286100	-2.40215100	1.57254100
H	3.55035000	-3.87563200	1.72830100
C	2.76754200	-3.74375000	-0.96107100
H	1.90204700	-4.28849200	-0.54974900
H	3.56167400	-4.46225800	-1.17547700
H	2.46520200	-3.27340100	-1.90044800
N	3.27103900	-2.73921500	-0.05228700
O	0.99727500	0.69969400	0.78884800
C	3.03248800	3.00449200	-1.02046400

C	3.37520000	3.31476500	0.45765100
B	1.86255500	1.65127400	0.34876800
O	2.19433200	1.85495000	-0.96730900
O	2.47201800	2.52000000	1.21834700
H	3.91890400	2.78316700	-1.61995900
H	2.48498500	3.82459700	-1.49664300
H	3.23578900	4.36937600	0.70842800
H	4.40205500	3.02957400	0.70903200
H	-1.53915500	0.97412600	1.22174400
C	-3.29503000	0.21271200	0.17702600
C	-4.00840100	0.02112500	1.36422300
C	-3.93069300	-0.09048200	-1.03271300
C	-5.31397200	-0.45877500	1.34674900
H	-3.52836600	0.25053400	2.31168000
C	-5.23491800	-0.57150600	-1.05240700
H	-3.40237300	0.04684200	-1.97306600
C	-5.93435100	-0.75834600	0.13747000
H	-5.84680400	-0.59906500	2.28220400
H	-5.70812400	-0.79983300	-2.00256100
H	-6.95273600	-1.13250000	0.12098000

## INT12

C	2.45965900	-0.31678200	1.24887200
C	1.20960200	-0.80676000	0.58552900
C	0.30728200	0.33665500	0.18812400
H	0.67270600	-1.47124200	1.27184500
H	1.45752400	-1.41083800	-0.29983800
H	0.78266400	1.23927100	-0.18509500
C	-1.02958300	0.33627300	0.27839800
C	-1.87984300	1.47009400	-0.05383700
H	-1.36735800	2.36126400	-0.39859800
C	-3.22155300	1.42514500	0.06424000
H	-3.68651700	0.52356000	0.45476000
C	-5.35940600	2.47704000	0.44664200
H	-6.10838500	3.01473000	-0.14117500
H	-5.72728000	1.46432900	0.62701500
H	-5.25002200	2.98261000	1.41812500
C	-3.57238700	3.68378800	-0.71413900
H	-3.02539100	4.19477800	0.09435100
H	-4.38762600	4.32833600	-1.04941300
H	-2.88546100	3.53174600	-1.55118200
N	-4.11392200	2.41197400	-0.29334300



H 2.10731400 2.93921900 0.29362900

**INT13**

C 1.43233500 0.00885600 -0.03000700  
C 0.92300000 0.38355900 -1.43625400  
C -0.55260500 0.66776900 -1.57311500  
H 1.18000900 -0.43590800 -2.11876100  
H 1.47185200 1.26377700 -1.78941600  
H -0.81639200 1.51671200 -2.19700100  
C -1.60445100 -0.00046100 -1.07402800  
C -2.98854900 0.40230300 -1.29495800  
H -3.13036100 1.33983500 -1.82053100  
C -4.03571400 -0.34242300 -0.89121400  
H -3.84814900 -1.27142000 -0.35748900  
C -6.29780800 -0.53958100 -0.09543400  
H -7.30631100 -0.59922600 -0.51302500  
H -6.00581700 -1.53870100 0.23730600  
H -6.32294000 0.12516500 0.78255500  
C -5.70658400 1.18586800 -1.72331900  
H -5.41340600 2.04120800 -1.09339100  
H -6.78360900 1.22831600 -1.89762600  
H -5.19830500 1.27715500 -2.68698500  
N -5.37263800 -0.08253400 -1.11489300  
O -1.48559900 -1.08726300 -0.21801600  
C 0.83209000 -3.55478300 -1.36825600  
C 0.44240700 -4.05091800 0.04285100  
B -0.65347200 -2.14311700 -0.43743600  
O -0.05602900 -2.46422000 -1.62587200  
O -0.34987600 -2.99854900 0.59325800  
H 0.69758600 -4.31897400 -2.13684400  
H 1.86370000 -3.18708700 -1.40020100  
H 1.31719400 -4.21751600 0.67645000  
H -0.15650800 -4.96678800 0.00971100  
H 0.68177100 -0.58524200 0.49189200  
C 2.68805200 -0.83131700 -0.04782700  
C 2.86175200 -1.80231300 0.94551000  
C 3.68429300 -0.67476600 -1.01527200  
C 3.99438100 -2.61176800 0.96021000  
H 2.08308300 -1.92603300 1.69697600  
C 4.81848400 -1.48367300 -1.00194500  
H 3.56835000 0.07833300 -1.79000600  
C 4.97429900 -2.45731500 -0.01870800

H 4.11124600 -3.36523700 1.73347700  
H 5.58104700 -1.35346800 -1.76326900  
H 5.85604500 -3.08986200 -0.01314800  
C -1.63492200 -0.63155800 2.89011300  
C -2.72927100 0.37929700 2.45674800  
B -0.70298900 1.11944200 1.81587300  
O -0.40126200 -0.04309900 2.47867000  
O -2.03068500 1.45143400 1.82569200  
C -0.04253100 3.01476000 0.42537000  
C 0.85400100 3.75959500 -0.24425200  
C 2.26140300 3.37427500 -0.15449600  
C 2.63179800 2.21931700 0.42757600  
C 1.60638000 1.23545600 0.91970700  
N 0.30349700 1.88659300 1.14766500  
H -1.09784000 3.26671000 0.46137900  
H 0.56037700 4.64806600 -0.78458200  
H 3.67828800 1.95012300 0.52372100  
H 1.94080900 0.82490000 1.87995500  
C 3.26269700 4.27432800 -0.66818400  
N 4.05219500 5.00463000 -1.09583100  
H -1.74140400 -1.59803800 2.39120700  
H -1.61200200 -0.78185700 3.97313800  
H -3.29469500 0.77300300 3.30649500  
H -3.42469300 -0.05384900 1.73249700

**INT14**

C 1.48961900 -0.55240800 -0.72304200  
C 1.57700100 0.18803200 -2.08493200  
C 0.47398000 -0.19004000 -3.05941300  
H 2.52210200 -0.04948300 -2.57748100  
H 1.55661400 1.27095600 -1.93540400  
H 0.75261400 -0.66540900 -3.99968000  
C -0.79435000 -0.01457800 -2.85455800  
C -2.08548100 0.09213200 -2.57442600  
H -2.64367500 0.98759800 -2.82328400  
C -2.63736800 -0.95546800 -1.76529500  
H -1.99352600 -1.79298900 -1.51639600  
C -4.19130200 -1.98767600 -0.26508300  
H -5.18054500 -2.37435300 -0.51809100  
H -3.45115200 -2.78504800 -0.27765400  
H -4.18527700 -1.50994800 0.71815400  
C -4.71950000 0.18853700 -1.30650400



H	-4.67902100	0.64686700	-2.29327000	C	-1.65950600	0.15505400	0.84308300
H	-4.40636600	0.88785900	-0.52573700	C	-1.42759700	1.19987100	1.94807700
H	-5.73533600	-0.15836600	-1.11898200	C	-0.03623600	1.32144800	2.53270200
N	-3.81779900	-0.96002900	-1.23558700	H	-2.10828000	0.96209000	2.76990700
H	0.73212700	-1.34065300	-0.79295500	H	-1.70493400	2.20413500	1.61128500
C	2.79857600	-1.19631400	-0.32111900	H	0.03382100	1.38177700	3.62042200
C	2.77920300	-2.42993900	0.33609800	C	1.10249300	1.43224100	1.92206800
C	4.03075200	-0.56308300	-0.51160000	C	2.33446300	1.45054000	1.41655900
C	3.95685600	-3.02559300	0.77586000	H	2.79773900	2.37214900	1.08055400
H	1.82223100	-2.91926100	0.50387600	C	2.92464100	0.16771000	1.20403500
C	5.21163800	-1.15531300	-0.07094600	H	2.35842800	-0.70550900	1.54569100
H	4.06732400	0.40937000	-0.99648000	C	4.51222000	-1.40357900	0.31215700
C	5.17916200	-2.39034000	0.57018000	H	5.43361900	-1.60495200	0.86446400
H	3.92074900	-3.98690400	1.27888000	H	3.71897300	-2.10998200	0.56181800
H	6.15827200	-0.64730000	-0.22599200	H	4.70867200	-1.48455800	-0.76032400
H	6.09975300	-2.85298500	0.91090200	C	4.80998200	1.06379800	0.00594800
C	-1.76405800	0.98948800	3.03273300	H	5.74593100	0.67882700	-0.39525200
C	-3.09109700	0.98575400	2.25305600	H	5.02755200	1.82092200	0.76131600
B	-1.40844900	-0.21105000	1.14484700	H	4.20666200	1.50607300	-0.79558400
O	-1.09702400	-0.15046000	2.56315800	N	4.05627200	-0.04093200	0.59654800
O	-2.78597800	0.34493500	1.02827300	O	0.62050200	-1.71798500	1.66223200
C	-0.77632600	1.89154400	-0.19411200	H	-1.40397400	-0.81759100	1.26514000
C	0.09217200	2.91342600	-0.44921700	C	-3.13000400	0.10063700	0.45365000
C	1.41979600	2.76667600	0.11265900	C	-3.62766300	-1.11594200	-0.03240800
C	1.84095300	1.58852100	0.62757200	C	-3.99186100	1.19700500	0.51035800
C	0.99373200	0.35503400	0.45617700	C	-4.94990900	-1.23027900	-0.44239500
N	-0.42612100	0.69788200	0.32935800	H	-2.94757000	-1.96385000	-0.08652900
H	-1.84531500	2.01046900	-0.35577000	C	-5.31937500	1.08318800	0.09728200
H	-0.24104700	3.85745200	-0.85465000	H	-3.64369300	2.15693600	0.88028600
H	2.78239200	1.51469200	1.16010600	C	-5.80324800	-0.12936100	-0.37833300
H	1.08262000	-0.26928500	1.35391600	H	-5.31850400	-2.18230200	-0.81217900
C	2.26475600	3.93118200	0.21448300	H	-5.97310600	1.94843100	0.14853400
N	2.93897800	4.87079500	0.27194000	H	-6.83679100	-0.21781200	-0.69787100
H	-1.90596200	0.93517900	4.11704000	C	-0.29083000	-3.19908700	-1.43311300
H	-1.19255600	1.90286000	2.80044400	C	1.20674600	-3.52763500	-1.28033400
H	-3.47666700	1.99975000	2.08172400	B	0.52017700	-1.87308900	0.22458300
H	-3.86123200	0.41323500	2.79326000	O	-0.64878200	-2.64154100	-0.19327700
O	-1.28363800	-1.57115600	0.62699600	O	1.68277200	-2.59630000	-0.33195500
C	-1.48000800	-2.59781900	1.56731900	C	1.44628100	-0.02909000	-1.25831100
H	-1.50161100	-3.55904800	1.03717300	C	1.54605600	1.21177100	-1.82922200
H	-0.67532400	-2.62544800	2.31006400	C	0.53833900	2.17084800	-1.44378200
H	-2.42446400	-2.48217100	2.11932200	C	-0.55396400	1.78437400	-0.74945700
				C	-0.80218000	0.32316100	-0.45303200
				N	0.47281300	-0.42082700	-0.41542900

INT15

H	2.21947800	-0.77679000	-1.41853000
H	2.33989200	1.46731900	-2.51702300
H	-1.30338300	2.51288000	-0.45721900
H	-1.41467300	-0.11584900	-1.26234100
C	0.75393700	3.56721400	-1.73031700
N	0.96228600	4.68356300	-1.95668600
H	-0.90226900	-4.08140200	-1.64944800
H	-0.43638800	-2.46893900	-2.24691300
H	1.74671200	-3.43727700	-2.23285500
H	1.34942100	-4.55095200	-0.90419100
H	0.53354000	-2.59768300	2.04559400

### INT16

C	-1.08535900	-1.14356400	-0.04145800
C	-0.41679300	-1.42434300	1.30252500
C	1.06099900	-1.19788100	1.18250100
H	-0.63923700	-2.44539100	1.62900400
H	-0.83134800	-0.74908700	2.06825700
H	1.74700400	-1.75294700	1.81002100
C	1.56497400	-0.25614600	0.36461400
C	3.00685000	0.01236000	0.24174000
H	3.34984400	1.03779700	0.33267500
C	3.88370800	-0.99833100	0.08695700
H	3.50372700	-2.00839100	-0.05754900
C	6.00312600	-1.87406200	-0.67027000
H	7.01745900	-1.96721800	-0.27351600
H	5.51991400	-2.85183300	-0.60763700
H	6.06797400	-1.58670200	-1.73029700
C	5.84733800	0.39788600	0.23716700
H	5.65076800	1.02358400	-0.64837500
H	6.92732400	0.29691800	0.36232000
H	5.44146200	0.90663700	1.11580700
N	5.25654900	-0.91634300	0.12335700
H	-0.62303600	-1.81718400	-0.77433000
C	-2.58409500	-1.36270900	-0.09598400
C	-3.20366500	-1.48007800	-1.34481500
C	-3.38015000	-1.43018300	1.04890200
C	-4.57818600	-1.65335200	-1.45017400
H	-2.59427200	-1.44140100	-2.24506300
C	-4.75934400	-1.60538700	0.94733600
H	-2.92692900	-1.35044400	2.03223300
C	-5.36279900	-1.71505800	-0.30032000

H	-5.03772800	-1.74483200	-2.42921700
H	-5.36114700	-1.65493300	1.84925300
H	-6.43656500	-1.85088000	-0.37828200
C	1.06709400	1.77751100	-0.90962500
C	0.18277600	2.80441200	-0.91161300
C	-1.03716300	2.64065200	-0.12796100
C	-1.46853700	1.40241100	0.19579000
C	-0.74583800	0.28094400	-0.50088100
N	0.69906700	0.54469200	-0.41494300
H	2.09073500	1.88338100	-1.25218800
H	0.44457100	3.76670300	-1.32969100
H	-2.29464400	1.22264800	0.87592200
H	-0.99154700	0.35714000	-1.57414700
C	-1.69399100	3.81523700	0.38280200
N	-2.21704500	4.76943900	0.77750000

### INT17

C	-1.09076900	-1.04825100	-0.31000400
C	-0.27535300	-1.95176300	0.62557300
C	1.19884000	-1.79361800	0.28721200
H	-0.58884100	-2.99311800	0.51628100
H	-0.46436700	-1.65858500	1.66415800
H	1.80070100	-2.20519300	1.10892400
C	1.60142000	-0.36003100	0.07584200
C	2.98783000	-0.03191700	-0.13223900
H	3.20503200	0.93276200	-0.57981900
C	4.00907900	-0.90045900	0.07955000
H	3.82763100	-1.85908100	0.55893700
C	6.33690800	-1.39918000	0.48811900
H	6.58062300	-0.86382500	1.41809700
H	5.98775300	-2.40092100	0.74918200
H	7.25019100	-1.49890500	-0.10390700
C	5.70422100	0.55963800	-0.84235100
H	5.08649400	0.79154500	-1.71446200
H	6.74719100	0.51538600	-1.16137900
H	5.59271900	1.37593600	-0.11064800
N	5.32110300	-0.72228200	-0.29572200
H	-0.77446000	-1.29495700	-1.33750700
C	-2.57656700	-1.30567600	-0.19973100
C	-3.30562800	-1.74164500	-1.30484100
C	-3.23961500	-1.13841900	1.02077200
C	-4.66890000	-2.01014100	-1.19829100

H	-2.80176800	-1.86981600	-2.25927600
C	-4.59938200	-1.40474700	1.13045400
H	-2.68683800	-0.77859700	1.88496900
C	-5.31842500	-1.84344400	0.01982100
H	-5.22204000	-2.34536800	-2.06986400
H	-5.10024700	-1.26501500	2.08305300
H	-6.38062400	-2.04837800	0.10480700
C	1.06617200	1.95834300	0.33396200
C	0.18379300	2.99491500	0.26660400
C	-1.18236300	2.77861500	0.02841500
C	-1.58273700	1.43452200	-0.10595600
C	-0.70709900	0.38640400	-0.05378500
N	0.68155700	0.61967200	0.12667000
H	2.09315500	2.10027500	0.62595100
H	0.56083700	3.99639400	0.44298500
H	-2.62734100	1.20126000	-0.27850900
C	-2.11485500	3.84905500	-0.04479900
N	-2.87483300	4.72505000	-0.10600200
H	1.45999900	-2.38209600	-0.60255100

**INT18**

C	-1.63495400	-0.86501200	-0.75727700
C	-1.21027800	-2.31340100	-0.44979700
C	0.10811500	-2.64804300	-1.15460900
H	-2.00487300	-2.99136300	-0.77204400
H	-1.09614900	-2.43554700	0.63363200
H	0.42923100	-3.67171300	-0.94937100
C	1.16685900	-1.68932000	-0.70616000
C	2.49319000	-1.80795900	-0.56699700
H	3.05435700	-2.69313200	-0.82999400
C	3.10424300	-0.48111400	-0.16178100
H	3.59057400	-0.00696200	-1.04559100
C	4.54691800	0.77183700	1.28353100
H	5.03581300	1.27639500	0.42816600
H	3.72767700	1.40588400	1.63330000
H	5.27475500	0.69248200	2.09455100
C	5.17353400	-1.42735100	0.61878500
H	4.82637700	-2.45291200	0.48057000
H	5.88328100	-1.42438600	1.44969600
H	5.71160900	-1.11099300	-0.29413400
N	4.05654600	-0.55513500	0.94332400
H	-1.79805400	-0.79773000	-1.84230800

C	-2.93984100	-0.51442800	-0.07205200
C	-4.12482200	-0.44606100	-0.80344400
C	-2.98698800	-0.31168800	1.31072200
C	-5.33737400	-0.18144400	-0.17007900
H	-4.09762200	-0.59812500	-1.87940900
C	-4.19505000	-0.04843700	1.94546100
H	-2.06533000	-0.34246200	1.88622300
C	-5.37493000	0.01659400	1.20592600
H	-6.25013600	-0.12609700	-0.75442000
H	-4.21628900	0.11135300	3.01863400
H	-6.31728100	0.22629800	1.70122400
C	1.85361900	0.33654400	0.24357700
C	1.75554000	1.76742500	-0.19633300
C	0.51560100	2.28433900	-0.34543000
C	-0.67819300	1.45457100	-0.28577900
C	-0.51883700	0.11010500	-0.42176700
N	0.74354600	-0.40563000	-0.36346100
H	1.75748700	0.24997200	1.34304800
H	2.64892900	2.36113500	-0.35490900
H	-1.66355800	1.89912000	-0.30260000
C	0.35847400	3.67915000	-0.67445300
N	0.22121600	4.79936200	-0.93080100
H	-0.02892300	-2.55924600	-2.23997600

**INT19**

C	-0.70015200	-1.06256300	-0.51260900
C	-0.43194800	-2.36941000	0.26210000
C	0.91348900	-2.97790600	-0.14362000
H	-1.24813700	-3.06893400	0.06447100
H	-0.43658400	-2.15701300	1.33719200
H	0.85240900	-3.33939800	-1.17866800
C	1.99485800	-1.95297100	-0.00747400
C	3.36019000	-2.03377700	0.21490100
H	3.90906000	-2.95863400	0.32465000
C	3.88872600	-0.73226100	0.27792300
H	4.91709800	-0.44905400	0.44372500
H	-0.67837600	-1.31431700	-1.58336100
C	-2.06801400	-0.49905000	-0.19339400
C	-3.07072000	-0.47990600	-1.16135400
C	-2.36096700	-0.03054300	1.09149500
C	-4.34528400	-0.00693700	-0.85568100
H	-2.85220400	-0.83805600	-2.16411900



C	2.02769900	-1.56313400	-0.38219800	H	2.46194500	3.14141500	0.23694900
C	1.42024700	-2.41004500	-1.45681300	H	-1.70369700	4.26208400	-0.08143500
C	1.26007700	-0.91272200	-1.51243400	H	-2.24461800	2.13729400	1.05328400
H	0.53008900	-2.97901100	-1.21337100	C	0.74663500	5.19211600	-0.34626400
H	2.08969000	-2.85456300	-2.18527600	N	1.05686400	6.26443400	-0.65107500
H	1.84566000	-0.36956200	-2.24743400	H	-0.56002700	-2.43737700	2.10182400
C	-0.03814300	-0.30730600	-1.17220800	H	-0.05342600	-2.15885700	3.80069800
C	-0.48704700	0.87370200	-1.61698300	H	-2.03129900	-0.81551900	4.23685100
H	0.07851900	1.47110400	-2.31989100	H	-2.71062500	-1.77410000	2.87797300
C	-1.71377500	1.42715900	-0.95916900	N	-2.79663100	0.34954700	-0.95844100
O	-0.76984400	-1.00334900	-0.25897600	C	-3.90685500	0.66873300	-0.02756500
C	-2.92210900	-3.25197700	-1.33506100	C	-3.36173300	0.34086200	-2.33721700
C	-3.65920400	-2.87219000	-0.04880400	H	-4.72478900	-0.02570500	-0.22560600
B	-2.16347900	-1.22166600	-0.60352000	H	-3.58115600	0.53252200	1.00062000
O	-2.37349100	-2.02816000	-1.77424400	H	-4.25213800	1.69334700	-0.20884100
O	-2.88508200	-1.81451300	0.48255200	H	-3.82999400	1.31015200	-2.53677000
H	-3.57902400	-3.67325600	-2.10280700	H	-4.09535100	-0.45853400	-2.41564300
H	-2.12405000	-3.97845100	-1.12193600	H	-2.55908000	0.14736000	-3.04719900
H	-3.72585400	-3.69144200	0.67429800	H	-2.13677100	2.24702500	-1.55511500
H	-4.68163900	-2.52667100	-0.27273800				
H	1.50180000	-1.56313600	0.57168200				
C	3.50836500	-1.36929000	-0.30025800	<b>INT-AB</b>			
C	4.07038300	-0.09409800	-0.39905500				
C	4.35278900	-2.46241000	-0.09374000	C	1.70979400	-0.55776300	-0.77069700
C	5.44635200	0.08648900	-0.28726600	C	2.08128800	0.13160100	-2.09052100
H	3.41475400	0.75668800	-0.57332600	C	1.08488300	1.05782800	-2.74882600
C	5.72814900	-2.28577100	0.01815000	H	2.30652600	-0.64672900	-2.82766300
H	3.91979800	-3.45675800	-0.02382700	H	3.00358500	0.71798000	-1.97828000
C	6.27853500	-1.00958600	-0.07726600	H	1.25855200	1.25365300	-3.80898600
H	5.86934000	1.08295200	-0.36929300	C	0.07552200	1.69229000	-2.23927200
H	6.37277500	-3.14478000	0.17727200	C	-0.95830300	2.35893200	-1.74761300
H	7.35166200	-0.87085900	0.00745300	H	-0.79147700	3.31749600	-1.26808000
C	-0.51397700	-1.70892100	2.91901400	C	-2.17445300	1.61914100	-1.59697000
C	-1.90379400	-1.11143400	3.18986200	H	-2.27740400	0.69643200	-2.16219800
B	-0.64033400	0.30393000	1.99034100	C	-4.23202500	0.94007100	-0.58171500
O	0.27237000	-0.59276800	2.48321500	H	-5.18788200	1.46685100	-0.55219400
O	-1.93384400	0.06642400	2.37661800	H	-4.22631900	0.20890700	-1.38983700
C	1.02967100	1.75332000	0.96656900	H	-4.03398600	0.44294600	0.37528300
C	1.41796900	2.89567400	0.36914800	C	-3.16876200	3.02243100	0.14707600
C	0.37313700	3.84958500	0.02294300	H	-3.05966900	2.59223700	1.14714000
C	-0.93075800	3.52455500	0.10772000	H	-4.12194100	3.54679600	0.05200300
C	-1.35304300	2.10824700	0.42164500	H	-2.35154900	3.71077100	-0.05122900
N	-0.29748500	1.43839600	1.18388400	N	-3.15535400	1.90689300	-0.79649800
H	1.73904600	1.02823100	1.35709700	O	-1.34381200	-0.53804900	-0.33452700

C	-3.94119700	-2.62387000	-1.52356300
C	-3.82952000	-3.07802100	-0.05442200
B	-2.30885500	-1.45010300	-0.45568600
O	-2.82436300	-1.76749300	-1.71662900
O	-2.98970700	-2.10810700	0.55411400
H	-4.86875000	-2.06202800	-1.70226200
H	-3.90332600	-3.45531000	-2.23164500
H	-3.36232400	-4.06575800	0.02841400
H	-4.79658300	-3.10719300	0.45480600
H	0.71169200	-0.98612600	-0.88629700
C	2.66102800	-1.70898100	-0.47523300
C	2.22699100	-2.69423400	0.42271400
C	3.94649300	-1.81564000	-1.00869700
C	3.05078000	-3.75961200	0.76189200
H	1.23695600	-2.59579300	0.86547300
C	4.77539200	-2.88477200	-0.66568600
H	4.32088400	-1.06755400	-1.70152500
C	4.33019100	-3.86128700	0.21617700
H	2.69406300	-4.51398400	1.45657700
H	5.77162600	-2.94922600	-1.09243300
H	4.97392800	-4.69413300	0.48084700
C	-0.81997200	-0.88053000	3.11435800
C	-2.13183300	-0.10683600	2.93784500
B	-0.86132000	-0.05636100	0.98749700
O	-0.42473800	-1.17777500	1.79729100
O	-1.96229700	0.59533600	1.71716600
C	0.18221400	2.25313900	1.07859300
C	1.15499600	3.19998900	1.00609100
C	2.47639800	2.73455600	0.62869100
C	2.72435800	1.42655100	0.41953600
C	1.64987700	0.37409100	0.50021700
N	0.31453100	0.94917600	0.74739700
H	-0.81497800	2.51486300	1.41782200
H	0.98247800	4.22619000	1.29542700
H	3.73121600	1.08317000	0.19686900
H	1.86824600	-0.30447600	1.33941400
C	3.55149300	3.68743600	0.50388500
N	4.39893400	4.46886900	0.39495900
H	-0.94356100	-1.80255900	3.69178600
H	-0.06859100	-0.24980900	3.61703800
H	-2.32484500	0.59314700	3.75956000
H	-2.97692500	-0.80336500	2.85164000

**INT-AC**

C	-0.63984500	-1.29383400	-0.31814900
C	-0.16868800	-2.20087600	0.83526600
C	1.21301100	-2.73989100	0.57384000
H	-0.89770300	-3.00076500	0.98708600
H	-0.13443600	-1.60639600	1.76182600
H	1.48643800	-3.75961700	0.81307100
C	2.11230900	-1.84904300	0.12220700
C	3.57026100	-1.82189300	-0.01359100
H	4.20888900	-2.67357900	0.17657800
C	3.95949700	-0.55812700	-0.29234300
H	4.97163100	-0.19135400	-0.39125400
H	-0.62293800	-1.92203200	-1.21631200
C	-2.04707100	-0.75185700	-0.17852000
C	-2.74675600	-0.39041400	-1.33408800
C	-2.65660400	-0.54603800	1.06106500
C	-4.01945800	0.16436800	-1.25716800
H	-2.28462200	-0.54929800	-2.30583700
C	-3.93326400	0.00623900	1.14145800
H	-2.13691500	-0.81556500	1.97505000
C	-4.61765400	0.36465600	-0.01546200
H	-4.54574700	0.43722000	-2.16622200
H	-4.39191400	0.15670100	2.11358700
H	-5.61119200	0.79586600	0.04996800
C	2.77024300	0.29192200	-0.35057500
C	2.55292100	1.63531300	-0.39546000
C	1.21046600	2.07025000	-0.03022300
C	0.15343100	1.22023500	-0.00125300
C	0.37563100	-0.14899500	-0.59810100
N	1.69924200	-0.54777000	-0.15444400
H	3.35483500	2.34914300	-0.51930700
H	-0.82351600	1.53304800	0.34912500
H	0.40378500	-0.01741300	-1.69744500
C	1.03686600	3.43660000	0.39483600
N	0.91098900	4.53810700	0.72696400

**INT-AD**

C	-0.71883200	-0.99632400	1.04265100
C	-1.60880100	-0.52052500	0.17055300
C	1.68158000	1.21367900	0.26885800
C	1.62130500	0.10230900	1.38904100
C	0.18567700	-0.16385100	1.90560200
H	1.35842200	0.21677500	-2.90623300

H	-0.61399800	-2.07685400	1.09883400
C	1.84460600	0.60001900	-2.00824800
C	3.08976600	1.71095000	0.17991600
H	-0.27173600	0.81003600	2.10224200
C	3.83356300	1.50590100	-0.94658300
C	3.23683000	0.89510500	-2.07691400
H	3.52743900	2.19405700	1.04836700
H	3.80516300	0.70636100	-2.97797900
N	1.08621300	0.76170300	-0.97059500
C	5.21166500	1.92735500	-0.99577800
N	6.31704700	2.26566800	-1.03727600
C	2.42062400	-1.12674700	1.01079600
C	3.61595500	-1.40067600	1.68210200
C	2.02045100	-1.99430500	-0.01429900
C	4.39148100	-2.50836500	1.35203400
H	3.94409100	-0.73298400	2.47554900
C	2.79439000	-3.10321900	-0.34450600
H	1.10121000	-1.79716900	-0.55468300
C	3.98076200	-3.36464200	0.33532200
H	5.31613500	-2.69919300	1.88737700
H	2.46642800	-3.76529400	-1.13982500
H	4.58176500	-4.22944900	0.07301200
H	2.14212600	0.56797900	2.23698500
H	0.29379500	-0.66378100	2.87505300
O	-2.25487800	-1.42799300	-0.66386900
C	-5.65197700	-2.31238100	-1.13179800
C	-5.75658800	-1.22941800	-0.03752900
H	-6.32391000	-2.13040100	-1.97405300
H	-5.85182400	-3.31332000	-0.73297500
H	-6.18193600	-0.29709100	-0.42625400
H	-6.34557000	-1.55106500	0.82472500
B	-3.60637400	-1.53578400	-0.62078600
O	-4.40915600	-0.99539100	0.35884100
O	-4.30014600	-2.24529700	-1.57039700
C	-1.92191500	0.88922200	-0.10927200
H	-1.67289600	1.24007800	-1.10595400
C	-2.47845300	1.68681000	0.81698400
H	-2.76728400	1.26262200	1.77786500
N	-2.70870500	3.04559900	0.70984900
C	-2.42770700	3.65831700	-0.56923300
H	-3.09854700	3.29660700	-1.36536100
H	-2.53867400	4.74140400	-0.48097500
H	-1.39813100	3.43297200	-0.86173200
C	-3.87756000	3.56143300	1.39674100

**TS10**

H	-3.77703600	4.64187700	1.53150400
H	-4.81258900	3.36356400	0.85016800
H	-3.95370400	3.09749600	2.38304600
H	1.03376500	2.01845900	0.65615200
C	-2.99046200	0.12655400	-0.17318300
C	-2.31791300	0.34631100	-1.48628600
C	-1.79580800	-0.72958900	-0.56192400
H	-1.68423900	1.22123200	-1.59059000
H	-2.83737700	0.01629200	-2.37973400
H	-1.99917300	-1.76415200	-0.81987000
C	-0.51441200	-0.45710900	0.13602900
C	0.44074200	-1.50654700	0.21564700
H	0.26469600	-2.42325700	-0.33263500
C	1.54968900	-1.33587100	1.01646600
H	1.57513500	-0.45896900	1.66136700
C	3.63921000	-1.96215100	2.09221300
H	4.62088100	-1.92338400	1.60953400
H	3.46351100	-1.02863000	2.62819700
H	3.62395700	-2.79526800	2.80311000
C	2.77533700	-3.23411200	0.14603100
H	2.21603900	-4.12176500	0.46283800
H	3.83769800	-3.47476900	0.07354900
H	2.42362300	-2.91765300	-0.83938600
N	2.60741600	-2.13574800	1.08382900
O	-0.32738300	0.69106000	0.62343500
H	-2.75503400	0.85698500	0.59605000
C	-4.34068600	-0.49132400	-0.07371100
C	-5.18506200	-0.11859400	0.97486800
C	-4.79967500	-1.44060600	-0.99290400
C	-6.45382700	-0.67505600	1.10444100
H	-4.83898600	0.61656500	1.69623600
C	-6.06606100	-2.00029600	-0.86387200
H	-4.16457500	-1.74862100	-1.82010900
C	-6.89951400	-1.61972500	0.18546500
H	-7.09326200	-0.37051300	1.92695500
H	-6.40465500	-2.73596600	-1.58678500
H	-7.88760600	-2.05692200	0.28480400
C	-0.86921300	3.64801900	-0.43341500
C	-0.52575500	3.63962600	1.07476800
B	0.76730700	2.16600500	0.02375400

O	-0.04162800	2.64111400	-1.00802400
O	0.72209000	2.96495000	1.15468900
C	3.10216200	1.49628400	0.57453800
C	4.20044700	0.72329700	0.37863700
C	4.28104400	-0.14048700	-0.76100700
C	3.22950900	-0.03884900	-1.72658000
C	2.16262600	0.76659500	-1.49040300
N	2.04207000	1.49576300	-0.31865900
H	2.98152200	2.15727500	1.42450600
H	5.01206900	0.75528700	1.09701500
H	3.27584600	-0.60905500	-2.64708900
H	1.33640100	0.87167700	-2.18398500
C	5.28809900	-1.12165800	-0.85733900
N	6.08933600	-1.97040600	-0.88461900
H	-0.63488000	4.60840300	-0.90510200
H	-1.92423600	3.41583500	-0.61592100
H	-0.42733800	4.64400800	1.49423500
H	-1.27580600	3.08280800	1.64850900

**TS11**

C	-3.09211700	0.46339600	0.14953900
C	-2.60842200	1.33734100	-0.96939900
C	-1.88811600	0.05000600	-0.70871900
H	-2.10278800	2.25856500	-0.71184300
H	-3.22398400	1.38606800	-1.86231200
H	-2.09580900	-0.76864500	-1.39332400
C	-0.56321900	-0.03990600	-0.07100200
C	0.17781300	-1.21880400	-0.07781400
H	-0.13208800	-1.97441900	-0.79494600
C	1.23568100	-1.48246500	0.77795900
H	1.42806800	-0.80857600	1.60727100
C	2.86086000	-2.95713100	1.81354900
H	3.81075000	-3.40962600	1.51181100
H	3.07265400	-2.09745400	2.45651500
H	2.28832700	-3.68998600	2.40063300
C	1.99517700	-3.45539900	-0.43425300
H	2.90755000	-4.05161800	-0.51543600
H	1.84453500	-2.91796700	-1.37729200
H	1.13904900	-4.13116600	-0.28488200
N	2.15034200	-2.50184800	0.63779800
O	-0.20890800	0.96068700	0.80674900
C	0.77783600	4.05550900	-0.68741900

C	0.92302100	4.30855900	0.82713000
B	0.36934400	2.15970000	0.42410200
O	0.07793800	2.82300500	-0.77035300
O	0.81342000	3.02268600	1.42159900
C	3.14955500	1.14483400	0.75706300
C	4.11481400	0.15816200	0.61934300
C	4.11887400	-0.58603000	-0.56336300
C	3.22557600	-0.26576900	-1.58676800
C	2.31049600	0.75490200	-1.35282700
N	2.26327100	1.42172000	-0.20194800
H	3.03975300	1.72333400	1.67139200
H	4.80865500	-0.06620200	1.42098500
H	3.21902800	-0.82304800	-2.51592700
H	1.55175000	1.02695200	-2.08272300
C	4.98142600	-1.73285000	-0.68593800
N	5.64426600	-2.67884400	-0.76166900
H	1.76101800	3.95023900	-1.16447200
H	0.21476600	4.83750600	-1.20252800
H	0.12060300	4.95116600	1.20860800
H	1.88464700	4.76429800	1.08261200
H	-2.81733000	0.79558700	1.14672100
C	-4.36494500	-0.29509600	0.07002200
C	-5.06368400	-0.59727800	1.24315800
C	-4.89817900	-0.73343000	-1.14804600
C	-6.25817500	-1.30920900	1.20403600
H	-4.66267900	-0.26363300	2.19639600
C	-6.09085600	-1.44700600	-1.18935400
H	-4.37785000	-0.51443700	-2.07739200
C	-6.77850500	-1.73806300	-0.01350300
H	-6.78355200	-1.52890200	2.12841100
H	-6.48606100	-1.77672700	-2.14540500
H	-7.70996700	-2.29365300	-0.04697600

**TS12**

C	-1.86711900	0.90447000	0.61132200
C	-1.05713100	1.70590100	-0.33804400
C	-0.51131700	0.36477500	-0.67937500
H	-0.35104100	2.38893300	0.13176900
H	-1.60008800	2.20549600	-1.13881100
H	-1.06662000	-0.22502000	-1.40068900
C	0.66152900	-0.17508900	-0.18532300
C	1.11871500	-1.49957800	-0.45586800



H	0.50194400	-2.08642700	-1.12821000	C	1.33027800	-0.32105200	-1.84694900
C	2.25565400	-2.01355100	0.08432200	C	2.65561400	-0.67770100	-1.64067100
H	2.81946600	-1.41612000	0.79556300	H	2.86633900	-1.21255500	-0.72280700
C	3.61293000	-3.86431100	0.83567000	C	3.64748900	-0.17829000	-2.44976600
H	4.30905100	-4.57756400	0.38592300	H	3.37987100	0.36434100	-3.35400500
H	4.19266400	-3.10032600	1.35839500	C	5.95518200	0.12417900	-3.17438200
H	2.99701100	-4.39692700	1.57600400	H	6.51605800	-0.73898500	-3.54743900
C	2.08320400	-4.13928100	-1.05838200	H	5.46737400	0.61469700	-4.01728600
H	1.14272000	-4.48291500	-0.59909100	H	6.65635300	0.82617800	-2.71372600
H	2.70451500	-5.00968200	-1.27945400	C	5.40752800	-0.91418700	-0.97437400
H	1.84433200	-3.63849100	-2.00049400	H	4.85449800	-0.49237600	-0.12896000
N	2.81708100	-3.23686500	-0.20110100	H	6.47211800	-0.71487100	-0.84914700
O	1.41256100	0.55739600	0.72109800	H	5.24649700	-1.99774100	-0.99678000
C	2.82134800	3.38612900	-0.92446200	N	4.95364400	-0.29030800	-2.20926500
C	3.47767800	3.42628700	0.47286100	O	1.26773300	1.39776900	-0.97018400
B	2.08936000	1.66609300	0.32348900	C	-0.97796100	4.16342300	-1.25526200
O	2.14854900	2.13101300	-0.96737100	C	-0.22066900	4.46290600	0.05682100
O	2.78132500	2.43670600	1.22411600	B	0.51516900	2.53136400	-0.84464800
H	3.54865600	3.44301800	-1.73761900	O	-0.28270800	3.05136500	-1.82739700
H	2.08627500	4.18825300	-1.05354600	O	0.55869700	3.29212100	0.29953300
H	3.37549000	4.39854200	0.96066500	H	-0.95558400	4.99981000	-1.95750300
H	4.54038900	3.16367800	0.43257900	H	-2.01584300	3.87403400	-1.06565500
H	-1.43594700	0.73815700	1.59284200	H	-0.90072200	4.62694400	0.89541800
C	-3.18262700	0.38940300	0.35094700	H	0.45204200	5.32224300	-0.03692000
C	-3.85916100	-0.34025200	1.35351200	H	-0.59225200	0.25592300	0.17754000
C	-3.84494700	0.56438100	-0.88409600	C	-2.44814100	1.25630900	-0.05975200
C	-5.12771000	-0.85228400	1.13824400	C	-2.26319800	1.96871000	1.13154600
H	-3.36785400	-0.49130000	2.31095500	C	-3.52739500	1.59503300	-0.88346500
C	-5.11371300	0.04276800	-1.09451400	C	-3.13229000	2.99893400	1.48434000
H	-3.35779800	1.11054500	-1.68687500	H	-1.42553200	1.71027200	1.77725500
C	-5.76820500	-0.66702500	-0.08879000	C	-4.39748000	2.62414100	-0.53026800
H	-5.62466900	-1.40280000	1.93146700	H	-3.68949500	1.04848900	-1.80860100
H	-5.59846800	0.19246700	-2.05478100	C	-4.20053900	3.33253200	0.65349000
H	-6.76064400	-1.07131200	-0.25721000	H	-2.97550100	3.54003200	2.41306900
				H	-5.23066000	2.87201400	-1.18046100
				H	-4.87830000	4.13413900	0.92920600
				C	1.68719000	-3.11949800	2.51332200
				C	2.32340000	-2.05986800	1.59002000
				B	0.00149900	-2.07253800	1.44136200
				O	0.42849600	-3.36228100	1.94716800
				O	1.23973100	-1.40418400	0.97337700
				C	-0.93529100	-3.21863300	-0.57657600
				C	-1.84091000	-3.48154200	-1.56282000
				C	-3.10062100	-2.77109600	-1.47384400
<b>TS13</b>							
C	-1.52316800	0.10813100	-0.38393700				
C	-1.18771900	0.03391500	-1.88936600				
C	0.11092500	-0.66877800	-2.15387600				
H	-1.13137800	1.04414000	-2.30109700				
H	-1.98183100	-0.49602500	-2.42091600				
H	0.07843600	-1.65424600	-2.62163900				

C	-3.27847400	-1.75477100	-0.60020300	C	-3.24217600	-1.58739000	-1.91798700
C	-2.11426300	-1.22670300	0.19358000	H	-2.90715900	-2.43775900	-2.50856300
N	-1.07108800	-2.24318500	0.34628300	C	-5.35877000	-2.77630100	-1.74496800
H	-0.04473900	-3.82849700	-0.44746800	H	-6.24332200	-2.40429700	-2.27210800
H	-1.71186500	-4.30591700	-2.24858300	H	-4.84013800	-3.48677900	-2.38948400
H	-4.24983200	-1.28913100	-0.47390500	H	-5.68383000	-3.29200100	-0.83643600
H	-2.46114600	-0.95230800	1.19468500	C	-4.95917600	-0.65239200	-0.50094000
C	-4.21321400	-3.21264500	-2.27934600	H	-4.18017300	-0.39607700	0.22457700
N	-5.09395000	-3.56232700	-2.94469000	H	-5.83989800	-1.03631400	0.01528700
H	1.58639500	-2.71950300	3.53727700	H	-5.23422600	0.25409400	-1.05157000
H	2.27180300	-4.04414100	2.56716900	N	-4.46628400	-1.68376300	-1.40767300
H	2.95573300	-2.54982000	0.82897000	O	-0.49654700	-2.11935200	-0.94745500
H	2.95874400	-1.34821000	2.13791900	C	2.77146700	-3.56289700	-0.92227700
O	-0.55659500	-1.19847800	2.50833400	C	2.16774600	-4.05071200	0.40876600
H	1.86173800	1.21072100	-0.11216900	B	0.67614500	-2.78420100	-0.71031400
O	2.66384900	1.04189100	1.03520400	O	1.65927900	-3.00754400	-1.63430900
H	2.00807700	0.75856700	1.75672000	O	0.94358600	-3.32237300	0.52789500
O	1.01868200	0.74420400	2.96405900	H	3.21277500	-4.36823200	-1.51264100
H	0.35897500	0.00166700	2.77702500	H	3.51692800	-2.77659800	-0.75927600
C	3.23152900	2.27403700	1.46103600	H	2.81058100	-3.82557000	1.26186900
H	4.09535500	2.08937700	2.10883700	H	1.94044200	-5.12203300	0.39394100
H	3.56432500	2.82584400	0.57750400	H	0.66638600	-0.40026000	0.23081100
H	2.49004600	2.87823100	1.98990400	C	2.77163800	-0.26243200	0.35289400
C	1.61050100	0.47416700	4.21660500	C	2.78811500	-0.94255900	1.57570700
H	2.09807600	-0.50972300	4.23819600	C	3.98765300	-0.03926700	-0.30217900
H	2.36515600	1.24022100	4.41687800	C	3.98167000	-1.41006100	2.11853800
H	0.86696600	0.50780400	5.02153200	H	1.84468000	-1.10752700	2.09208700
C	-1.43345700	-1.82083800	3.41834200	C	5.18361000	-0.50867100	0.23728200
H	-0.90408300	-2.54675500	4.04666400	H	4.00085900	0.50207800	-1.24381800
H	-1.88932900	-1.05295700	4.05093500	C	5.18400700	-1.20294400	1.44465400
H	-2.22861900	-2.35947400	2.88627000	H	3.97319200	-1.93765600	3.06789800

## TS13-2

C	1.45366000	0.22678300	-0.19993300	H	6.11692500	-0.32961100	-0.28715000
C	1.40886700	0.11576100	-1.74141900	H	6.11546300	-1.57067500	1.86282600
C	0.01120900	0.11547600	-2.29131500	C	-2.85716600	3.13315800	2.36157100
H	1.92314700	-0.79621700	-2.05812000	C	-3.53565300	2.55091500	1.11543500
H	1.94475300	0.95868500	-2.18526000	B	-1.33774500	1.75495400	1.27716600
H	-0.26027900	0.90218300	-2.99423100	O	-1.48978800	2.91202100	2.13997000
C	-1.03111300	-0.60245500	-1.95139900	O	-2.68291900	1.49971100	0.71872900
C	-2.39427000	-0.52488400	-1.69755700	C	-0.64007900	2.74200600	-0.90746200
H	-2.69830900	0.32002700	-1.08119400	C	0.23994300	3.39756300	-1.71587700
				C	1.61026200	3.46512700	-1.24661100
				C	2.03104000	2.71429800	-0.20486300
				C	1.12318000	1.65551800	0.36194500
				N	-0.29062400	1.98991900	0.16029000

H	-1.71346700	2.80986300	-1.07432800	H	4.25547100	-2.92220300	-0.39504100
H	-0.09369500	3.99629400	-2.55096600	N	4.52779700	-0.98953800	-1.20349300
H	3.01861500	2.84830600	0.22244900	O	1.05761700	1.51981900	-0.24977600
H	1.28785300	1.57347100	1.44111600	C	4.24315000	2.89980900	-0.97867400
C	2.50836000	4.42264800	-1.84375800	C	4.05780700	3.28332800	0.50165300
N	3.22661200	5.17910700	-2.34629300	B	2.24793300	2.14854200	-0.23332200
H	-3.20727000	2.60821500	3.26711800	O	2.96458300	2.42865200	-1.38587100
H	-3.05643800	4.20224400	2.49273300	O	2.91352000	2.54337000	0.91025500
H	-3.60596900	3.31312800	0.32328500	H	4.97586900	2.08800200	-1.09206400
H	-4.54602200	2.17173000	1.31594900	H	4.55087000	3.73975900	-1.60527100
O	-0.85981100	0.54469700	2.02768500	H	3.85800900	4.35372100	0.62038600
H	-1.06554900	-1.94211800	-0.04464000	H	4.91529100	3.01471900	1.12284000
O	-1.74639200	-1.61246500	1.08302400	H	-1.10958200	1.30748100	0.32935900
H	-1.42494100	-0.68258000	1.40499600	C	-3.12063500	1.67050100	-0.11172800
C	-1.55347100	-2.55128700	2.13357700	C	-3.28505100	2.34927800	1.10129900
H	-1.68971300	-3.55506100	1.72528600	C	-4.14730600	1.75288200	-1.05683700
H	-0.54182000	-2.48952800	2.54644500	C	-4.43049100	3.09246700	1.36259700
H	-2.28832900	-2.38205100	2.92648800	H	-2.49598700	2.28324300	1.84736000
C	-1.27044300	0.48307700	3.38045900	C	-5.29587000	2.49901700	-0.80037100
H	-2.35413400	0.30731700	3.45729500	H	-4.06599100	1.22469400	-2.00191800
H	-0.74620300	-0.34377600	3.86966700	C	-5.44144500	3.17292600	0.40785800
H	-1.03156000	1.41845500	3.89111000	H	-4.53295000	3.61102100	2.31072700

**TS13-3**

C	-1.86317300	0.84029700	-0.29694400	H	-6.08025400	2.54894300	-1.54907100
C	-1.35397200	0.88954200	-1.75227200	H	-6.33628000	3.75426600	0.60532900
C	-0.18073600	-0.00918600	-2.04626800	C	-0.19346300	-2.76736100	3.25701300
H	-1.07667300	1.92467600	-1.97436800	C	1.25898300	-2.79706600	2.75911700
H	-2.14851000	0.60328800	-2.44395500	B	0.03005400	-1.10001700	1.73241300
H	-0.35156200	-0.85087000	-2.72139200	O	-0.61396200	-1.45681000	2.97939800
C	1.02674200	-0.06694600	-1.56085000	O	1.26903200	-1.89636600	1.66801400
C	2.13903000	-0.77941000	-1.17531700	C	-0.62681300	-2.46624800	-0.28801400
H	1.99942800	-1.47300500	-0.34693900	C	-1.47917400	-2.96538000	-1.22205700
C	3.39417500	-0.48054900	-1.67306100	C	-2.81232300	-2.39346300	-1.24608600
H	3.49114400	0.22898700	-2.49099800	C	-3.13755400	-1.33816600	-0.47241100
C	5.79895300	-0.77292600	-1.87326900	C	-2.09381600	-0.59045500	0.31594600
H	6.17848300	-1.71173900	-2.28946400	N	-0.85627400	-1.37687400	0.48575400
H	5.66708600	-0.05560400	-2.68414600	H	0.32873100	-2.94631000	-0.10014900
H	6.53456700	-0.38166800	-1.16451100	H	-1.23944400	-3.84824900	-1.79619700
C	4.51729700	-1.90948800	-0.07016200	H	-4.15885300	-0.97648500	-0.42688900
H	3.78782200	-1.58284900	0.67541700	H	-2.48136700	-0.38842600	1.32580200
H	5.51269300	-1.92357100	0.37558200	C	-3.83072300	-3.02186700	-2.05109800
				N	-4.63114200	-3.52686500	-2.71826000
				H	-0.28596400	-2.98299900	4.32653400
				H	-0.79817300	-3.50153900	2.70020700
				H	1.57783700	-3.79744000	2.44030200

H	1.94763800	-2.44733700	3.54328500	C	-3.62401700	1.08639800	-0.89941200
H	0.75621600	1.00427300	0.67202300	C	-3.71114400	2.47694600	1.50857800
O	0.33546300	0.36672200	1.75795000	H	-1.87211700	1.44532800	1.97887900
C	1.03680300	0.79844300	2.91692200	C	-4.67820100	1.95830100	-0.63505100
H	1.30209700	1.84938300	2.78357100	H	-3.59905200	0.54502200	-1.84132600
H	0.40293300	0.66901500	3.79527200	C	-4.72330000	2.66024100	0.56771200
H	1.95439500	0.21216300	3.04324800	H	-3.74293800	3.01208900	2.45337100

**TS14**

C	-1.46875800	-0.07444900	-0.18882800	B	0.30382200	-1.88447000	1.78389400
C	-1.00684800	-0.11447600	-1.66010600	O	0.83518400	-3.08098400	2.41965100
C	0.39919200	-0.61762100	-1.81267300	O	1.49395500	-1.12824500	1.31856400
H	-1.06836900	0.88981600	-2.08597000	C	-0.29172400	-3.25379300	-0.22473400
H	-1.66787100	-0.76360200	-2.23996000	C	-1.06124900	-3.70657000	-1.25723900
H	0.54719100	-1.61082600	-2.24061700	C	-2.42398700	-3.21433300	-1.29769700
C	1.52774200	-0.07332500	-1.45311600	C	-2.84115000	-2.22031800	-0.48190600
C	2.89145200	-0.15946800	-1.21399000	C	-1.85592900	-1.48352100	0.38347400
H	3.19291400	-0.53906300	-0.24494500	N	-0.65611600	-2.28266200	0.63665500
C	3.78404300	0.39922100	-2.09781500	H	0.67798500	-3.69684400	-0.00973100
H	3.42450100	0.78301900	-3.05005400	H	-0.74372000	-4.52331000	-1.88853200
C	6.00353000	1.00577500	-2.90369300	H	-3.88186600	-1.91483400	-0.45927400
H	6.71364800	0.22452100	-3.19360700	H	-2.31862300	-1.26303800	1.35116300
H	5.43522500	1.30604100	-3.78455200	C	-3.37446800	-3.84999500	-2.17758500
H	6.56281300	1.86978300	-2.53258000	N	-4.12436400	-4.35232300	-2.90288300
C	5.65070000	0.10993000	-0.60154000	H	2.00899600	-2.24000500	3.90622200
H	5.09232300	0.58523400	0.21147600	H	2.72989300	-3.60944700	3.03445600
H	6.69475600	0.41973600	-0.55496400	H	3.21053000	-2.26336800	1.10262400
H	5.59339800	-0.97733100	-0.47930800	H	3.30022400	-0.96936800	2.32283800
N	5.09315200	0.51880900	-1.88315100	O	-0.42097400	-1.00188800	2.73335900
O	1.11693500	1.59758300	-0.56669600	H	1.68496800	1.52107900	0.31963000
C	-1.48599000	4.01808100	-0.94416700	H	-0.94183000	-1.54921900	3.33077800
C	-0.84214500	4.40349500	0.40757900	O	2.45390300	1.63391700	1.51462500
B	0.21083300	2.61309500	-0.47888900	H	2.03671600	1.11177400	2.27148300
O	-0.62865200	3.00818500	-1.48316900	H	2.32992400	2.55404600	1.78387300
O	0.11605500	3.37640700	0.66386700	O	1.37694200	0.64358800	3.65458100
H	-1.53318300	4.85708000	-1.64253400	H	0.64145000	0.03351500	3.35336700
H	-2.48682100	3.59796900	-0.81094800	H	1.97536200	0.07909000	4.15446000
H	-1.57474100	4.42486000	1.21793100				
H	-0.32467400	5.36757000	0.36377200				
H	-0.62528600	0.23832600	0.43699700	<b>TS14-2</b>			
C	-2.59912600	0.90061800	0.03431500				
C	-2.65956800	1.60265700	1.24427500	C	1.36392200	0.21170000	-0.14909600



H	3.86132900	-1.37036500	0.75031000	H	-0.72511800	-3.51082600	2.69278100
H	5.57270300	-1.76091400	0.42106200	H	1.62687500	-3.81806600	2.30073300
H	4.27225100	-2.73055100	-0.31501800	H	2.07214700	-2.53057100	3.44733800
N	4.58042700	-0.80997500	-1.14375300	O	0.33698500	0.37523300	1.79990600
O	1.06811800	1.62191200	-0.16233800	H	0.76572100	1.08951600	0.72870700
C	4.36144800	2.88177100	-0.60401400	H	0.76110200	0.58462600	2.63971800
C	4.19717500	2.91799300	0.92965500				
B	2.31069700	2.13766800	-0.03147100				
O	3.05928700	2.59137100	-1.09893300	<b>TS15</b>			
O	2.98393400	2.21318900	1.16883800				
H	5.04767000	2.08195300	-0.91489500	C	1.48164500	-0.82364300	-0.65573800
H	4.71650000	3.82744200	-1.01942200	C	1.47603800	-0.38149300	-2.11926900
H	4.09994600	3.94234300	1.30455600	C	0.09088400	-0.18181900	-2.67646200
H	5.01955400	2.42817500	1.45663100	H	1.96207900	-1.14410000	-2.73657100
H	-1.11047500	1.33326500	0.42416000	H	2.05405200	0.54327400	-2.25282200
C	-3.12491300	1.68210900	-0.00643500	H	-0.03320700	-0.32339700	-3.75221500
C	-3.29161800	2.34022700	1.21733900	C	-1.02613700	0.09451400	-2.06202000
C	-4.15406500	1.77053600	-0.94801400	C	-2.36597500	0.18884100	-1.88368900
C	-4.44215600	3.06976800	1.49308700	H	-2.84929100	1.15519600	-1.80039100
H	-2.50031200	2.26729500	1.96041400	C	-3.02014400	-0.98537100	-1.48629900
C	-5.30800800	2.50317100	-0.67695000	H	-2.46474600	-1.91710400	-1.52262000
H	-4.06945800	1.25723800	-1.90117900	C	-4.86179600	-2.33393400	-0.68592400
C	-5.45589300	3.15699500	0.54202400	H	-5.74797400	-2.52346100	-1.29849200
H	-4.54697500	3.57175200	2.44995500	H	-4.13981900	-3.13640300	-0.83616200
H	-6.09457300	2.55972800	-1.42306500	H	-5.15141200	-2.31200200	0.36806500
H	-6.35507800	3.72751400	0.75133600	C	-5.05911500	0.14628600	-0.86789700
C	-0.08772700	-2.80063800	3.24411500	H	-4.49373500	0.82715400	-0.22590300
C	1.34153200	-2.82824000	2.67996200	H	-5.99764800	-0.12850100	-0.38741600
B	0.07692300	-1.09458900	1.75781800	H	-5.27682200	0.61368300	-1.83272400
O	-0.50705100	-1.47768600	3.02676500	N	-4.26070700	-1.06236800	-1.05841800
O	1.32082300	-1.87657200	1.63415900	O	-1.31641700	-1.27503000	0.63906100
C	-0.60569800	-2.40892100	-0.29663100	H	0.66864500	-1.54285600	-0.51255100
C	-1.46761400	-2.87986300	-1.23805000	C	2.77210900	-1.48326000	-0.21938800
C	-2.81249000	-2.33761600	-1.20364700	C	2.73733500	-2.33195200	0.89267500
C	-3.13738300	-1.31693200	-0.38384600	C	4.00064600	-1.25126200	-0.84197900
C	-2.08086300	-0.57465200	0.39364100	C	3.89541300	-2.93664800	1.36688300
N	-0.84373000	-1.36474400	0.53244200	H	1.78268500	-2.51221400	1.38268000
H	0.36309500	-2.87699900	-0.14897600	C	5.16387400	-1.85628700	-0.36903900
H	-1.22363600	-3.73209900	-1.85522400	H	4.05836300	-0.58846500	-1.70100500
H	-4.16450000	-0.98134400	-0.29341100	C	5.11505100	-2.70086100	0.73497200
H	-2.44979200	-0.38474400	1.41227600	H	3.84717900	-3.59404900	2.22926700
C	-3.84168000	-2.96300600	-1.99733700	H	6.10975000	-1.66305900	-0.86516600
N	-4.65221900	-3.46373800	-2.65545100	H	6.02094000	-3.17193000	1.10240300
H	-0.13452500	-3.04899700	4.30954500	C	-1.51626700	1.45105800	2.87768000

C	-2.86895100	1.43755700	2.15201600	H	-4.66999100	0.71995200	-0.14022600
B	-1.29020600	0.12198500	1.02417800	H	-6.13076800	-0.20508300	-0.62135800
O	-0.87743000	0.29340800	2.40972900	H	-5.15157400	0.59231100	-1.86590000
O	-2.60013800	0.80025000	0.91892900	N	-4.30872500	-1.13156900	-1.01914000
C	-0.45103100	2.17359400	-0.21558600	O	-1.20466100	-1.70442500	0.51308700
C	0.50847600	3.10271300	-0.38916700	H	0.76859200	-1.59940000	-0.56477100
C	1.89225800	2.69972700	-0.16746100	C	2.85328800	-1.31717400	-0.26072400
C	2.19086600	1.43674400	0.18001300	C	2.91453700	-2.18630000	0.83425300
C	1.14237800	0.36192700	0.29259700	C	4.04710900	-0.95025900	-0.88548900
N	-0.24132500	0.83197400	0.04460200	C	4.13121000	-2.67953100	1.28962300
H	-1.50192700	2.43504400	-0.29492700	H	1.98696000	-2.47128200	1.32655400
H	0.26566300	4.12785200	-0.63069900	C	5.26967900	-1.44272900	-0.43119700
H	3.21443100	1.14771200	0.39742000	H	4.03159000	-0.27170400	-1.73393700
H	1.17104300	-0.03823500	1.31678600	C	5.31574100	-2.30911400	0.65548300
C	2.94016000	3.68178300	-0.28144400	H	4.15630300	-3.35434900	2.13948500
N	3.77084400	4.48109300	-0.38830700	H	6.18684600	-1.14537900	-0.92999800
H	-1.61536800	1.42304400	3.96810400	H	6.26759100	-2.69266300	1.00842900
H	-0.94839900	2.35587000	2.60468500	C	-1.61447000	0.74166200	3.02464700
H	-3.27135300	2.44612900	1.98964600	C	-2.98258200	0.69674900	2.32571900
H	-3.61158600	0.85857200	2.72323100	B	-1.33186500	-0.35990300	1.03512100
C	-2.09963100	-2.07018200	1.48711600	O	-0.89606600	-0.30419100	2.42458600
H	-2.19304100	-3.07265200	1.04949800	O	-2.71326600	0.17411100	1.04099800
H	-1.65616400	-2.16214100	2.48517200	C	-0.81113700	1.92406500	0.03569400
H	-3.10962800	-1.64500400	1.60939200	C	0.00214100	2.99212400	-0.07346800

**TS16**

C	1.49621000	-0.79008800	-0.67703900
C	1.44632800	-0.30467900	-2.12389700
C	0.05060200	-0.18092000	-2.67516400
H	1.98146800	-1.01245200	-2.76552000
H	1.95548200	0.66267300	-2.23464600
H	-0.05939300	-0.30379400	-3.75546900
C	-1.09260200	0.01340000	-2.07962400
C	-2.44068700	0.08999000	-1.94555200
H	-2.92786200	1.05800300	-1.90874400
C	-3.07621500	-1.06401900	-1.47200400
H	-2.48654100	-1.97070100	-1.39356000
C	-4.69310900	-2.24771200	-0.16716300
H	-5.72493500	-2.53955900	-0.37341200
H	-4.02855400	-3.09157900	-0.35143100
H	-4.58932500	-1.93708300	0.87821100
C	-5.11635300	0.07526500	-0.90521000

**TS17**

C	-1.10472400	0.50558600	-1.31177700
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C	0.20628200	1.11607900	-1.82756500	H	-0.88257500	1.80783700	0.32313200
C	1.33150500	1.12618600	-0.76135300	O	1.02242700	3.89702200	-0.06409200
H	0.00561400	2.15880100	-2.08386100	H	-0.05846400	3.70365400	-0.20286800
H	0.53633400	0.59134300	-2.72846600	C	-2.10084800	4.04841100	0.48973600
H	2.31438600	1.10620100	-1.23204500	H	-1.57925400	4.90072800	0.96055200
C	1.23043100	0.09898400	0.30149200	H	-3.01080700	4.45622700	0.01471300
C	2.35856000	-0.57485800	0.85720200	H	-2.45596700	3.41423400	1.33319600
H	2.25053600	-1.05647500	1.81952600	C	1.49340600	4.44796600	-1.25313600
C	3.58943100	-0.57474600	0.25105000	H	2.06853300	3.71862200	-1.85995300
H	3.72005000	-0.11722000	-0.72416800	H	0.67007900	4.80691300	-1.89042200
C	5.95985100	-1.10121500	0.02564400	H	2.16579900	5.29775300	-1.06528500
H	6.30457500	-2.12029500	-0.17537400				
H	5.82404100	-0.58397800	-0.92431800				
H	6.72657700	-0.57610000	0.60312500	<b>TS17-2</b>			
C	4.68240600	-1.75591200	2.05852400				
H	4.35986100	-1.04455300	2.82578800	C	1.18435800	-1.15477200	0.70650400
H	5.68575300	-2.10504000	2.30020000	C	-0.04574200	-2.04256200	0.40267700
H	3.99973800	-2.61296800	2.06225700	C	-1.34917800	-1.38463300	0.88206500
N	4.70181400	-1.12117500	0.75259800	H	0.07953300	-3.01837100	0.87824800
H	-1.93900700	1.11016100	-1.67835900	H	-0.09058400	-2.21620200	-0.67936200
C	-1.32788900	-0.95435300	-1.64312300	H	-2.21296800	-2.04413400	0.81074500
C	-2.63081100	-1.46221500	-1.67371900	C	-1.55680300	-0.10991500	0.19536400
C	-0.26734100	-1.84342600	-1.84632100	C	-2.82152100	0.35683100	-0.29077000
C	-2.86929100	-2.81523100	-1.89000900	H	-2.96076400	1.42177400	-0.42685600
H	-3.46759500	-0.78375500	-1.52693700	C	-3.86704400	-0.49365900	-0.51935700
C	-0.50120900	-3.19922000	-2.06209600	H	-3.72055700	-1.56624200	-0.43371200
H	0.75659500	-1.47636500	-1.83988200	C	-6.11471100	-1.11274000	-1.23994500
C	-1.80289100	-3.69036500	-2.08190000	H	-6.35223800	-1.04803400	-2.30772900
H	-3.88910700	-3.18569400	-1.91192400	H	-5.73995000	-2.11452000	-1.02742000
H	0.33635300	-3.87174000	-2.22009100	H	-7.03299600	-0.95597700	-0.66643200
H	-1.98656300	-4.74600600	-2.25326600	C	-5.44911900	1.27103400	-1.01057000
C	-0.30844900	-1.22820000	1.59598700	H	-5.18447200	1.81793100	-0.10037700
C	-1.53553000	-1.42346800	2.08840400	H	-6.52196700	1.36634800	-1.17817300
C	-2.61641200	-0.48770500	1.78412200	H	-4.91729900	1.72122900	-1.85797800
C	-2.39901700	0.48936600	0.88754000	N	-5.11339800	-0.13188900	-0.86541900
C	-1.09087000	0.71038000	0.23100900	H	1.59939400	-1.46543700	1.67261000
N	0.00490700	-0.11904400	0.78596700	C	2.26010700	-1.32515800	-0.34569900
H	0.48075300	-1.95290600	1.73022800	C	3.33093300	-2.19087900	-0.11953100
H	-1.73993800	-2.30732900	2.67905200	C	2.19268900	-0.65055900	-1.56938100
H	-3.17593800	1.19238300	0.60080000	C	4.31167500	-2.38430500	-1.08970700
C	-3.89485300	-0.66372100	2.41408400	H	3.39749800	-2.71543600	0.83050700
N	-4.91822400	-0.83218500	2.92801100	C	3.17188500	-0.83777300	-2.53869700
H	1.28478500	2.13165400	-0.25000500	H	1.37141600	0.03729900	-1.76046300
O	-1.30180800	3.35807700	-0.40517600	C	4.23469200	-1.70755700	-2.30264300



H	5.13892600	-3.05911900	-0.89361700	N	-4.63801400	0.68923700	0.76371100
H	3.10919400	-0.29891700	-3.47887200	H	2.01385000	-1.10902300	-1.98771200
H	5.00077800	-1.85039400	-3.05773000	C	1.39539000	0.89511400	-1.51023900
C	-0.43362200	1.81630500	-0.71754900	C	2.69461000	1.39697800	-1.37824100
C	0.57846300	2.69153900	-0.67725600	C	0.33723500	1.80859300	-1.55763800
C	1.72192500	2.45936200	0.19816500	C	2.93116000	2.76421000	-1.28587500
C	1.78997700	1.30139600	0.88705200	H	3.53042000	0.70217300	-1.34879200
C	0.71319200	0.30838000	0.93422400	C	0.56909000	3.17876700	-1.46346800
N	-0.46845600	0.66757400	0.09367900	H	-0.68279300	1.44945100	-1.67304800
H	-1.24297300	1.90903300	-1.42799700	C	1.86638900	3.66151200	-1.32426400
H	0.57489500	3.54491900	-1.34370100	H	3.94831900	3.12942600	-1.18634500
H	2.66762900	1.06679400	1.48333600	H	-0.26705800	3.87023900	-1.50360300
H	0.25909400	0.25077200	2.03396200	H	2.04841200	4.72895400	-1.25359600
C	2.78001000	3.42592000	0.24837400	C	0.32425200	0.43449900	1.71209200
N	3.62371400	4.21901700	0.27041300	C	1.53941400	0.49922500	2.26484500
H	-1.18570200	-1.05341800	2.02654700	C	2.62306900	-0.34834600	1.77060800
O	-0.58897700	-0.28828800	3.16904000	C	2.41868800	-1.07978300	0.66181600
C	0.20417600	-1.04615800	4.00838000	C	1.12725000	-1.13984800	-0.05103500
H	0.30444700	-2.10502100	3.68124700	N	0.02535400	-0.44818400	0.65547000
H	1.24082600	-0.65825000	4.08716900	H	-0.46673200	1.11225100	1.99712300
H	-0.18040800	-1.08380800	5.04280900	H	1.73175800	1.21657100	3.05236900

**TS18**

C	1.16987000	-0.60180500	-1.51099200
C	-0.12798400	-1.08011300	-2.17365400
C	-1.29213600	-1.25425200	-1.16733400
H	0.06765800	-2.06653000	-2.59976000
H	-0.41133500	-0.39451700	-2.97789200
H	-2.25965700	-1.07788300	-1.63917100
C	-1.18961000	-0.51871500	0.10375400
C	-2.32267700	0.02200600	0.79224300
H	-2.24190100	0.19776200	1.85672600
C	-3.51517200	0.26654800	0.16624100
H	-3.60515700	0.13584800	-0.90762500
C	-5.83263400	1.01362000	0.00520900
H	-6.07371200	2.07824000	0.09294900
H	-5.67090300	0.77863100	-1.04712300
H	-6.68417700	0.42904600	0.36605300
C	-4.66720300	0.89542800	2.19956200
H	-4.37271900	-0.02069000	2.72140200
H	-5.67958100	1.16277100	2.50146700
H	-3.98590600	1.70257900	2.49369500

N	-4.63801400	0.68923700	0.76371100
H	2.01385000	-1.10902300	-1.98771200
C	1.39539000	0.89511400	-1.51023900
C	2.69461000	1.39697800	-1.37824100
C	0.33723500	1.80859300	-1.55763800
C	2.93116000	2.76421000	-1.28587500
H	3.53042000	0.70217300	-1.34879200
C	0.56909000	3.17876700	-1.46346800
H	-0.68279300	1.44945100	-1.67304800
C	1.86638900	3.66151200	-1.32426400
H	3.94831900	3.12942600	-1.18634500
H	-0.26705800	3.87023900	-1.50360300
H	2.04841200	4.72895400	-1.25359600
C	0.32425200	0.43449900	1.71209200
C	1.53941400	0.49922500	2.26484500
C	2.62306900	-0.34834600	1.77060800
C	2.41868800	-1.07978300	0.66181600
C	1.12725000	-1.13984800	-0.05103500
N	0.02535400	-0.44818400	0.65547000
H	-0.46673200	1.11225100	1.99712300
H	1.73175800	1.21657100	3.05236900
H	3.19662400	-1.70980500	0.23946700
C	3.88593400	-0.35072900	2.45377600
N	4.89854700	-0.33186100	3.01461300
H	-1.32118300	-2.37249500	-0.89766500
O	1.20647700	-3.60068200	-1.16166300
H	0.93884900	-2.25476700	-0.21941700
H	1.72051400	-4.27046500	-0.69731800
O	-1.14988000	-4.04877500	-0.83914000
H	-1.49277800	-4.42743000	-1.65553400
H	-0.04440500	-3.93649600	-1.00121800

**TS18-2**

C	1.21237800	-1.04311500	1.07642300
C	-0.00557800	-1.98191400	0.89815200
C	-1.31941100	-1.28058100	1.26852600
H	0.13236500	-2.87996100	1.50634000
H	-0.03518100	-2.30940700	-0.14857100
H	-2.17978700	-1.94597300	1.32198600
C	-1.54446400	-0.12584700	0.41923300
C	-2.82500800	0.26717100	-0.10688300
H	-2.98631800	1.31384800	-0.33411100

C	-3.84127400	-0.62675500	-0.27000500
H	-3.65984500	-1.68493600	-0.10156000
C	-6.02823700	-1.37262200	-1.04650700
H	-6.13821200	-1.41096800	-2.13732400
H	-5.66116200	-2.33996000	-0.70056800
H	-7.01225800	-1.19693600	-0.60267100
C	-5.47244000	1.04210800	-0.91030900
H	-5.19676700	1.67619900	-0.06259500
H	-6.55162500	1.10176800	-1.05552800
H	-4.97225500	1.42346700	-1.81067400
N	-5.10446700	-0.33209200	-0.63828200
H	1.60845600	-1.18974600	2.08936000
C	2.30838400	-1.38086300	0.08766800
C	3.35051900	-2.23258600	0.45558700
C	2.28377400	-0.87885700	-1.21750300
C	4.34604900	-2.57968000	-0.45448600
H	3.38353500	-2.62391200	1.46978900
C	3.27718300	-1.22097200	-2.12829400
H	1.48434300	-0.20391900	-1.51795200
C	4.31191300	-2.07398300	-1.75002600
H	5.15184100	-3.23940500	-0.14803400
H	3.24782900	-0.81522000	-3.13473000
H	5.09003700	-2.33630900	-2.45959400
C	-0.46592400	1.66580700	-0.77473500
C	0.52471200	2.56131500	-0.87007100
C	1.68276000	2.47755600	0.01142700
C	1.78344500	1.41860300	0.84620400
C	0.73204900	0.43186200	1.05082100
N	-0.46800300	0.64241900	0.19177400
H	-1.28556000	1.63880400	-1.47927500
H	0.49270600	3.31246200	-1.64963500
H	2.68018300	1.28035600	1.44520600
H	0.26729200	0.52968600	2.20361500
C	2.72028600	3.46070200	-0.08321100
N	3.54916500	4.26455200	-0.17883900
H	-1.12379200	-0.73937700	2.38401700
O	-0.58339600	0.20113000	3.28207400
H	-0.09222000	-0.15784200	4.03126900

**TS19**

C	-1.58470000	0.05387200	-1.27594300
C	-1.14567200	-1.25050500	-1.97730800

C	0.23982300	-1.05127200	-2.59919300
H	-1.88839700	-1.54163000	-2.72483000
H	-1.09382800	-2.05890900	-1.23946400
H	0.55422200	-1.91372700	-3.18920800
C	1.22105600	-0.80818600	-1.48949500
C	2.52284900	-1.24650700	-1.46493300
H	2.98421700	-1.49241200	-2.41737900
C	3.32906900	-1.08617500	-0.30593400
H	4.34973100	-0.71540800	-0.41767400
C	3.96715000	-1.52574400	1.98152700
H	4.04941800	-2.39594900	2.63598900
H	4.97176300	-1.22836700	1.66811800
H	3.53295200	-0.69539400	2.55653200
C	1.98824100	-2.65907000	0.98698700
H	1.81701300	-3.24898300	0.08214000
H	1.08592900	-2.05182400	1.15861900
H	2.12733800	-3.32754400	1.83830500
N	3.19183900	-1.87420100	0.80847300
H	-2.05911700	0.70046500	-2.02390900
C	-2.61343400	-0.24927600	-0.19716100
C	-3.95541400	-0.40309200	-0.54905800
C	-2.23903100	-0.44428600	1.13394200
C	-4.90743600	-0.74434200	0.40739500
H	-4.25668500	-0.24719100	-1.58245200
C	-3.18868100	-0.78720300	2.09158900
H	-1.19980400	-0.30543300	1.42319700
C	-4.52546000	-0.93911800	1.73169700
H	-5.94824200	-0.85184800	0.11885000
H	-2.88470100	-0.92839900	3.12398500
H	-5.26600900	-1.20040000	2.48050200
C	1.73216600	0.50499000	0.47267800
C	1.74809700	1.89632000	0.68538100
C	0.80835200	2.73065400	0.11535600
C	-0.34796000	2.13121700	-0.49841400
C	-0.37684900	0.80603100	-0.75497500
N	0.80104300	0.05226900	-0.52295800
H	1.89252400	-0.13153600	1.33404600
H	2.49195500	2.30467200	1.36340600
H	-1.23092800	2.73168500	-0.68979500
C	0.87722600	4.14637600	0.29314200
N	0.93000300	5.29665500	0.43413300
H	0.21409700	-0.17302600	-3.26020400

**TS20**

C	-1.95061900	-0.16141500	-1.51239000	H	2.80569800	-1.33843700	0.72793600
C	-1.35865500	-1.49770500	-2.01120500	O	0.58335700	-0.32655200	1.88028900
C	-0.09716600	-1.28908500	-2.86130900	H	1.37092700	-1.52294900	1.91589500
H	-2.12717600	-2.03447600	-2.57375900	O	1.97229800	-2.30469200	1.58239200
H	-1.10225900	-2.11435600	-1.14218800	C	0.25923100	0.56949500	2.90703200
H	0.29836400	-2.23771400	-3.23159400	H	0.46991200	0.14086200	3.89563400
C	0.92108500	-0.60264700	-2.00503500	H	0.83561200	1.50613500	2.82049000
C	2.27162200	-0.72949300	-1.89608400	H	-0.80541000	0.84355100	2.87432000
H	2.88992500	-1.28887300	-2.58316800	C	1.14008900	-3.13836500	0.79478900
C	2.77187300	0.18307100	-0.81505900	H	0.08500600	-2.96464700	1.03550500
H	3.55345300	0.89734200	-1.13073300	H	1.28381500	-2.94338000	-0.27805800
C	3.88967600	0.27225500	1.42508300	H	1.37561200	-4.18828000	0.99292600
H	4.61061400	1.01243400	1.06733300				
H	2.99765200	0.76611500	1.81090200				
H	4.33589600	-0.33624000	2.21285100	<b>TS20-2</b>			
C	4.64722600	-1.36892200	-0.21176700				
H	4.29173400	-2.07655500	-0.95959600	C	-1.85879400	-0.36560200	-1.41002000
H	5.11392200	-1.91257400	0.61046300	C	-1.33167600	-1.76868000	-1.78562400
H	5.36744100	-0.67942200	-0.66062600	C	-0.05530700	-1.70454900	-2.63760500
N	3.49323900	-0.60960300	0.30648000	H	-2.12458400	-2.31325100	-2.30520900
H	-2.43621900	0.33349900	-2.36324600	H	-1.10745200	-2.31951300	-0.86548900
C	-2.99913300	-0.42191500	-0.44518600	H	0.28733000	-2.70267900	-2.91824400
C	-4.35567500	-0.40705100	-0.76180200	C	0.98784300	-1.00470200	-1.82513500
C	-2.60163900	-0.73942200	0.85944700	C	2.31715200	-1.22724300	-1.62960000
C	-5.31237700	-0.70312100	0.20828400	H	2.91707500	-1.91191700	-2.21163100
H	-4.66705800	-0.15737900	-1.77327700	C	2.84634000	-0.24897500	-0.63101900
C	-3.55736200	-1.03655100	1.82426700	H	3.72876800	0.32789400	-0.95717600
H	-1.54142000	-0.73108100	1.11877900	C	4.08108200	0.02136600	1.52322100
C	-4.91466400	-1.01928300	1.50258700	H	4.97418200	0.39205500	1.01193000
H	-6.36665600	-0.68111800	-0.04892000	H	3.39732300	0.85025000	1.71860800
H	-3.24077700	-1.27615600	2.83484300	H	4.36233900	-0.44435300	2.46935900
H	-5.65767100	-1.24599300	2.26050800	C	4.23840000	-2.12452200	0.36963700
C	1.50499400	0.82862700	-0.25701500	H	3.64236300	-2.86233400	-0.16504700
C	1.37030100	2.28526700	-0.14168700	H	4.61017100	-2.55347200	1.30154900
C	0.12680900	2.82577400	-0.17639700	H	5.08353600	-1.81140300	-0.25168600
C	-1.04645300	1.98479200	-0.45831900	N	3.39062400	-0.96195700	0.66915100
C	-0.85923300	0.76228800	-0.99719900	H	-2.34571600	0.06703500	-2.29306100
N	0.43887400	0.30466400	-1.12173800	C	-2.88552300	-0.47472300	-0.29680200
H	1.09992300	0.27619600	0.92406500	C	-4.24103400	-0.27568500	-0.54474200
H	2.24111400	2.90700300	0.05460400	C	-2.46818400	-0.81841100	0.99545700
H	-2.04556900	2.36488400	-0.28578800	C	-5.17667000	-0.41582800	0.48033300
C	-0.05388000	4.23122900	0.04045900	H	-4.56817000	-0.00544100	-1.54563500
N	-0.20746600	5.36600800	0.22029500	C	-3.40113000	-0.96134900	2.01436500
H	-0.33048200	-0.66285700	-3.73177100	H	-1.40564100	-0.96162400	1.19655600

C	-4.75860100	-0.75988100	1.76026000	H	5.51628600	-0.58882200	-0.45350100
H	-6.22997500	-0.25253700	0.27550500	N	3.63969200	-0.64356300	0.51091900
H	-3.06963000	-1.22667000	3.01354200	H	-2.30509100	-0.01043400	-2.23376000
H	-5.48429600	-0.86747800	2.56000300	C	-3.01347300	-0.48023900	-0.27561400
C	1.61905100	0.56671900	-0.22949000	C	-4.34521400	-0.41030000	-0.67956800
C	1.56781300	2.02377700	-0.20382000	C	-2.71628800	-0.68638000	1.07709300
C	0.35758000	2.63016900	-0.32170100	C	-5.37601300	-0.54329000	0.24946100
C	-0.85311700	1.83085900	-0.56233100	H	-4.57815100	-0.24649000	-1.72892200
C	-0.72438500	0.56022200	-0.99803200	C	-3.74612400	-0.82240700	2.00087100
N	0.55430200	0.04353500	-1.08842400	H	-1.67507000	-0.71999700	1.40017700
H	1.23407600	-0.06902100	0.94395400	C	-5.07765700	-0.75139300	1.59134300
H	2.46467400	2.61009600	-0.01593200	H	-6.40916900	-0.47991400	-0.07716000
H	-1.83350100	2.26901400	-0.42162800	H	-3.50953400	-0.97936300	3.04868200
C	0.25045200	4.05398500	-0.20745600	H	-5.87753600	-0.85256700	2.31793200
N	0.15652500	5.20564000	-0.11140100	C	1.57608300	0.65670500	-0.13566000
H	-0.24537800	-1.14302400	-3.56099400	C	1.44824400	2.11797100	-0.12065600
H	2.46641600	-1.22644700	1.22031200	C	0.20495000	2.65649700	-0.17330900
O	1.10085300	-0.97840300	1.74924300	C	-0.97165300	1.80021600	-0.38161400
C	0.97569400	-0.41559600	3.02927400	C	-0.79136900	0.54352900	-0.84197100
H	1.63958300	-0.90605300	3.75540600	N	0.50276500	0.08065100	-0.95949400
H	1.21955600	0.66082000	3.02683200	H	1.17581200	0.15283300	1.07977100
H	-0.05192600	-0.51135900	3.40395000	H	2.32216500	2.75141500	0.01476300

**TS21**

C	-1.89183400	-0.40177100	-1.29446600
C	-1.32791900	-1.80932300	-1.57902900
C	-0.06384400	-1.74745400	-2.44714200
H	-2.10545300	-2.40958700	-2.05900100
H	-1.08491100	-2.29025700	-0.62430000
H	0.31971800	-2.74511000	-2.67249700
C	0.96466400	-0.95580300	-1.70115700
C	2.31215500	-1.09024000	-1.57757400
H	2.91448700	-1.75045800	-2.18526100
C	2.83865600	-0.02600300	-0.65666900
H	3.57971300	0.65964400	-1.11044100
C	3.95588100	0.35534500	1.55335200
H	4.52734000	1.17706300	1.11218800
H	3.01924600	0.72237500	1.97107000
H	4.53959600	-0.12660300	2.33878800
C	4.85994100	-1.31762100	0.02985800
H	4.57756000	-2.09152100	-0.68276900
H	5.37189800	-1.77571500	0.87703500

**TS21-2**

C	-1.78029500	-0.48182000	-1.24177700
C	-1.24850000	-1.91258900	-1.47494700
C	0.04264700	-1.91800600	-2.30546300
H	-2.03101800	-2.50261300	-1.95959700
H	-1.04231200	-2.37656600	-0.50394400
H	0.39455200	-2.93518600	-2.49022700
C	1.07109600	-1.14440300	-1.54204900
C	2.40224900	-1.33432700	-1.33285400

H	3.00927000	-2.05405300	-1.86301300	C	1.49837800	-1.67775300	-1.81512100
C	2.92081000	-0.27912900	-0.40859300	C	1.29542700	-0.26404600	-1.32455300
H	3.78831800	0.29038300	-0.78624300	H	0.61996300	-2.31431700	-1.78556900
C	4.15310000	0.16641900	1.71001200	H	2.16114400	-1.80773800	-2.66358500
H	5.02543600	0.54064000	1.16606200	H	1.85265600	0.51001300	-1.84417100
H	3.44241800	0.98031400	1.86710500	C	-0.07740800	0.16682100	-0.98077300
H	4.46661400	-0.23245400	2.67646500	C	-0.96802100	0.69269000	-1.86523700
C	4.36890200	-2.04129700	0.69612900	H	-0.81152300	0.75968500	-2.92846100
H	3.79148500	-2.83252300	0.22049200	C	-2.15441400	1.11137600	-1.10895700
H	4.76321200	-2.39524300	1.65019700	O	-0.73266500	-0.97190200	0.05007600
H	5.19902200	-1.74748400	0.04512200	C	-2.14394000	-3.64703300	-1.06782700
N	3.48786800	-0.88883800	0.92702300	C	-3.05234800	-3.48636600	0.15463800
H	-2.21055200	-0.12026800	-2.18462200	B	-2.06114300	-1.48538300	-0.37039300
C	-2.87289900	-0.49388300	-0.18879400	O	-1.95845200	-2.32089700	-1.52551700
C	-4.20993200	-0.32176800	-0.53826200	O	-2.70263000	-2.21732900	0.67645600
C	-2.54043100	-0.72521000	1.15161900	H	-2.58402600	-4.26082400	-1.85979000
C	-5.20952900	-0.37878200	0.43260700	H	-1.17925900	-4.08769500	-0.77632100
H	-4.47175600	-0.13838000	-1.57731000	H	-2.89687000	-4.26058700	0.91202400
C	-3.53678800	-0.78564800	2.11745800	H	-4.11364000	-3.49916400	-0.13877000
H	-1.49351800	-0.84487700	1.43025500	H	1.61195700	-1.62435200	0.37911500
C	-4.87478500	-0.61228300	1.76116200	C	3.57768100	-1.04938400	-0.39177800
H	-6.24727900	-0.23731800	0.14778400	C	4.16222400	0.21687700	-0.34145600
H	-3.27092600	-0.96387600	3.15467600	C	4.40647300	-2.17245500	-0.30404300
H	-5.65024100	-0.65527800	2.51918500	C	5.54147900	0.36013900	-0.20461600
C	1.68071500	0.54296700	-0.05901200	H	3.53022400	1.09899100	-0.40880900
C	1.61567300	1.99659200	-0.13723400	C	5.78225900	-2.03378400	-0.16561700
C	0.40105600	2.58412200	-0.29724000	H	3.95794600	-3.16134300	-0.35027600
C	-0.80115500	1.76093900	-0.49530100	C	6.35526300	-0.76409000	-0.11560700
C	-0.65773100	0.46538400	-0.84684900	H	5.97889300	1.35307600	-0.16709600
N	0.62200300	-0.05197300	-0.88040400	H	6.41060700	-2.91681600	-0.10191500
H	1.31191600	-0.02368500	1.17433500	H	7.42981100	-0.65349000	-0.01027800
H	2.50713300	2.60254600	0.01047000	C	0.18327200	-0.75008600	3.43156500
H	-1.78632700	2.20146300	-0.40514300	C	-1.34273800	-0.84437700	3.33730100
C	0.28253000	4.01143700	-0.27932200	B	-0.52017000	-0.19014300	1.32404300
N	0.17931900	5.16621700	-0.25974000	O	0.59829300	-0.64246100	2.07930100
H	-0.13399800	-1.44314300	-3.27888900	O	-1.63912800	-0.05613200	2.19602600
H	2.55612800	-1.14470500	1.50601200	C	0.88657300	1.91187200	0.75627600
O	1.21376300	-0.94457100	1.97307900	C	0.97653400	3.21342100	0.47486900
H	1.10759700	-0.58126100	2.86028000	C	-0.20074700	3.91953000	-0.04516900
				C	-1.37893500	3.29145900	-0.16235100
				C	-1.54870700	1.83732500	0.15391900
<b>TS-AF</b>				N	-0.26398300	1.14025600	0.45994000
				H	1.69287900	1.32754200	1.18745800
C	2.09813700	-1.24109400	-0.51200800	H	1.88418600	3.76583100	0.68148700

H	-2.26406700	3.83285100	-0.48264400	C	-4.02054500	-0.24028700	-0.49058700
H	-2.19937100	1.74647900	1.02985500	C	-4.37043900	2.13670500	-0.38489600
C	-0.09064500	5.31811600	-0.36512100	C	-5.39489300	-0.44599000	-0.38692200
N	0.01261400	6.44242200	-0.61878100	H	-3.34481800	-1.08817400	-0.56380600
H	0.64296200	-1.62820000	3.89388800	C	-5.74138900	1.93391000	-0.27844000
H	0.48690800	0.14461500	3.99238700	H	-3.96483400	3.14501300	-0.39027300
H	-1.85738600	-0.43976800	4.21322000	C	-6.25807600	0.63944700	-0.27928600
H	-1.67240000	-1.87629700	3.16152800	H	-5.78915800	-1.45738100	-0.39023000
N	-3.01827600	-0.12152200	-0.76661200	H	-6.40927400	2.78598600	-0.19893300
C	-4.02642200	0.15744200	0.29054100	H	-7.32847200	0.47951300	-0.19849800
C	-3.76541000	-0.44158300	-2.01269400	C	0.42140000	1.26239400	3.54018300
H	-4.75210000	-0.65572400	0.29489100	C	1.92131600	1.23062800	3.22418300
H	-3.54501100	0.18910600	1.26478200	B	0.73580500	0.55060700	1.39711900
H	-4.53367200	1.10137600	0.05959400	O	-0.19292200	1.19776600	2.26426400
H	-4.46588900	0.37235000	-2.22749300	O	1.99832300	0.44023700	2.04860000
H	-4.31099200	-1.37390100	-1.86842700	C	-1.01220900	-1.28491300	1.18096300
H	-3.05593400	-0.57326200	-2.82673700	C	-1.42930500	-2.54320700	0.97732200
H	-2.83104200	1.80077900	-1.62777700	C	-0.49843700	-3.50096300	0.38057900

**TS-AG**

C	-2.02211600	1.31248400	-0.57216200	C	0.78586000	-3.16784300	0.17648100
C	-1.43322100	1.89202900	-1.82097400	C	1.31236300	-1.80851600	0.52610000
C	-1.15913700	0.44887800	-1.46063900	N	0.24883800	-0.82310700	0.78878200
H	-0.60486900	2.58507700	-1.73969200	H	-1.64670200	-0.52453600	1.62372700
H	-2.09940400	2.05096900	-2.66200500	H	-2.42481700	-2.85398500	1.26605500
H	-1.68757800	-0.30334100	-2.04058600	H	1.48236700	-3.86993700	-0.26836600
C	0.17012800	-0.00974400	-1.06257200	H	1.96204800	-1.85842600	1.41021800
C	1.14276900	-0.71248900	-1.62037700	C	-0.97295300	-4.81410200	0.03027700
H	1.02216000	-1.11087000	-2.62018100	N	-1.37419900	-5.86432400	-0.24482200
C	2.17412100	-1.21698100	-0.65829700	H	0.10843400	2.17263000	4.05966000
O	0.79139200	1.28463300	0.04817900	H	0.13028500	0.39218600	4.14578400
C	2.78505600	3.68208500	-1.66525900	H	2.51711000	0.77397600	4.02018600
C	3.33090000	3.77289000	-0.22301100	H	2.30290200	2.23850500	3.01795200
B	1.69183500	2.24013600	-0.33099000	N	3.09724200	-2.18958700	-1.22746000
O	1.90264200	2.56015100	-1.64686600	C	3.85790300	-1.58617300	-2.31481200
O	2.43215200	2.98026100	0.55161700	C	4.02525300	-2.67334000	-0.21149300
H	3.56969500	3.51648100	-2.40655700	H	4.53751200	-2.33157700	-2.73536800
H	2.21766600	4.57510500	-1.94626300	H	3.19005900	-1.24356600	-3.10632800
H	3.34254200	4.79479900	0.16211600	H	4.45588900	-0.72091300	-1.97408600
H	4.33747300	3.35109300	-0.13752400	H	4.56764700	-1.84928800	0.28605600
H	-1.55799800	1.63597300	0.35777600	H	4.75630000	-3.33561200	-0.68122700
C	-3.49463700	1.05204900	-0.48989400	H	3.50176800	-3.24866600	0.55621300

**TS-AH**

C	0.86016900	-1.03026700	-1.25365300	N	2.32975000	3.12402400	-0.36834200
C	1.68905600	-0.58898200	-0.30447500	C	2.00278600	3.51582100	0.98570000
C	-1.46362800	1.29901700	0.02052600	H	2.74416000	3.15577300	1.71696400
C	-1.53379600	-0.05064300	-1.54950200	H	1.95350500	4.60549000	1.04190900
C	-0.10062100	-0.18480000	-2.04310700	H	1.02653900	3.10530700	1.25994800
H	-1.69430200	-0.53436500	2.72388900	C	3.38992900	3.89145300	-0.99405000
H	0.86447700	-2.09984300	-1.44731300	H	3.13078500	4.95348200	-0.98091200
C	-2.02215600	0.10575000	1.90668800	H	4.36013800	3.76262000	-0.49050500
C	-2.78298600	1.84657900	-0.05508600	H	3.50006100	3.57691400	-2.03470800
H	0.29845300	0.82516100	-2.17154400	H	-0.65235600	1.84101300	-0.46579500
C	-3.74669700	1.35017200	0.79833500				
C	-3.38220800	0.41641400	1.78722200				
H	-3.03307200	2.57665500	-0.81742400	<b>TS-AI</b>			
H	-4.11866600	-0.00256700	2.46078700				
N	-1.07220200	0.56130800	1.10913200	C	0.56991800	-0.24229700	0.00536800
C	-5.11475300	1.78772000	0.67963800	C	-0.26578600	0.45468400	-1.08903800
N	-6.21442900	2.13271100	0.57822900	C	-1.53027500	1.13680700	-0.57516500
C	-2.34929400	-1.15604500	-1.05046500	H	-0.51874500	-0.24998000	-1.88621800
C	-3.72584500	-1.16131400	-1.34753500	H	0.34844200	1.23433700	-1.54433300
C	-1.85412800	-2.16315200	-0.19973100	H	-1.82463200	2.02238000	-1.14254400
C	-4.57253200	-2.13106100	-0.82892600	C	-2.68515700	0.37166800	-0.21157600
H	-4.12820000	-0.38294600	-1.99173000	C	-3.94804900	0.97702500	-0.05058700
C	-2.70352300	-3.13728700	0.31089500	H	-4.03001600	2.02519400	-0.30536900
H	-0.80961600	-2.15477200	0.08878100	C	-5.01501200	0.26211700	0.44920700
C	-4.06277700	-3.12493200	0.00453100	H	-4.86617800	-0.78357200	0.70544800
H	-5.63003900	-2.11002100	-1.07203300	C	-7.30185300	-0.09135900	1.20334200
H	-2.30221500	-3.90347100	0.96689600	H	-7.65514600	0.32081600	2.15312000
H	-4.72221400	-3.88376300	0.41349000	H	-8.14177300	-0.14054100	0.50412700
H	-2.09960000	0.59469700	-2.22581400	H	-6.92521800	-1.09967700	1.37495100
H	-0.17069100	-0.60416300	-3.05750600	C	-6.54442500	2.12960700	0.36336300
O	2.39957800	-1.53523300	0.42478000	H	-5.92235600	2.79348100	0.97173900
C	5.85560700	-2.15140700	0.90205000	H	-7.59329200	2.31893600	0.58863600
C	5.88050700	-0.93145300	-0.04329400	H	-6.36309400	2.34411600	-0.69425800
H	6.48220300	-2.01498000	1.78681300	N	-6.23838800	0.73696300	0.65694900
H	6.16609200	-3.06925700	0.39037700	O	-2.59466700	-0.89877300	0.18281100
H	6.20916800	-0.02205400	0.47256400	C	-1.00469100	-3.43499800	-1.79399400
H	6.51428900	-1.08626900	-0.91989700	C	-1.11088000	-4.07234400	-0.39142100
B	3.75711800	-1.50960900	0.41972800	B	-1.91921100	-1.98828700	-0.35350500
O	4.52548600	-0.77057900	-0.45056000	O	-1.75177800	-2.20940100	-1.68360700
O	4.49229700	-2.27251000	1.29225800	O	-1.52689600	-2.99862700	0.46421600
C	1.86545900	0.79430300	0.15980500	H	-1.45239300	-4.05035600	-2.57672200
H	1.60186500	0.97680500	1.19671400	H	0.02982700	-3.19340200	-2.05468300
C	2.28556800	1.77352500	-0.65813500	H	-0.15369300	-4.46106400	-0.04259400
H	2.59809200	1.52641300	-1.67212500	H	-1.86883100	-4.86101400	-0.34658600

H	-0.10117400	-0.69387200	0.75341400	H	2.30699000	0.64560000	-2.28636600
C	1.41179100	-1.36028700	-0.57019500	H	0.33503300	1.69807800	-2.76694200
C	1.71379700	-2.48582800	0.20588100	C	-0.90022100	0.93253200	-1.44807100
C	1.96634800	-1.27423900	-1.85398600	C	-2.05358600	1.55183900	-1.03728800
C	2.52800500	-3.50075100	-0.28930000	H	-1.96542900	2.25623100	-0.21603000
H	1.30174000	-2.56006100	1.20991900	C	-3.28862800	1.06024600	-1.43339000
C	2.78039100	-2.28741800	-2.35146500	H	-3.34874600	0.40181800	-2.29647700
H	1.76524400	-0.40060100	-2.46721800	C	-5.70982300	0.88640600	-1.33305100
C	3.05957300	-3.40971200	-1.57425600	H	-6.34147600	1.75716900	-1.53428800
H	2.75335100	-4.36225200	0.33291900	H	-5.55615500	0.34078300	-2.26493700
H	3.20119100	-2.19861800	-3.34861400	H	-6.22149500	0.23837400	-0.61530800
H	3.69571400	-4.19954900	-1.96081000	C	-4.41149800	1.99565200	0.48896900
C	1.12939200	4.39876700	-1.49728400	H	-3.62256600	1.56277500	1.11495800
C	2.64509800	4.57820000	-1.70659200	H	-5.38061200	1.85288000	0.96781300
B	2.24686400	2.64477500	-0.61286500	H	-4.23722900	3.06817300	0.35584700
O	1.01989800	3.29904000	-0.60702600	N	-4.42487700	1.30430500	-0.79879600
O	3.20092400	3.31817800	-1.36427000	O	-0.87897400	-0.70114100	-0.19980400
C	3.80098300	0.88858300	0.06998700	C	-3.55495900	-2.60888800	-1.52131400
C	4.23514200	0.23265100	1.15217800	C	-3.34529400	-3.27471800	-0.14905100
C	3.30372400	-0.02103000	2.25620800	B	-1.86799400	-1.58856300	-0.40938300
C	1.96758300	0.13962600	2.02047500	O	-2.43168000	-1.75093400	-1.67183100
C	1.44582900	0.75028600	0.82444800	O	-2.46598100	-2.39419100	0.53557900
N	2.48915500	1.42152700	0.03103300	H	-4.47432200	-2.00596800	-1.53764900
H	4.42250000	1.06308900	-0.80291700	H	-3.59386200	-3.32451600	-2.34589300
H	5.23828800	-0.17413700	1.19216200	H	-2.87205100	-4.25816100	-0.24597800
H	1.25107600	-0.25250700	2.74540800	H	-4.27440800	-3.38729200	0.41540100
H	0.33989000	1.76692600	1.39742300	H	1.17230500	-1.30303000	-0.24156900
C	3.76904700	-0.56188300	3.49224800	C	3.23564000	-1.22752100	-0.55140700
N	4.14406300	-1.01523900	4.49387900	C	3.48231600	-2.15084800	0.47423300
H	0.62068800	4.15654600	-2.44038900	C	4.24321100	-0.99847700	-1.48976200
H	0.65304000	5.28101300	-1.06111100	C	4.69664300	-2.81812000	0.56231500
H	3.05283100	5.34946800	-1.04202800	H	2.69476500	-2.33597400	1.20271000
H	2.90421800	4.83398400	-2.73789900	C	5.46317900	-1.67034100	-1.40543400
O	-0.59660000	2.23950300	1.69976000	H	4.09322100	-0.29736300	-2.30489900
H	-1.25009600	1.63554400	0.50629600	C	5.69534200	-2.57966000	-0.38106700
H	-0.84348800	1.78357100	2.51540400	H	4.86378400	-3.53066700	1.36409100
				H	6.23211600	-1.47850200	-2.14740600
				H	6.64494900	-3.10132300	-0.31737200
<b>TS-AJ</b>				C	-0.50708800	-1.29315200	3.23741800
				C	-1.87543300	-0.62190900	3.04723100
C	1.88345000	-0.53328900	-0.53308800	B	-0.50735400	-0.23477400	1.21901700
C	1.49134200	0.02072200	-1.91064900	O	0.02956100	-1.36637500	1.93656900
C	0.26480400	0.89336500	-2.03065100	O	-1.70133100	0.21697200	1.91791000
H	1.39531900	-0.81072900	-2.62020200	C	0.19282500	2.18754400	1.32662300



C	0.97211400	3.26787700	1.06804800
C	2.23621500	3.00768400	0.40446000
C	2.66654500	1.75142500	0.17486400
C	1.87277400	0.54300400	0.60374400
N	0.50788600	0.90443100	1.02322700
H	-0.78305000	2.29640200	1.79260000
H	0.67067300	4.27101300	1.32970500
H	3.61733600	1.57241100	-0.31953700
H	2.37503300	0.04954400	1.45417200
C	3.04024000	4.12008700	-0.03877500
N	3.66956500	5.02418900	-0.39556000
H	-0.58408600	-2.29528400	3.67187600
H	0.13404300	-0.67797000	3.88793300
H	-2.17652100	-0.02921800	3.91884900
H	-2.64826900	-1.37246200	2.83781400

**TS-AK**

C	1.44763700	-1.23195900	0.00348700
C	1.04992600	-1.74614000	-1.38216100
C	-0.40310000	-2.11556000	-1.36327100
H	1.67645800	-2.59721300	-1.66785800
H	1.22271000	-0.95345000	-2.12741000
H	-0.77098100	-2.94809000	-1.95116200
C	-1.27283700	-1.40031100	-0.63163700
C	-2.74748000	-1.49624100	-0.70607200
H	-3.20436900	-1.32444900	-1.67462600
C	-3.28930600	-1.01923600	0.42721400
H	-2.89073200	-1.23785200	1.40794000
C	-4.97833900	0.33482500	-0.75874700
H	-5.83548700	0.98222300	-0.57284600
H	-4.13260800	0.90498400	-1.14691800
H	-5.25466500	-0.47278900	-1.43588600
C	-5.62551000	-0.94680100	1.26648500
H	-5.95718500	-1.78937600	0.65947500
H	-6.44901300	-0.25405600	1.44273800
H	-5.22925400	-1.30856100	2.21484300
N	-4.54028700	-0.24714900	0.53415000
H	1.21068500	-2.03237000	0.71661900
C	2.91248400	-0.88552600	0.17383600
C	3.43838400	-0.76420700	1.46484600
C	3.76239800	-0.65887300	-0.91020700
C	4.76990900	-0.42253800	1.66812000

H	2.78900900	-0.94449700	2.31863500
C	5.09880900	-0.31729600	-0.71102800
H	3.38413300	-0.75074300	-1.92353300
C	5.60703600	-0.19698000	0.57745800
H	5.15690600	-0.33418900	2.67851900
H	5.74232200	-0.14400400	-1.56802300
H	6.64757700	0.06908900	0.73317900
C	-1.76884500	0.68745900	0.61135600
C	-1.24749900	1.95336300	0.68106700
C	0.01125200	2.26123200	0.00842400
C	0.89548900	1.27487400	-0.26783500
C	0.56531500	-0.03248600	0.38969800
N	-0.86384700	-0.29286700	0.15619200
H	-4.13356000	0.54380600	1.07186300
H	-1.85193400	2.78232500	1.03548300
H	1.77833600	1.41387000	-0.88265400
H	0.66008200	0.11512900	1.48245200
C	0.22247300	3.59902100	-0.48227200
N	0.36876300	4.68580100	-0.85654300

**TS-AL**

C	-1.60736100	-0.78697400	-0.85435100
C	-1.14471000	-2.23865800	-0.62543000
C	0.13806800	-2.52741100	-1.41013800
H	-1.94752900	-2.91655300	-0.92815900
H	-0.96957000	-2.39778000	0.44510900
H	0.48576700	-3.55066500	-1.24653100
C	1.19998300	-1.55776100	-0.98900500
C	2.56137200	-1.67132700	-0.97039400
H	3.11187700	-2.50746200	-1.37785500
C	3.17040100	-0.42258700	-0.44516000
H	3.99243800	0.00435900	-1.03685300
C	4.81008500	0.43311000	1.27808700
H	5.70723200	0.18652100	0.70125200
H	4.45481800	1.42508200	0.98569700
H	5.05642000	0.44468300	2.34146400
C	4.06419500	-1.88212700	1.51879300
H	3.22564100	-2.54290600	1.29635500
H	4.22985700	-1.83362500	2.59698200
H	4.96606000	-2.27177100	1.03393000
N	3.74179400	-0.54018000	1.02628000
H	-1.84690800	-0.69433600	-1.92354900

C	-2.87080800	-0.49204700	-0.07150200	H	-6.06092000	0.78257900	-0.51481300
C	-4.11294700	-0.50840000	-0.70452800	H	-5.14546200	1.50538200	-1.85204600
C	-2.82037400	-0.26671000	1.30732600	N	-4.37645800	-0.29783700	-1.09226000
C	-5.28489500	-0.30359100	0.02060800	O	-1.76646800	-0.65017800	0.63420700
H	-4.16233900	-0.67900300	-1.77718400	C	-1.38395200	-4.15260900	0.48032100
C	-3.98767200	-0.06361900	2.03392000	C	-0.01474000	-3.71830900	1.03117700
H	-1.85459100	-0.22885700	1.80462100	B	-1.32759200	-1.89180200	0.74487500
C	-5.22471200	-0.08171400	1.39219700	O	-2.00408800	-2.93278400	0.09566200
H	-6.24301400	-0.31268800	-0.48938600	O	-0.19902700	-2.35677800	1.40262200
H	-3.93243400	0.11623400	3.10288500	H	-1.99175500	-4.64291700	1.24992500
H	-6.13577200	0.08342200	1.95825400	H	-1.30229800	-4.82080600	-0.38078600
C	1.95092600	0.43827300	-0.09929100	H	0.76847200	-3.77850800	0.26409300
C	1.79130500	1.84799600	-0.31424400	H	0.30087100	-4.30139000	1.89978600
C	0.54654100	2.39619200	-0.40581300	H	0.73509700	-1.31568200	-0.80252000
C	-0.63492600	1.52818800	-0.43490200	C	2.83813100	-1.14078800	-0.51276300
C	-0.48533400	0.19461800	-0.56284600	C	2.94519500	-1.90435400	0.65706800
N	0.79565800	-0.34432300	-0.53367100	C	3.98936500	-0.93075600	-1.27426800
H	2.62835200	-0.01067300	1.22187700	C	4.16142900	-2.45909600	1.03859600
H	2.66774500	2.49138400	-0.31625200	H	2.06319800	-2.04243100	1.27714400
H	-1.62731000	1.96150700	-0.42187800	C	5.20941300	-1.48697900	-0.89244900
C	0.38849200	3.81357000	-0.49282500	H	3.95175100	-0.31862700	-2.16966900
N	0.25730400	4.96423700	-0.56528700	C	5.30007700	-2.25607700	0.26192100
H	-0.05580800	-2.41912900	-2.48505500	H	4.22079500	-3.04703200	1.94939700

**TS-AM**

C	1.49302100	-0.52229400	-0.85667300	H	6.09201600	-1.30752900	-1.49842000
C	1.43280100	0.08165200	-2.25934800	H	6.25082300	-2.68608900	0.56011800
C	0.02996800	0.29380200	-2.75898100	C	-1.19110800	2.08738900	2.77261000
H	1.93065100	-0.58485300	-2.96974000	C	-2.53674700	2.36659900	2.08526400
H	1.98006600	1.03493600	-2.28404600	B	-1.35720000	0.70254700	0.97801400
H	-0.14215200	0.16081300	-3.82848300	O	-0.84613700	0.80061300	2.32145900
C	-1.05503800	0.59266000	-2.09368600	O	-2.47465500	1.63742900	0.87348000
C	-2.39753800	0.77823200	-1.96196900	C	-0.20535800	2.52145200	-0.39814300
H	-2.80406500	1.78056700	-1.88739100	C	0.87140400	3.32485000	-0.43985600
C	-3.14473300	-0.33123600	-1.54765900	C	2.14144000	2.79319800	0.04650900
H	-2.67825600	-1.31198600	-1.57037300	C	2.24210400	1.50516900	0.41065200
C	-4.97163000	-1.48114700	-0.48613500	C	1.10739500	0.52944500	0.22468200
H	-5.92924200	-1.70921000	-0.96243300	N	-0.20256700	1.16505000	-0.07720000
H	-4.28332000	-2.32095400	-0.58246400	H	-1.19428200	2.90688800	-0.62367500
H	-5.13240900	-1.29117300	0.57931700	H	0.78661100	4.36255400	-0.73166400
C	-5.05989200	0.97762500	-0.89863800	H	3.15975600	1.11893200	0.84106000
H	-4.48271700	1.57485100	-0.18484500	H	0.98521900	-0.01789800	1.16782300
				C	3.26353000	3.68260300	0.20033800
				N	4.15667600	4.41180600	0.30376400
				H	-1.25698700	2.10231900	3.86534500
				H	-0.43916900	2.82928600	2.45833600

H	-2.69276400	3.43401500	1.88489400
H	-3.37335000	2.00448000	2.70068700

**TS-AN**

C	-1.71324200	-1.26496900	-0.02440200
C	-1.31135900	-1.80658800	1.34995900
C	0.12562400	-2.23571300	1.29681800
H	-1.96543000	-2.63662700	1.63506500
H	-1.44438100	-1.01754500	2.10667400
H	0.46082800	-3.11433500	1.83504600
C	1.01865700	-1.53092600	0.58510800
C	2.48042500	-1.68353400	0.60240600
H	2.96856700	-1.58920500	1.57112500
C	3.04885900	-1.08666400	-0.47783500
H	2.73410300	-1.25556200	-1.50079400
C	5.43555600	-1.60019800	-0.12007900
H	6.41521600	-1.13017100	-0.01717700
H	5.16209800	-2.12704600	0.79204100
H	5.43753700	-2.30004100	-0.95694600
C	4.75339300	0.26163300	-1.58622800
H	4.88269200	-0.40695600	-2.43940900
H	5.67246500	0.81569800	-1.39489900
H	3.91132900	0.93478300	-1.75196000
N	4.42007500	-0.54980000	-0.38700200
H	-1.50479500	-2.06374100	-0.74757500
C	-3.17008700	-0.87952900	-0.17669600
C	-3.70936700	-0.74857100	-1.46108600
C	-3.99866200	-0.62642800	0.91813300
C	-5.03414200	-0.37241400	-1.64788600
H	-3.07725300	-0.95040200	-2.32299500
C	-5.32812100	-0.25059000	0.73530300
H	-3.60916500	-0.72560300	1.92661600
C	-5.85015700	-0.12135900	-0.54693700
H	-5.43236000	-0.27756700	-2.65327600
H	-5.95541800	-0.05772300	1.60006500
H	-6.88534500	0.17150400	-0.68947500
C	1.53384200	0.57507100	-0.56686400
C	1.06375900	1.86295100	-0.67401800
C	-0.20762800	2.20539100	-0.03799400
C	-1.11320800	1.23672000	0.23054900
C	-0.80311400	-0.08614100	-0.40963600
N	0.61689600	-0.36938200	-0.14175300

H	4.35944700	0.14067900	0.41299700
H	1.70232900	2.66804400	-1.02604900
H	-2.00446500	1.40075300	0.82640800
H	-0.87837900	0.05193200	-1.50509100
C	-0.39954800	3.54998100	0.44092100
N	-0.52773000	4.64021100	0.81118200
O	3.76448100	1.49887900	1.12951300
H	2.90398800	1.47456000	0.64678700
H	3.53698200	1.56761700	2.06252700

**TS-AO**

C	0.66998100	-1.14765600	0.83764300
C	0.24270100	-2.51913000	0.22416400
C	-1.27198900	-2.69687500	0.01852700
H	0.62742300	-3.32121900	0.85914200
H	0.74747200	-2.61376600	-0.74489900
H	-1.56578600	-3.66542200	-0.37959200
C	-1.85687200	-1.57294200	-0.62306700
C	-2.96539100	-1.36557500	-1.52674000
H	-3.51678000	-2.16643300	-1.99918500
C	-3.16554200	-0.02306900	-1.68246000
H	-3.90522700	0.46837700	-2.29793900
H	0.89280800	-1.30706000	1.89835000
C	1.93111500	-0.63007700	0.17082400
C	3.17365700	-0.83344200	0.77041300
C	1.87800800	0.03705800	-1.05775100
C	4.34219600	-0.38321200	0.15928700
H	3.22570200	-1.34575000	1.72807700
C	3.04192100	0.48936100	-1.66842100
H	0.91398300	0.20664600	-1.53334800
C	4.27942000	0.27945100	-1.06157800
H	5.30071800	-0.54537400	0.64225200
H	2.98371800	1.01066600	-2.61872000
H	5.18743000	0.63612500	-1.53677100
C	-2.20032800	0.65853500	-0.86962600
C	-1.95679600	1.95807500	-0.55851300
C	-0.91860900	2.27126200	0.38588700
C	-0.20655700	1.26640300	0.99840100
C	-0.49521000	-0.12202800	0.80504400
N	-1.41228200	-0.35043500	-0.28276400
H	-2.54619900	2.75101400	-1.00422200
H	0.58842700	1.51961200	1.69447500

H	-1.16964800	-0.64005700	1.82011200	O	-3.46630000	-2.10391800	1.00478400
C	-0.64197500	3.64484800	0.69233800	H	-2.57766800	-2.32854900	0.44350100
N	-0.42585200	4.75746300	0.93083800	H	-4.19143800	-2.02256300	0.37341800
O	-1.72985000	-1.71542000	2.35015500	O	-2.74699300	-0.03757400	2.01133100
H	-1.71129600	-2.39091200	1.35373200	H	-3.15682500	-0.98111300	1.57103000
H	-2.62539000	-1.58819500	2.69454500	H	-2.63723300	-0.13327800	2.96600500

### TS-AP

C	0.40070000	-0.83772100	1.31804500
C	-0.31338900	-2.20565500	1.19436700
C	-1.05286400	-2.41211100	-0.13154100
H	-1.00284000	-2.30167900	2.04606000
H	0.43707800	-2.99152400	1.33438600
H	-0.99252600	-3.39887700	-0.58393200
C	-1.12156700	-1.32948700	-1.02511700
C	-1.50558600	-1.21738900	-2.41599800
H	-1.74952200	-2.06381600	-3.04336300
C	-1.49742800	0.10097900	-2.78177800
H	-1.73797100	0.51686900	-3.74969500
H	0.52853200	-0.60124800	2.38188900
C	1.78299800	-0.80941800	0.68248600
C	2.74594300	0.06156200	1.20231300
C	2.11888400	-1.58414800	-0.43022800
C	4.00812400	0.16214700	0.63010400
H	2.50147800	0.66674800	2.07284400
C	3.38380300	-1.48415300	-1.00669200
H	1.39058300	-2.27275900	-0.84710700
C	4.33118800	-0.61134900	-0.48269800
H	4.74018100	0.84261900	1.05339800
H	3.62680900	-2.09270800	-1.87227100
H	5.31459800	-0.53372900	-0.93497500
C	-1.10525900	0.87022500	-1.64209700
C	-0.91545200	2.19138300	-1.38450100
C	-0.47310500	2.59954200	-0.08181900
C	-0.19311200	1.64643400	0.88576900
C	-0.47168500	0.27403700	0.71219200
N	-0.88868200	-0.06860500	-0.61070700
H	-1.07833100	2.93081000	-2.15990100
H	0.21126400	1.96563000	1.84320000
H	-1.71839400	0.19290900	1.51286200
C	-0.28938500	3.98787100	0.20544100
N	-0.13964200	5.11456200	0.43559800

### TS-AQ

C	1.91480900	-0.80451600	1.00438000
C	1.47910200	-2.23750000	0.62905300
C	0.24412900	-2.67174600	1.42612700
H	2.31662400	-2.91698000	0.81215200
H	1.26773100	-2.27832700	-0.44653900
H	-0.08819300	-3.67019200	1.12994600
C	-0.86018800	-1.68259700	1.20639000
C	-2.21278500	-1.85186300	1.11636000
H	-2.72161900	-2.76324400	1.39720400
C	-2.90018700	-0.52930000	0.87247500
H	-3.58876200	-0.23903500	1.69780400
C	-4.52867600	0.72773500	-0.43913400
H	-5.11980400	0.92531100	0.47078400
H	-3.81707800	1.54956400	-0.56466200
H	-5.20578700	0.72122600	-1.29819700
C	-4.76142800	-1.64253400	-0.26612400
H	-4.22600800	-2.59287900	-0.30037400
H	-5.45624900	-1.60024600	-1.10933100
H	-5.34731200	-1.59942700	0.66773300
N	-3.80886800	-0.54095400	-0.35912500
H	2.18200800	-0.83649700	2.07154100
C	3.16625100	-0.42492000	0.23710700
C	4.41699200	-0.72365200	0.78128700
C	3.11381000	0.12687900	-1.04523500
C	5.58630200	-0.48143100	0.06684800
H	4.47265300	-1.15010900	1.78018100
C	4.28020100	0.37155300	-1.76366500
H	2.14823200	0.39984700	-1.46156700
C	5.52101900	0.06627100	-1.21107100
H	6.54862400	-0.71411200	0.51182500
H	4.21910200	0.80958700	-2.75509900
H	6.43096700	0.26318200	-1.76858200
C	-1.70537200	0.40257600	0.72367300
C	-1.56582500	1.77963500	0.92691900

C	-0.31460300	2.37574900	0.94330200
C	0.86542100	1.51858500	0.81252700
C	0.76423200	0.17389900	0.87165900
N	-0.51013600	-0.39198700	1.01014900
H	-1.51217800	0.29895200	-0.96447600
H	-2.45312300	2.40666200	0.98191300
H	1.84621100	1.97079700	0.71795500
C	-0.18225800	3.78560800	1.00863700
N	-0.07299600	4.94344400	1.05247000
H	0.49717100	-2.71589000	2.49299200
H	-2.67272000	-0.43214800	-1.74970600
C	-1.60900900	0.95890000	-2.98793100
H	-0.57845400	1.31545700	-3.04478400
H	-1.92484200	0.58977100	-3.96586000
H	-2.25298000	1.78330200	-2.67780600
C	-0.81134500	-1.26721500	-2.22170000
H	0.23102600	-0.95079600	-2.12822300
H	-1.04451200	-2.01696700	-1.46094100
H	-0.98424000	-1.67455700	-3.22069100
N	-1.68943300	-0.11092400	-1.98442100

**TS-AR**

C	-0.39796600	-1.26858300	0.94546400
C	-1.04193600	-0.45169200	0.02327000
C	1.41090900	0.88885500	0.27688600
C	1.78873100	-0.09334900	1.39458700
C	0.48481700	-0.70410700	2.01032300
H	-0.29970600	0.65835400	-2.56419200
H	-0.24776900	-2.30129400	0.64387600
C	0.45227300	1.03663600	-1.87308100
C	2.55783600	1.73624500	-0.22369600
H	-0.01931100	0.09875300	2.55556700
C	2.35712200	2.42363300	-1.36547400
C	1.15148300	2.17674000	-2.15096300
H	3.45863100	1.84241700	0.37257600
H	0.96902000	2.73932300	-3.05740300
N	0.74894400	0.21780900	-0.83289100
C	3.34661600	3.34439600	-1.85885900
N	4.12563800	4.10038500	-2.26103200
C	2.80866800	-1.14215900	1.00673700
C	3.96727700	-1.26941600	1.77864000
C	2.63161700	-2.01175700	-0.07761100

C	4.92802500	-2.23272000	1.48642100
H	4.11943800	-0.59992800	2.62218500
C	3.59275600	-2.97565800	-0.36968200
H	1.75310100	-1.90536100	-0.70472000
C	4.74133100	-3.09232500	0.40897200
H	5.82136800	-2.30763200	2.09860700
H	3.44316900	-3.63818600	-1.21672700
H	5.48708500	-3.84556000	0.17499100
H	2.23889900	0.51241700	2.19201600
H	0.76564500	-1.47705000	2.73057400
O	-1.51715700	-1.05581900	-1.13038300
C	-4.67384400	-2.37580100	-2.05632400
C	-4.93220100	-1.93063800	-0.60128800
H	-5.41761900	-1.98919800	-2.75662100
H	-4.63632000	-3.46642600	-2.14937400
H	-5.57371700	-1.04366800	-0.55401400
H	-5.37469700	-2.71834800	0.01271200
B	-2.81191000	-1.47234800	-1.18661300
O	-3.64127100	-1.59548100	-0.09712900
O	-3.39323300	-1.83724200	-2.37200600
C	-1.66947900	0.83710800	0.34052000
H	-1.63993100	1.60208200	-0.43017100
C	-2.31478700	1.02683400	1.51169000
H	-2.40897300	0.19172200	2.20432200
N	-2.86624500	2.19357200	1.95788700
C	-2.83123600	3.34853900	1.08811800
H	-3.48617400	3.23123300	0.21170200
H	-3.14833400	4.22968400	1.64924300
H	-1.80824300	3.50703200	0.73426200
C	-3.95335900	2.13138900	2.91460600
H	-3.96237600	3.04020400	3.52214700
H	-4.93363500	2.02705600	2.42842800
H	-3.80519900	1.27532200	3.57643400
H	0.69219800	1.61172600	0.72951400

**INT-AF**

C	-0.17965800	-0.22333200	0.28638500
C	0.27480200	-0.44078400	-1.17909200
C	1.67500000	-0.97789200	-1.31292000
H	0.21209500	0.49839300	-1.73883100
H	-0.39994800	-1.13890400	-1.68807800
H	1.82336600	-1.86438800	-1.92117800

C	2.78418400	-0.45702400	-0.76641700
C	4.11315600	-1.03767900	-0.91840700
H	4.17065000	-1.93411800	-1.52562800
C	5.20607300	-0.50506800	-0.34068700
H	5.09377100	0.37322000	0.28933000
C	7.39446600	-0.72336600	0.64584800
H	8.43487500	-0.76373200	0.31181400
H	7.20860500	0.26564100	1.07078900
H	7.25468000	-1.47202100	1.44089300
C	6.72827800	-2.16377600	-1.21258000
H	6.27637700	-3.03502100	-0.71084000
H	7.80176800	-2.33559000	-1.31677000
H	6.29343800	-2.08018500	-2.21229000
N	6.51127600	-0.93490200	-0.48481800
O	2.75551200	0.63866800	0.07718000
C	1.21663300	3.56171100	-1.28676300
C	1.23147100	3.83238200	0.23585300
B	2.15414300	1.82570400	-0.19502100
O	1.69243800	2.22539200	-1.42590400
O	1.99348500	2.76444800	0.79124500
H	1.88253500	4.23351800	-1.83844800
H	0.20939700	3.63457900	-1.70590600
H	0.22236300	3.80725000	0.65904700
H	1.70325100	4.78581600	0.48756900
H	0.70321500	-0.24372100	0.93582100
C	-0.90338700	1.07014800	0.55721600
C	-0.94066200	1.57442000	1.86869200
C	-1.65016900	1.74366400	-0.41819000
C	-1.71005300	2.68550300	2.19290500
H	-0.37195200	1.05940100	2.63690100
C	-2.41461900	2.86781800	-0.09849500
H	-1.65462500	1.37519500	-1.44101300
C	-2.45560500	3.34005500	1.20923500
H	-1.72380800	3.04913100	3.21591100
H	-2.98609200	3.36683400	-0.87601400
H	-3.05334400	4.21022900	1.46100700
C	-1.00837100	-2.80333100	2.73383000
C	-0.99024300	-3.66529900	1.46315400
B	-1.03467100	-1.48265900	0.85567600
O	-1.28334500	-1.49291000	2.27074100
O	-0.57136300	-2.77308600	0.44701300
C	-2.88589700	-1.96915000	-0.98631600
C	-4.08712100	-1.77104700	-1.64854000
C	-5.01424300	-0.89179600	-1.08305700

C	-4.71959800	-0.25419500	0.12274700
C	-3.49415600	-0.51046500	0.71896800
N	-2.60555600	-1.33983400	0.16000100
H	-2.11293700	-2.64628800	-1.33536200
H	-4.30074800	-2.28672000	-2.57630900
H	-5.42284700	0.42894500	0.58208100
H	-3.18656000	-0.05896900	1.65659000
C	-6.27353000	-0.65002900	-1.74070400
N	-7.28362500	-0.45647000	-2.26894600
H	-0.03056000	-2.82300300	3.23294500
H	-1.77001200	-3.12679200	3.45163700
H	-2.00029900	-4.05055400	1.24591000
H	-0.30301500	-4.51384300	1.52328500

### INT-AG

C	-0.06751000	-1.67114700	-0.54338300
C	-1.18058600	-1.63325500	-1.61319500
C	-2.49550200	-1.24101600	-1.00360300
H	-1.25288700	-2.61196100	-2.09860700
H	-0.92157600	-0.90657800	-2.38888100
H	-3.16755600	-2.01431600	-0.64611700
C	-2.85628400	0.03612500	-0.82016300
C	-4.09918800	0.47986600	-0.20782800
H	-4.73968500	-0.30362500	0.18153700
C	-4.44537500	1.77968600	-0.12792200
H	-3.80007200	2.52976400	-0.57914100
C	-6.09735300	3.53641900	-0.02377800
H	-6.69070900	4.03621600	0.74658900
H	-5.27946100	4.20081300	-0.31165400
H	-6.73626500	3.37370700	-0.90483900
C	-6.51976700	1.37096900	1.03884700
H	-7.01129100	0.77978900	0.24975200
H	-7.28289100	1.92318600	1.59116000
H	-6.02505600	0.68127600	1.72801900
N	-5.55116200	2.30214200	0.50670200
O	-2.02552200	1.05033300	-1.28710500
C	0.53468300	2.99082000	0.22032600
C	0.30940500	1.87745700	1.26220600
B	-1.09306800	1.60254100	-0.46840600
O	-0.24069600	2.58524700	-0.90634600
O	-0.90375900	1.25123000	0.85043100
H	1.58482500	3.09559200	-0.06586700

H	0.16541500	3.95964400	0.57525300	O	-2.26532500	-0.24849700	1.66422700
H	0.19983900	2.25797600	2.28015500	C	-4.89916800	-0.09598900	-0.06692000
H	1.11546700	1.13204300	1.24187100	C	-4.67774300	1.37354400	0.37870000
H	-0.14601600	-0.75601600	0.04952200	B	-3.14512400	0.79043200	-1.15750000
C	-0.25277100	-2.82641100	0.41826700	O	-3.90789900	-0.34211100	-1.05932600
C	-0.50366000	-2.55359700	1.76505000	O	-3.58316800	1.84411700	-0.40190500
C	-0.19694700	-4.16091600	0.00073900	C	-1.07621100	1.92497900	-1.81743700
C	-0.68674400	-3.58619800	2.68080400	C	0.24687500	1.75697100	-1.80378700
H	-0.56929500	-1.51629300	2.08483800	C	0.82633700	0.35516400	-1.73840700
C	-0.37070300	-5.19391600	0.91758300	C	-0.11668400	-0.57625000	-2.48302300
H	-0.01069400	-4.39750300	-1.04304000	C	-1.42738700	-0.33368900	-2.47961400
C	-0.61564300	-4.91068500	2.25935400	N	-1.96755900	0.85483700	-1.96962700
H	-0.88584400	-3.35523600	3.72264900	H	-1.54089200	2.90088700	-1.73113000
H	-0.31831200	-6.22428300	0.58026600	H	0.90415800	2.61572600	-1.76547600
H	-0.75465800	-5.71871900	2.97049500	H	0.28318800	-1.47167700	-2.94185000
C	5.55274500	2.61606900	1.56974600	H	-2.15162300	-1.03137300	-2.88548000
C	5.16520600	3.50219300	0.36762000	C	0.94122300	-0.12506400	-0.21524000
B	4.10351900	1.52528500	0.24453800	C	2.14949600	0.29952000	-2.38703900
O	5.00275200	1.33470400	1.26188100	N	3.17669800	0.26223800	-2.91661000
O	4.08134200	2.80692800	-0.25254100	H	-0.82676600	-0.66644700	4.52669600
C	2.40242100	0.70490500	-1.33979800	H	-2.68454900	0.50117800	3.54035700
C	1.56166400	-0.21924100	-1.80814200	H	-3.31147500	-1.13286100	3.21471600
C	1.37535500	-1.57856100	-1.15848100	H	-1.16417100	-2.14661000	3.59801300
C	2.42520400	-1.76315000	-0.07961700	H	-5.55120700	2.00445600	0.19077100
C	3.23716500	-0.78596700	0.32525600	H	-4.41019000	1.43932000	1.43691000
N	3.24915400	0.49528400	-0.24543200	H	-5.89026300	-0.25691500	-0.50078800
H	2.48074900	1.68500200	-1.79715600	H	-4.75077100	-0.79617600	0.75934700
H	0.96368400	0.02524700	-2.67766100	O	-0.41338200	-0.00670600	0.22374900
H	2.47946100	-2.73155000	0.40340100	C	1.36657700	-1.59451100	-0.16756300
H	3.95377500	-0.92774500	1.12604900	C	0.41515900	-2.61860000	-0.15584900
C	1.53869500	-2.62905100	-2.19120200	C	2.72194400	-1.92999300	-0.18445700
N	1.64940700	-3.44504400	-3.00365500	C	0.81393300	-3.95186600	-0.14583200
H	5.11070300	2.97708900	2.50420800	H	-0.64147300	-2.36969500	-0.17428700
H	6.63298000	2.52806000	1.70092100	C	3.11877100	-3.26403100	-0.18412700
H	5.98391200	3.59572300	-0.35279600	H	3.46541500	-1.13934300	-0.19541700
H	4.83739500	4.50097500	0.66243900	C	2.16688500	-4.27909600	-0.15939100
				H	0.06374900	-4.73632600	-0.13254800
				H	4.17602500	-3.50823000	-0.19895800
				H	2.47732200	-5.31902900	-0.15271600
				C	1.81887500	0.72869700	0.66647900
				H	1.72971000	0.46751400	1.71665900
				C	2.68046400	1.68290800	0.28214400
				H	2.80009200	1.95158000	-0.76351800
				N	3.54395800	2.37814300	1.10809500
<b>INT-AH</b>							
C	-1.13046700	-1.05285400	3.55145700				
C	-2.46520600	-0.45873100	3.05862900				
B	-0.89872500	-0.29514100	1.44368600				
O	-0.18432500	-0.66144400	2.56100600				

C	3.41191700	2.17774700	2.53315600
H	3.53426700	1.11748200	2.77035100
H	4.19485000	2.73906200	3.04695600
H	2.43075800	2.50439900	2.91396900
C	3.89110300	3.72603600	0.69906000
H	4.06052600	3.74562300	-0.38005000
H	3.10728200	4.46002100	0.94154500
H	4.81623900	4.03224400	1.19435000

**INT-AI**

C	-4.63598000	0.82268400	1.47140900
C	-5.45246400	0.65134100	0.17393500
B	-3.26801800	0.29659400	-0.23816200
O	-3.28148700	0.82396000	1.03707000
O	-4.52968400	0.10161400	-0.75711200
C	-0.85766400	0.03302900	-0.30462900
H	-4.85905100	1.75571800	1.99481200
H	-5.81916100	1.61276000	-0.20438800
H	-6.30378300	-0.02305300	0.29513500
H	-4.78981800	-0.01360900	2.16263900
O	-2.15639500	0.00147200	-0.94640700
C	-0.86231600	-1.00658100	0.81747400
C	-1.30721400	-2.30114100	0.49918500
C	-0.44073500	-0.76190300	2.12588500
C	-1.27802300	-3.32056200	1.44401200
H	-1.65383600	-2.49593800	-0.50906500
C	-0.40842600	-1.78626300	3.07256500
H	-0.16590000	0.24114100	2.42627000
C	-0.81402800	-3.07194600	2.73539500
H	-1.62113100	-4.31392000	1.17086700
H	-0.07636300	-1.56769900	4.08307300
H	-0.78677500	-3.86833400	3.47247800
C	-0.53830000	1.45978200	0.07493500
H	-1.22169700	2.18386500	-0.35705400
C	0.52609500	1.89266400	0.76601000
H	1.25156500	1.18995300	1.17485000
N	0.82614100	3.21828900	1.10404000
C	-0.04932700	4.22702900	0.54945200
H	-1.07728800	4.02824800	0.86283700
H	0.24782000	5.20686000	0.93005600
H	-0.02219100	4.25040000	-0.55340400
C	2.23405200	3.54960200	1.00703800

H	2.82668100	2.78411000	1.51751800
H	2.58676000	3.62035600	-0.03787200
H	2.42258200	4.50879200	1.49624100
C	0.14968800	-0.17472600	-3.83732300
C	-0.51799900	-1.50425600	-3.47734200
B	0.11491900	-0.41976500	-1.56650500
O	0.13478800	0.55044000	-2.62137600
O	-0.14141300	-1.71731500	-2.12864700
C	2.49318400	0.53338900	-1.14773800
C	3.75551300	0.56362800	-0.57441800
C	4.14511600	-0.51403800	0.22278200
C	3.27713500	-1.59379900	0.40661800
C	2.03804800	-1.55297500	-0.21186900
N	1.66720600	-0.50190000	-0.95511200
H	2.09178900	1.32190100	-1.77524900
H	4.41576700	1.40659700	-0.73672300
H	3.56115700	-2.44322500	1.01460700
H	1.30850600	-2.35184100	-0.12780100
C	5.44257400	-0.51444900	0.84982800
N	6.48343500	-0.51151700	1.35317100
H	1.18512500	-0.34193800	-4.17578600
H	-0.17892800	-2.33806000	-4.10060700
H	-1.60991200	-1.41979700	-3.55069400
H	-0.38394900	0.38403200	-4.61155000

**INT-AJ**

C	-4.85658900	-2.29864400	-0.23141800
C	-5.14457500	-2.40285300	1.28205300
B	-3.04758800	-1.67710800	0.94507500
O	-3.45519100	-2.05516200	-0.30969700
O	-4.02480700	-1.77773900	1.90285000
C	-0.89503700	-0.96664600	0.22518400
H	-5.10277200	-3.21346700	-0.77494300
H	-5.20325500	-3.44468800	1.61509100
H	-6.06267200	-1.88866800	1.57549200
H	-5.38936900	-1.45980100	-0.69212400
O	-1.79855800	-1.23464300	1.25167400
C	-1.33113800	0.12676900	-0.68058200
C	-2.07393300	1.19373000	-0.15834100
C	-1.05452000	0.11512600	-2.05457200
C	-2.47412000	2.25156600	-0.97075200
H	-2.32899700	1.19046000	0.89779100



C	-1.44316100	1.17745500	-2.86303400	C	-6.15104500	0.38938900	-0.07393300
H	-0.56264400	-0.74886400	-2.48890900	C	-6.49625800	0.28884100	1.42770100
C	-2.14150600	2.25700300	-2.32286200	B	-4.28504500	0.06292800	1.12897300
H	-3.03829500	3.07593500	-0.54498100	O	-4.78071000	0.00498100	-0.14838800
H	-1.22116700	1.15096800	-3.92527600	O	-5.23268800	0.31078600	2.08690200
H	-2.44956300	3.08190000	-2.95729600	C	6.77906600	1.60829600	-0.01376900
C	0.27529300	-1.61325200	0.23659300	C	6.08240500	2.49288300	1.04214500
H	0.38616600	-2.35844200	1.02254200	B	4.76862500	0.75343600	0.50438300
C	1.49551200	-1.35566600	-0.60292100	O	5.77142300	0.68613500	-0.42976800
H	1.21615600	-0.74424000	-1.46535100	O	4.93898500	1.73820300	1.44366700
N	2.00711900	-2.62794100	-1.15977400	C	2.63951600	-0.03664900	1.46876700
C	2.85109500	-3.37006600	-0.23766100	C	1.55715000	-0.81514400	1.47536400
H	2.37271600	-3.44326100	0.74200900	C	1.25486700	-1.79975400	0.36029400
H	3.00134000	-4.38260900	-0.62662800	C	2.49509700	-1.99508100	-0.48450500
H	3.84290700	-2.90601700	-0.09471600	C	3.55028800	-1.18163200	-0.41538700
C	2.69390000	-2.43234200	-2.42473400	N	3.64697700	-0.12795300	0.49947500
H	2.01455200	-1.96212700	-3.14413400	H	2.81748200	0.71039100	2.23362400
H	3.59844300	-1.80915500	-2.33611700	H	0.82755300	-0.71036000	2.26940100
H	2.98203900	-3.40855200	-2.82878200	H	2.51383700	-2.82869200	-1.17646300
C	4.75367800	0.06452500	0.59272700	H	4.41793300	-1.30554000	-1.05337800
C	4.27807700	-0.79182600	1.77725600	C	-2.00576700	-0.11055000	0.47065100
B	2.58339400	-0.49596500	0.24959400	C	0.87367100	-3.09884600	0.95988700
O	3.80954200	-0.20104200	-0.42882500	N	0.56256000	-4.10717600	1.43395600
O	2.87957300	-0.91906800	1.58938800	H	-6.75438800	-0.27633900	-0.69484000
C	1.71077000	1.84200000	-0.60445700	H	-7.00795200	-0.64939900	1.66716900
C	0.95814800	3.00356600	-0.56351800	H	-7.10839200	1.12240800	1.77920400
C	0.27827800	3.30033600	0.61938400	H	-6.25309600	1.41301500	-0.44979000
C	0.37733700	2.44244200	1.71561700	H	6.71263600	2.69181800	1.91139400
C	1.14363200	1.29450600	1.58285200	H	5.74846000	3.44680800	0.62115500
N	1.78857600	1.01834400	0.44571700	H	7.61917500	1.04921300	0.41092100
H	2.27905700	1.53376100	-1.47652400	H	7.13304500	2.17640100	-0.87652200
H	0.88433400	3.65002100	-1.42860900	O	-2.97443800	-0.11663500	1.45678900
H	-0.14742200	2.65325200	2.63911800	C	-1.95010700	1.13292500	-0.33317900
H	1.26941100	0.55940600	2.37054200	C	-1.68419200	1.09156400	-1.70578300
C	-0.55773400	4.47132800	0.69285100	C	-2.19546600	2.36562800	0.28284000
N	-1.23932200	5.40393600	0.74764300	C	-1.63241900	2.27145600	-2.44159400
H	4.74038700	1.13362100	0.85884000	H	-1.54816100	0.12479900	-2.18246600
H	4.49611100	-0.32828300	2.74551800	C	-2.14294300	3.54127600	-0.45719800
H	4.74443800	-1.78633200	1.75865500	H	-2.41447000	2.39408700	1.34623800
H	5.75953700	-0.19292700	0.24923800	C	-1.85681600	3.49740200	-1.82026400
				H	-1.43086300	2.23107100	-3.50747400
				H	-2.32359200	4.49391400	0.03042600
				H	-1.81823800	4.41571200	-2.39748100
				C	-1.18134500	-1.15862000	0.38839600

INT-AE

H	-1.38275600	-1.98891900	1.06234000
C	0.04051500	-1.23272400	-0.49545800
H	0.36044700	-0.21314900	-0.73836000
N	-0.24509600	-1.88075400	-1.76460700
C	-0.59680100	-3.28533100	-1.73245300
H	-1.28429600	-3.48265400	-0.90653800
H	-1.10108900	-3.54763900	-2.66851100
H	0.27166800	-3.95636600	-1.61805800
C	0.57389700	-1.52070100	-2.90475600
H	0.82273000	-0.45601800	-2.85672800
H	1.51498500	-2.08448100	-2.99252300
H	-0.00208700	-1.69625600	-3.82150800

**TS-INT-Z**

C	-1.93594100	1.74335900	-0.47115900
C	-1.56640200	2.35295900	-1.79059200
C	-1.12944500	0.94654400	-1.49504800
H	-0.80260400	3.12280700	-1.78150500
H	-2.35421400	2.49117200	-2.52355200
H	-1.67252600	0.14283700	-1.98321800
C	0.27334300	0.62639000	-1.20109300
C	0.86922100	-0.55315100	-1.52326000
H	0.27110000	-1.24434700	-2.11130200
C	2.09828600	-1.00477400	-0.98769000
H	2.62213300	-0.37461500	-0.27191000
C	3.90950600	-2.57049400	-0.77007000
H	4.70198600	-2.98072300	-1.40143200
H	4.34687000	-1.82180100	-0.10429800
H	3.50508100	-3.38714300	-0.15072200
C	2.33063700	-2.79536600	-2.62535400
H	1.58387500	-3.50280000	-2.23497000
H	3.13595000	-3.36578200	-3.09393100
H	1.85710400	-2.17588700	-3.39022000
N	2.89807900	-1.94790600	-1.59605600
O	0.92642500	1.61627300	-0.48127100
C	3.86666600	2.82773400	-2.10036200
C	3.98671500	3.38974800	-0.66633700
B	2.10747000	2.16725400	-0.86955500
O	2.76732800	1.92182700	-2.04173100
O	2.73351800	3.08433400	-0.05588200
H	4.76317000	2.29386200	-2.42231800
H	3.64239900	3.61242400	-2.82998700

H	4.15161800	4.46912000	-0.64604300
H	4.78632000	2.89988500	-0.10046500
H	-1.35600600	2.07970900	0.38248300
C	-3.32734400	1.33461200	-0.14838100
C	-3.75534200	1.36814600	1.18337600
C	-4.22517900	0.89186800	-1.12583400
C	-5.04200200	0.96640800	1.53036300
H	-3.05885800	1.70116600	1.94962000
C	-5.51122600	0.49139000	-0.78003800
H	-3.91840100	0.85312300	-2.16830200
C	-5.92607000	0.52637200	0.54959100
H	-5.35228500	0.99608800	2.57010600
H	-6.19211800	0.14799900	-1.55247300
H	-6.92897600	0.21102600	0.81747500
C	0.66507800	2.31606000	2.56659400
C	2.05583600	1.67831200	2.73299900
B	0.60643700	0.18144900	1.89063900
O	-0.20535600	1.21070200	2.30400200
O	1.95129200	0.41860900	2.06131900
C	-1.24588700	-1.21903800	1.06438000
C	-1.71041900	-2.29151000	0.40026000
C	-0.79529700	-3.34458300	-0.00012600
C	0.54234700	-3.21317600	0.36175600
C	1.02270700	-2.04815500	0.94397800
N	0.11762500	-1.04437000	1.34439700
H	-1.88913100	-0.41952500	1.40942900
H	-2.77076200	-2.37470000	0.19529100
H	1.24261600	-4.01586500	0.15311200
H	1.99731000	-2.00130400	1.41220300
C	-1.24263200	-4.48759700	-0.71214700
N	-1.59518300	-5.41903600	-1.31285000
H	0.64391600	2.99581100	1.70836200
H	0.32538800	2.84118000	3.46172100
H	2.30209000	1.49699300	3.78480200
H	2.83925900	2.27600900	2.26556000

**TS-INT-AA**

C	2.08303100	-1.42688600	-1.75532000
C	1.54831300	-1.83977100	-3.09529800
C	1.23793600	-0.46517000	-2.56429600
H	0.73079600	-2.55096400	-3.10999300
H	2.25263200	-1.89562500	-3.91776700

H	1.75328600	0.37229000	-3.02285800	H	-2.64685900	-2.29403300	3.93052000
C	-0.10529300	-0.15386700	-2.04652900	H	-2.02979800	-1.17344700	5.16407000
C	-0.57431900	1.12006600	-1.92146300	H	-3.73697200	0.37445200	4.55550100
H	0.05842600	1.93816600	-2.24179300	H	-4.27361700	-0.70032400	3.24688900
C	-1.78623900	1.39347400	-1.23140200	N	-2.76925000	0.29159400	-1.28498900
O	-0.80189900	-1.21895600	-1.64110600	C	-3.90477200	0.53672800	-0.36880100
C	-2.96454600	-3.16886100	-0.32198200	C	-3.30721300	0.19055800	-2.67896500
C	-2.67838600	-2.37936100	0.95999800	H	-4.59635300	-0.30292400	-0.46072700
B	-2.06967800	-1.15386000	-0.91464600	H	-3.54216000	0.60744100	0.65520400
O	-2.99024300	-2.17834000	-1.32426800	H	-4.40730500	1.46415500	-0.66084900
O	-1.91431300	-1.27445200	0.52174000	H	-3.75564900	1.14915900	-2.95310000
H	-3.91787600	-3.70545900	-0.29290400	H	-4.04343900	-0.61165800	-2.70884800
H	-2.16051100	-3.89291100	-0.51530200	H	-2.48189600	-0.03864500	-3.35145900
H	-2.11515400	-2.95248800	1.70391900	H	-2.26904800	2.36284300	-1.35740100
H	-3.61861600	-2.03026800	1.42077800				
H	1.55867500	-1.86362700	-0.90791900				
C	3.54294500	-1.17929500	-1.54742200	<b>TS-INT-AG</b>			
C	4.09134900	0.10415000	-1.58856700	C	-0.56748100	-1.41032500	0.22570700
C	4.38928900	-2.25967000	-1.27392100	C	-1.78320000	-1.45797300	-0.65137600
C	5.45061600	0.30803800	-1.35783900	C	-2.91900900	-0.72345000	0.01115600
H	3.45449300	0.96037600	-1.78879600	H	-2.07030100	-2.48588000	-0.88235900
C	5.74620700	-2.06051200	-1.04581500	H	-1.57114500	-0.96987300	-1.61035400
H	3.97167100	-3.26268600	-1.24381700	H	-3.56359100	-1.26379500	0.69703000
C	6.28189300	-0.77372200	-1.08651600	C	-3.14173200	0.58514500	-0.15773200
H	5.84801200	1.31779000	-1.38571700	C	-4.21142000	1.34372900	0.47626400
H	6.38853500	-2.91024700	-0.83595400	H	-4.80314100	0.80537500	1.20833300
H	7.34064900	-0.61800600	-0.90594000	C	-4.46916000	2.63111300	0.17221900
C	-2.31965500	-1.26663700	4.11379900	H	-3.89385800	3.11984600	-0.61162300
C	-3.40049900	-0.22988600	3.70916800	C	-5.98691300	4.49337800	-0.04589400
B	-1.50462400	0.11745200	2.53177200	H	-6.39817400	5.27803900	0.59479400
O	-1.19160600	-0.97692400	3.29308200	H	-5.21486300	4.93656500	-0.67911000
O	-2.76522600	0.61778000	2.75462400	H	-6.79126800	4.11643300	-0.69542600
C	0.72746900	0.29821800	1.53946800	C	-6.28382500	2.85671400	1.74922000
C	1.67850200	0.96482400	0.85859200	H	-6.95120000	2.10219700	1.30285200
C	1.35924700	2.26261100	0.30438500	H	-6.89375800	3.63872000	2.20619900
C	0.07877900	2.76616300	0.45940700	H	-5.69479900	2.37427500	2.53383900
C	-0.91900000	1.98181400	1.03613500	N	-5.39757200	3.45340200	0.77590600
N	-0.54537400	0.83107100	1.73224500	O	-2.34549600	1.31018900	-1.03936100
H	0.88977600	-0.67019400	1.99595000	C	0.01196700	3.88334600	-0.42193400
H	2.66214800	0.53443700	0.71735900	C	0.14745600	3.02071900	0.84755100
H	-0.18959300	3.72487800	0.02866400	B	-1.37776100	2.12090000	-0.53612800
H	-1.88721500	2.38439000	1.30218900	O	-0.77941400	3.09120900	-1.30780800
C	2.34580100	2.99461200	-0.41904700	O	-0.92524400	2.08795200	0.76071700
N	3.15471000	3.56300700	-1.02914300				

H	0.98053600	4.10818900	-0.87483600	H	0.13813200	0.35456100	-2.23174500
H	-0.51575800	4.82259300	-0.22233300	H	-0.42386100	-1.28509300	-1.94836500
H	0.05755600	3.60065600	1.76901100	H	1.86250400	-1.84350600	-2.16407900
H	1.09774900	2.47514500	0.86125400	C	2.66984000	-0.47433400	-0.84818400
H	-0.25257100	-0.41198500	0.52669600	C	4.01377000	-1.03809500	-0.87797700
C	0.04323400	-2.50539900	0.89726900	H	4.14831700	-1.91616500	-1.49964200
C	1.02861000	-2.24775000	1.88376200	C	5.03399900	-0.50321300	-0.17806700
C	-0.21446900	-3.85913500	0.56829900	H	4.84097600	0.35747900	0.45664200
C	1.70807700	-3.28022000	2.50969700	C	7.14204200	-0.66526400	0.99059800
H	1.23898300	-1.21451900	2.14745500	H	8.20336700	-0.65137000	0.72842100
C	0.47656300	-4.88365400	1.19517300	H	6.87905400	0.30918600	1.40778800
H	-0.93363900	-4.09703400	-0.20782900	H	6.98593300	-1.42779900	1.76860300
C	1.43833600	-4.60720800	2.17013200	C	6.67197800	-2.11040400	-0.93267800
H	2.45212700	-3.05398300	3.26762400	H	6.19971600	-3.00665800	-0.49934000
H	0.26914200	-5.91265000	0.91839400	H	7.75480100	-2.25037600	-0.93530000
H	1.97066300	-5.41681900	2.65826100	H	6.33429900	-2.01068000	-1.96787300
C	5.16621900	3.09009300	1.04657300	N	6.34886900	-0.90917500	-0.19829600
C	4.38745000	4.08002800	0.15637400	O	2.54118200	0.59899100	0.00843900
B	3.63873700	1.98788700	-0.17414900	C	1.06867500	3.48669600	-1.49833700
O	4.76586300	1.80014500	0.58044100	C	0.91419700	3.75181300	0.01694400
O	3.30676700	3.30667500	-0.37422700	B	1.91748500	1.76771200	-0.31646300
C	1.76587200	1.14425500	-1.53886300	O	1.56894400	2.15314200	-1.58698200
C	1.01612300	0.13486200	-2.03676100	O	1.64079500	2.69906200	0.64876200
C	1.30661900	-1.22526800	-1.68702500	H	1.78759600	4.16479300	-1.96980100
C	2.45992000	-1.45811900	-0.86947400	H	0.11405200	3.55307400	-2.02613300
C	3.18221200	-0.42166400	-0.38898900	H	-0.13345200	3.70048500	0.33052000
N	2.85900700	0.90608300	-0.69518500	H	1.33334400	4.71461800	0.31966300
H	1.57752000	2.18200000	-1.78089000	H	0.28050300	-0.41198000	0.68453300
H	0.18425800	0.37283200	-2.69086100	C	-1.15775000	1.03259700	0.03004900
H	2.73398600	-2.47122200	-0.59935300	C	-1.43016700	1.48543900	1.34760200
H	4.04476700	-0.54738600	0.25271500	C	-1.84381000	1.67783000	-1.03067600
C	0.63800800	-2.31161000	-2.30593000	C	-2.30110900	2.53911000	1.58282700
N	0.07635200	-3.21017000	-2.78619700	H	-0.92283800	0.99691700	2.17560100
H	4.89251500	3.18568300	2.10220700	C	-2.72146300	2.72389800	-0.78412800
H	6.24853700	3.19306600	0.94985400	H	-1.68379000	1.34612000	-2.05161600
H	4.99623000	4.45172000	-0.67367800	C	-2.95246700	3.17003200	0.51990500
H	3.98841800	4.93044500	0.71267200	H	-2.47378800	2.87402000	2.60122300
				H	-3.23951300	3.19467400	-1.61462300
				H	-3.63509100	3.99289800	0.70370300
				C	-0.31679500	-2.99077900	2.06318100
				C	0.15119500	-3.38489900	0.64510500
				B	-1.62111300	-2.03804300	0.50379100
				O	-1.33732200	-2.01225300	1.85342500
				O	-0.92527100	-2.98840700	-0.20864300
<b>TS-INTAF</b>							
C	-0.28813800	-0.07300900	-0.17917600				
C	0.21279300	-0.48905500	-1.53398400				
C	1.63276000	-0.99278300	-1.52956300				

C	-3.14830400	-1.49687300	-1.36719900
C	-4.18462800	-0.78724300	-1.89930300
C	-4.97432000	0.05216700	-1.07321000
C	-4.64414300	0.11878400	0.29783300
C	-3.59678500	-0.60508300	0.79142800
N	-2.82690100	-1.41339800	-0.02639000
H	-2.53456500	-2.17348900	-1.94822500
H	-4.40708400	-0.88309300	-2.95514800
H	-5.21228800	0.75140900	0.96897700
H	-3.31281800	-0.59955300	1.83455900
C	-6.03603100	0.82799800	-1.61363300
N	-6.89863900	1.46623400	-2.05829600
H	0.48881500	-2.55850600	2.66173300
H	-0.74808700	-3.83838000	2.60584200
H	0.32254000	-4.45776800	0.53563200
H	1.05473300	-2.83899100	0.34915500

**TS-INT-AJ**

C	-4.49012300	-2.29236200	0.20867900
C	-4.63938800	-2.12244100	1.73506400
B	-2.56826800	-1.55047400	1.09135600
O	-3.09155200	-2.14861200	-0.02604200
O	-3.45270500	-1.43978000	2.13298200
C	-0.51839800	-0.87759700	0.07361200
H	-4.82590500	-3.26873600	-0.14720400
H	-4.68716500	-3.08766800	2.25082600
H	-5.51424900	-1.53096500	2.01343500
H	-5.02308100	-1.51039500	-0.34295900
O	-1.28693000	-1.09922200	1.20479500
C	-1.10944600	0.01817600	-0.93089500
C	-2.04244700	0.99456700	-0.54752400
C	-0.82481800	-0.12196800	-2.30111200
C	-2.62786300	1.83733400	-1.48893100
H	-2.30051100	1.10335800	0.50196500
C	-1.40709200	0.71952600	-3.23614100
H	-0.16959400	-0.92207900	-2.62898400
C	-2.30137100	1.71391500	-2.83415100
H	-3.31577900	2.60846800	-1.15862600
H	-1.17769800	0.58924800	-4.28913800
H	-2.74855400	2.37648300	-3.56772900
C	0.67963900	-1.53486600	0.00304700
H	0.85844100	-2.28210900	0.77254700

C	1.76166000	-1.17592900	-0.84856100
H	1.64494800	-0.30760700	-1.49469000
N	2.66738800	-2.09950500	-1.32905300
C	2.79618800	-3.38478300	-0.68219500
H	1.82735900	-3.89819500	-0.66675800
H	3.50809000	-3.99601300	-1.24010200
H	3.14582400	-3.29643800	0.35586800
C	3.63245300	-1.70867500	-2.33294900
H	3.23315500	-0.86188600	-2.89639700
H	4.60082300	-1.40336900	-1.92037000
H	3.78875200	-2.53909300	-3.02889800
C	5.08911100	-0.98781800	0.67650200
C	4.39810600	-1.35929300	1.99845700
B	3.00086200	-0.12468800	0.72403900
O	4.24388100	-0.00349900	0.09463200
O	3.02944100	-1.03993000	1.78146000
C	2.16775800	2.02125100	-0.20617800
C	1.20753200	2.97769900	-0.32166800
C	0.10447100	2.99542500	0.57539400
C	0.06345500	2.00032800	1.57551300
C	1.02841400	1.03551800	1.63194400
N	2.10099600	1.02960000	0.75947300
H	3.03761400	1.97458800	-0.85018700
H	1.29518300	3.73116400	-1.09493200
H	-0.74961500	1.97025200	2.29171400
H	1.02531300	0.24421600	2.36993700
C	-0.93722800	3.95322700	0.45201300
N	-1.80332500	4.72107900	0.34542000
H	6.09063900	-0.57409600	0.81951600
H	4.78525300	-0.76547100	2.83502600
H	4.49928500	-2.42012500	2.24587900
H	5.16160100	-1.85886300	0.01123300

**TS3-iso2**

C	5.16612200	-0.41378300	1.23672900
C	5.02207200	-1.94753000	1.15112800
B	3.01393400	-0.96370200	0.94086900
O	3.82515200	0.06137600	1.34287000
O	3.67234200	-2.15148100	0.73026900
C	1.24096400	-2.87553900	-1.57039700
C	0.82548900	-3.69315900	-0.32530600
B	-0.65779800	-2.03529600	-0.69189200

O	0.30035100	-1.80417800	-1.65323500	C	-2.46913700	1.29274200	2.74375900
O	-0.44325800	-3.16727700	0.05548300	H	-2.51147900	0.20755500	2.60462100
C	-2.76342600	-1.57038800	0.47165600	H	-1.73572900	1.52856500	3.52663500
C	-3.85195400	-0.81700800	0.71545900	H	-3.45722800	1.62764200	3.06479800
C	-4.07063500	0.41868300	-0.01424800				
C	-3.11268000	0.77379700	-0.96132200				
C	-1.92323200	0.07931700	-1.05006300				
N	-1.80554000	-1.21248100	-0.49123900				
H	-2.57546300	-2.51296000	0.97102800	C	-4.95926600	0.37158100	1.13586200
H	-4.56918500	-1.14041400	1.46065300	C	-5.47153700	0.24173800	-0.31427400
H	-3.21432800	1.69974800	-1.51944300	B	-3.22723000	0.32480900	-0.28640300
H	-1.15488600	0.32992300	-1.77210000	O	-3.57109300	0.66194800	0.99643000
C	1.03123300	0.32362100	0.53593300	O	-4.29748700	-0.01075800	-1.08298300
C	-5.17791700	1.25562000	0.26792700	C	-0.84853600	0.31030900	0.06890200
N	-6.05507200	1.97269000	0.53765000	H	-5.45051900	1.17355700	1.69102700
H	5.74171900	-0.08747000	2.10503600	H	-5.93841400	1.16808600	-0.66644400
H	5.16734000	-2.42730900	2.12445000	H	-6.18005100	-0.57957100	-0.44265700
H	5.70375900	-2.40004800	0.42820600	H	-5.07053800	-0.56494200	1.69292800
H	5.61766600	0.00569200	0.33151800	O	-1.96637500	0.30347300	-0.78918400
H	0.72425700	-4.75988500	-0.54238300	C	-0.78725600	-0.82999400	0.97364100
H	1.53493200	-3.55633800	0.49477500	C	-1.51851000	-2.00431000	0.67315600
H	1.18858900	-3.46212000	-2.49314400	C	0.01900000	-0.85701900	2.12664200
H	2.25271800	-2.47319400	-1.45998800	C	-1.42708000	-3.13313100	1.46910600
O	1.66556400	-0.88475500	0.75671600	H	-2.14045700	-2.02981400	-0.21458500
C	1.68766700	1.23132800	-0.42573900	C	0.09833400	-1.99414200	2.92810500
C	2.25659800	0.72575200	-1.60190800	H	0.53974100	0.03580200	2.44566600
C	1.79140800	2.60216400	-0.15580100	C	-0.61041300	-3.14311200	2.60347400
C	2.89654000	1.57832900	-2.49534800	H	-1.99694700	-4.01800800	1.20290600
H	2.15359200	-0.33074300	-1.82453700	H	0.72066800	-1.96965600	3.81755200
C	2.42992800	3.45058100	-1.05188700	H	-0.54015100	-4.03007200	3.22406600
H	1.38981500	2.98756700	0.77635400	C	-0.28954200	1.61013400	0.22342900
C	2.98344900	2.94167700	-2.22548800	H	-0.81547900	2.36111300	-0.35825100
H	3.32073900	1.17723600	-3.41027200	C	0.85305900	1.99611700	0.87784300
H	2.51022000	4.50917700	-0.82687800	H	1.47707900	1.28832600	1.40944100
H	3.48395200	3.60487600	-2.92344100	N	1.24155700	3.30788800	1.06745700
C	-0.16075700	0.53644100	1.13971200	C	0.52799400	4.34732000	0.36240400
H	-0.48152100	-0.21833800	1.85260900	H	-0.53821400	4.29213000	0.59681100
C	-1.09133500	1.55157500	0.73785800	H	0.90420400	5.31921400	0.68759800
H	-0.77455400	2.26839500	-0.00941500	H	0.64821500	4.27015100	-0.73091700
N	-2.14765400	1.94141600	1.49153200	C	2.65081300	3.55983300	1.27422700
C	-2.76724700	3.22544800	1.22429000	H	3.08897000	2.74500700	1.85781400
H	-2.65983300	3.46293700	0.16299500	H	3.20525400	3.63794800	0.32458800
H	-3.83495900	3.18216800	1.45227800	H	2.78324000	4.49433300	1.82590900
H	-2.30197800	4.03044200	1.81016100	C	-0.98954400	-0.04889100	-3.50716900

### TS-INT-AI

C	-1.27765200	-1.48759200	-3.00127600
B	0.32286900	-0.53086300	-1.73766000
O	0.06614100	0.44145400	-2.68568600
O	-0.32532700	-1.72661500	-1.96726100
C	2.34739400	0.65517500	-1.04216800
C	3.51081300	0.76503600	-0.30771600
C	3.87233900	-0.24303200	0.58946600
C	3.04140300	-1.38949800	0.68315500
C	1.93863300	-1.49424000	-0.11403700
N	1.58501800	-0.48867500	-0.98602700
H	2.03871400	1.38288900	-1.77967400
H	4.13314400	1.64341400	-0.42764100
H	3.28353500	-2.19503300	1.36498200
H	1.28438500	-2.35814300	-0.11175400
C	5.05190600	-0.11947700	1.38572400
N	6.00444900	-0.00967900	2.03826600
H	-0.66035700	-0.03486200	-4.55104300
H	-1.14314400	-2.24083100	-3.78322900
H	-2.29005500	-1.56928300	-2.59370600
H	-1.86531000	0.59466400	-3.39502100

**TS-INT-AE**

C	-3.97911500	3.68527800	0.17946400
C	-4.28902800	3.35956200	1.65586800
B	-2.74095900	1.94390600	0.86169800
O	-3.18657700	2.58748300	-0.26483800
O	-3.29187200	2.41114000	2.02682300
C	4.12574600	3.98203300	0.88767100
C	3.36012900	3.99109000	2.23009300
B	2.98004200	2.06544900	1.13341100
O	3.98009500	2.65276400	0.39734100
O	2.53386200	2.83047400	2.18698800
C	1.44489900	0.19384300	1.60049800
C	0.93285400	-1.02139600	1.31897400
C	1.40390200	-1.78481100	0.19364600
C	2.57297700	-1.25056200	-0.47269500
C	3.04808800	-0.02695900	-0.16834900
N	2.49367700	0.75194400	0.85867000
H	1.08473200	0.80477900	2.41916900
H	0.11511500	-1.39550400	1.92409000
H	3.05800700	-1.82549600	-1.25446700
H	3.89478200	0.42149400	-0.67210800

C	-1.06627800	0.66065400	-0.24997100
C	1.01413900	-3.13094500	0.01306300
N	0.65307700	-4.21749300	-0.20939400
H	-4.87686000	3.76594400	-0.43716300
H	-5.27809400	2.90412200	1.77450800
H	-4.22479600	4.23432500	2.30675400
H	-3.39563100	4.60689600	0.07833000
H	4.03632300	3.91635700	3.08814900
H	2.73726000	4.88135000	2.35375600
H	5.18638500	4.21574700	1.00554300
H	3.68803900	4.67665500	0.16234200
O	-1.84043800	0.92126500	0.86671800
C	-0.26811100	1.78689700	-0.74325600
C	0.04873300	1.93580600	-2.10545800
C	0.14404300	2.79645700	0.14216100
C	0.78348100	3.02401500	-2.55127000
H	-0.31994800	1.20676000	-2.81904900
C	0.86135900	3.89840700	-0.31390800
H	-0.08301200	2.70503400	1.20065200
C	1.19997100	4.01316200	-1.65822800
H	1.01245500	3.11700600	-3.60809800
H	1.15976400	4.66605100	0.39540800
H	1.76690600	4.86793900	-2.01295500
C	-1.16453600	-0.59941400	-0.77901400
H	-1.93163200	-1.23458300	-0.34544000
C	-0.23016800	-1.18078100	-1.66445500
H	0.64409100	-0.61288000	-1.96453700
N	-0.48394900	-2.27759800	-2.41062100
C	-1.68894500	-3.05943400	-2.19507300
H	-2.56370800	-2.40257700	-2.23958500
H	-1.76721500	-3.80213700	-2.99061400
H	-1.66907800	-3.58189300	-1.23412400
C	0.57900600	-2.86736100	-3.20376400
H	1.33017600	-2.10152000	-3.41421300
H	1.05716600	-3.70310600	-2.68337500
H	0.17126300	-3.22230900	-4.15505000

**TS3-iso**

C	-1.65324900	1.44090100	3.42394600
C	-2.81018900	0.70196300	2.71559000
B	-0.82842100	0.03837000	1.85093400
O	-0.48736800	1.08073000	2.68889100

O	-2.17341500	-0.26974700	1.89274000	C	3.35133900	2.46675100	2.84874300
C	-5.41942500	-1.04292500	-0.61545700	H	2.95772600	1.78401400	3.60641700
C	-5.59380200	0.38710100	-0.06140500	H	4.05255400	3.15175100	3.32851600
B	-3.49447500	0.09098800	-0.81209300	H	2.50895800	3.04569600	2.43831400
O	-4.15099500	-1.02323900	-1.26723900	C	5.07711700	2.44345500	1.09850400
O	-4.27507700	0.93332600	-0.05444100	H	5.57519800	1.76497100	0.40431300
C	-1.47023400	1.45248600	-0.53305300	H	4.65965400	3.27576200	0.51513100
C	-0.13652400	1.63046600	-0.65351600	H	5.81670200	2.83658100	1.80103900
C	0.66976000	0.67472000	-1.36543600				
C	-0.04189900	-0.35722200	-2.07392900				
C	-1.37273300	-0.50624300	-1.91205800	<b>TS3</b>			
N	-2.13068600	0.37336200	-1.12970000				
H	-2.10910700	2.13603500	0.01422200	C	2.78265200	-0.97016700	2.58613700
H	0.33433200	2.47780900	-0.16817600	C	3.96218200	-0.31950300	1.84043300
H	0.50001100	-1.05567700	-2.69963300	B	2.00797000	0.46441300	1.02715500
H	-1.93827300	-1.30166500	-2.38072200	O	1.64156100	-0.22659100	2.16139300
C	1.31905300	-0.65750300	0.76924100	O	3.36131400	0.38395100	0.75824900
C	2.02204300	0.96352100	-1.64789700	C	3.86150200	-0.86084700	-2.06164100
N	3.15126400	1.20277900	-1.81094800	C	4.15567000	-2.09104500	-1.18025200
H	-1.77503900	2.52692600	3.40619100	B	1.99484200	-1.51570000	-1.00830500
H	-3.40125300	1.36805700	2.07992700	O	2.43657400	-0.76401000	-2.06641000
H	-3.47838300	0.20037600	3.42081200	O	2.97191800	-2.27286600	-0.39772700
H	-1.53074800	1.11925600	4.46340400	C	0.17205600	-2.34227200	0.45553800
H	-6.22999300	1.00328200	-0.70512300	C	-1.12631300	-2.39433000	0.80245200
H	-5.99992700	0.39966200	0.95304100	C	-2.10684700	-1.60453300	0.08605200
H	-6.19619200	-1.31712400	-1.33240000	C	-1.65786000	-0.84963600	-0.99886300
H	-5.39406300	-1.78885100	0.18543000	C	-0.31356000	-0.70870200	-1.24182000
O	0.00026100	-0.74930200	1.11948400	N	0.63087700	-1.51810900	-0.58402100
C	1.74363200	-1.82508400	0.00816400	H	0.93719400	-2.94108300	0.93392000
C	0.77215500	-2.75540500	-0.42486500	H	-1.43969200	-3.04097000	1.61286400
C	3.08713000	-2.08434500	-0.32929600	H	-2.34990600	-0.25224800	-1.58394900
C	1.12742100	-3.85475700	-1.19527500	H	0.06714300	-0.16264200	-2.09363500
H	-0.26096200	-2.60497200	-0.14160400	C	-0.14153000	1.36146000	0.17046000
C	3.43037000	-3.18392500	-1.10228000	C	-3.47559900	-1.64370900	0.45403300
H	3.87993600	-1.45398300	0.04416800	N	-4.58796300	-1.65340200	0.79496400
C	2.45516000	-4.07161200	-1.55383900	H	2.65513300	-2.01620400	2.29050600
H	0.35741300	-4.55144900	-1.51284400	H	4.66389100	-1.06307200	1.45616600
H	4.47444800	-3.35362900	-1.34538900	H	4.50592200	0.39304700	2.46996200
H	2.73025700	-4.92913300	-2.15898000	H	2.87507800	-0.90769300	3.67254700
C	2.10500300	0.32530900	1.44325200	H	4.32505200	-2.99429200	-1.77578400
H	1.57347600	0.86049100	2.21877600	H	5.01391300	-1.93767400	-0.52168700
C	3.37435100	0.74143800	1.14652200	H	4.22166900	-0.97968400	-3.08578100
H	3.92800600	0.35081400	0.30638200	H	4.27210400	0.05298300	-1.62513900
N	4.04667300	1.72061800	1.82386600	O	1.22386000	1.21497600	0.21417700



C	-0.54339600	2.25839300	-0.92527400	H	-5.59814700	1.53414200	-0.44408100
C	0.27788100	2.38047600	-2.06306200	H	-6.95353700	0.79246100	-1.33274000
C	-1.70637900	3.04161900	-0.86651400	H	-5.40042500	1.05735400	-2.14583200
C	-0.07880400	3.21521000	-3.11143900	N	-5.45481200	-0.55459000	-0.82565500
H	1.19657900	1.80337500	-2.11072300	O	-1.49636000	-1.59041600	-0.43832000
C	-2.06070600	3.87293900	-1.92421400	C	0.98318300	-3.51533200	-2.13978300
H	-2.31154200	3.04026000	0.03183000	C	0.75656400	-4.30548200	-0.83124800
C	-1.25767700	3.95942800	-3.05677700	B	-0.56846600	-2.48969200	-0.88386400
H	0.56820700	3.28595400	-3.98029000	O	-0.05616300	-2.53426500	-2.15354400
H	-2.96398600	4.47065600	-1.85082300	O	-0.11064500	-3.48002200	-0.05457700
H	-1.53724800	4.60743200	-3.88073700	H	0.90435100	-4.13891600	-3.03296700
C	-0.87826500	1.05291700	1.33844600	H	1.95225900	-3.00480300	-2.13869800
H	-0.28330000	0.77011800	2.19700200	H	1.68725500	-4.46890300	-0.28271900
C	-2.24710300	0.93537800	1.44621200	H	0.26653900	-5.26853400	-1.00882800
H	-2.90043700	1.15090400	0.60710400	H	0.55143800	-0.79435400	0.63174900
N	-2.90836700	0.57455200	2.57687600	C	2.54350300	-1.17602000	-0.10002600
C	-2.16304200	0.23737700	3.76739000	C	2.82301600	-2.13572600	0.90070600
H	-1.68091200	1.11717400	4.21888900	C	3.56299900	-0.87888600	-1.03437500
H	-2.84304500	-0.20451400	4.49740400	C	4.05234600	-2.77481000	0.95233000
H	-1.38521600	-0.49368500	3.52525900	H	2.04151000	-2.38387900	1.61499900
C	-4.32217300	0.85835600	2.72524300	C	4.79233600	-1.52128100	-0.97080300
H	-4.77583400	0.95725100	1.73891800	H	3.38498600	-0.12964100	-1.80069700
H	-4.81800200	0.02529200	3.22894900	C	5.04529500	-2.47429700	0.01646200
H	-4.49323900	1.78159900	3.29758900	H	4.24154800	-3.51439200	1.72459300

### TS-INT13

C	1.27158000	-0.52140500	-0.13380800	H	5.56284100	-1.27346700	-1.69420800
C	0.78113200	0.21419100	-1.34678000	H	6.00677500	-2.97471800	0.05932500
C	-0.70064300	0.47813800	-1.36912600	C	-2.29691800	0.04376900	2.40727000
H	1.05909300	-0.35627200	-2.24708200	C	-3.06349600	1.33658200	2.06253000
H	1.31037700	1.17528300	-1.44116900	B	-0.89630700	1.56537800	1.55059000
H	-1.01975000	1.43713200	-1.76793600	O	-0.91613300	0.40058400	2.26623200
C	-1.69790300	-0.34200700	-0.99154500	O	-2.12191200	2.13407000	1.33588300
C	-3.10356800	0.04575100	-1.04463000	C	0.33088300	3.29138600	0.29006700
H	-3.30119100	1.06409800	-1.36069300	C	1.44858200	3.74244100	-0.31487000
C	-4.10296200	-0.80290100	-0.72885100	C	2.69523100	3.03685200	-0.13087000
H	-3.85575100	-1.80602500	-0.38942200	C	2.71672400	1.95208700	0.75184500
C	-6.32496800	-1.24764000	0.10410800	C	1.55057900	1.48734800	1.32310900
H	-7.34160900	-1.27904400	-0.29613500	N	0.33934400	2.15471400	1.10065800
H	-5.97495600	-2.27427500	0.23262900	H	-0.63634900	3.76762400	0.18654000
H	-6.35768900	-0.76688400	1.09460100	H	1.40951600	4.62653900	-0.93827400
C	-5.87009400	0.77788900	-1.19914500	H	3.64153500	1.42283800	0.95220600
				H	1.54017800	0.74318000	2.10693500
				C	3.87612500	3.45923000	-0.80099800
				N	4.83519900	3.80680700	-1.35695200
				H	-2.51805500	-0.76141500	1.70087400

H	-2.47819700	-0.29864300	3.42815900
H	-3.37214900	1.88703900	2.95741900
H	-3.93393700	1.14261800	1.43205800