

*Supporting Information*

**A DFT Study of NHC-Catalyzed Reaction of [3 + 3] Annulation of 2-Bromo-enals  
and Thioamides: Mechanism, Regio- and Stereoselectivities**

**Yan Li\*, Lina Geng, Zhiyi Song, Zhiqiang Zhang\***

*School of Chemical Engineering, University of Science and Technology Liaoning,*

*Qianshan Road 185, Anshan 114051, China*

***Corresponding person: Yan Li***

***E-mail: [yanli@ustl.edu.cn](mailto:yanli@ustl.edu.cn)***

***[zzq@ustl.edu.com](mailto:zzq@ustl.edu.com)***

***Telephone: +86-412-5929627***

***Fax: +86-412-5929627***

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## 1. Computational Details

### (1) 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.

### (2) Distortion-interaction model

In distortion-interaction analysis, the transition state was divided into two fragments, followed by single point energy calculations on each fragment. The activation energy  $\Delta E^\ddagger$  was divided into  $\Delta E_{\text{dist}}^\ddagger$  and  $\Delta E_{\text{int}}^\ddagger$ , where  $\Delta E_{\text{dist}}^\ddagger$  and  $\Delta E_{\text{int}}^\ddagger$  are distortion energy and interaction energy, respectively. The distortion energy  $\Delta E_{\text{dist}}^\ddagger$  of each fragment is the energy difference between the distorted fragment and the corresponding optimized structure without the other fragment. The interaction energy  $\Delta E_{\text{int}}^\ddagger$  can be calculated using  $\Delta E_{\text{int}}^\ddagger = \Delta E^\ddagger - \Delta E_{\text{dist}}^\ddagger$ .

### (3) Global reactivity indexes (GRI) analysis

In global reactivity index (GRI) analysis, the electrophilicity index  $\omega$  which reflects the molecular global electrophilicity character can be measured with the expression  $\omega = (\mu^2/2\eta)$  (eV), where  $\mu$  is the electronic chemical potential and  $\eta$  is the chemical hardness. The values of  $\mu$  and  $\eta$  can be determined in terms of the one-electron energy of HOMO and LUMO ( $E_{\text{HOMO}}$  and  $E_{\text{LUMO}}$ ) using  $\mu \approx (E_{\text{HOMO}} - E_{\text{LUMO}})/2$  and  $\eta \approx (E_{\text{LUMO}} - E_{\text{HOMO}})$ . Within the Kohn–Sham scheme, the molecular nucleophilicity

character is reflected by the value of the nucleophilicity index  $N$  as defined in  $N = E_{\text{HOMO}}(\text{Nu}) - E_{\text{LUMO}}(\text{TCE})$ , where  $E_{\text{LUMO}}(\text{TCE})$  is the LUMO energy of tetracyanoethylene (TCE).

## 2. Test results at different levels

**Table S1** Comparisons of relative energies for stereoselective transition states. Energies (in kcal/mol) are based on SMD(mesitylene)M06-2X/6-31G(d,p)-optimized geometries.

	M06-2X-D3		B3LYP-D3		$\omega$ B97X-D	
	SMD	IEFPCM	SMD	IEFPCM	SMD	IEFPCM
<b>TS5R</b>	4.1	2.8	3.1	1.8	3.3	2.0
<b>TS5S</b>	0.0	0.0	0.0	0.0	0.0	0.0

**Table S2** Different computational levels.

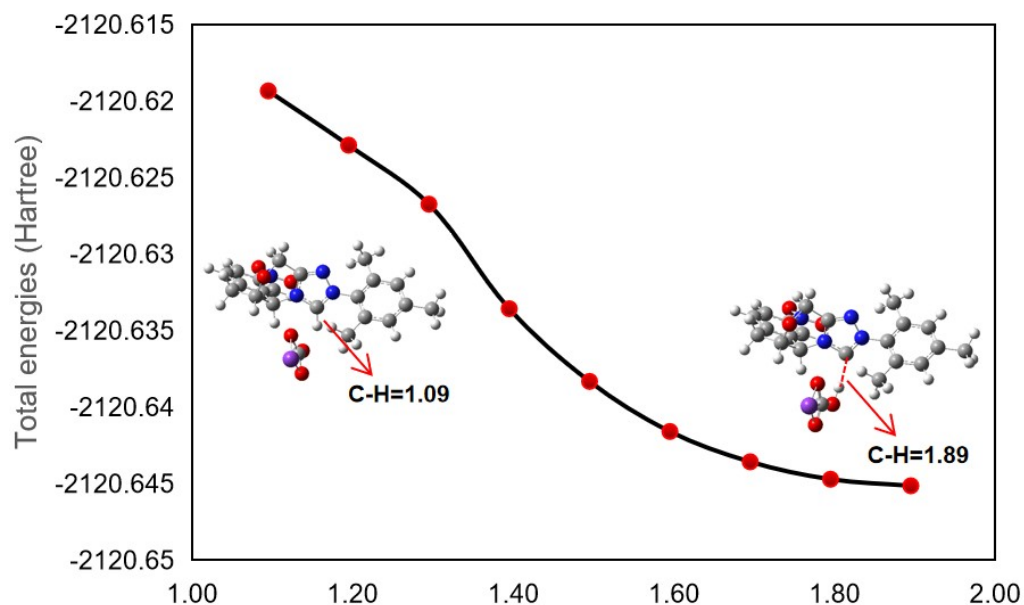
Different levels	Optimization		Single Point Energy		Solvation model
	Method	Basis set	Method	Basis set	
<b>L1</b>	M06-2X	6-31G(d,p)	M06-2X-D3	6-311++G(2df,2pd)	IEFPCM
<b>L2</b>	M06-2X	6-31G(d,p)	M06-2X-D3	6-311++G(2df,2pd)	SMD
<b>L3</b>	$\omega$ B97X-D	6-31G(d,p)	$\omega$ B97X-D	6-311++G(2df,2pd)	IEFPCM
<b>L4</b>	$\omega$ B97X-D	6-31G(d,p)	$\omega$ B97X-D	6-311++G(2df,2pd)	SMD

**Table S3** Comparisons of relative energies for stereoselective transition states with different Levels L1~L4. Energies are given in kcal/mol.

	<b>L1</b>	<b>L2</b>	<b>L3</b>	<b>L4</b>
<b>TS5R</b>	4.1	2.5	3.2	2.0
<b>TS5S</b>	0.0	0.0	0.0	0.0

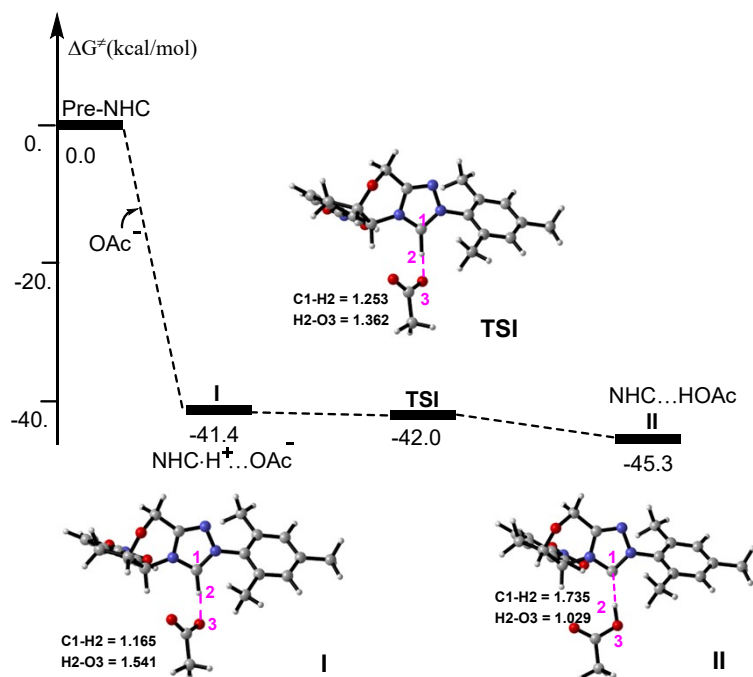
### 3. Generation of NHC.

**Fig. S1** The deprotonation of Pre-NHC by base ( $K_2CO_3$ ) generating NHC.

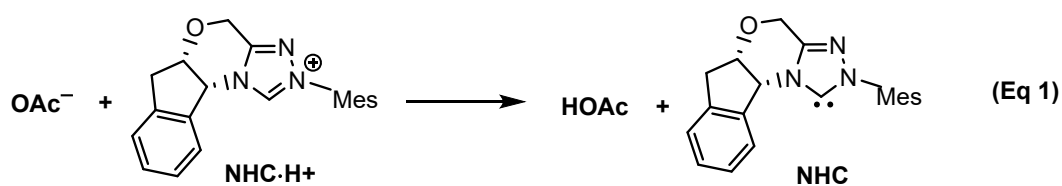


It should be noted that the **Pre-NHC** was firstly deprotonated by base ( $K_2CO_3$ ) or additive ( $LiOAc$ ) to generate the active catalyst **NHC**. However, for the deprotonation by  $KCO_3^-$ , we can not locate the transition state despite of lots of attempts. Then we scanned the changes of C-H bond (Fig. S1). Fig.S1 shows that this process has no energy barrier.

**Fig. S2** The deprotonation of Pre-NHC by additive (LiOAc) generating NHC.

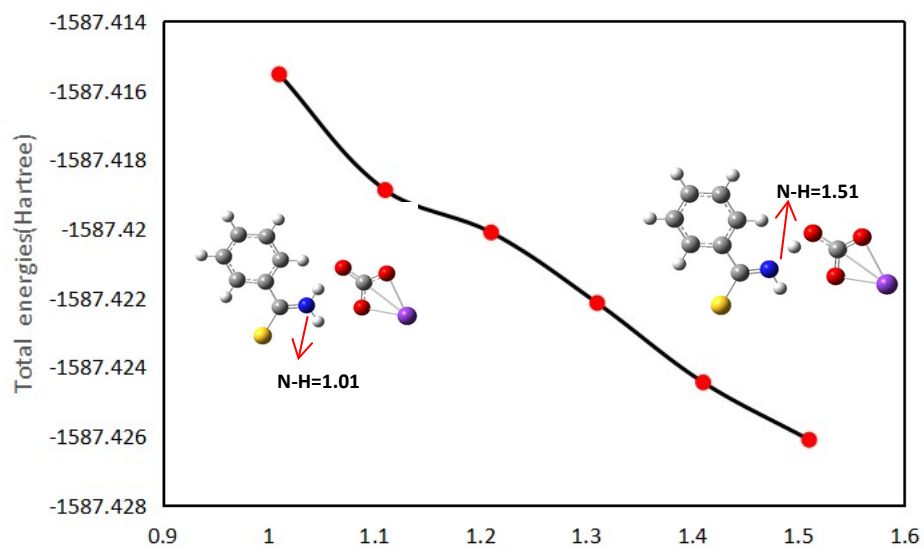


In addition, we examined the deprotonation of **Pre-NHC** by LiOAc. The deprotonation of **Pre-NHC** by base OAc<sup>-</sup> (derived from LiOAc) generates the active NHC (Equation 1). The corresponding energy profiles are provided in Fig. S2. As shown in Fig. S2, the active catalyst NHC could be easily formed.



#### 4. Generation of R2

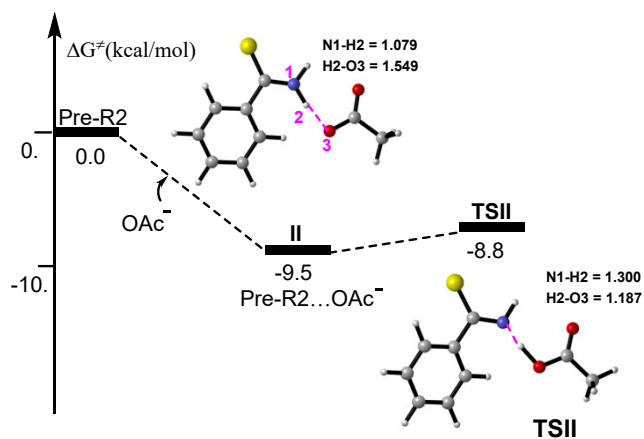
**Fig. S3** The deprotonation of Pre-R2 by base ( $K_2CO_3$ ) generating R2.



The **Pre-R2** was firstly deprotonated by base ( $K_2CO_3$ ) to generate the real reactant **R2**. However, for the deprotonation by  $KCO_3^-$ , we can not locate the transition state despite of lots of attempts. We scanned the changes of N - H bond. Fig.S3 shows that with the aid of  $KCO_3^-$ , formation of **R2** is barrierless.

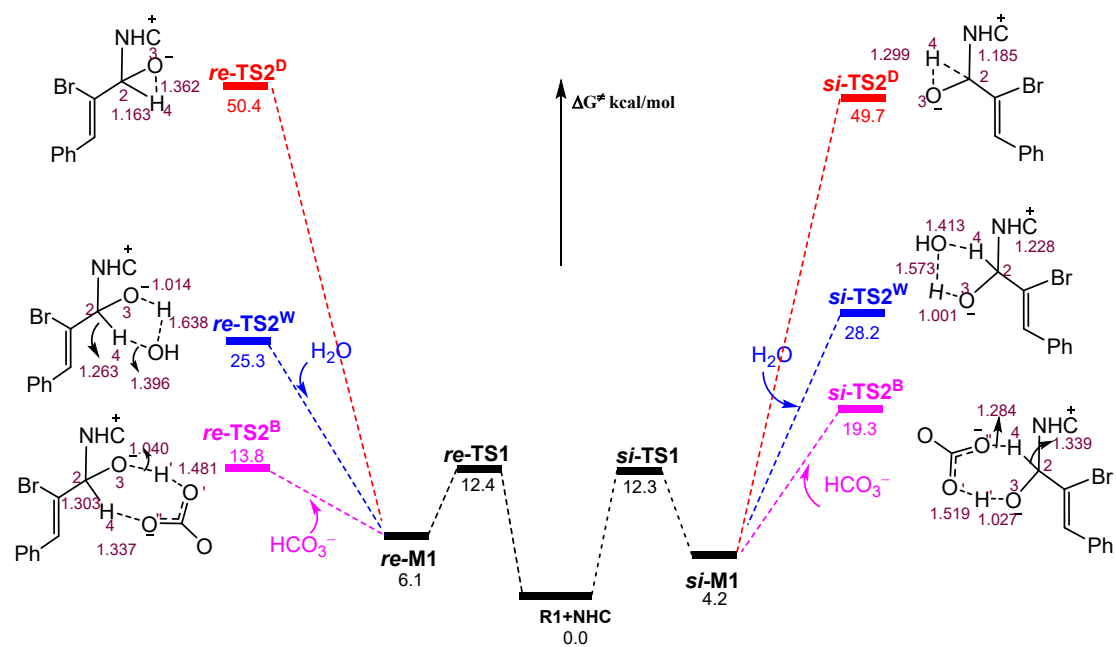


**Fig. S4** The deprotonation of Pre-R2 by additive (LiOAc) generating R2.

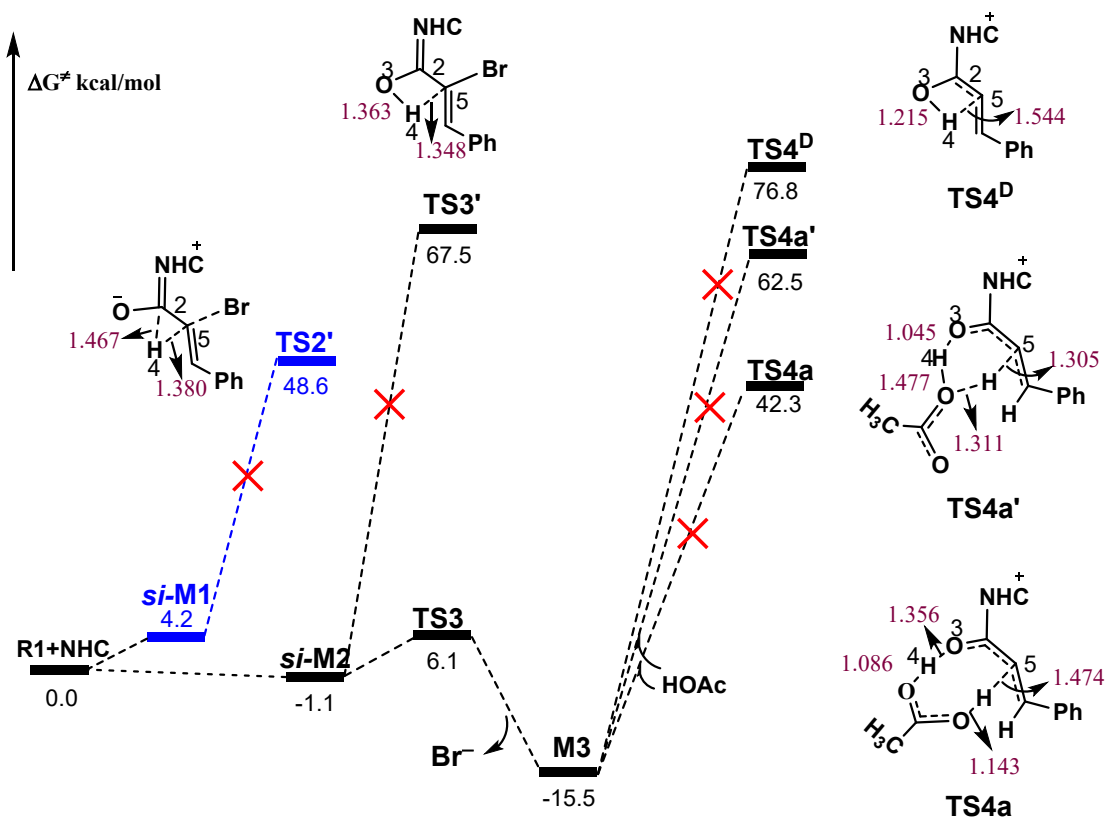


We then examined the deprotonation of **Pre-R2** by LiOAc. As shown in Fig. S4, the energy barrier is estimated to be 0.7 kcal/mol, indicating that this step can happen under the experimental condition.

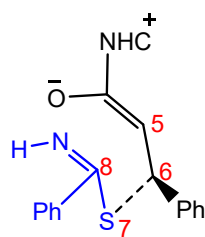
**Fig. S5** Unfavorable pathways and optimized structures for steps 1-2. Bond distances are given in Å.



**Fig. S6** Unfavorable pathways and optimized structures for steps 2-4. Bond distances are given in Å.



## Conformation search of TS5

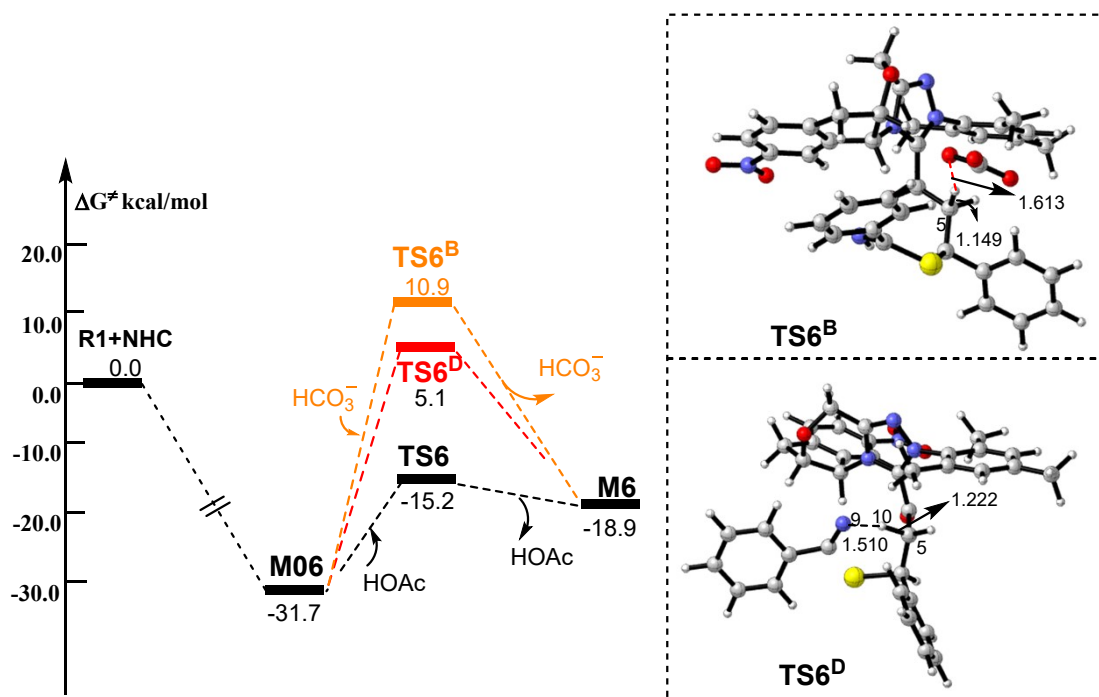


**TS5**

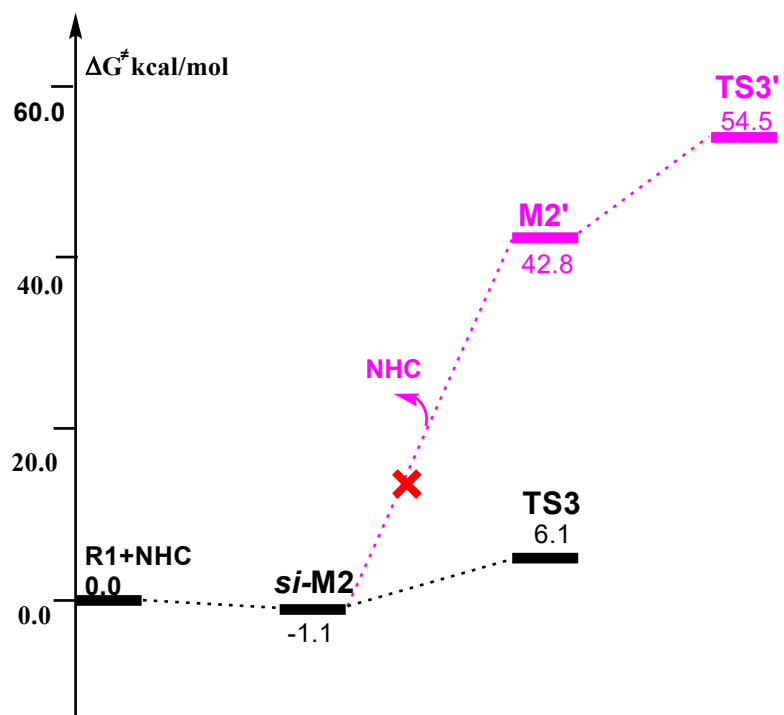
**Table S4. Energies of different conformations of the stereoselective transition states (TS5s).**

species	Dihedral angle C5-C6-S7-C8	Free energies (a.u.)	relative energies (kcal/mol)
<b>TS5R</b>	11.60	-2401.8367411	4.0
<b>TS5R'</b>	70.27	-2401.8289582	8.9
<b>TS5R''</b>	-81.88	-2401.8253568	11.2
<b>TS5R'''</b>	-165.38	-2401.8264793	10.5
<b>TS5S</b>	7.32	-2401.8431944	0.0
<b>TS5S'</b>	66.57	-2401.8369836	3.9
<b>TS5S''</b>	149.99	-2401.8304274	8.0
<b>TS5S'''</b>	-83.36	-2401.8306087	7.9

**Fig. S7** Possible pathways for 1,5-proton transfer. Bond distances are given in Å.



**Fig. S8** The pathways of debromination with/without NHC.



## Coordinates

### NHC

C	5.53451800	-0.11320600	1.21334700
C	4.45849800	-0.75240300	0.58926500
C	3.88155900	-1.89068100	1.13129700
C	4.43226600	-2.37011200	2.31425400
C	5.50781200	-1.76180200	2.95525600
C	6.06606100	-0.61757300	2.39712600
C	5.95162000	1.10771300	0.43760800
C	5.32428700	0.84663400	-0.95082600
C	4.07174900	-0.03120100	-0.67944900
H	3.03610800	-2.38679200	0.67042100
H	5.89234000	-2.18950500	3.87280800
H	6.90571500	-0.13026000	2.88191500
H	5.52939200	2.00502600	0.90583300
H	6.02053100	0.24051900	-1.53618700
H	7.03385200	1.24438000	0.38141000
H	3.85800300	-0.71064700	-1.50743400
N	2.90454600	0.83062700	-0.48809900
O	5.06616100	1.98126300	-1.74390600
C	1.66035800	0.40368900	-0.09898600
C	2.90177300	2.17673700	-0.74881500
N	0.99435300	1.57423700	-0.14199300
N	1.72482700	2.67728700	-0.53955700
C	4.14001200	2.89387100	-1.18660900
H	4.57782700	3.44340200	-0.34245400
H	3.89839100	3.61857300	-1.96582700
C	-0.38179200	1.77047700	0.20684100
C	-0.67548100	2.44589900	1.39400100
C	-1.37867800	1.30280000	-0.65472700
C	-2.01799900	2.64325000	1.71683400
C	-2.70562300	1.51714700	-0.28713500
C	-3.04377800	2.18358000	0.89194800
H	-2.26600200	3.16744500	2.63676100
H	-3.49603500	1.16052900	-0.94383300
C	-4.48914200	2.37659700	1.27046200
N	3.85923000	-3.58340300	2.91258700
O	2.95198900	-4.13523200	2.31665800
O	4.32594300	-3.97068100	3.96988800
H	-5.09329200	2.64846300	0.40050300
H	-4.90998500	1.45411700	1.68451100
H	-4.60234900	3.16018000	2.02328200
C	-1.02669200	0.59920000	-1.93696000
H	-1.92509000	0.40042600	-2.52486800

H	-0.34572300	1.20614600	-2.54239400
H	-0.52414200	-0.35098900	-1.73716600
C	0.42723400	2.93718000	2.29225800
H	0.99467800	3.74017400	1.81259200
H	0.02012700	3.31382800	3.23276700
H	1.13366700	2.13225700	2.51925000

**R1**

C	0.29596000	0.76569600	0.21390500
C	1.06527200	1.86712700	0.22877100
C	2.53051900	1.71892000	0.38236400
C	-1.14753600	0.54926300	0.10220700
C	-1.62671300	-0.70902100	0.50244400
C	-2.06496200	1.48936200	-0.39363600
C	-2.97991100	-1.01237800	0.44370400
C	-3.41715600	1.17693700	-0.46377100
H	-1.72364800	2.45580500	-0.73871400
C	-3.88086200	-0.06633400	-0.03957700
H	-3.33053200	-1.98615700	0.76953600
H	-4.11368200	1.91095600	-0.85569800
H	-0.92279600	-1.44969900	0.87225200
H	-4.93967400	-0.29925800	-0.09241500
Br	0.46715200	3.64925300	0.13077300
H	0.86660000	-0.15684200	0.33479400
O	3.31804800	2.62994600	0.43952000
H	2.85735500	0.66192600	0.44541500

**R2**

C	0.13104900	0.22815600	0.34699400
S	1.82184600	-0.13202000	0.59634600
N	-0.66889300	-0.36923700	-0.47338200
H	-0.12835500	-1.09371700	-0.95057600
C	-0.50899900	1.34661700	1.14887600
C	0.19959800	2.08866700	2.09704900
C	-1.85947800	1.65693000	0.94137200
C	-0.41921700	3.11019200	2.81483800
H	1.24468800	1.84562500	2.25699900
C	-2.47963000	2.67576700	1.65574900
H	-2.40586100	1.07706900	0.20582600
C	-1.76100200	3.41009200	2.59837000
H	0.15244900	3.67456100	3.54677600
H	-3.52790200	2.90019300	1.47651200
H	-2.24352500	4.20775500	3.15663500



**HOAc**

H	1.72054400	-0.80114900	-0.00000700
C	0.09155600	0.12185200	0.00001100
O	0.77851900	-1.03550500	-0.00001700
O	0.63855000	1.19662900	0.00004100
C	-1.39089700	-0.11237400	-0.00000400
H	-1.67201100	-0.69301400	0.88180800
H	-1.91045900	0.84385000	0.00006100
H	-1.67200800	-0.69288900	-0.88190000

**HCO<sub>3</sub><sup>-</sup>**

H	1.67806800	-0.43436400	0.00002300
C	-0.12892700	0.08075400	0.00000300
O	-1.29368100	-0.33372900	-0.00001300
O	0.34572600	1.23594000	0.00000800
O	0.85993600	-0.94507300	0.00001700

**H<sub>2</sub>CO<sub>3</sub>**

H	-1.52652600	-1.18854900	3.13453000
H	-2.46910000	0.08228500	1.81114200
C	-3.38074600	-1.43350000	2.61484900
O	-4.38343400	-2.07149500	2.71345400
O	-3.36055800	-0.22651300	2.01839000
O	-2.20391000	-1.87621400	3.09525000

**H<sub>2</sub>O**

O	0.02507700	0.00000000	0.01796700
H	0.06642800	0.00000000	0.98026500
H	0.94856500	0.00000000	-0.25635700

**HBr**

H	0.00000000	0.00000000	-1.37264400
Br	0.00000000	0.00000000	0.03921800

**re-TS1**

C	-4.99309000	0.50876400	0.43545300
C	-3.64436800	0.17090800	0.52300400
C	-3.17244000	-1.07168600	0.12102400
C	-4.11622400	-1.95817200	-0.37881500
C	-5.47391400	-1.65966300	-0.47302000
C	-5.91853900	-0.41028500	-0.05866300
C	-5.23070400	1.91163900	0.92738100
C	-3.82284100	2.53704700	1.08037300
C	-2.81870500	1.32583300	1.05099100

H	-2.12592500	-1.34818300	0.21678800
H	-6.15533400	-2.40034600	-0.87278800
H	-6.97097800	-0.15546300	-0.13174600
H	-5.84042600	2.51244800	0.24555800
H	-3.72729300	3.07997300	2.02112400
H	-5.74711700	1.89575500	1.89296100
H	-2.41360800	1.11379300	2.04294100
N	-1.70155400	1.61013600	0.16008300
O	-3.55197600	3.51188900	0.08581700
C	-0.44251000	1.11069800	0.19581100
C	-1.89626600	2.28331500	-1.01802700
N	0.04625000	1.50152400	-0.98777800
N	-0.83051600	2.24190200	-1.75407400
C	-3.19902400	2.99592000	-1.18628100
H	-3.97195900	2.32371400	-1.58462300
H	-3.08781900	3.83951600	-1.86848100
C	1.30848000	1.10538200	-1.54219100
C	1.48446500	-0.24554500	-1.86388000
C	2.29719900	2.07051700	-1.73562400
C	2.72122000	-0.62001000	-2.38442500
C	3.51415300	1.64593400	-2.27039900
C	3.74159500	0.30951100	-2.59862500
H	2.89600000	-1.66613500	-2.62489300
H	4.30352500	2.37779500	-2.42399000
C	5.06144800	-0.13952600	-3.16734600
C	2.20090100	-1.30872700	1.30070000
C	1.57225800	-0.15925600	1.55279600
H	1.51426100	-2.15641900	1.32153100
C	3.60565800	-1.63255900	1.02446200
C	4.01674800	-2.95706400	1.23397500
C	4.53882500	-0.71529200	0.51837400
C	5.32554100	-3.35060100	0.98242900
H	3.29548600	-3.67988300	1.60561500
C	5.84642200	-1.11317100	0.26068100
H	4.23812900	0.30337800	0.30714200
C	6.24762300	-2.42679800	0.49637800
H	5.62351600	-4.37901400	1.16110400
H	6.55443700	-0.39104100	-0.13530400
H	7.27066500	-2.72925400	0.29496800
Br	2.39441100	1.53628600	1.74840100
C	0.08456000	-0.11417600	1.81701200
H	-0.17282500	0.72590900	2.49325300
O	-0.60134200	-1.14139100	1.77239600
N	-3.65598600	-3.27359900	-0.84682500

O	-2.45550900	-3.47128100	-0.89156100
O	-4.50346800	-4.08845300	-1.17007900
H	5.83062200	0.62704800	-3.04403900
H	4.97268300	-0.35401100	-4.23780800
H	5.40486600	-1.05444900	-2.67550900
C	2.05891900	3.50484200	-1.35285100
H	1.25442400	3.94703900	-1.94754800
H	1.76663200	3.57214400	-0.30007500
H	2.96452000	4.09726000	-1.49814700
C	0.38213700	-1.25207500	-1.65545700
H	0.15422900	-1.39510800	-0.59261700
H	-0.54002100	-0.93108100	-2.15269400
H	0.66742000	-2.22096100	-2.07036600

**re-M1**

C	4.13161300	-4.44549000	0.23130900
C	3.44341800	-3.28074600	-0.10466200
C	2.95326400	-3.05812000	-1.38515600
C	3.17423200	-4.07067000	-2.30889400
C	3.86913800	-5.24224200	-2.01563800
C	4.35615200	-5.43154700	-0.72820000
C	4.53898800	-4.43060500	1.68086000
C	3.72054700	-3.28349800	2.31086700
C	3.30128100	-2.37254900	1.10183400
H	2.45365900	-2.12271000	-1.63309300
H	4.00784300	-5.98689200	-2.78949500
H	4.89225000	-6.34076100	-0.47597500
H	4.33849000	-5.37075200	2.20277600
H	4.30521900	-2.71421000	3.03428900
H	5.61126600	-4.22613400	1.77383300
H	3.93039200	-1.48409600	1.02006300
N	1.91955600	-1.93614000	1.27587600
O	2.61073800	-3.76633600	3.05739300
C	1.31280200	-0.79672300	0.89370000
C	0.96008500	-2.80075500	1.72128000
N	0.01239100	-1.03238900	1.08709600
N	-0.22227000	-2.27702400	1.62126000
C	1.44712000	-4.08409500	2.31297600
H	1.64368700	-4.82867300	1.52986500
H	0.70964500	-4.48920400	3.00616100
C	-1.10972300	-0.20531000	0.72719700
C	-1.40320400	-0.06324500	-0.63387800
C	-1.86519700	0.37811900	1.74413200
C	-2.47082200	0.76688400	-0.96417100

C	-2.93296500	1.18924500	1.35735800
C	-3.23765600	1.40549100	0.01376500
H	-2.70960400	0.91970300	-2.01379700
H	-3.53160000	1.66896600	2.12769800
C	-4.35056800	2.33311700	-0.39323500
C	1.04925200	2.24752300	-0.99932900
C	1.32441500	1.62174400	0.14162600
H	1.47078200	1.72110800	-1.85736000
C	0.30290500	3.48791300	-1.25819700
C	-0.79107200	3.88985100	-0.47858500
C	0.65856200	4.26808600	-2.36658500
C	-1.48153400	5.05859700	-0.78298800
H	-1.10546300	3.27746100	0.35945600
C	-0.02994200	5.43842900	-2.66627800
H	1.49031600	3.95128900	-2.98989800
C	-1.10193200	5.83967600	-1.87265300
H	-2.32528100	5.35692300	-0.16760300
H	0.26662000	6.03455200	-3.52369100
H	-1.64363900	6.75094200	-2.10621800
Br	0.92868800	2.30564000	1.87654600
C	2.13230700	0.32071800	0.18482000
H	2.93303400	0.53070700	0.94524300
O	2.53819500	-0.15277700	-0.97586500
N	2.63450800	-3.90432700	-3.66657600
O	1.89861000	-2.95721100	-3.87195500
O	2.94606900	-4.73262500	-4.50607700
H	-3.94070600	3.21667000	-0.89495300
H	-4.92900300	2.66884700	0.47044700
H	-5.03378900	1.84763200	-1.09621400
C	-1.54929500	0.13407100	3.19373400
H	-1.78645700	-0.89671500	3.47488300
H	-0.48874800	0.30237900	3.39982500
H	-2.13094200	0.80521400	3.82889800
C	-0.60660200	-0.78594200	-1.68637700
H	0.44942700	-0.48602200	-1.68512400
H	-0.64067500	-1.86893200	-1.51634100
H	-1.02214400	-0.59079300	-2.67685000

**si-TS1**

C	5.05110600	-0.08921700	0.27917300
C	3.68314700	0.14382100	0.40529100
C	3.06861200	1.23314700	-0.19748100
C	3.89109400	2.09769100	-0.90608700
C	5.26606700	1.91301100	-1.02928900

C	5.85195500	0.80234600	-0.43371800
C	5.45091100	-1.36652400	0.96833900
C	4.12625100	-2.02802600	1.43048200
C	3.00492300	-0.94800300	1.20148600
H	1.99676800	1.40809800	-0.14740000
H	5.84956600	2.62630200	-1.59827000
H	6.91850800	0.63031600	-0.53743100
H	6.00325600	-2.04450700	0.30939600
H	4.16690800	-2.28507700	2.48895000
H	6.09673600	-1.16072900	1.82776000
H	2.61098400	-0.58833700	2.15591300
N	1.88314900	-1.50047400	0.46057900
O	3.87098100	-3.26487900	0.78586500
C	0.61274700	-1.03427900	0.43281500
C	2.02419500	-2.51415100	-0.44743400
N	0.04617900	-1.82368000	-0.48566500
N	0.89769000	-2.75543100	-1.04371300
C	3.36519100	-3.16638100	-0.53374900
H	4.03690800	-2.58378700	-1.18153000
H	3.28204200	-4.17629100	-0.93624800
C	-1.32446900	-1.76604400	-0.90601000
C	-1.61650900	-1.20428600	-2.14953600
C	-2.30545000	-2.25843900	-0.04051600
C	-2.95819000	-1.14508900	-2.52858000
C	-3.63111100	-2.16378800	-0.45850900
C	-3.97374100	-1.61846400	-1.69757800
H	-3.21316300	-0.70854500	-3.49138800
H	-4.41759800	-2.52044600	0.20255600
C	-5.41837500	-1.54220400	-2.11436300
C	-2.43928200	0.56105500	1.88612600
C	-1.23535500	0.73045300	1.33869500
H	-2.38354000	0.01865700	2.83131800
C	-3.78166800	0.97721300	1.45983000
C	-4.77102600	1.10619000	2.44534400
C	-4.13703500	1.19812400	0.12167800
C	-6.06784200	1.48012600	2.11331000
H	-4.51054400	0.91507700	3.48298900
C	-5.43734500	1.56376300	-0.20942800
H	-3.40168700	1.06241300	-0.66208700
C	-6.40551600	1.71212800	0.78221000
H	-6.81642700	1.58447600	2.89243100
H	-5.69634500	1.72654500	-1.25153200
H	-7.41835100	1.99968900	0.51764000
Br	-0.85197500	1.72947500	-0.22742700

C	0.01808500	0.19214500	1.99464400
H	0.88270700	0.86071600	1.79411500
O	-0.03303100	-0.49727500	3.01725800
N	3.27289900	3.25051500	-1.57719700
O	2.05763600	3.32847500	-1.56012800
O	4.01196300	4.05667600	-2.11415600
H	-5.78066900	-2.52167100	-2.44513600
H	-5.55911500	-0.84006100	-2.93987600
H	-6.04828400	-1.22220800	-1.27941700
C	-1.93358500	-2.86415300	1.28607500
H	-1.24432200	-3.70434600	1.14721700
H	-1.43647800	-2.14087300	1.94309100
H	-2.82441200	-3.23582000	1.79685100
C	-0.52059600	-0.65941400	-3.02272100
H	0.00756100	0.14529900	-2.50018600
H	0.21100600	-1.43298800	-3.27355000
H	-0.92993200	-0.25409100	-3.95012100

**si-M1**

C	5.77207400	-0.56194700	0.52188800
C	4.46819000	-0.77956300	0.96001800
C	4.14926000	-0.86190500	2.30960400
C	5.19641600	-0.67826600	3.20105700
C	6.51248000	-0.44940100	2.80187000
C	6.80504000	-0.39702300	1.44529500
C	5.85195900	-0.57567100	-0.98077500
C	4.38579400	-0.65055400	-1.47723100
C	3.50871000	-0.92359100	-0.19656300
H	3.13515300	-1.11232500	2.61485000
H	7.28133900	-0.32060900	3.55344200
H	7.82514900	-0.22804200	1.11496600
H	6.34451200	0.31111700	-1.39333800
H	4.24539600	-1.46773100	-2.18503000
H	6.41961700	-1.44493100	-1.32725600
H	3.02350500	-1.90041800	-0.19218800
N	2.42168200	0.06562300	-0.10407400
O	4.01209400	0.50730000	-2.20938200
C	1.21021800	-0.03013000	0.46639300
C	2.53235200	1.32893600	-0.61804600
N	0.64400000	1.15940500	0.27370200
N	1.45426100	2.02508300	-0.40886200
C	3.76036600	1.64168900	-1.40493500
H	4.60564400	1.87122700	-0.74012700
H	3.58493500	2.49488400	-2.06059900

C	-0.67234300	1.55051600	0.69792100
C	-0.84954400	1.94140700	2.02731600
C	-1.70817700	1.50691900	-0.23858300
C	-2.14172300	2.28354800	2.42267300
C	-2.98034100	1.86182700	0.20774100
C	-3.21524100	2.24183500	1.53109800
H	-2.31198900	2.59190400	3.45117600
H	-3.80839500	1.83384500	-0.49655500
C	-4.60764900	2.57467500	1.99723100
C	-1.73163000	-1.79967800	0.35783300
C	-0.41496800	-1.80693600	0.14172200
H	-2.00695600	-1.39012300	1.33156200
C	-2.87757600	-2.16944600	-0.48948100
C	-2.83635300	-3.13993800	-1.49956700
C	-4.09279400	-1.51142500	-0.24533700
C	-3.97031500	-3.41671600	-2.25629000
H	-1.92282500	-3.69052900	-1.68316100
C	-5.22175800	-1.78271600	-1.00910000
H	-4.14074000	-0.77547800	0.55346200
C	-5.16231500	-2.73555900	-2.02326800
H	-3.92135100	-4.17713200	-3.02969000
H	-6.14977000	-1.25647100	-0.80755100
H	-6.04261600	-2.95646800	-2.61871500
Br	0.38755500	-2.35545700	-1.49906100
C	0.64574300	-1.31239000	1.15258200
H	0.02447200	-0.91071300	1.99529900
O	1.61057200	-2.14744800	1.44606500
N	4.90541800	-0.72744700	4.64083200
O	3.73878100	-0.79520100	4.98158800
O	5.84847300	-0.68765600	5.41332300
H	-4.59179800	3.34095500	2.77631900
H	-5.22812900	2.93327500	1.17264200
H	-5.09515700	1.68855000	2.41856900
C	-1.45711300	1.09529000	-1.66349200
H	-2.39572700	1.04924400	-2.21865600
H	-0.79345200	1.80775000	-2.16457200
H	-0.98298200	0.10994300	-1.72159100
C	0.30933200	1.99055200	2.98639500
H	1.15908200	2.52602000	2.55164200
H	0.02111600	2.49901400	3.90813100
H	0.65213200	0.98458300	3.25463800

**re-M02**

C	-2.15039400	3.28374600	1.11198600
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C	-1.20350600	2.54794000	0.39674000
C	-0.30129000	3.15498300	-0.46769300
C	-0.40723100	4.53570200	-0.58694400
C	-1.34208000	5.30215200	0.10311100
C	-2.22649400	4.66640400	0.96640500
C	-2.98983900	2.38611100	1.98297300
C	-2.23537400	1.04232600	2.00317600
C	-1.35398100	1.06958900	0.70546900
H	0.47408400	2.59949700	-0.99802900
H	-1.35984700	6.37553400	-0.03850100
H	-2.95847400	5.24380300	1.52157500
H	-3.12198500	2.76315400	3.00051300
H	-2.91538900	0.18839600	1.98554500
H	-3.98647800	2.25338500	1.54764600
H	-1.86093100	0.53931500	-0.10411400
N	-0.08799900	0.39380000	0.96486400
O	-1.47152000	0.87218400	3.19057800
C	0.61857800	-0.49816100	0.24911200
C	0.58259800	0.60963200	2.13688800
N	1.68752100	-0.77911400	0.99502500
N	1.66927900	-0.09571000	2.18377200
C	-0.14856400	1.39066800	3.17910900
H	-0.12267400	2.46692200	2.96966300
H	0.28635000	1.20719200	4.16139500
C	2.84755500	-1.59437100	0.70944500
C	4.08022800	-0.94151100	0.59395400
C	2.71135300	-2.98312400	0.63991900
C	5.19861000	-1.73808400	0.35045100
C	3.86410000	-3.72773000	0.39984700
C	5.11088000	-3.12486300	0.23953100
H	6.16623600	-1.25390500	0.24401800
H	3.77958200	-4.80949600	0.33318000
C	6.33204700	-3.94872300	-0.07041500
C	-1.72182700	-2.21194800	0.18092800
C	-1.07942700	-1.90477600	-0.95081900
H	-1.23766000	-1.87541200	1.09849400
C	-2.96121500	-2.97170800	0.42650000
C	-4.06121700	-2.97746300	-0.44183200
C	-3.05966000	-3.66915200	1.63899500
C	-5.20883700	-3.69248500	-0.11638900
H	-4.02105300	-2.41933400	-1.36890800
C	-4.20348700	-4.39117900	1.95715700
H	-2.22153400	-3.65086600	2.33103800
C	-5.28294500	-4.40637100	1.07719200



H	-6.05260000	-3.68629900	-0.79901700
H	-4.25440500	-4.93554000	2.89457900
H	-6.17968800	-4.96578200	1.32341000
Br	-1.63452600	-2.51749300	-2.65264200
C	0.19203800	-1.06673200	-1.09363100
H	1.78100900	-1.11831400	-2.24595900
O	1.19268800	-1.78859900	-1.67988400
N	0.52297900	5.22690600	-1.49446700
O	1.28049600	4.54274300	-2.15559600
O	0.47655400	6.44500800	-1.53223700
H	6.48295700	-4.01654600	-1.15294500
H	6.23442200	-4.96669800	0.31466700
H	7.23240400	-3.50262200	0.35941800
C	1.38363200	-3.66929900	0.78633800
H	0.75732600	-3.18558100	1.54266400
H	0.84734200	-3.64838400	-0.16703700
H	1.52457000	-4.71117700	1.08134500
C	4.23135800	0.54842600	0.75113500
H	3.41146700	1.08978200	0.27374500
H	4.25502700	0.82231600	1.81096200
H	5.17002800	0.87466600	0.29728800
C	2.56544700	0.94320400	-2.29730700
O	2.54280500	-0.14149500	-2.94615600
O	1.84684000	1.19802400	-1.29666400
H	-0.07339600	-0.17309800	-1.68408700
C	3.53746000	2.00367800	-2.78703500
H	3.21488900	2.35995100	-3.76963900
H	3.57889300	2.84744100	-2.09872400
H	4.52944600	1.56176000	-2.91053600

**re-TS2**

C	-2.06594000	3.43180000	1.51230000
C	-1.30790500	2.50224200	0.79961500
C	-0.58503200	2.86200900	-0.33299200
C	-0.66618100	4.19643200	-0.71325300
C	-1.42943200	5.14494800	-0.03824000
C	-2.13767500	4.75798100	1.09236400
C	-2.72421000	2.79226800	2.70672700
C	-2.04484000	1.41293500	2.85393300
C	-1.40619900	1.13464100	1.44735800
H	0.02050400	2.16827300	-0.91513700
H	-1.44707800	6.16595200	-0.39865000
H	-2.72532900	5.48512200	1.64338900
H	-2.60844000	3.37110800	3.62761400

H	-2.76551100	0.63114000	3.09680700
H	-3.79827300	2.66816200	2.53073700
H	-2.05944000	0.47756100	0.87586300
N	-0.10167700	0.49528000	1.58788900
O	-1.11154200	1.37899200	3.92124400
C	0.56436300	-0.42798500	0.84032300
C	0.74482800	0.91078200	2.58710900
N	1.77513300	-0.51478900	1.42981600
N	1.88531800	0.30956500	2.52384200
C	0.18810900	1.84642100	3.60794900
H	0.17713700	2.87985200	3.23622200
H	0.78728500	1.80559100	4.51801900
C	2.94650000	-1.26755800	1.05444000
C	3.92910600	-0.61924200	0.31077300
C	3.07831600	-2.57851100	1.51861000
C	5.08550400	-1.34301400	0.01125800
C	4.25095200	-3.25436300	1.20243500
C	5.26219400	-2.65357200	0.44605500
H	5.86409900	-0.86359100	-0.57669500
H	4.37836700	-4.27744200	1.54854700
C	6.50641700	-3.42570400	0.09395500
C	-1.85926000	-2.47111300	-0.27871900
C	-1.27270200	-1.32443100	-0.63796700
H	-1.16375300	-3.14244700	0.22705200
C	-3.19820000	-3.04687800	-0.47575200
C	-4.36211900	-2.31879400	-0.76606500
C	-3.31072100	-4.43714200	-0.31276700
C	-5.58330100	-2.96914800	-0.90857800
H	-4.31915200	-1.24393800	-0.87686100
C	-4.52958700	-5.08517700	-0.46327900
H	-2.42025700	-5.01228400	-0.07371900
C	-5.67414600	-4.35088700	-0.76442400
H	-6.47227100	-2.38780100	-1.13277200
H	-4.58643500	-6.16229600	-0.34169900
H	-6.63052400	-4.85074500	-0.88108600
Br	-2.17118500	0.02138800	-1.66980700
C	0.19091900	-1.05745700	-0.42059500
H	1.59554000	-1.94472700	-1.37609200
O	0.96992700	-2.19977900	-0.65367800
N	0.11086700	4.63811500	-1.88205400
O	0.91034100	3.85415400	-2.35583000
O	-0.08724900	5.76697500	-2.29951600
H	6.31728800	-4.10109400	-0.74700600
H	6.84385800	-4.03661900	0.93573500

H	7.32180700	-2.75792800	-0.19346400
C	1.97081800	-3.22930000	2.29544000
H	1.65317000	-2.60907700	3.13978400
H	1.10686600	-3.38084100	1.63974700
H	2.28576800	-4.20025100	2.68243100
C	3.77267400	0.81246900	-0.12332600
H	2.75610600	1.03130100	-0.46276800
H	3.99964400	1.49346300	0.70457800
H	4.45797200	1.03669000	-0.94375900
C	2.02961200	0.15406300	-2.77831400
O	2.47853500	-0.97365400	-2.53202600
O	0.99049700	0.66656300	-2.20662600
H	0.56855300	-0.13417100	-1.32680900
C	2.69467800	1.04981700	-3.79719500
H	1.97816300	1.28887200	-4.58734700
H	2.97232000	1.99420800	-3.32201000
H	3.57292000	0.56558500	-4.22314200

**re-TS2<sup>B</sup>**

C	3.75879200	-4.19097300	0.21569500
C	3.00761400	-3.07648100	-0.15462400
C	2.48913400	-2.93208400	-1.43413600
C	2.72817500	-3.97772900	-2.31650400
C	3.47229400	-5.10852000	-1.98294000
C	4.00049400	-5.21266100	-0.70195000
C	4.22044600	-4.06889400	1.64519600
C	3.37401300	-2.92189300	2.24271200
C	2.86271600	-2.11344400	1.00330000
H	1.96363700	-2.02041600	-1.71207800
H	3.62206900	-5.88346800	-2.72405900
H	4.58483400	-6.08397800	-0.42340400
H	4.09127300	-4.98519200	2.22885600
H	3.96013900	-2.26968800	2.89065500
H	5.28318800	-3.80413800	1.67396100
H	3.44739000	-1.20663800	0.85339600
N	1.47320900	-1.71967300	1.19980000
O	2.33322800	-3.41903400	3.08123300
C	0.80656600	-0.61427800	0.77931400
C	0.57597600	-2.55505200	1.79685500
N	-0.47574300	-0.86763600	1.11146300
N	-0.62559800	-2.06865600	1.77447100
C	1.13585500	-3.78899400	2.42564000
H	1.30440900	-4.56707400	1.66745400
H	0.44864500	-4.17835100	3.17777700

C	-1.63540600	-0.16995200	0.63924300
C	-1.84429500	-0.10648900	-0.74409900
C	-2.49096000	0.42227900	1.56826600
C	-2.92592500	0.65238000	-1.18596200
C	-3.57389900	1.14801100	1.07434300
C	-3.79098500	1.29234400	-0.29550900
H	-3.09779400	0.74561400	-2.25579700
H	-4.24583300	1.63290900	1.77848000
C	-4.91558400	2.14498000	-0.82097300
C	0.59675500	2.25064000	-1.40002600
C	0.69031700	1.69937500	-0.18446000
H	1.15674200	1.67808900	-2.13912100
C	-0.08203000	3.45908500	-1.88169400
C	-1.26390700	3.97436900	-1.32453700
C	0.44069800	4.09060100	-3.02071300
C	-1.86920500	5.10218700	-1.87224700
H	-1.70696400	3.48095900	-0.46611800
C	-0.16497600	5.21550300	-3.56554600
H	1.34394600	3.68778600	-3.47075900
C	-1.32437100	5.73059500	-2.99008900
H	-2.78024500	5.49022400	-1.42478800
H	0.26791500	5.68899000	-4.44184800
H	-1.80196800	6.60936700	-3.41283800
Br	0.02606900	2.55213400	1.39426200
C	1.50507500	0.48327500	0.09723800
H	3.60088700	0.36438400	-0.62255600
O	2.21197400	-0.01087000	-0.97315600
N	2.15536700	-3.89857700	-3.66630600
O	1.40380800	-2.97323100	-3.91339400
O	2.45245600	-4.77375100	-4.46489300
H	-4.51762000	3.04417800	-1.30401600
H	-5.58801100	2.46012300	-0.01948600
H	-5.50429400	1.60877400	-1.57130800
C	-2.21646400	0.31374300	3.04190200
H	-2.31583100	-0.71812300	3.39071200
H	-1.19367300	0.63820600	3.25788200
H	-2.90533100	0.94264000	3.61008000
C	-0.95993300	-0.84618700	-1.71488600
H	0.06672700	-0.46142800	-1.73157100
H	-0.91565500	-1.91062200	-1.45460500
H	-1.36502100	-0.76758600	-2.72596800
H	2.41484300	0.79289800	0.97854800
C	4.65525900	0.90453600	0.99292400
O	5.75152200	1.19042800	1.46641000

O	4. 57031000	0. 57477400	-0. 31059200
O	3. 54883500	0. 85864100	1. 68452600

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

C	4. 27803200	-2. 52497500	0. 27832800
C	3. 19923400	-1. 87018700	-0. 31417100
C	2. 79748400	-2. 15903800	-1. 61154200
C	3. 51464700	-3. 14035900	-2. 28302900
C	4. 59501900	-3. 81490800	-1. 72057600
C	4. 98330700	-3. 50051300	-0. 42416900
C	4. 51945100	-2. 02131900	1. 67552600
C	3. 31143700	-1. 11208800	2. 00503400
C	2. 59114200	-0. 85463400	0. 62865800
H	1. 96895700	-1. 64905400	-2. 09024500
H	5. 11037800	-4. 57095700	-2. 29981100
H	5. 82204300	-4. 01536900	0. 03322900
H	4. 59811200	-2. 82578400	2. 41358000
H	3. 63337100	-0. 16113400	2. 43084200
H	5. 45229300	-1. 44999300	1. 72105700
H	2. 79078000	0. 16127900	0. 28699000
N	1. 14640100	-1. 02125500	0. 76966600
O	2. 46709500	-1. 67312200	2. 99513200
C	0. 10715400	-0. 53403300	0. 01284100
C	0. 63319600	-1. 99892200	1. 58274000
N	-0. 97019900	-1. 22881500	0. 44578000
N	-0. 63904800	-2. 14382700	1. 42762000
C	1. 58196900	-2. 66949200	2. 51994900
H	2. 11832100	-3. 48470800	2. 01281500
H	1. 04482900	-3. 08186200	3. 37462800
C	-2. 34906000	-1. 09317100	0. 07589700
C	-2. 99694700	-2. 21428200	-0. 45444300
C	-2. 99888700	0. 12357600	0. 28913200
C	-4. 34862100	-2. 08992800	-0. 76407500
C	-4. 35282600	0. 19530600	-0. 03764000
C	-5. 04229600	-0. 89534300	-0. 56253400
H	-4. 87049600	-2. 94665400	-1. 18497000
H	-4. 87676300	1. 13502400	0. 11783400
C	-6. 50074500	-0. 79390200	-0. 92496200
C	1. 33595200	2. 25298300	0. 04726400
C	1. 20805800	1. 43160600	-1. 00233700
H	0. 62583500	2. 05735700	0. 85269800
C	2. 31766700	3. 31198200	0. 34018000
C	2. 71666600	3. 46892100	1. 67541500
C	2. 84279100	4. 18238000	-0. 62403200

C	3.64640500	4.43690000	2.03518200
H	2.28968900	2.81736400	2.43425300
C	3.76673900	5.15613200	-0.26028100
H	2.51652900	4.10586700	-1.65404000
C	4.17809300	5.28254800	1.06434100
H	3.94887100	4.53718600	3.07286800
H	4.16016200	5.82802900	-1.01651300
H	4.89961600	6.04497000	1.34083300
Br	2.39669600	1.50650300	-2.49910400
C	0.19111400	0.35363200	-1.10861400
H	0.06070200	-0.18839400	-2.12931100
O	-0.98772100	0.63996900	-1.86310600
N	3.10895200	-3.48509600	-3.65318200
O	2.14599000	-2.90490700	-4.11995500
O	3.75743100	-4.33375100	-4.23946700
H	-7.08330200	-1.58482100	-0.44294200
H	-6.64230100	-0.89694200	-2.00556500
H	-6.91893100	0.16863200	-0.62203700
C	-2.26639500	1.32609400	0.81445200
H	-1.62425200	1.06918800	1.66421700
H	-1.65332800	1.74018300	0.00564300
H	-2.97212000	2.09174300	1.14390300
C	-2.26661600	-3.50779700	-0.69955700
H	-1.29859300	-3.33469400	-1.18078700
H	-2.07447700	-4.04040300	0.23633800
H	-2.85742400	-4.15629600	-1.34961500

**re-TS2<sup>W</sup>**

C	3.67719700	-4.31745900	0.59175000
C	3.02918100	-3.18795400	0.09179700
C	2.55932300	-3.13824500	-1.21344400
C	2.75860600	-4.27197100	-1.98993400
C	3.40769200	-5.41317500	-1.52683800
C	3.87573600	-5.43408000	-0.21819900
C	4.07417100	-4.11491700	2.02985200
C	3.32023600	-2.84406800	2.48484200
C	2.90256900	-2.11651000	1.15567300
H	2.07344500	-2.25423800	-1.61528400
H	3.52777800	-6.26225900	-2.18841800
H	4.37606500	-6.31705000	0.16649300
H	3.81839800	-4.96112200	2.67445900
H	3.95566100	-2.18860300	3.08026500
H	5.15540800	-3.95985600	2.10806400
H	3.54810000	-1.24553800	0.96634300

N	1.51691200	-1.65382300	1.25111200
O	2.22772700	-3.14658300	3.34272100
C	0.89859800	-0.58651500	0.69615200
C	0.56683400	-2.40044600	1.88775700
N	-0.39928200	-0.76205100	0.99170500
N	-0.61289900	-1.87644600	1.76098400
C	1.04524900	-3.56554400	2.68965900
H	1.21349000	-4.44272100	2.04933000
H	0.30940300	-3.82157800	3.45291300
C	-1.53346600	-0.04215200	0.47917000
C	-1.77949700	-0.09838200	-0.89866200
C	-2.35770800	0.63624800	1.37763100
C	-2.87100400	0.62091900	-1.37685400
C	-3.44516300	1.33058100	0.84587200
C	-3.70675900	1.34546300	-0.52342700
H	-3.07772000	0.61208900	-2.44425100
H	-4.09532100	1.88051900	1.52173200
C	-4.84486100	2.14954100	-1.09138400
C	0.62255300	2.29060300	-1.46957000
C	0.83786500	1.72975700	-0.27738400
H	1.05462500	1.73290300	-2.30019800
C	-0.10320500	3.52955700	-1.79766600
C	-1.27716200	3.89654300	-1.12476300
C	0.34114400	4.33276200	-2.85575300
C	-1.96039000	5.05558400	-1.47643800
H	-1.65529800	3.26547900	-0.32781400
C	-0.34271800	5.49295800	-3.20488200
H	1.23681200	4.04564300	-3.39995700
C	-1.49455400	5.86063000	-2.51336200
H	-2.86497800	5.32623600	-0.93986000
H	0.02221300	6.10937800	-4.02059300
H	-2.03053000	6.76449900	-2.78548000
Br	0.37487700	2.58421800	1.36609900
C	1.61424500	0.48404900	-0.03227900
H	3.20273300	0.12832800	-0.90632300
O	2.24140200	-0.04555300	-1.17791700
N	2.24079500	-4.27059500	-3.36571000
O	1.58510600	-3.30849400	-3.72342500
O	2.49095600	-5.23552700	-4.06706700
H	-4.45854100	2.99133300	-1.67641800
H	-5.48638900	2.54934200	-0.30299500
H	-5.46183500	1.54333500	-1.76093600
C	-2.09770300	0.61390200	2.85832200
H	-2.47164600	-0.31430600	3.30169600

H	-1.02922500	0.67973200	3.07661500
H	-2.59951300	1.45302400	3.34497800
C	-0.92157500	-0.91749400	-1.82640800
H	0.07769700	-0.48914500	-1.95660000
H	-0.80232300	-1.93876600	-1.44799100
H	-1.38734600	-0.98167800	-2.81139200
O	4.06256300	0.51313500	0.43420300
H	4.53555200	1.35126900	0.42936900
H	2.69123700	0.73070900	0.58029000

**re-M2**

C	4.03049600	-3.63168700	-3.85967800
C	3.46220300	-2.35794400	-3.83679800
C	3.90292200	-1.35716600	-4.69497200
C	4.91507000	-1.69178100	-5.58360500
C	5.48774800	-2.95963600	-5.64660800
C	5.04104800	-3.94004200	-4.76991200
C	3.43957800	-4.51834400	-2.79697600
C	2.33724700	-3.67414900	-2.10864900
C	2.40802600	-2.23801500	-2.75774400
H	3.49123700	-0.35462100	-4.67891300
H	6.27408800	-3.15331400	-6.36568900
H	5.48373900	-4.93081300	-4.79230000
H	3.01487100	-5.44100400	-3.20732200
H	2.52714500	-3.58379300	-1.03868500
H	4.20352200	-4.81954900	-2.07393400
H	2.71555700	-1.51857000	-2.00015600
N	1.09434200	-1.84270900	-3.26228800
O	1.05955400	-4.27617300	-2.18501900
C	0.68945500	-0.60933400	-3.75750700
C	0.22905400	-2.78025800	-3.78996500
N	-0.42169700	-0.90321100	-4.51564900
N	-0.70597900	-2.26399000	-4.50524100
C	0.48892100	-4.21505900	-3.47460200
H	1.15417100	-4.65581100	-4.23248500
H	-0.44438600	-4.77932800	-3.46397600
C	-1.47295700	0.02394300	-4.80086800
C	-1.64583900	0.46658100	-6.11490200
C	-2.29248600	0.45202400	-3.75106000
C	-2.68226900	1.36248900	-6.36942300
C	-3.31188000	1.35662400	-4.05069700
C	-3.52063000	1.81951300	-5.35005700
H	-2.83604100	1.71716000	-7.38606300
H	-3.96385600	1.69887300	-3.25024400



C	-4.61124200	2.81585900	-5.64554200
C	3.28746600	1.77403000	-2.80942500
C	2.19258800	1.02199600	-2.59373500
H	3.49881000	1.91702800	-3.87043200
C	4.24772300	2.40509900	-1.89730900
C	5.57332300	2.52955900	-2.34231600
C	3.91687000	2.92543400	-0.63802400
C	6.54580300	3.11476900	-1.54156400
H	5.83470300	2.15118900	-3.32756000
C	4.89103000	3.51583300	0.15931600
H	2.89201200	2.88011700	-0.29013700
C	6.20887700	3.60692900	-0.28253600
H	7.56657700	3.19145300	-1.90293200
H	4.61442900	3.91698200	1.12960400
H	6.96488000	4.06828500	0.34505500
Br	1.67969100	0.48731800	-0.79751300
C	1.25926800	0.63218800	-3.62294300
O	1.00012900	1.54503900	-4.64133200
N	5.42777700	-0.64595400	-6.47934600
O	4.99327700	0.48399000	-6.34015300
O	6.26318900	-0.96653900	-7.30641400
H	-5.40709400	2.76632400	-4.89839000
H	-5.05394800	2.64099700	-6.62962800
H	-4.21709100	3.83791500	-5.64142300
C	-2.08516200	-0.06218600	-2.35119300
H	-2.84931600	0.33334600	-1.67874900
H	-2.14411100	-1.15541700	-2.32680600
H	-1.10362800	0.22073300	-1.95429200
C	-0.70864700	0.00134800	-7.19299500
H	0.30444700	0.35623000	-6.97767400
H	-0.67197500	-1.09107500	-7.24057700
H	-1.01479800	0.38303400	-8.16919800
H	0.43328900	2.24982700	-4.29751400

**si-M02**

C	2.11956400	-4.37890200	-0.92561600
C	1.76298500	-3.03259000	-1.00418400
C	1.95129100	-2.28909000	-2.16502000
C	2.49226200	-2.97722500	-3.24505300
C	2.84028200	-4.32534500	-3.20825200
C	2.65928300	-5.03468400	-2.02945700
C	1.86611700	-4.94001600	0.44655500
C	1.09495700	-3.83932800	1.20943300
C	1.23610000	-2.54023800	0.32661600

H	1.67267100	-1.23696500	-2.24681000
H	3.25126600	-4.79104500	-4.09547400
H	2.93609800	-6.08262300	-1.97344000
H	1.28182500	-5.86566100	0.43212000
H	1.52774500	-3.65809700	2.19360800
H	2.81134700	-5.16419800	0.95104100
H	1.91769600	-1.81926800	0.77286200
N	-0.06710400	-1.86448000	0.20270300
O	-0.24544900	-4.21679700	1.48099100
C	-0.41273700	-0.56573400	0.13138200
C	-1.23012200	-2.59021800	0.16120900
N	-1.74310500	-0.56093100	0.05558600
N	-2.27073500	-1.81757500	0.08218500
C	-1.12699700	-4.06119400	0.38507000
H	-0.76798700	-4.58042400	-0.51408300
H	-2.09885700	-4.46659100	0.66781100
C	-2.59027500	0.60274000	0.07337500
C	-2.83024700	1.27820400	-1.12418000
C	-3.11181500	0.99981500	1.30953900
C	-3.58909600	2.44575800	-1.04250300
C	-3.85452700	2.17591100	1.33296300
C	-4.08715300	2.91654600	0.17197200
H	-3.79117800	3.00100600	-1.95504700
H	-4.25547000	2.52530700	2.28107700
C	-4.83782500	4.21901200	0.23992800
C	0.40014400	1.18100200	2.54715700
C	0.19381300	1.56096500	1.28455500
H	0.77197200	0.15758200	2.63923000
C	0.17382300	1.87350300	3.82607000
C	-0.17301800	1.09196200	4.93815200
C	0.31195800	3.25723900	3.99707200
C	-0.41871600	1.67633400	6.17476700
H	-0.25723000	0.01393800	4.82298900
C	0.07550000	3.83864900	5.23822200
H	0.61833100	3.87618500	3.16324600
C	-0.29821600	3.05555800	6.32742400
H	-0.69590700	1.05529000	7.02068100
H	0.19346400	4.91128000	5.35603800
H	-0.48228200	3.51643500	7.29273000
Br	-0.47287100	3.25541600	0.77145700
C	0.51186700	0.64169200	0.09894000
H	0.24939100	1.16617000	-0.83131900
O	1.80992000	0.20143100	0.08473500
N	2.73278800	-2.25048500	-4.50028700

O	2. 74807800	-1. 03661900	-4. 45750800
O	2. 90942000	-2. 91293900	-5. 51047700
H	-5. 31983700	4. 45334900	-0. 71205500
H	-4. 14989200	5. 03881000	0. 47460200
H	-5. 60307400	4. 19859600	1. 01992700
C	-2. 90504500	0. 17803500	2. 55195100
H	-3. 12876400	0. 76783900	3. 44285800
H	-3. 55968100	-0. 70010200	2. 54700400
H	-1. 87443100	-0. 17942200	2. 63516700
C	-2. 30498600	0. 77010900	-2. 43814900
H	-1. 23833700	0. 98460000	-2. 57520500
H	-2. 43082800	-0. 31428800	-2. 51897500
H	-2. 84880500	1. 23582400	-3. 26266500
C	1. 98145100	1. 25037100	-2. 83437700
O	0. 88670700	0. 65329400	-2. 83243400
O	2. 77029700	1. 32934700	-1. 83194300
H	2. 29545600	0. 69551900	-0. 78230700
C	2. 44802600	1. 96948700	-4. 08559100
H	2. 43462300	3. 04883800	-3. 90529800
H	3. 47819400	1. 68562100	-4. 30990700
H	1. 80338400	1. 73060900	-4. 93096400

**si-TS2**

C	3. 64983200	-5. 00446600	-4. 79956900
C	3. 43519900	-3. 65539800	-4. 51773400
C	3. 79317300	-2. 66108600	-5. 42153500
C	4. 34213900	-3. 08543300	-6. 62488600
C	4. 54770800	-4. 42474000	-6. 94623400
C	4. 20350300	-5. 39679900	-6. 01704800
C	3. 23487900	-5. 88199200	-3. 65151600
C	2. 57758800	-4. 93789800	-2. 61589400
C	2. 83265500	-3. 47005500	-3. 14109600
H	3. 65153300	-1. 60241300	-5. 22523900
H	4. 97650500	-4. 68151100	-7. 90680300
H	4. 36740100	-6. 44624300	-6. 23951500
H	2. 52948600	-6. 66508200	-3. 94874500
H	3. 04327100	-5. 04489100	-1. 63618200
H	4. 10303100	-6. 38585500	-3. 21599100
H	3. 51519200	-2. 93553100	-2. 48626900
N	1. 58184800	-2. 69694600	-3. 17271800
O	1. 21598000	-5. 25514200	-2. 39173000
C	1. 33412900	-1. 36261600	-3. 03084200
C	0. 37012200	-3. 31808000	-3. 35612700
N	-0. 00902000	-1. 26317800	-3. 11923000

N	-0.61246700	-2.48091100	-3.31559000
C	0.35616900	-4.80668100	-3.42107900
H	0.68006300	-5.16463600	-4.40884400
H	-0.64727200	-5.18197400	-3.21971200
C	-0.82296900	-0.08143000	-3.05783400
C	-1.13373700	0.57904400	-4.24708800
C	-1.28709000	0.33850200	-1.80655700
C	-1.92218000	1.72575300	-4.15295500
C	-2.04194800	1.50601200	-1.76282100
C	-2.36296600	2.21351200	-2.92437100
H	-2.17466700	2.26287000	-5.06398900
H	-2.39670700	1.86699700	-0.80064600
C	-3.14526900	3.49641800	-2.84049500
C	2.17485900	0.97243500	-0.85013700
C	1.97391900	0.92209300	-2.17058000
H	2.50846300	0.02479100	-0.42437200
C	1.99295900	2.06166900	0.12425800
C	1.54250500	1.71957200	1.40749300
C	2.28712900	3.40467700	-0.14527800
C	1.34813000	2.69242500	2.38106600
H	1.33966400	0.67637900	1.63698600
C	2.10169700	4.37541100	0.83343600
H	2.67187300	3.68462300	-1.11805500
C	1.62445400	4.02723300	2.09475100
H	0.98963900	2.40730600	3.36519800
H	2.34112300	5.41040600	0.61032200
H	1.48055700	4.78980200	2.85363900
Br	1.39342700	2.44491900	-3.16188400
C	2.31062600	-0.29711900	-2.99060300
H	2.41944200	0.09580800	-4.29729600
O	3.58908000	-0.80592700	-2.68334300
N	4.73956800	-2.07091400	-7.61186300
O	4.73555800	-0.90619800	-7.26030000
O	5.05256700	-2.45663200	-8.72535200
H	-3.64854600	3.71982600	-3.78403900
H	-2.47653200	4.33361600	-2.61316200
H	-3.89831800	3.45407100	-2.04939300
C	-0.99342900	-0.45669500	-0.56507500
H	-1.45039100	0.01238000	0.30822100
H	-1.38139100	-1.47689200	-0.65342700
H	0.08403300	-0.52747600	-0.38788400
C	-0.58046300	0.12332300	-5.56726400
H	0.46117500	0.45161400	-5.67140600
H	-0.60895700	-0.96519600	-5.66770100

H	-1.15241200	0.55618700	-6.39065700
C	3.91569800	1.05781500	-5.32725300
O	2.74705100	0.50979400	-5.42137900
O	4.70635100	0.84539000	-4.39717800
H	4.19592700	-0.25616500	-3.25051300
C	4.25813700	2.03602800	-6.42137100
H	3.72491100	2.97001000	-6.21584500
H	5.32999500	2.23000200	-6.43980500
H	3.91991100	1.65649900	-7.38605500

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

C	4.37371100	-3.49141600	-3.82249800
C	3.65438100	-2.30912400	-3.98423000
C	3.80159100	-1.48971600	-5.10033000
C	4.71005200	-1.93671200	-6.05269400
C	5.44332700	-3.11638700	-5.93217300
C	5.27638000	-3.90375600	-4.80133700
C	4.03517000	-4.16682300	-2.52013200
C	2.83875700	-3.37538600	-1.93813400
C	2.73370900	-2.06929000	-2.80869600
H	3.22287400	-0.55757300	-5.21253100
H	6.12715800	-3.39710100	-6.72329000
H	5.83808000	-4.82588400	-4.68921900
H	3.76659200	-5.22157800	-2.64089600
H	3.00921700	-3.09919400	-0.89702800
H	4.88734200	-4.12952100	-1.83382200
H	3.04144600	-1.19675900	-2.23180800
N	1.35841000	-1.85091200	-3.24203400
O	1.64772300	-4.14574600	-1.90099600
C	0.72466700	-0.69827800	-3.57482600
C	0.51032600	-2.88759600	-3.50444900
N	-0.46946700	-1.10520400	-4.01625900
N	-0.62248700	-2.46398700	-3.97639500
C	0.97831800	-4.25690900	-3.14343300
H	1.63624000	-4.66283400	-3.92595200
H	0.13156700	-4.93139600	-3.01227700
C	-1.52478100	-0.24886200	-4.48614900
C	-1.51973700	0.12351300	-5.83064500
C	-2.44185700	0.23347500	-3.55336300
C	-2.48094600	1.04561500	-6.23137600
C	-3.38724800	1.14776900	-4.00633400
C	-3.39653800	1.58829000	-5.32978700
H	-2.46491800	1.40576400	-7.25668800
H	-4.08991400	1.57491000	-3.29490300

C	-4.28348900	2.72185800	-5.75832400
C	3.33368500	1.64312900	-2.63441600
C	2.15421600	1.01260000	-2.51933400
H	3.61207500	1.75926700	-3.68172300
C	4.28157100	2.13315500	-1.62997800
C	5.64848800	2.13135800	-1.95600600
C	3.91000200	2.64221200	-0.37526000
C	6.60821300	2.57519300	-1.05464900
H	5.95092000	1.76788600	-2.93470700
C	4.87177400	3.08518500	0.52643300
H	2.86010700	2.70418200	-0.11549900
C	6.22530200	3.04915700	0.19848600
H	7.65796300	2.55608600	-1.33358400
H	4.55692500	3.47699800	1.48944800
H	6.97112000	3.39997900	0.90529600
Br	1.41669400	0.50020700	-0.81019800
C	1.26334700	0.69116200	-3.65766400
H	0.30053200	1.62043200	-3.61108800
O	1.85025700	0.85379700	-4.89392100
N	4.91771400	-1.12508400	-7.26368900
O	4.30570400	-0.08112000	-7.35904300
O	5.69771700	-1.55065800	-8.10362300
H	-5.15682400	2.82577000	-5.10850600
H	-4.62666100	2.60097400	-6.78980700
H	-3.68048800	3.63546400	-5.69855500
C	-2.33737800	-0.15840400	-2.10583500
H	-3.17909300	0.24070900	-1.53605200
H	-2.31756400	-1.24629200	-1.98020200
H	-1.41377300	0.24167900	-1.67075100
C	-0.47332400	-0.40344200	-6.77128700
H	0.51496600	-0.06765600	-6.43521600
H	-0.48128300	-1.49923800	-6.79899200
H	-0.64477800	-0.02859000	-7.78208700
H	0.98274300	1.94417500	-5.49980000
C	-0.54047700	3.10711400	-4.99350000
O	-1.35175600	3.96438000	-5.34947500
O	-0.44797400	2.64959600	-3.78118500
O	0.31653700	2.61246100	-5.90636400

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

C	3.93103400	-4.82785000	-5.13813100
C	3.65465800	-3.46340200	-5.08145300
C	3.84669300	-2.63668800	-6.18061200
C	4.29403300	-3.24411800	-7.34532500

C	4. 56804900	-4. 60720600	-7. 44115800
C	4. 39173000	-5. 40743900	-6. 32028500
C	3. 69986900	-5. 48713200	-3. 80619600
C	3. 03752600	-4. 40907200	-2. 91372800
C	3. 16859200	-3. 05138200	-3. 70990200
H	3. 69307000	-1. 56570300	-6. 10528300
H	4. 91899100	-5. 01501300	-8. 38095000
H	4. 61007700	-6. 46942000	-6. 36974700
H	3. 05620300	-6. 37057500	-3. 86898700
H	3. 55188000	-4. 31099000	-1. 95746500
H	4. 64935800	-5. 81523600	-3. 37143000
H	3. 85923000	-2. 35508600	-3. 23452200
N	1. 87015200	-2. 36623900	-3. 76929200
O	1. 71014500	-4. 76033100	-2. 55852300
C	1. 58353200	-1. 04430800	-3. 69885500
C	0. 68130400	-3. 04573200	-3. 72584000
N	0. 24171000	-0. 99444100	-3. 62235700
N	-0. 32981500	-2. 23965700	-3. 62114400
C	0. 75375200	-4. 52744900	-3. 57696500
H	1. 03248500	-5. 01762700	-4. 52044400
H	-0. 20511400	-4. 92056200	-3. 23893700
C	-0. 55909900	0. 19145300	-3. 52825900
C	-0. 82960900	0. 90323000	-4. 69758700
C	-0. 98178500	0. 60544000	-2. 26138400
C	-1. 55173800	2. 09053500	-4. 57076800
C	-1. 70366100	1. 79364500	-2. 18798200
C	-1. 99528600	2. 54646800	-3. 32871700
H	-1. 77229600	2. 66954200	-5. 46425100
H	-2. 02722000	2. 15207500	-1. 21370800
C	-2. 77489100	3. 82969900	-3. 21168800
C	1. 92988500	2. 10732100	-2. 40755100
C	2. 48403600	0. 89844100	-2. 53443600
H	1. 48365600	2. 45289000	-3. 34086500
C	1. 74496000	3. 04001100	-1. 28421600
C	2. 44172000	3. 00229300	-0. 06745300
C	0. 80463900	4. 06664500	-1. 47560300
C	2. 19141500	3. 95043800	0. 91919900
H	3. 19079800	2. 24261200	0. 10655700
C	0. 55092800	5. 00769800	-0. 48598900
H	0. 26873900	4. 11627000	-2. 42047400
C	1. 24406700	4. 95138800	0. 72091900
H	2. 74779400	3. 90697100	1. 85035600
H	-0. 18159500	5. 79019600	-0. 65931700
H	1. 05581200	5. 68747900	1. 49609700

Br	3.31897100	-0.06806500	-1.07114500
C	2.52260500	0.05937300	-3.74571200
H	2.99292600	0.41263700	-4.77430100
O	3.85087300	-0.34697900	-4.16306100
N	4.49353300	-2.40802400	-8.53786800
O	4.21967000	-1.22471900	-8.45419100
O	4.91585000	-2.94841900	-9.54587600
H	-2.54077300	4.34845100	-2.27776000
H	-3.85235000	3.63342000	-3.21465300
H	-2.55911300	4.50367100	-4.04428700
C	-0.61051000	-0.17144500	-1.02907800
H	-0.90830800	-1.22108800	-1.11395700
H	0.47347700	-0.14754700	-0.86489900
H	-1.09267200	0.25575900	-0.14790700
C	-0.32431800	0.42045100	-6.02916300
H	0.76850400	0.49118800	-6.06883000
H	-0.59672900	-0.62529900	-6.20239000
H	-0.73510700	1.02229000	-6.84167400

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

C	6.46962200	1.05784000	-5.11633500
C	5.15198500	1.15462900	-4.66640100
C	4.41148400	2.32723900	-4.80015000
C	5.06869600	3.38598700	-5.41969600
C	6.38202100	3.32614500	-5.87914600
C	7.09396300	2.14460000	-5.72381500
C	7.04769800	-0.30261200	-4.83282100
C	5.84703600	-1.17486900	-4.40749800
C	4.71692700	-0.15017100	-4.02541000
H	3.38502500	2.45103000	-4.42218800
H	6.82186800	4.19702200	-6.34902400
H	8.11736100	2.07159700	-6.07778500
H	7.55097600	-0.75003000	-5.69521500
H	6.08632700	-1.80064300	-3.54710200
H	7.78178600	-0.24324900	-4.02203100
H	4.61908100	-0.05336800	-2.94563800
N	3.41899300	-0.61613900	-4.52786100
O	5.47396800	-2.09704700	-5.42116900
C	2.17080400	-0.57179700	-4.01250600
C	3.33597100	-1.25074900	-5.74304300
N	1.40381400	-1.16441300	-4.93939400
N	2.11961800	-1.60695900	-6.01506100
C	4.62351800	-1.57269200	-6.42473700
H	5.05408300	-0.68695100	-6.91085200



H	4.46746800	-2.34865600	-7.17441900
C	-0.01855900	-1.32067300	-4.84177900
C	-0.81274900	-0.20060100	-5.08852100
C	-0.51987900	-2.54217100	-4.37718900
C	-2.16538000	-0.30287100	-4.75684500
C	-1.87264100	-2.58660400	-4.05982900
C	-2.69885300	-1.46855200	-4.20885100
H	-2.81014000	0.55913100	-4.91132100
H	-2.29020700	-3.50809200	-3.66018900
C	-4.13358000	-1.53794600	-3.76231200
C	-0.53744800	-0.16641500	-1.76182800
C	0.69631000	-0.62593600	-1.99211100
H	-0.70700200	0.80539200	-2.22647900
C	-1.71402500	-0.68203400	-1.04526500
C	-2.76400900	0.22709100	-0.84046800
C	-1.89246200	-2.00533400	-0.61334300
C	-3.93620400	-0.15295600	-0.19856400
H	-2.64886300	1.24949100	-1.19059300
C	-3.07016900	-2.38639400	0.02241900
H	-1.11704800	-2.74090300	-0.77897200
C	-4.09288100	-1.46524700	0.24038400
H	-4.72730100	0.57434800	-0.04604000
H	-3.18769500	-3.41465900	0.35060900
H	-5.00573000	-1.76971100	0.74266300
Br	1.38585200	-2.26413500	-1.28058200
C	1.70268500	0.12721600	-2.79688100
H	1.30381800	1.22548000	-3.17359100
O	2.79382500	0.59149600	-2.03552700
N	4.33703100	4.64968800	-5.60681000
O	3.14783900	4.65789900	-5.35864200
O	4.96853100	5.61617700	-6.00563100
H	-4.18578500	-1.84464200	-2.71178200
H	-4.69500000	-2.27227900	-4.34911000
H	-4.63089500	-0.57033000	-3.85992200
C	0.35598400	-3.75892900	-4.25316300
H	0.48241200	-4.23201400	-5.23279500
H	1.34894300	-3.51664700	-3.87039600
H	-0.09575200	-4.48823300	-3.57731700
C	-0.23162000	1.06625200	-5.65934000
H	0.32656400	1.65693200	-4.91878700
H	0.45750100	0.84045500	-6.47960900
H	-1.03042000	1.69649900	-6.05643600
O	1.78436600	2.54515400	-3.32451700
H	2.69106100	1.57004000	-2.21985300

H	1. 26827300	3. 28775300	-2. 99699000
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**si-M2**

C	3. 73495600	-4. 18199100	0. 13317800
C	3. 12519300	-2. 96129700	-0. 15099200
C	2. 59306300	-2. 69032300	-1. 40442900
C	2. 69665900	-3. 69362200	-2. 35809700
C	3. 31196200	-4. 91930600	-2. 11312700
C	3. 83967400	-5. 16461400	-0. 85129100
C	4. 20528000	-4. 23343000	1. 56236100
C	3. 64079200	-2. 95627700	2. 23669000
C	3. 08983600	-2. 05763200	1. 06386600
H	2. 12475500	-1. 74170100	-1. 64115700
H	3. 36052700	-5. 65905500	-2. 90244800
H	4. 31529300	-6. 11655600	-0. 63783500
H	3. 85622200	-5. 12561900	2. 09219200
H	4. 42449800	-2. 41546100	2. 76779600
H	5. 29879900	-4. 24146800	1. 61084500
H	3. 72355200	-1. 18260600	0. 92620200
N	1. 74260100	-1. 59504300	1. 34901200
O	2. 68176000	-3. 24830100	3. 23513400
C	1. 04529000	-0. 49006000	0. 86975900
C	0. 85547700	-2. 36289700	2. 06304500
N	-0. 24417800	-0. 70525800	1. 33108800
N	-0. 32899500	-1. 86564400	2. 09970500
C	1. 40380200	-3. 58258100	2. 72524100
H	1. 46226500	-4. 41983400	2. 01384200
H	0. 77113900	-3. 87857800	3. 56213200
C	-1. 44997700	-0. 18247000	0. 77354900
C	-1. 69914100	-0. 30298600	-0. 60164000
C	-2. 36554600	0. 42636900	1. 64108600
C	-2. 86462000	0. 27938800	-1. 10145700
C	-3. 52614000	0. 97023700	1. 09635900
C	-3. 78284600	0. 92599800	-0. 27447100
H	-3. 06662900	0. 20781700	-2. 16808500
H	-4. 23942500	1. 45511400	1. 75876200
C	-5. 01361300	1. 56832200	-0. 85896400
C	0. 80978600	2. 30629100	-1. 46045500
C	0. 80428900	1. 74547300	-0. 23745400
H	1. 33756300	1. 71746600	-2. 21157000
C	0. 23999300	3. 57320900	-1. 93946500
C	-0. 98569000	4. 08027600	-1. 48244700
C	0. 90950300	4. 26535600	-2. 95938800
C	-1. 49740100	5. 26311800	-2. 00481000

H	-1.53944900	3.53640500	-0.72606100
C	0.39819200	5.44944600	-3.47690900
H	1.84583900	3.86698600	-3.34135700
C	-0.80718500	5.95645800	-2.99656400
H	-2.44892700	5.63923600	-1.64153700
H	0.93820800	5.97428800	-4.25888100
H	-1.21158900	6.87907300	-3.40076800
Br	0.06661000	2.66916200	1.27417700
C	1.51997000	0.52883100	0.09238200
H	3.28028600	1.04809600	-0.50132500
O	2.70030200	0.28236100	-0.61679000
N	2.11948800	-3.45022600	-3.68740100
O	1.53560400	-2.39605700	-3.86741100
O	2.25261200	-4.31811100	-4.53236700
H	-4.75384200	2.48556500	-1.39851300
H	-5.73403400	1.83077200	-0.08074800
H	-5.50823700	0.90199500	-1.57147400
C	-2.08209800	0.50285400	3.11490300
H	-2.14461500	-0.48512000	3.58087100
H	-1.06907900	0.87886700	3.28691200
H	-2.79311900	1.16725400	3.61081500
C	-0.77678500	-1.05173200	-1.52754700
H	0.04144500	-0.41538400	-1.88192000
H	-0.33467000	-1.92172800	-1.03170500
H	-1.32692300	-1.40478300	-2.40241700

**TS2'**

C	4.23527900	-3.41575300	0.26407000
C	3.25224900	-2.52748300	-0.16780600
C	2.76451200	-2.54051100	-1.46888900
C	3.32283100	-3.48266400	-2.32321700
C	4.32313400	-4.37017200	-1.93472600
C	4.78422900	-4.33859800	-0.62443800
C	4.54857100	-3.21835800	1.72315700
C	3.49329000	-2.21342400	2.24766500
C	2.80021500	-1.63085200	0.96042300
H	1.97600200	-1.87398100	-1.81673800
H	4.71395300	-5.07694500	-2.65614600
H	5.55164200	-5.03370300	-0.29958900
H	4.50068300	-4.14928400	2.29697400
H	3.95809500	-1.39823600	2.80248600
H	5.55694700	-2.81314300	1.85286200
H	3.08262500	-0.58526200	0.81743000
N	1.34622600	-1.66755900	1.09242200

O	2.59275700	-2.79355900	3.17577900
C	0.40744200	-0.91001500	0.50305300
C	0.69890900	-2.62757000	1.81858900
N	-0.75393500	-1.43469300	0.88013200
N	-0.59079100	-2.50318500	1.71572600
C	1.55312100	-3.56535200	2.60793000
H	1.93992400	-4.36624500	1.96133300
H	0.98130600	-4.01408500	3.42029300
C	-2.06908300	-1.01443800	0.46499400
C	-2.64148400	-1.67222400	-0.62662600
C	-2.69364600	0.01784100	1.16570200
C	-3.90747600	-1.25018200	-1.02289100
C	-3.95906200	0.40219200	0.72424200
C	-4.57610500	-0.21607400	-0.36358600
H	-4.37886800	-1.73453800	-1.87401900
H	-4.47158000	1.20765600	1.24392200
C	-5.95301300	0.20538100	-0.80301900
C	0.66103000	2.61347700	-0.93292900
C	0.92413200	1.48759300	-0.21897700
H	-0.17229400	2.50499200	-1.62412400
C	1.37070200	3.87555600	-0.91297900
C	2.63520100	4.04864700	-0.31676800
C	0.78922400	5.00104400	-1.53055500
C	3.26061300	5.29033100	-0.31171000
H	3.12800500	3.20046900	0.14638900
C	1.42239600	6.23516700	-1.53309100
H	-0.18124500	4.89004300	-2.00772100
C	2.66386600	6.39402100	-0.91671700
H	4.23444800	5.39314800	0.15937400
H	0.94366100	7.08156100	-2.01763500
H	3.15991800	7.35934900	-0.91536300
Br	1.52937800	1.59566600	1.74980400
C	0.52411300	0.13689500	-0.59931200
H	1.91988400	0.57084000	-0.48633400
O	0.11524200	-0.22808100	-1.71300300
N	2.81743800	-3.56190600	-3.70281900
O	1.86137900	-2.86836000	-3.99256000
O	3.38161300	-4.32393900	-4.46833500
H	-6.12352600	1.26650100	-0.60628700
H	-6.72175300	-0.35842800	-0.26363400
H	-6.09951900	0.02505800	-1.87056600
C	-2.02915200	0.69079500	2.33495900
H	-1.58609600	-0.03995800	3.01891100
H	-1.22622600	1.36094000	2.01124300

H	-2.75562000	1.28413100	2.89326400
C	-1.90253200	-2.76601600	-1.34555800
H	-0.99636900	-2.35906200	-1.80689700
H	-1.61273700	-3.56717500	-0.65765900
H	-2.52602600	-3.19881400	-2.12966700

**TS3**

C	2.07959800	-4.28917500	-2.20488000
C	1.84749500	-2.94668000	-1.90871800
C	2.14834100	-1.94138400	-2.81893100
C	2.68049100	-2.34135600	-4.03718000
C	2.92596600	-3.67272600	-4.36435800
C	2.62249300	-4.65865300	-3.43469300
C	1.68211800	-5.18007600	-1.06002500
C	0.99026600	-4.25643300	-0.02712600
C	1.24966200	-2.78134500	-0.52863800
H	1.99572300	-0.89108500	-2.59687000
H	3.34662000	-3.91429200	-5.33270500
H	2.80519700	-5.70247000	-3.66899100
H	1.00123700	-5.98227800	-1.36318300
H	1.43073600	-4.37353300	0.96292000
H	2.56157700	-5.65817900	-0.61754000
H	1.93191600	-2.26912000	0.14582600
N	0.00691100	-2.00728700	-0.56225200
O	-0.37454100	-4.58253800	0.15715200
C	-0.22956200	-0.67308200	-0.38588900
C	-1.20815800	-2.61347900	-0.76112700
N	-1.57383200	-0.56079600	-0.48351300
N	-2.18549700	-1.76981600	-0.70209200
C	-1.22585800	-4.10057800	-0.86459400
H	-0.89765500	-4.43327700	-1.86007500
H	-2.23136500	-4.47839500	-0.67809500
C	-2.35779800	0.63554800	-0.42243600
C	-2.59987900	1.32101100	-1.61430300
C	-2.82967100	1.06204100	0.82075800
C	-3.35147100	2.49237000	-1.53727800
C	-3.58094700	2.23556500	0.84552300
C	-3.85317200	2.95679200	-0.31909800
H	-3.55188500	3.05168500	-2.44807300
H	-3.94691800	2.60460100	1.80053400
C	-4.67291700	4.21958000	-0.26213300
C	0.06788400	2.75129600	0.48386800
C	0.48110900	1.49867300	0.47630100
H	-0.24737000	3.08183800	-0.51012800

C	-0.08941100	3.76841100	1.54377700
C	0.84238400	3.95424000	2.57086300
C	-1.17300900	4.65104500	1.44560800
C	0.65754600	4.96712600	3.50594000
H	1.70293000	3.30180400	2.63368900
C	-1.35977200	5.65665700	2.38776000
H	-1.87572500	4.53628300	0.62487500
C	-0.44535600	5.81354700	3.42655100
H	1.38886900	5.09993900	4.29689200
H	-2.21230900	6.32387400	2.30410600
H	-0.58377600	6.59954100	4.16234600
Br	1.41014900	0.71641800	2.62778900
C	0.72934800	0.36108600	-0.24420600
H	2.42558900	0.09102500	0.53466800
O	2.05366500	-0.03532000	-0.36528200
N	3.00165200	-1.30665300	-5.03098200
O	2.72307500	-0.15344100	-4.75745700
O	3.52410700	-1.66331800	-6.07250700
H	-4.32400800	4.95305500	-0.99399100
H	-4.62910200	4.67496600	0.73078800
H	-5.72494200	4.01034000	-0.48347500
C	-2.47807300	0.31298900	2.07486800
H	-2.69343500	-0.75542200	1.97246700
H	-1.40913300	0.41858500	2.30361100
H	-3.04300000	0.70011000	2.92487200
C	-2.03592800	0.81723900	-2.91489800
H	-0.94001900	0.84068900	-2.89824000
H	-2.34210800	-0.21673100	-3.10339000
H	-2.37456600	1.43376400	-3.74948700

### TS3'

C	1.56811900	-3.38749200	-2.72274400
C	1.65347800	-2.53256300	-1.62472800
C	2.07009700	-1.21448400	-1.76419900
C	2.33354900	-0.77479700	-3.05364900
C	2.25541700	-1.59982800	-4.17413200
C	1.88248300	-2.92725600	-4.00219900
C	1.12418400	-4.76439700	-2.30763700
C	0.79850700	-4.65752800	-0.79290300
C	1.15424500	-3.18856200	-0.35652000
H	2.21371100	-0.57298500	-0.90276900
H	2.48138100	-1.19562000	-5.15337100
H	1.82454400	-3.58941600	-4.86017500
H	0.25402400	-5.11612600	-2.87145900

H	1.41941100	-5.34674000	-0.22021900
H	1.92001800	-5.49627600	-2.47550700
H	1.89200100	-3.16649400	0.44294700
N	-0.04590300	-2.49286500	0.12551600
O	-0.52648300	-5.04335800	-0.48111000
C	-0.11393400	-1.19002200	0.61896200
C	-1.30533500	-2.82015000	-0.30940200
N	-1.44484200	-0.85109200	0.46424500
N	-2.16579300	-1.88054900	-0.12150500
C	-1.50604400	-4.14946000	-0.96198000
H	-1.45479600	-4.03819900	-2.05496600
H	-2.48571900	-4.55730400	-0.70930400
C	-2.05965700	0.43471800	0.52878000
C	-1.96289200	1.28515100	-0.58225100
C	-2.83430700	0.75279200	1.64732600
C	-2.66311700	2.48768900	-0.54482600
C	-3.51033000	1.97384900	1.64464400
C	-3.44604100	2.84313100	0.55618400
H	-2.59149000	3.16772100	-1.39072700
H	-4.11721400	2.24032000	2.50723000
C	-4.21824700	4.13587900	0.55401500
C	1.01829000	1.75947300	0.89739400
C	1.00869500	0.78217600	1.91525000
H	1.68106800	1.46691600	0.07982300
C	0.40457400	3.04817600	0.71045100
C	-0.39008100	3.71319000	1.66663300
C	0.61851900	3.67271600	-0.53962400
C	-0.94255600	4.95137100	1.37418400
H	-0.57608700	3.25729900	2.62901500
C	0.05247400	4.90421300	-0.82688400
H	1.23280800	3.16697300	-1.28134500
C	-0.73136300	5.54896700	0.13146700
H	-1.55076400	5.45359400	2.12023100
H	0.22347700	5.36695600	-1.79358900
H	-1.17116700	6.51766000	-0.08662100
Br	0.15920000	0.99957400	3.62703000
C	0.92975500	-0.55416200	1.26483900
H	2.19490200	0.14687100	1.99298000
O	2.18461500	-1.00847500	1.26933100
N	2.68628200	0.63571500	-3.24003800
O	2.60853000	1.37496000	-2.26867700
O	3.02379900	1.00209700	-4.35008500
H	-3.68913100	4.90982900	-0.00850900
H	-4.38572900	4.50264600	1.57013900

H	-5.20005800	4.00038900	0.08685400
C	-3.00199600	-0.23242800	2.77126200
H	-3.75084300	-0.98523600	2.50093200
H	-2.06980700	-0.75510300	2.99060400
H	-3.33777000	0.27164400	3.68059600
C	-1.11693500	0.90423000	-1.76709200
H	-0.05649300	0.83773800	-1.49209000
H	-1.41285800	-0.07343000	-2.16268900
H	-1.21427400	1.64363500	-2.56518600

**M3**

C	2.18888900	-4.23901900	-1.58113400
C	1.81119900	-2.89802800	-1.67631900
C	1.86682900	-2.21160800	-2.87884100
C	2.30850400	-2.92560900	-3.98670900
C	2.69399900	-4.26148500	-3.92726700
C	2.63516800	-4.92576500	-2.70692000
C	2.04740300	-4.73297400	-0.16434300
C	1.20761000	-3.65683000	0.55775400
C	1.39808500	-2.37262700	-0.32117000
H	1.58394700	-1.16940200	-2.97647200
H	3.02771800	-4.76012200	-4.82901000
H	2.92754100	-5.96881900	-2.64146300
H	1.56213100	-5.70977000	-0.08878600
H	1.55273700	-3.44122500	1.56944700
H	3.03420100	-4.81816600	0.30408100
H	2.16973700	-1.75051400	0.12421200
N	0.16306000	-1.58850200	-0.37565100
O	-0.14527500	-4.06377200	0.71043900
C	-0.10112700	-0.26939300	-0.26045200
C	-1.03973100	-2.23866300	-0.41724100
N	-1.43799800	-0.18172200	-0.26327200
N	-2.03245200	-1.40595500	-0.34854000
C	-1.01917700	-3.72906300	-0.34792000
H	-0.70855500	-4.16972500	-1.30499400
H	-2.01303400	-4.09822900	-0.09287000
C	-2.26945200	0.97825300	-0.06530300
C	-2.60588500	1.76169600	-1.17296100
C	-2.71074600	1.24093600	1.23148000
C	-3.38790800	2.88675500	-0.93824300
C	-3.49672200	2.38169800	1.41104800
C	-3.83434000	3.21417800	0.34795100
H	-3.65641900	3.52533400	-1.77685300
H	-3.83380200	2.62829400	2.41447600



C	-4.66091300	4.45266000	0.56751600
C	0.08698000	3.31916700	-0.01109900
C	0.48698000	2.08245600	-0.14755100
H	0.04766800	3.97893000	-0.87769900
C	-0.41511300	3.84172900	1.27609300
C	-0.26469800	3.11559100	2.46591000
C	-1.12119500	5.04709500	1.28596600
C	-0.84431500	3.58624500	3.63723500
H	0.29389400	2.17930300	2.47427300
C	-1.70187600	5.51215500	2.46210900
H	-1.23242900	5.60705500	0.36058700
C	-1.56980400	4.77871900	3.63847200
H	-0.72722600	3.01849400	4.55524100
H	-2.25789500	6.44469400	2.45860000
H	-2.02061600	5.13970300	4.55777700
Br	1.30325100	-0.68362900	2.68838600
C	0.87803400	0.82553400	-0.14263800
H	2.20196800	0.14685100	0.99756000
O	2.17606100	0.45737900	0.03751300
N	2.36489100	-2.23493600	-5.28243200
O	1.98311800	-1.07855400	-5.32307500
O	2.78608700	-2.85727600	-6.24064900
H	-4.16242300	5.33468100	0.15342500
H	-4.83556100	4.62968600	1.63091800
H	-5.63352100	4.36656500	0.07193600
C	-2.37684600	0.32745000	2.37773800
H	-2.93802100	-0.60979000	2.28972900
H	-1.31355800	0.06349400	2.41841100
H	-2.64781100	0.79699000	3.32575500
C	-2.09464700	1.41930200	-2.54478100
H	-1.01788200	1.61301600	-2.62092900
H	-2.26023700	0.36356800	-2.78059800
H	-2.59577100	2.02066200	-3.30539100

#### M04

C	4.93844100	-1.15803200	0.40176300
C	3.71761700	-0.48834800	0.47212900
C	3.57107200	0.81226100	0.01254300
C	4.69829800	1.41179000	-0.53288300
C	5.93425100	0.77622100	-0.61420700
C	6.05585200	-0.52509600	-0.13989100
C	4.82269100	-2.54837100	0.96879000
C	3.30728100	-2.78764300	1.17803100
C	2.64626000	-1.36417600	1.08170900

H	2. 63150300	1. 35263500	0. 06807000
H	6. 77472500	1. 30126900	-1. 05131400
H	7. 00995900	-1. 03830900	-0. 20193500
H	5. 23936100	-3. 31833900	0. 31218000
H	3. 09724700	-3. 22463500	2. 15408100
H	5. 35272700	-2. 61728700	1. 92425500
H	2. 32025900	-0. 98780500	2. 05255400
N	1. 46276100	-1. 40922400	0. 21823100
O	2. 77579800	-3. 72451600	0. 25575600
C	0. 36305800	-0. 62819700	0. 18858500
C	1. 42397500	-2. 20769500	-0. 89080800
N	-0. 28842300	-0. 98572600	-0. 92063400
N	0. 36297100	-1. 97611500	-1. 60187700
C	2. 51273200	-3. 22064800	-1. 03742200
H	3. 40459700	-2. 77221600	-1. 49773000
H	2. 17474500	-4. 04933800	-1. 66020000
C	-1. 52627400	-0. 46968900	-1. 44878700
C	-1. 43827800	0. 43663200	-2. 51173400
C	-2. 73202800	-0. 91082400	-0. 90952400
C	-2. 63116100	0. 90336000	-3. 04915100
C	-3. 90215700	-0. 41504700	-1. 49297000
C	-3. 87192900	0. 47992900	-2. 55757900
H	-2. 59512800	1. 61507400	-3. 87065700
H	-4. 85912600	-0. 73752800	-1. 09068300
C	-5. 14625400	0. 98060400	-3. 18249300
C	-1. 41139000	2. 42281600	0. 37619200
C	-0. 66473000	1. 43501000	0. 80521900
H	-0. 94255400	3. 31235900	-0. 04876900
C	-2. 89109200	2. 39847000	0. 39586800
C	-3. 59081700	1. 56046900	1. 27159900
C	-3. 60582600	3. 21256600	-0. 48788700
C	-4. 97944300	1. 51573000	1. 23961200
H	-3. 03979500	0. 95183400	1. 98503900
C	-4. 99638100	3. 16840800	-0. 51769000
H	-3. 06440500	3. 87211900	-1. 16167900
C	-5. 68590800	2. 31429200	0. 34033700
H	-5. 51129000	0. 86157700	1. 92374500
H	-5. 54325500	3. 80199500	-1. 20961700
H	-6. 77098400	2. 28208400	0. 31933500
C	0. 01038800	0. 37137400	1. 22961500
H	0. 13988100	-1. 38626700	2. 65715100
O	0. 44807100	0. 09476800	2. 44310200
N	4. 57289300	2. 77804900	-1. 06048000
O	3. 46083200	3. 27527800	-1. 07794000

O	5.58426500	3.32906500	-1.45511300
H	-5.06379200	2.03657800	-3.45400200
H	-5.99136600	0.86657200	-2.49998000
H	-5.37405100	0.42261100	-4.09738800
C	-2.79021600	-1.81774500	0.28675200
H	-1.94722300	-2.51215400	0.33331500
H	-2.78674900	-1.21737500	1.20307200
H	-3.71203400	-2.40240500	0.28816100
C	-0.10036500	0.91062400	-3.00926000
H	0.45424400	1.41490900	-2.20848900
H	0.51294900	0.07753500	-3.36642500
H	-0.22403100	1.62072800	-3.82880000
H	-1.05449000	-0.22268300	3.32674700
C	-1.55549200	-2.07709300	3.22419200
O	-2.36715200	-2.95190900	3.37511400
O	-1.83179900	-0.79396800	3.53357600
O	-0.33184400	-2.28489500	2.73605400

**E-TS4**

C	4.94026900	-0.64879100	0.16261700
C	3.63100200	-0.38308800	0.56139100
C	3.13488300	0.91215600	0.60847900
C	3.99522900	1.92726200	0.21562000
C	5.30733200	1.69852000	-0.18959900
C	5.78650200	0.39444800	-0.21117500
C	5.24271900	-2.12089700	0.21581500
C	3.90335200	-2.81439500	0.57106600
C	2.87963600	-1.65419600	0.88528200
H	2.13106900	1.15142000	0.94496800
H	5.92809900	2.53695400	-0.48056800
H	6.80728100	0.19590100	-0.52119200
H	5.63318700	-2.50630000	-0.73185000
H	4.00509000	-3.43738800	1.45931200
H	5.99741300	-2.33426800	0.97857700
H	2.52807500	-1.68730300	1.91634500
N	1.68629400	-1.77980500	0.03276000
O	3.46465400	-3.70937700	-0.43341100
C	0.45087700	-1.27298000	0.19826200
C	1.70890500	-2.38201000	-1.19372100
N	-0.21850500	-1.59235000	-0.90731300
N	0.54926800	-2.29639400	-1.78047200
C	2.96411800	-3.08226800	-1.59565900
H	3.68288900	-2.37056600	-2.02567800
H	2.74752700	-3.85384700	-2.33472300

C	-1.62091800	-1.35864700	-1.16068800
C	-1.97208800	-0.31693500	-2.01793200
C	-2.54143200	-2.14625600	-0.46580700
C	-3.33205000	-0.04248100	-2.14273900
C	-3.88587700	-1.81997900	-0.61579500
C	-4.29322400	-0.76333300	-1.43216800
H	-3.64078700	0.78591800	-2.77502800
H	-4.61856400	-2.36525400	-0.02745800
C	-5.74609700	-0.37728500	-1.49003900
C	-0.81306200	1.63803300	0.52244300
C	-1.05752400	0.48743800	1.17137100
H	0.20625900	1.92111700	0.23715500
C	-1.81618700	2.64000100	0.12135300
C	-3.19492200	2.38839200	0.18377400
C	-1.37557400	3.86916000	-0.38496200
C	-4.10067400	3.35186000	-0.24309600
H	-3.55254100	1.43389200	0.55933500
C	-2.28500700	4.83249900	-0.81018900
H	-0.30750700	4.07032500	-0.43342000
C	-3.65145900	4.57563400	-0.74079200
H	-5.16554800	3.14528000	-0.18898600
H	-1.92614400	5.78260400	-1.19391900
H	-4.36420900	5.32385900	-1.07404800
C	-0.02908000	-0.48397500	1.41663000
H	-1.68663600	-0.95564600	3.36682700
O	0.45351000	-0.83796700	2.48663100
N	3.48862300	3.30740500	0.21623000
O	2.30697200	3.47307900	0.46606500
O	4.27446600	4.19933300	-0.04074900
H	-5.91793400	0.42752200	-2.20843400
H	-6.07994300	-0.03603600	-0.50450800
H	-6.37375400	-1.22895500	-1.76828700
C	-2.09502100	-3.27356900	0.42701300
H	-1.39972100	-3.93831900	-0.09754700
H	-1.60117700	-2.90520500	1.33311200
H	-2.95650300	-3.85362400	0.75875500
C	-0.93124300	0.49668900	-2.73352500
H	-0.19335000	0.89856800	-2.02994500
H	-0.39327100	-0.10562500	-3.47309000
H	-1.39454700	1.34194800	-3.24555400
H	-2.29739200	0.13961100	1.68373400
C	-3.41234900	-1.37367800	2.60889600
O	-4.30649800	-2.19255200	2.53711700
O	-3.40066200	-0.18397800	2.09252100

0	-2.27548700	-1.72049000	3.29609000
<b>TS4<sup>a</sup></b>			
C	2.01798900	-3.69782800	-2.38908000
C	1.82935000	-2.67962100	-1.45488900
C	2.33967200	-1.40427700	-1.65537600
C	3.03735900	-1.18673700	-2.83435200
C	3.24854600	-2.18039800	-3.78681200
C	2.73530400	-3.45137600	-3.55928800
C	1.37902300	-4.98274800	-1.94061200
C	0.62957500	-4.64509400	-0.62742900
C	0.99155100	-3.14706700	-0.28642600
H	2.22539100	-0.59691100	-0.93845000
H	3.80551400	-1.94552300	-4.68570900
H	2.88812900	-4.23696900	-4.29164600
H	0.68827700	-5.39208800	-2.68492700
H	0.96989500	-5.27758900	0.19173100
H	2.13637700	-5.75101400	-1.76087100
H	1.49944000	-3.05542000	0.67364900
N	-0.23574000	-2.33381900	-0.19484300
O	-0.76223500	-4.88774800	-0.69948000
C	-0.41143100	-1.11116400	0.33506400
C	-1.38911400	-2.64687100	-0.85615400
N	-1.64182300	-0.73662200	-0.00675900
N	-2.26847900	-1.69226300	-0.74297200
C	-1.47214100	-3.98394300	-1.51760800
H	-1.06339100	-3.93317400	-2.53662300
H	-2.51007500	-4.31421200	-1.57169200
C	-2.34124000	0.48420900	0.32223000
C	-2.48758000	1.43223400	-0.69289600
C	-2.84839100	0.64094500	1.61294700
C	-3.17809900	2.59748200	-0.37286500
C	-3.53108500	1.82771500	1.87832100
C	-3.70636000	2.81058500	0.90217500
H	-3.28937400	3.36611400	-1.13356400
H	-3.93944100	1.98345600	2.87340900
C	-4.45098000	4.08102200	1.21067800
C	0.80580800	1.90292500	-0.02985000
C	0.63427400	1.02897400	0.97310000
H	1.29099500	1.58185200	-0.95677300
C	0.45215700	3.32343500	0.01349400
C	-0.37301800	3.84515800	1.02010800
C	0.90509300	4.16734000	-1.00784900
C	-0.72537800	5.18712800	1.00828600

H	-0.75691000	3.18556200	1.79421300
C	0.55277300	5.51280400	-1.01728700
H	1.54284800	3.76158300	-1.78946500
C	-0.26173500	6.02332600	-0.00970300
H	-1.36710500	5.58471800	1.78847400
H	0.91229300	6.16198900	-1.80880500
H	-0.53895700	7.07276100	-0.01674400
C	0.62329600	-0.34647100	1.10585800
H	1.96149700	-0.28042700	2.81627500
O	1.29082000	-1.05022300	1.92459600
N	3.56995400	0.15959000	-3.09012800
O	3.28720100	1.03938600	-2.29210700
O	4.25393000	0.31892200	-4.08068400
H	-4.01154800	4.92992100	0.68041800
H	-4.44314000	4.29779900	2.28135200
H	-5.49664100	4.00191300	0.89490900
C	-2.65862500	-0.40842600	2.67459000
H	-2.91408500	-1.40633000	2.30502800
H	-1.62187600	-0.43657600	3.03011100
H	-3.29300900	-0.19444400	3.53602800
C	-1.91647200	1.20412100	-2.06472900
H	-0.90339700	0.78879800	-2.01565700
H	-2.53313700	0.50018100	-2.63340200
H	-1.86885200	2.14333500	-2.61845500
H	0.65657700	1.50075700	2.36939300
C	1.87495900	1.35518500	3.99784800
O	0.85994200	1.86866400	3.43226700
O	2.44202800	0.28611900	3.60919600
C	2.45177000	2.06294000	5.17510500
H	1.64754000	2.41263200	5.82365100
H	3.13780800	1.41378000	5.71522000
H	2.99008600	2.94213400	4.80733800

**TS4<sup>b</sup>**

C	2.12522300	-3.83305300	-2.37625000
C	1.80086500	-2.77607700	-1.52794000
C	2.14552800	-1.46754800	-1.82739900
C	2.82377200	-1.25278100	-3.01671800
C	3.19456900	-2.28521700	-3.87393400
C	2.84215100	-3.59095400	-3.54798700
C	1.58402400	-5.13528100	-1.84818200
C	0.66031500	-4.75534100	-0.66369500
C	0.97098300	-3.24255600	-0.35328900
H	1.90564600	-0.62965100	-1.18045600

H	3.73252500	-2.05386100	-4.78571000
H	3.10647500	-4.40573900	-4.21375900
H	1.02564700	-5.70162200	-2.60006500
H	0.87535600	-5.35679500	0.21857200
H	2.39641700	-5.78106000	-1.50156400
H	1.46208800	-3.11429100	0.61228500
N	-0.27695400	-2.46027300	-0.32326100
O	-0.71091500	-4.99494200	-0.92375400
C	-0.50293000	-1.23456900	0.17912500
C	-1.33257500	-2.75481000	-1.13842400
N	-1.67126500	-0.83866800	-0.32731800
N	-2.20608800	-1.78697000	-1.14025900
C	-1.32094800	-4.08896600	-1.81655000
H	-0.79036600	-4.02681400	-2.77742600
H	-2.34072300	-4.42803200	-2.00245900
C	-2.37087700	0.40648700	-0.10318000
C	-2.50210200	1.27052600	-1.19497200
C	-2.84538700	0.69700900	1.17911200
C	-3.13743900	2.48862800	-0.96369200
C	-3.45619000	1.93774700	1.35290900
C	-3.60929300	2.84318600	0.30049600
H	-3.24403100	3.18844300	-1.78839100
H	-3.82627800	2.20037100	2.34096400
C	-4.29202100	4.16484700	0.52161100
C	0.42534900	1.71163800	0.04062800
C	0.55246500	0.84032800	1.09432300
H	0.69233600	1.38030100	-0.96929800
C	0.03200200	3.08408000	0.14993400
C	-0.40732700	3.62771700	1.37454300
C	-0.01672500	3.86533600	-1.02150500
C	-0.90020300	4.92032500	1.41392100
H	-0.35137600	3.02883000	2.27876600
C	-0.51069500	5.15854400	-0.97478800
H	0.33740600	3.43902400	-1.95725400
C	-0.95556800	5.68096700	0.24181100
H	-1.23757800	5.34597100	2.35283000
H	-0.54561100	5.76390300	-1.87383900
H	-1.33955600	6.69580500	0.28127000
C	0.38076500	-0.51231200	1.12067900
H	1.34063800	-0.67333800	2.74671800
O	0.83757100	-1.29566400	2.07411000
N	3.11915600	0.13575100	-3.39727500
O	2.59532300	1.02115200	-2.73803500
O	3.84816400	0.31959600	-4.34985800

H	-3.94931000	4.91103100	-0.19901500
H	-4.10539200	4.54390600	1.52934600
H	-5.37582100	4.05918200	0.40323900
C	-2.69258600	-0.25334800	2.33638300
H	-2.78239800	-1.29787000	2.02564400
H	-1.72479100	-0.12609600	2.83565900
H	-3.46659100	-0.06163000	3.08152300
C	-1.95427200	0.92492200	-2.55339600
H	-0.92137600	0.55848100	-2.49580800
H	-2.55038000	0.14324300	-3.03360500
H	-1.96361900	1.80376000	-3.20046000
H	1.02784100	1.09104000	2.28298500
C	2.78707700	1.27824200	3.48754700
O	1.62341700	0.64038600	3.36053100
O	3.01488900	2.32622400	2.92305900
C	3.76757300	0.58448800	4.40232000
H	3.98376000	-0.41845800	4.02337300
H	4.68932300	1.16058100	4.46850100
H	3.32587500	0.47072400	5.39537100

#### TS4<sup>D</sup>

C	2.26675300	-3.64270300	-2.24305900
C	1.84784600	-2.58730000	-1.43366400
C	2.17869900	-1.27159100	-1.72193900
C	2.94193400	-1.05303700	-2.85927000
C	3.39229900	-2.08194000	-3.68150100
C	3.05213800	-3.39318600	-3.36751500
C	1.75286200	-4.95941600	-1.72670600
C	0.72369100	-4.60267300	-0.62849000
C	0.96987500	-3.07938800	-0.30387500
H	1.87168700	-0.42782600	-1.11087500
H	3.98759500	-1.84317600	-4.55459500
H	3.38410600	-4.20762100	-4.00289200
H	1.28316600	-5.57316200	-2.50135400
H	0.87343100	-5.19558300	0.27328300
H	2.56954800	-5.55086900	-1.30097500
H	1.41357000	-2.94015100	0.68408300
N	-0.30701400	-2.34874300	-0.32196400
O	-0.61133500	-4.88059700	-1.01278200
C	-0.65022200	-1.18608400	0.25563100
C	-1.31293900	-2.67001700	-1.18827900
N	-1.83089200	-0.84877000	-0.26335000
N	-2.26278200	-1.77727100	-1.15516000
C	-1.18238000	-3.96517500	-1.92400900



H	-0.57292400	-3.83432900	-2.82957300
H	-2.16601400	-4.33772300	-2.21117300
C	-2.64024000	0.29990100	0.06567100
C	-2.86715600	1.24279000	-0.94447200
C	-3.12700500	0.42458900	1.36865100
C	-3.59040000	2.37742600	-0.59193900
C	-3.85088200	1.58087400	1.66054800
C	-4.08296300	2.56660700	0.70276700
H	-3.76934700	3.13798500	-1.34769900
H	-4.24121800	1.71049200	2.66624600
C	-4.87033000	3.80284000	1.04033700
C	0.31151300	1.83672200	0.29002700
C	0.44706500	0.94152700	1.31216600
H	0.04356100	1.48426300	-0.71266300
C	0.53421100	3.26074000	0.38375800
C	0.83639300	3.87417700	1.61294800
C	0.42218400	4.04687100	-0.77509400
C	1.01256200	5.24617700	1.67542900
H	0.92882100	3.25550900	2.50020400
C	0.60516100	5.42042900	-0.70901700
H	0.19941700	3.56475600	-1.72404700
C	0.89802400	6.01849500	0.51605000
H	1.24310400	5.72289000	2.62223900
H	0.52571100	6.02526200	-1.60590400
H	1.04363800	7.09285300	0.56925900
C	0.16881200	-0.41778100	1.20859800
H	1.09777900	0.08419300	2.41950200
O	0.76901800	-1.05484200	2.15381200
N	3.25840400	0.33712200	-3.22079000
O	2.71451500	1.22059300	-2.57955200
O	4.03005000	0.51953100	-4.14128900
H	-4.42525900	4.68896000	0.58072500
H	-4.91901700	3.96187400	2.11930400
H	-5.89591400	3.71965800	0.66613200
C	-2.88836300	-0.61855300	2.42806500
H	-2.92354400	-1.63334200	2.02102800
H	-1.92027300	-0.48160900	2.92289100
H	-3.65564300	-0.54451900	3.20035700
C	-2.36495300	1.04871500	-2.35001400
H	-1.33324500	0.68148500	-2.37712100
H	-2.98001700	0.31811800	-2.88422100
H	-2.40289500	1.99148700	-2.89834800

**E-M4**

C	4.91664400	-0.40486500	0.12386400
C	3.57348000	-0.24695100	0.46178300
C	2.97586500	1.00422400	0.50742800
C	3.77766000	2.09143500	0.19110100
C	5.12443100	1.97310300	-0.14070100
C	5.70116100	0.70915800	-0.17204200
C	5.31725400	-1.85467000	0.13768000
C	4.00843600	-2.65111800	0.36525200
C	2.90698600	-1.57868100	0.72000800
H	1.93502100	1.15704700	0.77745400
H	5.69470100	2.86406500	-0.37398700
H	6.74812400	0.59606500	-0.43399100
H	5.79580000	-2.17116800	-0.79476700
H	4.10686700	-3.34730500	1.19731200
H	6.02969100	-2.05268000	0.94405600
H	2.55353000	-1.68726400	1.74642200
N	1.73658800	-1.74294100	-0.15139200
O	3.66760700	-3.47232300	-0.73640300
C	0.46120600	-1.36345000	0.03586100
C	1.82835200	-2.22340600	-1.42735600
N	-0.16344800	-1.63504700	-1.10708500
N	0.67283200	-2.18076100	-2.02862600
C	3.14626600	-2.78180800	-1.85373900
H	3.81648800	-1.98196900	-2.19898600
H	3.00943300	-3.49968900	-2.66268500
C	-1.57976400	-1.47234200	-1.32294700
C	-2.01944200	-0.39822300	-2.10369800
C	-2.42542900	-2.31069800	-0.59766800
C	-3.38001400	-0.11494300	-2.05698800
C	-3.78060100	-1.98340700	-0.59158400
C	-4.26131700	-0.86871300	-1.27327300
H	-3.75476300	0.74195900	-2.61207200
H	-4.45319900	-2.56634600	0.02914800
C	-5.69445600	-0.44238900	-1.11204800
C	-0.86303000	1.21088600	0.34286900
C	-1.00114600	0.30585400	1.33139400
H	-0.07741500	1.06116300	-0.40156200
C	-1.65510100	2.42309900	0.13515600
C	-2.90843200	2.59737500	0.74315600
C	-1.16032600	3.40838000	-0.73012700
C	-3.63673200	3.75248600	0.48442600
H	-3.30895100	1.81910500	1.39403100
C	-1.89277900	4.56326500	-0.97675400
H	-0.18530400	3.27242000	-1.19160100

C	-3.13449300	4.73549600	-0.36887400
H	-4.60801600	3.88562000	0.95092300
H	-1.49676700	5.32554800	-1.64004700
H	-3.71216400	5.63411700	-0.56347400
C	-0.11956800	-0.85573200	1.36721600
H	-5.69883100	-0.70909300	2.26306300
O	0.24815100	-1.47756900	2.33978000
N	3.16418000	3.42736000	0.18915900
O	1.95958100	3.49142800	0.36100000
O	3.89283000	4.38420300	0.00543200
H	-6.07185700	0.05106000	-2.01154700
H	-5.77017300	0.26878000	-0.28220000
H	-6.33941300	-1.29198000	-0.87810100
C	-1.90495300	-3.48879700	0.17871300
H	-1.08308800	-3.98740600	-0.34515900
H	-1.58942700	-3.17539100	1.17744300
H	-2.70720500	-4.21450300	0.32330000
C	-1.08262600	0.42004300	-2.95215400
H	-0.09264900	0.53422800	-2.49945300
H	-0.93211000	-0.05623300	-3.92686500
H	-1.49610300	1.41659900	-3.12163000
H	-1.73666600	0.38106900	2.13397900
C	-3.83542400	-0.93903900	2.39658900
O	-2.90684000	-1.75507100	2.32381100
O	-3.81526300	0.28574300	2.66975800
O	-5.10766900	-1.46075400	2.13197700

#### Z-TS4

C	-4.30251000	-1.77978700	-0.16215400
C	-3.24617500	-0.88234400	-0.31338100
C	-3.41058400	0.48082100	-0.10927800
C	-4.67880100	0.90213500	0.26646400
C	-5.75709800	0.03567900	0.42252600
C	-5.56770200	-1.32288600	0.20121300
C	-3.86608100	-3.19053200	-0.44860700
C	-2.32389900	-3.13485900	-0.53929800
C	-1.97094800	-1.60570200	-0.68906500
H	-2.60451100	1.19275200	-0.24703400
H	-6.72015100	0.43440100	0.71679500
H	-6.39454800	-2.01546500	0.31903400
H	-4.17450200	-3.90429100	0.32139100
H	-1.95344000	-3.68284200	-1.40598000
H	-4.28958200	-3.53658400	-1.39713800
H	-1.64917700	-1.36471400	-1.70273000

N	-0.87704900	-1.24837000	0.22187000
O	-1.69123300	-3.75735800	0.56638000
C	0.12011900	-0.35268500	0.10948900
C	-0.75793300	-1.82649300	1.45342200
N	0.77898900	-0.40171100	1.26504500
N	0.24437800	-1.32251500	2.11268400
C	-1.65702800	-2.98209100	1.75006600
H	-2.65577800	-2.63975500	2.05403100
H	-1.23270000	-3.59531100	2.54512100
C	1.91316700	0.38835900	1.66904900
C	1.78608300	1.78160200	1.70297100
C	3.09383600	-0.29344100	1.98003500
C	2.93135600	2.50562600	2.02768300
C	4.20421600	0.48634000	2.29763700
C	4.14478100	1.88029700	2.31557200
H	2.87073200	3.59094100	2.04615100
H	5.14047000	-0.01289000	2.53343900
C	5.36108900	2.70509200	2.64079600
C	2.79573700	0.24890700	-1.55059300
C	1.66930300	0.96745200	-1.43033600
H	3.73424200	0.79416900	-1.65857000
C	2.93664300	-1.21602000	-1.52390900
C	1.86586600	-2.09169500	-1.76121000
C	4.18638900	-1.76463200	-1.20219500
C	2.02262900	-3.46535500	-1.60579100
H	0.92066300	-1.69715100	-2.12638600
C	4.34825200	-3.13791700	-1.06304400
H	5.02706600	-1.09559500	-1.03736200
C	3.26257000	-3.99193500	-1.24783700
H	1.18472600	-4.13078100	-1.79078400
H	5.32133500	-3.54375600	-0.80421700
H	3.38665400	-5.06435300	-1.13666100
C	0.35373600	0.49491900	-1.13021400
O	-0.68098500	0.81733700	-1.71881500
N	-4.89016800	2.33563900	0.52294300
O	-3.92256700	3.06920400	0.45002700
O	-6.01890200	2.69803300	0.80173800
H	5.62807400	3.34875400	1.79737300
H	6.22119100	2.07379700	2.87393800
H	5.17318300	3.35635600	3.49965200
C	3.17836700	-1.79702500	1.99543700
H	2.76177200	-2.19508800	2.92600100
H	2.62861500	-2.25235400	1.16633500
H	4.22032200	-2.11449900	1.92457400

C	0.50547600	2.50801500	1.38492800
H	0.49167100	2.83860600	0.33889800
H	-0.38370900	1.90338600	1.58598700
H	0.43397800	3.40863400	1.99867700
C	1.05754600	3.97252000	-2.79048500
O	1.50780200	3.54500400	-1.64815900
O	0.18291800	3.13644200	-3.43140500
H	-0.07465400	2.41141200	-2.84282200
O	1.33943300	5.02381100	-3.32925500
H	1.63181400	2.26802400	-1.56962200

**Z-M4**

C	4.17840600	1.30140000	0.05858100
C	2.95310400	0.64147300	-0.03620800
C	2.78091300	-0.64401100	0.45087800
C	3.88353900	-1.24531000	1.04202800
C	5.12435400	-0.62215600	1.14542600
C	5.27231900	0.66764900	0.64645800
C	4.08836400	2.67845900	-0.54621300
C	2.57686100	2.94368000	-0.75216900
C	1.92111600	1.51698000	-0.70613100
H	1.83992200	-1.17345000	0.37148500
H	5.94665500	-1.14537200	1.61778900
H	6.22923000	1.17311700	0.72692100
H	4.52822900	3.45687500	0.08380300
H	2.34085000	3.39606700	-1.71425300
H	4.61120500	2.70209300	-1.50857100
H	1.69534500	1.19136400	-1.72192800
N	0.66547900	1.52961700	0.05160100
O	2.07456000	3.86427300	0.20322100
C	-0.48852700	0.86335500	-0.11080600
C	0.48764500	2.39570800	1.08853200
N	-1.30647100	1.33142700	0.83120900
N	-0.71213200	2.29772100	1.58343700
C	1.61255500	3.31974300	1.41522100
H	2.40112500	2.77911300	1.95971200
H	1.25292200	4.13934900	2.03825200
C	-2.68351300	0.99297800	1.08632800
C	-2.97533800	-0.16720900	1.80274600
C	-3.65575500	1.88445000	0.61547400
C	-4.32340000	-0.45478300	2.01996800
C	-4.98377600	1.54719500	0.86264900
C	-5.33476000	0.38309900	1.55310300
H	-4.58381900	-1.35375300	2.57283300

H	-5.76576900	2.21361100	0.50674900
C	-6.78474600	0.04345600	1.77390700
C	-2.27782800	-2.15897800	-1.44114500
C	-2.00795700	-0.85333300	-1.28257400
H	-3.31603000	-2.39133600	-1.67589400
C	-1.41320200	-3.35076700	-1.34272100
C	-0.29433700	-3.44423900	-0.50347400
C	-1.77818800	-4.47686700	-2.09228400
C	0.44926400	-4.61531200	-0.43762800
H	-0.00470900	-2.60307700	0.11721000
C	-1.02556600	-5.64536800	-2.04134500
H	-2.65814100	-4.42776100	-2.72821500
C	0.09094800	-5.71697600	-1.21383800
H	1.30793800	-4.66321900	0.22436100
H	-1.31773800	-6.50212400	-2.64016500
H	0.67548200	-6.63022200	-1.16462700
C	-0.65945000	-0.28855200	-1.08005300
O	0.36658700	-0.73359100	-1.55477800
N	3.72174100	-2.59670700	1.59062000
O	2.59568900	-3.06875300	1.60919400
O	4.71369600	-3.16827300	2.00298000
H	-7.23960400	-0.32261600	0.84745400
H	-7.35116300	0.92379700	2.08938000
H	-6.90200900	-0.73192500	2.53400300
C	-3.26871300	3.13540600	-0.12262600
H	-2.72332900	3.82070200	0.53448800
H	-2.61466900	2.90230100	-0.97133200
H	-4.16068400	3.64780600	-0.48817800
C	-1.89926000	-1.09667700	2.29267900
H	-1.63203700	-1.81955100	1.51257700
H	-0.99474400	-0.55773100	2.58861900
H	-2.25063400	-1.66524900	3.15597500
C	-0.42834500	2.39539700	-2.55593600
O	-1.41850500	1.61826400	-2.42198200
O	0.46400900	2.03702200	-3.55845700
H	0.07925100	1.25020600	-3.96755400
O	-0.11587400	3.38149000	-1.88451600
H	-2.80789100	-0.12561900	-1.35385200

**re-TS5**

C	3.66636200	-3.42160400	-6.43787900
C	3.14449100	-2.25179700	-5.88126700
C	2.71503100	-1.19894800	-6.67435000
C	2.84139600	-1.36441700	-8.04794000

C	3.38173000	-2.50368600	-8.63541800
C	3.79912200	-3.54854100	-7.81753800
C	4.01132500	-4.41296900	-5.35717700
C	3.24719400	-3.90478300	-4.12079000
C	3.11047800	-2.36587900	-4.36899200
H	2.32212500	-0.28217300	-6.24846100
H	3.45521200	-2.56252900	-9.71435800
H	4.20698500	-4.45384700	-8.25504200
H	3.72432500	-5.44069000	-5.59247600
H	3.78439700	-4.09728300	-3.19076700
H	5.08984700	-4.40215900	-5.16195400
H	3.92374900	-1.82795400	-3.87704800
N	1.85829100	-1.88365400	-3.79418000
O	1.99520700	-4.56755300	-3.96556000
C	1.56183800	-0.79148000	-3.07043700
C	0.71278900	-2.61665000	-3.92668900
N	0.26101600	-0.90438800	-2.79682200
N	-0.28477200	-2.04310100	-3.32205900
C	0.85414800	-3.96562300	-4.55351600
H	0.93504500	-3.88787400	-5.64483700
H	-0.00793800	-4.58459700	-4.30370600
C	-0.54631400	-0.00845600	-2.01021300
C	-1.47164600	0.79311900	-2.67851500
C	-0.32665500	0.04320000	-0.62982100
C	-2.15349900	1.74223800	-1.91552900
C	-1.02974700	1.01091300	0.08172500
C	-1.92929700	1.87744500	-0.54556300
H	-2.86882600	2.39511800	-2.40889400
H	-0.86536900	1.09696500	1.15297400
C	-2.62323200	2.94439700	0.25674500
C	2.72323200	2.03294200	-0.93360300
C	2.09619500	1.45939900	-1.96580200
H	3.60690300	1.52985900	-0.54311500
C	2.33384300	3.28386400	-0.27210300
C	3.19203400	3.82795600	0.69126000
C	1.13364900	3.95387800	-0.55790200
C	2.87433600	5.01271700	1.34630400
H	4.12245000	3.31424000	0.91721000
C	0.81915500	5.14041800	0.09395700
H	0.44295000	3.54443700	-1.29069700
C	1.68647600	5.67395200	1.04828400
H	3.55613800	5.42025300	2.08592700
H	-0.10708700	5.65516600	-0.14443100
H	1.43576300	6.59990300	1.55618800

C	2. 60569500	0. 17349700	-2. 50315800
O	3. 60552100	-0. 41034800	-2. 06615600
N	2. 35745300	-0. 28642000	-8. 92273800
O	1. 74487300	0. 62905700	-8. 40380000
O	2. 58527900	-0. 37941900	-10. 11561200
H	-3. 17080700	2. 50986300	1. 09833400
H	-3. 32790500	3. 51174900	-0. 35482600
H	-1. 88928600	3. 64337800	0. 67178900
C	0. 62544600	-0. 90136800	0. 05378900
H	0. 42291900	-1. 93791200	-0. 23520800
H	1. 67038700	-0. 68213700	-0. 18980700
H	0. 51644000	-0. 82411900	1. 13696400
C	-1. 73595500	0. 62739000	-4. 15010500
H	-0. 80969300	0. 62431500	-4. 73188600
H	-2. 24957700	-0. 31979100	-4. 34344700
H	-2. 36532100	1. 43948300	-4. 51763700
H	1. 22982500	1. 90135500	-2. 44753200
C	3. 45066200	2. 11004400	-4. 58524100
S	4. 99772000	2. 73493100	-4. 86422300
N	3. 17639900	0. 82996400	-4. 36475000
H	4. 06286900	0. 31848600	-4. 36690200
C	2. 26807300	3. 02648800	-4. 58980900
C	2. 30783600	4. 25367500	-3. 92117500
C	1. 09350200	2. 64571200	-5. 24489700
C	1. 18345600	5. 07156800	-3. 88643500
H	3. 22459200	4. 54736200	-3. 42025100
C	-0. 02327100	3. 47855400	-5. 23266100
H	1. 07521400	1. 70911200	-5. 79519400
C	0. 01443400	4. 68769300	-4. 54281600
H	1. 22107000	6. 01126800	-3. 34374700
H	-0. 91841800	3. 18724700	-5. 77431700
H	-0. 85794000	5. 33394200	-4. 52799100

**si-TS5**

C	3. 76938400	-4. 84454600	-5. 19861400
C	3. 55814300	-3. 48025100	-5. 00345400
C	3. 60481800	-2. 57556100	-6. 05527200
C	3. 86174700	-3. 10119900	-7. 31359400
C	4. 08619500	-4. 45609500	-7. 54615000
C	4. 04194300	-5. 33871200	-6. 47357800
C	3. 66252200	-5. 60019900	-3. 90087600
C	3. 07934600	-4. 59075700	-2. 88433400
C	3. 25327800	-3. 17524500	-3. 55281100
H	3. 46486100	-1. 51101900	-5. 89805100



H	4. 28399000	-4. 79750400	-8. 55464800
H	4. 20821600	-6. 39888200	-6. 63435200
H	3. 02544600	-6. 48750900	-3. 96590000
H	3. 61543600	-4. 61933600	-1. 93532500
H	4. 65125300	-5. 93677400	-3. 57275300
H	4. 02606300	-2. 58271100	-3. 05877100
N	2. 00708600	-2. 41663600	-3. 44102500
O	1. 73372700	-4. 88587200	-2. 53389800
C	1. 79821700	-1. 09982300	-3. 31017200
C	0. 78322600	-3. 01625900	-3. 53828900
N	0. 47742500	-0. 94135600	-3. 39429200
N	-0. 17447900	-2. 13716200	-3. 51017500
C	0. 76386700	-4. 50910900	-3. 49434300
H	0. 96986600	-4. 93938500	-4. 48373900
H	-0. 20832300	-4. 86257200	-3. 14991000
C	-0. 25366500	0. 29377000	-3. 52617700
C	-0. 06881300	1. 04647600	-4. 69078700
C	-1. 10372800	0. 67439500	-2. 48674400
C	-0. 75151900	2. 25819600	-4. 77159700
C	-1. 77106300	1. 89088600	-2. 62514200
C	-1. 59476900	2. 69904100	-3. 74937500
H	-0. 61700700	2. 87534200	-5. 65623000
H	-2. 43219600	2. 21875400	-1. 82704300
C	-2. 26442400	4. 04285700	-3. 84631200
C	2. 94022100	2. 39945000	-3. 14886100
C	2. 47101800	1. 25217900	-2. 64870000
H	3. 67328800	2. 33190600	-3. 95159900
C	2. 54426100	3. 74688200	-2. 71834700
C	3. 34321600	4. 84247100	-3. 06618700
C	1. 36458500	3. 97763500	-1. 99581800
C	2. 99092300	6. 13187200	-2. 68011100
H	4. 25336800	4. 67423700	-3. 63529700
C	1. 01171800	5. 26537300	-1. 61243200
H	0. 71050400	3. 14439500	-1. 75371100
C	1. 82480200	6. 34742100	-1. 95121500
H	3. 62677500	6. 96883100	-2. 95071000
H	0. 09572300	5. 42787200	-1. 05231100
H	1. 54625300	7. 35294800	-1. 65226400
C	2. 89340300	-0. 04463600	-3. 23986900
O	3. 76131700	-0. 14872700	-4. 12054600
N	3. 88573800	-2. 17887200	-8. 45843500
O	3. 56533600	-1. 02130500	-8. 25804900
O	4. 21566500	-2. 62864200	-9. 54159600
H	-2. 63514800	4. 23050600	-4. 85727700

H	-1.54875600	4.83689300	-3.60614700
H	-3.10222300	4.12340500	-3.15024400
C	-1.26283400	-0.18856800	-1.26857400
H	-1.84930300	-1.08524600	-1.49339400
H	-0.29023800	-0.52386300	-0.89804600
H	-1.76515700	0.35928700	-0.46927700
C	0.83952500	0.59035900	-5.80156600
H	1.89281300	0.77079900	-5.55902500
H	0.71907700	-0.47859300	-6.00635800
H	0.61466000	1.13393900	-6.72071900
H	1.77314300	1.21428300	-1.81466500
C	3.51929400	-0.52021800	-0.31913000
S	4.56079800	0.31508400	0.71772700
N	3.77470500	-0.78567800	-1.59499900
H	4.68783300	-0.40249000	-1.84791400
C	2.22583100	-1.06535500	0.20890900
C	1.49638400	-0.39450200	1.19713800
C	1.76486200	-2.30983700	-0.23868400
C	0.33559600	-0.95610400	1.71937400
H	1.86546900	0.55968800	1.55918000
C	0.60663200	-2.87569400	0.28708200
H	2.35542100	-2.85647400	-0.96437800
C	-0.11249700	-2.19839600	1.26942400
H	-0.21974800	-0.42451500	2.48601600
H	0.28364500	-3.85249900	-0.06147400
H	-1.01274800	-2.63742400	1.68833900

**re-M5**

C	3.64519200	-3.30745500	-6.65020000
C	3.21040200	-2.12084400	-6.05888500
C	2.85289200	-1.02216600	-6.82584100
C	2.96522500	-1.15224900	-8.20279500
C	3.42404300	-2.30971900	-8.82347200
C	3.76465200	-3.40357300	-8.03500000
C	3.92054600	-4.35811200	-5.60754300
C	3.33601700	-3.79350600	-4.29227100
C	3.17068900	-2.25024500	-4.55205000
H	2.50291400	-0.09554700	-6.38821100
H	3.49286100	-2.34374300	-9.90383000
H	4.10585100	-4.32319400	-8.49940000
H	3.46308500	-5.32465900	-5.83839500
H	4.01096200	-3.95129100	-3.45081600
H	4.99819800	-4.52322500	-5.50307900
H	3.96610200	-1.70741900	-4.03646100

N	1.91622000	-1.75991400	-3.98816400
O	2.13678800	-4.45104100	-3.90972100
C	1.63666900	-0.60861300	-3.34154900
C	0.80189200	-2.54843400	-3.95212300
N	0.36949600	-0.75729700	-2.94208500
N	-0.16374400	-1.96680900	-3.30941500
C	0.94403000	-3.93933200	-4.47487900
H	0.96670500	-3.95076600	-5.57318200
H	0.11671400	-4.55989700	-4.12984900
C	-0.43222000	0.14566600	-2.15913100
C	-1.44968600	0.84551300	-2.80625300
C	-0.15134800	0.27131000	-0.79401300
C	-2.15727800	1.78314200	-2.05194500
C	-0.88378100	1.22272800	-0.08982100
C	-1.87421200	1.99527800	-0.70355500
H	-2.94452700	2.35754900	-2.53374900
H	-0.66940900	1.37426300	0.96542600
C	-2.60773900	3.03794200	0.09576200
C	2.73348100	2.07185400	-1.10737700
C	2.17573700	1.63427600	-2.23610300
H	3.59134000	1.51120700	-0.73842700
C	2.28934600	3.22395500	-0.30904600
C	3.01762900	3.57365400	0.83473100
C	1.15953000	3.98968300	-0.63963700
C	2.64145300	4.65655800	1.62359600
H	3.89294700	2.98696300	1.10034400
C	0.78721700	5.07516300	0.14476700
H	0.56998300	3.73708500	-1.51716600
C	1.52502800	5.41313000	1.28019300
H	3.22271300	4.91078200	2.50452000
H	-0.08171300	5.66505500	-0.13268100
H	1.23138200	6.26228100	1.88926900
C	2.76840800	0.41119500	-2.92345300
O	3.63136300	-0.29280900	-2.26215800
N	2.55227800	-0.01686200	-9.03931300
O	1.97433900	0.90480400	-8.49183500
O	2.79852700	-0.07206500	-10.23063800
H	-3.14023000	2.58431100	0.93738000
H	-3.33423400	3.57655400	-0.51654400
H	-1.90048500	3.76333400	0.51141700
C	0.87527800	-0.59697700	-0.11832000
H	0.55261300	-1.64433100	-0.13380000
H	1.85618300	-0.54227900	-0.60203100
H	0.99495000	-0.29409700	0.92394400

C	-1.79772700	0.56377300	-4.24218500
H	-0.91092300	0.55610800	-4.88214200
H	-2.27266400	-0.41867900	-4.33277500
H	-2.49318300	1.31340500	-4.62395400
H	1.30992800	2.11546400	-2.67953900
C	3.48964900	2.01250800	-4.93957200
S	4.79542000	2.43305000	-5.89274400
N	3.44430900	0.85257800	-4.26795500
H	4.33307900	0.35579900	-4.29891700
C	2.29425200	2.90005200	-4.87160900
C	2.38842300	4.15785900	-4.27082900
C	1.07700200	2.47230700	-5.40280300
C	1.26006200	4.96272300	-4.16724900
H	3.34127800	4.48422100	-3.86619500
C	-0.04385500	3.29622400	-5.32395500
H	1.01807800	1.51423600	-5.91346500
C	0.04055400	4.53314100	-4.69081200
H	1.33355200	5.92777300	-3.67557100
H	-0.98158000	2.97213200	-5.76410300
H	-0.83688200	5.16824900	-4.62047500

**si-M5**

C	3.83201400	-4.88021300	-5.11923900
C	3.63052500	-3.53396600	-4.81924800
C	3.74386600	-2.54038300	-5.78342100
C	4.05292300	-2.96432900	-7.06796200
C	4.27537000	-4.29767300	-7.40463200
C	4.16652200	-5.26839900	-6.41602700
C	3.63710900	-5.74208400	-3.89985900
C	2.98904400	-4.81466100	-2.84654800
C	3.25215100	-3.35249100	-3.36340700
H	3.61204300	-1.49150200	-5.52584900
H	4.51902100	-4.55465900	-8.42824600
H	4.32811100	-6.31367400	-6.65898800
H	3.00234900	-6.61481300	-4.08146300
H	3.43243900	-4.95140300	-1.85976600
H	4.60027200	-6.11302800	-3.53417800
H	4.03122000	-2.85089400	-2.78857100
N	2.02605600	-2.55976700	-3.24067200
O	1.60833500	-5.09102600	-2.65292100
C	1.84278200	-1.24426700	-3.02410400
C	0.80986400	-3.10067900	-3.55719100
N	0.54925900	-1.03166000	-3.27243600
N	-0.11506700	-2.19084600	-3.58510400
C	0.74951500	-4.59075500	-3.66299200

H	1.04315800	-4.93392900	-4.66391300
H	-0.26044800	-4.94350700	-3.45231000
C	-0.14455900	0.22440300	-3.43002900
C	0.08570500	0.94863300	-4.60378500
C	-1.01672000	0.63774000	-2.42568900
C	-0.58216100	2.16365600	-4.73283800
C	-1.67461200	1.85354900	-2.61298800
C	-1.45797000	2.63178800	-3.74985700
H	-0.40748200	2.76362100	-5.62258100
H	-2.35525600	2.20700500	-1.84228700
C	-2.11250900	3.97829900	-3.89955800
C	2.83776600	2.21339700	-2.90311300
C	2.47421400	1.09281900	-2.28019100
H	3.51657600	2.10017800	-3.74776000
C	2.41037700	3.57718000	-2.55171100
C	3.16931300	4.67056300	-2.98544300
C	1.24489100	3.82244800	-1.81281000
C	2.78870600	5.97203900	-2.67298500
H	4.06921300	4.49081500	-3.56760600
C	0.86028200	5.12223800	-1.50559900
H	0.62406900	2.98621000	-1.50377000
C	1.63301400	6.20272500	-1.93203000
H	3.39404500	6.80745600	-3.01106400
H	-0.05006500	5.29513900	-0.93866400
H	1.33166500	7.21765300	-1.69214100
C	3.00028200	-0.24576300	-2.78157000
O	3.74075400	-0.24072600	-3.85053400
N	4.12991800	-1.95218500	-8.13210200
O	3.79218200	-0.81559700	-7.85708200
O	4.51689300	-2.31287300	-9.23062300
H	-2.51917500	4.11400200	-4.90548700
H	-1.37794000	4.77334800	-3.73069000
H	-2.92367000	4.11097100	-3.17991200
C	-1.17910700	-0.17934100	-1.17729600
H	-1.52397400	-1.19314000	-1.40401400
H	-0.21946000	-0.27279300	-0.65808900
H	-1.89258000	0.28569200	-0.49413800
C	1.04520300	0.45481600	-5.65113600
H	2.07279100	0.44533500	-5.26557500
H	0.79595900	-0.56592500	-5.96349200
H	1.01266700	1.09374800	-6.53525100
H	1.83791400	1.09266100	-1.39495400
C	3.73652000	-0.90503700	-0.29133900
S	5.05605900	-0.85677200	0.73555600

N	3.86780700	-0.84172200	-1.62114800
H	4.82585000	-0.70536100	-1.93982700
C	2.37657600	-1.13322700	0.28712200
C	1.86839700	-0.26197100	1.25683300
C	1.67396400	-2.30432600	-0.01635400
C	0.67522200	-0.55745900	1.90643100
H	2.43064400	0.63181600	1.50870900
C	0.48935100	-2.60742900	0.65117200
H	2.08376700	-3.01289400	-0.72956000
C	-0.01230200	-1.73531200	1.61330300
H	0.28918800	0.12629200	2.65561300
H	-0.03122000	-3.53274600	0.42381800
H	-0.93290100	-1.97227700	2.13716300

**TS5R**

C	-5.36938500	-0.34017100	-0.65421600
C	-3.98041000	-0.21675400	-0.59187200
C	-3.35772700	1.01353300	-0.43688600
C	-4.19600900	2.12004200	-0.37306400
C	-5.58159800	2.04244800	-0.47250500
C	-6.17779000	0.79278300	-0.61069100
C	-5.76814900	-1.79179500	-0.73612400
C	-4.49856500	-2.56851300	-0.32535100
C	-3.32740100	-1.58450400	-0.64634000
H	-2.27631300	1.13908400	-0.37406800
H	-6.17072400	2.94976600	-0.41956100
H	-7.25841300	0.70752400	-0.66020600
H	-6.60509300	-2.05363900	-0.08338300
H	-4.38740800	-3.49658400	-0.88681800
H	-6.05198200	-2.05523800	-1.76098000
H	-2.87004400	-1.79683600	-1.61087500
N	-2.28001300	-1.68245700	0.37622400
O	-4.52906200	-2.97689400	1.03672600
C	-0.94244300	-1.50403600	0.33412300
C	-2.64648500	-1.74773300	1.69023700
N	-0.56845000	-1.44572600	1.61852100
N	-1.61753500	-1.60734700	2.47200200
C	-4.08339900	-2.03069800	1.98932000
H	-4.67278900	-1.10451700	1.97107800
H	-4.17451300	-2.48472000	2.97667400
C	0.71203500	-1.06152400	2.15788900
C	0.89872000	0.29915100	2.40946100
C	1.69004000	-2.03730500	2.35798200
C	2.16916200	0.68934900	2.83295800

C	2. 93681900	-1. 59374100	2. 79121900
C	3. 19732100	-0. 23582500	3. 01038800
H	2. 35945500	1. 74532800	3. 00320100
H	3. 73018200	-2. 32239100	2. 94200200
C	4. 57685000	0. 21285900	3. 41261600
C	2. 01660200	-1. 48875700	-2. 04154200
C	1. 28048500	-1. 40377500	-0. 88376600
H	1. 49909200	-1. 82323100	-2. 93506600
C	3. 48876100	-1. 53034700	-2. 07580000
C	4. 14363900	-1. 59530700	-3. 31289300
C	4. 26162700	-1. 54040400	-0. 90656000
C	5. 52876900	-1. 65542300	-3. 38349000
H	3. 54984600	-1. 57592200	-4. 22282400
C	5. 64996500	-1. 59733700	-0. 97744900
H	3. 77830100	-1. 51392300	0. 06613100
C	6. 28831100	-1. 65301400	-2. 21386100
H	6. 01867400	-1. 69796200	-4. 35097700
H	6. 23474400	-1. 60493500	-0. 06251300
H	7. 37155200	-1. 69716000	-2. 26701500
C	-0. 13134300	-1. 55876400	-0. 95784400
O	-0. 79088900	-1. 81988200	-1. 96818800
N	-3. 58236300	3. 43799900	-0. 15339000
O	-2. 41767600	3. 46259400	0. 19982500
O	-4. 27921700	4. 42285700	-0. 32369100
H	4. 91840100	-0. 31387000	4. 30877000
H	4. 60189800	1. 28584100	3. 61345700
H	5. 29616600	0. 00257700	2. 61432300
C	1. 42340400	-3. 48135800	2. 03519500
H	0. 46352200	-3. 81380800	2. 44125900
H	1. 39966800	-3. 63057000	0. 94882600
H	2. 20918100	-4. 11873400	2. 44427300
C	-0. 21294700	1. 29050400	2. 20151400
H	-0. 45453000	1. 37832300	1. 13437600
H	-1. 11392100	0. 98903000	2. 74618600
H	0. 08766900	2. 27732600	2. 55604000
H	1. 73688500	-1. 07502000	0. 03868500
C	0. 96158800	1. 46354300	-1. 65750400
S	1. 66327800	0. 90604000	-3. 14337700
N	-0. 24807500	1. 20159200	-1. 27398000
H	-0. 70641700	0. 69175500	-2. 03559300
C	1. 82198900	2. 22638600	-0. 69593800
C	3. 17623700	1. 91687800	-0. 53566500
C	1. 26363100	3. 25570000	0. 06909000
C	3. 95543400	2. 61483800	0. 38279800

H	3.61252800	1.13433700	-1.14917600
C	2.04994100	3.97091000	0.96890400
H	0.21099600	3.49149500	-0.06078000
C	3.39735600	3.65008100	1.13136300
H	5.00457400	2.35925400	0.50104100
H	1.61064900	4.78427400	1.53942900
H	4.01075200	4.21030500	1.83133500

**TS5R'**

C	5.62100100	0.21859000	-0.72364800
C	4.22969200	0.17391800	-0.79558800
C	3.54444100	-1.01806000	-0.98940600
C	4.31751800	-2.16536800	-1.09574200
C	5.70923500	-2.15771700	-1.04340700
C	6.36974700	-0.94966700	-0.85646300
C	6.10908100	1.62453000	-0.49871700
C	4.84466300	2.45430200	-0.17285300
C	3.62898100	1.54918000	-0.59710400
H	2.46312600	-1.05560400	-1.07222100
H	6.24941100	-3.09137500	-1.14107100
H	7.45333400	-0.92412000	-0.80378300
H	6.83397600	1.70458300	0.31742500
H	4.82158200	3.38639000	-0.73752500
H	6.59552400	2.01205200	-1.39950200
H	3.13441300	1.91388200	-1.49678800
N	2.62571600	1.50909000	0.47352300
O	4.79956200	2.86805300	1.18336900
C	1.29873200	1.29332200	0.42571100
C	2.98297600	1.54184700	1.79288800
N	0.91497200	1.17752100	1.69685800
N	1.95403600	1.34242800	2.56391700
C	4.40795200	1.86680000	2.10178700
H	5.03449700	0.96671500	2.02998300
H	4.49539600	2.27643900	3.10834100
C	-0.38174200	0.76051200	2.16327700
C	-0.79381300	-0.54058300	1.86109400
C	-1.17482000	1.69104400	2.83887400
C	-2.08198200	-0.89654800	2.25280900
C	-2.46327100	1.28866700	3.18328000
C	-2.93700800	0.00946300	2.88013000
H	-2.43519400	-1.90105400	2.03706600
H	-3.11756100	1.99635200	3.68638500
C	-4.36203700	-0.37777700	3.15835300
C	-1.61068000	1.56101600	-1.95370700



C	-0.83262600	1.62697600	-0.80477300
H	-1.08654600	1.32079900	-2.87376200
C	-2.89062400	2.27092300	-2.10910700
C	-3.46156400	2.36774300	-3.38561500
C	-3.54830900	2.87717400	-1.02959300
C	-4.65280700	3.05224800	-3.58175500
H	-2.96791300	1.87662600	-4.21943000
C	-4.74545100	3.55733600	-1.22580900
H	-3.14110100	2.79589400	-0.02660800
C	-5.29976800	3.64927700	-2.50017600
H	-5.08372500	3.11393100	-4.57589900
H	-5.24910300	4.01365900	-0.37958700
H	-6.23595600	4.17782500	-2.64982700
C	0.49963600	1.17611700	-0.85433800
O	1.13575000	0.73039200	-1.82331400
N	3.62879100	-3.45538100	-1.25618800
O	2.41743400	-3.46574000	-1.13979300
O	4.31378200	-4.43685500	-1.48356400
H	-4.80874500	0.25022200	3.93311500
H	-4.43521600	-1.42434800	3.46574800
H	-4.94219900	-0.26236600	2.23504500
C	-0.66598800	3.07530200	3.13872400
H	0.16018600	3.04862300	3.85584700
H	-0.29665800	3.56916900	2.23275700
H	-1.46269600	3.69195400	3.55840500
C	0.06998500	-1.50753200	1.09527100
H	-0.07484800	-1.37656000	0.01410500
H	1.13360700	-1.38959400	1.32672100
H	-0.21362700	-2.53448300	1.33406100
H	-1.23964700	1.97309800	0.13582900
C	-3.50006600	-1.18500200	-0.91807400
S	-2.34741800	-0.92487200	-2.22806400
N	-4.35047700	-0.33665400	-0.46575300
H	-4.31028500	0.52075100	-1.01726600
C	-3.49548100	-2.53862600	-0.25531100
C	-2.42723000	-3.43174300	-0.36998200
C	-4.58695600	-2.89597600	0.54740300
C	-2.43252500	-4.63680100	0.33103400
H	-1.58548200	-3.16936500	-1.00251400
C	-4.59449500	-4.09898200	1.24351000
H	-5.42119600	-2.20646100	0.61502100
C	-3.51092400	-4.97183900	1.14536800
H	-1.58959600	-5.31515200	0.23750800
H	-5.44945300	-4.35989900	1.86062000

H	-3.51393400	-5.91083400	1.69068200
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**TS5R"**

C	-4.54331300	-0.99465000	-1.05121200
C	-3.22413100	-0.63340000	-0.77810400
C	-2.86762200	0.01823800	0.39351100
C	-3.89383300	0.26308700	1.29620500
C	-5.22665400	-0.04376300	1.04143600
C	-5.55790200	-0.67697300	-0.15185000
C	-4.63006200	-1.74690800	-2.35357700
C	-3.17585900	-2.16399900	-2.66716100
C	-2.29069400	-1.16318600	-1.84685500
H	-1.84946000	0.33276800	0.60865000
H	-5.97773800	0.19163300	1.78586500
H	-6.58873700	-0.94703600	-0.35706400
H	-5.27701500	-2.62723300	-2.30925800
H	-2.95007600	-2.08615700	-3.73083400
H	-5.01254600	-1.09624900	-3.14731700
H	-1.86514100	-0.37588100	-2.46717600
N	-1.18921900	-1.87848100	-1.18714900
O	-2.92166000	-3.52662400	-2.35259800
C	0.02446000	-1.46347900	-0.78486200
C	-1.40248200	-3.10755900	-0.62938400
N	0.48220100	-2.43215000	0.01228700
N	-0.39415300	-3.47227200	0.10693900
C	-2.67289300	-3.80798300	-0.98972700
H	-3.49215300	-3.47768000	-0.33596300
H	-2.55220200	-4.88656900	-0.88451300
C	1.66338900	-2.40858300	0.83690500
C	1.75346300	-1.42854800	1.83431000
C	2.66587000	-3.34497500	0.57557600
C	2.93523000	-1.39538700	2.57140200
C	3.82220800	-3.26765600	1.35086000
C	3.97744800	-2.29691600	2.34198000
H	3.04450900	-0.63672300	3.34226100
H	4.62320400	-3.97852600	1.16606600
C	5.25119700	-2.19465300	3.13734800
C	2.67181600	1.17693400	-1.36596300
C	2.03812400	-0.01743900	-1.11884500
H	2.11547100	1.93303400	-1.91088800
C	4.11958600	1.36263900	-1.24347800
C	4.72434100	2.44114500	-1.90274800
C	4.92161700	0.48985500	-0.49484500
C	6.09878100	2.62789500	-1.84148600

H	4. 10028100	3. 13735700	-2. 45640400
C	6. 29622700	0. 68068200	-0. 42987800
H	4. 46405600	-0. 32655300	0. 05836000
C	6. 88875500	1. 74582500	-1. 10623500
H	6. 55508500	3. 46615100	-2. 35800000
H	6. 90827700	0. 00229500	0. 15652800
H	7. 96256200	1. 89520600	-1. 05077400
C	0. 62530100	-0. 12323300	-1. 16853400
O	-0. 19750400	0. 74488100	-1. 45808600
N	-3. 54986700	0. 83622100	2. 60191900
O	-2. 39599900	0. 73018400	2. 97402900
O	-4. 44122900	1. 36528400	3. 24240300
H	5. 93316500	-3. 01584200	2. 90743300
H	5. 04634700	-2. 20875300	4. 21156100
H	5. 76484800	-1. 25260300	2. 91860300
C	2. 51723800	-4. 38110500	-0. 50593400
H	1. 77321300	-5. 13442700	-0. 23132300
H	2. 19568800	-3. 93282700	-1. 45149900
H	3. 46898300	-4. 88642600	-0. 67861500
C	0. 65853700	-0. 42731700	2. 09111800
H	0. 75954400	0. 45475600	1. 44145500
H	-0. 33603200	-0. 86160500	1. 95114400
H	0. 71422700	-0. 06563900	3. 11946400
H	2. 60535700	-0. 87429300	-0. 77816000
C	0. 33895700	3. 49740900	-0. 71990100
S	1. 74553200	3. 18805200	0. 29223700
N	0. 39814400	3. 85096600	-1. 95710000
H	1. 38177300	3. 94341100	-2. 22184300
C	-1. 04598600	3. 40350400	-0. 13773300
C	-1. 27901600	3. 47350700	1. 23629200
C	-2. 14557200	3. 32760100	-1. 00452900
C	-2. 58141900	3. 50826900	1. 73406800
H	-0. 42888600	3. 51927500	1. 90944600
C	-3. 44272800	3. 34676400	-0. 50849900
H	-1. 95095400	3. 27161500	-2. 06982700
C	-3. 66732200	3. 44941100	0. 86555700
H	-2. 74804400	3. 56775100	2. 80613000
H	-4. 28473900	3. 28786900	-1. 19314500
H	-4. 68034000	3. 46896800	1. 25823300

**TS5R'''**

C	0. 49942200	-4. 27551400	-0. 31476900
C	0. 46211100	-2. 89104100	-0. 17076200
C	0. 19628100	-2. 28807000	1. 04965100

C	-0.02042700	-3.13448900	2.12666000
C	-0.00852400	-4.52273300	2.01810900
C	0.25491400	-5.10097600	0.78206200
C	0.80300400	-4.66004300	-1.73879000
C	1.22345400	-3.34738600	-2.44123000
C	0.76030400	-2.19436800	-1.47858100
H	0.12943700	-1.21132600	1.17163900
H	-0.20007500	-5.12537100	2.89756600
H	0.27505000	-6.18097300	0.67994200
H	1.59497500	-5.40992900	-1.82869000
H	0.74123500	-3.23698100	-3.41190200
H	-0.09062100	-5.07300200	-2.21769100
H	-0.10557300	-1.64208400	-1.85798300
N	1.85293800	-1.23441800	-1.29178900
O	2.61387800	-3.30381100	-2.73677800
C	1.79606800	0.05961300	-0.95134700
C	3.16378400	-1.61441300	-1.22725100
N	3.04747900	0.41896700	-0.69448500
N	3.92388800	-0.61707900	-0.87692300
C	3.46369400	-3.02021700	-1.64373700
H	3.30892800	-3.71416400	-0.80571400
H	4.49546600	-3.10559600	-1.98589000
C	3.50567000	1.72369300	-0.29465200
C	3.87098400	1.90461300	1.04012000
C	3.57170000	2.72880300	-1.26322400
C	4.31561500	3.17394500	1.40630800
C	4.02111700	3.97769500	-0.84253100
C	4.39342100	4.21696500	0.48278900
H	4.60502700	3.35080700	2.43877700
H	4.08608500	4.78360100	-1.56941900
C	4.85602400	5.58693800	0.90103700
C	-1.35573800	1.52282800	0.38086500
C	-0.00216900	1.25753100	0.28435200
H	-1.88633400	1.70879600	-0.54883500
C	-2.06116800	1.85541800	1.61374400
C	-3.32694900	2.45256900	1.53209300
C	-1.51558900	1.58451000	2.87904000
C	-4.02157000	2.79326700	2.68908300
H	-3.76721300	2.63722200	0.55655900
C	-2.21371100	1.91628600	4.02893000
H	-0.55929300	1.07814900	2.96135700
C	-3.46666900	2.52781800	3.93645200
H	-5.00194500	3.25163500	2.61143600
H	-1.78949600	1.68777400	5.00152800

H	-4.01305200	2.78277700	4.83924100
C	0.49309100	0.83680700	-0.97129100
O	-0.06000200	0.84342800	-2.07296600
N	-0.25593100	-2.53258200	3.44459600
O	-0.04096800	-1.33842900	3.56700400
O	-0.62976300	-3.26217400	4.34400200
H	5.59518900	5.98351200	0.19963600
H	5.30239000	5.57001400	1.89740600
H	4.01575700	6.28849300	0.92042900
C	3.18183300	2.46430900	-2.69282700
H	3.71705200	1.59619100	-3.09154600
H	2.10904300	2.26503200	-2.78989700
H	3.42005500	3.32688500	-3.31695100
C	3.79244100	0.77466500	2.03080100
H	2.77689600	0.36800900	2.10139400
H	4.45533400	-0.04750300	1.74405600
H	4.08226000	1.11754500	3.02516700
H	0.64179700	1.17841900	1.15458500
C	-4.07667800	-0.11453800	-0.33191800
S	-2.51922900	-0.90118400	-0.08894900
N	-4.98110200	0.00085800	0.57309900
H	-4.64870900	-0.45392500	1.42614700
C	-4.37793200	0.53040000	-1.66151500
C	-3.39747200	0.71631700	-2.64038800
C	-5.67762300	0.99010200	-1.91573500
C	-3.70749900	1.35236500	-3.84143300
H	-2.38673200	0.37043600	-2.44735100
C	-5.98777800	1.61337300	-3.11792200
H	-6.43195800	0.84606900	-1.14999900
C	-5.00158400	1.79916700	-4.08720100
H	-2.93023200	1.49658000	-4.58621700
H	-7.00189100	1.95649200	-3.30163200
H	-5.24294800	2.29047000	-5.02527400

### TS5S

C	5.19590500	0.38164600	-0.45817100
C	3.93041000	-0.15687500	-0.68873600
C	3.76082300	-1.43163700	-1.21011000
C	4.91819300	-2.15335200	-1.47050000
C	6.19812500	-1.64873700	-1.25343600
C	6.33888800	-0.36252800	-0.74564900
C	5.09602500	1.78311400	0.08433900
C	3.60214100	1.98751900	0.43077300
C	2.84666200	0.82427500	-0.30573600

H	2.77833300	-1.83754000	-1.42683500
H	7.05875500	-2.26453500	-1.48369300
H	7.32811700	0.04837600	-0.57168200
H	5.71664800	1.95043300	0.97005400
H	3.21988800	2.94265500	0.07110500
H	5.41296700	2.50717400	-0.67337700
H	2.29723100	1.19731200	-1.16702400
N	1.86926200	0.20825900	0.59221100
O	3.37794400	2.02154600	1.83369800
C	0.65996700	-0.31950200	0.35015900
C	2.11094500	0.07691000	1.92934100
N	0.23460100	-0.77930500	1.52865300
N	1.12698000	-0.52563700	2.52994600
C	3.32964700	0.75596000	2.46327200
H	4.23268000	0.16080700	2.26974800
H	3.23307000	0.91412400	3.53764400
C	-0.97443500	-1.50873100	1.81119800
C	-1.09543600	-2.81394400	1.32535200
C	-1.97341100	-0.85781700	2.53835700
C	-2.29252200	-3.47573000	1.58669500
C	-3.15132200	-1.56793300	2.77096100
C	-3.32915600	-2.86942700	2.30018800
H	-2.41999000	-4.49067800	1.21837400
H	-3.95113300	-1.08364500	3.32508400
C	-4.61953200	-3.60912300	2.53310900
C	-2.09095000	0.08303700	-2.17639800
C	-1.39786100	-0.18180400	-1.00606500
H	-1.52991200	-0.01031500	-3.10233200
C	-3.55804800	-0.04687700	-2.29424900
C	-4.16609100	0.15199400	-3.54033100
C	-4.36027400	-0.40592700	-1.20450900
C	-5.53895400	0.01040600	-3.69233100
H	-3.54838200	0.43448200	-4.38903400
C	-5.73565300	-0.54456800	-1.35608700
H	-3.90810100	-0.59430000	-0.23523100
C	-6.33045900	-0.33530600	-2.59782700
H	-5.99433500	0.17061300	-4.66450800
H	-6.34425600	-0.82360100	-0.50134000
H	-7.40405000	-0.44574100	-2.71470100
C	0.00487200	-0.34519200	-1.01669600
O	0.78165500	-0.48220700	-1.97327000
N	4.78355800	-3.51883500	-1.99823500
O	3.66074700	-3.98194600	-2.08617200
O	5.80198300	-4.10971900	-2.31110600

H	-4.43544100	-4.59680100	2.96547100
H	-5.15245000	-3.76051200	1.58882500
H	-5.27833600	-3.05839800	3.20770400
C	-1.79725200	0.55895500	3.01043700
H	-1.02535700	0.62641100	3.78339900
H	-1.49409100	1.21664600	2.18775200
H	-2.73198600	0.94366900	3.42119700
C	0.00130400	-3.47225000	0.53205800
H	0.01970200	-3.10471400	-0.50040100
H	0.98596000	-3.29229500	0.97473000
H	-0.15637100	-4.55131400	0.49141600
H	-1.89293600	-0.08832400	-0.04657600
C	-0.91760300	2.78421100	-1.08032600
S	-2.01789000	2.59308200	-2.42236900
N	0.32463700	2.43707400	-1.12067400
H	0.52364900	2.11956600	-2.07383400
C	-1.43387400	3.26022600	0.24819300
C	-2.80001500	3.28466400	0.54343100
C	-0.52140800	3.64223800	1.24194200
C	-3.24429100	3.68570300	1.80168000
H	-3.50587300	2.98587900	-0.22460300
C	-0.96606200	4.04810400	2.49485000
H	0.53897300	3.61023800	1.01435100
C	-2.33152700	4.07219900	2.77906400
H	-4.30878100	3.69849900	2.01582600
H	-0.24769800	4.35113400	3.25095300
H	-2.67979200	4.39357100	3.75616800

**TS5S'**

C	-4.76666300	0.09195600	0.04896100
C	-3.50373300	-0.38778300	0.39430900
C	-3.34502600	-1.46835900	1.25098000
C	-4.50691800	-2.05059000	1.73929000
C	-5.78361200	-1.59458800	1.42073000
C	-5.91420200	-0.50804900	0.56510200
C	-4.66553800	1.27863900	-0.87106700
C	-3.17471700	1.36711100	-1.27270900
C	-2.41535700	0.43035000	-0.26039100
H	-2.36424500	-1.81971300	1.55099100
H	-6.64759500	-2.09290000	1.84281000
H	-6.89998600	-0.13832900	0.30173600
H	-5.29192900	1.18639500	-1.76389600
H	-2.78624300	2.38146600	-1.17734800
H	-4.97334900	2.19186800	-0.35185200

H	-1.85262400	1.03417700	0.46075400
N	-1.45747600	-0.42035400	-0.97878500
O	-2.97114300	1.03601200	-2.63965200
C	-0.23870000	-0.86282300	-0.62731500
C	-1.69524600	-0.86045300	-2.25043600
N	0.20523700	-1.55320800	-1.67717200
N	-0.69433200	-1.55606700	-2.70560900
C	-2.92991900	-0.34912400	-2.91786600
H	-3.82233600	-0.87525900	-2.54974500
H	-2.85882300	-0.47929900	-3.99804300
C	1.46320000	-2.23834700	-1.81628600
C	1.65559600	-3.43938100	-1.13050100
C	2.43371100	-1.64638400	-2.62955700
C	2.89325200	-4.06235300	-1.28506700
C	3.65082000	-2.31294600	-2.75088600
C	3.89537100	-3.51951000	-2.09055200
H	3.07619500	-4.99841300	-0.76355400
H	4.42764400	-1.87556500	-3.37294300
C	5.20661000	-4.23671800	-2.26797500
C	2.27819900	0.40433900	1.82012400
C	1.76025100	-0.28978300	0.72138500
H	1.60031400	0.56263500	2.65575500
C	3.71525100	0.41735100	2.16554300
C	4.14479600	1.10680600	3.30754800
C	4.65823300	-0.28751100	1.40969400
C	5.48135000	1.09841200	3.68021000
H	3.41720400	1.66588100	3.88952600
C	5.99943200	-0.29264300	1.78165800
H	4.34222400	-0.85552600	0.53987400
C	6.41530400	0.40045600	2.91457400
H	5.79680100	1.63978300	4.56645900
H	6.71949800	-0.84669400	1.18757800
H	7.46154900	0.39510200	3.20403100
C	0.38488300	-0.56959600	0.71372400
O	-0.42718600	-0.52095500	1.65808700
N	-4.38241900	-3.20627800	2.63840000
O	-3.27023100	-3.67116200	2.81194500
O	-5.39969400	-3.63634100	3.15326600
H	5.47878400	-4.79406100	-1.36849800
H	6.01370400	-3.53727400	-2.49845300
H	5.14421500	-4.95356000	-3.09385300
C	2.18404800	-0.32623400	-3.30752800
H	1.31624800	-0.37525600	-3.97155300
H	1.99424200	0.46491500	-2.57228500



H	3.05319800	-0.03091200	-3.89738100
C	0.58693200	-4.02598700	-0.24873000
H	0.52392200	-3.49014600	0.70513000
H	-0.39736500	-3.98190400	-0.72486200
H	0.80865900	-5.07072200	-0.02501400
H	2.34787200	-0.43803900	-0.17586700
C	0.48552700	3.10976100	0.90960900
S	2.21109200	2.79681700	1.03624600
N	-0.47267500	2.44494100	1.44823100
H	-0.11963700	1.68146500	2.02594300
C	0.08063300	4.27056500	0.03965300
C	0.86598800	4.70866600	-1.02934100
C	-1.13484300	4.91687900	0.29491500
C	0.44144300	5.76275600	-1.83344700
H	1.81093000	4.21410700	-1.22786800
C	-1.55286000	5.97773300	-0.50174500
H	-1.73672500	4.57628400	1.13110300
C	-0.76671800	6.40242300	-1.57160200
H	1.05983200	6.08556700	-2.66544900
H	-2.49102600	6.47985400	-0.28447300
H	-1.09159400	7.23109200	-2.19337300

**TS5S"**

C	-3.42939200	-2.08590700	-1.33471800
C	-2.27791100	-1.79082600	-0.60372000
C	-2.06864700	-2.30502500	0.66824500
C	-3.05868500	-3.14134700	1.16999000
C	-4.22593200	-3.44658800	0.47450600
C	-4.41464900	-2.90844400	-0.79364100
C	-3.41403800	-1.38406500	-2.66651900
C	-1.96589200	-0.87795300	-2.84043600
C	-1.37953000	-0.86183600	-1.38755700
H	-1.19329800	-2.05082900	1.25507300
H	-4.96013900	-4.10108600	0.92776100
H	-5.31594800	-3.13709400	-1.35288300
H	-3.70225900	-2.02350800	-3.50522400
H	-1.93508500	0.12947000	-3.25728600
H	-4.10387700	-0.53298300	-2.64249800
H	-1.38445000	0.16206000	-0.99115600
N	0.00812600	-1.32489600	-1.40183800
O	-1.21836400	-1.66666400	-3.76259100
C	1.06868900	-0.91198400	-0.69300800
C	0.44236800	-2.29979500	-2.25336500
N	2.09047700	-1.64889300	-1.11567100

N	1. 71668600	-2. 52206500	-2. 10089000
C	-0. 56099300	-2. 80469700	-3. 24009500
H	-1. 25701000	-3. 50471700	-2. 75792800
H	-0. 06209300	-3. 31238600	-4. 06579100
C	3. 43243200	-1. 64066000	-0. 59768100
C	3. 64178300	-2. 10125000	0. 70376100
C	4. 45752200	-1. 18184600	-1. 43243100
C	4. 95366300	-2. 07376200	1. 17860600
C	5. 74612200	-1. 18085800	-0. 90806800
C	6. 01116800	-1. 62035000	0. 39222200
H	5. 14902000	-2. 42245300	2. 18910000
H	6. 56467200	-0. 82587400	-1. 52948700
C	7. 42049000	-1. 61145000	0. 92109500
C	1. 22332600	2. 45627000	0. 80948300
C	1. 74233000	1. 29842400	0. 24105600
H	0. 45084800	2. 31099900	1. 55778400
C	1. 86074800	3. 77836300	0. 80546900
C	1. 23000400	4. 82559700	1. 49326900
C	3. 08105800	4. 02637100	0. 16566700
C	1. 79961500	6. 09125100	1. 53078000
H	0. 27563300	4. 63965300	1. 98006500
C	3. 65259100	5. 29275300	0. 20785800
H	3. 59178500	3. 22636600	-0. 36091100
C	3. 01363800	6. 32816200	0. 88712000
H	1. 29771200	6. 89374300	2. 06175000
H	4. 60038400	5. 47285600	-0. 28968700
H	3. 46173300	7. 31644400	0. 91772000
C	0. 93660100	0. 14963600	0. 37061000
O	-0. 01667400	-0. 03587700	1. 13993800
N	-2. 86190800	-3. 73383200	2. 50087100
O	-1. 79163600	-3. 54647600	3. 05062200
O	-3. 77708800	-4. 38521400	2. 97274300
H	8. 04035900	-2. 33934600	0. 38800100
H	7. 44762000	-1. 85936700	1. 98412700
H	7. 88300300	-0. 62932100	0. 78761100
C	4. 17436600	-0. 71111900	-2. 83336700
H	3. 89976400	-1. 54840100	-3. 48190600
H	3. 34653400	0. 00513500	-2. 85851000
H	5. 05529700	-0. 22538600	-3. 25623500
C	2. 51557000	-2. 61129700	1. 56364600
H	1. 90046600	-1. 79494600	1. 95722200
H	1. 85803400	-3. 28526500	1. 00480300
H	2. 91493600	-3. 16235700	2. 41656400
H	2. 53994100	1. 30696600	-0. 49347400

C	-2.07419500	3.54306300	0.06558000
S	-0.74083700	2.74646300	-0.78032200
N	-2.09520900	4.77679200	0.41637800
H	-1.23912900	5.22846400	0.08317000
C	-3.28406600	2.71479600	0.38639000
C	-3.18708200	1.36702300	0.75050700
C	-4.54706800	3.31020000	0.31897300
C	-4.33601700	0.62850000	1.02339600
H	-2.20417400	0.91252300	0.85133800
C	-5.69455300	2.56803100	0.58067800
H	-4.60971400	4.35984400	0.05027600
C	-5.59282100	1.22290200	0.92949500
H	-4.24796100	-0.41448300	1.31767100
H	-6.67010600	3.04012300	0.51105800
H	-6.48763500	0.64348200	1.13656100

**TS5S'''**

C	2.93522300	3.15931800	-0.24290700
C	1.79205100	2.58646700	0.31290200
C	1.15771500	3.13985400	1.41666100
C	1.71557800	4.30310400	1.93183000
C	2.85702300	4.90207600	1.40455200
C	3.47546600	4.32127400	0.30427900
C	3.43367700	2.35178000	-1.41001100
C	2.30778800	1.34351000	-1.72566800
C	1.39759200	1.33633400	-0.44069800
H	0.28328900	2.68065600	1.86762600
H	3.24076000	5.80838300	1.85632300
H	4.36471100	4.77378200	-0.12240900
H	3.66567600	2.95457100	-2.29305000
H	2.69963400	0.34155600	-1.90669700
H	4.34391000	1.80910500	-1.13405700
H	1.55677300	0.42543300	0.15489100
N	-0.01192800	1.37581300	-0.83665500
O	1.61156800	1.67404600	-2.92236100
C	-1.07371100	0.76333700	-0.29980100
C	-0.44976400	2.05581700	-1.93881600
N	-2.10684100	1.09658000	-1.06496400
N	-1.73178600	1.90338000	-2.10444000
C	0.60803900	2.66290400	-2.80091400
H	0.98680000	3.59593100	-2.36103300
H	0.21421800	2.87089300	-3.79611900
C	-3.47777100	0.69831700	-0.88959600
C	-4.18469100	1.20372700	0.20356700

C	-4.02838900	-0.17563700	-1.83229000
C	-5.50693400	0.78405300	0.34668100
C	-5.35363100	-0.55642200	-1.64304200
C	-6.10499700	-0.08896400	-0.56209200
H	-6.08293100	1.15458300	1.19054200
H	-5.80786700	-1.24054200	-2.35539600
C	-7.54434400	-0.49886300	-0.40259300
C	-0.67559100	-2.35386600	1.67834200
C	-1.18096100	-1.46899000	0.73366900
H	-0.51946000	-1.95676700	2.67581600
C	-0.77957700	-3.81380500	1.57959900
C	-0.53095400	-4.58663900	2.72304100
C	-1.09469500	-4.46473200	0.37987700
C	-0.60369700	-5.97177400	2.67209800
H	-0.25984500	-4.08503300	3.64802600
C	-1.16739600	-5.85235800	0.32921700
H	-1.25739600	-3.89032500	-0.52618300
C	-0.92164100	-6.60866500	1.47241000
H	-0.40321100	-6.55662900	3.56402800
H	-1.40012400	-6.34575200	-0.60885300
H	-0.96931800	-7.69214300	1.42798300
C	-0.96799700	-0.09463900	0.94236900
O	-0.53109700	0.48769800	1.94217100
N	1.06318800	4.93684900	3.08600300
O	0.01407000	4.45790400	3.47633000
O	1.60550900	5.90934800	3.58135900
H	-8.19134300	0.11797500	-1.03532800
H	-7.87985800	-0.38165700	0.63012100
H	-7.69365600	-1.54083900	-0.69667800
C	-3.22430400	-0.67894200	-3.00046300
H	-3.04391000	0.11951800	-3.72641900
H	-2.24553300	-1.05709300	-2.68658900
H	-3.75316100	-1.48881600	-3.50578200
C	-3.55715700	2.16305700	1.17992900
H	-2.81299400	1.67242400	1.81608100
H	-3.05725200	2.98710700	0.66012100
H	-4.32075700	2.59065300	1.83172200
H	-1.52156200	-1.79622800	-0.24242900
C	2.36627200	-2.93766400	0.25315800
S	1.85649500	-1.93758800	1.61613700
N	2.06549300	-4.16149700	0.02066800
H	1.49140400	-4.52653800	0.78326200
C	3.24739100	-2.26647000	-0.76590000
C	4.25998200	-1.38053300	-0.38355500

C	3.08888200	-2.56645800	-2.12220300
C	5.11234200	-0.82757300	-1.33683200
H	4.38737500	-1.14884000	0.66961100
C	3.91233600	-1.97878500	-3.07936500
H	2.31466100	-3.27115600	-2.40901600
C	4.93304200	-1.11316700	-2.68957200
H	5.92159300	-0.17475100	-1.02126700
H	3.76628000	-2.20765900	-4.13082100
H	5.58932000	-0.67178700	-3.43350300

**M5R**

C	-4.12784000	-2.94964700	-0.09221300
C	-2.93813300	-2.43098700	0.41537500
C	-2.39770300	-2.87650800	1.61496800
C	-3.09883200	-3.87779000	2.27319400
C	-4.29306900	-4.41708500	1.79868300
C	-4.81556500	-3.94416600	0.60185600
C	-4.49846800	-2.29258700	-1.39414200
C	-3.26374800	-1.45395800	-1.79932100
C	-2.36305900	-1.37967400	-0.50907300
H	-1.48938700	-2.43754900	2.01838800
H	-4.78974200	-5.19493000	2.36536100
H	-5.74308100	-4.35218500	0.21335600
H	-4.74391700	-3.00970000	-2.18390000
H	-3.54311600	-0.44601000	-2.10566100
H	-5.37153300	-1.64521500	-1.26261900
H	-2.37260800	-0.38249200	-0.06017800
N	-0.97466900	-1.69088300	-0.85528900
O	-2.59708500	-1.99174400	-2.93267500
C	0.16825400	-1.21556200	-0.33660300
C	-0.64057400	-2.58569300	-1.83356800
N	1.14057400	-1.85517000	-0.98717100
N	0.64968100	-2.70778200	-1.94035400
C	-1.76504300	-3.10599300	-2.66830600
H	-2.30316800	-3.91141500	-2.14958200
H	-1.39178500	-3.48412100	-3.62004600
C	2.55113700	-1.77366900	-0.71802100
C	3.02235900	-2.27925400	0.49639100
C	3.37287400	-1.16999100	-1.67366900
C	4.38968800	-2.15578600	0.74456800
C	4.72989200	-1.07383700	-1.37529900
C	5.25420200	-1.56134100	-0.17524500
H	4.78541600	-2.53403900	1.68358700
H	5.39361100	-0.60275000	-2.09612900

C	6. 73047200	-1. 46394100	0. 10626900
C	1. 16434900	1. 93947700	1. 53908900
C	1. 09554900	0. 81512700	0. 57318800
H	0. 52641700	1. 70503200	2. 39876400
C	2. 56251100	2. 27305500	2. 04259600
C	2. 74889400	3. 30297100	2. 97174900
C	3. 67402900	1. 53973400	1. 62294600
C	4. 01561900	3. 59716100	3. 46294300
H	1. 89003300	3. 87598100	3. 31166500
C	4. 94366700	1. 83426300	2. 11574500
H	3. 54689400	0. 72023900	0. 92131300
C	5. 12066400	2. 86437500	3. 03323300
H	4. 14006700	4. 39742400	4. 18590200
H	5. 79585600	1. 24961900	1. 78048700
H	6. 11024200	3. 09266300	3. 41696200
C	0. 22949500	-0. 21777100	0. 77566400
O	-0. 60957100	-0. 42661800	1. 71631100
N	-2. 55014400	-4. 40083000	3. 53263400
O	-1. 44992300	-4. 01041200	3. 87724000
O	-3. 22495600	-5. 20249400	4. 15599300
H	7. 26950500	-2. 28688100	-0. 37535500
H	6. 93501300	-1. 51633700	1. 17820500
H	7. 14613400	-0. 52996500	-0. 28109700
C	2. 80629900	-0. 63247600	-2. 95977200
H	2. 41591800	-1. 44015500	-3. 58602500
H	1. 98059200	0. 06217400	-2. 77144500
H	3. 57564600	-0. 10037600	-3. 52178400
C	2. 09906600	-2. 90776400	1. 50546300
H	1. 51344800	-2. 14987800	2. 03804400
H	1. 39554200	-3. 59915100	1. 03009800
H	2. 67221200	-3. 46692200	2. 24702700
H	1. 70057100	0. 85814900	-0. 32675900
C	-1. 19383500	3. 06047200	0. 37220100
S	0. 49222300	3. 51014700	0. 78546500
N	-1. 84482200	2. 04109200	0. 75531600
H	-1. 34332500	1. 40225200	1. 38101700
C	-1. 87243100	4. 06659700	-0. 50697700
C	-1. 17661900	4. 87791400	-1. 40706700
C	-3. 26539600	4. 17498000	-0. 42712200
C	-1. 86399500	5. 78135900	-2. 21366300
H	-0. 09812000	4. 79353900	-1. 49267300
C	-3. 94794700	5. 08028600	-1. 22923500
H	-3. 79288100	3. 53932400	0. 27616900
C	-3. 24849600	5. 88670200	-2. 12617200

H	-1.31296500	6.40107000	-2.91406500
H	-5.02788500	5.16178100	-1.15253900
H	-3.78195400	6.59529800	-2.75228400

**M5S**

C	2.08676900	-4.11018200	-2.40974400
C	1.75432000	-2.93449200	-1.74017600
C	1.33636100	-1.79603100	-2.41759600
C	1.24989200	-1.89883200	-3.79874800
C	1.58692500	-3.05181600	-4.50486400
C	2.01476000	-4.17113600	-3.80128600
C	2.48964400	-5.18865000	-1.43891400
C	2.08888400	-4.65438100	-0.04234800
C	1.84594500	-3.11482700	-0.23942400
H	1.11234400	-0.86966500	-1.89486400
H	1.49975000	-3.05851200	-5.58447400
H	2.27097200	-5.08204600	-4.33274600
H	2.00180200	-6.14926900	-1.63084100
H	2.88008900	-4.81267000	0.69052300
H	3.56992100	-5.36136200	-1.48374500
H	2.62616900	-2.49426600	0.19889300
N	0.57195700	-2.71745400	0.37217800
O	0.97148900	-5.34278800	0.50043800
C	0.15482000	-1.51032800	0.80256900
C	-0.51524400	-3.54634100	0.35227500
N	-1.16150600	-1.65312300	1.00142900
N	-1.58994600	-2.92629100	0.73680800
C	-0.27979200	-4.96887000	-0.04003800
H	-0.30690300	-5.07680800	-1.13383900
H	-1.04318900	-5.61563400	0.39359600
C	-2.12754400	-0.60228800	1.19860100
C	-2.48825300	0.15070800	0.07941300
C	-2.63672000	-0.37929600	2.47978700
C	-3.37467300	1.20882700	0.28832700
C	-3.51860600	0.68613200	2.63307000
C	-3.88309300	1.49765200	1.55313400
H	-3.65985600	1.82839800	-0.55991500
H	-3.92641800	0.89279500	3.61992100
C	-4.79460300	2.67720800	1.76245700
C	1.43798300	1.89926100	1.96274500
C	0.67073600	0.63341100	1.82920400
H	2.34861500	1.83568700	1.36075100
C	1.80776100	2.25695400	3.38818000
C	3.13732800	2.50984900	3.72577600

C	0.82987800	2.33272900	4.38573000
C	3.48963700	2.82189600	5.03685900
H	3.90115600	2.45794100	2.95445600
C	1.17973400	2.64836200	5.69400600
H	-0.21161100	2.14947000	4.13093300
C	2.51173400	2.89262200	6.02415900
H	4.52930500	3.01333200	5.28427800
H	0.41105200	2.70734200	6.45869900
H	2.78378800	3.13886200	7.04583600
C	1.04663900	-0.30979200	0.91635000
O	2.05650500	-0.32359600	0.13223200
N	0.75054500	-0.73839000	-4.55089400
O	0.27269100	0.18199000	-3.91351900
O	0.83236200	-0.77227300	-5.76704400
H	-5.65453200	2.40988100	2.38352100
H	-5.16269800	3.06518300	0.81013400
H	-4.26268000	3.48780000	2.27227200
C	-2.20347500	-1.23159900	3.64195900
H	-2.31582900	-2.29681700	3.41908800
H	-1.14896900	-1.05506100	3.88564200
H	-2.79567200	-1.00066400	4.52943400
C	-1.92825000	-0.14059400	-1.28622200
H	-0.93635900	0.31377800	-1.40596800
H	-1.84662300	-1.21793500	-1.46672200
H	-2.57417300	0.28294900	-2.05841600
H	-0.22629900	0.51666000	2.42177200
C	0.03757900	2.83213400	-0.33577300
S	0.43647500	3.35023200	1.33869500
N	0.66316500	1.97255400	-1.02545200
H	1.46395000	1.52937000	-0.56837700
C	-1.17906200	3.48230200	-0.92466800
C	-2.01750900	4.32625800	-0.19156300
C	-1.51022100	3.18161200	-2.25260400
C	-3.16820500	4.85642800	-0.77039300
H	-1.78773000	4.56153200	0.84233500
C	-2.66519600	3.70252800	-2.82413400
H	-0.85208200	2.52772200	-2.81653500
C	-3.50031300	4.54082100	-2.08483700
H	-3.80814100	5.51107500	-0.18645500
H	-2.91270400	3.45740700	-3.85254600
H	-4.40025100	4.95020500	-2.53363000

**TS6R**

C	-3.88307900	-1.36736900	-0.48624500
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C	-2.64378500	-1.20820900	0.13092800
C	-2.39628000	-1.67273200	1.41592200
C	-3.44586100	-2.32166400	2.05054400
C	-4.70025000	-2.49598400	1.46846500
C	-4.92261000	-2.01041800	0.18626600
C	-3.89250600	-0.75506200	-1.86129000
C	-2.43783200	-0.29593500	-2.12554900
C	-1.68760600	-0.45105300	-0.75588800
H	-1.44179900	-1.52736600	1.91362100
H	-5.47630000	-3.00712500	2.02438500
H	-5.89273100	-2.13828400	-0.28296100
H	-4.21778000	-1.45659000	-2.63657000
H	-2.38659000	0.75193800	-2.42785400
H	-4.56957700	0.10442600	-1.89493100
H	-1.44817100	0.52766600	-0.34291700
N	-0.42730000	-1.17414400	-0.93985200
O	-1.82625800	-1.00856700	-3.19153900
C	0.72742600	-1.08496300	-0.27082300
C	-0.26646000	-2.14899600	-1.88199800
N	1.51639400	-2.02283200	-0.77470100
N	0.91301000	-2.69198700	-1.80067100
C	-1.37972400	-2.31084400	-2.86587300
H	-2.18632100	-2.92658000	-2.44292400
H	-1.01286500	-2.78126300	-3.77795400
C	2.81031900	-2.42026600	-0.28030800
C	2.84996600	-3.14644700	0.91570900
C	3.94519600	-2.10256100	-1.03067900
C	4.10689300	-3.51796900	1.38836800
C	5.17540200	-2.50112900	-0.50935800
C	5.27598700	-3.19457000	0.69733500
H	4.17125200	-4.08126900	2.31571400
H	6.07817100	-2.26271000	-1.06592700
C	6.62211000	-3.57553400	1.25304200
C	1.45506800	2.36335700	1.32516200
C	1.36117200	1.22967900	0.31537700
H	1.41014100	1.97411700	2.34651800
C	2.70892900	3.19520300	1.17300800
C	3.51627300	3.47385900	2.27541900
C	3.06656600	3.70220200	-0.08102600
C	4.67389500	4.23485700	2.12761900
H	3.23805900	3.08891700	3.25277700
C	4.22102900	4.46248600	-0.22844700
H	2.42881200	3.49903000	-0.93880700
C	5.02876100	4.72929700	0.87627300

H	5.29712500	4.44105900	2.99209500
H	4.49037800	4.84963200	-1.20604600
H	5.93038700	5.32243000	0.76066500
C	0.97520200	-0.05682000	0.83156600
O	0.66967500	-0.38698600	1.97088900
N	-3.22237900	-2.85416900	3.40170900
O	-2.09686600	-2.77977300	3.86020600
O	-4.17403300	-3.34685900	3.98247500
H	6.56684600	-4.50579400	1.82351900
H	6.99262700	-2.79623000	1.92747800
H	7.35927000	-3.70150900	0.45670100
C	3.84189300	-1.39856400	-2.35383300
H	3.47061700	-2.08703700	-3.12071900
H	3.13937200	-0.56251800	-2.32353900
H	4.82322200	-1.03770700	-2.66780700
C	1.59290200	-3.53676400	1.64726600
H	1.12024200	-2.67195300	2.12346100
H	0.86459300	-3.98603100	0.96367200
H	1.82082100	-4.26801900	2.42445000
H	2.22207900	1.13365900	-0.35620600
C	-1.37666400	2.49629800	1.18910300
S	0.05033000	3.58508200	1.12746100
N	-1.47638300	1.46062900	1.92093700
H	-0.66605000	1.31237100	2.52294500
C	-2.51513600	2.82556700	0.27627800
C	-2.35916500	3.61184600	-0.86859600
C	-3.76462300	2.25093900	0.55131000
C	-3.44019200	3.82570200	-1.72129800
H	-1.38344400	4.01390200	-1.11290600
C	-4.83999200	2.46772600	-0.30178500
H	-3.87140200	1.63717600	1.43990200
C	-4.67981800	3.25691000	-1.44201700
H	-3.30807100	4.43319000	-2.61097200
H	-5.80548000	2.02529200	-0.07468500
H	-5.52018800	3.42935600	-2.10761300
H	0.55386000	1.50095600	-0.68999900
C	0.38505200	1.24217200	-2.81128500
O	-0.11401700	1.84117800	-1.78023400
O	1.22457700	0.33622800	-2.76108000
C	-0.15870200	1.69265700	-4.15511200
H	-0.71401300	2.62729400	-4.06861100
H	0.66254800	1.80217800	-4.86648400
H	-0.82101900	0.90677800	-4.53119600

**TS6S**

C	-5.40745100	0.70602000	-0.50824600
C	-4.01702800	0.76432000	-0.61367100
C	-3.37366000	1.85626100	-1.17900700
C	-4.18522800	2.89111500	-1.62745200
C	-5.57468300	2.86494200	-1.54154300
C	-6.19393100	1.75647100	-0.97642200
C	-5.84544800	-0.58572100	0.13140900
C	-4.55609000	-1.21576200	0.70556000
C	-3.38851700	-0.49021300	-0.05064000
H	-2.29527000	1.90583600	-1.28063200
H	-6.14555900	3.70722900	-1.91170500
H	-7.27544100	1.71904800	-0.89682500
H	-6.58604700	-0.44660100	0.92414700
H	-4.48145700	-2.28544800	0.51656200
H	-6.29020100	-1.24812100	-0.61892000
H	-2.97898300	-1.14077100	-0.82120700
N	-2.29638900	-0.18747200	0.87177100
O	-4.49989500	-1.10046500	2.12142500
C	-0.96728000	-0.28323300	0.72236100
C	-2.53687200	0.13740500	2.17124500
N	-0.45371900	0.01854100	1.91368000
N	-1.42481300	0.27489700	2.83613700
C	-3.95894900	0.10463300	2.62405800
H	-4.50557400	0.98975500	2.27092200
H	-4.00696200	0.06808300	3.71255600
C	0.92998100	0.14594800	2.29891700
C	1.52644400	1.40268400	2.18396100
C	1.58054900	-0.98450300	2.80311400
C	2.86990900	1.49682600	2.54701400
C	2.91997200	-0.83164100	3.15280400
C	3.58021900	0.39304000	3.01792600
H	3.37270100	2.45629600	2.44496600
H	3.46146000	-1.69171800	3.53926300
C	5.04080600	0.50936900	3.36248400
C	1.68301500	-1.32908400	-1.93589500
C	0.90402500	-1.36262300	-0.62736900
H	1.05416100	-0.89508500	-2.71946500
C	2.18795100	-2.67022600	-2.43311500
C	2.21040200	-2.93410900	-3.80388000
C	2.68270900	-3.63004500	-1.54806500
C	2.70671400	-4.14200000	-4.28469200
H	1.83454900	-2.18560900	-4.49696800
C	3.17974000	-4.83782000	-2.02732700

H	2.65731700	-3.44030300	-0.47899800
C	3.19320000	-5.09686400	-3.39575300
H	2.71181000	-4.33689600	-5.35250800
H	3.55226900	-5.58056400	-1.32905800
H	3.57873700	-6.04103700	-3.76757200
C	-0.30934200	-0.58486600	-0.61405600
O	-0.95842300	-0.20101800	-1.58341900
N	-3.54538000	4.07519400	-2.21918100
O	-2.32884400	4.10966300	-2.23992000
O	-4.26978600	4.95519700	-2.65082600
H	5.26555500	0.00373300	4.30579500
H	5.34605900	1.55462400	3.44712100
H	5.65603800	0.04168000	2.58597200
C	0.87854000	-2.31064200	2.91978700
H	-0.14648900	-2.19500800	3.28349800
H	0.83144400	-2.82296900	1.95067400
H	1.41561400	-2.96019700	3.61386900
C	0.76075500	2.59774100	1.68634700
H	0.60169800	2.53492000	0.60308800
H	-0.21258100	2.67772200	2.18040400
H	1.32170000	3.51231100	1.88799200
H	1.52218400	-1.22050600	0.25961500
C	2.60031400	1.29652400	-1.31033300
S	3.22522800	-0.30641700	-1.79944700
N	1.41591000	1.72251300	-1.49476100
H	0.82745900	1.07384800	-2.01690900
C	3.59812200	2.18417300	-0.63503600
C	4.81657800	1.71128900	-0.13817000
C	3.27726200	3.53814600	-0.47689400
C	5.69540000	2.57603100	0.50942100
H	5.07572600	0.66215400	-0.23457700
C	4.14906500	4.39574700	0.18333200
H	2.33669800	3.89919300	-0.87905600
C	5.36200000	3.91705200	0.67918200
H	6.63937000	2.19661800	0.88810400
H	3.88776300	5.44269800	0.30152400
H	6.04669000	4.58921300	1.18703200
H	0.42887500	-2.54660600	-0.41701500
C	-1.14880300	-3.81939500	0.36369800
O	-1.90410900	-2.83140400	0.37182400
O	0.05652200	-3.81758600	-0.06656100
C	-1.62942400	-5.14246400	0.93457300
H	-2.71102900	-5.13554300	1.07170900
H	-1.33172800	-5.96568600	0.28220900

H	-1.14803100	-5.30122800	1.90501000
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**M6R**

C	-3.87071700	-0.89091900	-0.98143900
C	-2.65631400	-0.86262000	-0.29827300
C	-2.54999100	-1.29988700	1.01497000
C	-3.71833000	-1.73291800	1.62442900
C	-4.95514900	-1.74377700	0.98383100
C	-5.02998800	-1.32481200	-0.33831300
C	-3.71494700	-0.41772800	-2.40039000
C	-2.20355700	-0.14374500	-2.58938300
C	-1.56084400	-0.28284100	-1.15945800
H	-1.62078400	-1.27992300	1.57113800
H	-5.82992000	-2.08746000	1.52231000
H	-5.98028800	-1.34118500	-0.86244200
H	-4.05888300	-1.16279900	-3.12622700
H	-2.00053300	0.86779300	-2.94122400
H	-4.29414300	0.49423300	-2.57358700
H	-1.22621500	0.70302100	-0.83010900
N	-0.37992400	-1.14334200	-1.19617500
O	-1.61574100	-0.99028200	-3.56559000
C	0.74475500	-1.11433600	-0.47655500
C	-0.25320300	-2.16870900	-2.08601600
N	1.47722700	-2.13913700	-0.89550500
N	0.87534700	-2.79745300	-1.92413600
C	-1.32493800	-2.29869200	-3.11885200
H	-2.21070800	-2.79749400	-2.69841100
H	-0.95983300	-2.87623400	-3.96836200
C	2.73686000	-2.59459500	-0.36058000
C	2.70186500	-3.39041800	0.79172800
C	3.91117300	-2.26516100	-1.03955400
C	3.92436000	-3.81327900	1.30409600
C	5.10723400	-2.71678000	-0.47774000
C	5.13404200	-3.47462700	0.69150300
H	3.93177800	-4.42895600	2.20006100
H	6.04067100	-2.47128000	-0.97780200
C	6.43920100	-3.92376200	1.29225600
C	1.51071000	2.30025800	1.30040900
C	1.42700200	1.25169800	0.18651400
H	1.66932200	1.82535700	2.27308000
C	2.61791400	3.30277800	1.05442600
C	3.48961800	3.65979900	2.08206900
C	2.76104100	3.89163500	-0.20683700
C	4.50577800	4.58413700	1.85294200

H	3.37332200	3.20915300	3.06423200
C	3.77581100	4.81552200	-0.43306600
H	2.07246600	3.62357000	-1.00675200
C	4.65046500	5.16234300	0.59519500
H	5.18277200	4.85157100	2.65816600
H	3.88303000	5.26667500	-1.41440100
H	5.44154200	5.88372700	0.41627500
C	1.12634800	-0.13899500	0.63390800
O	1.22062400	-0.57696500	1.75650700
N	-3.64291200	-2.19777600	3.01495200
O	-2.53796300	-2.32653800	3.51028200
O	-4.69075900	-2.43268700	3.59247200
H	6.38627600	-4.96697500	1.61541700
H	6.68602200	-3.32096300	2.17248200
H	7.25998600	-3.82544400	0.57852800
C	3.89509300	-1.51680200	-2.34307400
H	3.66967200	-2.20967200	-3.16202100
H	3.13615900	-0.72988100	-2.37960300
H	4.87701000	-1.07992200	-2.53739900
C	1.40126100	-3.79373500	1.43209700
H	0.93192200	-2.94596900	1.93901200
H	0.69714100	-4.17758500	0.68664600
H	1.57079100	-4.57836800	2.17138500
H	2.39328400	1.15236800	-0.33440300
C	-1.29011500	2.05947000	1.63347600
S	-0.03687500	3.31379800	1.35932000
N	-1.16231200	1.02703800	2.36603600
H	-0.25594200	0.98575000	2.83613600
C	-2.58267800	2.28822800	0.92661900
C	-2.62249200	2.80922900	-0.37157700
C	-3.76640800	1.88014700	1.55289500
C	-3.84534900	2.91707400	-1.03215700
H	-1.70075600	3.07676400	-0.88367800
C	-4.98273900	2.00558100	0.89323100
H	-3.71175800	1.46841000	2.55594200
C	-5.02368500	2.52497000	-0.40123000
H	-3.87191500	3.31139300	-2.04368200
H	-5.89924500	1.69779200	1.38712400
H	-5.97494200	2.62340100	-0.91611400
H	0.75262700	1.55454800	-0.63269600
C	0.65663500	1.33346600	-3.06879800
O	-0.09219500	2.05222400	-2.34618100
O	1.38803200	0.39578600	-2.66346500
C	0.62000300	1.58820600	-4.57500200

H	0.27112500	2.59810900	-4.79670400
H	1.60228800	1.41658800	-5.01994000
H	-0.07736300	0.86973500	-5.02031900

**M6S**

C	-5.42168000	0.49359000	-0.43142000
C	-4.03585800	0.62994400	-0.53249000
C	-3.45537900	1.72193700	-1.16034500
C	-4.32335200	2.67547700	-1.67883900
C	-5.70907700	2.56977900	-1.59957800
C	-6.26543400	1.46260300	-0.96904400
C	-5.78298500	-0.78259200	0.28463600
C	-4.46592400	-1.27117000	0.92685600
C	-3.34295600	-0.55181700	0.10578300
H	-2.38174500	1.83807500	-1.25486800
H	-6.32674000	3.35083800	-2.02499800
H	-7.34339600	1.36453300	-0.89317100
H	-6.55425000	-0.64985900	1.04814900
H	-4.32130000	-2.34823200	0.84613700
H	-6.15307300	-1.52444300	-0.43151100
H	-2.92310500	-1.24798400	-0.61877100
N	-2.25123600	-0.14726900	0.98658500
O	-4.43419200	-1.00566100	2.32417800
C	-0.92200000	-0.25857700	0.84843700
C	-2.49071800	0.26543700	2.26084600
N	-0.40578600	0.13372900	2.01083700
N	-1.37890500	0.45092900	2.91357600
C	-3.91243800	0.24916400	2.71588200
H	-4.47337500	1.08983700	2.28595700
H	-3.96007600	0.30727000	3.80324600
C	0.97723700	0.25642000	2.40269700
C	1.58924600	1.50509400	2.28018900
C	1.60361100	-0.87489800	2.93714400
C	2.92891900	1.58717100	2.66084600
C	2.94044700	-0.73303100	3.30136500
C	3.61780100	0.48121900	3.15825700
H	3.44572200	2.53852700	2.55366400
H	3.46396000	-1.59316500	3.71145300
C	5.07257600	0.58405400	3.53086200
C	1.74506200	-1.31093200	-1.84345800
C	1.02736700	-1.36385000	-0.48442500
H	1.10056900	-0.82041300	-2.57932000
C	2.14454600	-2.65493600	-2.42698000
C	2.30766000	-2.75690000	-3.81251200

C	2. 38985700	-3. 77374600	-1. 62973700
C	2. 70073400	-3. 95592200	-4. 39465000
H	2. 12212100	-1. 88556900	-4. 43613700
C	2. 77937900	-4. 97675000	-2. 21564300
H	2. 24221100	-3. 73163700	-0. 55593300
C	2. 93823800	-5. 07178500	-3. 59417700
H	2. 81709400	-4. 02049700	-5. 47187200
H	2. 95142100	-5. 84330300	-1. 58537700
H	3. 23983900	-6. 01180600	-4. 04546800
C	-0. 27362700	-0. 62725000	-0. 47074600
O	-0. 89595400	-0. 28525300	-1. 45544600
N	-3. 74913700	3. 85522200	-2. 34185700
O	-2. 53571500	3. 94954300	-2. 37666000
O	-4. 51995600	4. 67122300	-2. 81556400
H	5. 26268200	0. 12161100	4. 50364500
H	5. 39935800	1. 62535400	3. 57179000
H	5. 69560700	0. 06392800	2. 79509400
C	0. 86994200	-2. 17808300	3. 08657800
H	-0. 11735700	-2. 02692400	3. 53394000
H	0. 71682500	-2. 68378600	2. 12378200
H	1. 43606900	-2. 85382000	3. 73068700
C	0. 84273600	2. 70499200	1. 76510400
H	0. 67387200	2. 62463800	0. 68517600
H	-0. 12485000	2. 81186700	2. 26530300
H	1. 42238400	3. 61229000	1. 94599800
H	1. 66614000	-1. 01138400	0. 33050000
C	2. 71312600	1. 25209400	-1. 19381200
S	3. 31447500	-0. 34507000	-1. 73628100
N	1. 52488100	1. 68480100	-1. 34153400
H	0. 93314700	1. 05734400	-1. 88428400
C	3. 72915700	2. 11895200	-0. 52543600
C	4. 92709400	1. 61547300	-0. 00972500
C	3. 44731100	3. 48453500	-0. 39416600
C	5. 82711100	2. 46456900	0. 62922500
H	5. 15113300	0. 55623400	-0. 08269600
C	4. 34122700	4. 32656800	0. 25593000
H	2. 52130100	3. 86698500	-0. 81011700
C	5. 53479200	3. 81854700	0. 76956900
H	6. 75479600	2. 06326500	1. 02482400
H	4. 11303400	5. 38336100	0. 35244000
H	6. 23679100	4. 47837600	1. 26984700
H	0. 73949000	-2. 39871300	-0. 21377400
C	-1. 10269500	-3. 85585400	0. 54109600
O	-1. 59274900	-2. 68579400	0. 54677500



O	0.11471800	-4.13714000	0.54728600
C	-2.11358100	-5.00245000	0.53738600
H	-2.78233500	-4.89877300	-0.32212800
H	-1.61405100	-5.97088700	0.49880100
H	-2.72979200	-4.94439400	1.43986200

**TS7R**

C	-4.92558100	1.02351500	0.47085800
C	-3.75770500	0.26458600	0.54302300
C	-3.76811200	-1.04404900	1.00579100
C	-5.00137000	-1.56159800	1.37945200
C	-6.18678000	-0.83272900	1.31924500
C	-6.14726400	0.47799000	0.86090700
C	-4.63924800	2.41068400	-0.03881900
C	-3.18067600	2.36899000	-0.54978300
C	-2.56271600	1.06598100	0.07776100
H	-2.85863900	-1.62805900	1.09134500
H	-7.11421600	-1.29877200	1.62839500
H	-7.05980000	1.06288000	0.80709700
H	-5.31243300	2.72369700	-0.84254200
H	-2.60367500	3.23274600	-0.22014900
H	-4.73925000	3.14101100	0.77109800
H	-1.87565500	1.31321200	0.88903800
N	-1.77347200	0.35145800	-0.92021300
O	-3.11538900	2.42781100	-1.96794700
C	-0.59740500	-0.28219100	-0.79343700
C	-2.08835900	0.36634000	-2.24789300
N	-0.26816900	-0.65989500	-2.02776600
N	-1.18460400	-0.24287600	-2.95673400
C	-3.26451800	1.19432500	-2.64443300
H	-4.20694900	0.69011400	-2.38891700
H	-3.24556300	1.39380500	-3.71600000
C	0.89617600	-1.39539300	-2.43941300
C	0.90877000	-2.77875100	-2.26110900
C	1.96990700	-0.66841500	-2.95927500
C	2.07691200	-3.45148100	-2.61780000
C	3.11233000	-1.38837600	-3.30123300
C	3.18469600	-2.77362600	-3.12978300
H	2.12179900	-4.52981200	-2.48816200
H	3.97027000	-0.85331000	-3.70062900
C	4.45178800	-3.51674300	-3.46009500
C	2.18963800	-0.34790800	1.83919200
C	1.53046200	-0.89214400	0.56397900
H	1.42552100	-0.30526000	2.62081300

C	3. 33372200	-1. 21311300	2. 31979000
C	3. 50454800	-1. 44660100	3. 68538400
C	4. 24228200	-1. 77831500	1. 41921600
C	4. 55431600	-2. 23698900	4. 14499800
H	2. 80446200	-1. 00620000	4. 39054600
C	5. 29051200	-2. 57017900	1. 87662700
H	4. 12903700	-1. 59415500	0. 35340300
C	5. 44925000	-2. 80297200	3. 24117100
H	4. 67085300	-2. 41307500	5. 20993900
H	5. 98749200	-3. 00444900	1. 16612200
H	6. 26717400	-3. 42171500	3. 59692200
C	0. 06793900	-0. 53392800	0. 53375700
O	-0. 69200800	-0. 75092400	1. 47672600
N	-5. 05917500	-2. 94841300	1. 86301600
O	-4. 02811400	-3. 59605400	1. 85187000
O	-6. 13660400	-3. 37206900	2. 24363400
H	5. 12683800	-3. 52328800	-2. 59726300
H	4. 98268900	-3. 04505000	-4. 29039700
H	4. 24553800	-4. 55600500	-3. 72621900
C	1. 88922500	0. 82730300	-3. 09404700
H	1. 13562500	1. 11305200	-3. 83501800
H	1. 60327800	1. 29512100	-2. 14358400
H	2. 85158400	1. 23732500	-3. 40446900
C	-0. 28069100	-3. 50078600	-1. 68715900
H	-0. 41743400	-3. 27122100	-0. 62377400
H	-1. 20227000	-3. 22033600	-2. 20683900
H	-0. 15272200	-4. 58078200	-1. 77682700
H	1. 59127600	-1. 98958400	0. 57913700
C	1. 46373000	2. 21848400	0. 70620500
S	2. 86972600	1. 33513600	1. 61007900
N	0. 41493300	1. 71609600	0. 27651100
H	2. 05077100	-0. 53403800	-0. 32553800
C	1. 80044600	3. 68359300	0. 59112100
C	3. 10912200	4. 15729000	0. 46842300
C	0. 74520200	4. 60022400	0. 57111900
C	3. 35433100	5. 52163500	0. 32859800
H	3. 94187000	3. 46050200	0. 46547900
C	0. 99013900	5. 96172800	0. 44331400
H	-0. 26592500	4. 21679600	0. 66111900
C	2. 29839800	6. 42763800	0. 31972600
H	4. 37553300	5. 87568400	0. 22555900
H	0. 16064700	6. 66266300	0. 44077100
H	2. 49220000	7. 49095700	0. 21713500

**TS7S**

C	-5.06575500	-1.23285100	-0.71905200
C	-3.70164200	-0.95871400	-0.80021200
C	-3.22193500	0.27397000	-1.22960400
C	-4.18423900	1.21677200	-1.56792200
C	-5.55557500	0.98072600	-1.49512600
C	-6.00289900	-0.26213000	-1.06800300
C	-5.31589200	-2.63730600	-0.24001800
C	-3.93256300	-3.18497800	0.18511500
C	-2.88286100	-2.15900800	-0.38410100
H	-2.15829400	0.50156100	-1.28079100
H	-6.24528100	1.76809500	-1.77254700
H	-7.06673000	-0.46779800	-1.00625300
H	-6.01423400	-2.68483700	0.60191900
H	-3.74632000	-4.16882000	-0.24634700
H	-5.73971800	-3.24911600	-1.04276400
H	-2.33123600	-2.57019700	-1.22608200
N	-1.89257100	-1.79915700	0.64238200
O	-3.84242400	-3.39651800	1.58441500
C	-0.60175600	-1.41708200	0.54988800
C	-2.24406500	-1.75173200	1.96367800
N	-0.22726800	-1.18123100	1.81486800
N	-1.24237000	-1.39167600	2.70404300
C	-3.61053800	-2.22122500	2.33514400
H	-4.36049200	-1.44413900	2.12946300
H	-3.64739000	-2.47858000	3.39395700
C	1.03396800	-0.71114800	2.32968900
C	1.13502500	0.63110700	2.71138300
C	2.06851100	-1.63592600	2.49711700
C	2.38321900	1.06464900	3.15734300
C	3.29233900	-1.14991600	2.95433500
C	3.47386600	0.19992000	3.26050200
H	2.49933300	2.10973500	3.43487300
H	4.11824400	-1.84555800	3.08025800
C	4.81926500	0.71805400	3.69230400
C	2.22493100	-0.59305900	-1.96125700
C	1.59793000	-1.44731100	-0.85462300
H	1.49698400	-0.50334500	-2.77322300
C	3.50751100	-1.18621600	-2.49822100
C	3.71494100	-1.28016300	-3.87483800
C	4.50429200	-1.64554300	-1.63095700
C	4.89049300	-1.83102000	-4.37908000
H	2.94689200	-0.91902800	-4.55350800
C	5.67763900	-2.19837800	-2.13289200

H	4.36058700	-1.55978000	-0.55610600
C	5.87397800	-2.29304000	-3.50946600
H	5.03688200	-1.89898800	-5.45270700
H	6.44265200	-2.55324900	-1.44897600
H	6.79079000	-2.72243000	-3.90122700
C	0.10086500	-1.23529100	-0.80194100
O	-0.59560500	-1.49568300	-1.79541200
N	-3.73768600	2.53608900	-2.03691700
O	-2.54846700	2.69034200	-2.24712900
O	-4.58390400	3.40001000	-2.19273000
H	5.34168000	1.17244300	2.84345500
H	5.45052500	-0.08463000	4.08069200
H	4.71954900	1.48447800	4.46522900
C	1.86605600	-3.09963400	2.20752400
H	2.71775800	-3.67869100	2.56916200
H	0.96347200	-3.47454100	2.70048300
H	1.76287800	-3.29608400	1.13527200
C	-0.05485500	1.55047800	2.70905600
H	0.26789800	2.58921500	2.81173500
H	-0.62216500	1.45506900	1.77930300
H	-0.71225000	1.30602700	3.55092400
H	1.74218800	-2.50527500	-1.11135200
C	1.01754400	1.53377700	-0.53791400
S	2.61543600	1.08486000	-1.35410100
N	0.01566400	0.80940600	-0.36970700
H	2.09026500	-1.24471200	0.09585900
C	1.06260100	2.95767400	-0.05580800
C	2.21003900	3.49854700	0.53041600
C	-0.10423700	3.72555600	-0.11421500
C	2.18689500	4.78784300	1.05932100
H	3.11704700	2.90371000	0.59233000
C	-0.12022500	5.01649000	0.40079600
H	-0.98871100	3.29085200	-0.56961800
C	1.02349900	5.54965200	0.99497100
H	3.08091800	5.19628900	1.52105700
H	-1.02777400	5.60964000	0.33976400
H	1.00787000	6.55642400	1.40126800

### M7R

C	4.39830900	-4.35046700	-6.22342500
C	4.15487900	-3.06264300	-5.74711200
C	4.63401200	-1.92669200	-6.39368700
C	5.37481100	-2.15922400	-7.54733500
C	5.64776400	-3.42993900	-8.04862700

C	5. 15147000	-4. 54168700	-7. 37946800
C	3. 75898900	-5. 38785900	-5. 33888800
C	2. 84716300	-4. 59884700	-4. 36863900
C	3. 32744800	-3. 10767000	-4. 48219300
H	4. 43163200	-0. 91640600	-6. 01615500
H	6. 23137600	-3. 52820200	-8. 95565200
H	5. 34286300	-5. 53927000	-7. 76191500
H	3. 17126900	-6. 12622800	-5. 89334800
H	2. 96547000	-4. 94481400	-3. 34144700
H	4. 52311300	-5. 93748700	-4. 77902700
H	3. 91572600	-2. 81378400	-3. 61442100
N	2. 18964000	-2. 18274600	-4. 55927500
O	1. 46819700	-4. 79090000	-4. 64437500
C	2. 03126700	-0. 89144800	-4. 17975800
C	1. 05092100	-2. 56750700	-5. 21634000
N	0. 80116500	-0. 57597300	-4. 60628300
N	0. 17634700	-1. 61286100	-5. 24661600
C	0. 95893400	-3. 98110300	-5. 68474000
H	1. 51446400	-4. 11695700	-6. 62374700
H	-0. 08352700	-4. 25499100	-5. 85011800
C	0. 09872200	0. 67903500	-4. 52932800
C	0. 26741200	1. 59237100	-5. 57075000
C	-0. 74645300	0. 90090300	-3. 43788900
C	-0. 41332000	2. 80658300	-5. 46149100
C	-1. 40351600	2. 12561400	-3. 37950200
C	-1. 23743400	3. 09380700	-4. 37488500
H	-0. 29141300	3. 54476800	-6. 24983100
H	-2. 05726900	2. 33364000	-2. 53565000
C	-1. 94942300	4. 41597500	-4. 26687300
C	3. 76693700	2. 20090400	-2. 56448900
C	2. 66076300	1. 16847000	-2. 74717100
H	4. 05605300	2. 52389700	-3. 56769700
C	3. 34706500	3. 39250200	-1. 73700200
C	3. 31326600	4. 65915100	-2. 32114800
C	2. 95236300	3. 25221300	-0. 40273400
C	2. 89030500	5. 76687100	-1. 58966900
H	3. 61970200	4. 77440700	-3. 35729000
C	2. 52971100	4. 35624600	0. 32887800
H	2. 98958300	2. 27160100	0. 06515200
C	2. 49780400	5. 61799700	-0. 26330800
H	2. 87129400	6. 74643300	-2. 05748000
H	2. 22808400	4. 23407700	1. 36470900
H	2. 17257400	6. 48074600	0. 30974500
C	3. 17203600	0. 11347900	-3. 75777800

O	3.62167800	0.60955300	-4.88771800
N	5.88879000	-1.00129400	-8.29650500
O	5.52576200	0.10468400	-7.94799900
O	6.64510400	-1.22059200	-9.22950600
H	-1.63658900	4.95292400	-3.36603100
H	-3.03264600	4.27369600	-4.20395700
H	-1.73926900	5.05177800	-5.12949400
C	-0.90906400	-0.13460300	-2.35870000
H	-1.09994700	-1.12495300	-2.78250700
H	-0.00658100	-0.20536900	-1.74153200
H	-1.74205600	0.12446600	-1.70256300
C	1.15283700	1.27576300	-6.74240100
H	2.18494800	1.13987400	-6.39579400
H	0.83036500	0.34911800	-7.22990300
H	1.11574500	2.08010400	-7.47963800
H	1.80543900	1.70303200	-3.16327500
C	5.07916300	-0.26484300	-2.34736900
S	5.25620200	1.42854600	-1.81669200
N	4.17498200	-0.76080600	-3.08462300
H	2.36890600	0.71537500	-1.79127400
C	6.17156000	-1.15364300	-1.84908000
C	6.71730800	-1.01989900	-0.56995500
C	6.65446700	-2.15203100	-2.70166900
C	7.72246100	-1.88459500	-0.14561500
H	6.34625000	-0.25033400	0.10009900
C	7.66278000	-3.00910300	-2.27720700
H	6.24284600	-2.22491900	-3.70465400
C	8.19673900	-2.87939500	-0.99602700
H	8.13528300	-1.77936200	0.85264000
H	8.04158200	-3.77178800	-2.95051800
H	8.98559000	-3.54730500	-0.66450200

### M7S

C	3.71393700	-3.58063200	-4.94913200
C	3.34418600	-2.30816800	-4.52010700
C	3.39487100	-1.20390500	-5.36314900
C	3.80708700	-1.44563600	-6.66609100
C	4.18795100	-2.70374400	-7.13094700
C	4.14576500	-3.78404400	-6.25997400
C	3.58378700	-4.59090800	-3.84115500
C	2.90568100	-3.83890400	-2.66786700
C	2.89018900	-2.32011400	-3.07885500
H	3.15628400	-0.20812000	-4.99477300
H	4.50574200	-2.81602500	-8.16008700

H	4.43880200	-4.77136100	-6.60239300
H	2.98714500	-5.46339800	-4.12747600
H	3.47463300	-3.95339500	-1.74508200
H	4.56683200	-4.96473800	-3.53862700
H	3.52062500	-1.68298700	-2.46012700
N	1.52757000	-1.76935700	-2.97298700
O	1.62746600	-4.36932600	-2.35239600
C	1.11512700	-0.49506100	-2.85004300
C	0.41754300	-2.54628100	-3.16708700
N	-0.21436600	-0.55659200	-2.97037200
N	-0.66790000	-1.83354800	-3.15958400
C	0.61687400	-4.02173000	-3.27585900
H	0.88715800	-4.30111200	-4.30445600
H	-0.29609000	-4.54998000	-2.99876000
C	-1.13661400	0.55012500	-2.98949700
C	-1.37865700	1.17818600	-4.21720500
C	-1.74712300	0.93622400	-1.79697100
C	-2.19373700	2.30523400	-4.20129800
C	-2.56187400	2.07033100	-1.83683200
C	-2.77357600	2.77680700	-3.01963600
H	-2.37010900	2.83568100	-5.13444600
H	-3.03974100	2.40496600	-0.91952100
C	-3.61454100	4.02541300	-3.04194400
C	2.69018900	2.47236200	-0.94821100
C	1.77018200	1.28927200	-1.20924900
H	3.70607800	2.14774000	-1.18772400
C	2.62107500	2.98794800	0.46939400
C	3.76580900	2.99029900	1.26759200
C	1.41561700	3.44391300	1.01436600
C	3.71015000	3.43301100	2.58765500
H	4.70594400	2.64087100	0.84917200
C	1.35842200	3.88603600	2.33081300
H	0.52139800	3.45932500	0.39563800
C	2.50689300	3.88222200	3.12209100
H	4.60962200	3.43023800	3.19549700
H	0.41744100	4.24015500	2.74068800
H	2.46199600	4.23075000	4.14914500
C	2.08477000	0.73536500	-2.62596500
O	3.32959100	0.37607900	-2.79019000
N	3.83678300	-0.32118900	-7.61202900
O	3.38264100	0.74642500	-7.24137100
O	4.30433400	-0.52208800	-8.71982500
H	-3.00472600	4.89346900	-3.31235500
H	-4.06938100	4.21946100	-2.06809800

H	-4.41439400	3.94723400	-3.78426200
C	-1.57410300	0.13886800	-0.53197100
H	-2.08228800	-0.82738200	-0.61838100
H	-0.52344200	-0.06634300	-0.31004000
H	-2.00037100	0.67222300	0.31994500
C	-0.79099100	0.64458600	-5.49323200
H	-1.14356900	1.22486800	-6.34807000
H	0.30059300	0.70415300	-5.45963100
H	-1.07868600	-0.40189600	-5.64283000
H	2.00389400	0.50739300	-0.47729400
C	1.66045300	2.93231600	-3.52148400
S	2.26593000	3.84012000	-2.10168200
N	1.59884700	1.67705100	-3.67574300
H	0.72193700	1.58767400	-1.09779900
C	1.16999000	3.81304000	-4.62360300
C	0.46683100	4.99265400	-4.36295200
C	1.36820700	3.40714000	-5.94710700
C	-0.03980900	5.75152700	-5.41471200
H	0.29534400	5.30620300	-3.33743900
C	0.86748500	4.17222800	-6.99426100
H	1.92726300	2.49644500	-6.13796300
C	0.15888800	5.34375100	-6.73094000
H	-0.59208800	6.66199600	-5.20303700
H	1.03781200	3.85586900	-8.01878900
H	-0.23185400	5.93964400	-7.55012900

**TS8R**

C	4.10639300	-4.62176800	-5.89820400
C	3.83456900	-3.29988400	-5.54356200
C	4.29719500	-2.22733800	-6.29943200
C	5.04403600	-2.55265100	-7.42732200
C	5.33095100	-3.85987000	-7.81238900
C	4.85676300	-4.90961700	-7.03605400
C	3.49817700	-5.58207900	-4.91054800
C	2.53913400	-4.72653200	-4.05292800
C	3.01109100	-3.24496400	-4.27300600
H	4.09467900	-1.18827000	-6.03254900
H	5.91334300	-4.03475400	-8.70839300
H	5.06536800	-5.93622600	-7.32018200
H	2.95354900	-6.40441600	-5.38348500
H	2.60610200	-4.98732000	-2.99578700
H	4.27802300	-6.02497700	-4.28109300
H	3.62160900	-2.89504900	-3.43914400
N	1.86922900	-2.34554900	-4.38900100



O	1. 17753200	-4. 95666100	-4. 38696700
C	1. 70737700	-1. 06140300	-3. 97394900
C	0. 73508000	-2. 75958100	-5. 03907500
N	0. 46819600	-0. 78595400	-4. 40582000
N	-0. 15997100	-1. 82268800	-5. 05757200
C	0. 67423800	-4. 18756800	-5. 46617300
H	1. 24900100	-4. 34912400	-6. 38896100
H	-0. 35894700	-4. 49116700	-5. 63764100
C	-0. 21180800	0. 47109400	-4. 27781900
C	-0. 20995900	1. 33799600	-5. 37404400
C	-0. 83728700	0. 77520800	-3. 06685300
C	-0. 84486900	2. 56932500	-5. 21496700
C	-1. 45367400	2. 02070500	-2. 95579800
C	-1. 45993100	2. 92969400	-4. 01489200
H	-0. 85328700	3. 26571100	-6. 05000600
H	-1. 94293000	2. 28530300	-2. 02144400
C	-2. 09149400	4. 28748500	-3. 85470800
C	3. 81498800	2. 27090100	-2. 59097300
C	2. 68087700	1. 29074700	-2. 89368200
H	4. 18797600	2. 66214900	-3. 54132800
C	3. 39203200	3. 42386300	-1. 71093500
C	3. 41741800	4. 72357400	-2. 21770000
C	2. 93296000	3. 21218800	-0. 40740400
C	2. 98954000	5. 79593300	-1. 43833500
H	3. 77423500	4. 89373800	-3. 22990800
C	2. 50667600	4. 28196500	0. 37179600
H	2. 91925000	2. 20425700	-0. 00042000
C	2. 53377100	5. 57746200	-0. 14223400
H	3. 01738500	6. 80210800	-1. 84472800
H	2. 15508500	4. 10582000	1. 38368500
H	2. 20516300	6. 41273900	0. 46814100
C	3. 20632000	0. 27709300	-3. 90333500
O	3. 34101400	0. 60916000	-5. 09330300
N	5. 56053400	-1. 45908900	-8. 26542600
O	5. 29048400	-0. 31966200	-7. 93973100
O	6. 23120700	-1. 75993800	-9. 23996600
H	-1. 35841500	5. 01023900	-3. 48049000
H	-2. 91891100	4. 25940300	-3. 14136100
H	-2. 47054300	4. 66487900	-4. 80755700
C	-0. 83021000	-0. 20513500	-1. 92525600
H	-1. 18059900	-1. 18992400	-2. 24966300
H	0. 17874900	-0. 33718200	-1. 52058700
H	-1. 47662700	0. 14143500	-1. 11665500
C	0. 46929200	0. 95183900	-6. 65828200

H	1. 53503200	0. 77341400	-6. 47832500
H	0. 03367800	0. 03633100	-7. 07119700
H	0. 36735400	1. 74634700	-7. 40026300
H	1. 85800900	1. 84503400	-3. 35188900
C	5. 06084400	-0. 24629400	-2. 52190700
S	5. 21498500	1. 37931600	-1. 79362900
N	4. 20297600	-0. 63962900	-3. 37219000
H	2. 33069800	0. 80707700	-1. 97645800
C	6. 10314200	-1. 20881500	-2. 05532100
C	6. 63521100	-1. 15735500	-0. 76457500
C	6. 53986400	-2. 20038200	-2. 94086200
C	7. 58667000	-2. 09037500	-0. 36341400
H	6. 29391300	-0. 40119100	-0. 06423900
C	7. 49531900	-3. 12569800	-2. 53853800
H	6. 13221000	-2. 21670200	-3. 94747600
C	8. 01973900	-3. 07407200	-1. 24793900
H	7. 98831300	-2. 04761100	0. 64387000
H	7. 83972100	-3. 88278500	-3. 23624500
H	8. 76728900	-3. 79573000	-0. 93364900

**TS8S**

C	3. 54910000	-3. 74097500	-5. 11575400
C	3. 18038700	-2. 47197400	-4. 67109100
C	3. 33352500	-1. 34378300	-5. 46876800
C	3. 85247000	-1. 55784300	-6. 74081600
C	4. 22301000	-2. 81323500	-7. 21952000
C	4. 07379200	-3. 91901500	-6. 39484000
C	3. 31784800	-4. 77985100	-4. 05185300
C	2. 51538800	-4. 06133100	-2. 94177500
C	2. 63633000	-2. 52461400	-3. 25948700
H	3. 08216100	-0. 34734500	-5. 11050700
H	4. 62203600	-2. 90238900	-8. 22199300
H	4. 36130900	-4. 90472600	-6. 74635300
H	2. 76506300	-5. 65274000	-4. 41338400
H	2. 92836800	-4. 26743300	-1. 95397500
H	4. 27389900	-5. 14289700	-3. 66033600
H	3. 30260300	-2. 00541200	-2. 56908100
N	1. 32943200	-1. 88148800	-3. 15903500
O	1. 17665400	-4. 52793600	-2. 86386100
C	1. 02552300	-0. 61974700	-2. 78240000
C	0. 18084700	-2. 53204200	-3. 53040300
N	-0. 30126400	-0. 58077900	-2. 95225800
N	-0. 85306900	-1. 75776700	-3. 40640200
C	0. 29990900	-3. 98783000	-3. 83865900

H	0.67268700	-4.15153400	-4.85974900
H	-0.66539400	-4.48385300	-3.73333900
C	-1.12270100	0.57904600	-2.74747500
C	-1.40127800	1.39602300	-3.84668100
C	-1.58816200	0.85351600	-1.45864700
C	-2.13183700	2.56024100	-3.61035600
C	-2.31252900	2.03054300	-1.27340800
C	-2.57867300	2.90063700	-2.33301300
H	-2.34740000	3.21902200	-4.44837200
H	-2.68197500	2.26990500	-0.27867800
C	-3.31722500	4.19181900	-2.09959200
C	2.65968100	2.69094600	-0.97192100
C	2.02740300	1.31989000	-1.19262700
H	3.73728200	2.62299400	-1.14713000
C	2.40883500	3.24320200	0.41201200
C	3.48226700	3.61172600	1.22327500
C	1.10680600	3.36616500	0.90982200
C	3.26404900	4.08557800	2.51513800
H	4.49511900	3.52234600	0.83971500
C	0.88865900	3.83771300	2.19915200
H	0.26182700	3.09756700	0.27904900
C	1.96729700	4.19812100	3.00607300
H	4.10905100	4.36713400	3.13555500
H	-0.12544400	3.92830400	2.57602900
H	1.79542600	4.56782700	4.01210600
C	2.45143700	0.76974300	-2.55135500
O	3.54931900	0.20255200	-2.67794100
N	4.03349000	-0.40678500	-7.63594300
O	3.70795400	0.69296300	-7.22566100
O	4.49802600	-0.61377600	-8.74346600
H	-2.61976600	4.98963600	-1.82114000
H	-4.04573200	4.09497700	-1.29049400
H	-3.84530900	4.51459900	-3.00017700
C	-1.31487100	-0.08858900	-0.31676900
H	-1.55668900	-1.11946000	-0.59253800
H	-0.26048100	-0.06963500	-0.02006900
H	-1.91250000	0.18400700	0.55537700
C	-0.94125100	1.01838300	-5.22725900
H	-1.13657800	1.82966000	-5.93253700
H	0.13283400	0.80827800	-5.23414700
H	-1.46539800	0.12094900	-5.57364800
H	2.38538000	0.62624200	-0.42620500
C	1.75781900	2.78625100	-3.62536700
S	1.97699400	3.86481800	-2.21266100

N	1. 98195800	1. 53714500	-3. 69890100
H	0. 94070600	1. 41232400	-1. 12752900
C	1. 27973100	3. 50406300	-4. 84272100
C	0. 36571400	4. 55834400	-4. 76863900
C	1. 73086300	3. 06503200	-6. 09073200
C	-0. 10203200	5. 15641900	-5. 93626500
H	-0. 00429900	4. 89342000	-3. 80374100
C	1. 27028800	3. 67200500	-7. 25266200
H	2. 43878400	2. 24482400	-6. 13203400
C	0. 34933500	4. 71620300	-7. 17827400
H	-0. 82167800	5. 96679000	-5. 87334300
H	1. 63361500	3. 32733000	-8. 21576000
H	-0. 01403500	5. 18747200	-8. 08634600

**PR**

C	2. 68655800	2. 89664000	-0. 98634300
C	2. 27183700	1. 46022400	-1. 30723800
H	3. 77850400	2. 96717700	-1. 01145400
C	2. 20259300	3. 37503400	0. 36408500
C	3. 12744200	3. 78975100	1. 32214800
C	0. 84062100	3. 38670800	0. 67968400
C	2. 70131000	4. 20196100	2. 58270700
H	4. 18695000	3. 78653800	1. 08062300
C	0. 41513000	3. 79734100	1. 93775800
H	0. 11118600	3. 08067900	-0. 06600800
C	1. 34522400	4. 20521800	2. 89260200
H	3. 43035600	4. 52237900	3. 32019900
H	-0. 64437200	3. 80183000	2. 17330700
H	1. 01155600	4. 52741000	3. 87380600
C	2. 88303500	1. 03890600	-2. 62785900
O	3. 62521300	0. 08934100	-2. 72633300
H	2. 64173700	0. 79096400	-0. 52832200
C	2. 11852900	2. 99286300	-3. 71779200
S	2. 05882300	4. 03965600	-2. 28204300
N	2. 52469000	1. 77907300	-3. 76358200
H	1. 17990700	1. 38208300	-1. 35913500
C	1. 65720600	3. 63735600	-4. 97954200
C	0. 98964400	4. 86650100	-4. 99470400
C	1. 90359400	2. 97489500	-6. 18865000
C	0. 57226600	5. 42100200	-6. 19954500
H	0. 77591900	5. 39410300	-4. 07041000
C	1. 48706100	3. 53376100	-7. 38921100
H	2. 42643400	2. 02546600	-6. 16414600
C	0. 82075000	4. 75779200	-7. 39806600

H	0.04979200	6.37189000	-6.19980500
H	1.68557400	3.01461300	-8.32125200
H	0.49506900	5.19378900	-8.33734700

**PS**

C	3.46449700	1.92937000	-2.07466900
C	2.99189800	0.74493900	-2.91853300
H	4.51176200	1.77365500	-1.79709300
C	3.34719500	3.25793500	-2.78703800
C	4.49447500	4.01313700	-3.02866900
C	2.11087900	3.72947100	-3.23882000
C	4.41229800	5.22219500	-3.71546300
H	5.45693200	3.65107400	-2.67731400
C	2.02841500	4.93675600	-3.92315700
H	1.20978700	3.15373500	-3.04335600
C	3.17950000	5.68528000	-4.16399600
H	5.31256800	5.79988000	-3.89919000
H	1.06421000	5.29538900	-4.26899000
H	3.11288100	6.62810800	-4.69754900
C	3.24245800	-0.54641800	-2.16666100
O	3.94148200	-1.42912900	-2.60709900
H	3.55724300	0.71378900	-3.85188700
C	2.21236400	0.27899000	-0.20645700
S	2.51475400	2.00514300	-0.50347100
N	2.59706900	-0.70471600	-0.93085200
H	1.92510500	0.84498700	-3.14834800
C	1.45646500	-0.00899600	1.04375700
C	0.71853500	0.97153900	1.71525700
C	1.49387500	-1.31208900	1.55455100
C	0.02780600	0.65185300	2.87892600
H	0.66106000	1.98410100	1.32806200
C	0.80686700	-1.62468700	2.72005100
H	2.07121600	-2.06224400	1.02583600
C	0.07239700	-0.64439700	3.38485600
H	-0.54702200	1.41800200	3.38855000
H	0.84704100	-2.63549900	3.11269200
H	-0.46477700	-0.89041100	4.29538500

**E-M4\_Li<sup>+</sup>**

C	4.04477100	0.80011400	-1.67569000
C	3.16341400	0.47159500	-0.64743300
C	2.39160300	1.44153200	-0.02369000
C	2.49956100	2.73596500	-0.51054200
C	3.37169700	3.10167400	-1.53423400

C	4. 16062800	2. 11949500	-2. 11701400
C	4. 78845500	-0. 40663500	-2. 17432900
C	4. 22497500	-1. 60844900	-1. 37408100
C	3. 17041700	-1. 01040000	-0. 35529000
H	1. 70961600	1. 22218600	0. 78790000
H	3. 40849600	4. 13388800	-1. 86235800
H	4. 84950700	2. 37842900	-2. 91458900
H	4. 65411000	-0. 56756500	-3. 24957100
H	5. 01250400	-2. 09739200	-0. 80078100
H	5. 86520600	-0. 30381400	-2. 00833100
H	3. 43866700	-1. 23183800	0. 67832100
N	1. 84550100	-1. 62696300	-0. 57611700
O	3. 71633900	-2. 63014200	-2. 20249500
C	0. 78019200	-1. 71109100	0. 23742000
C	1. 47561300	-2. 21652100	-1. 75215000
N	-0. 15038500	-2. 37803300	-0. 43424100
N	0. 27200500	-2. 70835800	-1. 68080200
C	2. 49417500	-2. 30970900	-2. 83484500
H	2. 54091500	-1. 35871100	-3. 38338800
H	2. 24864500	-3. 11654700	-3. 52485000
C	-1. 43209700	-2. 80588800	0. 05971700
C	-2. 57930200	-2. 40543400	-0. 64155600
C	-1. 46998800	-3. 59338700	1. 21698000
C	-3. 80532300	-2. 79401200	-0. 10994000
C	-2. 73004600	-3. 95042700	1. 69708800
C	-3. 90361000	-3. 55985300	1. 05519200
H	-4. 71365400	-2. 49314900	-0. 62637900
H	-2. 79064300	-4. 56346900	2. 59261600
C	-5. 24967900	-3. 98551000	1. 57793000
N	1. 62216200	3. 76030900	0. 05338100
O	0. 66104900	3. 37325500	0. 73832300
O	1. 86544100	4. 91676200	-0. 16038100
H	-5. 61148300	-4. 86203100	1. 02998400
H	-5. 99081900	-3. 19174800	1. 45386600
H	-5. 20056300	-4. 25065800	2. 63628600
C	-0. 23080500	-4. 08091400	1. 92917900
H	0. 58698100	-4. 29374100	1. 23418900
H	0. 13337200	-3. 36164300	2. 67127900
H	-0. 45678000	-5. 00494400	2. 46490300
C	-2. 50723400	-1. 59904300	-1. 91178400
H	-1. 77352000	-0. 79214100	-1. 83139500
H	-2. 21238800	-2. 23342100	-2. 75301600
H	-3. 48616300	-1. 17005000	-2. 13646300
H	0. 92615400	1. 28283600	-3. 55708800

C	0.07660600	1.30506200	-1.88483000
O	-0.27417100	0.62978400	-0.87851500
O	0.75492600	0.63663500	-2.85162600
O	-0.13156500	2.53209400	-2.01794100
C	-0.54501300	0.86075200	2.51288000
C	-0.56066700	-0.25161600	1.75564800
H	0.32622400	1.04533400	3.14140100
C	-1.54439600	1.92749800	2.44686600
C	-1.36789100	3.06819400	3.24118700
C	-2.60831400	1.90199600	1.52182200
C	-2.22476000	4.15718500	3.12178900
H	-0.54185500	3.10141800	3.94594100
C	-3.45512200	2.99806300	1.39593500
H	-2.78019600	1.02329900	0.90337300
C	-3.26334000	4.12852300	2.19510300
H	-2.07330900	5.03350500	3.74281000
H	-4.27157000	2.96927700	0.68134600
H	-3.92495700	4.98218400	2.09235300
C	0.67490100	-1.00886000	1.57304800
O	1.66704500	-0.97878000	2.27422900
H	-1.37550500	-0.47097000	1.07750700
Li	-0.77763900	2.41842400	-0.18673000

**TS5R\_Li<sup>+</sup>**

C	-5.50133500	0.07963300	0.46583000
C	-4.11882200	-0.07293300	0.43088800
C	-3.52502000	-1.09892600	-0.27250100
C	-4.35262900	-2.06572300	-0.80910000
C	-5.74253300	-1.96907100	-0.78601600
C	-6.31868200	-0.86097000	-0.16851000
C	-5.88065600	1.31152300	1.24597000
C	-4.55016600	1.88877500	1.80586100
C	-3.41837500	0.88746900	1.34928900
H	-2.45569200	-1.14220600	-0.38998500
H	-6.34901300	-2.75259500	-1.22621300
H	-7.39832700	-0.75753400	-0.14991900
H	-6.37298100	2.05653900	0.61086800
H	-4.57211700	1.90999100	2.89566900
H	-6.57501800	1.07972800	2.05758600
H	-3.01445800	0.34684300	2.20584400
N	-2.28610600	1.57494500	0.71650400
O	-4.31493300	3.23111900	1.43552000
C	-0.97257000	1.25791400	0.64056400
C	-2.44856000	2.78655700	0.11079000

N	-0.40333700	2.29773300	0.02039700
N	-1.30892300	3.25377800	-0.31036400
C	-3.80971000	3.40231000	0.12738300
H	-4.45461600	2.93565400	-0.63095000
H	-3.74096400	4.47112900	-0.07547000
C	0.98513900	2.51429400	-0.31337800
C	1.38885500	2.25634400	-1.62314300
C	1.83464900	2.99907200	0.68725900
C	2.74321900	2.43433300	-1.90570300
C	3.17752300	3.14747700	0.35110200
C	3.64990300	2.85114500	-0.93232900
H	3.09406600	2.23555600	-2.91362400
H	3.87021700	3.51401400	1.10470400
C	5.11559600	2.96703200	-1.24982400
C	1.48588400	-1.33319000	1.88901000
C	1.00134100	-0.16380300	1.30925400
H	0.75936800	-1.98785200	2.35911300
C	2.87250500	-1.53542700	2.29460800
C	3.20642400	-2.71756900	2.97266200
C	3.87226300	-0.57479200	2.06385400
C	4.50508400	-2.94132600	3.40627600
H	2.43681600	-3.46611900	3.14147500
C	5.16999200	-0.80008500	2.50170700
H	3.63915900	0.35066900	1.54385500
C	5.48862000	-1.98147800	3.17143500
H	4.75299800	-3.86021400	3.92648000
H	5.93614300	-0.05211900	2.32574100
H	6.50504700	-2.15333700	3.51091000
C	-0.38025300	-0.04482100	1.12731500
O	-1.22105000	-0.95941800	1.36264000
N	-3.69565600	-3.27358300	-1.29910500
O	-2.53677900	-3.48663500	-0.90635000
O	-4.30036900	-4.02014400	-2.02377100
H	5.28110700	3.08741200	-2.32272400
H	5.64532300	2.06207300	-0.93165500
H	5.56972800	3.81560700	-0.73190300
C	1.32267700	3.31387000	2.06698000
H	0.46315900	3.99102500	2.02746000
H	1.00978400	2.40330500	2.59220200
H	2.10227800	3.79030200	2.66338000
C	0.41213700	1.81322300	-2.67549100
H	0.06569000	0.78896300	-2.48885500
H	-0.45726600	2.47750500	-2.70594400
H	0.88721300	1.83203000	-3.65795600



H	1.67456200	0.60508700	0.96271800
C	0.99367900	-1.94029800	-1.37611100
S	1.06178500	-3.11861200	-0.05429500
N	-0.08984600	-1.50995200	-1.92144900
H	-0.89824700	-2.04481200	-1.60135500
C	2.28255400	-1.39449500	-1.90502400
C	3.46083000	-1.41964500	-1.15610300
C	2.31396900	-0.86848500	-3.20371400
C	4.63932200	-0.88839200	-1.67338700
H	3.46047400	-1.87877900	-0.17482200
C	3.49784300	-0.36667500	-3.73104700
H	1.40520500	-0.88447800	-3.79564600
C	4.66248600	-0.36274000	-2.96211900
H	5.54486200	-0.91053100	-1.07426700
H	3.51598500	0.01628400	-4.74714300
H	5.58700000	0.03086500	-3.37418700
Li	-1.21647900	-2.74442400	0.55735700

**TS5S\_Li<sup>+</sup>**

C	4.93201800	-1.17039200	0.06056300
C	3.72062300	-0.62782300	0.49160100
C	3.67458200	0.34665300	1.48005000
C	4.88890600	0.75666500	2.01219500
C	6.11550200	0.24267800	1.60029100
C	6.13547200	-0.73563400	0.61377300
C	4.72379800	-2.21456400	-1.00090400
C	3.21093600	-2.18964700	-1.32279700
C	2.55080000	-1.23622300	-0.24996200
H	2.74177500	0.77302900	1.83044900
H	7.02851500	0.60938800	2.05350900
H	7.08037200	-1.15132100	0.27958100
H	5.30910200	-2.02284600	-1.90610300
H	2.77193800	-3.18325700	-1.22330100
H	5.02008000	-3.20331000	-0.63884200
H	1.87739100	-1.80562200	0.39702500
N	1.74095200	-0.20448700	-0.91881000
O	2.93830800	-1.80783300	-2.65869900
C	0.62796000	0.43706200	-0.52217800
C	2.05047200	0.27335200	-2.16286500
N	0.33214700	1.29131400	-1.50087300
N	1.20580600	1.19047900	-2.53771100
C	3.13247300	-0.42918500	-2.91518800
H	4.12619700	-0.08151400	-2.60159500
H	3.01747300	-0.25728500	-3.98580500

C	-0.73085100	2.26502900	-1.54096200
C	-0.68980400	3.34263100	-0.65224100
C	-1.74776300	2.07245800	-2.48140000
C	-1.74287400	4.25402500	-0.72206000
C	-2.77307200	3.01299600	-2.50443200
C	-2.78632300	4.10806800	-1.63681100
H	-1.74114600	5.10434400	-0.04534300
H	-3.58028800	2.88798800	-3.22166600
C	-3.89282000	5.12414500	-1.71289100
C	-2.29158600	-0.12835700	1.78462600
C	-1.51233800	0.14024200	0.64430700
H	-1.84900800	0.13163200	2.74322000
C	-3.75554700	-0.14041300	1.77089300
C	-4.43673500	-0.11933900	2.99708000
C	-4.49639400	-0.15105400	0.57921400
C	-5.82329900	-0.10961300	3.03598500
H	-3.86505200	-0.11652700	3.92173200
C	-5.88473100	-0.14145800	0.62081200
H	-3.99269200	-0.16813000	-0.38175800
C	-6.54954200	-0.12230300	1.84564900
H	-6.33956900	-0.09292500	3.98980100
H	-6.45173400	-0.14678400	-0.30430500
H	-7.63443900	-0.11571400	1.87285100
C	-0.12906100	0.17791500	0.74038200
O	0.58168900	-0.06532600	1.76421900
N	4.87128500	1.78281200	3.06652600
O	3.78354600	2.17800700	3.44992500
O	5.94070300	2.17402800	3.49264600
H	-3.96759700	5.70130100	-0.78888500
H	-4.85714000	4.64511400	-1.89970900
H	-3.71016000	5.82681600	-2.53247700
C	-1.74022200	0.89846800	-3.42153500
H	-1.01051100	1.04271600	-4.22424900
H	-1.47753900	-0.03194000	-2.90775000
H	-2.72470400	0.76851800	-3.87520800
C	0.42653400	3.51860700	0.34280200
H	0.32585600	2.83073700	1.19077500
H	1.40640900	3.35183700	-0.11571900
H	0.41521500	4.53296900	0.74437000
H	-1.96883700	0.24056700	-0.33291400
C	-0.73799300	-3.00851400	1.11627100
S	-1.71957400	-2.46554800	2.50188400
N	0.46030300	-3.46127200	1.21205800
H	0.74583900	-3.55928000	2.19014500

C	-1.33683100	-2.89073900	-0.24779100
C	-2.71879000	-2.80728600	-0.43347800
C	-0.49586800	-2.87503000	-1.36869100
C	-3.25021500	-2.71019300	-1.71781100
H	-3.37872200	-2.82279800	0.42847500
C	-1.02554100	-2.76414600	-2.64819700
H	0.57502100	-2.96629300	-1.22638100
C	-2.40793700	-2.68276100	-2.82583000
H	-4.32668200	-2.65832400	-1.84895400
H	-0.36007400	-2.74774900	-3.50596500
H	-2.82400200	-2.60130800	-3.82523400
Li	0.25312800	-1.29702300	3.05804100