

Electronic Supplementary Material (ESI) for New Journal of Chemistry.

*Supporting Information*

**Mechanism of [3+2] Annulations between Indole-2-formaldehydes and Isatins  
Mediated by N-Heterocyclic Carbene: A DFT Study**

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## Computational Details

### 1. Distortion-interaction model

In the distortion–interaction model, each transition state is divided into two parts (*i.e.* M4-and R2-part), followed by single point energy calculations at the IEF-PCM(THF)/M06-2X-D3/6-311++G(2df,2pd) level of theory. The distortion energies of M4 (R2), denoted as  $\Delta E_{\text{dist}}(\text{M4})$  ( $\Delta E_{\text{dist}}(\text{R2})$ ), is defined as the energy difference between the distorted and the corresponding optimized M4 (R2), *i.e.*  $E_{\text{dist}}(\text{M4/R2}) = E_{(\text{M4/R2})} - E_{(\text{M4/R2\_in TS5})}$ . The total distortion energy  $E_{\text{dist\_total}}$  can be obtained through  $E_{\text{dist\_total}} = E_{\text{dist\_M4}} + E_{\text{dist\_R2}}$ . The activation energy ( $\Delta E_{\text{act}}$ ) can be written as  $\Delta E_{\text{act}} = \Delta E_{\text{dist}} - \Delta E_{\text{int}}$ .

### 2. Global reactivity indexes (GRI) analysis

To disclose the role of the NHC, we performed the global reactivity index (GRI) analyses. The molecular global electrophilicity character is described with the electrophilicity index  $\omega$ , which can be calculated from the expression  $\omega = (\mu^2/2\eta)$  (eV), in which  $\mu$  and  $\eta$  are the electronic chemical potential and the chemical hardness, respectively. The values of  $\mu$  and  $\eta$  can be calculated from the following expressions  $\mu \approx (E_{\text{H}} + E_{\text{L}})/2$  and  $\eta \approx (E_{\text{H}} - E_{\text{L}})$ , in which  $E_{\text{H}}$  is and  $E_{\text{L}}$  are the one-electron energies of the frontier molecular orbital HOMO and LUMO, respectively. Within the Kohn–Sham scheme, Domingo and coworkers introduce relative nucleophilicity index  $N$ , defined as  $N = E_{\text{H}}(\text{Nu}) - E_{\text{H}}(\text{TCE})$ . This nucleophilicity scale takes tetracyanoethylene (TCE) as a reference.

### 3. Calculation of enantiomeric excess (ee)

The extent of enantioselectivity, in terms of enantiomeric excess (ee %), was calculated by using the Boltzmann distribution of diastereomeric transition states with the following equations:

$$\frac{[R]}{[S]} = \frac{\exp(-G_{[R]}^\ddagger)}{\exp(-G_{[S]}^\ddagger)} = \exp(\Delta G^\ddagger / RT) \quad (1)$$

$$ee = \frac{[R]-[S]}{[R]+[S]} \times 100\% = \frac{\frac{[R]}{[S]} - 1}{\frac{[R]}{[S]} + 1} \times 100\% \quad (2)$$

Where  $G^\ddagger$  is the Gibbs free energy barrier of the competing diastereomeric transition state and  $\Delta G^\ddagger$  is the Gibbs free energy difference between the two diastereomeric transition states.

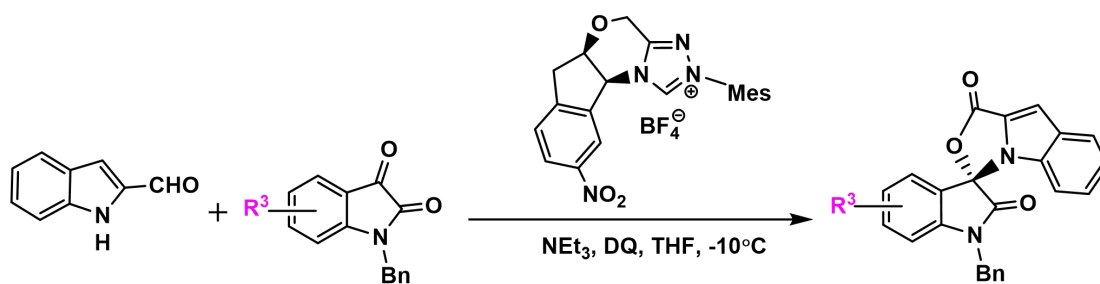
**Table S1.** Different computational levels.

<b>Level</b>	<b>Optimization</b>	<b>Single point Energy</b>	<b>Solvation model</b>
<b>L1</b>	M062X/6-31G(d,p)	M062X-D3/6-311++G(2df,2pd)	IEFPCM
<b>L2</b>	M062X/6-31G(d,p)	M062X-D3/6-311++G(2df,2pd)	SMD
<b>L3</b>	$\omega$ B97X-D/6-31G(d,p)	$\omega$ B97X-D/6-311++G(2df,2pd)	IEFPCM
<b>L4</b>	B3LYP-D3/6-31G(d,p)	B3LYP-D3/6-311++G(2df,2pd)	IEFPCM
<b>L5</b>	M062X/6-31G(d,p)	M062X-D3/6-311++G(d,p)	IEFPCM
<b>L6</b>	M062X/6-31G(d,p)	M062X/6-311++G(2df,2pd)	IEFPCM

**Table S2** Relative energies (kcal/mol) at different computational levels.

<b>Species</b>	<b>L1</b>	<b>L2</b>	<b>L3</b>	<b>L4</b>	<b>L5</b>	<b>L6</b>
<b>TS5(S)</b>	0.0	0.0	0.0	0.0	0.0	0.0
<b>TS5(R)</b>	6.8	6.1	7.1	8.2	6.9	6.8

**Table S3** Relative energy barriers (kcal/mol)  $\Delta\Delta G = \Delta G(\text{TS5}(\text{R})) - \Delta G(\text{TS5}(\text{S}))$  of the NHC-catalyzed reaction.



entry	$\text{R}^3$	$\Delta\Delta G$ (kcal/mol)	<i>ee</i> % in experiment
1	5-MeO	7.9	91
2	5-Me	7.7	89
3	5-F	9.2	95
4	5-Br	8.5	91
5	4-Br	9.4	98

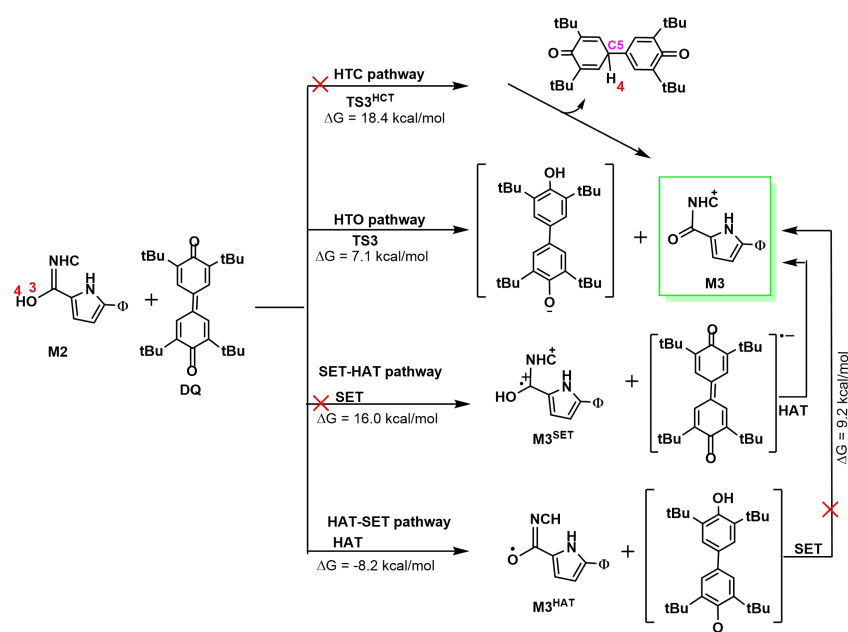
### Possible pathways for the oxidation process (M2 → M3).

For the transformation of M2 to M3, we have investigated four possible pathways including HTO (hydride transfer to the oxygen), HTC (hydride transfer to the carbon), SET-HAT (single electron transfer-hydrogen atom transfer), and HAT-SET (hydrogen atom transfer-single electron transfer) pathways (Scheme S1). As presented in Scheme S2, four possible HTC pathways corresponding to the hydride H5 transfers from the O4 atom to four different types of carbon atoms (C2, C3, C4 and C5) of DQ have been investigated. The energy barriers are calculated to be 49.5 ( $TS3^{HCT\_C2}$ ), 20.4 ( $TS3^{HCT}$ ), 31.4 ( $TS3^{HCT\_C4}$ ) and 18.4 ( $TS3^{HCT}$ ), which are much higher than the HTO pathway ( $TS3$ , 7.1 kcal/mol). Therefore, the HCT pathways can be ruled out.

In addition, the energy barrier of SET-HAT pathway (16.0 kcal/mol) is much higher than the HCT pathways (7.1 kcal/mol), thus can be ruled out.

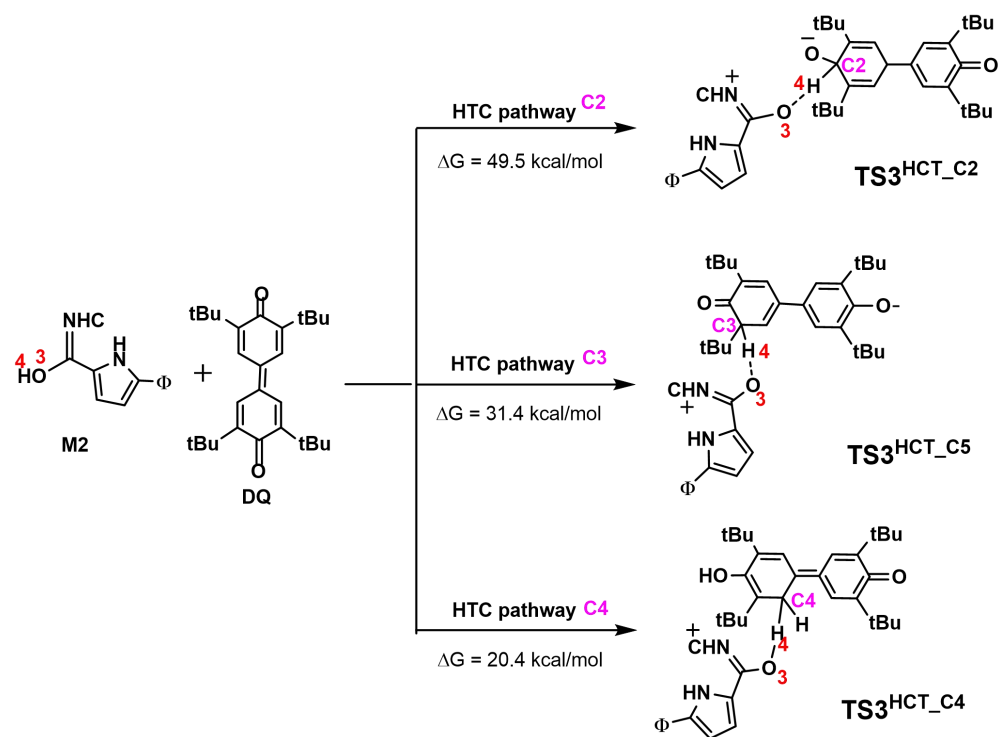
For HAT-SET pathway, the HAT process is exothermic, indicating this process can be take place very easily. However, the SET process needs to absorb 9.2 kcal/mol energy, which is higher than the energy barrier of  $TS3$  (7.1 kcal/mol). Therefore, the HAT-SET pathway can be neglected. Taken together, the HTO pathway (shown in Fig. 1) is the most energetically pathway among the four possibilities.

### Scheme S1. Possible pathways for the oxidation process.

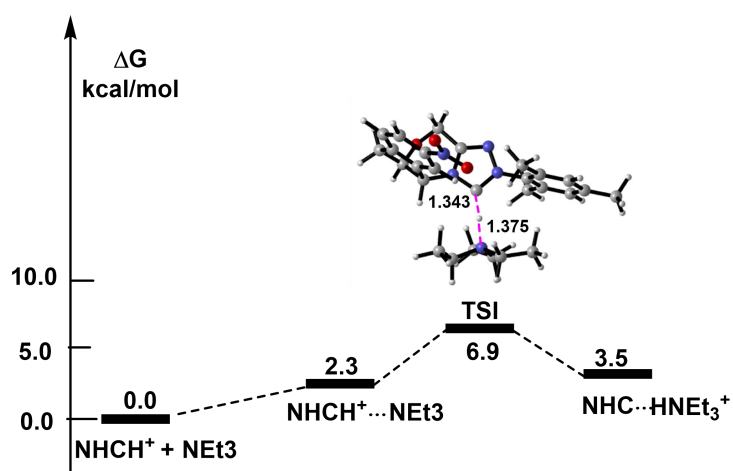




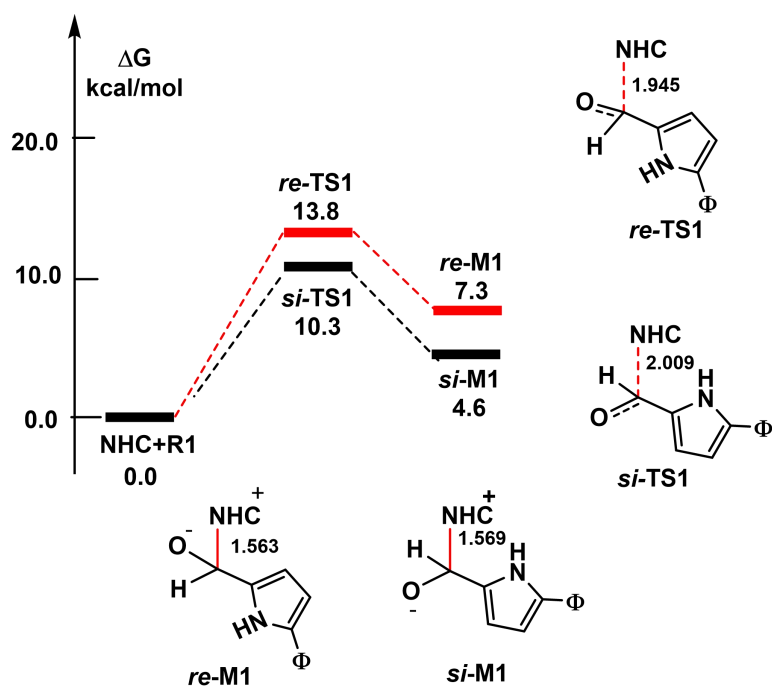
Scheme S2. Other possible HCT pathways.



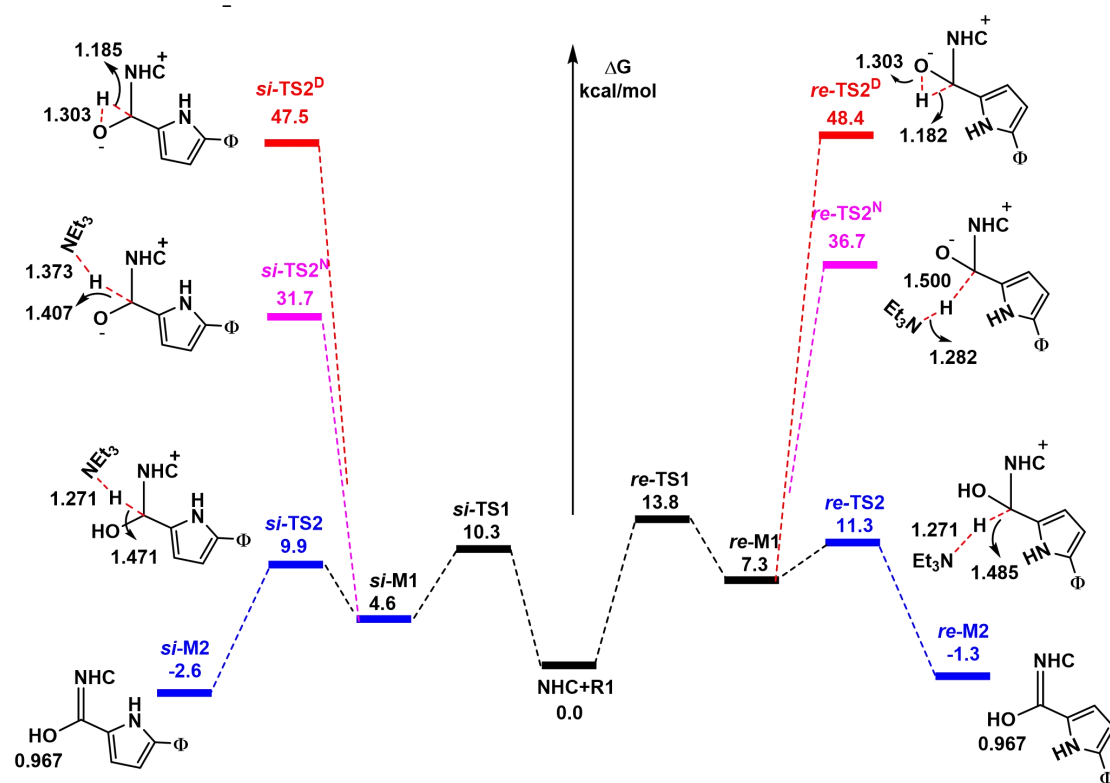
**Fig. S1** The deprotonation of pre-NHC by base  $\text{NEt}_3$  to generate NHC.



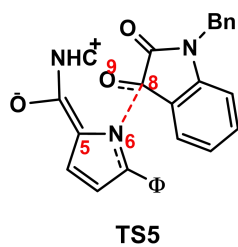
**Fig. S2** Free energy (kcal/mol) profiles for step 1.



**Fig. S3** Possible pathways for the formation of **M2**. Energies are given in kcal/mol.



**Fig. S4** Conformational search of **TS5**.



**Table S4. Energies of different conformations of the stereoselective transition states.**

species	Dihedral angle C5-C6-N8-O9	Free energies (a.u.)	relative energies (kcal/mol)
<b>TS5R</b>	6.42	-2515.4192092	0.0
<b>TS5R'</b>	-53.14	-2515.4112696	5.0
<b>TS5R''</b>	139.18	-2515.3992312	12.5
<b>TS5R'''</b>	-62.68	-2515.4131211	3.9
<b>TS5S</b>	17.23	-2515.4083092	6.8
<b>TS5S'</b>	54.81	-2515.4069197	7.7
<b>TS5S''</b>	141.95	-2515.3968339	14.0
<b>TS5S'''</b>	-150.02	-2515.4041551	9.4

## Coordinates

### NHC

C	-1.57720000	-1.28610300	-0.26344600
C	-3.32070900	-2.59395400	0.34098500
C	-3.57573400	-0.20983600	0.84228900
H	-2.88718500	0.56688900	1.18157700
N	-2.52887400	-3.40723400	-0.28305100
N	-1.47864700	-2.57887400	-0.64353600
N	-2.78229600	-1.33579900	0.38935900
C	-4.63328400	-2.81159300	1.02002600
H	-4.75361400	-3.85354500	1.31576600
H	-5.46496100	-2.53547600	0.35536100
C	-4.57584400	-0.62340100	1.98310800
O	-4.63052300	-2.02431700	2.19980900
C	-5.79974400	0.37483400	0.13105500
C	-4.46986300	0.28360600	-0.27327300
C	-4.07991700	0.55933500	-1.57453000
C	-5.07898300	0.95303100	-2.45428000
C	-6.41646500	1.07510900	-2.08196300
C	-6.78160200	0.77980600	-0.77332900
C	-5.94905800	-0.02941900	1.57426300
H	-3.04968500	0.45744600	-1.89881400
H	-7.14793300	1.38272400	-2.81837400
H	-7.82093200	0.85175300	-0.47121200
H	-6.74244800	-0.76682700	1.72924000
H	-6.19023800	0.83893600	2.19523500
C	-0.41759300	-3.12819900	-1.43050200
C	-0.30541800	-2.74058000	-2.76940700
C	0.45516900	-4.04705700	-0.84002200
C	0.72994200	-3.29817700	-3.52034800
C	1.47114400	-4.58053700	-1.63133600
C	1.62567200	-4.21552600	-2.96998600
H	0.83285500	-3.01314800	-4.56469000
H	2.16054100	-5.29631600	-1.18971600
C	0.29735900	-4.43795700	0.60526900
H	-0.60523500	-5.03765500	0.75221100
H	0.19983500	-3.55081800	1.23830400
H	1.15876600	-5.01618600	0.94362100
C	2.75292700	-4.78135400	-3.79529200
H	3.00136100	-5.79768500	-3.48095500
H	3.65609600	-4.17227500	-3.68568000
H	2.49465100	-4.80066000	-4.85643500
C	-1.26333200	-1.75164200	-3.38136100
H	-2.29908800	-1.98435400	-3.11530600

H	-1.17486500	-1.75404300	-4.46916000
H	-1.05942900	-0.73898300	-3.02114900
H	-4.24014300	-0.21753700	2.93724500
N	-4.70838600	1.23248600	-3.84631400
O	-5.58015500	1.62542700	-4.60212500
O	-3.54744700	1.05327500	-4.17290000
<b>R1</b>			
C	-0.23307600	1.06972500	-0.44478600
C	-1.54671800	1.20311000	0.08001900
C	-1.97061800	2.46233200	0.55174700
C	-1.09477400	3.52531600	0.48891000
C	0.20939300	3.36878500	-0.03869400
C	0.65869100	2.15180100	-0.50995800
C	-1.23299800	-0.92950700	-0.56595900
C	-2.16102300	-0.07980500	-0.00851600
H	-2.96999900	2.58582600	0.95705800
H	-1.40444500	4.50126200	0.84760900
H	0.87124600	4.22819300	-0.07220800
H	1.65794900	2.03291000	-0.91527200
N	-0.06927700	-0.23174600	-0.82869100
H	0.76794400	-0.62292900	-1.23486600
H	-3.15880600	-0.36218700	0.29382000
C	-1.36094400	-2.35306400	-0.86912700
H	-0.46785000	-2.82842700	-1.32076600
O	-2.36876400	-2.99417500	-0.64852900
<b>R2</b>			
C	-0.26248700	1.07002200	-0.44039400
C	-1.54960400	1.24362100	0.09197800
C	-1.97153700	2.47714400	0.56634100
C	-1.08170100	3.54832600	0.50221000
C	0.19751800	3.36374000	-0.02745900
C	0.63385300	2.12426600	-0.50773800
C	-1.17881400	-1.02297000	-0.61915600
C	-2.22660400	-0.05788400	0.02152700
H	-2.97066900	2.59102400	0.97442200
H	-1.37876900	4.52576900	0.86417300
H	0.88002800	4.20658900	-0.06731200
H	1.63440800	1.99619500	-0.90515700
N	-0.06601900	-0.25825000	-0.86292100
O	-1.32503600	-2.20186200	-0.84740300
C	1.15562800	-0.76479100	-1.45992300
H	1.39956800	-0.16560700	-2.34379100
H	0.92004700	-1.77926100	-1.79514800
C	2.32062200	-0.77487100	-0.49234200

C	3.56474800	-0.28064300	-0.88176700
C	2.16361900	-1.29822800	0.79297200
C	4.64383500	-0.31235000	-0.00026300
H	3.69014900	0.13328100	-1.87934300
C	3.23867300	-1.32765000	1.67495900
H	1.19506100	-1.68465200	1.10084700
C	4.48209500	-0.83490900	1.27968300
H	5.60744400	0.07637200	-0.31342700
H	3.10767900	-1.73712500	2.67140200
H	5.32011700	-0.85690600	1.96866100
O	-3.33338100	-0.39801200	0.35808800

**NEt<sub>3</sub>**

N	-0.00044900	-0.00049400	-0.17731600
C	-1.10400600	0.84414900	0.28186700
C	-1.04083500	2.27575600	-0.24149500
H	-1.15798700	0.85203200	1.38911800
H	-2.03469600	0.39649100	-0.07477500
H	-1.99897900	2.77278500	-0.07124200
H	-0.27082600	2.87275000	0.25169900
H	-0.84069300	2.27298100	-1.31683100
C	-0.17993100	-1.37804600	0.28326000
C	-1.44990300	-2.04099900	-0.24119400
H	-0.16162000	-1.42715300	1.39061200
H	0.67400000	-1.96024500	-0.07119600
H	-1.40239000	-3.11843800	-0.06519000
H	-2.35346800	-1.66975800	0.24699800
H	-1.54384900	-1.87206200	-1.31778300
C	1.28269300	0.53310500	0.28197600
C	2.49139300	-0.23407500	-0.24513400
H	1.31766400	0.57260300	1.38931500
H	1.35890200	1.56406000	-0.07164300
H	3.40073900	0.34586800	-0.06943600
H	2.62263900	-1.20285400	0.24150400
H	2.39057200	-0.39823800	-1.32185500

**HNEt<sub>3</sub><sup>+</sup>**

N	-0.00078800	-0.00144400	-0.20292800
C	-0.07836800	1.43949900	0.24005300
C	1.13335400	2.26199000	-0.16052300
H	-0.21663700	1.41344600	1.32382600
H	-0.97907300	1.84791600	-0.21570700
H	0.90032300	3.31151000	0.02617400
H	2.02216100	2.01200700	0.41920500
H	1.35620700	2.15661200	-1.22590600
C	-1.20856900	-0.78656800	0.24764900



C	-2.52566200	-0.14891600	-0.15832800
H	-1.11551400	-0.88489100	1.33237300
H	-1.11306500	-1.77366100	-0.20245500
H	-3.31957600	-0.87442100	0.02584100
H	-2.75526200	0.74746000	0.41820200
H	-2.54019400	0.09459500	-1.22455000
C	1.28500000	-0.65374000	0.24363800
C	1.39500300	-2.11202100	-0.16390700
H	1.32624600	-0.52577700	1.32827800
H	2.09138200	-0.07660500	-0.20652300
H	2.41618700	-2.43876600	0.03882400
H	0.72220400	-2.75987000	0.39828600
H	1.21178300	-2.24265800	-1.23388100
H	-0.00449700	-0.00444000	-1.22987000
<b>DQ</b>			
C	-2.80856700	1.28200600	-0.00297800
C	-1.45945600	1.23519800	0.03357600
C	-0.69348900	0.00002000	0.01190100
C	-1.45945800	-1.23515600	0.03363100
C	-2.80856900	-1.28196300	-0.00292100
C	-3.56965500	0.00002000	-0.08946300
H	-0.91807200	2.16744100	0.09051500
H	-0.91807600	-2.16739700	0.09061200
C	0.69347000	0.00001800	-0.01199500
C	1.45943800	-1.23516100	-0.03367200
C	1.45944100	1.23519300	-0.03372600
C	2.80854800	-1.28197000	0.00290100
H	0.91805300	-2.16740200	-0.09063100
C	2.80855100	1.28199900	0.00284500
H	0.91806000	2.16743400	-0.09072500
C	3.56963500	0.00001500	0.08941000
O	4.78991500	0.00001700	0.22173900
O	-4.78993900	0.00001900	-0.22175100
C	3.58585400	-2.59771300	-0.02875600
C	4.55427600	-2.60437200	-1.22727000
C	4.37260600	-2.77527800	1.28383000
C	2.64843000	-3.80158300	-0.17949400
H	4.00441100	-2.48412500	-2.16641600
H	5.29346500	-1.80764000	-1.14664700
H	5.07889400	-3.56478500	-1.26325500
H	3.69142400	-2.78332300	2.14077600
H	4.90056600	-3.73447900	1.26162100
H	5.10281500	-1.97842400	1.42094300
H	3.24718300	-4.71591100	-0.21419100

H	1. 95772300	-3. 88983300	0. 66561300
H	2. 06451200	-3. 74895000	-1. 10431400
C	3. 58586100	2. 59773800	-0. 02886900
C	4. 37260600	2. 77536300	1. 28371400
C	4. 55429100	2. 60433900	-1. 22737800
C	2. 64844200	3. 80160400	-0. 17967100
H	3. 69141800	2. 78345400	2. 14065500
H	5. 10280800	1. 97851100	1. 42087000
H	4. 90057100	3. 73456000	1. 26146100
H	4. 00443200	2. 48404500	-2. 16652100
H	5. 07890800	3. 56475100	-1. 26340600
H	5. 29348100	1. 80761200	-1. 14671200
H	3. 24719700	4. 71592900	-0. 21440700
H	2. 06453000	3. 74892800	-1. 10449200
H	1. 95772800	3. 88989600	0. 66542700
C	-3. 58587100	2. 59775100	0. 02867200
C	-4. 55431000	2. 60441300	1. 22717200
C	-2. 64844500	3. 80161800	0. 17942500
C	-4. 37260400	2. 77531700	-1. 28392500
H	-5. 29351800	1. 80769900	1. 14652600
H	-4. 00446000	2. 48413700	2. 16632400
H	-5. 07890700	3. 56483700	1. 26316500
H	-1. 95774000	3. 88987800	-0. 66568300
H	-3. 24719600	4. 71594600	0. 21413600
H	-2. 06452400	3. 74897000	1. 10424200
H	-4. 90056600	3. 73451800	-1. 26172100
H	-3. 69141100	2. 78336500	-2. 14086200
H	-5. 10280800	1. 97846200	-1. 42104900
C	-3. 58587500	-2. 59770500	0. 02878700
C	-4. 55430400	-2. 60431700	1. 22729600
C	-4. 37261900	-2. 77532300	-1. 28379700
C	-2. 64845200	-3. 80156900	0. 17958100
H	-4. 00444700	-2. 48400600	2. 16643800
H	-5. 29351000	-1. 80760500	1. 14662500
H	-5. 07890300	-3. 56473800	1. 26333100
H	-3. 69143300	-2. 78340100	-2. 14073900
H	-4. 90057700	-3. 73452500	-1. 26155200
H	-5. 10282800	-1. 97847600	-1. 42094400
H	-3. 24720500	-4. 71589500	0. 21432100
H	-1. 95774400	-3. 88985900	-0. 66552200
H	-2. 06453300	-3. 74889200	1. 10439800
<b>DQH<sup>-</sup></b>			
H	-2. 99768600	3. 20904600	12. 87291000
C	-2. 88312000	2. 01102000	10. 72712100

C	-2.91072700	1.12040000	9.65189600
C	-3.30726100	-0.21449900	9.77807300
C	-3.70113200	-0.64368000	11.05141200
C	-3.71952300	0.19430900	12.16577600
C	-3.30122400	1.52788400	11.98351000
H	-2.63268100	1.47214100	8.66621800
H	-3.97890400	-1.68421900	11.16714300
C	-3.30060600	-1.13417900	8.62070900
C	-4.21990700	-2.18777100	8.50959400
C	-2.36769800	-0.99410300	7.58279300
C	-4.22869200	-3.07849400	7.44515400
H	-4.97456700	-2.28202400	9.28607600
C	-2.31654000	-1.84285800	6.48647000
H	-1.63491600	-0.19633400	7.66888100
C	-3.24842200	-2.95084100	6.38154700
O	-3.32305100	2.33412400	13.09874400
O	-3.21065600	-3.77047900	5.40025800
C	-4.16147400	-0.32509500	13.54394100
C	-3.00934300	-0.20565200	14.55886100
C	-5.38977300	0.46027600	14.03981200
C	-4.56358500	-1.80573200	13.49048100
H	-2.14887900	-0.79481900	14.22514500
H	-2.69239900	0.82885000	14.69018200
H	-3.33156900	-0.59773700	15.53013100
H	-6.21823800	0.35167800	13.33215800
H	-5.71682900	0.06307600	15.00744400
H	-5.16997400	1.52132800	14.15642000
H	-4.87950200	-2.12403000	14.48880200
H	-5.39877000	-1.97712800	12.80404200
H	-3.72849100	-2.44365500	13.18494400
C	-2.41879100	3.46670100	10.53149100
C	-3.55845400	4.45777500	10.85397400
C	-1.15883400	3.75318700	11.37832900
C	-2.01606000	3.74686100	9.07582500
H	-4.39019900	4.29509800	10.16243300
H	-3.96957200	4.37205300	11.86335800
H	-3.20456900	5.48607300	10.72787000
H	-0.34007900	3.10975600	11.04367800
H	-0.85106300	4.79551600	11.24692900
H	-1.27502400	3.57740400	12.45123400
H	-1.68299500	4.78586400	8.99248200
H	-1.19277700	3.10265100	8.75378100
H	-2.85567900	3.60705000	8.38923600
C	-1.27848300	-1.63984100	5.37598200

C	-1.99697100	-1.42117400	4.03186300
C	-0.38155100	-0.42091100	5.62287100
C	-0.36670100	-2.87502200	5.27409500
H	-2.65154300	-2.26775000	3.82274500
H	-2.59900800	-0.50616400	4.06972700
H	-1.26633300	-1.31316400	3.22021600
H	0.19936500	-0.52224000	6.54602900
H	0.32595300	-0.31695200	4.79280800
H	-0.96297300	0.50553200	5.68633900
H	0.35946500	-2.75039200	4.46067800
H	0.19085400	-3.01100700	6.20775500
H	-0.97113500	-3.76298600	5.08946900
C	-5.26642400	-4.20478000	7.36234700
C	-6.08550000	-4.06902400	6.06619000
C	-4.55544500	-5.56960500	7.37744200
C	-6.25373300	-4.18495200	8.53515600
H	-6.64639900	-3.12755800	6.07118000
H	-5.41656100	-4.07966100	5.20537900
H	-6.80627000	-4.89222500	5.98132800
H	-4.02301600	-5.70753900	8.32517700
H	-5.28585100	-6.38269300	7.27762700
H	-3.84009500	-5.62192700	6.55669700
H	-6.97019500	-5.00586400	8.41993200
H	-5.74783900	-4.31590000	9.49798100
H	-6.82103600	-3.24861900	8.57253900

**re-TS1**

C	-4.52742200	-6.61944000	1.11489700
C	-5.69986900	-8.26168800	2.04380700
C	-5.45050700	-6.18490300	3.40679100
H	-4.51384900	-5.71311900	3.71333400
N	-5.43343700	-8.69153700	0.84750900
N	-4.71430600	-7.65457800	0.29245900
N	-5.15754800	-7.02344600	2.24640200
C	-6.48111200	-8.89776400	3.14757200
H	-6.35120200	-9.97999800	3.13377100
H	-7.55009700	-8.67552100	3.02614700
C	-6.08473000	-7.02517400	4.57293700
O	-5.98229400	-8.42325700	4.38312200
C	-7.70321300	-5.39968300	3.75279300
C	-6.52955200	-5.19984000	3.03102500
C	-6.46340400	-4.28313700	1.99609300
C	-7.61097800	-3.56417300	1.70820500
C	-8.79374000	-3.70898600	2.43042500
C	-8.83772400	-4.63728100	3.46530100

C	-7.54128600	-6.51266000	4.75351100
H	-5.56129600	-4.14322200	1.41705200
H	-9.66003600	-3.11709500	2.16210200
H	-9.75768500	-4.78084100	4.02181100
H	-8.26574300	-7.31563400	4.58414100
H	-7.70007500	-6.15964400	5.77583600
C	-4.29951600	-7.74978200	-1.08111500
C	-5.12837000	-7.20740600	-2.06167600
C	-3.07949000	-8.36745300	-1.36617200
C	-4.69848200	-7.29699800	-3.38706800
C	-2.69809300	-8.44007800	-2.70204400
C	-3.49229600	-7.90738100	-3.72221200
H	-5.31553900	-6.86327700	-4.16991200
H	-1.74726200	-8.90531000	-2.95321600
C	-2.20514800	-8.86384800	-0.24721600
H	-2.72336600	-9.61959000	0.35189400
H	-1.94450200	-8.03215100	0.42009900
H	-1.28772600	-9.30456600	-0.64183500
C	-3.03805300	-7.98763700	-5.15629900
H	-3.02572800	-9.02447200	-5.50713000
H	-2.02512000	-7.58844500	-5.26193500
H	-3.69610900	-7.41075600	-5.80961500
C	-6.42746300	-6.53832000	-1.69871000
H	-7.05469900	-7.19671200	-1.08959200
H	-6.98220800	-6.26335200	-2.59732800
H	-6.24921600	-5.62697400	-1.11644500
H	-5.50840400	-6.83579300	5.47830300
N	-7.57292000	-2.64829700	0.56579400
O	-8.51286500	-1.89654500	0.40132700
O	-6.59731700	-2.69630700	-0.17310700
C	-3.59896300	-4.24524800	-2.23976200
C	-2.34972400	-4.88939000	-2.42591500
C	-1.82450400	-4.98128900	-3.72435400
C	-2.54740400	-4.45310000	-4.78116900
C	-3.78948700	-3.81996000	-4.57007000
C	-4.33004700	-3.70109800	-3.29958700
C	-2.91263300	-5.01920100	-0.24876200
C	-1.93190000	-5.36050200	-1.13706900
H	-0.87241200	-5.47609900	-3.89599200
H	-2.15655400	-4.52938300	-5.79117300
H	-4.33186800	-3.41693500	-5.41976000
H	-5.28809300	-3.21883000	-3.12892000
N	-3.90979100	-4.32366300	-0.90372700
H	-4.72876500	-3.90302900	-0.48500000

H	-1.04889000	-5.93174900	-0.89014100
C	-3.02110200	-5.39191800	1.19804300
H	-3.56642200	-4.61375500	1.78042000
O	-2.09990600	-6.03746100	1.75282500
<b>si-TS1</b>			
C	-4.74320000	-6.90185400	0.80066800
C	-6.54976600	-8.16271700	1.09193800
C	-6.47005200	-6.17227800	2.53762100
H	-5.65007200	-5.62091600	2.99774800
N	-5.88776900	-8.77193900	0.15683300
N	-4.78130300	-7.96850600	-0.00756000
N	-5.88688900	-7.03966200	1.51399500
C	-7.78604300	-8.55051400	1.83200900
H	-8.01355600	-9.60446100	1.67471600
H	-8.64634900	-7.94725900	1.51008200
C	-7.28908100	-7.01172200	3.58756100
O	-7.49693400	-8.36350000	3.20666500
C	-8.69274800	-5.27172100	2.63355800
C	-7.48471900	-5.22516600	1.94086800
C	-7.30004800	-4.39016100	0.84867800
C	-8.38507900	-3.60546000	0.47852400
C	-9.60757300	-3.62528600	1.14823800
C	-9.76279700	-4.46881200	2.24077700
C	-8.62257000	-6.24776900	3.77719300
H	-6.35480300	-4.34817600	0.31725400
H	-10.41253400	-2.98719800	0.80644500
H	-10.70714000	-4.50137500	2.77372300
H	-9.46200600	-6.94946600	3.79354200
H	-8.62662100	-5.71605300	4.73392100
C	-3.78194900	-8.33732100	-0.96727800
C	-3.97550900	-7.97131200	-2.30161400
C	-2.64379600	-9.00767500	-0.51669100
C	-2.97802300	-8.31242900	-3.21095500
C	-1.66150100	-9.30992500	-1.46200900
C	-1.81571100	-8.97641000	-2.80875500
H	-3.09582400	-8.02317100	-4.25236700
H	-0.76029900	-9.82457300	-1.13828400
C	-2.48286800	-9.36874200	0.93665500
H	-3.35950600	-9.91087900	1.30313600
H	-2.37226700	-8.47318400	1.55721100
H	-1.60126200	-9.99475400	1.08171400
C	-0.75815100	-9.33841000	-3.81875300
H	-1.02370500	-10.26499900	-4.33772400
H	0.21188700	-9.48996700	-3.34088600

H	-0.65388800	-8.55815200	-4.57734400
C	-5.18051000	-7.16731500	-2.70469100
H	-6.10777800	-7.70177900	-2.47740200
H	-5.15516200	-6.94225000	-3.77216300
H	-5.20041300	-6.21846400	-2.15408600
H	-6.73231100	-7.07814200	4.52230400
N	-8.23885800	-2.70783400	-0.67311900
O	-9.19665800	-2.02338300	-0.98983100
O	-7.16742100	-2.69400300	-1.25546800
C	-2.57763300	-4.90628500	-2.46632600
C	-3.52352500	-3.85086700	-2.41382800
C	-3.75663300	-3.09065800	-3.57262500
C	-3.05985100	-3.39769400	-4.72827200
C	-2.12296800	-4.45200900	-4.75643200
C	-1.86756600	-5.21793100	-3.63157200
C	-3.44760400	-4.85548900	-0.39685400
C	-4.05308700	-3.83340000	-1.08136700
H	-4.47936100	-2.28016200	-3.55707800
H	-3.23488400	-2.82165300	-5.63127700
H	-1.59203800	-4.66693300	-5.67837400
H	-1.14956500	-6.03235700	-3.64740700
N	-2.54063300	-5.48656100	-1.22203400
H	-2.01061300	-6.31338400	-0.98316800
H	-4.77902200	-3.14745900	-0.67089700
C	-3.63821200	-5.24087400	1.04038200
H	-2.77144300	-5.80606600	1.43996800
O	-4.29695900	-4.47198400	1.77828400

**re-M1**

C	-4.68457200	-6.31908100	0.77325000
C	-6.10326100	-7.77171800	1.61111800
C	-5.44910900	-5.94553600	3.14855100
H	-4.49436700	-5.41476200	3.23333400
N	-5.84993100	-8.21486600	0.41637200
N	-4.96976500	-7.28968600	-0.09835700
N	-5.40988400	-6.62494000	1.86304200
C	-6.85572300	-8.35486300	2.76147600
H	-7.09085700	-9.40238500	2.57779600
H	-7.78696200	-7.80200200	2.94575100
C	-5.61645600	-6.99241000	4.31372200
O	-5.97338000	-8.29396600	3.87024100
C	-7.35497300	-5.30447200	4.45548500
C	-6.66603600	-5.05581200	3.26867000
C	-7.11913400	-4.11870900	2.35223200
C	-8.27922500	-3.42885000	2.68178400

C	-8.98247600	-3.64226400	3.86429700
C	-8.51466800	-4.59523400	4.76134100
C	-6.67670000	-6.38062500	5.25866200
H	-6.61666100	-3.92435500	1.41053900
H	-9.88221900	-3.07316300	4.06066900
H	-9.05518200	-4.78735800	5.68195400
H	-7.36612600	-7.15441000	5.60787100
H	-6.19490600	-5.95027200	6.14244600
C	-4.37124900	-7.54661600	-1.38479200
C	-5.06242000	-7.18787900	-2.53887100
C	-3.11933700	-8.16858500	-1.39669600
C	-4.44166100	-7.44915900	-3.76187400
C	-2.54489700	-8.40995300	-2.64013200
C	-3.18569100	-8.04803400	-3.82893200
H	-4.94602200	-7.15540300	-4.67870800
H	-1.56183400	-8.87324300	-2.68393400
C	-2.42862500	-8.52131400	-0.10655700
H	-3.01680100	-9.25240600	0.45953200
H	-2.30210200	-7.63460900	0.52941200
H	-1.44719500	-8.95551200	-0.30600700
C	-2.52324000	-8.30829800	-5.15646100
H	-2.56895700	-9.37122300	-5.41555500
H	-1.46960000	-8.01832100	-5.12459400
H	-3.00680700	-7.74071000	-5.95444500
C	-6.41778800	-6.53998600	-2.46362000
H	-7.16209100	-7.23325100	-2.05955500
H	-6.74614400	-6.21934000	-3.45363500
H	-6.39947900	-5.66438800	-1.80702700
H	-4.66082000	-7.13385600	4.81768900
N	-8.79151200	-2.43603100	1.73003600
O	-9.79334700	-1.81507700	2.03721300
O	-8.18676000	-2.28794900	0.68176700
C	-3.39401100	-4.37797800	-2.73420400
C	-2.10741200	-4.94977800	-2.56537800
C	-1.30956900	-5.15794100	-3.70084000
C	-1.80262200	-4.80150900	-4.94574700
C	-3.08103000	-4.22540100	-5.08548400
C	-3.89137400	-4.00047800	-3.98370700
C	-3.13348700	-4.89643500	-0.56163000
C	-1.96290900	-5.24814200	-1.16776200
H	-0.32594700	-5.60909400	-3.60303000
H	-1.19861200	-4.97095800	-5.83196400
H	-3.43836100	-3.95529500	-6.07428200
H	-4.88197600	-3.56772700	-4.08692500



N	-3.99202800	-4.34931100	-1.49562400
H	-4.87302200	-3.90589900	-1.28312000
H	-1.13565600	-5.73655100	-0.67404600
C	-3.60898100	-5.18703900	0.84461500
H	-4.22898100	-4.29514000	1.15011600
O	-2.70291900	-5.58892000	1.72330300
<b>si-M1</b>			
C	-4.78674000	-6.72157100	0.84203900
C	-6.48385100	-8.03881300	1.27278600
C	-6.41902500	-6.00379400	2.69245100
H	-5.57236300	-5.47071900	3.12132800
N	-5.85717800	-8.62767700	0.29912900
N	-4.80671500	-7.79205500	0.04279300
N	-5.85916900	-6.87768300	1.64367100
C	-7.65259500	-8.49341100	2.07993100
H	-7.80015900	-9.56626300	1.96095900
H	-8.56938500	-7.97031500	1.77450500
C	-7.24102100	-6.85214500	3.73812800
O	-7.32160000	-8.23453100	3.43003800
C	-8.67714800	-5.17794300	2.71044400
C	-7.42993600	-5.04766800	2.10454200
C	-7.19692300	-4.12471500	1.09386700
C	-8.28758900	-3.37030300	0.68552900
C	-9.55619400	-3.48497000	1.25389500
C	-9.75075100	-4.39407200	2.28570500
C	-8.64140400	-6.19240800	3.82027700
H	-6.18893400	-3.99108500	0.70766900
H	-10.36278800	-2.86252900	0.88791300
H	-10.72651300	-4.48990800	2.74978000
H	-9.42524500	-6.95143800	3.73292200
H	-8.77904200	-5.70451400	4.78957700
C	-3.88055500	-8.09943700	-1.01157100
C	-4.23371800	-7.75473600	-2.32014500
C	-2.66655200	-8.69552300	-0.67232500
C	-3.28355400	-7.98277300	-3.31081900
C	-1.75084200	-8.90774700	-1.70490800
C	-2.03775800	-8.54568800	-3.02128000
H	-3.51174000	-7.69078900	-4.33332100
H	-0.79239200	-9.36425800	-1.47130900
C	-2.35463600	-9.07887400	0.75106900
H	-3.18036200	-9.63987000	1.19774900
H	-2.18290300	-8.19627700	1.37726500
H	-1.45625000	-9.69626200	0.79099300
C	-1.03187400	-8.74783700	-4.12358100

H	-1.38875800	-9.48741700	-4.84653400
H	-0.07298500	-9.09102800	-3.73021900
H	-0.87098900	-7.80984600	-4.66353800
C	-5.58475200	-7.17773100	-2.64479700
H	-6.33848400	-7.97031100	-2.69358500
H	-5.55438200	-6.66742100	-3.60905600
H	-5.90208200	-6.45471800	-1.88944000
H	-6.73149800	-6.82067800	4.70052100
N	-8.09541700	-2.39583500	-0.39491200
O	-9.03876400	-1.68623700	-0.70036600
O	-7.00362300	-2.34911400	-0.93597900
C	-2.12631800	-5.04423500	-2.35093200
C	-3.33746500	-4.35836700	-2.62205700
C	-3.53617300	-3.82613500	-3.90837600
C	-2.54968000	-3.99116000	-4.86598300
C	-1.35032200	-4.67217200	-4.56853200
C	-1.12044100	-5.20262200	-3.30977500
C	-3.40596800	-5.13420500	-0.50422100
C	-4.12413000	-4.41383300	-1.42316500
H	-4.45500100	-3.29778000	-4.14548700
H	-2.69582800	-3.58841400	-5.86316800
H	-0.59444100	-4.78216800	-5.33992400
H	-0.20292900	-5.73479800	-3.07626800
N	-2.19220900	-5.48613400	-1.05361700
H	-1.50397100	-6.07218300	-0.60494500
H	-5.10283100	-3.98078700	-1.26492400
C	-3.78309800	-5.51878300	0.92648000
H	-2.86589400	-6.01547300	1.35247600
O	-4.30350300	-4.54027900	1.64946000

**M02**

C	0.17011700	-0.22824100	0.44131900
C	-1.08317800	-1.73622400	1.39647700
C	-1.47038100	0.53098400	2.29984600
H	-0.80520000	1.36431300	2.51728600
N	-0.42688700	-2.38100400	0.47924600
N	0.34249400	-1.42858200	-0.11246200
N	-0.74464100	-0.40673000	1.41516000
C	-2.01231000	-2.24418500	2.44850300
H	-1.86159000	-3.31333800	2.59287600
H	-3.05930900	-2.06397400	2.17036500
C	-1.93490000	-0.19041000	3.62637800
O	-1.65417700	-1.57717600	3.64258900
C	-3.85973900	0.72343900	2.45200700
C	-2.75563200	0.97191800	1.63871400

C	-2.89148100	1.53352500	0.37877500
C	-4.17994300	1.82748500	-0.04024500
C	-5.30693200	1.59662200	0.74478900
C	-5.14344000	1.04022700	2.00816800
C	-3.44560000	0.11976300	3.76555000
H	-2.03756100	1.75058500	-0.24948100
H	-6.28681800	1.84816200	0.35866200
H	-6.00869900	0.84713800	2.63295500
H	-4.00066500	-0.79053600	4.01179700
H	-3.61370700	0.82668800	4.58313600
C	1.15037300	-1.76765200	-1.25927800
C	0.53323400	-1.76357600	-2.51408600
C	2.49933300	-2.05825700	-1.05831900
C	1.34970800	-2.01377500	-3.61366700
C	3.26939100	-2.30578700	-2.19487300
C	2.71488200	-2.27497400	-3.47521800
H	0.91118200	-1.97977700	-4.60830900
H	4.32693400	-2.52460200	-2.07318200
C	3.08779100	-2.09884800	0.32524200
H	2.66653400	-2.93242800	0.89833300
H	2.87813700	-1.18148100	0.88834200
H	4.17002400	-2.23105400	0.28017200
C	3.56066300	-2.52140500	-4.69566000
H	3.38678000	-1.74149200	-5.44233200
H	3.30625200	-3.48167700	-5.15444200
H	4.62358200	-2.53515000	-4.44707200
C	-0.94276500	-1.52403600	-2.68487500
H	-1.49163100	-2.46685100	-2.59396700
H	-1.14050000	-1.10343100	-3.67273100
H	-1.34316200	-0.83131800	-1.94020500
H	-1.36951500	0.21053600	4.46823100
N	-4.35459900	2.40523100	-1.37864800
O	-5.47934400	2.71414200	-1.72371000
O	-3.36025500	2.54020100	-2.07351500
C	2.08670100	1.19823900	-3.39537800
C	0.73407500	1.55800000	-3.60223000
C	0.27484800	1.76658800	-4.91580900
C	1.16178200	1.60631200	-5.96274400
C	2.50958600	1.24982200	-5.73117500
C	2.99279200	1.04389300	-4.45248700
C	1.06720800	1.22908200	-1.40378400
C	0.10675800	1.58650200	-2.31496700
H	-0.76012800	2.03961800	-5.09730200
H	0.82339900	1.75635500	-6.98248200

H	3.17966800	1.13274500	-6.57691500
H	4.02489200	0.75960800	-4.27233600
N	2.26738300	1.02516100	-2.04673700
H	3.12114900	0.70329300	-1.61546900
H	-0.92936500	1.82099400	-2.10828400
C	0.91786600	1.04501500	0.07989400
H	0.51618900	2.92862500	0.32520600
O	0.16197600	2.08936500	0.65113200
N	2.65369200	0.09559000	2.98915200
C	2.41590100	1.50930800	3.27451400
C	2.15267700	1.90925900	4.73036200
H	1.55375500	1.84083400	2.67743100
H	3.28036500	2.06350900	2.88932500
H	2.01336900	2.99242500	4.79324300
H	1.23903000	1.43814500	5.10723200
H	2.97539200	1.63117800	5.39254700
C	1.67721600	-0.83670000	3.54248700
C	1.93713000	-1.43110800	4.92937000
H	1.55944600	-1.67443900	2.83558000
H	0.71430800	-0.31518200	3.56179800
H	1.09307600	-2.06947300	5.20698500
H	2.83857400	-2.05023800	4.93192100
H	2.04968200	-0.65852100	5.69351100
C	4.05003200	-0.33533400	3.05015900
C	4.85852300	0.03096000	4.29882000
H	4.56956700	0.08213900	2.17603700
H	4.05762600	-1.42414700	2.91843300
H	5.86578900	-0.38710300	4.21419600
H	4.96090500	1.11534600	4.39848200
H	4.40463700	-0.35560300	5.21395200
H	1.90430800	0.95456000	0.56843200
<b>re-TS2</b>			
C	-0.20742900	1.06259900	0.31899200
C	-1.40342500	2.32384300	1.67844300
C	-2.55779900	1.88565800	-0.42819700
H	-2.26117300	1.67178100	-1.45129100
N	-0.32109800	2.07770300	2.34170100
N	0.41226400	1.28848900	1.49442600
N	-1.38285400	1.73630600	0.43416300
C	-2.54824400	3.23036600	1.99302300
H	-2.28373400	3.88970000	2.81892000
H	-3.44612400	2.65960300	2.26273800
C	-3.16474200	3.32961800	-0.31925400
O	-2.74949200	4.03049400	0.84163100

C	-4.89849600	1.67012700	0.03002400
C	-3.68528800	0.98214500	0.01404000
C	-3.59842400	-0.34853100	0.38229900
C	-4.78515600	-0.97962400	0.73295800
C	-6.01704000	-0.33227900	0.73985400
C	-6.07330800	1.01324800	0.38938400
C	-4.69546900	3.11079600	-0.36059000
H	-2.65843900	-0.88514300	0.41912200
H	-6.90512200	-0.88078100	1.02767300
H	-7.02109600	1.54019700	0.40835600
H	-5.19711000	3.81387200	0.30972900
H	-5.07701800	3.29032200	-1.37106800
C	1.65186900	0.72250000	1.94057800
C	1.61185600	-0.54989000	2.51753300
C	2.83189700	1.45129600	1.77406100
C	2.83048200	-1.13582000	2.86135500
C	4.02206200	0.83185800	2.15300700
C	4.04225700	-0.46159700	2.67968900
H	2.83217400	-2.13381200	3.29344600
H	4.95824000	1.36636700	2.01429600
C	2.81868100	2.82305100	1.15980300
H	2.08081000	3.46540500	1.64853500
H	2.55969600	2.76509800	0.09664500
H	3.80087500	3.28921300	1.24759800
C	5.34246000	-1.10371800	3.08535200
H	5.28285900	-2.19211900	3.01931500
H	5.58576200	-0.84687000	4.12119600
H	6.16660400	-0.75833300	2.45726700
C	0.29768500	-1.23940500	2.77434000
H	-0.26910300	-0.70598200	3.54349200
H	0.45537700	-2.26528100	3.11326900
H	-0.32641500	-1.26676800	1.87407400
H	-2.82330300	3.94635100	-1.15072500
N	-4.72783100	-2.39410200	1.11691300
O	-5.76533500	-2.94422300	1.43283900
O	-3.63698900	-2.94398300	1.09531000
C	3.89098900	0.38840200	-1.38920900
C	3.46750700	1.38869500	-2.29674400
C	4.43466500	2.07308400	-3.05321400
C	5.76896000	1.75688500	-2.87248000
C	6.16803200	0.76854800	-1.94814200
C	5.24012200	0.07266500	-1.19339600
C	1.65076000	0.55318200	-1.23665000
C	2.04031800	1.47696000	-2.17689600

H	4.13648300	2.84204600	-3.75914000
H	6.52747600	2.27986300	-3.44549100
H	7.22410000	0.55132800	-1.82621000
H	5.54055400	-0.68770100	-0.47916800
N	2.76639900	-0.13671900	-0.79897000
H	2.77711200	-0.74539600	0.00942200
H	1.39275800	2.16169800	-2.70943900
C	0.27246600	0.20294100	-0.76747100
H	-0.35297800	0.71961600	-2.56545300
O	-0.67955000	0.17963800	-1.83255900
N	0.34910300	-2.47497100	-0.99539600
C	1.38453300	-3.09473200	-0.12613900
C	1.21494700	-4.56587900	0.22828200
H	1.39929900	-2.50930200	0.80005500
H	2.34626100	-2.93179200	-0.62207400
H	2.04690800	-4.85829600	0.87361600
H	0.29008500	-4.74175200	0.78271100
H	1.22684500	-5.21163300	-0.65135200
C	-1.05925500	-2.83422400	-0.67904300
C	-1.63284900	-4.09545900	-1.31236500
H	-1.65067900	-1.97634400	-1.01591300
H	-1.13942800	-2.88606300	0.41158100
H	-2.65595100	-4.20908500	-0.94584400
H	-1.67517900	-4.01229600	-2.40080500
H	-1.07710800	-4.99582900	-1.04847600
C	0.67610600	-2.49577900	-2.45006400
C	1.17559600	-3.82154700	-3.01258200
H	1.44252300	-1.72813300	-2.60281000
H	-0.22175100	-2.15750700	-2.97210200
H	1.36121300	-3.68920700	-4.08120500
H	2.11926400	-4.12687400	-2.55430400
H	0.45243300	-4.62987800	-2.89424300
H	0.35542000	-1.24877400	-0.66226400
<b>si-TS2</b>			
C	-4.63344100	-6.32694800	0.80438200
C	-5.82861500	-7.86547300	1.83842800
C	-6.29556200	-5.58030400	2.63614800
H	-5.68298900	-4.70113000	2.82178800
N	-5.21908900	-8.51301800	0.90145300
N	-4.49521100	-7.54571400	0.24111600
N	-5.50940000	-6.52842700	1.83387300
C	-6.74172500	-8.35787400	2.91257000
H	-6.55150400	-9.41127700	3.11517700
H	-7.79231000	-8.23847100	2.61353000

C	-6.76850300	-6.24414500	3.98406000
O	-6.43619000	-7.61739000	4.07784400
C	-8.69456700	-5.48937400	2.70182800
C	-7.57574000	-5.23362900	1.91127100
C	-7.69033400	-4.77113200	0.60872000
C	-8.97770400	-4.58532900	0.12620800
C	-10.12011400	-4.82542600	0.88678800
C	-9.97615300	-5.27967400	2.19270500
C	-8.29437200	-5.98632000	4.06521500
H	-6.82480900	-4.55091600	-0.00651000
H	-11.09635600	-4.66196500	0.44820700
H	-10.85344100	-5.47872800	2.79849100
H	-8.82010900	-6.89991700	4.35867800
H	-8.51220000	-5.23351900	4.82835000
C	-3.88087200	-7.85800800	-1.01601200
C	-4.49310200	-7.37787700	-2.17879900
C	-2.70023800	-8.60298200	-1.02311900
C	-3.83224400	-7.60735300	-3.38370600
C	-2.08697200	-8.81859000	-2.25661200
C	-2.62550800	-8.30849600	-3.43998100
H	-4.27293700	-7.23042600	-4.30315100
H	-1.16272600	-9.38980900	-2.29164700
C	-2.08456100	-9.10212900	0.25838900
H	-2.82278800	-9.59800100	0.89305300
H	-1.65984600	-8.27424500	0.84095900
H	-1.27541100	-9.80240700	0.04796100
C	-1.91144100	-8.48537900	-4.75276800
H	-1.36719400	-7.56808200	-5.00249300
H	-2.61729600	-8.68331100	-5.56272000
H	-1.19201600	-9.30530900	-4.70806400
C	-5.80564900	-6.63928400	-2.13105100
H	-6.49857100	-7.09901400	-1.41896200
H	-6.27678100	-6.63887100	-3.11507900
H	-5.65701100	-5.59462400	-1.83838800
H	-6.24321800	-5.78162100	4.81942600
N	-9.13524900	-4.12432100	-1.25901300
O	-10.26366900	-3.91126100	-1.66391400
O	-8.12580500	-3.98469700	-1.92894900
C	-1.61791300	-5.08195700	-2.32806800
C	-2.53151100	-4.08074100	-2.73602800
C	-2.33998500	-3.45404600	-3.97926700
C	-1.27237500	-3.84487000	-4.76848400
C	-0.38051900	-4.85135300	-4.34351800
C	-0.53873100	-5.48425300	-3.12124200

C	-3.19051700	-4.88744900	-0.72940300
C	-3.51525700	-3.96962900	-1.69839000
H	-3.02595400	-2.68303600	-4.31609800
H	-1.11610100	-3.37334700	-5.73304700
H	0.44489800	-5.13713100	-4.98762300
H	0.14013000	-6.26598300	-2.79407300
N	-2.01267600	-5.51871600	-1.08492900
H	-1.62206000	-6.32475900	-0.62103200
H	-4.37419000	-3.31404000	-1.67463200
C	-3.88157500	-5.11135100	0.56737200
H	-4.15500200	-3.21355500	0.90340100
O	-4.71490900	-4.00109100	0.89597000
N	-2.14051700	-5.15900800	2.68010600
C	-2.54536200	-3.91803000	3.39543100
C	-2.17832800	-3.82124200	4.87069200
H	-3.63356300	-3.84886000	3.29520600
H	-2.12006600	-3.08247900	2.83033300
H	-2.52445700	-2.85567000	5.24650300
H	-2.67447300	-4.59822700	5.45686100
H	-1.10361000	-3.88504700	5.04387800
C	-2.48449600	-6.42757700	3.37767900
C	-1.43456600	-7.00940400	4.31477500
H	-2.70204000	-7.16282400	2.59184900
H	-3.42467900	-6.25123600	3.91174400
H	-1.83476600	-7.92880300	4.74789900
H	-0.51957900	-7.26963700	3.77740200
H	-1.18147000	-6.33202400	5.13168100
C	-0.78408800	-5.11457700	2.06784800
C	0.35889700	-4.60925400	2.93852300
H	-0.87286800	-4.47251400	1.18501600
H	-0.57315100	-6.12724600	1.70695400
H	1.27984400	-4.66186500	2.35332800
H	0.21155900	-3.56454900	3.22146600
H	0.49846200	-5.20340200	3.84252200
H	-2.90409700	-5.18866700	1.66417000
<b>re-TS2<sup>D</sup></b>			
C	0.03062000	0.26728600	-0.43585600
C	1.20431000	0.07042500	-2.29239300
C	2.24382300	1.57461600	-0.62824600
H	1.81355300	2.23622800	0.12044800
N	0.15225900	-0.65303800	-2.50773600
N	-0.57109400	-0.53212900	-1.34545900
N	1.17664200	0.66347300	-1.05515500
C	2.30097800	0.47929300	-3.21639600



H	2.04861600	0.22097800	-4.24415600
H	3.25127300	-0.00205300	-2.94616700
C	2.82979400	2.36500500	-1.86130000
O	2.37981600	1.89089800	-3.12077600
C	4.61558400	1.19351400	-0.69894700
C	3.42878100	0.81815000	-0.07241500
C	3.41044500	-0.13139300	0.93818900
C	4.62770500	-0.70786800	1.27479000
C	5.83142200	-0.36364500	0.66307600
C	5.82530900	0.60412900	-0.33353300
C	4.36895400	2.26549800	-1.72527300
H	2.49700100	-0.38890900	1.45948100
H	6.74587500	-0.85304700	0.97365300
H	6.75161500	0.88998700	-0.82057100
H	4.81904500	2.04192900	-2.69735700
H	4.78659200	3.21896900	-1.38719800
C	-1.75061500	-1.31284300	-1.13199500
C	-1.61170500	-2.52896500	-0.45450900
C	-2.98413400	-0.80282500	-1.53915200
C	-2.77671800	-3.23892800	-0.16529900
C	-4.11937200	-1.55666400	-1.24328400
C	-4.03546400	-2.76720800	-0.55307500
H	-2.70052200	-4.18063900	0.37267500
H	-5.09449100	-1.17264800	-1.53211900
C	-3.08437400	0.55600100	-2.17390800
H	-2.34160600	0.68465600	-2.96540800
H	-2.90515200	1.32962400	-1.41650500
H	-4.07867800	0.71250300	-2.59467000
C	-5.27657900	-3.56351600	-0.24470200
H	-5.18600700	-4.07843500	0.71460800
H	-5.44469500	-4.32469200	-1.01322400
H	-6.15942500	-2.92115100	-0.21408900
C	-0.25327300	-3.01122500	-0.02064200
H	0.44047200	-3.04003900	-0.86611800
H	-0.31689600	-4.00985500	0.41323500
H	0.16766400	-2.33320200	0.73067200
H	2.49171900	3.40035400	-1.82582000
N	4.64667100	-1.72834800	2.32906500
O	5.72494100	-2.19718600	2.65145100
O	3.58228300	-2.05613800	2.82421200
C	-3.98531800	0.71367600	1.52455800
C	-3.69709000	2.10240200	1.46974200
C	-4.75597800	3.01531400	1.61771100
C	-6.04136200	2.53312700	1.79645000

C	-6.30406900	1.14785800	1.83154100
C	-5.28385100	0.22118700	1.69512900
C	-1.77813200	0.94770200	1.15550500
C	-2.28759300	2.22127500	1.23877000
H	-4.56617900	4.08413700	1.58458200
H	-6.86537100	3.23085000	1.90721600
H	-7.32412000	0.80237500	1.96602500
H	-5.47747400	-0.84744800	1.71620200
N	-2.79980600	0.04381100	1.36812300
H	-2.70071000	-0.95992700	1.29800600
H	-1.70700500	3.12805200	1.15083300
C	-0.36859200	0.54150000	0.91832700
H	0.25929300	0.01617000	1.77099700
O	0.63795100	1.26045800	1.69481200

**si-TS2<sup>D</sup>**

C	-4.78465000	-6.72457400	0.89617900
C	-6.17393500	-8.26666900	1.63291800
C	-6.34846600	-6.04543900	2.79155100
H	-5.53446800	-5.52763600	3.29608900
N	-5.59111000	-8.82455900	0.62115700
N	-4.73697700	-7.85601500	0.15231700
N	-5.72522900	-6.98595600	1.84835200
C	-7.20222500	-8.84455200	2.54928100
H	-7.01532300	-9.90908600	2.69324200
H	-8.20408500	-8.72733700	2.11708100
C	-7.30175300	-6.81487200	3.77367400
O	-7.08917700	-8.21412600	3.80712300
C	-8.60190800	-5.29560500	2.40911600
C	-7.26481100	-5.07697000	2.07826200
C	-6.88488500	-4.07525200	1.19286500
C	-7.91260700	-3.32614400	0.63286700
C	-9.25980700	-3.52619400	0.92940400
C	-9.60772100	-4.51841900	1.83598500
C	-8.75255000	-6.40496600	3.41265200
H	-5.83082500	-3.86977800	1.00400600
H	-10.00789600	-2.90243000	0.45681400
H	-10.64938000	-4.68175100	2.09154600
H	-9.31838400	-7.24563200	2.99864500
H	-9.29572600	-6.07419000	4.30151300
C	-3.80374300	-8.12979600	-0.89817200
C	-4.18636500	-7.90288500	-2.22382800
C	-2.52028400	-8.54559200	-0.53835700
C	-3.21342700	-8.06733800	-3.20658300
C	-1.58344900	-8.70796800	-1.56002000

C	-1.91004300	-8.45999100	-2.89368000
H	-3.47188400	-7.85749300	-4.24225200
H	-0.57438100	-9.02214900	-1.30426200
C	-2.16148000	-8.75845100	0.90842400
H	-2.87623800	-9.42616700	1.39862500
H	-2.17916800	-7.80532800	1.44995400
H	-1.16328300	-9.18899500	1.00115800
C	-0.88413000	-8.60209000	-3.98742900
H	-1.12358700	-9.44740000	-4.63984700
H	0.11501700	-8.76248600	-3.57698600
H	-0.86448800	-7.70060400	-4.60685700
C	-5.59321000	-7.50036600	-2.57185400
H	-6.25210400	-8.37497200	-2.57889000
H	-5.62223000	-7.03761200	-3.56032700
H	-5.99165600	-6.78619900	-1.84747400
H	-7.06586700	-6.48143600	4.78464200
N	-7.56690100	-2.25722800	-0.31234500
O	-8.47742400	-1.61283200	-0.80596800
O	-6.38769900	-2.07009000	-0.55748300
C	-2.26861500	-4.94986500	-2.40257400
C	-3.54988300	-4.43728200	-2.72930000
C	-3.78325800	-3.98640000	-4.04051100
C	-2.76171500	-4.06495700	-4.97089100
C	-1.49518400	-4.57993700	-4.62157700
C	-1.22976300	-5.02424200	-3.33750000
C	-3.57691700	-5.14308900	-0.58227700
C	-4.35735300	-4.56373300	-1.55208300
H	-4.75535900	-3.58897800	-4.31774500
H	-2.93225800	-3.72474600	-5.98734300
H	-0.71456600	-4.62997000	-5.37448500
H	-0.25917100	-5.42812700	-3.06496800
N	-2.30751200	-5.33969000	-1.09011900
H	-1.58444100	-5.85495600	-0.61085300
H	-5.38987600	-4.26646900	-1.43185100
C	-3.93151800	-5.57989100	0.79196800
H	-3.15488900	-5.46315800	1.67914000
O	-4.08436300	-4.56175100	1.82563500
<b>re-TS2<sup>N</sup></b>			
C	-3.71447900	-0.92571500	0.51250200
C	-5.07066300	-1.16523800	0.30655200
C	-6.01618700	-0.70351800	1.22305500
C	-5.58416800	-0.00505700	2.34301000
C	-4.21627700	0.20188400	2.52347600
C	-3.25146600	-0.25013900	1.63267200

C	-2.86859700	-1.50507400	-0.59758000
C	-3.91662700	-2.01067200	-1.66133100
C	-5.29296400	-1.96078000	-0.95128100
H	-7.07494400	-0.88327600	1.06857500
H	-6.28231900	0.37519000	3.07787600
H	-2.18166600	-0.14067600	1.78939500
H	-3.66388100	-3.02584300	-1.96746200
H	-6.04210000	-1.51666700	-1.61425900
H	-2.22664800	-2.29657400	-0.21506900
H	-5.63752600	-2.97073100	-0.70768200
C	-2.40283300	0.33215300	-2.17188300
C	-0.64033500	-0.26124300	-0.95681700
N	-1.45207700	1.08010700	-2.62766200
N	-1.97458700	-0.49760700	-1.17334200
N	-0.35593700	0.71881600	-1.86649200
C	-3.78480800	0.12769100	-2.69166000
H	-4.53747400	0.52599800	-1.99698900
H	-3.90133200	0.61036600	-3.66142500
O	-3.92685000	-1.27048500	-2.87327000
C	0.76975400	1.59890100	-1.91007100
C	0.78279400	2.67949200	-1.01895800
C	1.73166400	1.44303600	-2.91394900
C	1.85712000	3.56319800	-1.08366800
C	2.80003400	2.34246600	-2.92756100
C	2.88566000	3.39519500	-2.01505700
H	1.89086900	4.40552600	-0.39609500
H	3.57233900	2.22631600	-3.68387800
C	-0.37348500	2.89040700	-0.07886400
H	-1.28206600	3.12077000	-0.64518700
H	-0.57821500	1.98662100	0.50540200
H	-0.17718600	3.71634000	0.60767300
C	4.06818000	4.32755100	-2.02319200
H	4.84383700	3.96501100	-1.34007600
H	4.51114300	4.39898900	-3.01872400
H	3.78261400	5.32971400	-1.69575100
C	1.59307900	0.37426900	-3.96693400
H	2.55160100	0.18629700	-4.45467000
H	1.22267200	-0.56337800	-3.54616600
H	0.87767500	0.69622400	-4.73039400
C	0.13372500	-0.90024000	0.10182800
O	-0.64154300	-1.57303100	0.98613500
H	0.90259700	-0.01018200	1.03398400
N	1.45495100	0.33942000	2.13660700
C	0.29766700	0.61332900	3.03104700

C	0.65609300	1.07615700	4.43741400
H	-0.29895100	-0.29832600	3.03715600
H	-0.30628100	1.37745400	2.53128600
H	-0.26428400	1.13663400	5.02208600
H	1.32943100	0.37415600	4.93801400
H	1.12190400	2.06452900	4.44607800
C	2.32043800	-0.78633000	2.60371200
C	1.55740900	-1.97163900	3.17367400
H	3.02966700	-0.38432500	3.34062500
H	2.89358500	-1.11087800	1.73141500
H	2.24753700	-2.81506300	3.25866500
H	1.16063600	-1.75926500	4.17073200
H	0.73497400	-2.23308900	2.50103100
C	2.27038700	1.56220600	1.93050700
C	3.39498100	1.39335600	0.92135800
H	2.68676000	1.86685700	2.89770800
H	1.58675200	2.35098000	1.60256200
H	3.88385300	2.36019200	0.77708800
H	4.14887800	0.67935700	1.25853100
H	3.01076900	1.06873600	-0.04764900
N	-3.77872900	0.92409000	3.72220100
O	-4.63268600	1.34759300	4.48267900
O	-2.57960400	1.06808800	3.89901400
C	3.28946800	-2.14472700	-1.38513700
C	2.86593100	-3.30739300	-0.68822500
C	3.69309400	-4.44178900	-0.72700500
C	4.88698100	-4.39003700	-1.43422800
C	5.28188400	-3.22458300	-2.11451500
C	4.48481600	-2.08588600	-2.10033400
C	1.29885300	-1.68833100	-0.40758500
C	1.60601800	-2.99099000	-0.08097400
H	3.40093300	-5.34974500	-0.20695100
H	5.52935700	-5.26488300	-1.46416000
H	6.22051200	-3.21335700	-2.65934900
H	4.77928600	-1.18107500	-2.62478500
N	2.31862000	-1.18534000	-1.19951000
H	2.38543000	-0.23323600	-1.52137800
H	0.98603600	-3.61956400	0.53850300
<b>si-TS2<sup>N</sup></b>			
C	-4.57044000	-6.36525900	0.76466100
C	-5.52297200	-7.97713800	1.95936600
C	-6.16424000	-5.69275700	2.67031700
H	-5.57738500	-4.78332300	2.78266100
N	-4.89585100	-8.62108800	1.03366900

N	-4.32214700	-7.61595300	0.26198500
N	-5.37382200	-6.62000500	1.85812900
C	-6.30287200	-8.50557800	3.11609200
H	-5.97149500	-9.51250600	3.36922500
H	-7.37505900	-8.53585900	2.87559700
C	-6.54824100	-6.34654600	4.05073900
O	-6.04206800	-7.66093900	4.22061400
C	-8.56431200	-5.77661000	2.80719100
C	-7.48865400	-5.40848700	2.00406100
C	-7.65751100	-4.87911600	0.73168700
C	-8.96695000	-4.77106600	0.28527900
C	-10.07310800	-5.13550100	1.05409900
C	-9.87000800	-5.63634700	2.33416700
C	-8.09673900	-6.28385800	4.14584200
H	-6.78395500	-4.53819500	0.17297900
H	-11.06780400	-5.02282600	0.64168700
H	-10.71901700	-5.91953600	2.94740200
H	-8.50711100	-7.26811600	4.39433500
H	-8.40410400	-5.60446900	4.94627200
C	-3.91306500	-7.92244200	-1.07009100
C	-4.58879600	-7.32964300	-2.14451200
C	-2.80058500	-8.75550200	-1.25013100
C	-4.05844200	-7.52323700	-3.42028900
C	-2.32050500	-8.92774300	-2.54678900
C	-2.91471500	-8.29052400	-3.63854000
H	-4.55265000	-7.05192100	-4.26644400
H	-1.44563600	-9.55427000	-2.70490700
C	-2.10439500	-9.38670400	-0.07171500
H	-2.77639600	-10.04977600	0.47850300
H	-1.76363700	-8.62540400	0.64078000
H	-1.23435200	-9.95653400	-0.40146900
C	-2.30819100	-8.39710200	-5.01239300
H	-1.56342600	-7.60498400	-5.15089100
H	-3.06469800	-8.28074700	-5.79151000
H	-1.80590700	-9.35696100	-5.15340800
C	-5.82624200	-6.48933100	-1.95472600
H	-6.45219700	-6.87211200	-1.14210400
H	-6.41959700	-6.48493300	-2.87125100
H	-5.56977400	-5.45069500	-1.71668500
H	-6.08530400	-5.77615500	4.85700600
N	-9.20071300	-4.25212200	-1.06738000
O	-10.35474300	-4.07095300	-1.42082000
O	-8.22990200	-4.03542600	-1.77166100
C	-1.48532900	-5.08319600	-2.20518200

C	-2.11746200	-3.83793000	-2.45453100
C	-1.64905200	-3.04876400	-3.51757100
C	-0.60217800	-3.51595600	-4.29735200
C	-0.00309600	-4.76435400	-4.04049800
C	-0.43588400	-5.56442600	-2.99172000
C	-3.17120900	-4.84951900	-0.71968300
C	-3.17103500	-3.71133900	-1.49084000
H	-2.11119000	-2.08910500	-3.73047000
H	-0.23958400	-2.91451300	-5.12515800
H	0.80982000	-5.10702200	-4.67305200
H	0.01313300	-6.53352600	-2.79303200
N	-2.11232200	-5.65075500	-1.12117800
H	-1.94707000	-6.59727000	-0.81826300
H	-3.86716800	-2.89874500	-1.35476500
C	-4.04680800	-5.05533100	0.47256600
H	-3.06731700	-5.07133000	1.48187900
O	-4.84154700	-4.01600900	0.77355200
N	-2.17572600	-4.80498100	2.49171200
C	-2.22518800	-3.37351100	2.88640700
C	-3.57095100	-2.91686300	3.42557200
H	-1.99971300	-2.79286100	1.99067400
H	-1.42167800	-3.19654900	3.61811800
H	-3.52153300	-1.83929600	3.60139400
H	-4.32981400	-3.11673800	2.66109500
H	-3.83270200	-3.39097400	4.37518300
C	-2.59189500	-5.68002300	3.61442300
C	-2.42708600	-7.16994700	3.34398400
H	-3.64537100	-5.46623600	3.81156900
H	-2.02480300	-5.39221500	4.51213300
H	-2.96344400	-7.72685100	4.11595700
H	-2.85128600	-7.45479100	2.37694200
H	-1.38054600	-7.48198500	3.36397400
C	-0.82295100	-5.17510400	2.00214800
C	-0.21342300	-4.17776000	1.02400600
H	-0.92029400	-6.15069300	1.51671000
H	-0.16053500	-5.30375400	2.87116700
H	0.63311700	-4.65298900	0.52276900
H	-0.93142100	-3.87551200	0.25653700
H	0.15656600	-3.28535300	1.53275300
<b>re-M2</b>			
C	0.03006900	1.07609500	-0.82128200
C	1.19394800	0.50874900	-2.63931800
C	2.51118100	1.77080400	-0.97330700
H	2.29284900	2.64482000	-0.36131700

N	0.06057000	-0.06291300	-2.83227800
N	-0.71523700	0.30455200	-1.72362000
N	1.24871600	1.25289200	-1.48160900
C	2.40681500	0.52079000	-3.50802400
H	2.13901800	0.31638500	-4.54441600
H	3.12819000	-0.23963000	-3.17316900
C	3.47596100	2.15031300	-2.16289000
O	2.96311800	1.82112700	-3.44158800
C	4.54716000	0.50958500	-0.71865000
C	3.27381300	0.72241800	-0.19186800
C	2.81003300	-0.00952500	0.89321000
C	3.66045100	-0.98289900	1.40141800
C	4.93623700	-1.22482700	0.89548300
C	5.38691100	-0.46192100	-0.17472100
C	4.82241500	1.44133600	-1.86732200
H	1.83839600	0.17190100	1.33765900
H	5.54986200	-1.99826300	1.33983900
H	6.37721300	-0.63087500	-0.58450700
H	5.18419700	0.92171800	-2.76030800
H	5.58895900	2.17228700	-1.59204600
C	-1.73641100	-0.60695200	-1.29970200
C	-1.38194500	-1.75007600	-0.57458100
C	-3.07285500	-0.30276000	-1.58780600
C	-2.40500300	-2.58124900	-0.11197400
C	-4.06109400	-1.15024100	-1.09421400
C	-3.74718500	-2.28931200	-0.34897700
H	-2.14301000	-3.47152000	0.45572900
H	-5.10514500	-0.90969400	-1.28436000
C	-3.42373700	0.90203200	-2.41723100
H	-3.19735200	0.72103800	-3.47332700
H	-2.84418100	1.77195400	-2.10289100
H	-4.48718200	1.13454300	-2.32774800
C	-4.84612100	-3.16332700	0.19664700
H	-4.44159000	-4.04712100	0.69472400
H	-5.51845400	-3.49536500	-0.59978100
H	-5.44585500	-2.60449200	0.92230900
C	0.05634300	-2.05190500	-0.24019800
H	0.72618200	-1.80407000	-1.06828100
H	0.18150800	-3.10935900	0.00244700
H	0.38445200	-1.47115700	0.63019800
H	3.60177800	3.23251800	-2.19356800
N	3.18428100	-1.79957000	2.52273800
O	3.95750600	-2.60333700	3.01469500
O	2.03597200	-1.63653400	2.90131300



C	-3.51931000	0.49093700	1.88704400
C	-3.96148600	1.66740800	1.22961700
C	-5.32921100	1.99092400	1.26378300
C	-6.20231100	1.14965500	1.93052400
C	-5.73891300	-0.01551100	2.57792900
C	-4.39804400	-0.35911100	2.56922200
C	-1.73768800	1.42875600	0.87865000
C	-2.80747100	2.24821100	0.61106400
H	-5.69322400	2.88490000	0.76553800
H	-7.26140200	1.38505800	1.95867100
H	-6.44924400	-0.65686900	3.09062800
H	-4.03991500	-1.26042500	3.05751900
N	-2.16870600	0.39109500	1.68873700
H	-1.60251300	-0.41032200	1.92362500
H	-2.76899500	3.14399400	0.00728100
C	-0.35312800	1.53299600	0.39641200
H	0.32842200	3.03669900	1.40266000
O	0.60539300	2.12734900	1.22770000

**si-M2**

C	-4.67884800	-6.34488300	0.89009300
C	-5.81406800	-7.92115700	1.99678600
C	-6.38743600	-5.64222500	2.70697400
H	-5.81533500	-4.74078300	2.91204300
N	-5.20440200	-8.58664900	1.08353200
N	-4.49448200	-7.62293000	0.37121000
N	-5.52670000	-6.57491900	1.98466800
C	-6.74980100	-8.41837200	3.04857900
H	-6.53316200	-9.45919400	3.28891400
H	-7.79078700	-8.34821200	2.69899900
C	-6.90336300	-6.28133700	4.05139100
O	-6.54284200	-7.64176500	4.21165800
C	-8.79355600	-5.60594600	2.67353300
C	-7.64754100	-5.33449200	1.92711500
C	-7.72774000	-4.88551000	0.61521200
C	-9.00176300	-4.74169300	0.08070400
C	-10.16684100	-5.00351000	0.79849700
C	-10.05995000	-5.43667800	2.11453600
C	-8.43899000	-6.06931800	4.06097600
H	-6.84734000	-4.64921000	0.02829000
H	-11.12956600	-4.87033300	0.32152200
H	-10.95423700	-5.64992600	2.69062100
H	-8.95016600	-6.99469900	4.34453000
H	-8.71638100	-5.31191000	4.80068500
C	-3.96058700	-7.95206600	-0.90184900

C	-4.53480300	-7.41542400	-2.06241000
C	-2.81591400	-8.76238600	-0.94596300
C	-3.87200700	-7.62833500	-3.27128600
C	-2.19748100	-8.95757300	-2.17990300
C	-2.69212300	-8.36858400	-3.34646100
H	-4.28901100	-7.19876900	-4.17952300
H	-1.29719600	-9.56595500	-2.22715500
C	-2.25358900	-9.35616400	0.31913800
H	-2.95581800	-10.06911500	0.75959800
H	-2.08160600	-8.58155300	1.07427000
H	-1.30993400	-9.86676200	0.12003200
C	-1.95493100	-8.50247300	-4.65268100
H	-2.64816700	-8.58224300	-5.49355600
H	-1.30249900	-9.37840400	-4.65486900
H	-1.33199100	-7.61661600	-4.82108600
C	-5.80742400	-6.61128700	-2.02257200
H	-6.45997400	-6.93496900	-1.20585700
H	-6.35002300	-6.71751200	-2.96433000
H	-5.59345500	-5.54713400	-1.87759800
H	-6.43203800	-5.77728300	4.89488900
N	-9.12315800	-4.29857700	-1.31284400
O	-10.24321400	-4.13300200	-1.76507800
O	-8.09668900	-4.12353600	-1.94743100
C	-1.55055200	-5.02542800	-2.06110500
C	-2.20091700	-3.79087800	-2.31547600
C	-1.72645600	-2.98378000	-3.36341500
C	-0.65396700	-3.42463700	-4.12170700
C	-0.03379000	-4.66228200	-3.85872600
C	-0.47324200	-5.47899400	-2.82673500
C	-3.26763700	-4.84170100	-0.61189400
C	-3.27921500	-3.69295900	-1.38148300
H	-2.20343800	-2.03247000	-3.58022300
H	-0.28539700	-2.81038400	-4.93723300
H	0.80143700	-4.98222600	-4.47364500
H	-0.00792500	-6.43909300	-2.62255000
N	-2.18814400	-5.61509400	-0.99768300
H	-1.98908300	-6.54444200	-0.66135000
H	-4.00815200	-2.90050800	-1.29699000
C	-4.18087100	-5.14137900	0.47725300
H	-4.08405100	-3.41378200	1.32974000
O	-4.78630200	-4.00879600	1.03393600
<b>TS3</b>			
C	-4.30663600	-5.63788500	0.98797500
C	-5.15532700	-7.40119500	2.01514400

C	-6.25209200	-5.31529300	2.68955800
H	-5.88552300	-4.31844200	2.90888900
N	-4.29160000	-7.90022200	1.19078400
N	-3.78005400	-6.81119100	0.53453700
N	-5.21363100	-6.03883400	1.94044300
C	-5.99382400	-8.10098800	3.03129500
H	-5.55868200	-9.07163900	3.26786400
H	-7.01567000	-8.25088000	2.65434500
C	-6.62018500	-6.05605800	4.03272000
O	-5.97299900	-7.30402300	4.19683900
C	-8.60351800	-5.79907000	2.64195000
C	-7.53761900	-5.29734100	1.89789700
C	-7.69147900	-4.89237800	0.57981100
C	-8.96278600	-5.01612400	0.03666700
C	-10.05493200	-5.50178900	0.75262600
C	-9.87326000	-5.89589800	2.07271100
C	-8.16579000	-6.17941700	4.03104000
H	-6.86844100	-4.48823900	0.00095900
H	-11.02066000	-5.57342400	0.26833200
H	-10.70978800	-6.28478300	2.64346800
H	-8.46631600	-7.19473600	4.30843800
H	-8.60218600	-5.50267000	4.77147300
C	-2.98466100	-7.06582500	-0.62862900
C	-3.53347200	-6.80958100	-1.88903700
C	-1.68004400	-7.53546500	-0.44212000
C	-2.70068600	-6.98778100	-2.99229800
C	-0.89220100	-7.70480400	-1.58009700
C	-1.37824900	-7.41348300	-2.85734200
H	-3.09409700	-6.77713100	-3.98376700
H	0.12825200	-8.06267500	-1.46665700
C	-1.12415900	-7.74830800	0.94246700
H	-1.75223400	-8.42360600	1.52888700
H	-1.07680000	-6.79624100	1.49019400
H	-0.11421800	-8.15850600	0.89227200
C	-0.48518800	-7.51574100	-4.06484100
H	-1.00636100	-7.98106200	-4.90497800
H	0.41484100	-8.09462300	-3.84756300
H	-0.17538700	-6.51379700	-4.38360200
C	-4.94307800	-6.30718400	-2.05924400
H	-5.62718600	-6.75728300	-1.33342200
H	-5.30767700	-6.53729600	-3.06155400
H	-4.98391600	-5.21933800	-1.93032700
H	-6.27101600	-5.45791700	4.87444100
N	-9.15843000	-4.62941800	-1.36562900

O	-10.29245400	-4.65372600	-1.81109500
O	-8.17401600	-4.31107400	-2.01035100
C	-1.40208200	-3.73217800	-1.78030100
C	-2.19418400	-2.57485300	-2.01952700
C	-1.80238000	-1.69670600	-3.05913400
C	-0.68426500	-2.00484300	-3.80192000
C	0.07914500	-3.17656700	-3.54895300
C	-0.28381100	-4.05961900	-2.55326700
C	-3.14731500	-3.79983400	-0.35609100
C	-3.27245800	-2.62333600	-1.11060400
H	-2.38616300	-0.80711300	-3.27494500
H	-0.38404500	-1.34591000	-4.61067100
H	0.95207000	-3.38811500	-4.15983500
H	0.28174100	-4.96267800	-2.34920900
N	-1.98511200	-4.43147600	-0.76451000
H	-1.55364100	-5.22290700	-0.31655800
H	-4.10564700	-1.94092400	-1.03906500
C	-4.08598600	-4.26044100	0.61945400
H	-4.57416500	-2.99028400	2.17829000
O	-4.97736800	-3.41677000	1.11098300
C	-2.45670200	-1.44257800	1.94838900
C	-1.34600800	-1.50648200	1.13915900
C	-0.42431300	-2.59441800	1.17302900
C	-0.61617300	-3.55574100	2.20484600
C	-1.73866800	-3.57739200	3.00074400
C	-2.76353500	-2.59571200	2.73811400
H	-1.16886400	-0.70804800	0.43201500
H	0.17446800	-4.26984800	2.39506400
C	0.66146500	-2.68523100	0.24999300
C	1.41219600	-3.89984700	0.12984900
C	1.06801800	-1.59069400	-0.57178500
C	2.47585100	-4.04883100	-0.70778600
H	1.07353000	-4.75584600	0.70199500
C	2.14170800	-1.64012700	-1.41506200
H	0.51948400	-0.66179300	-0.48873400
C	2.92951300	-2.88697800	-1.50303300
O	3.95109900	-2.95820400	-2.20924800
O	-3.99444400	-2.74823500	3.18308300
C	3.22068800	-5.37771100	-0.84627100
C	3.19291000	-5.85528300	-2.31091400
C	4.68045400	-5.21089200	-0.38375100
C	2.57942200	-6.47717000	0.00798400
H	2.16608400	-6.07158400	-2.63030100
H	3.61909600	-5.10523700	-2.97693300

H	3. 77003100	-6. 78185800	-2. 40639200
H	4. 71242000	-4. 89574300	0. 66446600
H	5. 20599700	-6. 16876400	-0. 46768700
H	5. 19608400	-4. 46736200	-0. 99112400
H	3. 11534500	-7. 41839300	-0. 14961500
H	2. 61902500	-6. 24289300	1. 07722500
H	1. 53103400	-6. 63583200	-0. 27063400
C	2. 62270600	-0. 40830800	-2. 18745300
C	3. 98991600	0. 02771800	-1. 62551700
C	2. 76396100	-0. 69981600	-3. 69272000
C	1. 64782700	0. 76626500	-2. 04150600
H	3. 90668600	0. 26980500	-0. 56073900
H	4. 72898900	-0. 76521700	-1. 74984700
H	4. 33976300	0. 92261800	-2. 15248500
H	1. 78964400	-0. 94321000	-4. 12464800
H	3. 14522800	0. 19372700	-4. 20005700
H	3. 44944800	-1. 52680900	-3. 87171200
H	2. 00317200	1. 60640500	-2. 64617100
H	0. 64625000	0. 49330400	-2. 39248300
H	1. 57214600	1. 11319500	-1. 00575900
C	-3. 32976400	-0. 17859600	2. 02941400
C	-3. 30997400	0. 29138400	3. 49656600
C	-2. 74783400	0. 94403500	1. 16002400
C	-4. 79549100	-0. 37208600	1. 59883000
H	-3. 72768400	-0. 47800700	4. 15072900
H	-2. 28733900	0. 51065700	3. 81987500
H	-3. 90811200	1. 20283800	3. 60537700
H	-2. 78707100	0. 68892100	0. 09490100
H	-3. 33737500	1. 85372700	1. 30685500
H	-1. 71022200	1. 17051800	1. 42483200
H	-5. 28641900	0. 60728300	1. 58296500
H	-4. 86841800	-0. 80762500	0. 60057100
H	-5. 34063700	-1. 01406200	2. 29004300
C	-1. 85317300	-4. 51259900	4. 21355900
C	-2. 14708900	-3. 65511800	5. 45934100
C	-2. 97750100	-5. 54087300	4. 03951400
C	-0. 54827000	-5. 27706800	4. 46823800
H	-1. 35461500	-2. 91561400	5. 61277800
H	-3. 09889800	-3. 13034300	5. 35511900
H	-2. 19582600	-4. 29428500	6. 34733400
H	-2. 78412200	-6. 18550600	3. 17269900
H	-3. 04424600	-6. 18135100	4. 92580800
H	-3. 93210600	-5. 03298600	3. 90473200
H	-0. 66074500	-5. 88024500	5. 37408700

H	-0.30270200	-5.95994900	3.64773800
H	0.29640400	-4.59755300	4.61727700
<b>M3</b>			
C	-4.53426100	-9.89362100	-0.01589300
C	-5.17896700	-11.60317700	1.16469400
C	-6.29976100	-9.49963100	1.80878700
H	-6.00024000	-8.45124000	1.80140500
N	-4.35519100	-12.09390600	0.28005100
N	-3.96948600	-11.02143100	-0.45547100
N	-5.32457000	-10.25511700	1.00690600
C	-5.85230700	-12.22792100	2.34308400
H	-5.35952400	-13.16297200	2.60691100
H	-6.91126100	-12.42534100	2.13029300
C	-6.35522100	-10.08096500	3.27399700
O	-5.67266100	-11.31676900	3.41046300
C	-8.56753100	-10.11606600	2.27963600
C	-7.69800600	-9.70885900	1.26801500
C	-8.12313100	-9.55937100	-0.04377800
C	-9.45671900	-9.84520500	-0.30037800
C	-10.35488100	-10.24997800	0.68348900
C	-9.90488600	-10.38400000	1.99148000
C	-7.85982000	-10.19578300	3.60492000
H	-7.46755300	-9.22712900	-0.83925400
H	-11.38271500	-10.45851600	0.41395100
H	-10.58660400	-10.70389300	2.77195200
H	-8.05929800	-11.12418200	4.14755000
H	-8.16895500	-9.36831600	4.25090600
C	-3.09338600	-11.18823600	-1.58955900
C	-3.58715300	-10.89838900	-2.86271900
C	-1.77513200	-11.58318900	-1.33660900
C	-2.67414400	-10.95735300	-3.91673200
C	-0.91264600	-11.63017500	-2.42641300
C	-1.33701000	-11.29639500	-3.71594400
H	-3.02350100	-10.72794100	-4.91997800
H	0.12400000	-11.91274900	-2.26185200
C	-1.29707100	-11.91761500	0.05177200
H	-0.20758000	-11.88524800	0.09514700
H	-1.62303000	-12.91975300	0.34454200
H	-1.69286000	-11.22784500	0.80484600
C	-0.35379700	-11.26362500	-4.85411000
H	-0.85096800	-11.40441900	-5.81572900
H	0.41215400	-12.03347300	-4.73823900
H	0.15066100	-10.29106900	-4.87440700
C	-5.03156700	-10.54752400	-3.11623400

H	-5.70591900	-11.07447000	-2.43531000
H	-5.30457500	-10.82344200	-4.13575800
H	-5.21397200	-9.47180000	-3.01528400
H	-5.83834200	-9.40896200	3.95789500
N	-9.93667300	-9.72025700	-1.68322500
O	-11.11671900	-9.93100500	-1.89642800
O	-9.12461400	-9.41673100	-2.53979500
C	-1.11106600	-8.13798100	-1.87916300
C	-1.83474700	-7.39847200	-2.85036500
C	-1.16392400	-6.92299800	-3.99751700
C	0.18137700	-7.18554500	-4.12767100
C	0.88647100	-7.91359700	-3.13575100
C	0.26300000	-8.39467600	-2.00315700
C	-3.24640300	-8.05897400	-1.22919100
C	-3.18406500	-7.34212900	-2.40860400
H	-1.70339500	-6.36575400	-4.75608700
H	0.71869900	-6.83329800	-5.00143800
H	1.94564500	-8.10211100	-3.27770900
H	0.80083300	-8.96168500	-1.25066500
N	-1.98937900	-8.53513200	-0.90973600
H	-1.72215500	-8.95925300	-0.03301800
H	-4.03290600	-6.90584000	-2.91625200
C	-4.47445300	-8.49469700	-0.59691100
O	-5.51364500	-7.86065100	-0.57599200

**TS3<sup>HCT\_C2</sup>**

C	-4.90590800	-5.77313800	1.05071200
C	-6.75226100	-6.18471700	2.19604800
C	-5.98574000	-3.87060700	2.47333100
H	-5.00835200	-3.36365700	2.58700700
N	-6.52842100	-7.29188500	1.55102600
N	-5.38494400	-7.03457700	0.81995100
N	-5.81390100	-5.22436600	1.92684100
C	-7.82725100	-5.87279600	3.18682300
H	-8.24389300	-6.79809600	3.58936700
H	-8.63919800	-5.30280500	2.71020100
C	-6.62137100	-3.91650600	3.91100800
O	-7.23334000	-5.16459300	4.26075000
C	-7.90473700	-2.42813200	2.47879300
C	-6.96757400	-3.06041600	1.65077000
C	-7.01262500	-2.91186100	0.26901200
C	-8.03712900	-2.12710800	-0.25870700
C	-8.98148500	-1.48172100	0.54263100
C	-8.91022400	-1.63192300	1.92646000
C	-7.62518100	-2.73354800	3.92984300

H	-6.28117300	-3.36535800	-0.38697400
H	-9.75223200	-0.88241100	0.07415200
H	-9.63977800	-1.13858000	2.56257200
H	-8.51723300	-2.98963900	4.51174400
H	-7.15769200	-1.86782000	4.41621300
C	-4.98024000	-8.02880200	-0.13675900
C	-5.11542200	-7.76303100	-1.51054200
C	-4.52462600	-9.26916200	0.35347900
C	-4.71994300	-8.76778400	-2.39923400
C	-4.14584400	-10.23293700	-0.58466600
C	-4.22354500	-9.99917000	-1.96289600
H	-4.81132700	-8.57966000	-3.46612500
H	-3.78541500	-11.19442800	-0.22658000
C	-4.44291300	-9.56421900	1.83365500
H	-5.44175000	-9.62847700	2.27750300
H	-3.90321900	-8.78295600	2.38241300
H	-3.92811800	-10.51306900	2.00619700
C	-3.76795900	-11.04486000	-2.95157500
H	-2.69234700	-10.95026300	-3.14992400
H	-4.28578600	-10.94216500	-3.91020800
H	-3.94290900	-12.05754600	-2.57427000
C	-5.66640100	-6.46022300	-2.03811900
H	-6.53329900	-6.11835600	-1.46307700
H	-5.98186800	-6.57534600	-3.07830500
H	-4.91563700	-5.66161000	-2.01112100
H	-5.83365600	-3.78343400	4.65231500
N	-8.13095400	-1.98379400	-1.72011200
O	-8.99293500	-1.22852900	-2.16821400
O	-7.34680800	-2.63664100	-2.40988100
C	-0.93516000	-7.10039400	-0.62874300
C	-0.55741600	-5.81572000	-1.11839100
C	0.66170400	-5.67935900	-1.81623100
C	1.44172100	-6.80555700	-2.01997200
C	1.04086000	-8.07224700	-1.53339000
C	-0.14556400	-8.23897200	-0.83191800
C	-2.57256200	-5.64111300	-0.07939300
C	-1.59782800	-4.91695000	-0.75891000
H	0.97916300	-4.70733700	-2.18171800
H	2.37960800	-6.71869000	-2.56018800
H	1.67881100	-8.93367100	-1.71104700
H	-0.44865600	-9.21245700	-0.45614900
N	-2.14008300	-6.96450800	0.02048400
H	-2.70179600	-7.74318500	0.32675000
H	-1.64814800	-3.85546100	-0.94976200



C	-3.76628700	-5.04176700	0.49224900
H	-2.93644400	-3.02166200	1.71626600
O	-3.85074900	-3.77621800	0.54796000
C	-2.20971100	-1.13660200	1.97244100
C	-1.03440100	-1.12339900	1.28273900
C	-0.04263600	-2.16500100	1.37553200
C	-0.24227800	-3.14202900	2.41471800
C	-1.40326400	-3.26482600	3.11532300
C	-2.61320200	-2.41820800	2.70604700
H	-0.77601800	-0.24841100	0.70250500
H	0.57534500	-3.81173400	2.63794500
C	1.09570400	-2.18274300	0.52997100
C	2.23259500	-3.02273900	0.78989900
C	1.16090400	-1.35755800	-0.64605900
C	3.35349000	-3.04552900	0.01018900
H	2.21123400	-3.63835500	1.67835800
C	2.22195300	-1.34193200	-1.50598500
H	0.29469600	-0.75269600	-0.87795400
C	3.39944200	-2.19488500	-1.20548400
O	4.39608600	-2.19858900	-1.95374800
O	-3.68042300	-2.40913600	3.49776400
C	4.57729700	-3.91027600	0.36313300
C	4.86488800	-4.91883600	-0.77695800
C	5.81496600	-3.00330000	0.57878600
C	4.36065100	-4.72023300	1.65668300
H	4.01159500	-5.59312600	-0.91824400
H	5.06422200	-4.40073200	-1.71581900
H	5.73885900	-5.53141500	-0.52074300
H	5.64395200	-2.30372200	1.40625900
H	6.68782600	-3.61781400	0.83375700
H	6.04226100	-2.43086500	-0.32142600
H	5.25497400	-5.31986200	1.86082400
H	4.19494200	-4.07310700	2.52637500
H	3.51320900	-5.41116900	1.57382200
C	2.23546000	-0.46876900	-2.77283200
C	3.41120400	0.53859000	-2.70394500
C	2.38899600	-1.36120100	-4.03000500
C	0.93497000	0.34340600	-2.93378600
H	3.30327200	1.20170100	-1.83677000
H	4.36707000	0.01895800	-2.62908300
H	3.41948700	1.16405400	-3.60571000
H	1.54390100	-2.05592100	-4.11765400
H	2.40216300	-0.73691200	-4.93242100
H	3.31417200	-1.93746900	-3.99060800

H	0.99694700	0.94565500	-3.84718400
H	0.05216000	-0.30081300	-3.02571800
H	0.77168700	1.03354800	-2.09740900
C	-3.14804900	0.07519800	1.97751800
C	-3.28402600	0.57443000	3.43908000
C	-2.61556700	1.24230800	1.12169400
C	-4.54139700	-0.31070600	1.43180000
H	-3.64766100	-0.22950500	4.08163900
H	-2.31790400	0.92548000	3.82125500
H	-3.98771900	1.41595900	3.47999600
H	-2.52596800	0.97126500	0.06317600
H	-3.31660400	2.08211300	1.18737200
H	-1.64097700	1.60206800	1.47039300
H	-5.18843500	0.57528200	1.40776000
H	-4.47028100	-0.70755600	0.41254200
H	-4.99941200	-1.06460200	2.06954900
C	-1.52549400	-4.25640900	4.28126800
C	-1.79116400	-3.44595200	5.57640900
C	-2.68699800	-5.25067400	4.04957600
C	-0.24338400	-5.08690000	4.49494200
H	-0.94215700	-2.78936600	5.80024900
H	-2.68852900	-2.83535200	5.46376000
H	-1.92091700	-4.13016400	6.42502700
H	-2.51367800	-5.84624700	3.14389400
H	-2.76051000	-5.94224800	4.89827600
H	-3.62909100	-4.71216100	3.95417100
H	-0.38724000	-5.75371500	5.35290700
H	-0.00526600	-5.71214300	3.62620800
H	0.62552700	-4.45685400	4.71453400

**TS3<sup>HCT\_C3</sup>**

C	-2.56994900	-4.52127900	-0.75383700
C	-2.19389700	-6.54622200	0.01778800
C	-3.59309800	-5.18847200	1.51120200
H	-3.60314200	-4.14141400	1.80610400
N	-1.72663100	-6.57363500	-1.18955400
N	-1.98053900	-5.32052100	-1.67780200
N	-2.72002200	-5.32402200	0.33803600
C	-2.19902600	-7.60783600	1.06608300
H	-1.36909300	-8.29811400	0.90875300
H	-3.14004300	-8.17487200	1.03981600
C	-3.08463100	-6.11045200	2.67875700
O	-2.00943300	-6.95552800	2.30555400
C	-5.37138800	-6.69367000	2.09720800
C	-4.97452800	-5.71237800	1.19054800

C	-5.77804300	-5.33636100	0.12395200
C	-6.98846800	-6.00157100	-0.00849000
C	-7.41893000	-6.98657700	0.87719600
C	-6.60173400	-7.33320800	1.94697500
C	-4.32537500	-6.90190800	3.15998100
H	-5.49238600	-4.55457900	-0.57041800
H	-8.37591200	-7.46678100	0.71640400
H	-6.91847200	-8.09970600	2.64604600
H	-4.06988400	-7.95446900	3.31576700
H	-4.67658100	-6.51408500	4.12187100
C	-1.83903200	-5.08586700	-3.08770500
C	-2.98550700	-4.80686900	-3.83989500
C	-0.55572700	-5.13918400	-3.64037900
C	-2.78937200	-4.42859300	-5.16770100
C	-0.41863800	-4.76188600	-4.97413100
C	-1.51740300	-4.36014000	-5.73716700
H	-3.65835200	-4.17860700	-5.77149100
H	0.57304900	-4.76808500	-5.42066800
C	0.61479100	-5.60894400	-2.82416100
H	0.63659400	-6.70304800	-2.79192000
H	0.54399700	-5.26901400	-1.78760200
H	1.56042200	-5.26161200	-3.24019600
C	-1.33687200	-3.84423200	-7.13894000
H	-1.27772700	-2.74989500	-7.12020600
H	-2.17890600	-4.12293700	-7.77672400
H	-0.41591800	-4.22274100	-7.58764300
C	-4.37853400	-4.93116900	-3.27599500
H	-4.44517600	-5.74009900	-2.54110000
H	-5.08569400	-5.14992500	-4.07810600
H	-4.70971800	-4.00574200	-2.79388500
H	-2.67073100	-5.48702800	3.46943300
N	-7.84807900	-5.65302400	-1.14648300
O	-8.93615500	-6.19450800	-1.22699800
O	-7.42153900	-4.84407700	-1.95306000
C	-1.41709500	-1.46430200	-3.69091700
C	-2.73599900	-0.95596500	-3.81905200
C	-3.03450800	-0.09763500	-4.89402000
C	-2.03422600	0.22002500	-5.79281100
C	-0.72970600	-0.30103900	-5.64681300
C	-0.40241000	-1.14815500	-4.60210800
C	-2.65684000	-2.33617000	-2.03356400
C	-3.50116800	-1.51461100	-2.75086500
H	-4.03675900	0.30198500	-5.01262700
H	-2.25001300	0.87818100	-6.62795800

H	0.03159500	-0.03761700	-6.37422200
H	0.59660300	-1.55969100	-4.49986600
N	-1.38919400	-2.27328500	-2.58218200
H	-0.57660500	-2.77581500	-2.24649500
H	-4.55276300	-1.37634300	-2.54334700
C	-3.02664100	-3.15276500	-0.88546300
H	-3.46680800	-1.83743400	0.64102400
O	-3.99579500	-2.76282100	-0.12271700
C	-2.59254100	-1.08266000	1.27201900
C	-1.42144600	-1.68355600	0.71723000
C	-0.74457500	-2.75259700	1.31745900
C	-1.17012800	-3.14992600	2.65828800
C	-2.15634800	-2.53542000	3.35474800
C	-2.97765300	-1.49142700	2.66285300
H	-1.04334000	-1.29135300	-0.21692200
H	-0.56669900	-3.90097300	3.15633300
C	0.40571600	-3.35676700	0.73284000
C	0.85107300	-4.65689100	1.10871900
C	1.16616200	-2.66621000	-0.25989300
C	1.92202600	-5.27855300	0.52415500
H	0.27137300	-5.19600200	1.85156800
C	2.26333600	-3.19978600	-0.87463300
H	0.89604700	-1.63722800	-0.46916800
C	2.65606500	-4.58857900	-0.55520200
O	3.57117500	-5.15440500	-1.18313500
O	-3.95875500	-1.00109200	3.21368800
C	2.34168000	-6.69536800	0.91889200
C	2.08856400	-7.65014300	-0.26156600
C	3.83128800	-6.72674800	1.31055800
C	1.54476500	-7.21178600	2.12258500
H	1.02267300	-7.65052400	-0.52130800
H	2.66240200	-7.34198800	-1.13728200
H	2.37707200	-8.67149800	0.01210500
H	4.01191700	-6.07659100	2.17326900
H	4.11410300	-7.74726000	1.59168600
H	4.46137700	-6.40022600	0.48456200
H	1.89898000	-8.21352200	2.38446500
H	1.67542200	-6.56813800	2.99950100
H	0.47247700	-7.28085300	1.91333300
C	3.11424100	-2.38503100	-1.85206100
C	4.56377400	-2.31498200	-1.33582600
C	3.10117400	-3.02624800	-3.25125700
C	2.59924400	-0.94712700	-1.99409600
H	4.59446200	-1.84076600	-0.34927600

H	4.99707900	-3.31261800	-1.26108400
H	5.17239300	-1.71394000	-2.02019500
H	2.07672000	-3.08306000	-3.63955200
H	3.69158900	-2.41552300	-3.94348200
H	3.51952700	-4.03258600	-3.21989700
H	3.23205300	-0.40783800	-2.70533500
H	1.57117500	-0.91134100	-2.37354700
H	2.63091000	-0.40813100	-1.04157200
C	-2.95353200	0.38331800	0.87624500
C	-2.54537900	1.33453300	2.01635500
C	-2.18870800	0.83120800	-0.37649100
C	-4.45741500	0.51994700	0.59738000
H	-3.14448600	1.17204200	2.91346800
H	-1.48827900	1.19558100	2.26985800
H	-2.68331800	2.37169400	1.69326300
H	-2.37265800	0.17471400	-1.23236600
H	-2.52414100	1.83603700	-0.65156900
H	-1.10960900	0.88078900	-0.19613600
H	-4.70292400	1.56453600	0.37759400
H	-4.73986800	-0.08661000	-0.26950100
H	-5.04245000	0.19509200	1.45909800
C	-2.40984600	-2.78666600	4.84339400
C	-2.22412100	-1.45833700	5.60691300
C	-3.83774100	-3.31125700	5.08555400
C	-1.40848000	-3.78812800	5.43324600
H	-1.22211800	-1.05279100	5.43353900
H	-2.96253200	-0.71721100	5.30071500
H	-2.33556800	-1.64000000	6.68081400
H	-4.00791900	-4.26361500	4.57200700
H	-3.98324800	-3.48602400	6.15658400
H	-4.58196000	-2.59544300	4.73941400
H	-1.62101400	-3.91596800	6.49827500
H	-1.46694700	-4.77828300	4.96922800
H	-0.37910400	-3.42868900	5.33753000

**TS3<sup>HCT\_C4</sup>**

C	-2.85270500	-4.88709000	-0.18987800
C	-4.20544500	-5.89995300	1.21732400
C	-4.48869000	-3.46657200	1.22520400
H	-3.81091500	-2.61309700	1.21954700
N	-3.65098300	-6.86259300	0.54799600
N	-2.82747100	-6.23336400	-0.33629600
N	-3.75181300	-4.67232700	0.81828800
C	-5.23327700	-5.96737300	2.29776500
H	-5.16302700	-6.91871000	2.82492900

H	-6.23983400	-5.87623300	1.86385200
C	-5.10998900	-3.62776400	2.66160000
O	-4.95375600	-4.92719100	3.20643400
C	-6.85913500	-3.13241800	1.04607000
C	-5.67947600	-3.26641400	0.31358700
C	-5.68450600	-3.25249500	-1.07464400
C	-6.91691100	-3.10428900	-1.69578800
C	-8.11166600	-2.95430200	-0.99631200
C	-8.07986100	-2.96603100	0.39309400
C	-6.59267700	-3.20680300	2.52378300
H	-4.78108000	-3.34200100	-1.66543500
H	-9.04039400	-2.84112300	-1.54124200
H	-8.99989300	-2.86115200	0.95812000
H	-7.24534400	-3.91906900	3.03842100
H	-6.74701500	-2.23034100	2.99440200
C	-2.20877600	-7.01137600	-1.37118300
C	-2.72067900	-6.92073900	-2.66775700
C	-1.11609400	-7.80728200	-1.02503300
C	-2.01813200	-7.59451200	-3.66587600
C	-0.45685400	-8.46961000	-2.05810500
C	-0.87778200	-8.34913300	-3.38485000
H	-2.36839900	-7.51974900	-4.69254700
H	0.41353600	-9.07769900	-1.82308100
C	-0.67086000	-7.90661900	0.40842900
H	-1.43624900	-8.39073500	1.02195500
H	-0.50308500	-6.91054700	0.83670700
H	0.25414200	-8.47994700	0.49018600
C	-0.12660900	-9.03119900	-4.49729500
H	0.89240200	-9.27687000	-4.19051200
H	-0.07405500	-8.38546600	-5.37729900
H	-0.62530700	-9.96054400	-4.79077600
C	-3.96722900	-6.13343300	-2.98057600
H	-4.70828700	-6.22237100	-2.17992400
H	-4.41973700	-6.49909700	-3.90388800
H	-3.74532000	-5.07132900	-3.12358100
H	-4.58951100	-2.96738700	3.35335900
N	-6.95426700	-3.11864900	-3.16304900
O	-8.02712200	-2.93127900	-3.70833600
O	-5.90892700	-3.32391400	-3.75739400
C	0.30574400	-5.10597500	-3.28826900
C	-0.44960900	-4.28184700	-4.16178600
C	-0.11343000	-4.24974900	-5.52910500
C	0.96009600	-5.00067700	-5.96764900
C	1.71627200	-5.79005800	-5.07120200

C	1.40349000	-5.85658500	-3.72614600
C	-1.30465300	-4.12482100	-2.08274900
C	-1.44894900	-3.64362900	-3.36730100
H	-0.68514300	-3.63716300	-6.21929500
H	1.23541700	-4.98447400	-7.01715600
H	2.55812300	-6.36145500	-5.44934400
H	1.97515600	-6.46874900	-3.03581900
N	-0.24301700	-4.99988900	-2.03834800
H	0.16772700	-5.36078400	-1.18751200
H	-2.23047000	-2.97187800	-3.69438000
C	-2.20587600	-3.83460200	-0.96879900
H	-2.13078800	-1.87761700	0.17270200
O	-2.68887900	-2.66132700	-0.82714300
C	-2.48889900	-0.69614300	1.95641500
C	-1.51336200	-1.28935500	1.08655700
C	-0.72239300	-2.44831700	1.50822100
C	-0.98560400	-2.94942300	2.81616700
C	-1.87791600	-2.36990000	3.67994200
C	-2.78170900	-1.28025800	3.22423700
H	-0.99320100	-0.58466400	0.44008200
H	-0.37579400	-3.76479200	3.17834300
C	0.23194200	-3.02756800	0.64180500
C	0.99227300	-4.19668000	1.01779300
C	0.67805200	-2.31709100	-0.53256600
C	2.11102400	-4.60432800	0.35915800
H	0.66606200	-4.75628200	1.88611100
C	1.80040400	-2.63049500	-1.22887100
H	0.09989400	-1.46049500	-0.85109700
C	2.57324900	-3.83194000	-0.82728600
O	3.57812400	-4.18256900	-1.45387600
O	-3.73324700	-0.89649500	3.96495500
C	2.94354200	-5.80373400	0.81877200
C	2.96802800	-6.87663200	-0.28550400
C	4.38352600	-5.35500900	1.13821000
C	2.37961900	-6.43561600	2.09717500
H	1.94845000	-7.18212400	-0.55531200
H	3.46865100	-6.49949700	-1.17817900
H	3.50026800	-7.76616800	0.06883000
H	4.37866700	-4.60063900	1.93181500
H	4.96036100	-6.21559700	1.49358600
H	4.87610100	-4.94053800	0.25989300
H	3.01900400	-7.27257300	2.39250600
H	2.36221200	-5.72028800	2.92617700
H	1.36877600	-6.82837700	1.95818200

C	2. 35554200	-1. 72707500	-2. 33376500
C	3. 68980000	-1. 13759900	-1. 83399400
C	2. 59890400	-2. 47904100	-3. 65502800
C	1. 40225700	-0. 56523800	-2. 63775400
H	3. 53984900	-0. 57205100	-0. 90836900
H	4. 42023400	-1. 92755500	-1. 65003700
H	4. 09639300	-0. 45604800	-2. 58897200
H	1. 65952400	-2. 84912100	-4. 07247000
H	3. 04030000	-1. 78353600	-4. 37812100
H	3. 27434600	-3. 32166600	-3. 51793600
H	1. 82742200	0. 04476800	-3. 44014600
H	0. 42554600	-0. 93193600	-2. 97358700
H	1. 25345200	0. 08603300	-1. 76984400
C	-3. 28697300	0. 51540800	1. 47446000
C	-4. 75789900	0. 09634700	1. 27614000
C	-3. 20549900	1. 65453300	2. 50624000
C	-2. 77445700	1. 05658400	0. 13306000
H	-4. 84116700	-0. 62352900	0. 45276900
H	-5. 14994200	-0. 34966100	2. 19331600
H	-5. 36825500	0. 96910300	1. 01719500
H	-2. 16756100	1. 98138800	2. 62910200
H	-3. 79270300	2. 51227900	2. 15950000
H	-3. 58854000	1. 32429700	3. 47163900
H	-3. 40325300	1. 89692700	-0. 17695200
H	-1. 74541800	1. 42554600	0. 20709800
H	-2. 81629200	0. 29939700	-0. 65792600
C	-1. 90736100	-2. 77866000	5. 15761400
C	-1. 59218700	-1. 52245600	5. 99469200
C	-3. 27586400	-3. 34222700	5. 58142400
C	-0. 85024500	-3. 83970100	5. 48947700
H	-0. 60275200	-1. 12835100	5. 74030100
H	-2. 34071900	-0. 74934800	5. 82032600
H	-1. 59112100	-1. 78573700	7. 05789000
H	-3. 53271300	-4. 22962000	4. 99418400
H	-3. 22783500	-3. 63663500	6. 63582100
H	-4. 05546700	-2. 59074800	5. 46012500
H	-0. 89153800	-4. 05663500	6. 56081000
H	-1. 03172700	-4. 77886200	4. 95562900
H	0. 16331500	-3. 49687800	5. 25768000
<b>TS3<sup>HCT</sup></b>			
C	-1. 13520200	-4. 95080100	-1. 67804200
C	-0. 75244500	-7. 11389000	-1. 58684100
C	-1. 83826500	-6. 26313300	0. 44208200
H	-1. 75119500	-5. 35550600	1. 03672700



N	-0.42621300	-6.77863000	-2.79617300
N	-0.68143300	-5.43509600	-2.85170600
N	-1.17801600	-6.03982600	-0.85452700
C	-0.73646200	-8.45610700	-0.93291600
H	-0.00444100	-9.10172400	-1.41815900
H	-1.72870300	-8.92366800	-1.00795900
C	-1.20253100	-7.48322900	1.20466800
O	-0.33767100	-8.27502300	0.40843100
C	-3.58781700	-7.82659000	0.94313100
C	-3.28132100	-6.66996600	0.22731300
C	-4.21529100	-6.05659900	-0.59464200
C	-5.46422400	-6.65630500	-0.67693100
C	-5.80814200	-7.80523400	0.03078300
C	-4.85719900	-8.39567300	0.85482900
C	-2.40349800	-8.29297700	1.74524400
H	-4.00014200	-5.14973300	-1.14635000
H	-6.80098800	-8.22284100	-0.07914000
H	-5.10089700	-9.29583500	1.40849100
H	-2.20967100	-9.36495300	1.64914300
H	-2.55628800	-8.08204400	2.80856000
C	-0.70426200	-4.78774500	-4.13362400
C	-1.94724600	-4.46189600	-4.68711500
C	0.51428300	-4.49801500	-4.75270300
C	-1.93687600	-3.73290700	-5.87461400
C	0.46644500	-3.76139900	-5.93618200
C	-0.74594400	-3.35063500	-6.49529000
H	-2.88620500	-3.44752500	-6.32125500
H	1.40040700	-3.49892900	-6.42700300
C	1.81591300	-4.94050300	-4.14553100
H	1.91803000	-6.02917800	-4.20063000
H	1.87748400	-4.66968800	-3.08726900
H	2.66101600	-4.48303700	-4.66148200
C	-0.77781500	-2.49475200	-7.73318000
H	-1.54808100	-2.83678200	-8.42881000
H	0.18506000	-2.50142400	-8.24756900
H	-1.01268600	-1.45920300	-7.46325700
C	-3.25014500	-4.84658900	-4.03334900
H	-3.17383200	-5.79809900	-3.49781600
H	-4.03255500	-4.94876600	-4.78729000
H	-3.57979700	-4.07787200	-3.32501300
H	-0.56590700	-7.12097400	2.01464000
N	-6.46207800	-6.05154500	-1.56778800
O	-7.57747800	-6.54018600	-1.58987000
O	-6.11699700	-5.09606500	-2.24234000

C	-1.16367700	-0.94075300	-3.76302900
C	-2.39998000	-0.55811700	-3.18281400
C	-3.05155200	0.59388300	-3.66489700
C	-2.46608900	1.31161400	-4.68957400
C	-1.23598600	0.90738700	-5.25563600
C	-0.56937600	-0.21823400	-4.80626500
C	-1.67593600	-2.45501500	-2.18966200
C	-2.70351100	-1.53015500	-2.18334500
H	-3.99860600	0.90683500	-3.23596100
H	-2.95545900	2.20104400	-5.07236200
H	-0.80554200	1.49218800	-6.06222600
H	0.37344700	-0.53390900	-5.24365600
N	-0.74119100	-2.07947100	-3.12920000
H	0.15362800	-2.52544200	-3.26752100
H	-3.57792600	-1.58520900	-1.55134200
C	-1.64011000	-3.62875400	-1.31838400
H	-1.64350400	-3.05021400	0.67916300
O	-2.39959300	-3.61373700	-0.28328000
C	-1.67782200	-0.47347900	2.17384700
C	-1.14304900	-1.13265500	1.12499900
C	-0.62185800	-2.50592100	1.18577400
C	-0.59782400	-3.09245900	2.53226400
C	-1.11964100	-2.50216600	3.62827600
C	-1.67668400	-1.12453900	3.51151400
H	-1.17704500	-0.68103600	0.14024400
H	-0.15354500	-4.07593300	2.62924200
C	0.43507400	-2.89920800	0.22622200
C	1.13024800	-4.14208500	0.37455000
C	1.03943800	-1.94110700	-0.64491000
C	2.31566700	-4.43193600	-0.24235400
H	0.70608300	-4.88470200	1.04363000
C	2.20677900	-2.15656600	-1.32503100
H	0.55668400	-0.97639900	-0.74626900
C	2.90023800	-3.44686600	-1.17314800
O	3.93689800	-3.70517900	-1.81496800
O	-2.12980400	-0.54273600	4.49950000
C	3.08900500	-5.72399500	0.03321100
C	3.17761600	-6.57200600	-1.24751600
C	4.50642600	-5.38956700	0.53660800
C	2.41201000	-6.56966200	1.11497100
H	3.70045000	-6.02813900	-2.03548000
H	3.71382600	-7.50517300	-1.04153900
H	2.17326000	-6.83133700	-1.60635000
H	4.45338900	-4.80301300	1.45999600

H	5.04252300	-6.31926000	0.75727600
H	5.06768300	-4.82610100	-0.20703700
H	3.01778800	-7.46044700	1.30850500
H	2.31400900	-6.01930900	2.05794600
H	1.42506900	-6.91370400	0.79616700
C	2.84904400	-1.07385600	-2.19782300
C	4.24868000	-0.73293500	-1.65179600
C	2.97957400	-1.56692400	-3.65104600
C	2.02969400	0.22198300	-2.20301500
H	4.17115300	-0.33616500	-0.63423000
H	4.88915000	-1.61446900	-1.63922900
H	4.71348900	0.03467800	-2.28055400
H	2.00021600	-1.83167200	-4.07205000
H	3.39964400	-0.77305900	-4.27897900
H	3.62383600	-2.44472100	-3.70249000
H	2.52926500	0.95885900	-2.83961500
H	1.02048500	0.07185900	-2.59898200
H	1.94590500	0.65064200	-1.19873200
C	-2.28620100	0.92409200	2.02912500
C	-1.51805900	1.92807000	2.90780000
C	-2.21348100	1.42051000	0.57931100
C	-3.76981300	0.89530000	2.44021600
H	-1.57534200	1.65545800	3.96140900
H	-0.46510100	1.96802100	2.60972500
H	-1.94510200	2.92871900	2.77986100
H	-2.76252800	0.76498300	-0.10592300
H	-2.66045300	2.41727300	0.51925800
H	-1.17930400	1.49728000	0.22524000
H	-4.20550000	1.89268500	2.31663200
H	-4.32879500	0.20087400	1.80384800
H	-3.88551600	0.59069300	3.48032600
C	-1.12991700	-3.19043100	4.99625000
C	-0.29161300	-2.38081800	6.00210800
C	-2.57734800	-3.32059900	5.50541000
C	-0.53669300	-4.60300900	4.92166300
H	0.73911500	-2.28077300	5.64651900
H	-0.71085000	-1.38592000	6.15038600
H	-0.26939400	-2.90114500	6.96584500
H	-3.17618500	-3.91724200	4.80897800
H	-2.57967100	-3.82944200	6.47557700
H	-3.04255700	-2.34216300	5.62143500
H	-0.58487100	-5.06356400	5.91277400
H	-1.09803500	-5.24191400	4.22952600
H	0.51331800	-4.59115500	4.61028700

**M3<sup>SET</sup>**

C	0.01507700	0.63589000	-0.65635300
C	1.21411300	0.37321300	-2.47616700
C	2.38584000	1.66945700	-0.73953100
H	2.05123300	2.38325800	0.01161400
N	0.11772700	-0.28213000	-2.71028900
N	-0.61807500	-0.13987100	-1.56977000
N	1.20734300	0.95173800	-1.23835700
C	2.36924500	0.68043300	-3.37072600
H	2.09661000	0.50730100	-4.41108100
H	3.23862700	0.05866300	-3.11807000
C	3.12525000	2.40958600	-1.92208800
O	2.63257500	2.06023800	-3.20264700
C	4.66544300	0.92039200	-0.77495500
C	3.41598700	0.70202300	-0.19520900
C	3.21348200	-0.30807100	0.73430400
C	4.31373200	-1.09147600	1.05482700
C	5.57589900	-0.89962600	0.49854200
C	5.75369200	0.12167000	-0.42680400
C	4.62332800	2.06536100	-1.74915400
H	2.25540000	-0.48804900	1.20626900
H	6.39249400	-1.54762800	0.79078800
H	6.72691400	0.28433400	-0.87696100
H	5.06896500	1.81896500	-2.71756600
H	5.16885100	2.92707000	-1.35265300
C	-1.83671600	-0.88423100	-1.41815200
C	-1.88784100	-1.90349500	-0.46421400
C	-2.91778500	-0.54436200	-2.23862900
C	-3.10845300	-2.55933800	-0.30269100
C	-4.10896900	-1.23514700	-2.03964700
C	-4.22836300	-2.23029900	-1.06555600
H	-3.18022600	-3.35290500	0.43650000
H	-4.96923200	-0.98358200	-2.65450900
C	-2.80495300	0.53707900	-3.28042000
H	-2.18519400	0.20753900	-4.11888500
H	-2.33817800	1.44243100	-2.87724600
H	-3.79183600	0.80073300	-3.66280100
C	-5.54837300	-2.91703000	-0.83563500
H	-5.41222900	-3.88983500	-0.35934100
H	-6.08675000	-3.06055600	-1.77521200
H	-6.18130200	-2.30905700	-0.18101400
C	-0.69385800	-2.28874400	0.36996000
H	0.24167600	-2.19536300	-0.18932400
H	-0.78802400	-3.32336600	0.70307200

H	-0.61417900	-1.66228200	1.26567300
H	2.94817500	3.48178200	-1.84569500
N	4.13080000	-2.17719700	2.02669200
O	5.10411600	-2.84559800	2.32362500
O	3.01267900	-2.34936700	2.48119900
C	-3.37966600	0.98631100	2.64985400
C	-3.97677500	1.25402200	1.38951900
C	-5.37626100	1.41091700	1.30453000
C	-6.12304000	1.28517300	2.45575000
C	-5.50681800	1.01011200	3.69965600
C	-4.13782600	0.85737600	3.81901800
C	-1.74395900	1.03884600	1.10986100
C	-2.93281400	1.29710600	0.43248900
H	-5.84566800	1.61686900	0.34810300
H	-7.20098600	1.39685100	2.41565900
H	-6.12715500	0.91878200	4.58511000
H	-3.67115900	0.64924000	4.77535600
N	-2.02248800	0.89227100	2.46253600
H	-1.37533600	0.52008200	3.14370000
H	-3.02240400	1.53588200	-0.61646400
C	-0.40477400	1.00398700	0.64901300
H	0.34981100	1.89696000	2.17693400
O	0.61658100	1.24337300	1.51179700
<b>M3<sup>HAT</sup></b>			
C	-4.37089300	-9.83115600	0.31622000
C	-5.02865200	-11.59000800	1.48866000
C	-6.27812700	-9.53146900	2.01934300
H	-5.97814200	-8.49076800	2.12815900
N	-4.17049500	-12.08101500	0.65474700
N	-3.76495700	-10.99568900	-0.09702700
N	-5.18775100	-10.24025000	1.35267400
C	-5.80641700	-12.26881700	2.56727500
H	-5.29721300	-13.17635900	2.89109100
H	-6.81043200	-12.53565100	2.20600900
C	-6.60706300	-10.19697800	3.40819100
O	-5.86539500	-11.37808800	3.66420100
C	-8.58537500	-10.21103400	1.98967900
C	-7.55602800	-9.66886100	1.22252700
C	-7.72853100	-9.36713000	-0.12133000
C	-8.97380700	-9.64809500	-0.66624500
C	-10.02816600	-10.18382800	0.07053100
C	-9.83182700	-10.46562100	1.41712700
C	-8.13704800	-10.44544900	3.40781200
H	-6.93808400	-8.92088500	-0.71465200

H	-10.97545700	-10.37618900	-0.41733800
H	-10.63818100	-10.88905700	2.00666100
H	-8.35852600	-11.45644000	3.76407900
H	-8.63697300	-9.74995800	4.08886700
C	-3.03996100	-11.21277400	-1.30784700
C	-3.65548900	-10.93853000	-2.53303900
C	-1.71248200	-11.65145300	-1.21256300
C	-2.86635000	-11.03402700	-3.68181600
C	-0.97640500	-11.75124000	-2.38839600
C	-1.52687500	-11.41163100	-3.62758200
H	-3.31699400	-10.80234900	-4.64410100
H	0.06220500	-12.06975400	-2.33467200
C	-1.09634600	-11.96744300	0.12472500
H	-0.01644800	-12.09251600	0.02970100
H	-1.51794300	-12.88496300	0.54498800
H	-1.29280600	-11.17560300	0.85630500
C	-0.67048300	-11.40835200	-4.86577600
H	-1.27683400	-11.48130700	-5.77121800
H	0.04640300	-12.23312700	-4.85768900
H	-0.10180200	-10.47248700	-4.91621600
C	-5.10980000	-10.55520200	-2.63699200
H	-5.70752100	-11.01565500	-1.84438700
H	-5.51348200	-10.87677600	-3.59929400
H	-5.24064800	-9.47004000	-2.56903600
H	-6.31732000	-9.52003100	4.21140900
N	-9.18309400	-9.37441800	-2.09249100
O	-10.30642300	-9.51907700	-2.54355600
O	-8.22011200	-9.02256300	-2.75253000
C	-1.18034700	-8.10911900	-2.07839700
C	-2.05548300	-7.34650100	-2.89401300
C	-1.55553500	-6.79508500	-4.08768500
C	-0.23329800	-7.01718200	-4.42856100
C	0.61678200	-7.78119900	-3.60000500
C	0.15824600	-8.33517500	-2.41668000
C	-3.21058300	-8.12142900	-1.11591200
C	-3.33468700	-7.35831900	-2.25249100
H	-2.20243700	-6.20746300	-4.73216900
H	0.16179400	-6.60020100	-5.34933900
H	1.64846300	-7.93945700	-3.89809000
H	0.80251000	-8.93333900	-1.77975400
N	-1.90235000	-8.54263800	-0.99645400
H	-1.54132400	-9.10734300	-0.24329000
H	-4.25322000	-6.90522400	-2.59665100
C	-4.27944800	-8.49169200	-0.16699400

O	-5.16603900	-7.64636700	0.15566100
<b>DQ·radical</b>			
C	2.83921100	1.23725800	0.19923300
C	1.46825200	1.19479000	0.18849500
C	0.71865800	-0.00001500	-0.00004700
C	1.46824800	-1.19480000	-0.18873400
C	2.83920800	-1.23722600	-0.19973900
C	3.60175400	0.00002600	-0.00031900
H	0.91847000	2.10874900	0.37681000
H	0.91845300	-2.10877300	-0.37694800
C	-0.71865300	-0.00002600	0.00008200
C	-1.46822500	-1.19478700	0.18899100
C	-1.46826500	1.19473200	-0.18869000
C	-2.83918400	-1.23723400	0.19999100
H	-0.91841500	-2.10871400	0.37738300
C	-2.83922500	1.23717500	-0.19944700
H	-0.91849400	2.10866200	-0.37717400
C	-3.60174900	-0.00003200	0.00032800
O	4.86018800	0.00004200	-0.00043200
O	-4.86018300	-0.00003800	0.00042400
C	3.59977300	-2.54782300	-0.42566900
C	4.48597700	-2.43693200	-1.67975600
C	4.47625700	-2.85839800	0.80176000
C	2.65527800	-3.73811000	-0.63177900
H	3.86988500	-2.24001600	-2.56392200
H	5.21054100	-1.63083500	-1.56834900
H	5.02093000	-3.37986900	-1.84307200
H	3.85189800	-2.98060300	1.69362100
H	5.02481600	-3.79404800	0.64147800
H	5.18884500	-2.05290300	0.97737400
H	3.24940700	-4.64608200	-0.77758500
H	2.00638900	-3.89979000	0.23566500
H	2.02272500	-3.60822100	-1.51631600
C	3.59977600	2.54788500	0.42498300
C	4.48622700	2.43706200	1.67890100
C	4.47601100	2.85844700	-0.80262800
C	2.65528400	3.73814900	0.63123900
H	3.87031600	2.24014800	2.56319400
H	5.21079900	1.63099000	1.56737700
H	5.02117600	3.38002300	1.84208600
H	3.85146900	2.98060800	-1.69436800
H	5.02458000	3.79411500	-0.64248400
H	5.18858000	2.05296100	-0.97835600
H	3.24941400	4.64614700	0.77688800

H	2.00621000	3.89977700	-0.23607600
H	2.02291900	3.60827500	1.51591200
C	-3.59980700	2.54774800	-0.42545600
C	-4.47610000	2.85851500	0.80206200
C	-2.65532900	3.73799600	-0.63188300
C	-4.48620000	2.43668700	-1.67939200
H	-5.18865600	2.05304400	0.97790900
H	-3.85159800	2.98085700	1.69380500
H	-5.02468400	3.79414000	0.64172200
H	-2.02293300	3.60798500	-1.51651400
H	-3.24947200	4.64595700	-0.77770600
H	-2.00628600	3.89978200	0.23542500
H	-5.02115100	3.37961400	-1.84277500
H	-3.87025000	2.23961200	-2.56362000
H	-5.21077300	1.63063200	-1.56775300
C	-3.59972800	-2.54780100	0.42616300
C	-4.48591800	-2.43670000	1.68024000
C	-4.47622400	-2.85861200	-0.80120000
C	-2.65521300	-3.73803800	0.63247500
H	-3.86982100	-2.23959400	2.56436000
H	-5.21051100	-1.63064900	1.56869200
H	-5.02083900	-3.37962200	1.84374300
H	-3.85187300	-2.98097700	-1.69304500
H	-5.02477300	-3.79423700	-0.64073700
H	-5.18882000	-2.05315500	-0.97695200
H	-3.24932800	-4.64599400	0.77844400
H	-2.00632700	-3.89986200	-0.23494400
H	-2.02265800	-3.60798600	1.51698600

**DQH·radical**

C	2.85049500	-1.22804300	-0.31958600
C	1.47882500	-1.17982500	-0.30706200
C	0.75915900	-0.00019100	0.00098900
C	1.48081800	1.17812000	0.30939100
C	2.85253100	1.22432300	0.32150800
C	3.60267800	-0.00238200	0.00076200
H	0.90958800	-2.06081400	-0.57693000
H	0.91295800	2.06009600	0.57865300
C	-0.70844600	0.00238100	-0.00055200
C	-1.42771500	1.16630900	-0.30491700
C	-1.43189800	-1.15661000	0.30276000
C	-2.81661000	1.20656300	-0.31944000
H	-0.87320400	2.05620700	-0.57279200
C	-2.82335700	-1.18907600	0.31296700
H	-0.88216000	-2.04846500	0.57349000



C	-3.50137800	0.00989000	-0.00568100
O	4.85252700	-0.00330900	0.00025700
O	-4.86106500	0.07610500	-0.02810600
C	3.61576300	2.50165700	0.66825100
C	4.49021700	2.27120800	1.91527100
C	4.50014300	2.92029800	-0.52253800
C	2.66454600	3.66546100	0.97441500
H	3.87110000	1.97554200	2.76851200
H	5.23663100	1.49806600	1.73649300
H	5.00316400	3.20311400	2.17609400
H	3.88579800	3.10318100	-1.41030200
H	5.02443700	3.84987100	-0.27635100
H	5.23670300	2.15158800	-0.75454200
H	3.25613300	4.55574100	1.20633100
H	2.02348700	3.90447800	0.11953100
H	2.02782800	3.45458000	1.83966400
C	3.61197200	-2.50595600	-0.66805300
C	4.48467900	-2.27547200	-1.91632300
C	4.49787800	-2.92634100	0.52095900
C	2.65917900	-3.66859100	-0.97363400
H	3.86452500	-1.97834900	-2.76830000
H	5.23221200	-1.50329900	-1.73808600
H	4.99621500	-3.20770400	-2.17876300
H	3.88487800	-3.10923000	1.40966200
H	5.02089400	-3.85623100	0.27325200
H	5.23554300	-2.15849400	0.75224600
H	3.24951500	-4.55939900	-1.20669300
H	2.01892800	-3.90726100	-0.11802700
H	2.02169300	-3.45655000	-1.83803300
C	-3.58079300	-2.48240700	0.66503600
C	-4.43451500	-2.95489300	-0.53255300
C	-2.61592500	-3.63564500	0.97849000
C	-4.43684600	-2.28754500	1.93534900
H	-5.16927900	-2.22905200	-0.89141600
H	-3.78313300	-3.18579400	-1.38017700
H	-4.97881900	-3.86437800	-0.26093100
H	-1.98313500	-3.41060400	1.84184200
H	-3.19843100	-4.53015600	1.21587800
H	-1.97445000	-3.87195200	0.12433500
H	-4.96881100	-3.21545000	2.16603900
H	-3.78869200	-2.04470600	2.78209300
H	-5.18346100	-1.49115600	1.87333000
C	-3.57170700	2.49943400	-0.66747900
C	-4.43875400	2.29523000	-1.92332100

C	-4.44787900	2.94060000	0.52029600
C	-2.60329800	3.65199500	-0.96846300
H	-3.81462200	2.00059500	-2.77303900
H	-5.20279700	1.53351400	-1.77143100
H	-4.93589000	3.23699700	-2.17945200
H	-3.82789400	3.11572600	1.40550400
H	-4.95392300	3.87937800	0.27086700
H	-5.20463200	2.19595000	0.76600200
H	-3.18427500	4.54866200	-1.20219400
H	-1.96376500	3.88431400	-0.11077100
H	-1.96576900	3.43513900	-1.83139500
H	-5.24381800	-0.77614800	0.20019400
<b>TS4</b>			
C	0.49475300	-0.14908000	0.16749700
C	1.67576400	-0.69744000	1.91109900
C	2.62894300	-1.50783000	-0.22447400
H	2.19796400	-1.83667400	-1.17336800
N	0.74046400	0.08790100	2.36847600
N	0.01606100	0.43052900	1.26994400
N	1.56828400	-0.85350900	0.55672400
C	2.73497600	-1.49355600	2.60378500
H	2.46009700	-1.66970700	3.64309600
H	3.70020100	-0.97073800	2.57046100
C	3.24179600	-2.70433000	0.59996500
O	2.77961400	-2.74468200	1.94160100
C	4.98244600	-1.11411700	0.02352300
C	3.78435800	-0.54782700	-0.40809600
C	3.72022200	0.75204400	-0.88776600
C	4.90966700	1.46485200	-0.90963600
C	6.12794100	0.93097100	-0.49720300
C	6.16477100	-0.37644600	-0.02645900
C	4.77424200	-2.52405300	0.50627300
H	2.79869400	1.19868900	-1.24195100
H	7.02012400	1.54318000	-0.53854300
H	7.10142300	-0.80688800	0.31066500
H	5.23751800	-2.71993400	1.47750000
H	5.19716300	-3.23960100	-0.20505100
C	-0.97996600	1.47865700	1.33821200
C	-0.67269400	2.69689700	0.72508200
C	-2.18096100	1.23734300	2.01501100
C	-1.65556700	3.68693000	0.75808900
C	-3.12224300	2.26108100	2.01503000
C	-2.88654800	3.48171000	1.37741500
H	-1.44607000	4.64334600	0.28651700

H	-4.07321600	2.09393000	2.51399900
C	-2.47090900	-0.07903000	2.67924700
H	-1.66452700	-0.38180000	3.35280400
H	-2.58859100	-0.85610500	1.91701500
H	-3.39762100	-0.01887000	3.25171000
C	-3.95570600	4.54024500	1.35237600
H	-3.55969000	5.49942300	1.01403600
H	-4.40000700	4.67523200	2.34176500
H	-4.75575800	4.23991600	0.66825100
C	0.65186700	2.96658100	0.05444800
H	1.48412400	2.47077100	0.56430100
H	0.85784900	4.03790200	0.05719600
H	0.65254300	2.64412100	-0.99344700
H	2.91767500	-3.65440500	0.17551700
N	4.86843500	2.85683200	-1.37751300
O	5.92494000	3.45152200	-1.48611500
O	3.77593000	3.33865100	-1.62359800
C	-3.46252700	0.09078900	-0.69449000
C	-3.36174700	1.21932400	-1.56333600
C	-4.46263400	2.08844200	-1.72460800
C	-5.62458700	1.81588600	-1.03744500
C	-5.72054400	0.68650600	-0.18467000
C	-4.66438800	-0.18194300	-0.00907900
C	-1.40584200	0.15997200	-1.41705000
C	-2.03007400	1.22845800	-2.04708800
H	-4.38679900	2.95737900	-2.37136600
H	-6.48194500	2.47314200	-1.14018400
H	-6.64772700	0.51177200	0.35219200
H	-4.74117800	-1.02484400	0.67203700
N	-2.25916700	-0.55338600	-0.59791500
H	-2.13535600	-1.87271700	-0.57423600
H	-1.54903900	1.96963400	-2.67101400
C	0.02691600	0.04899800	-1.26475800
O	0.89181800	0.19744600	-2.11242400
N	-2.01650900	-3.13395500	-0.64006200
C	-0.72229700	-3.50445200	-0.01239500
C	-0.62814200	-3.14977200	1.46319100
H	0.05825200	-2.97168900	-0.56364700
H	-0.55317500	-4.57788900	-0.16876100
H	0.39747000	-3.32047700	1.80172900
H	-0.87636200	-2.09677600	1.62968900
H	-1.29028000	-3.75754800	2.08209900
C	-3.16065600	-3.70676500	0.12673400
C	-4.49733800	-3.62642300	-0.59822600

H	-3.21484100	-3.15135800	1.06822400
H	-2.92415400	-4.75040300	0.37135200
H	-5.29092000	-3.86089800	0.11452600
H	-4.68697100	-2.62488100	-0.99323200
H	-4.56309300	-4.34312900	-1.41838300
C	-2.05887800	-3.55176000	-2.07076300
C	-0.85613100	-3.11175100	-2.89263500
H	-2.96198500	-3.11242100	-2.49763100
H	-2.16462100	-4.64380700	-2.10487200
H	-1.06387500	-3.33182900	-3.94172900
H	-0.68232300	-2.03495200	-2.81369800
H	0.05762300	-3.64441500	-2.62210000

**M4**

C	0.43725700	-0.15269300	0.23667500
C	1.64595500	-0.73169100	1.95332700
C	2.54993600	-1.53116900	-0.20567800
H	2.10308900	-1.83496000	-1.15515000
N	0.72885100	0.05839200	2.43621700
N	-0.01219200	0.42086500	1.35342600
N	1.51042200	-0.87290800	0.59973400
C	2.70959800	-1.54752600	2.61543100
H	2.45711300	-1.72784600	3.65937800
H	3.68104000	-1.03860400	2.56255200
C	3.15266600	-2.75030000	0.59053300
O	2.72148900	-2.79431100	1.94264400
C	4.91474000	-1.18901100	0.00553200
C	3.72061400	-0.58917600	-0.39135500
C	3.67501400	0.72155100	-0.84356000
C	4.87957300	1.40862800	-0.87392700
C	6.09374500	0.84095700	-0.49555300
C	6.11159000	-0.47642300	-0.05222100
C	4.68603700	-2.60401500	0.46328600
H	2.75567600	1.19352200	-1.16970300
H	6.99768400	1.43488200	-0.54380100
H	7.04486700	-0.93424700	0.25642900
H	5.16789400	-2.83275900	1.41790400
H	5.07401800	-3.31275600	-0.27437900
C	-0.99719600	1.47456500	1.45359500
C	-0.70644000	2.69109300	0.83059800
C	-2.17590800	1.23637900	2.16909100
C	-1.68326400	3.68651800	0.90062900
C	-3.10931300	2.26579700	2.20867700
C	-2.89089800	3.48718000	1.56485400
H	-1.48579300	4.64233800	0.42299600

H	-4.04166700	2.10290000	2.74301100
C	-2.45575900	-0.08837200	2.82004100
H	-1.63163700	-0.41217600	3.46115700
H	-2.60342400	-0.84182000	2.03953000
H	-3.36292300	-0.03110300	3.42348800
C	-3.95511500	4.55184200	1.57738500
H	-3.54892900	5.52411200	1.29272900
H	-4.41307000	4.64022800	2.56545500
H	-4.74836300	4.29593300	0.86778300
C	0.59482600	2.95809300	0.11491000
H	1.44089100	2.45276700	0.59139800
H	0.80752700	4.02806600	0.11817900
H	0.55255100	2.64142500	-0.93318200
H	2.79931800	-3.68910500	0.16441100
N	4.86193400	2.80942700	-1.31661100
O	5.92946400	3.38417900	-1.42651700
O	3.77750900	3.31789800	-1.54275900
C	-3.52325000	0.08283800	-0.71651000
C	-3.45582400	1.02620300	-1.79724200
C	-4.61647400	1.73664500	-2.19061800
C	-5.79284700	1.50413100	-1.51962900
C	-5.85422000	0.57268900	-0.44468600
C	-4.74844200	-0.13826000	-0.04047300
C	-1.46164700	0.14877100	-1.35059500
C	-2.10965100	1.03714100	-2.21434400
H	-4.57142800	2.45407600	-3.00450400
H	-6.69319900	2.03984700	-1.80203900
H	-6.79824000	0.43318300	0.07297800
H	-4.80007600	-0.82724200	0.79876600
N	-2.30679900	-0.45699600	-0.44523000
H	-2.23231600	-2.12049900	-0.50407200
H	-1.64057700	1.65615100	-2.96681700
C	-0.03803200	0.05547300	-1.19108500
O	0.83547600	0.19472100	-2.03838300
N	-2.12568600	-3.19631700	-0.59861800
C	-0.78682200	-3.53141100	-0.02238100
C	-0.66814600	-3.22712700	1.46141200
H	-0.06203200	-2.93464600	-0.58106500
H	-0.58771900	-4.58573000	-0.23828800
H	0.37545900	-3.35912800	1.75987600
H	-0.96071000	-2.19314100	1.67194800
H	-1.27586300	-3.89252300	2.07606200
C	-3.23744900	-3.82994000	0.18737300
C	-4.60503600	-3.68620400	-0.46110400

H	-3.23323800	-3.34688300	1.16619600
H	-2.97438300	-4.88406600	0.32387500
H	-5.35667400	-4.00340100	0.26429400
H	-4.81730800	-2.64813600	-0.73072900
H	-4.71194500	-4.31362100	-1.34698000
C	-2.21139600	-3.54873600	-2.05658600
C	-1.03110800	-3.07556300	-2.88929400
H	-3.12854700	-3.08854900	-2.42514100
H	-2.32172200	-4.63617700	-2.11458400
H	-1.26640000	-3.27129900	-3.93717500
H	-0.86624000	-2.00012300	-2.78539500
H	-0.10882200	-3.61025800	-2.65495200

**TS5(R)**

C	1.89281700	1.37068100	0.24316400
C	3.68443300	0.59482900	1.21362600
C	1.69449700	-0.64467000	1.85647400
H	0.61047700	-0.52812500	1.80834600
N	4.11432800	1.53549400	0.41986200
N	2.98750800	1.99802900	-0.18652700
N	2.33140400	0.44239000	1.11194100
C	4.36659400	-0.16937400	2.30492600
H	5.30721800	0.31767200	2.56053300
H	4.56725700	-1.20397200	2.00561100
C	2.20090900	-0.61292100	3.32909400
O	3.52050700	-0.08163200	3.44155800
C	2.34830600	-2.84746800	2.47878800
C	2.12475300	-2.01946800	1.37481200
C	2.28639500	-2.48038100	0.07658700
C	2.66702000	-3.81008200	-0.06403200
C	2.87246800	-4.66962600	1.01134600
C	2.71120600	-4.17991500	2.30277200
C	2.14152800	-2.08666100	3.76370800
H	2.10107600	-1.85552800	-0.78727000
H	3.16406200	-5.69548700	0.82605100
H	2.88245400	-4.82574300	3.15705700
H	2.89356800	-2.29964500	4.52626200
H	1.15574600	-2.31222800	4.18653300
C	3.08922100	3.01974700	-1.19752900
C	2.86550500	2.64822400	-2.52642000
C	3.44049300	4.30796000	-0.79579200
C	3.01263900	3.64483400	-3.48695600
C	3.57207000	5.26655700	-1.79989700
C	3.36182000	4.95380200	-3.14324600

H	2. 84945900	3. 39258300	-4. 53141400
H	3. 84258500	6. 28171900	-1. 52218800
C	3. 65768000	4. 64789400	0. 65476100
H	4. 55439500	4. 15837600	1. 04457900
H	2. 81162600	4. 32109500	1. 26808500
H	3. 77114500	5. 72546900	0. 77852200
C	3. 48187000	6. 01246200	-4. 20788900
H	4. 08349900	6. 85528900	-3. 86219200
H	2. 49288300	6. 39508000	-4. 47894300
H	3. 93718300	5. 60784900	-5. 11477000
C	2. 47545800	1. 24202700	-2. 89512300
H	3. 15587800	0. 51028300	-2. 44704800
H	2. 50640300	1. 11396900	-3. 97790600
H	1. 46145900	1. 01014100	-2. 54973000
H	1. 57172400	0. 03728400	3. 93942300
N	2. 86338900	-4. 33443400	-1. 42215100
O	3. 14192000	-5. 51500800	-1. 54223700
O	2. 74125700	-3. 55987700	-2. 35417800
C	-2. 07053800	0. 32461300	2. 06777300
C	-1. 43816900	1. 15645700	3. 04334100
C	-1. 88388700	1. 14090200	4. 37990000
C	-2. 92198900	0. 29983600	4. 72673700
C	-3. 53521500	-0. 53040500	3. 75999500
C	-3. 12751800	-0. 53187500	2. 43980800
C	-0. 48909900	1. 42474000	1. 04207600
C	-0. 39974600	1. 85096700	2. 35512000
H	-1. 41729100	1. 78407400	5. 12093600
H	-3. 27778500	0. 27362300	5. 75194900
H	-4. 34923900	-1. 18202100	4. 06281100
H	-3. 61481500	-1. 17051800	1. 71049900
N	-1. 48774900	0. 51839800	0. 83701000
H	0. 30074300	2. 57052200	2. 75936600
C	0. 46144400	1. 80819600	-0. 03096700
O	0. 23952100	2. 52169200	-0. 97535000
C	-2. 99863900	-1. 89041300	-0. 72047300
C	-1. 71343500	-1. 92471400	-0. 16333500
C	-1. 34585100	-2. 94012800	0. 69835900
C	-2. 28687800	-3. 92736900	1. 01072700
C	-3. 56544900	-3. 87832800	0. 45809500
C	-3. 94565800	-2. 85898600	-0. 42261600
C	-1. 98055900	-0. 04665300	-1. 63567300
C	-0. 98162500	-0. 71545700	-0. 65296900
H	-0. 34824400	-2. 96303900	1. 12797500
H	-2. 02345300	-4. 73213700	1. 68807100

H	-4.28735100	-4.64729700	0.71349300
H	-4.94611400	-2.82016000	-0.84022400
N	-3.14300400	-0.78194200	-1.56833800
O	-1.78074500	0.91073300	-2.34953900
C	-4.37231800	-0.41403200	-2.23594000
H	-4.71062600	-1.24038100	-2.87152100
H	-4.11525400	0.42569400	-2.88896800
C	-5.46292800	-0.02595800	-1.25651800
C	-6.79523800	-0.34028800	-1.52543200
C	-5.14384100	0.65442700	-0.07966200
C	-7.80017800	0.02785500	-0.63330200
H	-7.04686000	-0.87995700	-2.43512700
C	-6.14617600	1.01168700	0.81801100
H	-4.10474100	0.89018500	0.14029700
C	-7.47700600	0.70241200	0.54200900
H	-8.83354200	-0.22223900	-0.85159100
H	-5.88289900	1.52633300	1.73691600
H	-8.25788300	0.98009900	1.24260000
O	0.24700400	-0.57501300	-0.77731800

#### TS5(S)

C	-1.35207900	0.47272700	-0.18533200
C	-1.95796000	-0.87312400	-1.77524200
C	-2.44800700	-1.71203000	0.49206200
H	-1.94889000	-1.55332800	1.44915000
N	-1.44551900	0.15570200	-2.38969600
N	-1.07382400	0.99096400	-1.37983200
N	-1.94307600	-0.69839700	-0.42366000
C	-2.40501800	-2.20959500	-2.26896000
H	-2.05910200	-2.37195400	-3.28907000
H	-3.50016500	-2.29061600	-2.24122000
C	-2.14168100	-3.14800900	-0.06723400
O	-1.77738700	-3.16905900	-1.43929300
C	-4.51038400	-2.92527400	0.40982600
C	-3.95547900	-1.65783900	0.58417300
C	-4.74173300	-0.53651000	0.80093600
C	-6.11545500	-0.74038900	0.82815100
C	-6.70597700	-1.99077000	0.66020400
C	-5.89243800	-3.09850300	0.45120300
C	-3.43270100	-3.95661700	0.20063400
H	-4.31350900	0.44906200	0.94972100
H	-7.78461400	-2.07818800	0.69067800
H	-6.33417300	-4.07960700	0.31397200
H	-3.63678200	-4.63384600	-0.63311500



H	-3.31694200	-4.56912500	1.10088500
C	-0.55856900	2.31340600	-1.64075800
C	-1.39554200	3.39816400	-1.36249000
C	0.74645900	2.45734400	-2.12531600
C	-0.86292100	4.67649600	-1.52656500
C	1.22486100	3.75721800	-2.26958900
C	0.44951700	4.87314700	-1.95229500
H	-1.49095500	5.53626200	-1.30758000
H	2.24361900	3.89794400	-2.62378900
C	1.63402200	1.28865000	-2.45516200
H	1.06735400	0.39428400	-2.71405100
H	2.25899300	1.04800200	-1.58829700
H	2.29270600	1.54910100	-3.28676600
C	1.03594700	6.25575200	-2.05885100
H	0.27067600	7.02464300	-1.93685100
H	1.52589200	6.40301400	-3.02502400
H	1.79285000	6.40033600	-1.28110600
C	-2.81543800	3.21964900	-0.88575800
H	-3.29100400	2.34277800	-1.33491300
H	-3.40885000	4.09698900	-1.14810800
H	-2.86263400	3.10495300	0.20263500
H	-1.27713700	-3.56386300	0.45044400
N	-6.98691500	0.42205100	1.03816700
O	-8.19011900	0.23243400	1.08383000
O	-6.45983400	1.51471900	1.15279500
C	2.16516100	2.25862900	0.91181600
C	1.57819200	3.47649900	1.37667300
C	2.34317800	4.65737000	1.42635900
C	3.66740800	4.60918200	1.03894800
C	4.24890300	3.39586200	0.60287000
C	3.52286500	2.22162800	0.53921300
C	0.06730200	1.83765000	1.34354900
C	0.21959700	3.17183800	1.67144700
H	1.89321000	5.58918300	1.75806200
H	4.27393800	5.50889300	1.06529200
H	5.29312000	3.38978400	0.30478400
H	3.98299400	1.30325000	0.18969400
N	1.21895700	1.26863600	0.86759400
H	-0.56796400	3.84730400	1.97759300
C	-1.20900800	1.16203100	1.15980800
O	-2.20334400	1.22530400	1.85786500
C	3.53754100	-1.05416400	1.08222600
C	2.56488300	-0.67213200	2.01149500
C	2.90328000	-0.43318900	3.32852100

C	4. 24178600	-0. 57595600	3. 71015000
C	5. 20294300	-0. 95556000	2. 77556300
C	4. 86762700	-1. 20530500	1. 43947900
C	1. 59382900	-1. 09549200	-0. 13254300
C	1. 24629500	-0. 60958900	1. 29738300
H	2. 13924800	-0. 13667400	4. 04090600
H	4. 53429800	-0. 39234900	4. 73830400
H	6. 23674600	-1. 06575000	3. 08678000
H	5. 61917300	-1. 51467800	0. 72086500
N	2. 95759700	-1. 22681400	-0. 19278300
O	0. 81073600	-1. 36253000	-1. 02588200
C	3. 67039500	-1. 68311700	-1. 37151400
H	4. 54891900	-1. 04576000	-1. 52313700
H	2. 98673200	-1. 52540700	-2. 21145800
C	4. 07493900	-3. 13918700	-1. 28223300
C	5. 40438600	-3. 52658400	-1. 43588600
C	3. 09925700	-4. 11234700	-1. 04735300
C	5. 76145200	-4. 87190400	-1. 35346500
H	6. 16590000	-2. 77254100	-1. 62011600
C	3. 45411600	-5. 45407000	-0. 96317100
H	2. 06032900	-3. 80868200	-0. 93894900
C	4. 78727300	-5. 83639500	-1. 11504600
H	6. 80024200	-5. 16327000	-1. 47117600
H	2. 69117300	-6. 20461700	-0. 78282000
H	5. 06336000	-6. 88380200	-1. 04822000
O	0. 13224600	-0. 87198100	1. 79519800

### 5(R)

C	-1. 00248300	0. 32306600	-0. 39734400
C	-1. 40046300	-1. 01519800	-2. 07540300
C	-1. 13996200	-2. 18248600	0. 07936700
H	-0. 54129200	-1. 98956200	0. 96918300
N	-1. 51955000	0. 17809000	-2. 57461300
N	-1. 28908600	1. 00319200	-1. 50390500
N	-1. 10581600	-0. 97073900	-0. 74196600
C	-1. 44329400	-2. 36326600	-2. 71773200
H	-1. 22897000	-2. 28378100	-3. 78301200
H	-2. 42891000	-2. 82995500	-2. 58470300
C	-0. 60019400	-3. 41147700	-0. 73836100
O	-0. 41231400	-3. 12924700	-2. 11841700
C	-2. 85245600	-3. 86524600	0. 04376600
C	-2. 57381400	-2. 54638000	0. 39643600
C	-3. 54061200	-1. 70607500	0. 93140000
C	-4. 80977700	-2. 24863500	1. 08054400

C	-5.12755600	-3.56338200	0.74375300
C	-4.13442900	-4.38397300	0.22251400
C	-1.62820800	-4.54505700	-0.50938200
H	-3.29958000	-0.68741800	1.23038900
H	-6.13936900	-3.92118800	0.88641200
H	-4.36282800	-5.40867900	-0.05053800
H	-1.81736100	-5.08160900	-1.44404100
H	-1.23668900	-5.27230100	0.20884500
C	-1.55628300	2.41330700	-1.62483900
C	-2.80076700	2.86382700	-1.18008900
C	-0.57982100	3.24962600	-2.16785000
C	-3.05490600	4.23220400	-1.28736900
C	-0.88498500	4.60437300	-2.25754600
C	-2.11021700	5.11237300	-1.81645100
H	-4.01343000	4.61547700	-0.94729100
H	-0.14098700	5.28418400	-2.66573800
C	0.77126600	2.71759300	-2.55135000
H	0.69613300	1.77357400	-3.09582400
H	1.35938500	2.51550700	-1.64853600
H	1.31073400	3.44418200	-3.16121500
C	-2.38818000	6.59137700	-1.89064400
H	-3.45402400	6.80143600	-1.78246600
H	-2.04573700	7.00835600	-2.84101500
H	-1.85915100	7.12026200	-1.09125200
C	-3.80367600	1.91791700	-0.57295100
H	-3.95473700	1.03691600	-1.20642700
H	-4.76688600	2.41235700	-0.43937800
H	-3.44878100	1.56967000	0.40409900
H	0.39395600	-3.68623800	-0.38524800
N	-5.87507200	-1.38720500	1.60879400
O	-6.96946000	-1.88822900	1.80574000
O	-5.61103400	-0.21581700	1.81519800
C	2.16253000	2.99761900	1.03791600
C	1.21761300	4.05896100	0.95285700
C	1.69580600	5.37714400	0.86726300
C	3.06230500	5.59840000	0.87731100
C	3.97627800	4.52895000	0.97358300
C	3.54480500	3.21549200	1.05566000
C	0.08913200	2.12523400	1.02387100
C	-0.09786400	3.47556800	0.96035700
H	0.99844600	6.20642200	0.79122900
H	3.44277000	6.61246300	0.80941800
H	5.04078700	4.73948800	0.98143300
H	4.24631000	2.39010500	1.12973400

N	1. 42799400	1. 83886400	1. 08692500
H	-1. 04325300	3. 99259500	0. 87221800
C	-0. 72551400	0. 83945700	1. 04438300
O	-1. 74626500	0. 71757200	1. 78741300
C	3. 79815400	-0. 63724300	1. 37898700
C	2. 79504600	0. 01013900	2. 10617900
C	2. 90483400	0. 18413300	3. 47102100
C	4. 04739600	-0. 30645300	4. 11293000
C	5. 03894700	-0. 95571800	3. 38099500
C	4. 93280000	-1. 13615500	1. 99699200
C	2. 23987200	-0. 10869900	-0. 20987600
C	1. 69639200	0. 41570000	1. 15871900
H	2. 11791200	0. 68975000	4. 02234900
H	4. 16132700	-0. 18399000	5. 18421100
H	5. 91768700	-1. 33552900	3. 89201600
H	5. 70764800	-1. 65206000	1. 44093400
N	3. 46334600	-0. 66837700	0. 00871300
O	1. 65929700	-0. 03660500	-1. 27828600
C	4. 26801300	-1. 25730300	-1. 05223800
H	5. 32055700	-1. 05189400	-0. 83791500
H	3. 99619300	-0. 72336300	-1. 96686400
C	4. 02353500	-2. 74044600	-1. 21941500
C	5. 00971100	-3. 67602300	-0. 91357700
C	2. 78435900	-3. 17932300	-1. 69775300
C	4. 76441200	-5. 03909400	-1. 08040200
H	5. 97853400	-3. 34001200	-0. 55191500
C	2. 54002200	-4. 53840400	-1. 86594300
H	2. 01155300	-2. 45328100	-1. 94250300
C	3. 53005100	-5. 47157000	-1. 55605600
H	5. 53921900	-5. 76030500	-0. 84081300
H	1. 57590600	-4. 86210100	-2. 24853300
H	3. 34048300	-6. 53172400	-1. 69025100
O	0. 45302200	-0. 13462100	1. 45266200

**5(S)**

C	1. 29824600	0. 09493200	0. 21882700
C	2. 26697200	-0. 36622800	2. 12953700
C	1. 57464600	-2. 36990100	0. 87875800
H	0. 74708600	-2. 58104400	0. 20371300
N	2. 32817700	0. 92772200	2. 03606600
N	1. 73249000	1. 19646300	0. 83280100
N	1. 64453600	-0. 91449700	1. 03964900
C	2. 62454100	-1. 28767900	3. 24965500
H	2. 71370600	-0. 73220500	4. 18268600
H	3. 57220600	-1. 80518900	3. 04792900

C	1. 37953200	-3. 07145700	2. 27281600
O	1. 53991300	-2. 18954800	3. 37317900
C	3. 36228700	-3. 93733300	1. 16395700
C	2. 89375900	-2. 89683200	0. 36476900
C	3. 60090900	-2. 42841900	-0. 73435200
C	4. 81116200	-3. 05916900	-0. 99278800
C	5. 31088700	-4. 10841000	-0. 22342700
C	4. 57631700	-4. 55480000	0. 86871300
C	2. 40352800	-4. 23278400	2. 28710800
H	3. 21981300	-1. 62079300	-1. 36008300
H	6. 26392400	-4. 55186700	-0. 48296100
H	4. 95315700	-5. 36410700	1. 48487700
H	2. 89206900	-4. 29785400	3. 26401800
H	1. 89620100	-5. 18731000	2. 11593000
C	1. 69849600	2. 55309700	0. 35115900
C	2. 69514100	2. 95298900	-0. 53676800
C	0. 66933400	3. 38768100	0. 79372900
C	2. 62636600	4. 26589300	-1. 00997200
C	0. 65112500	4. 68673300	0. 30014600
C	1. 61610300	5. 13861600	-0. 60657500
H	3. 38305100	4. 61041800	-1. 70989000
H	-0. 14601400	5. 35710000	0. 61203900
C	-0. 41263600	2. 86571300	1. 69806400
H	0. 00436600	2. 39110600	2. 59163900
H	-1. 01896500	2. 11850800	1. 17057000
H	-1. 07539800	3. 67346800	2. 01164000
C	1. 55378900	6. 54932000	-1. 13183000
H	2. 32601800	6. 72783900	-1. 88221500
H	1. 68990800	7. 27178200	-0. 32171200
H	0. 57932500	6. 74955600	-1. 58666000
C	3. 77660700	2. 00087700	-0. 97346000
H	4. 29002600	1. 57071300	-0. 10701600
H	4. 51501700	2. 51742100	-1. 58817500
H	3. 34266600	1. 17712100	-1. 55206200
H	0. 35339200	-3. 42936400	2. 36426300
N	5. 61192000	-2. 58325200	-2. 12828000
O	6. 62543100	-3. 20018500	-2. 41018700
O	5. 22304000	-1. 59412500	-2. 72307200
C	-2. 53912200	1. 52659900	-1. 07470900
C	-1. 90658800	2. 65283800	-1. 66820000
C	-2. 67621400	3. 80376700	-1. 90141800
C	-4. 02156900	3. 79107700	-1. 56991400
C	-4. 62557600	2. 65353400	-0. 99750900
C	-3. 89403800	1. 50624200	-0. 73403900

C	-0.37221600	1.03778900	-1.42295900
C	-0.52320200	2.30924500	-1.88926600
H	-2.22095900	4.68723200	-2.33943300
H	-4.62567700	4.67405400	-1.75196400
H	-5.68165000	2.67832900	-0.74795000
H	-4.35131500	0.63411600	-0.27446500
N	-1.56150000	0.57480100	-0.91643400
H	0.25457900	2.94935200	-2.28196800
C	0.69564100	-0.02700500	-1.22927400
O	1.61274500	-0.23443200	-2.07711000
C	-3.05555600	-2.19542600	0.55464600
C	-1.99512000	-1.29465400	0.69855800
C	-1.50594600	-0.98348100	1.95433100
C	-2.07972800	-1.59872200	3.07295000
C	-3.13589300	-2.49288000	2.91421800
C	-3.64967500	-2.80210600	1.65032500
C	-2.59183800	-1.57159400	-1.60288800
C	-1.55724400	-0.85256600	-0.68150200
H	-0.70025500	-0.26461800	2.07865700
H	-1.70189800	-1.37427000	4.06414800
H	-3.57874000	-2.95777000	3.78890600
H	-4.48280600	-3.48703400	1.53829900
N	-3.37671500	-2.36202400	-0.80588800
O	-2.67508700	-1.44134200	-2.80386800
C	-4.50130500	-3.13418400	-1.30839500
H	-4.49477900	-4.12019700	-0.83377500
H	-4.31700400	-3.26832400	-2.37760400
C	-5.81838500	-2.42613200	-1.07362900
C	-6.82132400	-2.99827300	-0.29434700
C	-6.02532700	-1.16498700	-1.64142200
C	-8.01861000	-2.31712100	-0.07564100
H	-6.66973600	-3.98276000	0.14192200
C	-7.21543700	-0.48134700	-1.41829100
H	-5.24600200	-0.72330500	-2.25913400
C	-8.21508400	-1.05726900	-0.63315600
H	-8.79363900	-2.77023600	0.53411700
H	-7.36519700	0.49813400	-1.86190600
H	-9.14483000	-0.52528500	-0.45943600
O	-0.26628300	-1.24610100	-1.04225600
<b>TS6(R)</b>			
C	-0.98041100	0.11152000	-0.41636100
C	-1.04781800	-1.10948000	-2.26413500
C	-1.07192400	-2.38994500	-0.14478700
H	-0.51781100	-2.23810400	0.78355000

N	-1.07797500	0.11525400	-2.69412600
N	-1.04732700	0.85071100	-1.52942600
N	-0.99770300	-1.14791900	-0.89979100
C	-0.98481000	-2.41128600	-2.99170600
H	-0.59563600	-2.27326500	-4.00002400
H	-1.98070100	-2.87288400	-3.05469300
C	-0.49381000	-3.59433300	-0.97518300
O	-0.07620200	-3.24004800	-2.28441800
C	-2.81676000	-4.02684500	-0.38534500
C	-2.51515800	-2.75833700	0.10331700
C	-3.47553100	-1.95021400	0.69554700
C	-4.76040400	-2.47089800	0.76780900
C	-5.10054000	-3.73751500	0.29481100
C	-4.11569900	-4.52623400	-0.28689400
C	-1.59886800	-4.68290200	-0.97999000
H	-3.23061200	-0.96925100	1.09544600
H	-6.12314600	-4.08209800	0.38216900
H	-4.36299200	-5.51199900	-0.66655100
H	-1.76957700	-5.04899000	-1.99762200
H	-1.29094700	-5.54407200	-0.37931200
C	-1.17417000	2.27896700	-1.57166200
C	-2.30246900	2.85338000	-0.97847400
C	-0.15770200	3.04257600	-2.15658400
C	-2.39621500	4.24598200	-0.98257000
C	-0.29789100	4.42739600	-2.12994800
C	-1.40389400	5.04620900	-1.54618900
H	-3.26060400	4.71354900	-0.51705100
H	0.49504700	5.04066600	-2.55250500
C	1.05044900	2.40323200	-2.78414500
H	0.81008400	2.00322100	-3.77448300
H	1.40887300	1.56891800	-2.17780400
H	1.84962300	3.13953400	-2.89230800
C	-1.50298900	6.54928700	-1.52311500
H	-2.32288000	6.88469000	-0.88446400
H	-1.67238200	6.94721600	-2.52853100
H	-0.57238400	6.98870300	-1.15089300
C	-3.35078300	2.01465800	-0.29366600
H	-3.64620300	1.15577300	-0.90478400
H	-4.24003900	2.61217800	-0.08466600
H	-2.97214400	1.61899900	0.65697900
H	0.41743900	-3.95572800	-0.49754400
N	-5.81411200	-1.64001700	1.36232600
O	-6.92214400	-2.13110400	1.49771300
O	-5.52678400	-0.50015900	1.68397200

C	1. 78880500	2. 93658300	0. 72725600
C	0. 77597100	3. 86428500	1. 09325900
C	1. 03475600	5. 23558300	0. 94388100
C	2. 26544900	5. 63550800	0. 45184500
C	3. 25707200	4. 69413000	0. 10691900
C	3. 03777100	3. 33267500	0. 24145200
C	-0. 02138400	1. 80311800	1. 41564000
C	-0. 36858300	3. 11303100	1. 54532300
H	0. 27319900	5. 96620000	1. 20136300
H	2. 47594800	6. 69290600	0. 32728800
H	4. 21211900	5. 04395900	-0. 27118500
H	3. 79673200	2. 60341100	-0. 02678800
N	1. 25418300	1. 68404900	0. 91978700
H	-1. 32163800	3. 50206600	1. 87145700
C	-0. 55603600	0. 42217900	1. 56621900
O	-1. 49501400	0. 02625900	2. 23681600
C	3. 99295500	-0. 41118700	1. 37537500
C	2. 94009000	0. 22267300	2. 03738400
C	3. 06137300	0. 62643500	3. 35166400
C	4. 26956300	0. 37850500	4. 01159900
C	5. 31234600	-0. 26307900	3. 34655400
C	5. 19443100	-0. 67179000	2. 01337600
C	2. 34407400	-0. 29651100	-0. 21570000
C	1. 77109100	0. 34056400	1. 09293000
H	2. 23504900	1. 12248300	3. 85284000
H	4. 39500500	0. 68356100	5. 04427600
H	6. 24294700	-0. 45341100	3. 87102400
H	6. 01438800	-1. 17111200	1. 50987900
N	3. 62584600	-0. 68602100	0. 04200900
O	1. 75483500	-0. 44185800	-1. 26833800
C	4. 43904100	-1. 38175700	-0. 94866200
H	5. 48600500	-1. 12588200	-0. 76649300
H	4. 15168800	-0. 97354200	-1. 92109600
C	4. 22806000	-2. 87981300	-0. 92481400
C	5. 16040800	-3. 72830200	-0. 32877500
C	3. 07396400	-3. 42266800	-1. 49932200
C	4. 94515300	-5. 10556800	-0. 30241700
H	6. 06586800	-3. 31451400	0. 10791300
C	2. 86227700	-4. 79794800	-1. 47712600
H	2. 33805700	-2. 76795600	-1. 95922300
C	3. 79644100	-5. 64233400	-0. 87703700
H	5. 67767400	-5. 75799600	0. 16186700
H	1. 96761000	-5. 20660000	-1. 93913600
H	3. 63159200	-6. 71490900	-0. 86229000



O	0.64563900	-0.38967000	1.53749300
<b>TS6(S)</b>			
C	1.33533300	0.16124700	0.39184000
C	2.31266800	-0.24508100	2.34694000
C	1.56569300	-2.26160000	1.14138600
H	0.71361400	-2.45801000	0.48934600
N	2.37462300	1.04551100	2.22244200
N	1.77518400	1.26670800	1.00181000
N	1.69429400	-0.81293700	1.26353200
C	2.64605100	-1.14362400	3.49159900
H	2.74591600	-0.57263500	4.41416200
H	3.57960000	-1.69323300	3.30765500
C	1.37294300	-2.92760800	2.55591200
O	1.53891300	-2.01927300	3.63316700
C	3.29950200	-3.89535200	1.42960500
C	2.83544900	-2.87729100	0.59953500
C	3.50269400	-2.51389500	-0.56303800
C	4.66635600	-3.21730100	-0.84841600
C	5.16271900	-4.23951100	-0.04148800
C	4.46867300	-4.58457800	1.11150500
C	2.38643400	-4.09773900	2.60868200
H	3.13184600	-1.73300100	-1.22526200
H	6.07767800	-4.74487000	-0.32329900
H	4.83972600	-5.37608100	1.75384800
H	2.91816600	-4.09645700	3.56539000
H	1.86748100	-5.05805100	2.53153700
C	1.68703800	2.60729700	0.49375800
C	2.66841400	3.04037800	-0.39730100
C	0.59874900	3.39387600	0.87598000
C	2.54456000	4.33549200	-0.90366700
C	0.51946200	4.67971600	0.34855000
C	1.48326000	5.16598600	-0.53882900
H	3.29163100	4.69991700	-1.60438800
H	-0.32737600	5.30693200	0.61675900
C	-0.48904600	2.82741700	1.74641800
H	-0.08258700	2.36317800	2.65006600
H	-1.04529700	2.05813300	1.19538800
H	-1.19625500	3.60532500	2.03909500
C	1.37826800	6.56782000	-1.08194300
H	1.95054800	6.67884400	-2.00530700
H	1.76625900	7.29227800	-0.35876100
H	0.33738900	6.83239200	-1.28512500
C	3.77836500	2.11710000	-0.82483100
H	4.28294500	1.67973000	0.04230800

H	4. 51734300	2. 65356700	-1. 42199200
H	3. 37233400	1. 29386200	-1. 42432900
H	0. 34490900	-3. 27805600	2. 65617300
N	5. 41309900	-2. 86304800	-2. 06218300
O	6. 41779200	-3. 50396700	-2. 32232100
O	4. 99074200	-1. 94622700	-2. 74349000
C	-2. 44073900	1. 51947200	-1. 10328500
C	-1. 79131500	2. 66893500	-1. 63318400
C	-2. 52547000	3. 86179100	-1. 73559300
C	-3. 85285600	3. 86856500	-1. 34060000
C	-4. 47488500	2. 70834900	-0. 83534600
C	-3. 77997800	1. 51739400	-0. 70205300
C	-0. 30902600	0. 99744600	-1. 58024100
C	-0. 43055700	2. 30614300	-1. 94072700
H	-2. 05520700	4. 76155600	-2. 12157100
H	-4. 43003600	4. 78421000	-1. 41773900
H	-5. 51704200	2. 75048200	-0. 53530500
H	-4. 25020700	0. 62516800	-0. 29768800
N	-1. 48982400	0. 53092200	-1. 06564500
H	0. 34996500	2. 95135000	-2. 31803300
C	0. 67465800	-0. 12309100	-1. 50138500
O	1. 67351300	-0. 29888400	-2. 18334300
C	-3. 00381400	-2. 26210800	0. 30820500
C	-1. 94963700	-1. 36269700	0. 50249100
C	-1. 53831400	-1. 03212200	1. 78212900
C	-2. 17073500	-1. 64235100	2. 87081500
C	-3. 21090200	-2. 54523300	2. 66128500
C	-3. 65462500	-2. 86383900	1. 37405200
C	-2. 46957400	-1. 61456400	-1. 82263900
C	-1. 47739400	-0. 89425000	-0. 85434000
H	-0. 74770100	-0. 30575500	1. 94185400
H	-1. 85241500	-1. 40414500	3. 87961700
H	-3. 69920000	-3. 00609400	3. 51354500
H	-4. 48173300	-3. 54793700	1. 22071000
N	-3. 27238700	-2. 42105900	-1. 06465400
O	-2. 50771600	-1. 46007900	-3. 02214500
C	-4. 39188100	-3. 17206100	-1. 61025800
H	-4. 39882500	-4. 17176600	-1. 16566400
H	-4. 18925100	-3. 27607400	-2. 67956900
C	-5. 70865000	-2. 46244800	-1. 37617900
C	-6. 74814200	-3. 07641200	-0. 68081800
C	-5. 88066400	-1. 16242100	-1. 86099700
C	-7. 94815100	-2. 39911200	-0. 46574200
H	-6. 62176300	-4. 08920500	-0. 30584400

C	-7.07366800	-0.48283100	-1.64065000
H	-5.07457200	-0.68624700	-2.41544300
C	-8.11081500	-1.10155300	-0.94138900
H	-8.75190800	-2.88535200	0.07758200
H	-7.19608200	0.52696900	-2.01964000
H	-9.04287800	-0.57288400	-0.77019300
O	-0.16216300	-1.27012400	-1.20833100
<b>P(R)</b>			
C	4.59294500	3.65551700	3.13200300
C	3.70023900	4.74811200	2.94076900
C	4.22631500	6.05431400	2.95372100
C	5.58344400	6.22374700	3.14151200
C	6.44629300	5.11876100	3.32241700
C	5.97054600	3.82185100	3.32337000
C	2.51501100	2.85962900	2.86064100
C	2.37682500	4.21730800	2.76819700
H	3.57139100	6.90847500	2.81482200
H	6.00243300	7.22430500	3.15088800
H	7.50705300	5.29503600	3.46631700
H	6.62768000	2.97055400	3.47003800
N	3.82390800	2.52433800	3.10119300
H	1.46251000	4.76642200	2.60275000
C	1.77157700	1.59760000	2.79914200
O	0.60809400	1.36357700	2.64447600
C	5.94749300	-0.18673500	3.41122800
C	4.90710800	0.48058900	4.06400800
C	4.82656400	0.50436500	5.44321100
C	5.81230700	-0.16682400	6.17267000
C	6.84248400	-0.83561600	5.51297300
C	6.93156400	-0.85895800	4.11717800
C	4.72932100	0.69669500	1.68403100
C	4.02856700	1.10027900	3.02109600
H	4.01791000	1.03088900	5.94039400
H	5.77551200	-0.16862800	7.25594000
H	7.59872500	-1.35383100	6.09328100
H	7.73148700	-1.38789600	3.61097100
N	5.82814200	-0.04342900	2.01342100
O	4.33226400	0.99870200	0.58276700
C	6.71707000	-0.65032600	1.04115900
H	7.74069100	-0.30743400	1.22702700
H	6.40360500	-0.25981500	0.06829000
C	6.65531600	-2.16425100	1.06189600
C	7.81058800	-2.91054400	0.82960500
C	5.44657400	-2.82565300	1.28467300

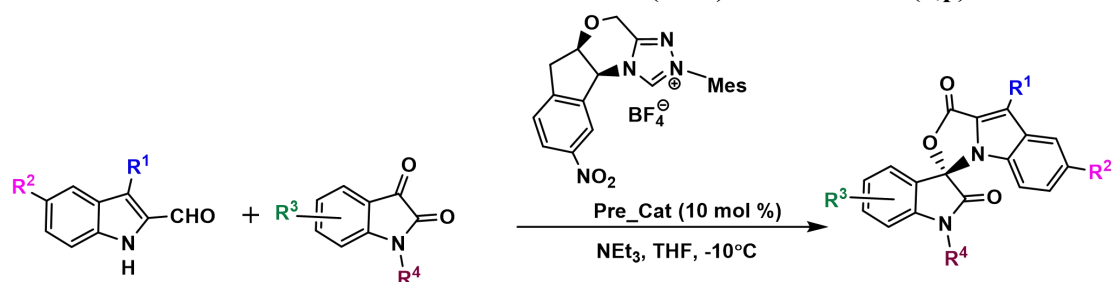
C	7. 75762800	-4. 30249200	0. 80772800
H	8. 75632000	-2. 40051000	0. 66483000
C	5. 39391200	-4. 21620400	1. 26828700
H	4. 54403800	-2. 25140100	1. 47804000
C	6. 54895800	-4. 95798300	1. 02765900
H	8. 66259600	-4. 87302900	0. 62520100
H	4. 44949200	-4. 72074200	1. 44469300
H	6. 50724500	-6. 04219100	1. 01628600
O	2. 69872400	0. 59120100	2. 99283800

**P(S)**

C	-2. 52332400	1. 80339400	-0. 40226800
C	-2. 00016800	2. 98534000	-0. 99910300
C	-2. 85915800	4. 08912100	-1. 16308800
C	-4. 17374900	3. 97609000	-0. 75606500
C	-4. 66710300	2. 78492100	-0. 17568700
C	-3. 85448400	1. 68437400	0. 01788200
C	-0. 37011000	1. 46241700	-0. 92362700
C	-0. 62164400	2. 74631900	-1. 32536400
H	-2. 49046900	5. 00787900	-1. 60771800
H	-4. 84816100	4. 81638400	-0. 88187300
H	-5. 70755600	2. 73474000	0. 12885200
H	-4. 22804200	0. 77017200	0. 46959600
N	-1. 48693900	0. 91294100	-0. 34804300
H	0. 07295000	3. 42893500	-1. 79064300
C	0. 65750300	0. 41602700	-0. 90251700
O	1. 80128000	0. 41263300	-1. 25396300
C	-2. 85846500	-1. 91273300	0. 95605400
C	-1. 83252700	-0. 99851900	1. 21117000
C	-1. 48334300	-0. 65406100	2. 50236500
C	-2. 18129300	-1. 25275500	3. 55559600
C	-3. 20840100	-2. 15733700	3. 29299800
C	-3. 57109000	-2. 50312200	1. 98665200
C	-2. 15436100	-1. 32044700	-1. 14149200
C	-1. 32056200	-0. 50007300	-0. 10601800
H	-0. 68968500	0. 06321600	2. 68686000
H	-1. 92824100	-1. 00723900	4. 58063800
H	-3. 74666900	-2. 60702600	4. 12080300
H	-4. 37986800	-3. 19899700	1. 79459100
N	-3. 01992000	-2. 10075000	-0. 43243900
O	-2. 04990600	-1. 22060900	-2. 34294700
C	-4. 06619900	-2. 90446200	-1. 04573000
H	-4. 06331200	-3. 89917100	-0. 58977200
H	-3. 78542200	-3. 01057500	-2. 09712200
C	-5. 42247700	-2. 24548000	-0. 90801500

C	-6.48333200	-2.89985100	-0.28515900
C	-5.60982700	-0.95187100	-1.40306900
C	-7.71975200	-2.26852700	-0.15284800
H	-6.34402300	-3.90728700	0.09937700
C	-6.83943300	-0.31736800	-1.26428400
H	-4.78676400	-0.44055700	-1.89831500
C	-7.89796200	-0.97640400	-0.63796100
H	-8.53940300	-2.78495000	0.33602500
H	-6.97181400	0.68919900	-1.64852000
H	-8.85832100	-0.48293900	-0.52957100
O	0.06549000	-0.69971500	-0.33818200

**Coordinates for different substituents at the IEFPCM(THF)//M062X/6-31G(d,p) level**



**H/H/5-MeO/Bn**

**TS5(R)**

C	1.89367500	1.36547900	0.27202300
C	3.69800200	0.57674400	1.20716600
C	1.71818200	-0.67172900	1.86314000
H	0.63350800	-0.55465100	1.83134700
N	4.11775400	1.52389300	0.41557300
N	2.98272700	1.99405700	-0.16915300
N	2.34327000	0.42724800	1.12481900
C	4.39582900	-0.19996300	2.27957300
H	5.33976400	0.28520600	2.52740300
H	4.59295900	-1.23101000	1.96530200
C	2.24532200	-0.65841200	3.32871400
O	3.56569800	-0.12617400	3.42897400
C	2.38311000	-2.88111500	2.44877900
C	2.14301600	-2.04032100	1.35818900
C	2.28669100	-2.48728600	0.05272200
C	2.66824800	-3.81436200	-0.10797500
C	2.89083200	-4.68538000	0.95445300
C	2.74626600	-4.21045500	2.25315100
C	2.19351300	-2.13717400	3.74565000
H	2.08628800	-1.85440800	-0.80208900
H	3.18096100	-5.70889300	0.75373300

H	2. 93026000	-4. 86557700	3. 09777300
H	2. 95648500	-2. 35809300	4. 49516900
H	1. 21369100	-2. 36953000	4. 17873000
C	3. 07027700	3. 01851900	-1. 17901900
C	2. 82378600	2. 65134100	-2. 50347300
C	3. 42789400	4. 30694800	-0. 77902300
C	2. 95311500	3. 65247500	-3. 46417500
C	3. 54194900	5. 26763500	-1. 78119200
C	3. 30771900	4. 95880600	-3. 12303200
H	2. 77054200	3. 40332100	-4. 50608600
H	3. 81646000	6. 28262400	-1. 50565700
C	3. 66533200	4. 64153000	0. 66947800
H	4. 56246300	4. 14397600	1. 04815900
H	2. 82314300	4. 32025100	1. 29109400
H	3. 78898000	5. 71798700	0. 79450200
C	3. 40968200	6. 02779200	-4. 17930300
H	4. 22938300	6. 71727400	-3. 96444600
H	2. 48650300	6. 61469800	-4. 21823600
H	3. 56978200	5. 59275300	-5. 16779600
C	2. 42498900	1. 24776300	-2. 87227600
H	3. 09457600	0. 51004100	-2. 41739800
H	2. 46347000	1. 11744700	-3. 95469100
H	1. 40629400	1. 02559200	-2. 53405500
H	1. 62462700	-0. 01669100	3. 95645500
N	2. 84563600	-4. 32251600	-1. 47472700
O	3. 14141700	-5. 49698300	-1. 61219000
O	2. 69139300	-3. 54176300	-2. 39696200
C	-2. 09709300	0. 28853300	2. 05677800
C	-1. 46463500	1. 08303900	3. 06286500
C	-1. 92568500	1. 03550200	4. 39306200
C	-2. 97801000	0. 19811700	4. 70451300
C	-3. 59096700	-0. 59576600	3. 70787800
C	-3. 16827500	-0. 56456700	2. 39263400
C	-0. 49008600	1. 39415000	1. 08105000
C	-0. 40908300	1. 78250500	2. 40625000
H	-1. 45917100	1. 65087300	5. 15759200
H	-3. 34551100	0. 14725600	5. 72473700
H	-4. 41748000	-1. 24413900	3. 98295900
H	-3. 65591900	-1. 17324800	1. 63780200
N	-1. 49868300	0. 50871100	0. 83779500
H	0. 29412800	2. 48403200	2. 83666800
C	0. 46020200	1. 80675900	0. 02001000
O	0. 22821100	2. 53902500	-0. 90751500
C	-2. 99062800	-1. 86692400	-0. 78036400

C	-1.71386900	-1.91302400	-0.20432900
C	-1.35490100	-2.92638700	0.65447500
C	-2.30467400	-3.91672500	0.95646500
C	-3.57818700	-3.86684300	0.38784000
C	-3.93340200	-2.83563300	-0.49571000
C	-1.94870300	-0.02144000	-1.66866700
C	-0.96920000	-0.70330000	-0.67578400
H	-0.36935600	-2.97469300	1.10851100
H	-4.31468300	-4.62624800	0.61953400
H	-4.93033600	-2.80138800	-0.92254300
N	-3.11360700	-0.74806900	-1.62614800
O	-1.72354800	0.93828700	-2.37411600
C	-4.33151400	-0.36830800	-2.30600100
H	-4.66386100	-1.18546800	-2.95705700
H	-4.06291200	0.47919500	-2.94442000
C	-5.43416500	0.00988000	-1.33623800
C	-6.76481400	-0.28965800	-1.62927000
C	-5.12663400	0.66478300	-0.14217900
C	-7.77929800	0.06973000	-0.74458800
H	-7.00749700	-0.81123100	-2.55190400
C	-6.13862800	1.01359000	0.74776800
H	-4.08846900	0.88719100	0.09640200
C	-7.46775200	0.72021100	0.44720300
H	-8.81152600	-0.16847700	-0.98151400
H	-5.88456700	1.50900300	1.67989400
H	-8.25669300	0.99114400	1.14157100
O	0.26015000	-0.56622300	-0.77799400
O	-1.88665700	-4.88266800	1.82017800
C	-2.81646800	-5.88931000	2.17105000
H	-2.30162900	-6.54947500	2.86794400
H	-3.69967100	-5.46177500	2.65938600
H	-3.13192900	-6.46332700	1.29238500

**TS5(S)**

C	-1.35712700	0.45702100	-0.18706500
C	-1.98123800	-0.85446900	-1.79844900
C	-2.47521500	-1.72762100	0.45424700
H	-1.97375600	-1.59037900	1.41350000
N	-1.45689900	0.17814800	-2.39629600
N	-1.07391700	0.99156000	-1.37309500
N	-1.96254400	-0.70279200	-0.44423200
C	-2.44728100	-2.17584600	-2.31460900
H	-2.10681200	-2.32410200	-3.33868600
H	-3.54331200	-2.24271000	-2.28483200

C	-2.18215000	-3.15619700	-0.12977700
O	-1.83009700	-3.15919200	-1.50537300
C	-4.54632400	-2.92432200	0.36179600
C	-3.98214000	-1.66300900	0.55030500
C	-4.76000500	-0.53891400	0.78236500
C	-6.13512500	-0.73361900	0.81013400
C	-6.73465600	-1.97781100	0.62906900
C	-5.92931900	-3.08861200	0.40492900
C	-3.47614900	-3.96014900	0.13656500
H	-4.32469800	0.44190500	0.94174400
H	-7.81378900	-2.05810300	0.66120100
H	-6.37809200	-4.06500000	0.25729900
H	-3.68853800	-4.62727200	-0.70314400
H	-3.35938000	-4.58232900	1.03007200
C	-0.54227700	2.31143300	-1.61277200
C	-1.36608600	3.40204600	-1.31847500
C	0.76543800	2.44626800	-2.09218200
C	-0.81648700	4.67582200	-1.45970500
C	1.26088500	3.74210300	-2.21414000
C	0.49968300	4.86248200	-1.87884100
H	-1.43358300	5.53995500	-1.22728400
H	2.28235700	3.87521700	-2.56349500
C	1.63920500	1.27165800	-2.43762400
H	1.06260900	0.38442300	-2.69884900
H	2.26773800	1.01862200	-1.57682900
H	2.29455200	1.53224200	-3.27190200
C	1.10513900	6.23878200	-1.95591300
H	0.34717700	7.01555800	-1.83797200
H	1.61559300	6.39278700	-2.91029800
H	1.84836000	6.36334600	-1.16143000
C	-2.78900800	3.23326800	-0.84722800
H	-3.27343400	2.36783100	-1.30889700
H	-3.37202600	4.12056700	-1.09929800
H	-2.83995200	3.10491600	0.23951300
H	-1.31593300	-3.58540800	0.37391900
N	-6.99820100	0.43237500	1.03460000
O	-8.20258400	0.25047000	1.08074200
O	-6.46341900	1.52013600	1.15973800
C	2.17608800	2.19160500	0.93834800
C	1.60115200	3.40672600	1.42504600
C	2.37731700	4.57933800	1.49458300
C	3.70054500	4.52561900	1.10447800
C	4.27005000	3.31462900	0.64633900
C	3.53306300	2.14849900	0.56351400



C	0.07526000	1.78282700	1.36450800
C	0.24026800	3.10967800	1.71604700
H	1.93684600	5.50927800	1.84379700
H	4.31543500	5.41911800	1.14545800
H	5.31382100	3.30408500	0.34669400
H	3.98357500	1.23135400	0.19851700
N	1.22095400	1.21125900	0.87737800
H	-0.54041200	3.78691400	2.03559400
C	-1.20789900	1.12445400	1.16857100
O	-2.20286900	1.18767800	1.86584000
C	3.51702000	-1.13340800	1.05425700
C	2.54957900	-0.75629700	1.99313100
C	2.88307800	-0.53256500	3.30811000
C	4.22694400	-0.68169400	3.69167200
C	5.19046800	-1.05646300	2.75438800
C	4.83981000	-1.28994600	1.41570700
C	1.56808300	-1.14839400	-0.15520800
C	1.22794600	-0.67950700	1.28251400
H	2.13923300	-0.23851300	4.04177700
H	6.22570500	-1.17880100	3.04699700
H	5.59521700	-1.59452000	0.69892200
N	2.92768200	-1.28844700	-0.22236900
O	0.77606100	-1.39624400	-1.04772600
C	3.63516300	-1.73625800	-1.40640800
H	4.51238300	-1.09681600	-1.55867300
H	2.94753100	-1.57591900	-2.24261400
C	4.04311100	-3.19201700	-1.32522500
C	5.37264200	-3.57693400	-1.48421500
C	3.06977400	-4.16748200	-1.09058400
C	5.73192700	-4.92206000	-1.40762800
H	6.13244200	-2.82095800	-1.66777300
C	3.42663300	-5.50900200	-1.01241100
H	2.03093200	-3.86545600	-0.97687200
C	4.75989300	-5.88886500	-1.16978400
H	6.77078800	-5.21149800	-1.52956000
H	2.66533500	-6.26126100	-0.83222200
H	5.03770600	-6.93610800	-1.10761100
O	0.11444400	-0.93653600	1.78074900
O	4.49016200	-0.44173800	5.00552100
C	5.83276700	-0.56073100	5.43375600
H	6.48437500	0.13820100	4.89680100
H	5.83655000	-0.31614300	6.49510200
H	6.20685000	-1.58144800	5.29394500

**H/H/5-Me/Bn**

**TS5(R)**

C	1. 89793700	1. 38512100	0. 22840600
C	3. 67452500	0. 59046000	1. 21201800
C	1. 66834100	-0. 62978000	1. 83514500
H	0. 58558400	-0. 50119900	1. 78057400
N	4. 11917500	1. 53192200	0. 42691400
N	3. 00126900	2. 00590000	-0. 18729100
N	2. 32160200	0. 45065700	1. 09781300
C	4. 34238100	-0. 19526600	2. 29671100
H	5. 28797500	0. 27715000	2. 56230200
H	4. 53251500	-1. 22752800	1. 98166400
C	2. 16170200	-0. 60915300	3. 31024700
O	3. 49569100	-0. 11682100	3. 43379100
C	2. 25296300	-2. 84721100	2. 46128900
C	2. 07927400	-2. 01047900	1. 35554200
C	2. 24402600	-2. 47429700	0. 05879000
C	2. 56930400	-3. 81883800	-0. 07882400
C	2. 71693000	-4. 68867600	0. 99778300
C	2. 55868300	-4. 19425000	2. 28812200
C	2. 05318700	-2. 08053900	3. 74387400
H	2. 09325900	-1. 84217100	-0. 80703700
H	2. 96378500	-5. 72673100	0. 81440600
H	2. 68748600	-4. 84917200	3. 14316300
H	2. 78874100	-2. 31612300	4. 51594500
H	1. 05501400	-2. 27563000	4. 15371400
C	3. 11845800	3. 03141100	-1. 19293100
C	2. 93282300	2. 65771200	-2. 52668400
C	3. 44441500	4. 32239600	-0. 78121100
C	3. 08847500	3. 65669700	-3. 48285400
C	3. 58792200	5. 28378700	-1. 78156600
C	3. 41253300	4. 96984500	-3. 12928000
H	2. 95367900	3. 40394500	-4. 53138400
H	3. 83994300	6. 30193000	-1. 49732300
C	3. 62510300	4. 66070400	0. 67453100
H	4. 51197700	4. 17057900	1. 08600700
H	2. 76397700	4. 33362400	1. 26641500
H	3. 73604600	5. 73813300	0. 80283200
C	3. 54683800	6. 02919700	-4. 19161200
H	4. 08157400	6. 90322300	-3. 81475400
H	2. 55954000	6. 35882200	-4. 52994800
H	4. 08032800	5. 64423100	-5. 06415400
C	2. 57981100	1. 24341900	-2. 90136300
H	3. 27742600	0. 52910500	-2. 45089000
H	2. 61903800	1. 11817300	-3. 98421800

H	1. 57100700	0. 98339100	-2. 56161800
H	1. 54508100	0. 05864800	3. 91464300
N	2. 76352700	-4. 34894400	-1. 43504300
O	2. 98701600	-5. 54122100	-1. 55406200
O	2. 69449900	-3. 56719600	-2. 36653300
C	-2. 05196900	0. 35136600	2. 05588500
C	-1. 41717600	1. 19145300	3. 02307700
C	-1. 85271000	1. 17838100	4. 36321600
C	-2. 88106200	0. 33043500	4. 72188600
C	-3. 49468400	-0. 50984800	3. 76394800
C	-3. 09751700	-0. 51372500	2. 44067400
C	-0. 48534100	1. 45420000	1. 01274200
C	-0. 38752100	1. 88703700	2. 32405100
H	-1. 38585700	1. 82867800	5. 09805400
H	-3. 22857300	0. 30619800	5. 75007900
H	-4. 30024000	-1. 16746400	4. 07664400
H	-3. 58271800	-1. 16178600	1. 71769000
N	-1. 48044500	0. 54153700	0. 81998700
H	0. 31464300	2. 60982900	2. 72000400
C	0. 46955400	1. 82772000	-0. 06100400
O	0. 25859900	2. 53321400	-1. 01352800
C	-2. 99223200	-1. 89476800	-0. 71416200
C	-1. 69695900	-1. 91178800	-0. 18151600
C	-1. 30029800	-2. 91763500	0. 67450800
C	-2. 20789100	-3. 92995500	1. 02380900
C	-3. 49571700	-3. 88738400	0. 48740600
C	-3. 91227400	-2. 87749800	-0. 39050000
C	-2. 01599500	-0. 03615400	-1. 64801500
C	-0. 98678900	-0. 69900700	-0. 69130300
H	-0. 29308000	-2. 92506600	1. 08368800
H	-4. 20318500	-4. 66600300	0. 75966200
H	-4. 92321400	-2. 86123600	-0. 78426900
N	-3. 16521700	-0. 78805500	-1. 56178500
O	-1. 84587800	0. 92962400	-2. 35890400
C	-4. 40693900	-0. 44285900	-2. 21735200
H	-4. 73807800	-1. 27775300	-2. 84591000
H	-4. 16968000	0. 39823800	-2. 87638100
C	-5. 49384200	-0. 06747100	-1. 22980900
C	-6. 82470600	-0. 39532200	-1. 48909600
C	-5. 17304700	0. 61563800	-0. 05524400
C	-7. 82683800	-0. 03644200	-0. 59046100
H	-7. 07732000	-0. 93840600	-2. 39650000
C	-6. 17242700	0. 96409000	0. 84891900
H	-4. 13441200	0. 86142900	0. 15639500

C	-7.50213000	0.64205700	0.58210800
H	-8.85941600	-0.29631800	-0.80159500
H	-5.90776200	1.48259500	1.76534300
H	-8.28114200	0.91307800	1.28758100
O	0.23681700	-0.54509500	-0.83415000
C	-1.77851500	-5.03083500	1.96004700
H	-0.96233600	-5.61734600	1.52604900
H	-1.41488600	-4.61955000	2.90703400
H	-2.60437700	-5.71050500	2.17997500
<b>TS5(S)</b>			
C	-1.35048800	0.47075900	-0.18479200
C	-1.95712500	-0.87300300	-1.77611700
C	-2.44273200	-1.71629400	0.49034800
H	-1.94224500	-1.55838600	1.44690200
N	-1.44603100	0.15711100	-2.38953200
N	-1.07384700	0.99104400	-1.37877100
N	-1.94098500	-0.70031600	-0.42435500
C	-2.40394500	-2.20891800	-2.27150300
H	-2.05958800	-2.36917900	-3.29247100
H	-3.49898700	-2.29070700	-2.24216600
C	-2.13500000	-3.15085500	-0.07166700
O	-1.77439900	-3.16963500	-1.44474400
C	-4.50311200	-2.93299700	0.41009900
C	-3.95014600	-1.66474600	0.58475000
C	-4.73802400	-0.54486400	0.80300500
C	-6.11138000	-0.75109200	0.83160500
C	-6.69998600	-2.00236300	0.66352700
C	-5.88482000	-3.10860600	0.45291200
C	-3.42379400	-3.96219300	0.19864700
H	-4.31124800	0.44134900	0.95171500
H	-7.77844500	-2.09159000	0.69508300
H	-6.32504700	-4.09034900	0.31539900
H	-3.62815000	-4.63975600	-0.63474600
H	-3.30495200	-4.57447100	1.09866800
C	-0.55960100	2.31406600	-1.63865700
C	-1.39743800	3.39795400	-1.35967500
C	0.74518800	2.45926600	-2.12342300
C	-0.86612700	4.67682900	-1.52367500
C	1.22227900	3.75965600	-2.26765100
C	0.44593600	4.87477800	-1.95000700
H	-1.49486400	5.53597000	-1.30424000
H	2.24080000	3.90144100	-2.62212400
C	1.63376600	1.29138600	-2.45340000
H	1.06784400	0.39630100	-2.71147400

H	2. 25938300	1. 05155300	-1. 58674600
H	2. 29172400	1. 55219000	-3. 28547500
C	1. 03097700	6. 25797800	-2. 05667400
H	0. 26498600	7. 02612700	-1. 93450400
H	1. 52056900	6. 40574200	-3. 02294900
H	1. 78791000	6. 40331900	-1. 27909700
C	-2. 81683500	3. 21775400	-0. 88213500
H	-3. 29186100	2. 34081000	-1. 33172100
H	-3. 41125800	4. 09478600	-1. 14322900
H	-2. 86306000	3. 10196900	0. 20619700
H	-1. 26825400	-3. 56562700	0. 44319000
N	-6. 98458800	0. 40973600	1. 04316700
O	-8. 18743300	0. 21809500	1. 08992700
O	-6. 45926400	1. 50324500	1. 15792300
C	2. 16444600	2. 26129000	0. 91366600
C	1. 57510000	3. 47801400	1. 37870900
C	2. 33800300	4. 66023100	1. 42921300
C	3. 66257600	4. 61443300	1. 04272900
C	4. 24653900	3. 40211200	0. 60699100
C	3. 52262800	2. 22663500	0. 54238300
C	0. 06749700	1. 83627000	1. 34491600
C	0. 21711000	3. 17070100	1. 67327800
H	1. 88620100	5. 59116700	1. 76092500
H	4. 26755300	5. 51518400	1. 06972800
H	5. 29110400	3. 39785900	0. 31005200
H	3. 98466500	1. 30863900	0. 19436500
N	1. 22017200	1. 26960100	0. 86892900
H	-0. 57184800	3. 84449300	1. 97953600
C	-1. 20760800	1. 15843800	1. 16112800
O	-2. 20175800	1. 21935500	1. 85973000
C	3. 54140600	-1. 05253700	1. 07293400
C	2. 57182200	-0. 67105500	2. 00584200
C	2. 91270400	-0. 42991800	3. 31952200
C	4. 25251700	-0. 56442700	3. 72025400
C	5. 20187600	-0. 94382200	2. 77020800
C	4. 86877300	-1. 19786400	1. 43319200
C	1. 59429700	-1. 09495100	-0. 13625800
C	1. 25065500	-0. 60908700	1. 29523200
H	2. 14705400	-0. 13190800	4. 03208800
H	6. 23824300	-1. 05006200	3. 07868300
H	5. 62494800	-1. 50466500	0. 71813200
N	2. 95671600	-1. 22585000	-0. 20101700
O	0. 80721300	-1. 36222500	-1. 02672500
C	3. 66683300	-1. 68305400	-1. 38053500

H	4. 54531100	-1. 04600500	-1. 53417200
H	2. 98182200	-1. 52659400	-2. 21962000
C	4. 07171100	-3. 13895700	-1. 28985500
C	5. 40170800	-3. 52623200	-1. 43862300
C	3. 09536600	-4. 11216200	-1. 05771200
C	5. 75870100	-4. 87147200	-1. 35418100
H	6. 16367000	-2. 77212200	-1. 62062200
C	3. 45007800	-5. 45379300	-0. 97162300
H	2. 05613300	-3. 80820100	-0. 95284700
C	4. 78383200	-5. 83599900	-1. 11873700
H	6. 79794000	-5. 16279200	-1. 46805300
H	2. 68666100	-6. 20439700	-0. 79349000
H	5. 05983800	-6. 88334100	-1. 05046000
O	0. 13800800	-0. 87291900	1. 79576700
C	4. 64400800	-0. 31138600	5. 15401000
H	4. 19717100	-1. 05517700	5. 82113500
H	5. 72784100	-0. 35399000	5. 28079800
H	4. 30048400	0. 67207500	5. 48730700

**H/H/5-F/Bn**

**TS5(R)**

C	1. 89947900	1. 37167700	0. 27998300
C	3. 70904900	0. 59597200	1. 21621800
C	1. 73404100	-0. 64774500	1. 89492900
H	0. 64938200	-0. 53028200	1. 86842100
N	4. 12378600	1. 53450500	0. 41178400
N	2. 98577100	1. 99626200	-0. 17344200
N	2. 35411200	0. 44391500	1. 14175600
C	4. 41283600	-0. 16790400	2. 29402900
H	5. 35719700	0. 32124000	2. 53217200
H	4. 61012200	-1. 20210100	1. 99030300
C	2. 26829400	-0. 61848800	3. 35789500
O	3. 58765900	-0. 08240600	3. 44620500
C	2. 40464200	-2. 85032200	2. 50057200
C	2. 15747500	-2. 02143000	1. 40225800
C	2. 29873600	-2. 48137100	0. 10094200
C	2. 68364900	-3. 80898800	-0. 04764900
C	2. 91300200	-4. 66824700	1. 02278800
C	2. 77166500	-4. 18037200	2. 31714400
C	2. 22119900	-2. 09293600	3. 79047300
H	2. 09654300	-1. 85779500	-0. 76021200
H	3. 20645100	-5. 69267300	0. 83165100
H	2. 96205200	-4. 82577500	3. 16781500
H	2. 98918400	-2. 30473700	4. 53744700
H	1. 24472000	-2. 32201100	4. 23266700

C	3. 06789900	3. 00930300	-1. 19532200
C	2. 81847000	2. 62563100	-2. 51592000
C	3. 42454700	4. 30163000	-0. 81180700
C	2. 94392000	3. 61453100	-3. 48775700
C	3. 53399800	5. 25159800	-1. 82650700
C	3. 29724200	4. 92675500	-3. 16262600
H	2. 75969400	3. 35322000	-4. 52660800
H	3. 80712900	6. 26998100	-1. 56317100
C	3. 66735300	4. 65451500	0. 63139500
H	4. 56989000	4. 16732700	1. 01078600
H	2. 83080400	4. 33513500	1. 26147300
H	3. 78477900	5. 73312200	0. 74321200
C	3. 39245800	5. 97641100	-4. 23852700
H	4. 01103900	6. 81729700	-3. 91875400
H	2. 39830400	6. 36526200	-4. 48110400
H	3. 81534300	5. 56155200	-5. 15644600
C	2. 42105600	1. 21688600	-2. 86613300
H	3. 09175400	0. 48559900	-2. 40259000
H	2. 45835900	1. 07274400	-3. 94681700
H	1. 40292500	0. 99845800	-2. 52403300
H	1. 64923200	0. 02831900	3. 98202000
N	2. 85829100	-4. 33018800	-1. 41000700
O	3. 16046400	-5. 50410800	-1. 53642700
O	2. 69502500	-3. 55975300	-2. 33932800
C	-2. 09089200	0. 31444400	2. 08526900
C	-1. 44976300	1. 11239300	3. 08315900
C	-1. 90539200	1. 07748600	4. 41554300
C	-2. 96110800	0. 24855400	4. 73781100
C	-3. 58284100	-0. 54905500	3. 74978000
C	-3. 16543400	-0. 52985400	2. 43263000
C	-0. 48190300	1. 40432700	1. 09523700
C	-0. 39297900	1. 80102000	2. 41742900
H	-1. 43221700	1. 69605200	5. 17331600
H	-3. 32462700	0. 20754400	5. 75983900
H	-4. 41216400	-1. 19023200	4. 03280800
H	-3. 66188500	-1. 14053800	1. 68530600
N	-1. 49712600	0. 52322900	0. 86181200
H	0. 31547300	2. 50203800	2. 84005900
C	0. 46412300	1. 80583300	0. 02681700
O	0. 22608800	2. 52074500	-0. 91267900
C	-2. 99776000	-1. 86139300	-0. 73294000
C	-1. 72043800	-1. 90906200	-0. 16151900
C	-1. 35899100	-2. 92390000	0. 70299700
C	-2. 32710500	-3. 88258600	0. 98612100

C	-3.60012000	-3.84879000	0.43697800
C	-3.95476000	-2.82352900	-0.44626500
C	-1.94876200	-0.03023300	-1.63983900
C	-0.96962200	-0.70920300	-0.64558100
H	-0.37309200	-2.98135800	1.15400700
H	-4.30697300	-4.62664200	0.70264600
H	-4.95065100	-2.78111800	-0.87362000
N	-3.12032700	-0.74954500	-1.58291700
O	-1.72263500	0.91871400	-2.35725100
C	-4.33859400	-0.36987200	-2.26428300
H	-4.67256900	-1.18883000	-2.91201200
H	-4.06702700	0.47376100	-2.90644600
C	-5.43904100	0.01539200	-1.29517500
C	-6.76976500	-0.28920200	-1.58261200
C	-5.12952400	0.68063500	-0.10730200
C	-7.78259300	0.07520200	-0.69816700
H	-7.01386700	-0.81861600	-2.50035200
C	-6.14000500	1.03429000	0.78247700
H	-4.09133500	0.90783600	0.12675200
C	-7.46921600	0.73564100	0.48764900
H	-8.81490000	-0.16693600	-0.93052800
H	-5.88464500	1.53787600	1.70980200
H	-8.25686200	1.01043300	1.18192400
O	0.25925200	-0.58121900	-0.74778200
F	-2.01464600	-4.88446500	1.82987200

**TS5(S)**

C	-1.35583100	0.46972800	-0.18445800
C	-1.96494400	-0.87622900	-1.77307800
C	-2.45954600	-1.71149900	0.49467600
H	-1.96234300	-1.55382800	1.45280200
N	-1.45055300	0.15119800	-2.38833200
N	-1.07668700	0.98637400	-1.37940800
N	-1.94925600	-0.70057500	-0.42150500
C	-2.41497300	-2.21214800	-2.26571200
H	-2.06853100	-2.37653700	-3.28531200
H	-3.51032100	-2.29045600	-2.23883500
C	-2.15759100	-3.14915800	-0.06305400
O	-1.79027300	-3.17191600	-1.43418100
C	-4.52613000	-2.91736700	0.41044100
C	-3.96698700	-1.65184200	0.58490900
C	-4.74951100	-0.52788500	0.80161700
C	-6.12390700	-0.72710100	0.82823200
C	-6.71860200	-1.97545600	0.66000800
C	-5.90875500	-3.08592400	0.45133800



C	-3.45220600	-3.95273300	0.20228400
H	-4.31824500	0.45619200	0.95122800
H	-7.79753100	-2.05924700	0.69019600
H	-6.35362200	-4.06560800	0.31414300
H	-3.65770200	-4.62849800	-0.63231700
H	-3.34038300	-4.56644700	1.10218400
C	-0.55917000	2.30789200	-1.64086500
C	-1.39255900	3.39447500	-1.35876200
C	0.74460800	2.44910300	-2.12961200
C	-0.85699100	4.67158900	-1.52289000
C	1.22591600	3.74788400	-2.27397800
C	0.45455600	4.86544600	-1.95259100
H	-1.48220900	5.53269100	-1.30118400
H	2.24368000	3.88638900	-2.63184200
C	1.62851600	1.27865100	-2.46284600
H	1.05963600	0.38562400	-2.72154900
H	2.25446200	1.03600400	-1.59732900
H	2.28617300	1.53840100	-3.29547200
C	1.04391300	6.24676800	-2.05950600
H	0.28028000	7.01723600	-1.93725800
H	1.53376700	6.39287700	-3.02588200
H	1.80135800	6.38991800	-1.28204500
C	-2.81213900	3.21966400	-0.87960600
H	-3.29061700	2.34368500	-1.32738900
H	-3.40375700	4.09819300	-1.14202500
H	-2.85828800	3.10636200	0.20895500
H	-1.29592700	-3.56828100	0.45678200
N	-6.99144400	0.43831700	1.03820200
O	-8.19527800	0.25280400	1.08326500
O	-6.46054400	1.52906900	1.15337900
C	2.16406800	2.25237500	0.90373600
C	1.58173200	3.46653500	1.38401900
C	2.34833200	4.64611100	1.44021400
C	3.66986000	4.60027000	1.04356600
C	4.24685900	3.39085200	0.59090800
C	3.51896500	2.21821600	0.52033000
C	0.06885000	1.82966100	1.34370800
C	0.22477900	3.16065600	1.68403100
H	1.90179900	5.57508400	1.78411800
H	4.27762500	5.49895700	1.07468000
H	5.28868400	3.38695500	0.28459800
H	3.97501100	1.30376300	0.15540200
N	1.21699400	1.26337900	0.85525300
H	-0.55993100	3.83410400	2.00173200

C	-1.20955700	1.15893200	1.16037600
O	-2.20213400	1.22165600	1.86105500
C	3.53671800	-1.05132100	1.07651200
C	2.56168300	-0.67788200	2.00631800
C	2.88494000	-0.44127200	3.32718100
C	4.22386800	-0.58304600	3.67974400
C	5.20555900	-0.95001700	2.77175100
C	4.86700800	-1.19438100	1.43659900
C	1.59252900	-1.10624600	-0.13829300
C	1.24181900	-0.62930100	1.29298500
H	2.13842200	-0.15308000	4.05946800
H	6.22861600	-1.04803700	3.11610700
H	5.62412700	-1.49629700	0.72116000
N	2.95701200	-1.22491500	-0.19941400
O	0.80976400	-1.37477100	-1.03104500
C	3.67409800	-1.67704900	-1.37731800
H	4.54640700	-1.03163600	-1.53117800
H	2.98853500	-1.52751200	-2.21717800
C	4.09155000	-3.12926600	-1.28349300
C	5.42375800	-3.50670700	-1.43835200
C	3.12403600	-4.10907600	-1.04270700
C	5.79133500	-4.84893300	-1.35107900
H	6.17908600	-2.74774800	-1.62791100
C	3.48937500	-5.44755700	-0.95380600
H	2.08290600	-3.81347500	-0.93347900
C	4.82523900	-5.81999900	-1.10673600
H	6.83211500	-5.13258700	-1.46989100
H	2.73258600	-6.20322000	-0.76904700
H	5.10974600	-6.86488600	-1.03621700
O	0.13276900	-0.89040800	1.79476000
F	4.58180900	-0.36340500	4.95882300

**H/H/5-Br/Bn**

**TS5(R)**

C	1.91059700	1.41108500	0.20916700
C	3.67392000	0.59967000	1.20460400
C	1.65742200	-0.61142600	1.80026600
H	0.57590800	-0.47566800	1.73816600
N	4.13046600	1.54617100	0.43165400
N	3.02073900	2.02983600	-0.19009100
N	2.32225400	0.46788400	1.07516900
C	4.32799100	-0.21363100	2.27787200
H	5.27671500	0.24372600	2.55838900
H	4.51106500	-1.23911100	1.93699400
C	2.12993100	-0.60220300	3.27859600

O	3.48063900	-0.15952700	3.41617300
C	2.15782500	-2.84252200	2.43213100
C	2.05357500	-1.99693300	1.32386000
C	2.23514800	-2.46411300	0.03093500
C	2.49356100	-3.82379200	-0.10194300
C	2.55464000	-4.70400700	0.97452800
C	2.38739300	-4.20477400	2.26212200
C	1.95856000	-2.06824000	3.71065100
H	2.14524700	-1.82482100	-0.83784000
H	2.74302500	-5.75461800	0.79375800
H	2.44572300	-4.86916300	3.11738300
H	2.66783200	-2.33158900	4.49811200
H	0.94447100	-2.22798100	4.09691500
C	3.14952100	3.06304400	-1.18612100
C	2.96817500	2.70243300	-2.52467300
C	3.48159100	4.34788300	-0.76083300
C	3.13457200	3.70946600	-3.47010600
C	3.63578000	5.31790600	-1.75158000
C	3.46554000	5.01741400	-3.10266900
H	3.00322900	3.46783800	-4.52174200
H	3.89216500	6.33174500	-1.45640500
C	3.65792000	4.67172100	0.69876700
H	4.54323800	4.17685300	1.10787800
H	2.79486300	4.33951100	1.28496800
H	3.76952600	5.74770100	0.83786700
C	3.61823000	6.08195200	-4.15731200
H	4.05650000	6.99169700	-3.74292500
H	2.64469500	6.33924300	-4.58578700
H	4.25299700	5.73255400	-4.97576800
C	2.61010500	1.29387500	-2.91653100
H	3.29242400	0.57008700	-2.45802200
H	2.67051800	1.17656700	-3.99934900
H	1.59195900	1.04061000	-2.60007700
H	1.52856800	0.08846300	3.87308000
N	2.70200800	-4.35966100	-1.45393400
O	2.87055100	-5.56081600	-1.57092100
O	2.69980800	-3.57277800	-2.38379300
C	-2.03551700	0.38922900	2.03458600
C	-1.38631600	1.22158800	2.99863000
C	-1.80517900	1.20437100	4.34399200
C	-2.83194000	0.35853200	4.71167700
C	-3.46084400	-0.47399300	3.75730100
C	-3.08017600	-0.47213400	2.42936700
C	-0.47154300	1.48462300	0.98055400

C	-0.35882800	1.91213300	2.29228100
H	-1.32600000	1.84905800	5.07574300
H	-3.16614000	0.32985800	5.74408500
H	-4.26482400	-1.13041100	4.07619100
H	-3.58060800	-1.11288400	1.71088800
N	-1.47602700	0.57972200	0.79230700
H	0.35332800	2.62739000	2.68426800
C	0.48264300	1.84908200	-0.09535800
O	0.26862600	2.53028100	-1.06471400
C	-2.95827600	-1.91303800	-0.68323700
C	-1.65635800	-1.89534200	-0.16845900
C	-1.22075900	-2.87359700	0.69908100
C	-2.12362800	-3.87363600	1.05663200
C	-3.42194500	-3.89796500	0.56011600
C	-3.85847500	-2.90828500	-0.32867300
C	-2.02146100	-0.05957200	-1.66766600
C	-0.96885100	-0.68608300	-0.71509500
H	-0.21441400	-2.87000100	1.09968000
H	-4.09948800	-4.68845500	0.86247300
H	-4.87437400	-2.91810800	-0.70858800
N	-3.16080800	-0.82938500	-1.54687300
O	-1.87649600	0.89027500	-2.40213300
C	-4.41582500	-0.52103100	-2.19890600
H	-4.73255900	-1.37306500	-2.81121600
H	-4.20004400	0.31348400	-2.87333300
C	-5.50086900	-0.15244800	-1.20753700
C	-6.82118300	-0.54247900	-1.43094600
C	-5.18831300	0.58702800	-0.06496500
C	-7.82196600	-0.19035100	-0.52811000
H	-7.06709700	-1.12746800	-2.31376900
C	-6.18589000	0.92881600	0.84359400
H	-4.15707100	0.88237800	0.11853700
C	-7.50548800	0.54385300	0.61272700
H	-8.84645600	-0.49889900	-0.71089200
H	-5.92746900	1.49156600	1.73522100
H	-8.28301200	0.80972700	1.32173300
O	0.24866100	-0.52242300	-0.87102800
Br	-1.53202700	-5.22062400	2.25397600
<b>TS5(S)</b>			
C	-1.35853900	0.46668500	-0.18463500
C	-1.96687800	-0.88118100	-1.77204800
C	-2.46581300	-1.71247200	0.49670200
H	-1.96938800	-1.55456900	1.45515000
N	-1.45138400	0.14522200	-2.38814100

N	-1.07801700	0.98156800	-1.38003500
N	-1.95210100	-0.70388200	-0.42054500
C	-2.41690200	-2.21763700	-2.26325900
H	-2.06901900	-2.38393400	-3.28205100
H	-3.51231400	-2.29549500	-2.23776800
C	-2.16662000	-3.15163500	-0.05923200
O	-1.79369000	-3.17582200	-1.42876600
C	-4.53553600	-2.91298100	0.41006400
C	-3.97320500	-1.64908000	0.58579400
C	-4.75301100	-0.52341200	0.80372200
C	-6.12786000	-0.71924100	0.83018800
C	-6.72567700	-1.96592800	0.66068800
C	-5.91858900	-3.07812800	0.45079600
C	-3.46466300	-3.95127200	0.20125800
H	-4.31945100	0.45941500	0.95474600
H	-7.80479900	-2.04711100	0.69103300
H	-6.36581800	-4.05661500	0.31278000
H	-3.67088900	-4.62380500	-0.63582000
H	-3.35692500	-4.56824800	1.09937800
C	-0.55996100	2.30286300	-1.64177300
C	-1.39210200	3.38997000	-1.35788300
C	0.74381000	2.44345000	-2.13076900
C	-0.85492100	4.66671400	-1.51982500
C	1.22671900	3.74184200	-2.27288800
C	0.45687500	4.85979300	-1.94900900
H	-1.47905800	5.52815900	-1.29644200
H	2.24460400	3.87973200	-2.63062900
C	1.62655800	1.27262800	-2.46593900
H	1.05711600	0.38029200	-2.72584700
H	2.25267400	1.02873200	-1.60093100
H	2.28414400	1.53288300	-3.29844500
C	1.04812300	6.24055100	-2.05239700
H	0.28530100	7.01171600	-1.92951700
H	1.53945800	6.38803100	-3.01780200
H	1.80467400	6.38111000	-1.27358500
C	-2.81199800	3.21653100	-0.87909800
H	-3.29112000	2.34067800	-1.32641100
H	-3.40275900	4.09535400	-1.14246300
H	-2.85876400	3.10431300	0.20953400
H	-1.30842200	-3.57335800	0.46418300
N	-6.99244600	0.44811900	1.04174200
O	-8.19669400	0.26548200	1.08705700
O	-6.45877200	1.53740500	1.15788400
C	2.16259700	2.24786300	0.89900600

C	1. 58330000	3. 46033900	1. 38679000
C	2. 35165700	4. 63847100	1. 44744100
C	3. 67225500	4. 59277500	1. 04762300
C	4. 24639300	3. 38501400	0. 58727800
C	3. 51643800	2. 21394400	0. 51218700
C	0. 06791100	1. 82588100	1. 34187000
C	0. 22660200	3. 15486100	1. 68853000
H	1. 90737500	5. 56620700	1. 79744000
H	4. 28147600	5. 49032000	1. 08223300
H	5. 28748100	3. 38110200	0. 27856600
H	3. 97071000	1. 30136000	0. 14030700
N	1. 21412800	1. 26014700	0. 84748400
H	-0. 55615800	3. 82780500	2. 01202500
C	-1. 21137400	1. 15710800	1. 15952800
O	-2. 20313700	1. 22020000	1. 86130300
C	3. 53633500	-1. 05177100	1. 07984600
C	2. 55916200	-0. 67674100	2. 00723600
C	2. 88276800	-0. 42631800	3. 32401600
C	4. 22351100	-0. 55524500	3. 69036000
C	5. 20244100	-0. 92978500	2. 77695100
C	4. 86626800	-1. 18869300	1. 44408200
C	1. 59424800	-1. 11320400	-0. 13606300
C	1. 23951000	-0. 63513000	1. 29342100
H	2. 12350700	-0. 13369100	4. 04137200
H	6. 23179800	-1. 02431200	3. 10275900
H	5. 62690300	-1. 49381700	0. 73375000
N	2. 96158900	-1. 23244800	-0. 19267400
O	0. 81689100	-1. 38245000	-1. 03183300
C	3. 68294300	-1. 67768200	-1. 37164500
H	4. 55436600	-1. 02977400	-1. 51899600
H	2. 99933600	-1. 52403700	-2. 21230900
C	4. 10165600	-3. 12967600	-1. 28442400
C	5. 43518100	-3. 50418800	-1. 43486500
C	3. 13390700	-4. 11218900	-1. 05576800
C	5. 80378900	-4. 84661500	-1. 35523800
H	6. 19052600	-2. 74318300	-1. 61577300
C	3. 50039000	-5. 45078300	-0. 97440400
H	2. 09181100	-3. 81876000	-0. 95016000
C	4. 83750000	-5. 82048000	-1. 12304400
H	6. 84545700	-5. 12824800	-1. 47081900
H	2. 74355700	-6. 20858000	-0. 79901900
H	5. 12287000	-6. 86552300	-1. 05876400
O	0. 13093000	-0. 89617100	1. 79399500
Br	4. 72114400	-0. 20526700	5. 48831200

**H/H/4-Br/Bn****TS5(R)**

C	1. 90004000	1. 37382500	0. 29195800
C	3. 71412400	0. 60052600	1. 22128200
C	1. 74298300	-0. 64380600	1. 91033000
H	0. 65821300	-0. 52734200	1. 88845200
N	4. 12492000	1. 53681400	0. 41231700
N	2. 98414900	1. 99711800	-0. 16863300
N	2. 35877500	0. 44806500	1. 15371500
C	4. 42308900	-0. 16007300	2. 29800800
H	5. 36782400	0. 33069000	2. 53128000
H	4. 62034400	-1. 19483800	1. 99617500
C	2. 28411900	-0. 61270900	3. 37096300
O	3. 60201600	-0. 07241600	3. 45296300
C	2. 42175400	-2. 84467900	2. 51405300
C	2. 16599400	-2. 01731100	1. 41655600
C	2. 30247800	-2. 47773700	0. 11487300
C	2. 69135800	-3. 80408700	-0. 03477300
C	2. 92985500	-4. 66170500	1. 03498700
C	2. 79322600	-4. 17337600	2. 32969400
C	2. 24395000	-2. 08705700	3. 80456000
H	2. 09407000	-1. 85535300	-0. 74566600
H	3. 22715600	-5. 68487900	0. 84303400
H	2. 99167000	-4. 81697900	3. 17991700
H	3. 01741300	-2. 29595900	4. 54670300
H	1. 27120100	-2. 31863400	4. 25350900
C	3. 06240600	3. 00443100	-1. 19668800
C	2. 80821400	2. 61254000	-2. 51431700
C	3. 42013000	4. 29880700	-0. 82265200
C	2. 93018200	3. 59506500	-3. 49249700
C	3. 52548000	5. 24283000	-1. 84384600
C	3. 28465600	4. 90962900	-3. 17679200
H	2. 74214200	3. 32740200	-4. 52911800
H	3. 79866400	6. 26296100	-1. 58755200
C	3. 66827300	4. 66072200	0. 61734000
H	4. 57305300	4. 17700900	0. 99588900
H	2. 83475500	4. 34392800	1. 25265700
H	3. 78476400	5. 74012100	0. 72223800
C	3. 37966300	5. 94955300	-4. 26218800
H	3. 93623500	6. 82599000	-3. 92477500
H	2. 38072900	6. 28024400	-4. 56336600
H	3. 87198100	5. 54532600	-5. 15009400
C	2. 40854500	1. 20191000	-2. 85401100
H	3. 08038300	0. 47290100	-2. 38846300

H	2.44132800	1.05088200	-3.93389300
H	1.39177200	0.98625400	-2.50622800
H	1.66621700	0.03244500	3.99790900
N	2.86108900	-4.32557200	-1.39769800
O	3.16361700	-5.49933400	-1.52482000
O	2.69348000	-3.55558200	-2.32655300
C	-2.09690900	0.30934300	2.09009600
C	-1.45816700	1.10275900	3.09306900
C	-1.91852400	1.06365400	4.42357900
C	-2.97694200	0.23539000	4.73896400
C	-3.59694400	-0.55708300	3.74582600
C	-3.17468600	-0.53371900	2.43023100
C	-0.48291900	1.40163900	1.10963600
C	-0.39850500	1.79326100	2.43340400
H	-1.44707500	1.67867800	5.18529200
H	-3.34429000	0.19138300	5.75948900
H	-4.42901600	-1.19715500	4.02309400
H	-3.67116100	-1.14007500	1.67934800
N	-1.49853400	0.52246700	0.86956600
H	0.30858000	2.49258200	2.86102100
C	0.46425500	1.80842000	0.04386700
O	0.22559400	2.52857300	-0.89154600
C	-2.99824800	-1.84681000	-0.74847400
C	-1.72291000	-1.90803700	-0.17031100
C	-1.38268200	-2.94353200	0.67666600
C	-2.33330700	-3.93078100	0.95741700
C	-3.59198200	-3.84132900	0.37352800
C	-3.96323600	-2.80818500	-0.49031900
C	-1.93860100	-0.01389200	-1.62808200
C	-0.96706200	-0.70533200	-0.63538400
H	-0.39268400	-2.99120800	1.12214200
H	-4.95770600	-2.76448300	-0.91848200
N	-3.11802400	-0.72841800	-1.57949300
O	-1.70988000	0.93726300	-2.33940100
C	-4.33370900	-0.33567600	-2.26047200
H	-4.66657200	-1.14436800	-2.92124000
H	-4.05691700	0.51608300	-2.88929900
C	-5.43478100	0.03790900	-1.28780600
C	-6.76364300	-0.27664100	-1.57259700
C	-5.12679100	0.70129200	-0.09838200
C	-7.77667400	0.07666900	-0.68382900
H	-7.00617400	-0.80524900	-2.49116900
C	-6.13744600	1.04397600	0.79533700
H	-4.08975700	0.93514500	0.13451100



C	-7.46505200	0.73571800	0.50309600
H	-8.80757400	-0.17351700	-0.91368100
H	-5.88350100	1.54605200	1.72383200
H	-8.25279100	1.00137300	1.20078700
O	0.26287800	-0.57847500	-0.73241900
H	-2.10033200	-4.75667700	1.61834000
Br	-4.87296000	-5.18769600	0.74864100
<b>TS5(S)</b>			
C	-1.35851000	0.46681500	-0.18489700
C	-1.96611900	-0.87979700	-1.77364500
C	-2.46384600	-1.71336500	0.49474400
H	-1.96598300	-1.55599100	1.45258700
N	-1.45093500	0.14733000	-2.38876800
N	-1.07805700	0.98298800	-1.37979700
N	-1.95147800	-0.70373400	-0.42200700
C	-2.41542200	-2.21609000	-2.26596500
H	-2.06765000	-2.38135700	-3.28495700
H	-3.51077800	-2.29466200	-2.24025800
C	-2.16473500	-3.15191800	-0.06286400
O	-1.79146100	-3.17456400	-1.43232300
C	-4.53355200	-2.91405800	0.40789400
C	-3.97117500	-1.65039700	0.58515000
C	-4.75099600	-0.52504500	0.80474400
C	-6.12581800	-0.72094200	0.83156400
C	-6.72366200	-1.96744600	0.66080100
C	-5.91659500	-3.07932100	0.44910200
C	-3.46278700	-3.95196000	0.19660900
H	-4.31743400	0.45765700	0.95655700
H	-7.80277000	-2.04871300	0.69148200
H	-6.36386000	-4.05763100	0.30995000
H	-3.66948200	-4.62275300	-0.64176000
H	-3.35470400	-4.57085700	1.09335900
C	-0.56063500	2.30471600	-1.64074900
C	-1.39376700	3.39113900	-1.35707400
C	0.74313200	2.44652300	-2.12943300
C	-0.85770900	4.66836200	-1.51884900
C	1.22494400	3.74535900	-2.27132900
C	0.45402700	4.86261800	-1.94775900
H	-1.48268800	5.52926000	-1.29570100
H	2.24279300	3.88412000	-2.62884100
C	1.62707300	1.27676500	-2.46527300
H	1.05842800	0.38359800	-2.72393800
H	2.25529000	1.03423400	-1.60134200
H	2.28294900	1.53760300	-3.29893400

C	1.04411900	6.24385600	-2.05130700
H	0.28069900	7.01444000	-1.92850500
H	1.53528300	6.39157800	-3.01676000
H	1.80067300	6.38511800	-1.27260700
C	-2.81349100	3.21631000	-0.87832200
H	-3.29203900	2.34052800	-1.32639000
H	-3.40489300	4.09497300	-1.14076900
H	-2.85999500	3.10297500	0.21022300
H	-1.30658000	-3.57416900	0.46018600
N	-6.99033200	0.44617100	1.04476200
O	-8.19456500	0.26349700	1.09028200
O	-6.45662600	1.53533700	1.16201100
C	2.16370900	2.24682100	0.90127000
C	1.58271700	3.46080700	1.38288800
C	2.35021500	4.63955700	1.44050800
C	3.67185100	4.59306400	1.04400400
C	4.24752600	3.38394900	0.58956100
C	3.51823400	2.21218100	0.51730100
C	0.06753300	1.82592200	1.34227700
C	0.22522900	3.15613300	1.68305800
H	1.90437400	5.56846200	1.78544500
H	4.28046200	5.49110400	1.07637100
H	5.28925000	3.37909200	0.28311200
H	3.97415400	1.29900100	0.14912300
N	1.21503900	1.25868000	0.85272600
H	-0.55849600	3.83034400	2.00155100
C	-1.21131200	1.15541200	1.16014000
O	-2.20285300	1.21853100	1.86206800
C	3.53553200	-1.05239800	1.07706400
C	2.55934000	-0.67699300	2.00636000
C	2.89630600	-0.43316400	3.32140200
C	4.23378300	-0.55779500	3.71110600
C	5.18235600	-0.92949500	2.76571900
C	4.86806500	-1.19192300	1.42969300
C	1.59507600	-1.10749100	-0.13789700
C	1.24171100	-0.62602300	1.29115500
H	2.13362400	-0.14212000	4.03693800
H	5.63176700	-1.49593300	0.72350500
N	2.96328200	-1.23045600	-0.19540200
O	0.81873200	-1.37697700	-1.03406200
C	3.68329200	-1.67958400	-1.37399800
H	4.55561500	-1.03333400	-1.52344700
H	2.99917600	-1.52634300	-2.21426500
C	4.09924900	-3.13208900	-1.28327000

C	5.43298800	-3.50861700	-1.42623500
C	3.12887700	-4.11269200	-1.05734000
C	5.79931600	-4.85137300	-1.34182200
H	6.19039700	-2.74915100	-1.60493000
C	3.49311100	-5.45159600	-0.97142000
H	2.08673800	-3.81739500	-0.95729900
C	4.83047900	-5.82335600	-1.11255600
H	6.84121400	-5.13460800	-1.45097200
H	2.73442600	-6.20802700	-0.79815100
H	5.11409900	-6.86862700	-1.04439500
O	0.13035700	-0.88984300	1.78920200
H	4.53538400	-0.36837200	4.73411600
Br	6.99281700	-1.08625500	3.30781400

**Et/H/H/Bn**

**R1**

C	-0.20458500	1.13149600	-0.45858200
C	-1.52313700	1.32286200	0.03027200
C	-1.93983200	2.61809200	0.39742400
C	-1.05021900	3.66401400	0.26869300
C	0.25980000	3.45065000	-0.22355100
C	0.70145900	2.19582700	-0.59182700
C	-1.23466800	-0.85733400	-0.43107000
C	-2.17055500	0.04759700	0.03590400
H	-2.94323600	2.78439900	0.77842700
H	-1.35135800	4.66806600	0.54796900
H	0.93384700	4.29660700	-0.31246000
H	1.70572600	2.03538700	-0.96949800
N	-0.05452100	-0.19560100	-0.73407000
H	0.78334500	-0.63018800	-1.09063100
C	-1.36279600	-2.29273300	-0.63209700
H	-0.47985500	-2.78997900	-1.08181000
O	-2.35544700	-2.93515200	-0.34002300
C	-3.56373000	-0.25390900	0.49755300
H	-4.02140400	-0.97798700	-0.18204400
H	-4.15948300	0.66373400	0.45133900
C	-3.58534200	-0.81957000	1.92213700
H	-3.12582400	-0.11884300	2.62490700
H	-3.02958200	-1.75984300	1.95560100
H	-4.61042900	-1.01288600	2.24906000

**si-M2**

C	-4.73399200	-6.18888000	0.96775800
C	-5.84966900	-7.84305400	1.97535600
C	-6.43245700	-5.60762200	2.82271300
H	-5.85420400	-4.72768500	3.09552000

N	-5.24631100	-8.44154600	1.01328200
N	-4.54689800	-7.42884400	0.35826500
N	-5.56801200	-6.49687200	2.05218000
C	-6.77832700	-8.41216100	2.99691600
H	-6.54492100	-9.46027800	3.18432600
H	-7.81901800	-8.34254200	2.64657000
C	-6.97575600	-6.33460600	4.11059400
O	-6.59156600	-7.69471900	4.20119500
C	-8.83875900	-5.56406800	2.74325900
C	-7.67627800	-5.23351300	2.04818100
C	-7.72620800	-4.67021300	0.77998800
C	-8.98668600	-4.47146100	0.23268200
C	-10.16821800	-4.78880500	0.89951300
C	-10.09197500	-5.33797900	2.17376600
C	-8.51591100	-6.15021500	4.09142500
H	-6.83149500	-4.39781800	0.23231300
H	-11.11978800	-4.60731400	0.41611600
H	-10.99960400	-5.59436400	2.70994300
H	-9.01715800	-7.10728100	4.26826300
H	-8.83158900	-5.47418100	4.89173400
C	-4.03346200	-7.67215800	-0.94450700
C	-4.63039100	-7.06566500	-2.05628400
C	-2.89670200	-8.48497400	-1.06655000
C	-4.00058900	-7.21441500	-3.29388900
C	-2.31747100	-8.62137100	-2.32450600
C	-2.83546400	-7.96304400	-3.44317800
H	-4.43723200	-6.72795700	-4.16348200
H	-1.42312300	-9.23182100	-2.43023700
C	-2.30486800	-9.15650200	0.14473700
H	-2.97088200	-9.93604900	0.52567300
H	-2.16612400	-8.44463300	0.96612300
H	-1.34025800	-9.60753900	-0.09508000
C	-2.12469500	-8.02829400	-4.76884900
H	-2.81623800	-7.87130700	-5.59990200
H	-1.62554900	-8.99040900	-4.90794500
H	-1.35998100	-7.24440100	-4.81734700
C	-5.90823600	-6.27884000	-1.93993300
H	-6.55158200	-6.67888200	-1.14955800
H	-6.45833100	-6.30745600	-2.88306300
H	-5.70562600	-5.22971400	-1.70150200
H	-6.53861600	-5.87290100	4.99580800
N	-9.07380400	-3.90398100	-1.11736000
O	-10.18241500	-3.71309700	-1.58701300
O	-8.03194800	-3.65628900	-1.70188900

C	-1.46447400	-5.03588700	-1.73868200
C	-2.19427200	-3.94829100	-2.28170800
C	-1.72198900	-3.33930600	-3.45752200
C	-0.56737300	-3.82438600	-4.05040000
C	0.13707300	-4.91156000	-3.49346200
C	-0.30148900	-5.53229600	-2.33405000
C	-3.29089700	-4.71189500	-0.45959000
C	-3.35453500	-3.75751900	-1.45688200
H	-2.26084900	-2.50511700	-3.89932000
H	-0.19623400	-3.36477300	-4.96104800
H	1.03713400	-5.27032300	-3.98307300
H	0.22653000	-6.37947800	-1.90685400
N	-2.12556500	-5.44637000	-0.61247500
H	-1.87189400	-6.23884100	-0.04385100
C	-4.23004000	-4.96902400	0.62379400
H	-4.04278500	-3.35617800	1.66971300
O	-4.77037100	-3.84746800	1.26561800
C	-4.43035900	-2.73312900	-1.65904600
C	-4.04875700	-1.35623100	-1.10492000
H	-5.35625500	-3.06905900	-1.17873800
H	-4.64662800	-2.64794300	-2.73140300
H	-4.83006900	-0.61654500	-1.30095300
H	-3.89802000	-1.41780600	-0.02338100
H	-3.11717100	-0.99947000	-1.55475200

**TS5(S)**

C	-1.34311400	0.50313700	-0.23504200
C	-1.96995000	-0.88845700	-1.77699100
C	-2.42562600	-1.66403800	0.52065800
H	-1.91235000	-1.47850800	1.46524200
N	-1.47312300	0.12499000	-2.42934600
N	-1.09150800	0.98891200	-1.44852200
N	-1.93336000	-0.67645100	-0.43017600
C	-2.41694300	-2.24071400	-2.22561800
H	-2.08429900	-2.43109600	-3.24534900
H	-3.51121000	-2.32644100	-2.18079500
C	-2.12727400	-3.11530200	-0.00308400
O	-1.77336800	-3.17226500	-1.37663400
C	-4.49088400	-2.87611600	0.49409800
C	-3.93155300	-1.60631300	0.63257300
C	-4.71253700	-0.47934800	0.83866500
C	-6.08600700	-0.67957600	0.88944700
C	-6.68116800	-1.93189600	0.75533300
C	-5.87259300	-3.04546700	0.55846800
C	-3.41793300	-3.91434400	0.29494500

H	-4.27992300	0.50775600	0.96399600
H	-7.75945900	-2.01646700	0.80245900
H	-6.31780000	-4.02836400	0.44793100
H	-3.63223000	-4.60852200	-0.52219500
H	-3.29456500	-4.50843300	1.20642700
C	-0.58839000	2.31267400	-1.72001000
C	-1.45405900	3.38406200	-1.47102200
C	0.73615700	2.47437800	-2.13167300
C	-0.92350800	4.66849200	-1.56570700
C	1.21493100	3.78174300	-2.20365000
C	0.41684400	4.88192500	-1.89362300
H	-1.57017300	5.51932100	-1.36625000
H	2.25300900	3.93763500	-2.48969600
C	1.63735700	1.32107400	-2.47910500
H	1.08479600	0.39464100	-2.63165700
H	2.35754200	1.15491800	-1.67118300
H	2.19728300	1.55542100	-3.38814600
C	1.00545600	6.26709400	-1.88655100
H	0.22776700	7.03346300	-1.90582500
H	1.66980300	6.42140200	-2.74053900
H	1.60078400	6.40749800	-0.97727000
C	-2.90669800	3.16443400	-1.12555200
H	-3.35870500	2.41250600	-1.78001400
H	-3.46263100	4.09589500	-1.24232700
H	-3.04141400	2.82714000	-0.09238700
H	-1.25969700	-3.51942800	0.51886700
N	-6.95187800	0.48894300	1.08841200
O	-8.15459700	0.30308500	1.15646700
O	-6.42088200	1.58255400	1.17187700
C	2.21975200	2.27574100	0.83557200
C	1.65163300	3.50589700	1.28578100
C	2.43453900	4.67265100	1.35532100
C	3.76518600	4.60245600	0.99190300
C	4.32911900	3.37864400	0.56275100
C	3.58278100	2.21728300	0.48461900
C	0.10927400	1.90162300	1.24295700
C	0.27529600	3.24440300	1.55710300
H	1.99604100	5.61095300	1.68732900
H	4.38878000	5.48975700	1.03300400
H	5.37799200	3.35276300	0.28230300
H	4.03355300	1.29213300	0.14108600
N	1.25663500	1.30468500	0.78067900
C	-1.17733900	1.25541200	1.07396800
O	-2.17783400	1.39364800	1.75894000

C	3.54818400	-1.03543700	1.06377100
C	2.58015000	-0.63159000	1.98897800
C	2.92309800	-0.37491800	3.30152500
C	4.26134800	-0.52099400	3.68274200
C	5.21778900	-0.92250400	2.75243400
C	4.87782500	-1.19096400	1.42109500
C	1.60117800	-1.08338800	-0.14560900
C	1.26110900	-0.57630200	1.27782300
H	2.16275700	-0.06201900	4.01084900
H	4.55721400	-0.32322800	4.70732100
H	6.25138300	-1.03550100	3.06337400
H	5.62558000	-1.51732300	0.70608500
N	2.96417800	-1.22352000	-0.20676600
O	0.81467600	-1.35779200	-1.03420900
C	3.67220100	-1.69667800	-1.38139500
H	4.55145500	-1.06326000	-1.54510000
H	2.98594700	-1.54931900	-2.22107100
C	4.07504800	-3.15208400	-1.27366400
C	5.40316300	-3.54337600	-1.42911100
C	3.09972900	-4.12053700	-1.01903500
C	5.75926800	-4.88772100	-1.32886400
H	6.16451300	-2.79291900	-1.62818800
C	3.45358500	-5.46133900	-0.91712900
H	2.06175800	-3.81411400	-0.90910300
C	4.78545800	-5.84743800	-1.07071600
H	6.79710600	-5.18197500	-1.44784800
H	2.69081800	-6.20828300	-0.72154900
H	5.06076600	-6.89404600	-0.98967300
O	0.14657800	-0.80837600	1.78425300
C	-0.76281500	4.22525700	2.00159300
C	-0.87717000	4.29079700	3.52916400
H	-1.73714500	3.94743100	1.58256100
H	-0.51330800	5.21453700	1.59929200
H	-1.61652600	5.03499000	3.83751400
H	-1.18095200	3.31612600	3.91975700
H	0.08515000	4.55324500	3.97812200

**Bn/H/H/Bn**

**R1**

C	-0.31574500	1.00018000	-0.46573100
C	-1.59761300	1.25660900	0.08686800
C	-1.94319300	2.57728000	0.43924900
C	-1.02052100	3.58228100	0.23714800
C	0.25308200	3.30305300	-0.31378700
C	0.62420700	2.02270400	-0.67157300

C	-1.42292000	-0.94337400	-0.34587700
C	-2.29149300	0.00856200	0.15424500
H	-2.92017900	2.79604100	0.86166800
H	-1.26808800	4.60474000	0.50187000
H	0.95523300	4.11761800	-0.45886100
H	1.60053800	1.81198000	-1.09496200
N	-0.23476500	-0.33730400	-0.72011300
H	0.56197500	-0.81168700	-1.11820800
C	-1.62208100	-2.37499700	-0.52165300
H	-0.76930200	-2.91889900	-0.97480000
O	-2.64022400	-2.96497100	-0.21027300
C	-3.66744300	-0.22883800	0.70684700
H	-4.18902700	-0.96607900	0.09214500
H	-4.23256200	0.70857700	0.65529300
C	-3.62624700	-0.71525200	2.14401400
C	-3.14712900	0.12219900	3.15613400
C	-4.05320200	-2.00055200	2.47855000
C	-3.10381600	-0.31262500	4.47674800
H	-2.80251600	1.12228700	2.90196300
C	-4.01120400	-2.43883200	3.80161800
H	-4.40732200	-2.66071500	1.69284300
C	-3.53811600	-1.59688300	4.80394600
H	-2.73236400	0.35069600	5.25175400
H	-4.34733100	-3.44148300	4.04753200
H	-3.50579700	-1.93778200	5.83390300
<b>si-M2</b>			
C	-4.63037100	-6.24055900	0.90708500
C	-5.81946600	-7.80561000	1.96878800
C	-6.21931900	-5.52263200	2.81501700
H	-5.55602900	-4.70287100	3.08244900
N	-5.29014400	-8.45209200	0.99363000
N	-4.55077900	-7.49428700	0.30298300
N	-5.45286500	-6.47912300	2.01896400
C	-6.74318300	-8.31119800	3.02683600
H	-6.55624100	-9.36705600	3.22275100
H	-7.78909300	-8.19474400	2.70616600
C	-6.79756400	-6.21153400	4.11007500
O	-6.48488200	-7.58828100	4.21406500
C	-8.61723500	-5.29107300	2.77758500
C	-7.44230300	-5.02550300	2.07508400
C	-7.46950500	-4.39918900	0.83521100
C	-8.71851100	-4.07463700	0.32384600
C	-9.91163400	-4.33163600	0.99640500
C	-9.85781100	-4.94338600	2.24245700



C	-8.32569800	-5.94447400	4.10117700
H	-6.56382000	-4.15639300	0.29227500
H	-10.85313600	-4.05071300	0.54148400
H	-10.77378500	-5.14981500	2.78603000
H	-8.88012500	-6.87790000	4.24282500
H	-8.60492700	-5.28391000	4.92727900
C	-4.10276100	-7.76679900	-1.01584100
C	-4.69302000	-7.10926400	-2.10272200
C	-3.02034900	-8.64353600	-1.17964100
C	-4.10116800	-7.26790800	-3.35688600
C	-2.48084500	-8.79015000	-2.45468800
C	-2.98504300	-8.08062600	-3.54792600
H	-4.52982100	-6.74218400	-4.20740500
H	-1.63006800	-9.45344000	-2.59485800
C	-2.43932000	-9.36553000	0.00779400
H	-3.16272800	-10.06849700	0.43013600
H	-2.18574000	-8.66556900	0.81204400
H	-1.53937200	-9.91433900	-0.27496300
C	-2.31535400	-8.16452000	-4.89375600
H	-3.03039200	-8.00739300	-5.70470400
H	-1.83122900	-9.13320200	-5.03896600
H	-1.54480600	-7.38899800	-4.97351300
C	-5.92069400	-6.25340200	-1.93784200
H	-6.55615500	-6.62298400	-1.12674400
H	-6.50355800	-6.24612200	-2.86148500
H	-5.65337100	-5.21849900	-1.70018400
H	-6.33156300	-5.76341200	4.98745900
N	-8.78067900	-3.42472200	-0.98915800
O	-9.87661700	-3.12714000	-1.42985100
O	-7.72995900	-3.21712500	-1.57685000
C	-1.45355200	-5.18297900	-2.00936800
C	-2.12032500	-3.99856000	-2.41317400
C	-1.65706500	-3.31381200	-3.55004500
C	-0.57647900	-3.82593300	-4.24866300
C	0.06127800	-5.01398700	-3.83652100
C	-0.36688300	-5.70795000	-2.71476300
C	-3.17097400	-4.83275200	-0.59290900
C	-3.21217100	-3.79334000	-1.50657100
H	-2.14380000	-2.39881200	-3.87738900
H	-0.21258200	-3.30855400	-5.13070700
H	0.90335400	-5.39201500	-4.40783700
H	0.11357300	-6.62865300	-2.39740500
N	-2.08272500	-5.63690900	-0.88020300
H	-1.85896100	-6.49199200	-0.39621700

C	-4.05681200	-5.05975000	0.53803900
H	-3.77742900	-3.28828700	1.26403400
O	-4.51203300	-3.91402000	1.19779500
C	-4.23839200	-2.69954200	-1.57146600
H	-5.24040800	-3.10605700	-1.39053900
H	-4.25658600	-2.30207000	-2.59466200
C	-4.01890100	-1.54768800	-0.60702800
C	-2.73563900	-1.07839100	-0.31485700
C	-5.11514900	-0.93134700	0.00297700
C	-2.55306200	-0.00872600	0.56001500
H	-1.87761300	-1.56096900	-0.77659700
C	-4.93592900	0.13728600	0.87715500
H	-6.11445600	-1.30659100	-0.20801900
C	-3.65262600	0.60299900	1.15806600
H	-1.54970300	0.34560900	0.77597500
H	-5.79780300	0.60211500	1.34613300
H	-3.51042700	1.43224700	1.84368900

**TS5(S)**

C	-1.32043000	0.55339400	-0.23110500
C	-1.97947800	-0.87335700	-1.72630300
C	-2.41040800	-1.58393400	0.59698900
H	-1.88361000	-1.37755400	1.52985800
N	-1.48350900	0.11858800	-2.41211300
N	-1.08138400	1.00448900	-1.46015300
N	-1.92345600	-0.62571000	-0.38633000
C	-2.44270300	-2.23336500	-2.13281500
H	-2.12536800	-2.45338100	-3.15143400
H	-3.53689100	-2.30931000	-2.07143900
C	-2.12846300	-3.05061600	0.10864000
O	-1.79432800	-3.14658300	-1.26774300
C	-4.48317100	-2.78223100	0.63147700
C	-3.91449500	-1.51260600	0.72590900
C	-4.68619000	-0.37527200	0.90928900
C	-6.05992600	-0.56546400	0.98488100
C	-6.66402500	-1.81744500	0.89654600
C	-5.86469500	-2.94110100	0.72025900
C	-3.41968800	-3.83274300	0.44606800
H	-4.24741200	0.61293400	0.99967500
H	-7.74201900	-1.89416000	0.96130600
H	-6.31690500	-3.92403700	0.64354200
H	-3.64946000	-4.54714600	-0.34908300
H	-3.28730700	-4.40279000	1.37151100
C	-0.57901800	2.31927900	-1.77150200
C	-1.43647900	3.39857800	-1.53266500

C	0.74092600	2.46595300	-2.20601500
C	-0.90221200	4.67914000	-1.66383100
C	1.22412200	3.76870300	-2.31016000
C	0.43411900	4.87932100	-2.01297200
H	-1.54303200	5.53671300	-1.47423800
H	2.25934400	3.91455000	-2.61180100
C	1.63014300	1.29939600	-2.54043200
H	1.06992700	0.37290500	-2.66147700
H	2.36234000	1.14751500	-1.74070600
H	2.17623000	1.50824100	-3.46396400
C	1.03016600	6.26098600	-2.04926500
H	0.26156600	7.03120500	-1.95935600
H	1.58545900	6.42942100	-2.97581300
H	1.73398400	6.37937500	-1.21803800
C	-2.88232500	3.19571700	-1.15037300
H	-3.32703300	2.35904200	-1.69783900
H	-3.45750800	4.09441200	-1.37850000
H	-3.00251100	2.99218900	-0.08071500
H	-1.25602500	-3.44601300	0.62921000
N	-6.91597800	0.61411500	1.16045800
O	-8.11781700	0.43724400	1.25948100
O	-6.37789900	1.70690800	1.19412800
C	2.27294000	2.32681300	0.73730500
C	1.72545300	3.57379900	1.16286400
C	2.52001700	4.73410200	1.18818800
C	3.84332300	4.63977900	0.80359500
C	4.38773400	3.39907600	0.39856500
C	3.62886000	2.24357800	0.36591800
C	0.16467400	1.98384900	1.18443400
C	0.35126800	3.33255100	1.45847900
H	2.09719700	5.68452200	1.50547800
H	4.47667100	5.52100700	0.81213600
H	5.43139000	3.35482100	0.10163600
H	4.06396900	1.30400600	0.04174800
N	1.29929500	1.36451000	0.72319700
C	-1.12700800	1.33257400	1.05741500
O	-2.11069200	1.47448800	1.76575300
C	3.57468600	-0.99234800	1.04844500
C	2.62112000	-0.55205500	1.97215900
C	2.98151000	-0.25668100	3.27186100
C	4.32252400	-0.40416900	3.64226100
C	5.26416000	-0.84457900	2.71424000
C	4.90675300	-1.15014000	1.39552200
C	1.61394000	-1.05455900	-0.13832600

C	1. 29506800	-0. 50846500	1. 27528100
H	2. 23285400	0. 08816800	3. 97877100
H	4. 63225600	-0. 17657900	4. 65643600
H	6. 30008000	-0. 95842000	3. 01702700
H	5. 64283300	-1. 50565800	0. 68233100
N	2. 97444000	-1. 21172300	-0. 20975600
O	0. 81427400	-1. 34140500	-1. 01097200
C	3. 66421800	-1. 72621800	-1. 37758600
H	4. 54030100	-1. 09942300	-1. 57903800
H	2. 96423800	-1. 60885400	-2. 21070400
C	4. 07127900	-3. 17665300	-1. 22445800
C	5. 39282900	-3. 57442200	-1. 41657400
C	3. 10896300	-4. 13353600	-0. 89081800
C	5. 75459900	-4. 91353900	-1. 27564900
H	6. 14467600	-2. 83275200	-1. 67611000
C	3. 46857400	-5. 46909600	-0. 74767300
H	2. 07565100	-3. 82391200	-0. 75067100
C	4. 79365800	-5. 86160300	-0. 93868500
H	6. 78735800	-5. 21239600	-1. 42397500
H	2. 71541400	-6. 20672900	-0. 48914300
H	5. 07359800	-6. 90388200	-0. 82464700
O	0. 18410800	-0. 71359400	1. 79932100
C	-0. 66600300	4. 35137700	1. 87322700
H	-1. 66925800	3. 99276900	1. 61502700
H	-0. 49713200	5. 27874800	1. 31284600
C	-0. 60850300	4. 64039000	3. 36207400
C	-0. 21189700	5. 88762900	3. 84263800
C	-0. 94349100	3. 63728600	4. 27680300
C	-0. 15019100	6. 13398800	5. 21419100
H	0. 04694100	6. 67499500	3. 13863500
C	-0. 88693300	3. 88136700	5. 64459700
H	-1. 25409800	2. 66589600	3. 89878200
C	-0. 48776900	5. 13181700	6. 11824800
H	0. 16221000	7. 10967100	5. 57347400
H	-1. 15426300	3. 09572000	6. 34474800
H	-0. 44138800	5. 32156300	7. 18589500

**H/Me/H/Bn**

**R1**

C	-0. 23585400	1. 06483400	-0. 45143000
C	-1. 54377600	1. 19695800	0. 08095900
C	-1. 96907500	2. 45660400	0. 55490300
C	-1. 11067500	3. 53578100	0. 49581400
C	0. 19368000	3. 36523000	-0. 04489500
C	0. 64797300	2. 15396300	-0. 51933600

C	-1.22994500	-0.93586200	-0.56639500
C	-2.15601300	-0.08643400	-0.00289700
H	-2.96867900	2.57343400	0.96480000
H	0.85280000	4.22867800	-0.08238900
H	1.64618500	2.04457200	-0.92995800
N	-0.07012100	-0.23599900	-0.83687000
H	0.76525000	-0.62502300	-1.24828300
H	-3.15111900	-0.37081900	0.30634600
C	-1.35540400	-2.35896500	-0.86774900
H	-0.46304000	-2.83098900	-1.32461500
O	-2.35917000	-3.00463500	-0.64096600
C	-1.52389000	4.89699900	0.99575800
H	-0.89470000	5.21683500	1.83246100
H	-1.42507900	5.65185400	0.20967400
H	-2.56175900	4.89424500	1.33531200

**si-M2**

C	-4.68054200	-6.34296600	0.88834900
C	-5.81301800	-7.92010600	1.99690900
C	-6.38430600	-5.64155900	2.71025900
H	-5.81158600	-4.74006400	2.91367700
N	-5.20578700	-8.58515100	1.08174400
N	-4.49750100	-7.62106700	0.36781300
N	-5.52587500	-6.57386200	1.98503900
C	-6.74517600	-8.41800100	3.05156100
H	-6.52754300	-9.45888500	3.29075300
H	-7.78737800	-8.34790700	2.70562900
C	-6.89571900	-6.28142800	4.05608500
O	-6.53446500	-7.64189900	4.21438900
C	-8.79065200	-5.60690900	2.68448200
C	-7.64715400	-5.33397400	1.93473100
C	-7.73170900	-4.88458600	0.62326900
C	-9.00746900	-4.74256600	0.09238800
C	-10.17011500	-5.00631900	0.81341700
C	-10.05888100	-5.43935800	2.12915100
C	-8.43135600	-6.06993000	4.07080200
H	-6.85311900	-4.64696300	0.03417200
H	-11.13436000	-4.87461700	0.33911300
H	-10.95119500	-5.65399000	2.70777400
H	-8.94127700	-6.99538500	4.35634900
H	-8.70645800	-5.31235900	4.81120700
C	-3.97111600	-7.94866000	-0.90875300
C	-4.54828000	-7.40672300	-2.06536300
C	-2.82964800	-8.76308100	-0.96042100
C	-3.89119300	-7.61825300	-3.27768000

C	-2.21702500	-8.95666300	-2.19739900
C	-2.71392900	-8.36173100	-3.35996200
H	-4.31056300	-7.18448700	-4.18283400
H	-1.31881900	-9.56772300	-2.25009800
C	-2.26350300	-9.36199900	0.30058100
H	-2.96619000	-10.07329800	0.74296100
H	-2.08522300	-8.58976800	1.05679500
H	-1.32263000	-9.87550800	0.09582500
C	-1.98051800	-8.49207700	-4.66866700
H	-2.67557200	-8.55149800	-5.50967700
H	-1.34140400	-9.37771600	-4.68161500
H	-1.34394500	-7.61408100	-4.82726700
C	-5.81826100	-6.59889000	-2.01819000
H	-6.47051600	-6.92593100	-1.20251400
H	-6.36280900	-6.69706200	-2.95969600
H	-5.60066400	-5.53645500	-1.86598800
H	-6.42178800	-5.77772700	4.89833200
N	-9.13357200	-4.29940600	-1.30069700
O	-10.25519900	-4.13699200	-1.75020400
O	-8.10918300	-4.12110600	-1.93774800
C	-1.54391400	-5.03321600	-2.05399700
C	-2.18890600	-3.80007800	-2.31410200
C	-1.70855900	-2.99397600	-3.36188600
C	-0.63422800	-3.42005700	-4.12852500
C	-0.02611000	-4.66678700	-3.84916000
C	-0.46562900	-5.48415200	-2.82043800
C	-3.26472300	-4.84429400	-0.61166800
C	-3.27074900	-3.69724000	-1.38511700
H	-2.18575700	-2.04115600	-3.57801500
H	0.81155100	-4.98835800	-4.46296300
H	0.00191500	-6.44392600	-2.61942800
N	-2.18613400	-5.62064300	-0.99099700
H	-1.99086600	-6.54972900	-0.65212500
H	-3.99814900	-2.90277100	-1.30528200
C	-4.18191100	-5.14028400	0.47532600
H	-4.08296200	-3.41033400	1.32244300
O	-4.78600300	-4.00662000	1.03114500
C	-0.10335500	-2.57589400	-5.26130600
H	-0.15689700	-3.11133700	-6.21463900
H	-0.67289100	-1.64928700	-5.36298200
H	0.94631400	-2.31016300	-5.09941700
<b>TS5(S)</b>			
C	-1.35500000	0.46684100	-0.17635100
C	-1.96270400	-0.86652800	-1.77661300

C	-2.45840900	-1.71894300	0.48406500
H	-1.96046100	-1.56770200	1.44306600
N	-1.44439900	0.16398500	-2.38322100
N	-1.07151300	0.99142700	-1.36734500
N	-1.94979200	-0.70053000	-0.42400600
C	-2.41582100	-2.19732200	-2.27994700
H	-2.07019700	-2.35422000	-3.30100900
H	-3.51136000	-2.27308400	-2.25338200
C	-2.15422500	-3.15182500	-0.08389200
O	-1.79345400	-3.16607800	-1.45710500
C	-4.52214700	-2.92898500	0.39502100
C	-3.96598600	-1.66280900	0.57464300
C	-4.75128400	-0.54136500	0.79436300
C	-6.12527500	-0.74400200	0.81956900
C	-6.71694600	-1.99317000	0.64680800
C	-5.90436900	-3.10099500	0.43457000
C	-3.44529600	-3.96055900	0.18263100
H	-4.32207500	0.44326000	0.94667800
H	-7.79569300	-2.07956100	0.67605800
H	-6.34693500	-4.08117200	0.29342500
H	-3.65022500	-4.63546400	-0.65274300
H	-3.32932300	-4.57525400	1.08139200
C	-0.54257100	2.31064900	-1.61868600
C	-1.36722200	3.40319300	-1.33250900
C	0.76566600	2.44431900	-2.09627400
C	-0.81636900	4.67605200	-1.47506400
C	1.26416100	3.73946300	-2.21560600
C	0.50350900	4.86083900	-1.88460200
H	-1.43406600	5.54111100	-1.24729600
H	2.28810600	3.87016800	-2.55863400
C	1.63949200	1.26982200	-2.44117400
H	1.06362800	0.38161700	-2.70045200
H	2.27045600	1.01965600	-1.58160800
H	2.29308700	1.52988800	-3.27703900
C	1.11594600	6.23473000	-1.94061600
H	0.35253800	7.01508800	-1.91415700
H	1.71736200	6.36483700	-2.84399900
H	1.77850600	6.37661400	-1.07901000
C	-2.79095300	3.23586400	-0.86337300
H	-3.27355700	2.36710800	-1.32069700
H	-3.37443100	4.12117000	-1.12139500
H	-2.84350400	3.11352600	0.22406700
H	-1.28879800	-3.57129400	0.42933600
N	-6.99586600	0.41851900	1.03269700

O	-8.19933100	0.22992400	1.07624900
O	-6.46791700	1.51027200	1.15190400
C	2.14690500	2.25123800	0.90444000
C	1.55953600	3.46853000	1.36279500
C	2.31148200	4.66050300	1.37347900
C	3.62754800	4.64332500	0.95417100
C	4.20454900	3.41516500	0.53331100
C	3.49915800	2.22931600	0.50916900
C	0.05863200	1.81954100	1.36437500
C	0.20888500	3.15843800	1.68127800
H	1.85288400	5.59249400	1.69755200
H	5.24351200	3.41845700	0.21133800
H	3.97046200	1.31271300	0.16895600
N	1.20735600	1.25429600	0.87943500
H	-0.57989700	3.83279800	1.98715400
C	-1.21684700	1.14703700	1.17487500
O	-2.21548600	1.20705900	1.86768200
C	3.53419600	-1.05220600	1.08984400
C	2.55957800	-0.68089900	2.02144200
C	2.89771500	-0.44139900	3.33841600
C	4.23805500	-0.57270100	3.71774600
C	5.20124000	-0.94145700	2.78090400
C	4.86615600	-1.19169100	1.44482500
C	1.58878200	-1.10905800	-0.12194100
C	1.23981200	-0.62927400	1.30920300
H	2.13191500	-0.15386800	4.05257500
H	4.53044200	-0.38864300	4.74586400
H	6.23649300	-1.04277000	3.09031700
H	5.61942500	-1.49297800	0.72455000
N	2.95361100	-1.22939600	-0.18425700
O	0.80627600	-1.38031800	-1.01457300
C	3.66832400	-1.68106500	-1.36363600
H	4.54359100	-1.03918600	-1.51514000
H	2.98362900	-1.52628600	-2.20329900
C	4.07977900	-3.13527600	-1.27513800
C	5.41099100	-3.51710600	-1.42743200
C	3.10787600	-4.11264400	-1.04197000
C	5.77338700	-4.86104600	-1.34524800
H	6.16967900	-2.75995900	-1.61055400
C	3.46800400	-5.45292000	-0.95807800
H	2.06765500	-3.81318700	-0.93452000
C	4.80291600	-5.82968800	-1.10854800
H	6.81350900	-5.14806500	-1.46189600
H	2.70787400	-6.20662300	-0.77903700



H	5.08328300	-6.87597400	-1.04197200
O	0.12745900	-0.89562800	1.80671800
C	4.46169300	5.89994500	0.92856100
H	5.33028300	5.81601100	1.58990000
H	4.84213000	6.10214100	-0.07823400
H	3.87781800	6.76660400	1.24807700

**H/Cl/H/Bn**

**R1**

C	-0.23306100	1.07032500	-0.44547700
C	-1.54618100	1.20323000	0.07867700
C	-1.97812900	2.45769500	0.55274300
C	-1.09084800	3.50653400	0.48293600
C	0.21448700	3.37193700	-0.04033000
C	0.65663200	2.15313300	-0.50974900
C	-1.23215200	-0.92617200	-0.56581500
C	-2.16171400	-0.07853100	-0.00904500
H	-2.97351000	2.59348100	0.96038100
H	0.86398000	4.23917100	-0.06731700
H	1.65645100	2.04033100	-0.91392200
N	-0.06934100	-0.23004300	-0.82857900
H	0.76828400	-0.62166700	-1.23368800
H	-3.15940800	-0.35996400	0.29328900
C	-1.36053600	-2.35239600	-0.86830700
H	-0.46806400	-2.82979500	-1.31771500
O	-2.37020100	-2.98800200	-0.64703700
Cl	-1.58345200	5.08543900	1.06394800

**si-M2**

C	-4.68633300	-6.33775500	0.87289100
C	-5.81309800	-7.91222400	1.98842000
C	-6.38759800	-5.63206600	2.69579700
H	-5.81592700	-4.72825200	2.89141400
N	-5.20064100	-8.57953900	1.07790100
N	-4.49832800	-7.61552200	0.35942000
N	-5.53313600	-6.56495100	1.96624300
C	-6.74135100	-8.40732100	3.04774300
H	-6.52235500	-9.44745600	3.28875600
H	-7.78480000	-8.33815400	2.70562400
C	-6.88715300	-6.26768600	4.04809700
O	-6.52516400	-7.62782300	4.20724200
C	-8.79367300	-5.60191300	2.68847800
C	-7.65673900	-5.33287600	1.92756300
C	-7.75188100	-4.89755900	0.61223500
C	-9.03174400	-4.76336000	0.08958300
C	-10.18831000	-5.02143900	0.82226600

C	-10.06635000	-5.44170400	2.14124700
C	-8.42237300	-6.05484800	4.07499800
H	-6.87832400	-4.66479800	0.01375600
H	-11.15634200	-4.89615600	0.35395300
H	-10.95382500	-5.65319600	2.72837300
H	-8.93020300	-6.97785400	4.37186700
H	-8.68986000	-5.29157300	4.81230400
C	-3.96482200	-7.94903300	-0.91319200
C	-4.54204400	-7.41759200	-2.07470000
C	-2.81951000	-8.75875300	-0.95562200
C	-3.88164600	-7.63566200	-3.28407400
C	-2.20325000	-8.95808100	-2.19007300
C	-2.70117500	-8.37519000	-3.35841000
H	-4.30182800	-7.21182100	-4.19349500
H	-1.30302000	-9.56651300	-2.23664800
C	-2.25480500	-9.34915100	0.31005500
H	-2.95079200	-10.07075900	0.74625000
H	-2.09301500	-8.57512500	1.06794500
H	-1.30548900	-9.84962800	0.11243500
C	-1.96882200	-8.51795000	-4.66653300
H	-2.66564400	-8.60578200	-5.50357700
H	-1.31520700	-9.39290900	-4.66432900
H	-1.34764700	-7.63325400	-4.84652400
C	-5.81568900	-6.61483200	-2.03697500
H	-6.46547900	-6.93229800	-1.21570000
H	-6.36124800	-6.73002300	-2.97591200
H	-5.60385000	-5.54883300	-1.90217800
H	-6.40552000	-5.76165600	4.88449100
N	-9.16864300	-4.33669500	-1.30766100
O	-10.29349300	-4.17473300	-1.74882300
O	-8.14913800	-4.17133000	-1.95602100
C	-1.53954100	-5.02576500	-2.05470100
C	-2.17507100	-3.78160000	-2.30470500
C	-1.68507600	-2.96390100	-3.33637900
C	-0.60913300	-3.42574700	-4.07034700
C	0.00788200	-4.66514400	-3.83095900
C	-0.45949600	-5.48170900	-2.81166800
C	-3.26948000	-4.83562500	-0.62383800
C	-3.26109400	-3.67874000	-1.38408700
H	-2.13861900	-2.00457500	-3.56044100
H	0.84589000	-4.97349700	-4.44512500
H	-0.00324100	-6.44723200	-2.61586500
N	-2.19579900	-5.61744300	-1.00582800
H	-2.00449200	-6.54867400	-0.66993000

H	-3.98137100	-2.87882800	-1.30169400
C	-4.19367700	-5.13206200	0.45383700
H	-4.11957300	-3.41003400	1.32220700
O	-4.81246000	-3.99933800	0.99425000
Cl	0.02404400	-2.42494700	-5.37115900
<b>TS5(S)</b>			
C	-1.35484800	0.46941500	-0.17027600
C	-1.95810200	-0.85932900	-1.77536000
C	-2.45040100	-1.72249800	0.48264200
H	-1.95168800	-1.57348200	1.44170500
N	-1.44206000	0.17491900	-2.37772300
N	-1.07154100	0.99954800	-1.35907300
N	-1.94607700	-0.69851900	-0.42213400
C	-2.40479600	-2.19033100	-2.28400700
H	-2.05785000	-2.34155600	-3.30543900
H	-3.49988200	-2.27182100	-2.25796200
C	-2.14246700	-3.15224400	-0.09208900
O	-1.77723200	-3.15810500	-1.46398700
C	-4.51155600	-2.93653000	0.38558500
C	-3.95806900	-1.67044200	0.57378100
C	-4.74590800	-0.55188000	0.79894300
C	-6.11949200	-0.75719900	0.82132400
C	-6.70848200	-2.00645900	0.64055400
C	-5.89350400	-3.11140900	0.42259900
C	-3.43285400	-3.96468100	0.16652000
H	-4.31991400	0.43326300	0.95644400
H	-7.78710300	-2.09507200	0.66791000
H	-6.33404500	-4.09153100	0.27493400
H	-3.63593300	-4.63300900	-0.67460800
H	-3.31707900	-4.58669900	1.06019800
C	-0.54276600	2.31975400	-1.60688200
C	-1.36745900	3.41102100	-1.31780100
C	0.76609500	2.45503600	-2.08426100
C	-0.81599100	4.68473500	-1.45533600
C	1.26562800	3.75013600	-2.19612500
C	0.50388100	4.87108200	-1.86356900
H	-1.43396800	5.54893400	-1.22544300
H	2.28916500	3.88246000	-2.54009600
C	1.63793700	1.28195000	-2.44011500
H	1.06049700	0.39683100	-2.70608700
H	2.27218900	1.02195300	-1.58593000
H	2.28987800	1.54865700	-3.27504800
C	1.11356100	6.24580000	-1.93236300
H	0.35996800	7.02415200	-1.79783800

H	1. 61364300	6. 40787600	-2. 89097500
H	1. 86796800	6. 35989100	-1. 14581700
C	-2. 79034300	3. 24134600	-0. 84711300
H	-3. 27382200	2. 37527800	-1. 30848700
H	-3. 37413300	4. 12821100	-1. 09876400
H	-2. 84149600	3. 11324300	0. 23993900
H	-1. 27775800	-3. 57265900	0. 42152300
N	-6. 99243700	0. 40267200	1. 03949900
O	-8. 19549400	0. 21161000	1. 08083000
O	-6. 46642400	1. 49470800	1. 16470800
C	2. 14649400	2. 26177700	0. 89480200
C	1. 54372000	3. 48505400	1. 32258600
C	2. 26900600	4. 68947300	1. 28791600
C	3. 57070700	4. 63456700	0. 84364700
C	4. 19262500	3. 42923100	0. 45586700
C	3. 49391100	2. 23819200	0. 48927200
C	0. 06190800	1. 82466000	1. 37029500
C	0. 19648900	3. 17015200	1. 65362300
H	1. 81597200	5. 63192700	1. 57847900
H	5. 22508600	3. 45068900	0. 12508600
H	3. 97447200	1. 31614300	0. 17973300
N	1. 21588700	1. 25861500	0. 90186700
H	-0. 59797400	3. 84570700	1. 93995400
C	-1. 21216600	1. 13639000	1. 18693000
O	-2. 20221300	1. 18668600	1. 88917400
C	3. 54196100	-1. 05089800	1. 08638100
C	2. 57089300	-0. 67049000	2. 01793400
C	2. 91139000	-0. 43164700	3. 33438100
C	4. 25071600	-0. 57368700	3. 71343800
C	5. 21056200	-0. 95069200	2. 77653400
C	4. 87311400	-1. 19959900	1. 44076300
C	1. 59612200	-1. 09297400	-0. 12476000
C	1. 25034000	-0. 60281000	1. 30519800
H	2. 14833000	-0. 13646600	4. 04836800
H	4. 54492400	-0. 39109300	4. 74125500
H	6. 24510700	-1. 05969500	3. 08554800
H	5. 62375000	-1. 50766900	0. 72069700
N	2. 95944600	-1. 22473100	-0. 18793800
O	0. 80986400	-1. 36089200	-1. 01485200
C	3. 66828500	-1. 69182100	-1. 36543900
H	4. 54812100	-1. 05803300	-1. 52395800
H	2. 98284700	-1. 53816900	-2. 20464800
C	4. 06919200	-3. 14819100	-1. 26650400
C	5. 39789800	-3. 53912700	-1. 41738800

C	3.09138300	-4.11782300	-1.02604300
C	5.75219400	-4.88461400	-1.32665000
H	6.16095300	-2.78784600	-1.60632400
C	3.44353200	-5.45972800	-0.93351300
H	2.05294200	-3.81157300	-0.92024000
C	4.77596400	-5.84560300	-1.08264900
H	6.79038300	-5.17884700	-1.44234500
H	2.67902500	-6.20766400	-0.74903600
H	5.04984200	-6.89314900	-1.00941100
O	0.13581000	-0.87278200	1.80250100
Cl	4.50203000	6.12158700	0.73314300

**H/Br/H/Bn**

**R1**

C	-0.23130300	1.06988200	-0.44214200
C	-1.54413800	1.20209100	0.08309300
C	-1.97602600	2.45693100	0.55557000
C	-1.09040400	3.50692200	0.48307300
C	0.21477000	3.37272200	-0.03961500
C	0.65786600	2.15323000	-0.50714600
C	-1.23159100	-0.92613100	-0.56456000
C	-2.16029800	-0.07929500	-0.00560000
H	-2.97174400	2.59175800	0.96237200
H	0.86453600	4.23940700	-0.06982000
H	1.65763500	2.04070300	-0.91168600
N	-0.06837500	-0.22998200	-0.82687100
H	0.76837900	-0.62123800	-1.23416700
H	-3.15812300	-0.36037800	0.29661400
C	-1.36244000	-2.35133300	-0.87135100
H	-0.47158700	-2.82889100	-1.32366900
O	-2.37301800	-2.98567200	-0.65076200
Br	-1.63371600	5.21891300	1.10125400

**si-M2**

C	-4.68588200	-6.34478300	0.86895700
C	-5.81590300	-7.91272800	1.99067700
C	-6.38263000	-5.63021100	2.69348100
H	-5.80975600	-4.72691300	2.88700200
N	-5.20947700	-8.58378900	1.07890000
N	-4.50536300	-7.62391000	0.35715700
N	-5.52964600	-6.56677600	1.96615200
C	-6.74506900	-8.40282500	3.05163400
H	-6.52887900	-9.44309700	3.29463200
H	-7.78839800	-8.33154000	2.70952900
C	-6.88377500	-6.26072700	4.04732400
O	-6.52663700	-7.62178100	4.20949100

C	-8.78838400	-5.59354700	2.68568600
C	-7.65067400	-5.33084700	1.92375000
C	-7.74434800	-4.90131400	0.60640700
C	-9.02380800	-4.76624500	0.08289400
C	-10.18112400	-5.01770000	0.81667100
C	-10.06052600	-5.43222500	2.13760200
C	-8.41818400	-6.04180000	4.07408600
H	-6.87006500	-4.67415600	0.00668800
H	-11.14876600	-4.89204500	0.34764800
H	-10.94870100	-5.63865800	2.72548400
H	-8.92956400	-6.96135600	4.37548100
H	-8.68201300	-5.27396900	4.80798000
C	-3.96894100	-7.96487100	-0.91210400
C	-4.54377100	-7.44034300	-2.07813600
C	-2.82368600	-8.77491600	-0.94695700
C	-3.88234700	-7.66777300	-3.28498100
C	-2.20525900	-8.98246600	-2.17928600
C	-2.70211800	-8.40879400	-3.35251500
H	-4.30078200	-7.24981500	-4.19793200
H	-1.30500700	-9.59112100	-2.22024200
C	-2.26117200	-9.35630400	0.32368300
H	-2.96050000	-10.07059400	0.76651700
H	-2.09548400	-8.57570300	1.07376400
H	-1.31418300	-9.86274100	0.13025300
C	-1.97238900	-8.56507300	-4.66076800
H	-2.67057200	-8.71873400	-5.48730500
H	-1.27772200	-9.40724500	-4.63142000
H	-1.39645700	-7.65936800	-4.88078300
C	-5.81448100	-6.63280500	-2.04644500
H	-6.46551700	-6.94192200	-1.22304100
H	-6.36026000	-6.75228500	-2.98469300
H	-5.59886500	-5.56657000	-1.91903500
H	-6.39999800	-5.75448000	4.88234400
N	-9.15944900	-4.34657600	-1.31659600
O	-10.28381200	-4.18375200	-1.75866200
O	-8.13944400	-4.18771600	-1.96578600
C	-1.55483200	-5.01142100	-2.07955700
C	-2.17435100	-3.75195600	-2.29080100
C	-1.67483900	-2.91145100	-3.29896300
C	-0.60733300	-3.36612400	-4.04956100
C	-0.00865000	-4.62117900	-3.85118500
C	-0.48493200	-5.46096500	-2.85467900
C	-3.27155800	-4.83562400	-0.63072600
C	-3.25283900	-3.65923000	-1.36064000

H	-2.11293700	-1.93817100	-3.48978100
H	0.82305400	-4.92411700	-4.47593100
H	-0.04115600	-6.43780300	-2.68805200
N	-2.21253700	-5.62246800	-1.04323100
H	-2.02688200	-6.56270200	-0.72968600
H	-3.96120200	-2.85201700	-1.25230500
C	-4.19103000	-5.13999700	0.44863000
H	-4.10233700	-3.42690500	1.33333700
O	-4.80038000	-4.00768300	1.00088000
Br	0.09787000	-2.23888800	-5.41516300

**TS5(S)**

C	-1.35518600	0.46724000	-0.15850600
C	-1.95843600	-0.84547000	-1.77709600
C	-2.45673500	-1.72726300	0.47230400
H	-1.95872500	-1.58707500	1.43324100
N	-1.43470300	0.19109400	-2.36861700
N	-1.06353000	1.00591600	-1.34210500
N	-1.95051000	-0.69587100	-0.42278500
C	-2.41084300	-2.16964900	-2.29827800
H	-2.06412800	-2.31308200	-3.32089200
H	-3.50629400	-2.24621000	-2.27346100
C	-2.14842500	-3.15204300	-0.11394800
O	-1.78814600	-3.14819900	-1.48734400
C	-4.51659700	-2.94224600	0.36899300
C	-3.96451200	-1.67643800	0.56349700
C	-4.75379900	-0.56014800	0.79487700
C	-6.12709500	-0.76757500	0.81762000
C	-6.71454400	-2.01669000	0.63120600
C	-5.89822200	-3.11931000	0.40655800
C	-3.43671000	-3.96782700	0.14361400
H	-4.32927500	0.42485500	0.95683900
H	-7.79300000	-2.10697600	0.65955500
H	-6.33752800	-4.09930500	0.25443000
H	-3.64019800	-4.63291200	-0.69991600
H	-3.31815800	-4.59317600	1.03463700
C	-0.52013100	2.32226000	-1.58285500
C	-1.33034000	3.42211100	-1.28600700
C	0.78928100	2.44564400	-2.06301500
C	-0.76245100	4.69001100	-1.41465700
C	1.30537200	3.73487800	-2.16545300
C	0.55919200	4.86339200	-1.82352500
H	-1.36869700	5.55985600	-1.17486700
H	2.33240400	3.85652800	-2.50313300
C	1.64721100	1.26534400	-2.42804600

H	1. 06021400	0. 38812400	-2. 69887200
H	2. 28060300	0. 99350200	-1. 57714200
H	2. 30076600	1. 53055300	-3. 26221600
C	1. 18185600	6. 23209400	-1. 90719300
H	0. 51201000	6. 99799800	-1. 51098700
H	1. 41953200	6. 48952700	-2. 94397500
H	2. 11723500	6. 26340700	-1. 33895900
C	-2. 75432100	3. 26595300	-0. 81388000
H	-3. 24894100	2. 41025800	-1. 28282200
H	-3. 32767100	4. 16222300	-1. 05611000
H	-2. 80627900	3. 12783300	0. 27198900
H	-1. 28121700	-3. 57461000	0. 39363200
N	-7. 00153100	0. 38984100	1. 04283900
O	-8. 20425200	0. 19676300	1. 08457800
O	-6. 47705000	1. 48201400	1. 17315500
C	2. 12471000	2. 26051500	0. 89574800
C	1. 51281500	3. 48065300	1. 32022800
C	2. 21276800	4. 69652700	1. 23754200
C	3. 49739800	4. 65651000	0. 74644400
C	4. 13457500	3. 45555000	0. 37169700
C	3. 46281600	2. 25142900	0. 45884300
C	0. 05086100	1. 80583000	1. 40255200
C	0. 17532200	3. 15388800	1. 67647800
H	1. 74688900	5. 63710800	1. 51293700
H	5. 15452100	3. 48947800	0. 00577800
H	3. 95341100	1. 33110300	0. 15916000
N	1. 20514000	1. 24820100	0. 92494200
H	-0. 62279600	3. 82457100	1. 96413100
C	-1. 22037600	1. 11641600	1. 20878700
O	-2. 21443800	1. 15694500	1. 90574400
C	3. 54123600	-1. 04748600	1. 09451100
C	2. 56966000	-0. 67534800	2. 02888700
C	2. 91107300	-0. 43876400	3. 34551000
C	4. 25184800	-0. 57443400	3. 72180600
C	5. 21225900	-0. 94257900	2. 78198700
C	4. 87387000	-1. 18920700	1. 44603800
C	1. 59326000	-1. 09921300	-0. 11273700
C	1. 24748700	-0. 61253600	1. 31824400
H	2. 14747600	-0. 15074200	4. 06184400
H	4. 54677300	-0. 39376300	4. 74976000
H	6. 24797900	-1. 04651200	3. 08879000
H	5. 62495700	-1. 49101900	0. 72377600
N	2. 95706100	-1. 22385400	-0. 17886500
O	0. 80611300	-1. 37061700	-1. 00102800



C	3.66533800	-1.69045400	-1.35701400
H	4.54352900	-1.05487400	-1.51749800
H	2.97832000	-1.53915100	-2.19537400
C	4.06938700	-3.14590500	-1.25704100
C	5.39864600	-3.53463300	-1.40872000
C	3.09354200	-4.11706200	-1.01472600
C	5.75533300	-4.87943600	-1.31695700
H	6.16025000	-2.78228400	-1.59922400
C	3.44807300	-5.45823200	-0.92111500
H	2.05468100	-3.81252300	-0.90835300
C	4.78104900	-5.84190700	-1.07107000
H	6.79392500	-5.17195600	-1.43337100
H	2.68500800	-6.20728800	-0.73520400
H	5.05686100	-6.88889000	-0.99703900
O	0.13426000	-0.88919800	1.81526500
Br	4.44174100	6.29390300	0.51724900

**Coordinates for rate-determining step catalyzed by different catalysts at the IEFPCM(THF)//M062X/6-31G(d,p) level**

*NHC<sub>A</sub>*

*si-M2*

C	-4.66212500	-6.09745800	0.90552000
C	-5.68792500	-7.81881700	1.88994300
C	-6.46466300	-5.62834100	2.69122600
H	-5.97275600	-4.67872100	2.89853300
N	-4.98834100	-8.39969000	0.98203900
N	-4.32952200	-7.33952700	0.33445500
N	-5.53006800	-6.45559500	1.93711700
C	-6.59459900	-8.42206800	2.91333200
H	-6.31931100	-9.45920300	3.10448400
H	-7.63652000	-8.38949600	2.56301200
C	-6.87122200	-6.34422400	4.03224800
O	-6.42524300	-7.69005000	4.11166300
C	-8.85906100	-5.77537300	2.75143700
C	-7.77096500	-5.42875400	1.95454000
C	-7.93992800	-4.98942800	0.64428100
C	-9.23456900	-4.90005500	0.13829100
C	-10.33175200	-5.24121600	0.93418800
C	-10.15294000	-5.68029300	2.24437600
C	-8.41278600	-6.22525800	4.11999700
H	-7.07934000	-4.72985600	0.03376000
H	-11.33412300	-5.16685300	0.52442500
H	-11.00839500	-5.95125500	2.85618100
H	-8.84537600	-7.18524400	4.42021300

H	-8.69466900	-5.49437600	4.88472200
C	-3.91438200	-7.53132300	-0.99206700
C	-4.48724400	-6.83833100	-2.05702200
C	-2.80609100	-8.33781500	-1.25506600
C	-3.92411500	-6.88302000	-3.32585200
C	-2.26497500	-8.42645500	-2.52593600
C	-2.81576200	-7.68085700	-3.56172400
H	-6.38473500	-5.85280800	4.87503700
C	-1.41089500	-5.13271800	-1.72418800
C	-2.17575600	-4.17702800	-2.44215400
C	-1.74881400	-3.80242100	-3.72803100
C	-0.60155100	-4.37556300	-4.24974000
C	0.14474900	-5.31797300	-3.51320000
C	-0.24564700	-5.70734100	-2.24194400
C	-3.24406300	-4.64823500	-0.50621400
C	-3.32674700	-3.87734400	-1.64404500
H	-2.32169700	-3.08420800	-4.30685900
H	-0.26964600	-4.09977400	-5.24542800
H	1.03770200	-5.75087100	-3.95214500
H	0.31527000	-6.44620100	-1.67734200
N	-2.06127400	-5.36550500	-0.53772000
H	-1.75932700	-5.99738400	0.18931500
H	-4.16145200	-3.24323600	-1.90479800
C	-4.22447200	-4.86231100	0.54868100
H	-4.29065500	-3.13527400	1.40091800
O	-4.92495000	-3.75682500	1.01994200
H	-9.39397600	-4.56318300	-0.88092000
F	-5.56576300	-6.08254700	-1.86260500
F	-4.44853700	-6.16158400	-4.31251000
F	-2.26748900	-7.72176400	-4.77060700
F	-1.17908700	-9.16502000	-2.74620900
F	-2.20903300	-8.97426900	-0.24963800

**TS5(R)**

C	-1.50186700	0.11324400	-0.07130300
C	-1.81081900	-1.26600500	-1.72243700
C	-2.20131600	-2.24936300	0.51308200
H	-1.77210300	-2.01175600	1.48807000
N	-1.44372700	-0.15698300	-2.29496100
N	-1.25630200	0.69746100	-1.25041500
N	-1.88244100	-1.12564500	-0.36520600
C	-1.96966500	-2.65199500	-2.25417900
H	-1.57826300	-2.71503900	-3.26861400
H	-3.02360200	-2.95932100	-2.24747300
C	-1.57326800	-3.57009300	-0.06532600

O	-1.16644800	-3.46954600	-1.42403500
C	-3.94627000	-3.87123100	0.33148700
C	-3.68745300	-2.52088600	0.55419700
C	-4.71174600	-1.60914600	0.78729100
C	-6.02367400	-2.07695400	0.78316000
C	-6.29304800	-3.42939600	0.55753600
C	-5.25859900	-4.33600800	0.33389900
C	-2.66706100	-4.64393600	0.12994900
H	-4.48603800	-0.56330300	0.97368200
H	-7.32100900	-3.77748300	0.55575000
H	-5.47307200	-5.38572800	0.15790400
H	-2.69152800	-5.31199000	-0.73567400
H	-2.44212800	-5.25601600	1.00951000
C	-0.82663700	2.02938400	-1.48824100
C	-1.60028600	3.09752700	-1.04860000
C	0.39610500	2.28086600	-2.10517600
C	-1.16494800	4.40199100	-1.21587700
C	0.82928500	3.58555200	-2.28982500
C	0.05148800	4.64402700	-1.83931900
H	-0.65549400	-3.80236500	0.47513100
C	1.46819800	2.61506600	0.90960300
C	0.64850600	3.65298200	1.45315500
C	1.08050900	4.99255100	1.39646700
C	2.30271500	5.27121200	0.81781700
C	3.11756600	4.23426600	0.30422400
C	2.72671700	2.90994700	0.35140400
C	-0.42084600	1.69542600	1.51628500
C	-0.56386800	3.02724000	1.86301900
H	0.44810200	5.78983700	1.77670300
H	2.64624800	6.29801000	0.74644500
H	4.06843100	4.49029200	-0.15293800
H	3.34314800	2.12681200	-0.07752100
N	0.79318300	1.42607000	0.94418500
H	-1.46632300	3.49530200	2.23271500
C	-1.51753700	0.75615700	1.31090000
O	-2.49212000	0.55653500	2.00379200
C	3.61881000	-0.25656300	0.98460400
C	2.59811600	-0.16247600	1.93619100
C	2.89149400	0.07574500	3.26390000
C	4.23213800	0.22784300	3.63491400
C	5.24101700	0.13537600	2.67794000
C	4.95269900	-0.11171600	1.33052600
C	1.72108700	-0.69069500	-0.22483600
C	1.28765400	-0.37542100	1.23158700

H	2.09056100	0.14452700	3.99399500
H	4.48942700	0.41657800	4.67151200
H	6.27683000	0.25152800	2.98029000
H	5.74390000	-0.20135200	0.59368400
N	3.07725300	-0.49937900	-0.29537200
O	1.00776100	-1.08906500	-1.12537700
C	3.85880600	-0.74271000	-1.49321100
H	4.58309400	0.06976800	-1.61723000
H	3.14976000	-0.69503700	-2.32479800
C	4.56144600	-2.08369300	-1.46673100
C	5.93526800	-2.18124000	-1.67861500
C	3.81919400	-3.24525000	-1.23482700
C	6.56537700	-3.42511700	-1.66031900
H	6.51636600	-1.27987800	-1.85940800
C	4.44671700	-4.48561600	-1.21285800
H	2.74519900	-3.16934700	-1.08046900
C	5.82251400	-4.57799500	-1.42557600
H	7.63629600	-3.49043800	-1.82396500
H	3.86388000	-5.38311000	-1.03147400
H	6.31190100	-5.54651100	-1.40670800
O	0.28338300	-0.94304700	1.71803500
H	-6.84215400	-1.38664400	0.95834600
F	-2.74459700	2.86121900	-0.41264000
F	-1.88618400	5.41249300	-0.74461900
F	0.47687600	5.88890000	-1.99324400
F	2.00141000	3.82242000	-2.86714500
F	1.17856400	1.28365400	-2.48790700

***NHC<sub>B</sub>***

***si-M2***

C	-4.72055800	-6.34364300	0.82609200
C	-5.84554100	-7.92155700	1.93771300
C	-6.41657800	-5.64645400	2.66631300
H	-5.83536700	-4.74560300	2.84885500
N	-5.22081800	-8.59083000	1.03581000
N	-4.52086900	-7.62366600	0.31809000
N	-5.57849200	-6.57423300	1.90882800
C	-6.76123700	-8.41812700	3.00663100
H	-6.55090200	-9.46399700	3.23043500
H	-7.80999700	-8.32791800	2.68701000
C	-6.86581400	-6.28845500	4.03347700
O	-6.50871100	-7.65464500	4.16980600
C	-8.81645800	-5.59656400	2.75416700
C	-7.71199700	-5.33802800	1.94647000
C	-7.86295900	-4.87951800	0.63978700

C	-9.15214900	-4.69380000	0.14586700
C	-10.26434000	-4.95579700	0.95048000
C	-10.10470100	-5.40431700	2.25982800
C	-8.39635400	-6.06675100	4.12330300
H	-6.99095100	-4.66481700	0.02822100
H	-11.26243000	-4.80837900	0.55010400
H	-10.97130200	-5.60811400	2.88213500
H	-8.89168300	-6.99369700	4.43069600
H	-8.62756500	-5.31434500	4.88398000
C	-3.95712000	-7.96397700	-0.93813400
C	-4.51092600	-7.44524700	-2.11643200
C	-2.80630800	-8.76727400	-0.95100800
C	-3.82433600	-7.66713700	-3.31007500
C	-2.16207000	-8.97065300	-2.17041700
C	-2.63748500	-8.39876100	-3.35338600
H	-4.22694900	-7.25144100	-4.23120600
H	-1.25675800	-9.57284600	-2.19336700
C	-2.26403600	-9.34342000	0.33077700
H	-2.96955600	-10.05665500	0.76521700
H	-2.11240000	-8.55957700	1.08059600
H	-1.31276000	-9.84839300	0.15502800
C	-1.87390100	-8.54192500	-4.64337500
H	-2.55014600	-8.63980800	-5.49617200
H	-1.21270900	-9.41100400	-4.62189500
H	-1.25672000	-7.65210500	-4.81185100
C	-5.78904600	-6.64932000	-2.10725200
H	-6.45380800	-6.97025200	-1.30008000
H	-6.31092100	-6.76764000	-3.05924900
H	-5.57895700	-5.58407900	-1.96268100
H	-6.34607300	-5.79377800	4.85423600
C	-1.53789400	-5.01991300	-2.06830900
C	-2.17183300	-3.77658700	-2.32308500
C	-1.66626300	-2.96258800	-3.35085200
C	-0.58080300	-3.40503800	-4.09015100
C	0.02188100	-4.65107500	-3.82789100
C	-0.44815800	-5.47495300	-2.81467800
C	-3.28684400	-4.83784900	-0.65536500
C	-3.27014300	-3.68007100	-1.41285100
H	-2.12893300	-2.00404800	-3.56730000
H	-0.18799800	-2.78469700	-4.88966300
H	0.86779700	-4.97177900	-4.42762700
H	0.00419100	-6.44135300	-2.61049600
N	-2.20512800	-5.61568000	-1.02645500
H	-2.01859900	-6.54888400	-0.69392800

H	-3.99153800	-2.88042900	-1.33336000
C	-4.22494200	-5.13791100	0.41088700
H	-4.15496900	-3.41855100	1.27936900
O	-4.84822700	-4.00407500	0.94559500
H	-9.29469700	-4.33962800	-0.87009100
<b>TS5(S)</b>			
C	-1.35879900	0.48086100	-0.17231000
C	-1.96695200	-0.86336800	-1.76089900
C	-2.46347400	-1.70559200	0.50232800
H	-1.97635100	-1.53909400	1.46414000
N	-1.45246900	0.16419200	-2.37686400
N	-1.07853800	0.99879700	-1.36773200
N	-1.95158100	-0.68868500	-0.40979100
C	-2.41025000	-2.20150700	-2.25357100
H	-2.06620600	-2.36111300	-3.27494000
H	-3.50450000	-2.28717200	-2.22077100
C	-2.13198200	-3.13761700	-0.05007800
O	-1.77444100	-3.15743700	-1.42657200
C	-4.50461400	-2.94429000	0.40295300
C	-3.97310700	-1.66796100	0.57090700
C	-4.78499300	-0.55657200	0.76900700
C	-6.16518000	-0.74507300	0.79026300
C	-6.70799600	-2.02159000	0.62116400
C	-5.88408800	-3.12950900	0.42978600
C	-3.40805800	-3.96517300	0.22410300
H	-4.34426500	0.42696900	0.90827400
H	-7.78541900	-2.15140500	0.63716000
H	-6.31224800	-4.11844400	0.29663000
H	-3.58697200	-4.66243100	-0.59913700
H	-3.28281000	-4.55885800	1.13594300
C	-0.56010000	2.31920200	-1.63120200
C	-1.39385700	3.40687700	-1.35492500
C	0.74414700	2.46033600	-2.11879900
C	-0.85942400	4.68396900	-1.52197400
C	1.22504100	3.75910400	-2.26609800
C	0.45288900	4.87732000	-1.94962600
H	-1.48559800	5.54537800	-1.30389600
H	2.24353200	3.89691700	-2.62227500
C	1.62875600	1.28990800	-2.45026100
H	1.05944100	0.39611000	-2.70490200
H	2.25720700	1.04982800	-1.58575900
H	2.28420000	1.54816600	-3.28516300
C	1.04222500	6.25853100	-2.05876400
H	0.27845000	7.02924300	-1.93851800

H	1. 53281400	6. 40308100	-3. 02502100
H	1. 79915300	6. 40321400	-1. 28101000
C	-2. 81332700	3. 23089800	-0. 87657000
H	-3. 29133600	2. 35731200	-1. 32945300
H	-3. 40424900	4. 11164200	-1. 13341100
H	-2. 85787000	3. 10986500	0. 21124400
H	-1. 25600800	-3. 53601000	0. 46287600
C	2. 17452700	2. 26054300	0. 91206500
C	1. 58991900	3. 48135100	1. 37195100
C	2. 35722100	4. 66078100	1. 41631200
C	3. 68130900	4. 60872400	1. 02829000
C	4. 26019900	3. 39278900	0. 59658600
C	3. 53167900	2. 21964600	0. 53827600
C	0. 07554700	1. 84495500	1. 34660500
C	0. 23062600	3. 18005800	1. 66817800
H	1. 90928800	5. 59488900	1. 74446800
H	4. 28941400	5. 50750800	1. 05082200
H	5. 30415100	3. 38345700	0. 29762900
H	3. 98973800	1. 29906400	0. 19188800
N	1. 22621400	1. 27210900	0. 87351600
H	-0. 55566400	3. 85836500	1. 97130200
C	-1. 20499400	1. 17135000	1. 17112600
O	-2. 19260500	1. 24333700	1. 87686300
C	3. 54022800	-1. 05463400	1. 08210700
C	2. 57090200	-0. 66800400	2. 01295600
C	2. 91304800	-0. 42889200	3. 32886200
C	4. 25189400	-0. 57587900	3. 70802500
C	5. 20974700	-0. 95982500	2. 77187200
C	4. 87062000	-1. 21000300	1. 43681600
C	1. 59308000	-1. 09007900	-0. 12821600
C	1. 25002200	-0. 60065800	1. 30191100
H	2. 15146900	-0. 12889800	4. 04245600
H	4. 54719100	-0. 39226500	4. 73540600
H	6. 24384400	-1. 07336500	3. 08097600
H	5. 61947300	-1. 52290300	0. 71690000
N	2. 95696600	-1. 22602600	-0. 19120700
O	0. 80849600	-1. 35524700	-1. 02036000
C	3. 66533700	-1. 68423400	-1. 37166100
H	4. 54505400	-1. 04911300	-1. 52609200
H	2. 97954900	-1. 52506400	-2. 20961000
C	4. 06682800	-3. 14122700	-1. 28385000
C	5. 39529300	-3. 53120400	-1. 43952000
C	3. 08947100	-4. 11256000	-1. 04831700
C	5. 74984400	-4. 87727400	-1. 35851600

H	6.15800700	-2.77844700	-1.62415700
C	3.44182400	-5.45506600	-0.96559100
H	2.05130300	-3.80687900	-0.93820700
C	4.77401700	-5.83996300	-1.11953100
H	6.78789400	-5.17065900	-1.47784400
H	2.67759600	-6.20419100	-0.78478700
H	5.04804100	-6.88799600	-1.05387300
O	0.13723900	-0.86119600	1.80372800
H	-6.82415700	0.10408400	0.93963300