

Competing Mechanisms and Origins of Chemo- and Stereo-Selectivities of NHC-Catalyzed Reactions of Enals with 2-Aminoacrylates

Yang Wang,^a Yanyan Wang,^b Xinghua Wang,^b Xue Li,^b Ling-Bo Qu,^{*,b} and Donghui Wei^{*,b},

^a Department of Material and Chemical Engineering, Zhengzhou University of Light Industry, Zhengzhou, Henan Province, 450002, P.R. China

^b College of Chemistry and Molecular Engineering, Zhengzhou University, Zhengzhou, Henan Province, 450001, P.R. China

Content

1. Computational Details	S2
2. EPS analysis of 2-aminoacrylates	S4
3. Transition states involved in reaction between 2-aminoacrylate and Breslow intermediate ...	S5
4. Energy profile of [3 + 2] Annulation reaction involved in another three pathways	S6
5. Nucleophilic and electrophilic Parr function analysis of Si-M2 , R2 , and R2'	S7
6. IRC plots of stereochemical transition states	S8
7. Energy profile of [3 + 3] annulation reaction involved in another three pathways	S9
8. Entire Energy profile of Cross-coupling and Stetter reaction	S10
9. EPS analysis for the chemoselective transition states	S11
10. Cartesian coordinates of the optimized structures	S12

* Corresponding Author: donghuiwei@zzu.edu.cn (D. H. Wei) and qulingbo@zzu.edu.cn (L.-B. Qu)

1. Computational Details

All the calculations involved in the reaction were performed by using density functional theory with the Gaussian 09 suite of programs, which has been identified to be a powerful and widely used method for exploring the mechanisms of organic, biological as well as transition metal-catalyzed reactions. The solution-phase structure optimization of all the stationary points was carried out at M06-2X/6-31G(d, p) level in THF solvent using the integral equation formalism polarizable continuum model (IEF-PCM). The M06-2X/6-31G(d, p) harmonic frequencies were performed at 298.15 K and 1 atm to provide the thermal corrections for Gibbs free energies and make sure that the local minima had no imaginary frequencies, while the transition states had one and only one imaginary frequency. Non-covalent interaction (NCI) analysis was plotted by using NCIPLOT and the computed 3D-structures were rendered using the CYLView software.

Moreover, we further refined the energy by employing the single-point energy calculations at the M06-2X-D3/6-31++G (2df, 2pd)/IEF-PCM_{THF} level based on the M06-2X/6-31G(d, p)/IEF-PCM_{THF} optimized structures. The energies discussed in this work were obtained by the addition of the thermal correction at the M06-2X/6-31G(d, p)/IEF-PCM_{THF} level to the corresponding single-point energy at the M06-2X-D3/6-31++G (2df, 2pd)/IEF-PCM_{THF} level.

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

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

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

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.

For analyzing the local nucleophilicity and electrophilicity, we have also performed the Parr function analysis. Pioneered by Domingo and coworkers, the nucleophilic (P_k^-) and electrophilic (P_k^+) Parr functions which allow for the characterization of the nucleophilic and electrophilic sites of a molecule, can be obtained through the analysis of Mulliken atomic spin density (ASD) of the

corresponding radical cations (RC) or anions (RA) of the studies molecules, separately. According to Domingo's definition, the Parr functions can be expressed by the following equations:

$$P^{-}(r) = \rho_S^{rc}(r) \text{ for the electrophilic attacks} \quad (3)$$

$$P^{+}(r) = \rho_S^{ra}(r) \text{ for the nucleophilic attacks} \quad (4)$$

where $\rho_S^{rc}(r)$ is the ASD of the radical cation and $\rho_S^{ra}(r)$ is the ASD of the radical anion. Each ASD condensed at the different atoms of the radical cation and radical anion provides the local nucleophilic P_k^{-} and electrophilic P_k^{+} Parr functions of the neutral system, respectively.

2. EPS analysis of 2-aminoacrylates

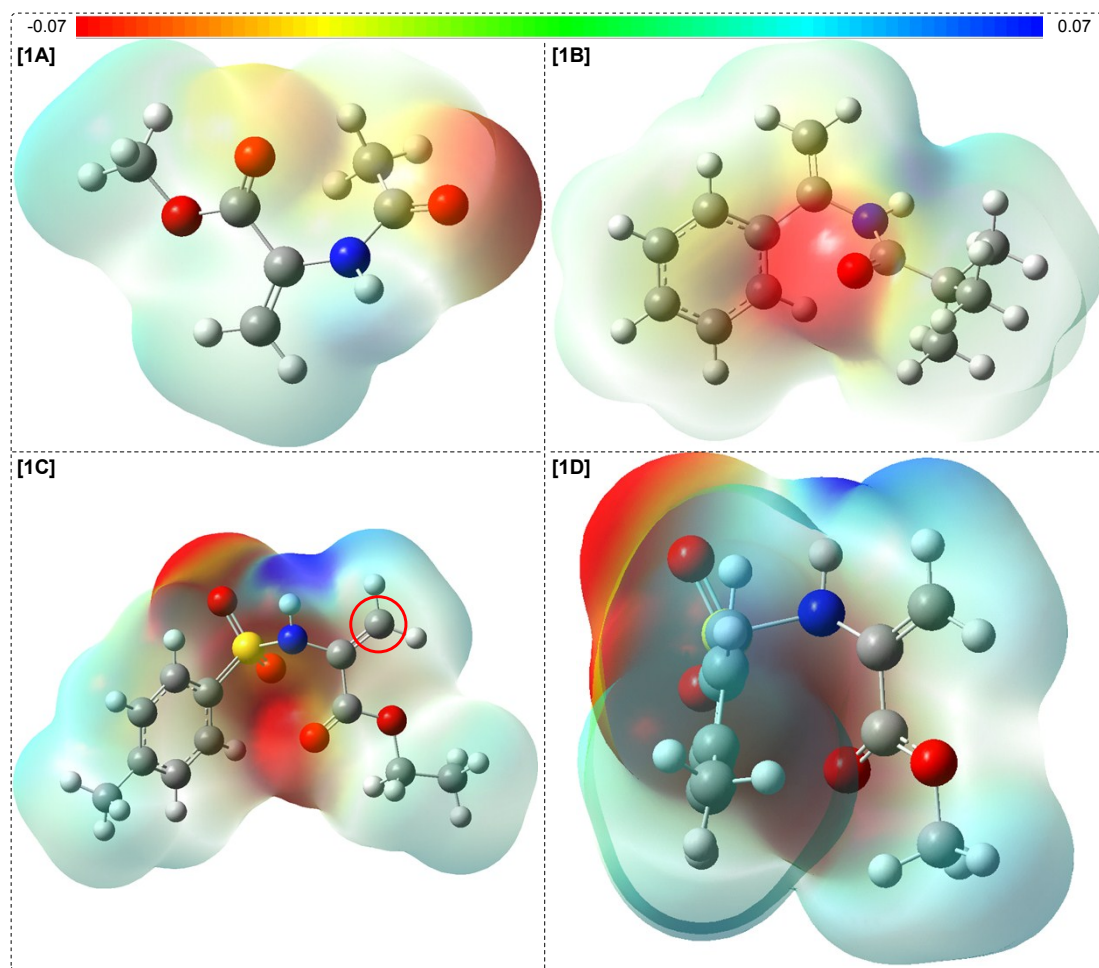


Fig. S1 Electron cloud distribution of the four representative 2-aminoacrylates

The electrostatic potential surface (EPS) analyses of 2-aminoacrylates involved in the works of Glorius,¹ Wang,² and Qi³ have been carried out. As shown in **Fig. S1C**, one can easily find that the positive charge center is located on the β -carbon of 2-aminoacrylate involved in Qi's work,^{3a} thus, the β -carbon would be electrophilic, then it reacts with acyl intermediate via the [3 + 3] annulation reaction.

1 T. Jousseume, E. Wurz Nathalie, F. Glorius, *Angew. Chem. Int. Ed.* 2011, **50**, 1410-1414.

2 J. Wu, C. Zhao, J. Wang, *J. Am. Chem. Soc.* 2016, **138**, 4706-4709.

3 a) L.-L. Zhao, X.-S. Li, L.-L. Cao, R. Zhang, X.-Q. Shi, J. Qi, *Chem. Commun.* 2017, **53**, 5985-5988; b) X.-S. Li, L.-L. Zhao, X.-K. Wang, L. L. Cao, X.-Q. Shi, R. Zhang, J. Qi, *Org. Lett.* 2017, **19**, 3943-3946.

3. Transition states involved in reaction between 2-aminoacrylate and Breslow intermediate

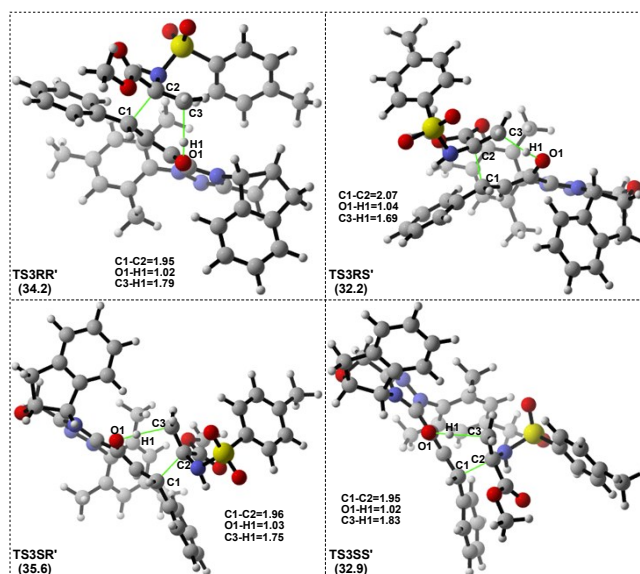


Fig. S2 3D-structures and energy barriers of transition states involved in the reaction pathway between 2-aminoacrylate **R2** and Breslow intermediate **Si-M2** (Distance in Å and energy in kcal/mol)

4. Energy profile of [3 + 2] Annulation reaction involved in another three pathways

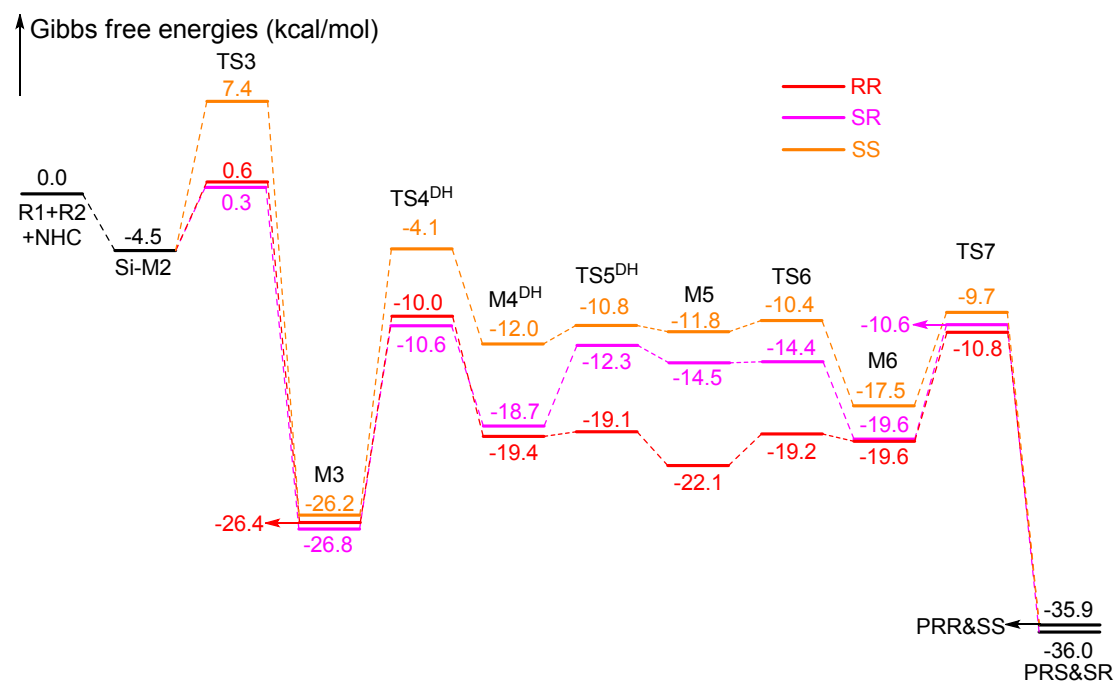


Fig. S3 The energy profile of [3 + 2] annulation reaction involved in another three pathways

5. Nucleophilic and electrophilic Parr function analysis of Si-M2, R2, and R2'

Table S1 Nucleophilic and electrophilic Parr function analysis of **Si-M2**, **R2**, and **R2'**

		Si-M2	R2	R2'
P_k^-	C1	0.40	–	–
	C2	–	0.04	0.02
	C3	–	0.47	0.00
	C4	0.33	–	–
	N1	–	0.39	–0.00
P_k^+	C1	0.07	–	–
	C2	–	0.11	0.55
	C3	–	0.47	–
	C4	–0.12	–	–
	N1	–	0.00	0.13

Note: The label C4 represents the carbonyl carbon atom of **Si-M2**.

6. IRC plots of stereochemical transition states

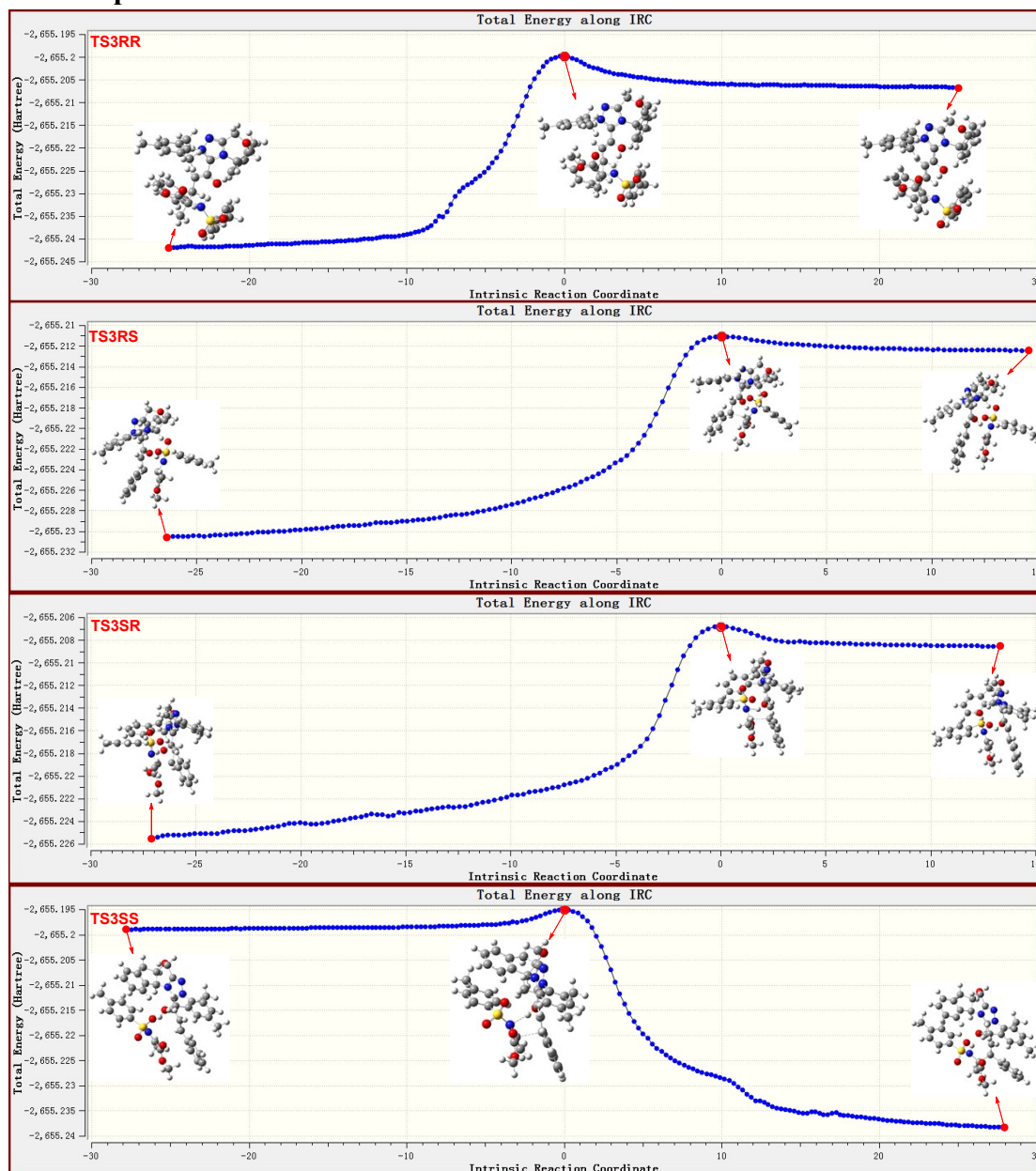


Fig. S4 IRC plots of stereochemical transition states

7. Energy profile of [3 + 3] annulation reaction involved in another three pathways

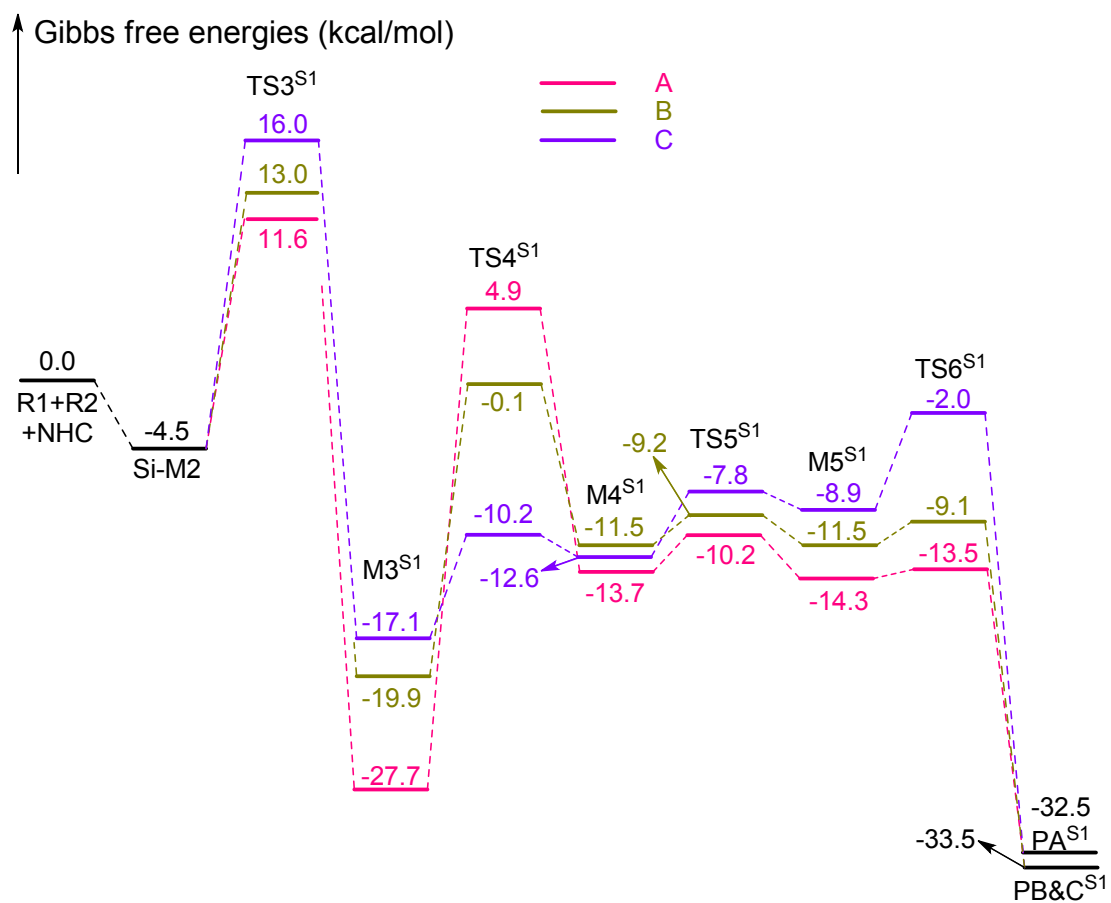


Fig. S5 The energy profile of [3 + 3] annulation reaction involved in another three pathways

8. Entire Energy profile of Cross-coupling and Stetter reaction

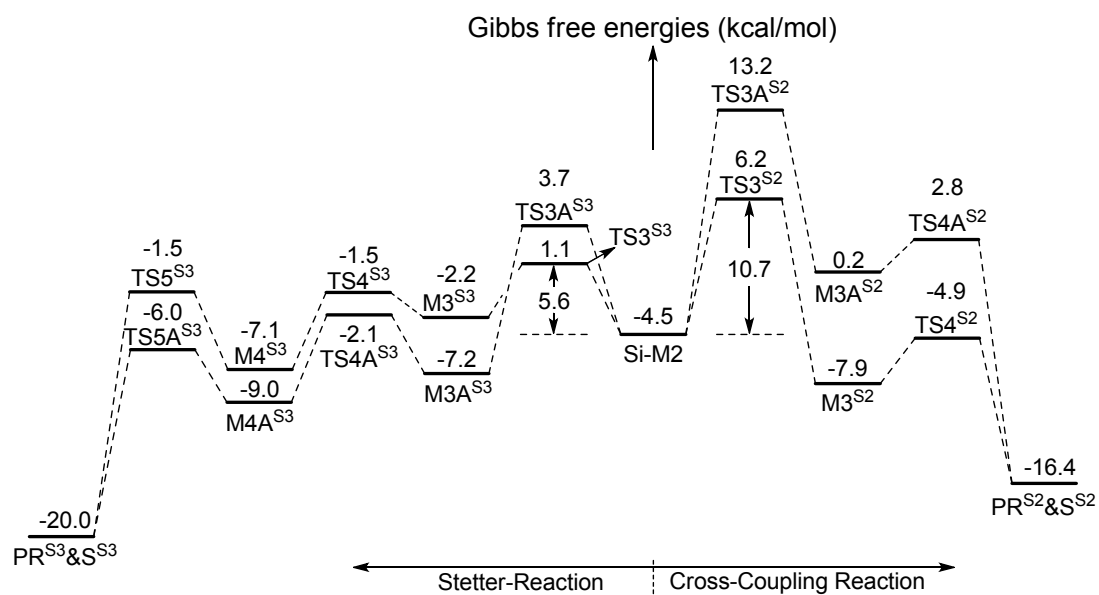


Fig. S6 The entire energy profiles of Cross-Coupling and Stetter reactions (Energy in kcal/mol)

9. EPS analysis for the chemoselective transition states

As shown in **Fig. S7**, the four transition states **TS3**, **TS3^{S1}**, **TS3^{S2}**, and **TS3^{S3}** are all polar molecules, and the dipole moment of **TS3RS** is extremely lower than that of **TS3^{S1}**, **TS3^{S2}**, and **TS3^{S3}** in THF solvent, which has the quite weaker polarity. This phenomenon reveal that the transition state **TS3RS** would be more stable in weaker polarity solvent. Moreover, the nucleophilicity of β -carbon of Breslow intermediate is stronger than that of the carbonyl atom, which would also be responsible for the preference of [3 + 2] annulation stage.

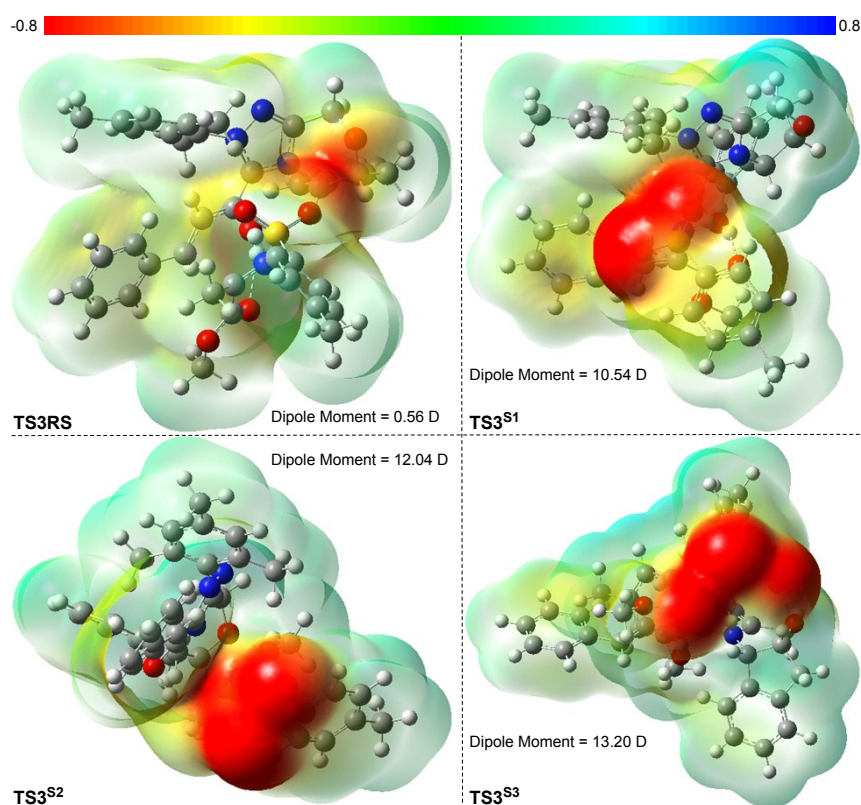


Fig. S7 The electrostatic potential surface of the chemoselective transition states **TS3**, **TS3^{S1}**, **TS3^{S2}**, and **TS3^{S3}**

10. Cartesian coordinates of the optimized structures

R1

C	-3.40880900	0.38469500	0.00000500
O	-3.84909500	-0.74895200	-0.00000900
H	-4.09916000	1.24915500	-0.00001100
C	-1.97265600	0.71940800	0.00000200
C	-1.05283900	-0.25950800	0.00000600
H	-1.71171500	1.77327900	-0.00000500
H	-1.43058200	-1.28195700	0.00001100
C	0.40448900	-0.11271400	0.00000300
C	1.19504200	-1.26997600	0.00000200
C	1.04074400	1.13810100	0.00000100
C	2.58334000	-1.18485600	-0.00000100
H	0.71009100	-2.24228200	0.00000400
C	2.42602000	1.22326400	-0.00000200
H	0.45050900	2.04877200	0.00000300
C	3.20172200	0.06244100	-0.00000400
H	3.18088600	-2.09033400	-0.00000200
H	2.90589800	2.19645500	-0.00000300
H	4.28450600	0.13339500	-0.00000600

R2

C	-1.55927500	1.10247800	2.31347400
C	-1.61339800	0.74761700	1.02827000
H	-1.87100400	0.42315100	3.09966800
H	-1.23100900	2.09562400	2.58839300
N	-2.16348200	-0.48196900	0.59543100
H	-2.57009000	-1.01948800	1.35720600
S	-1.29591900	-1.58159200	-0.37006400
O	-1.68823500	-1.44936400	-1.76131000
O	-1.50906100	-2.85934000	0.30550800
C	0.39895800	-1.09528400	-0.20867000
C	1.01913700	-0.41690400	-1.25186000
C	2.34721000	-0.02979700	-1.09701000
C	3.04738800	-0.31077300	0.07872300
C	2.39216700	-0.99664900	1.11086900
C	1.06977000	-1.39203600	0.97750000
H	0.46268700	-0.19453700	-2.15570500
H	2.84793300	0.49469700	-1.90512700
H	2.93082300	-1.22536100	2.02572900
H	0.56383100	-1.93221300	1.77168900
C	4.48155800	0.11317300	0.24921700
H	5.10589900	-0.73893700	0.53111700
H	4.88050400	0.54422900	-0.67041700

H	4.57024800	0.85974900	1.04401300
C	-1.20270600	1.67895900	-0.06998000
O	-1.43595500	1.47731500	-1.23856100
O	-0.54070800	2.74105800	0.38881000
C	-0.11468300	3.66653300	-0.61770300
H	0.56338000	3.17071100	-1.31513400
H	-0.97581900	4.05442100	-1.16424900
H	0.39662400	4.46595900	-0.08673100

R2'

C	-2.48890100	-0.01866400	-2.60047000
C	-1.86445900	-0.18341100	-1.25054600
H	-2.05619800	-0.72412200	-3.30772400
H	-3.56833200	-0.17772800	-2.51763700
N	-0.93876600	-1.04417000	-1.07925500
S	-0.26186300	-1.25063700	0.47085800
O	-0.08330200	-2.68709300	0.62003700
O	-1.02822000	-0.51593200	1.47735200
C	1.31124400	-0.47508200	0.26597100
C	2.41854500	-1.25562100	-0.04602700
C	3.64896600	-0.62688800	-0.20676400
C	3.77382400	0.75788200	-0.06480000
C	2.63616800	1.51301800	0.24948500
C	1.39853800	0.90797100	0.41714200
H	2.31453800	-2.33064200	-0.14674100
H	4.52612300	-1.22141300	-0.44318400
H	2.72671400	2.58869700	0.36907400
H	0.51355800	1.48896100	0.65983600
C	5.10213500	1.43759300	-0.26413700
H	5.25039400	2.23094300	0.47213700
H	5.92724700	0.72770800	-0.18278900
H	5.15006000	1.89693000	-1.25662900
C	-2.38561000	0.80991000	-0.21578500
O	-1.85464000	1.87760400	-0.03445200
O	-3.52394200	0.39947300	0.31549000
C	-4.07342200	1.27105400	1.31787400
H	-3.36234400	1.36657100	2.14008200
H	-4.27824700	2.25288700	0.88922000
H	-4.99087800	0.79339600	1.65187100
H	-2.33281100	1.00819600	-2.94553400

NHC

C	-3.78602100	0.57335300	-0.36891400
C	-2.93119000	0.62786100	0.73446100
C	-2.73823500	1.80973100	1.43962300

C	-3.42789000	2.94963700	1.02988700
C	-4.29164800	2.89780000	-0.06633500
C	-4.47633200	1.71086500	-0.77427100
C	-3.79271600	-0.80766800	-0.97495500
C	-3.22896000	-1.66894000	0.17653200
C	-2.30396600	-0.72215500	0.98473400
H	-2.05966100	1.84004700	2.28588900
H	-3.29651200	3.88316200	1.56726000
H	-4.82690400	3.79222300	-0.36929800
H	-5.14836600	1.67645600	-1.62657100
H	-3.13764000	-0.83447100	-1.85379900
H	-4.05515800	-1.95108300	0.83379300
H	-4.78124400	-1.14648900	-1.29256300
H	-2.26339000	-0.99102100	2.04293200
N	-0.94250200	-0.80315600	0.44698100
O	-2.61695000	-2.88888300	-0.18785000
C	0.10232800	0.00867800	0.81076600
C	-0.53769500	-1.74182300	-0.46599400
N	1.07823900	-0.51878100	0.04411300
N	0.72069200	-1.59344300	-0.74719000
C	-1.48754700	-2.75385800	-1.02823600
H	-1.77793700	-2.47140100	-2.04841200
H	-1.00521100	-3.73167000	-1.07496700
C	2.43045600	-0.05309500	-0.00742600
C	2.70047200	1.16002100	-0.64617600
C	3.43457000	-0.83480400	0.57059300
C	4.02650800	1.59106500	-0.68828200
C	4.74598100	-0.36748900	0.49833400
C	5.05941700	0.84273700	-0.12280100
H	4.25769800	2.53135700	-1.18326600
H	5.54124100	-0.96180400	0.94262000
C	3.09873600	-2.13393400	1.25302300
H	2.76033200	-2.88087100	0.52940200
H	2.28682500	-1.99366100	1.97334400
C	1.59226300	1.96498800	-1.27151800
H	0.87949900	2.30099400	-0.51339300
H	1.03073200	1.35901300	-1.98964800
H	1.99500100	2.83636300	-1.79076900
H	3.96916400	-2.52846500	1.78016700
C	6.48130500	1.34170600	-0.15656200
H	6.72045400	1.89184900	0.75938100
H	7.18901300	0.51302700	-0.23587200
H	6.64363900	2.01709800	-0.99964700

DBU

C	2.78376900	-0.05205000	0.34661000
C	1.89157400	-1.28072200	0.52479300
C	0.85123800	-1.44036600	-0.59117700
C	2.03913200	1.28293900	0.34449900
C	0.94971200	1.40170500	-0.73540900
C	-0.34011800	0.71995400	-0.33267600
H	3.32219900	-0.15387000	-0.60596300
H	1.36957600	-1.24125200	1.48976200
H	0.53410500	-2.48459500	-0.65141200
H	2.76707000	2.08688600	0.19408500
H	1.32214100	1.01174700	-1.69030300
C	-1.51495400	-1.36401800	0.14753700
H	-1.36494100	-1.57020800	1.21885200
C	-2.53460100	0.85843900	0.52679900
C	-2.76926500	-0.53021600	-0.05610400
H	-3.62787800	-1.01751900	0.41391500
H	-2.97224600	-0.44964300	-1.12947800
H	-2.51852900	0.79899600	1.62457400
H	-1.60354500	-2.32855200	-0.36215200
H	-3.36709900	1.52260100	0.26986500
N	-1.29707200	1.47997300	0.07000100
N	-0.36714600	-0.65772800	-0.40993800
H	1.31099800	-1.20169600	-1.55853200
H	2.52409000	-2.17506100	0.54088300
H	3.54494000	-0.03738400	1.13419500
H	1.57675400	1.45832700	1.32410300
H	0.69296700	2.45151300	-0.88206700

DBU·H⁺

C	2.83746100	-0.01146600	0.29245900
C	1.99700600	-1.27207700	0.49289500
C	0.90246400	-1.45927200	-0.55844000
C	2.05123100	1.29742600	0.35095300
C	0.93982400	1.40184400	-0.71154700
C	-0.29869900	0.65228700	-0.31011800
H	3.33944800	-0.07667500	-0.68162000
H	1.53498200	-1.27899600	1.48762000
H	0.57772700	-2.49941200	-0.58089800
H	2.73797600	2.13212100	0.18939300
H	1.29431500	1.01991500	-1.67461500
C	-1.51392200	-1.40948500	0.14212400
H	-1.40753900	-1.66724000	1.20171200
C	-2.61635100	0.78433600	0.52129100

C	-2.76947000	-0.59014100	-0.10693500
H	-3.62972100	-1.10458300	0.32355900
H	-2.93527300	-0.48786700	-1.18294200
H	-2.60558900	0.72088600	1.61376000
H	-1.54378900	-2.33588300	-0.43341800
H	-3.42205900	1.45429200	0.22047300
N	-1.35428400	1.36211400	0.05927800
N	-0.31357100	-0.66870900	-0.28584500
H	1.27292200	-1.21554900	-1.55967200
H	2.65422000	-2.14526600	0.44264400
H	3.62683300	0.01717100	1.04925000
H	1.61187000	1.43791400	1.34536900
H	0.66296400	2.44662500	-0.86646300
H	-1.27156900	2.36799500	0.01572100

Re-TS1

C	-2.98649000	-2.83397000	-0.00587200
C	-2.01280500	-1.93795500	-0.43952600
C	-1.53679300	-1.94634700	-1.74840200
C	-2.08264200	-2.87378100	-2.63522000
C	-3.07166600	-3.76625900	-2.21399500
C	-3.52851000	-3.75603100	-0.89729100
C	-3.29527200	-2.63908800	1.45710700
C	-2.20364400	-1.67508600	1.97806600
C	-1.57040700	-1.03376300	0.69039200
H	-0.75050900	-1.26008200	-2.06692300
H	-1.73158500	-2.90689700	-3.66151000
H	-3.48127300	-4.48340700	-2.91834000
H	-4.28534800	-4.46261000	-0.56956400
H	-3.27454100	-3.57083200	2.03048800
H	-2.62623200	-0.89691600	2.61449400
H	-4.28728200	-2.19636400	1.59399500
H	-1.92526800	-0.00793500	0.55987700
N	-0.11936300	-0.97716800	0.79554700
O	-1.25407300	-2.32689200	2.81147300
C	0.74875100	-0.08406400	0.26464800
C	0.57912800	-1.98336600	1.41067300
N	1.93283500	-0.60701500	0.60280300
N	1.85841500	-1.78030800	1.32384200
C	-0.21971200	-3.01912300	2.13138500
H	-0.62147400	-3.76189700	1.42846400
H	0.38871700	-3.52821300	2.87856200
C	3.21006900	-0.03456900	0.29176000
C	3.95237500	-0.58903600	-0.75323600

C	3.65204300	1.05504000	1.04558600
C	5.19388400	-0.01870400	-1.02990200
C	4.89743600	1.59483900	0.72718100
C	5.67873100	1.07119000	-0.30410600
H	5.79415900	-0.43248600	-1.83668200
H	5.26653200	2.44167300	1.30066300
C	2.80407500	1.62323000	2.15271200
H	2.48991300	0.84016300	2.84931900
H	1.89431600	2.08300200	1.75171200
C	3.40151400	-1.73908500	-1.55139500
H	2.45023500	-1.43768400	-2.00303200
H	3.21642100	-2.60868200	-0.91399800
H	4.09696700	-2.02771300	-2.34142900
H	3.35547600	2.38323500	2.70851300
C	7.00830700	1.69071700	-0.64984600
H	6.88552800	2.46044600	-1.41872300
H	7.46302600	2.16464700	0.22294000
H	7.70294400	0.94351800	-1.04022500
C	0.59463800	1.07804000	-1.36568600
O	0.87157300	0.32383600	-2.32690500
H	1.35082200	1.79299700	-0.97958200
C	-0.80838500	1.58785300	-1.20232000
C	-1.09891100	2.70302900	-0.52639200
H	-1.57428300	1.00036500	-1.70831200
H	-0.27192700	3.26062800	-0.08206500
C	-2.43731200	3.27254500	-0.30251500
C	-2.54814600	4.56431200	0.22751700
C	-3.61523700	2.56426800	-0.58448000
C	-3.79382000	5.14117300	0.45539300
H	-1.64355500	5.12024600	0.45919700
C	-4.85961000	3.13925100	-0.35677200
H	-3.55904800	1.55275500	-0.97745700
C	-4.95489400	4.43077700	0.16208700
H	-3.85768500	6.14479100	0.86358500
H	-5.76021600	2.57650600	-0.58099300
H	-5.92823600	4.87642400	0.33982200
Si-TS1			
C	5.36256000	0.65043800	-0.42869700
C	3.99892800	0.92122600	-0.34743100
C	3.50288700	1.96901500	0.42282100
C	4.41840600	2.75460700	1.12129300
C	5.78882600	2.49262700	1.04525700
C	6.27166000	1.44042600	0.26967600

C	5.63181500	-0.52850600	-1.32903200
C	4.24714000	-1.16518100	-1.58536600
C	3.20224600	-0.05712300	-1.18453700
H	2.43106200	2.16241300	0.47935100
H	4.06384600	3.57776600	1.73336500
H	6.48483500	3.11353700	1.60064700
H	7.33689200	1.23559500	0.21764100
H	6.30699400	-1.26831300	-0.88871500
H	4.11679000	-1.44360300	-2.63177200
H	6.07897800	-0.20236700	-2.27409900
H	2.78395800	0.41500900	-2.07746400
N	2.09173800	-0.64283300	-0.44532200
O	4.07803200	-2.38518100	-0.87481000
C	0.77594700	-0.31251200	-0.44384400
C	2.30894300	-1.65794200	0.44852500
N	0.27721600	-1.16044900	0.46530000
N	1.20165300	-2.01455400	1.02487900
C	3.67935300	-2.24896000	0.48038500
H	4.37297600	-1.61392500	1.04754200
H	3.66040800	-3.24411100	0.92424100
C	-1.10871900	-1.26013700	0.82089400
C	-1.56739000	-0.56462600	1.93725600
C	-1.95042000	-1.98980100	-0.02212900
C	-2.94005400	-0.59066900	2.18803300
C	-3.31040800	-1.99334500	0.27286900
C	-3.82335900	-1.28015400	1.35839000
H	-3.32879000	-0.03727900	3.03987700
H	-3.99094100	-2.53913400	-0.37709800
C	-1.40118600	-2.70753700	-1.22610300
H	-0.55644000	-3.34781000	-0.95506800
H	-1.03764000	-1.99147000	-1.97121600
C	-0.61923700	0.24368900	2.78012500
H	-0.24073900	1.08551900	2.18837000
H	0.23738600	-0.35701100	3.09986100
H	-1.12521000	0.62809000	3.66782200
H	-2.17133400	-3.32515900	-1.69137400
C	-5.31036000	-1.20862200	1.57798600
H	-5.54970100	-0.87627200	2.59057500
H	-5.75010600	-0.49412500	0.87227600
H	-5.78516500	-2.17866500	1.40848700
C	0.04305800	1.55226300	-0.78652600
O	0.26628500	2.19702100	0.26182600
H	0.71284900	1.68466400	-1.66072100
C	-1.35595200	1.18897900	-1.19248000

C	-2.40218500	1.63443400	-0.49093300
H	-1.46206500	0.59266800	-2.09751400
H	-2.17590900	2.24496400	0.38269900
C	-3.82652500	1.40889400	-0.77990900
C	-4.78502100	2.16970700	-0.09864500
C	-4.27242600	0.46607600	-1.71820000
C	-6.14411300	2.02057200	-0.36398900
H	-4.45315500	2.89456500	0.64019500
C	-5.62798200	0.31041600	-1.98022100
H	-3.55080200	-0.16473700	-2.23012900
C	-6.57078300	1.09293100	-1.31056800
H	-6.86830900	2.62758700	0.17023600
H	-5.95462300	-0.42602200	-2.70808600
H	-7.62872900	0.97064500	-1.51946200

Re-M1

C	-2.87719200	-3.08351300	0.05917100
C	-1.97266100	-2.15898900	-0.45552500
C	-1.43919700	-2.27504600	-1.73699100
C	-1.85213500	-3.35759100	-2.51218100
C	-2.76739900	-4.28815700	-2.01155200
C	-3.28586900	-4.15981400	-0.72431900
C	-3.28359500	-2.73291000	1.46753100
C	-2.35499900	-1.56775200	1.88758400
C	-1.66977700	-1.07711000	0.55578300
H	-0.71173800	-1.54157600	-2.09863500
H	-1.45515600	-3.48245600	-3.51458300
H	-3.07282700	-5.12602100	-2.63050800
H	-3.98926300	-4.89071200	-0.33669100
H	-3.17339500	-3.56659100	2.16839400
H	-2.91799700	-0.74682300	2.33166900
H	-4.33029500	-2.41567000	1.50865400
H	-2.06895200	-0.10368300	0.26547000
N	-0.22473300	-0.91520000	0.74122900
O	-1.43284600	-1.94177600	2.90002700
C	0.66718500	-0.11593500	0.12232100
C	0.47318300	-1.74456400	1.58003600
N	1.84713900	-0.47967400	0.62802800
N	1.74623700	-1.49320500	1.54360400
C	-0.31764300	-2.67835500	2.43416100
H	-0.62202900	-3.56569500	1.86227700
H	0.26739200	-2.99302400	3.29780400
C	3.13674000	0.04667900	0.27418500
C	3.86004100	-0.61064500	-0.72256900

C	3.61062900	1.16550800	0.96150100
C	5.12010200	-0.09981400	-1.03090100
C	4.87361100	1.63962600	0.61348800
C	5.63743900	1.02114400	-0.37934900
H	5.70969800	-0.58975000	-1.80170400
H	5.27130500	2.50911700	1.13102300
C	2.77765800	1.82204400	2.02978800
H	2.48898800	1.10179200	2.80127300
H	1.85425900	2.23563700	1.60917200
C	3.27578000	-1.80439700	-1.42490700
H	2.33045200	-1.50223900	-1.89315100
H	3.07078300	-2.61219600	-0.71480400
H	3.96371400	-2.17822200	-2.18512400
H	3.32844900	2.63554200	2.50369400
C	6.98716500	1.57368400	-0.75764900
H	6.88347000	2.33982100	-1.53282600
H	7.47906500	2.03723100	0.10052500
H	7.63912100	0.79088100	-1.15120800
C	0.51386900	0.79116100	-1.12759500
O	0.72329500	0.02079500	-2.19569500
H	1.28029800	1.58655600	-0.93853500
C	-0.84209300	1.48968800	-1.09739400
C	-1.08176100	2.63997800	-0.46131900
H	-1.61276200	0.98215400	-1.67872300
H	-0.25139400	3.11604300	0.06450900
C	-2.36244300	3.36412000	-0.37725000
C	-2.40257200	4.58817000	0.30182000
C	-3.55245800	2.87512600	-0.93685500
C	-3.58866600	5.30684700	0.41913100
H	-1.48819300	4.97805900	0.74135000
C	-4.73679000	3.59265000	-0.82272400
H	-3.55351900	1.92707400	-1.46659300
C	-4.76133700	4.81142800	-0.14399700
H	-3.59590300	6.25322600	0.95054700
H	-5.64753300	3.19888700	-1.26296400
H	-5.68902800	5.36747100	-0.05554000
Si-M1			
C	5.31963300	0.66666000	-0.38216700
C	3.95982400	0.95873600	-0.32479100
C	3.45729300	2.00176400	0.44829300
C	4.36804700	2.75626900	1.18532300
C	5.73600000	2.47165300	1.13947500
C	6.22307400	1.42862700	0.35436100

C	5.59499600	-0.49046900	-1.30760100
C	4.20757100	-1.08726700	-1.63809700
C	3.16547900	0.01151200	-1.19785800
H	2.38244700	2.19908000	0.45008600
H	4.01343100	3.57619000	1.80188600
H	6.42757800	3.07087700	1.72360600
H	7.28641800	1.21071300	0.32199400
H	6.23511100	-1.26017500	-0.86526900
H	4.09886100	-1.29832600	-2.70204800
H	6.08727600	-0.14869800	-2.22388200
H	2.73694900	0.51110200	-2.06963100
N	2.06137000	-0.60794700	-0.46253900
O	3.99985800	-2.34479500	-1.00979000
C	0.75827200	-0.27339600	-0.37750600
C	2.28240500	-1.65542700	0.38996900
N	0.25360800	-1.13168000	0.51332300
N	1.18955300	-2.00806100	0.99685600
C	3.64075400	-2.27383600	0.35901900
H	4.35798500	-1.68118300	0.94233300
H	3.60795800	-3.28875000	0.75399600
C	-1.11499500	-1.19899900	0.94717600
C	-1.52663300	-0.34236500	1.96619600
C	-1.97982600	-2.04580500	0.25156900
C	-2.89161300	-0.30875300	2.24869100
C	-3.33176900	-1.97975400	0.57579700
C	-3.80589900	-1.09264600	1.54486500
H	-3.25222100	0.37329900	3.01489300
H	-4.03606800	-2.60512600	0.03219600
C	-1.46617100	-2.95482200	-0.83284900
H	-0.68132800	-3.61676800	-0.45517600
H	-1.03356100	-2.37853300	-1.65857300
C	-0.54151500	0.55946600	2.65546300
H	-0.13886400	1.26811500	1.91858600
H	0.29283200	-0.01494600	3.07122300
H	-1.02496100	1.10506000	3.46792200
H	-2.27401300	-3.56837100	-1.23468700
C	-5.28495100	-0.93279900	1.76846800
H	-5.67756700	-0.18821000	1.06509900
H	-5.81970200	-1.86985400	1.59550900
H	-5.50182800	-0.58730700	2.78189100
C	0.12374000	1.02044400	-0.95273600
O	0.36474900	1.98984800	-0.07209500
H	0.64096000	1.12845100	-1.94345700
C	-1.33781600	0.75378200	-1.30525200

C	-2.31268000	1.47084300	-0.74570500
H	-1.53737900	-0.02526200	-2.04270800
H	-1.99103200	2.23519000	-0.03862500
C	-3.76173400	1.32671900	-0.96235000
C	-4.63070800	2.26394300	-0.38876700
C	-4.32274400	0.27771300	-1.70703900
C	-6.00930300	2.17593900	-0.56870100
H	-4.21216600	3.07516700	0.20139300
C	-5.69743900	0.18548400	-1.88659100
H	-3.67570100	-0.48220100	-2.13633100
C	-6.54902500	1.13777800	-1.32318000
H	-6.66109000	2.91869000	-0.11905000
H	-6.11014100	-0.63471900	-2.46637200
H	-7.62236200	1.06390600	-1.46604600

Re-M02^D

C	-3.13468600	-3.49034500	-0.75459500
C	-2.69286000	-2.17623900	-0.61013400
C	-3.51595900	-1.09811700	-0.92230100
C	-4.81766900	-1.35807100	-1.34885900
C	-5.27315600	-2.67206700	-1.47110300
C	-4.43341200	-3.74685000	-1.18194700
C	-2.03806700	-4.46732500	-0.41240500
C	-0.75053000	-3.61729300	-0.39599400
C	-1.25165800	-2.15535800	-0.13445900
H	-3.15617000	-0.07473300	-0.84335400
H	-5.47671300	-0.53141100	-1.59267900
H	-6.28723400	-2.85852600	-1.80974300
H	-4.78392600	-4.76752500	-1.30113800
H	-1.93990400	-5.28334600	-1.13313200
H	-0.06491800	-3.92819300	0.39332000
H	-2.20589900	-4.91415900	0.57361500
H	-1.16007600	-1.93079200	0.93165800
N	-0.45393000	-1.18567400	-0.86955400
O	-0.00033300	-3.76117200	-1.59662600
C	-0.06356200	0.07029100	-0.56872100
C	-0.01615000	-1.47775900	-2.12810900
N	0.58328200	0.48433200	-1.66195400
N	0.62687600	-0.47644400	-2.64234200
C	-0.28533800	-2.85130300	-2.64584300
H	-1.32521300	-2.93707300	-2.98827400
H	0.38354000	-3.08331400	-3.47414600
C	1.18276700	1.75781400	-1.97557800
C	2.56119900	1.80620000	-2.17015100

C	0.34287100	2.85503200	-2.19381100
C	3.11107500	3.03572000	-2.54680300
C	0.93809900	4.05063700	-2.57775000
C	2.32204200	4.16344400	-2.74846300
H	4.18702100	3.10180500	-2.69103900
H	0.30694000	4.91985700	-2.74831500
C	-1.14124700	2.74456900	-1.99258300
H	-1.33711800	2.62790900	-0.92242200
H	-1.55537200	1.87616300	-2.51682200
C	3.43973600	0.59076800	-2.02889000
H	3.57341400	0.10786700	-3.00279700
H	3.01368100	-0.14743500	-1.34567100
H	4.42762500	0.88134000	-1.66181400
H	-1.64847600	3.63999000	-2.35654100
C	2.93509000	5.48504500	-3.13349800
H	2.38812800	5.94728900	-3.95986700
H	2.90609400	6.18471000	-2.29215200
H	3.97789300	5.36557000	-3.43498200
C	-0.21076600	0.84409600	0.78077900
O	0.34863100	2.03355100	0.73436800
C	-1.69710300	0.81700700	1.17806000
C	-2.32823700	1.95098900	1.49013100
H	-2.20422400	-0.14246000	1.27258400
H	-1.72759600	2.85771200	1.42550400
C	-3.72807300	2.09380800	1.92521200
C	-4.16705400	3.33605400	2.40201700
C	-4.65465900	1.04103400	1.87287500
C	-5.47971800	3.52163800	2.82607500
H	-3.46280800	4.16275900	2.44195200
C	-5.96630400	1.22486400	2.29365600
H	-4.35101100	0.07160000	1.48756400
C	-6.38545300	2.46554300	2.77495600
H	-5.79560300	4.49244900	3.19512400
H	-6.66752400	0.39758400	2.24127500
H	-7.41041600	2.60679700	3.10256200
C	3.69403300	1.06349700	3.85877000
C	4.54327200	-0.20053600	4.00660900
C	5.25326700	-0.62790000	2.71533900
C	2.57351400	0.94155800	2.82882100
C	3.06385300	0.60927700	1.41020500
C	3.28771700	-0.86869600	1.21752500
H	4.35403500	1.89259000	3.56739700
H	3.92504800	-1.03820700	4.35506400
H	6.09816800	-1.27375600	2.96722500

H	1.99805600	1.86942400	2.76420000
H	3.98218300	1.16952400	1.19069200
C	4.71833700	-2.81604000	1.66524700
H	4.36852300	-3.35783800	2.55700800
C	2.58560900	-2.97124300	0.42650300
C	4.05587200	-3.37196500	0.41611700
H	4.17443400	-4.45824500	0.37854300
H	4.54071600	-2.94769800	-0.47052900
H	2.08120500	-3.48853600	1.25840500
H	5.80504200	-2.94159700	1.61311800
H	2.08892400	-3.29915800	-0.49276100
N	2.39103600	-1.53200900	0.56331100
N	4.42807800	-1.39122800	1.78210800
H	5.67682300	0.25422400	2.21782800
H	5.30677000	-0.02765000	4.77348700
H	3.27194900	1.32991600	4.83430500
H	1.86724500	0.16212900	3.14607300
H	2.29993700	0.93934000	0.70369300
H	0.28288400	0.09057600	1.46167700

Re-M02^{DH}

C	4.75060200	-1.69283200	1.61969400
C	3.53919100	-1.07956600	1.31365200
C	2.65385800	-0.66454000	2.30464800
C	3.00972700	-0.88443500	3.63304600
C	4.22282600	-1.50129100	3.95136200
C	5.10189200	-1.90706600	2.95016600
C	5.53177700	-2.02838700	0.37608500
C	4.57320500	-1.74355400	-0.80421800
C	3.36421900	-0.94458900	-0.18105600
H	1.71173000	-0.18471100	2.04610200
H	2.34012000	-0.57402500	4.42829800
H	4.48197400	-1.66744500	4.99204000
H	6.04248800	-2.38723500	3.20207300
H	5.86397100	-3.07084600	0.34310900
H	5.05041300	-1.13871000	-1.57452900
H	6.42689000	-1.40441300	0.29574800
H	3.37006100	0.09593000	-0.50879500
N	2.08457800	-1.53253300	-0.61514200
O	4.17836600	-2.92477100	-1.48354100
C	0.85929600	-1.00268500	-0.75600700
C	1.95917800	-2.88387100	-0.80893600
N	0.05739800	-2.02863600	-1.03068000
N	0.72839400	-3.21297900	-1.07400100

C	3.21254900	-3.69594000	-0.79643400
H	3.51874200	-3.92162200	0.23411000
H	3.06585000	-4.62899100	-1.33957900
C	-1.36940500	-1.97473000	-1.22040600
C	-1.86316000	-1.69556500	-2.49451600
C	-2.17867700	-2.21791900	-0.10682400
C	-3.25047800	-1.65773000	-2.64007000
C	-3.55642400	-2.17000300	-0.30769100
C	-4.10643300	-1.89029700	-1.56256300
H	-3.66954000	-1.44120300	-3.61937800
H	-4.21912400	-2.37373500	0.53111200
C	-1.56120600	-2.54583200	1.22580700
H	-0.87443800	-1.75044400	1.53566100
H	-0.98917400	-3.47696200	1.16581700
C	-0.93510600	-1.42627800	-3.64873700
H	-0.17349800	-2.20603500	-3.73722800
H	-0.41563800	-0.46881100	-3.52301400
H	-1.49256600	-1.38062800	-4.58478100
H	-2.32898600	-2.66451800	1.99146000
C	-5.60020600	-1.88263000	-1.75507600
H	-5.87914700	-1.36147400	-2.67340700
H	-5.98224300	-2.90615600	-1.82163900
H	-6.10484100	-1.40047000	-0.91381700
C	0.37092900	0.41560300	-0.56112200
O	0.01563100	0.55791300	0.77572200
H	-0.90693300	1.05321600	0.76129800
C	1.37021200	1.43515900	-1.05394700
C	1.79907600	2.42543900	-0.26672000
H	1.67982300	1.33960900	-2.09396500
H	1.41247000	2.44895600	0.75078000
C	2.74031100	3.49830300	-0.62597100
C	2.95243100	4.53057700	0.29573100
C	3.43777400	3.53075800	-1.84190100
C	3.82700000	5.57472900	0.01144600
H	2.42106000	4.51043400	1.24325600
C	4.31283800	4.57183000	-2.12591900
H	3.30199800	2.73616600	-2.56970300
C	4.50916600	5.59873700	-1.20163100
H	3.97610600	6.36673100	0.73797600
H	4.84724700	4.58312700	-3.07038100
H	5.19371400	6.40991200	-1.42696400
C	-5.34026200	1.04110900	3.44221600
C	-6.09987500	1.50411700	2.19867100
C	-5.77794500	0.69849700	0.93624500

C	-3.81878100	1.13368000	3.33663200
C	-3.23200300	0.31899500	2.17032500
C	-3.33979500	1.05490700	0.85819700
H	-5.61322200	-0.00321500	3.64624200
H	-5.89864700	2.56303700	1.99444700
H	-6.58235500	0.82534100	0.20771700
H	-3.37873800	0.76606300	4.26841400
H	-3.72638200	-0.65711700	2.11318600
C	-4.71163200	1.70563500	-1.07669900
H	-5.23873200	2.66458300	-0.98940100
C	-2.39546800	2.50222200	-0.74924500
C	-3.36369500	1.89424200	-1.75546600
H	-3.48287500	2.52735400	-2.63784500
H	-2.97582600	0.92212000	-2.08054000
H	-2.75861400	3.49010700	-0.43349100
H	-5.34399400	1.03223200	-1.66697400
H	-1.40235100	2.65434300	-1.18393700
N	-2.26481000	1.63862800	0.41860900
N	-4.55135500	1.11861200	0.25696900
H	-5.73362300	-0.37400800	1.17278000
H	-7.17387400	1.41418700	2.39167900
H	-5.67579100	1.62471600	4.30548100
H	-3.50473800	2.17924400	3.22991500
H	-2.16743000	0.14288700	2.33811300
H	-0.52779900	0.47693900	-1.20177700

Re-TS2

C	-2.03645400	3.28808100	0.62585800
C	-1.50012400	2.00397300	0.59503300
C	-1.15531800	1.31866900	1.75946400
C	-1.37434700	1.95915100	2.97754800
C	-1.92215500	3.24460400	3.02110500
C	-2.25583400	3.91853400	1.84877300
C	-2.30724200	3.81237200	-0.76180700
C	-1.73001300	2.74767900	-1.72847000
C	-1.32793700	1.52452200	-0.82761200
H	-0.71553800	0.31790900	1.73344400
H	-1.11581900	1.45405100	3.90263600
H	-2.08308300	3.72533100	3.98091400
H	-2.67256100	4.92058100	1.88799700
H	-1.84109800	4.78572500	-0.94827600
H	-2.47680400	2.42916500	-2.45537000
H	-3.38002300	3.93839600	-0.93541700
H	-1.95388300	0.66087000	-1.04833200

N	0.07359400	1.14940300	-1.06076900
O	-0.66055300	3.23283400	-2.52591500
C	0.73055200	0.07184300	-0.55066100
C	1.01689700	2.10949800	-1.32671600
N	2.02683600	0.42761400	-0.57553700
N	2.21605700	1.69781300	-1.05749500
C	0.54129400	3.43987100	-1.81580900
H	0.39977700	4.11964900	-0.96306300
H	1.26771600	3.88211400	-2.49783200
C	3.14564100	-0.38618700	-0.20255500
C	3.67604800	-1.25504700	-1.15755700
C	3.65994100	-0.25862700	1.08994200
C	4.78383900	-2.01623000	-0.78548600
C	4.77237300	-1.03302600	1.41079100
C	5.34359900	-1.91454700	0.48902200
H	5.22033600	-2.69919200	-1.50987000
H	5.20056600	-0.95044000	2.40679900
C	2.99510300	0.65018500	2.08457500
H	1.98481700	0.26870500	2.27435700
H	2.90694700	1.66931200	1.69602800
C	3.05427200	-1.36282500	-2.52394200
H	2.98321600	-0.38208700	-3.00404200
H	2.03875600	-1.76687500	-2.44631900
H	3.64043400	-2.02244500	-3.16522500
H	3.55620000	0.67992100	3.01993400
C	6.52814000	-2.76096600	0.87811100
H	6.20108600	-3.65361700	1.42093800
H	7.08456900	-3.09146100	-0.00151800
H	7.20789500	-2.20971900	1.53222200
C	0.20607300	-1.16834600	-0.03661100
O	0.62704600	-1.45736200	1.33513200
H	1.04335400	-1.97465400	0.21320400
C	-1.14012800	-1.57038100	-0.42737100
C	-1.97571200	-2.21122200	0.41116700
H	-1.42287400	-1.38209100	-1.46399400
H	-1.62040500	-2.36548800	1.42741800
C	-3.31565500	-2.71505000	0.09275300
C	-4.11539600	-3.21825900	1.13035000
C	-3.85044900	-2.72246400	-1.20667400
C	-5.39825000	-3.69803100	0.88776700
H	-3.71759700	-3.22660900	2.14177000
C	-5.13232800	-3.19967100	-1.44999600
H	-3.25400300	-2.36221100	-2.03975400
C	-5.91606800	-3.68997000	-0.40506400

H	-5.99429300	-4.07985800	1.71110200
H	-5.52163300	-3.19585000	-2.46367900
H	-6.91559200	-4.06552500	-0.59878100

Re-TS2^D

C	-4.71281000	0.27419800	0.44164300
C	-3.52128400	0.93690700	0.13031800
C	-3.27073500	1.38753100	-1.16233700
C	-4.22759100	1.15088500	-2.14850000
C	-5.41239600	0.47963600	-1.84319200
C	-5.66594300	0.04163400	-0.54431700
C	-4.76273900	-0.11425800	1.89657200
C	-3.62959000	0.73816700	2.50955200
C	-2.63082600	1.01764400	1.35285700
H	-2.34735700	1.90629200	-1.40189400
H	-4.04785000	1.49304100	-3.16252800
H	-6.14727800	0.30467400	-2.62263800
H	-6.59305100	-0.47060000	-0.30504200
H	-4.57305100	-1.18760400	2.01137500
H	-4.03836200	1.70243600	2.81981800
H	-5.72553600	0.09517200	2.36834300
H	-2.13450800	1.97897300	1.48336600
N	-1.61300500	-0.06824900	1.35310300
O	-3.00333100	0.21005000	3.65866900
C	-0.88851300	-0.48519100	0.25029500
C	-1.81213300	-1.19474700	2.13371000
N	-0.80055400	-1.83630500	0.39179100
N	-1.34979300	-2.26553000	1.58548700
C	-2.47006300	-1.08535600	3.47652900
H	-3.23235700	-1.86557200	3.58527600
H	-1.72492000	-1.22831600	4.26335800
C	-0.40566600	-2.81001800	-0.57466700
C	0.58405400	-3.73682800	-0.23939900
C	-1.08207600	-2.84283600	-1.80382900
C	0.91613600	-4.70412200	-1.19196400
C	-0.71335800	-3.82625500	-2.71547500
C	0.28750900	-4.76068500	-2.43233200
H	1.69122000	-5.42854900	-0.95171300
H	-1.22311500	-3.86832800	-3.67573700
C	-2.15231800	-1.83790300	-2.13344500
H	-1.67299500	-0.86923100	-2.30877400
H	-2.87231700	-1.71946500	-1.31446900
C	1.27139500	-3.71395900	1.09992600
H	0.65749300	-4.20272500	1.86266700

H	1.44794900	-2.68504900	1.42520900
H	2.22795400	-4.23923400	1.04192200
H	-2.69802600	-2.13825400	-3.03068800
C	0.67696500	-5.79394600	-3.45809900
H	-0.20542400	-6.28690200	-3.87581200
H	1.21485100	-5.33107800	-4.29166600
H	1.32479000	-6.55890400	-3.02448600
C	0.00126900	0.31013600	-0.60267800
O	0.40962800	-0.15590600	-1.75532600
C	-0.06426800	1.78968600	-0.38566400
C	0.31867400	2.64164700	-1.34848300
H	-0.29635800	2.15118000	0.61555600
H	0.60230800	2.19506000	-2.30012000
C	0.41717700	4.10337900	-1.23500900
C	1.09563100	4.82316100	-2.22900700
C	-0.14958400	4.82602200	-0.17285600
C	1.22142800	6.20729200	-2.15903200
H	1.53406600	4.28131800	-3.06303000
C	-0.02330300	6.20775300	-0.09961100
H	-0.70811400	4.30116700	0.59701800
C	0.66527000	6.90721000	-1.09118200
H	1.75441900	6.73956500	-2.94086700
H	-0.47303300	6.74419500	0.73043700
H	0.75912600	7.98688400	-1.03415100
C	5.16088600	0.63180900	-1.49141100
C	5.77384400	0.85846400	-0.10813900
C	5.62455500	-0.33831300	0.83863200
C	3.65890000	0.34972400	-1.49224200
C	3.24710100	-0.87112500	-0.65304000
C	3.16701300	-0.53345500	0.81380300
H	5.67691600	-0.21866500	-1.95880700
H	5.32782900	1.73958100	0.37114600
H	6.37380200	-0.27679300	1.63129300
H	3.32188300	0.17912700	-2.51862700
H	3.94581000	-1.70109000	-0.81446100
C	4.28904600	-0.00116800	2.91666900
H	4.38958800	1.09055400	2.99900800
C	1.82136100	0.02078800	2.70704500
C	2.98907300	-0.46517700	3.55554700
H	2.91894300	-0.08669400	4.57829700
H	2.97854100	-1.55985600	3.59698800
H	1.72631500	1.11292900	2.78565300
H	5.14792400	-0.45169300	3.42283600
H	0.87715400	-0.40635900	3.06694800

N	1.98162200	-0.35764800	1.31091800
N	4.32798800	-0.40827000	1.51323900
H	5.81741300	-1.27187800	0.29658100
H	6.84257200	1.06781500	-0.22725400
H	5.36812300	1.50384500	-2.12128900
H	3.09483400	1.22022700	-1.13224900
H	2.24466700	-1.17574300	-0.96711700
H	0.82041600	0.02338700	0.33867900

Re-TS2^{DH}

C	5.24578500	-1.11359200	0.35207200
C	3.92522000	-0.70568200	0.51667600
C	3.35372500	-0.55390300	1.77752500
C	4.14457500	-0.82187600	2.89188800
C	5.47326000	-1.22801400	2.73754700
C	6.03333900	-1.37546700	1.47074600
C	5.62176300	-1.20043800	-1.10512200
C	4.30848100	-0.95743900	-1.88861500
C	3.25623400	-0.48139100	-0.81820400
H	2.31734800	-0.23917800	1.89290000
H	3.72697600	-0.71461200	3.88746200
H	6.07461700	-1.43573500	3.61674100
H	7.06441300	-1.69624600	1.35768700
H	6.04863800	-2.17045700	-1.38021500
H	4.43301400	-0.18101700	-2.64260200
H	6.36432700	-0.44090700	-1.36668200
H	2.99729400	0.56455200	-0.97508300
N	2.02267100	-1.28008100	-0.91233000
O	3.88524200	-2.09200600	-2.62705500
C	0.79317100	-1.04945600	-0.38817100
C	2.08421500	-2.61119100	-1.23481700
N	0.17766500	-2.24057700	-0.44012700
N	0.97189000	-3.22144300	-0.96461100
C	3.35322400	-3.12867100	-1.82997900
H	4.04860000	-3.43546400	-1.03554200
H	3.15071600	-3.98635700	-2.47124500
C	-1.18432000	-2.53260800	-0.09378200
C	-2.15570100	-2.37288700	-1.08604900
C	-1.46139300	-3.02224600	1.18416500
C	-3.47006700	-2.69110200	-0.74986500
C	-2.79096100	-3.33393600	1.46859800
C	-3.80296700	-3.16986500	0.51984400
H	-4.24887400	-2.57098000	-1.49905800
H	-3.03972300	-3.71884000	2.45426100

C	-0.36158600	-3.20962100	2.19304200
H	0.13088300	-2.25382100	2.39526400
H	0.39542800	-3.90442500	1.81666000
C	-1.77477600	-1.91119300	-2.46604500
H	-1.06842800	-2.60964100	-2.92544000
H	-1.29232400	-0.92852200	-2.43421700
H	-2.65575600	-1.84321300	-3.10638500
H	-0.76095000	-3.60730500	3.12701000
C	-5.23785200	-3.46509000	0.87045900
H	-5.80036900	-3.79064800	-0.00707900
H	-5.30862800	-4.23858000	1.63785900
H	-5.72931900	-2.56669100	1.26260800
C	0.20806900	0.18411200	0.13344500
O	-0.04893500	-0.00411300	1.52331800
H	-0.77234600	0.59061800	1.76717300
C	0.92007900	1.43463500	-0.18835100
C	1.18571900	2.40792700	0.69776800
H	1.11755100	1.59868400	-1.24921100
H	1.00707700	2.20604200	1.75241200
C	1.74323700	3.72873300	0.37278100
C	2.37333600	4.47091800	1.38130700
C	1.66832700	4.28612200	-0.91269500
C	2.93450800	5.71472100	1.11179300
H	2.43041700	4.05699000	2.38456200
C	2.23089700	5.52818300	-1.18322600
H	1.14570700	3.75280400	-1.70196400
C	2.86943800	6.24775400	-0.17357900
H	3.42331600	6.26849000	1.90712700
H	2.15903500	5.94368500	-2.18355700
H	3.30318900	7.21963000	-0.38507800
C	-4.97647400	1.59893500	2.44551900
C	-5.63881500	2.27595600	1.24452000
C	-5.71685200	1.39694300	-0.00743300
C	-3.53274500	1.15070600	2.21478800
C	-3.38940300	0.15028900	1.05267800
C	-3.33397300	0.85400600	-0.27664800
H	-5.57119600	0.71760500	2.72070000
H	-5.11309900	3.20374500	0.98700100
H	-6.47791500	1.78773600	-0.68485300
H	-3.16262500	0.67279700	3.12711900
H	-4.21738500	-0.56380500	1.07115000
C	-4.46116000	2.10294200	-2.04989600
H	-4.43137100	3.17978900	-1.84081000
C	-2.00922500	1.76788600	-2.06263000

C	-3.27443100	1.68483400	-2.90304000
H	-3.20650600	2.33091300	-3.78050500
H	-3.41572400	0.65501400	-3.24733000
H	-1.78116800	2.81121700	-1.80976200
H	-5.39920700	1.88831800	-2.56807300
H	-1.14491500	1.37108900	-2.60732100
N	-2.16323700	0.99378000	-0.83759100
N	-4.47084600	1.36087500	-0.78413000
H	-6.02201300	0.37694100	0.25370600
H	-6.66001300	2.55600200	1.52186000
H	-5.00934200	2.27797000	3.30297500
H	-2.89075700	2.02225700	2.02617700
H	-2.47166200	-0.43473100	1.14786200
H	-1.06777400	0.45976000	-0.42893700

Si-M02^D

C	-5.39356800	-0.77235100	-0.48400900
C	-4.00259300	-0.77467300	-0.47164000
C	-3.27400500	-1.88404000	-0.05741200
C	-3.97370100	-3.01071500	0.36673900
C	-5.37185900	-3.01799300	0.36264900
C	-6.09105900	-1.90356500	-0.06539800
C	-5.93147700	0.53876600	-0.99853100
C	-4.69882400	1.47029600	-1.12354600
C	-3.44199900	0.53933100	-0.95288100
H	-2.18775400	-1.85679600	-0.07714700
H	-3.43090600	-3.89056200	0.69773800
H	-5.90422100	-3.90343200	0.69583100
H	-7.17697200	-1.91656700	-0.06734400
H	-6.67531100	0.99078400	-0.33419300
H	-4.66174800	1.95559600	-2.09886000
H	-6.41021200	0.41023600	-1.97412800
H	-2.84749100	0.42334000	-1.85991800
N	-2.51366200	1.09718900	0.04494100
O	-4.74693800	2.55217400	-0.20165100
C	-1.18551300	0.94634500	0.19132300
C	-2.96692300	1.83004300	1.10883200
N	-0.89263400	1.60650700	1.31609700
N	-1.99526100	2.17088300	1.90096400
C	-4.41464000	2.19271200	1.12468700
H	-5.02162300	1.35010700	1.48462400
H	-4.58515900	3.05564200	1.76795800
C	0.40498400	1.80791000	1.90015600
C	1.19681200	2.85590800	1.42840700

C	0.78996400	0.96250100	2.94861500
C	2.44082800	3.03455300	2.04021600
C	2.04609000	1.17209200	3.50881400
C	2.88322500	2.20175700	3.06539400
H	3.07888100	3.84541400	1.69642600
H	2.37486300	0.52727900	4.31999300
C	-0.12711800	-0.12589600	3.44044900
H	-0.37600000	-0.82889300	2.63675800
H	-1.06774500	0.29398400	3.80901300
C	0.75508000	3.74690400	0.29944100
H	-0.33060300	3.87227800	0.28263400
H	1.07946300	3.32838000	-0.66421400
H	1.21103500	4.73401100	0.40358700
H	0.34368300	-0.68500700	4.25031900
C	4.24924100	2.38334800	3.67343800
H	4.63912500	3.38515600	3.48266500
H	4.22554200	2.21816300	4.75332400
H	4.95555600	1.66249400	3.24739500
C	-0.24503100	0.19197600	-0.78621100
O	-0.90458700	-0.24020800	-1.85444200
C	0.47452800	-0.88127800	0.03621700
C	0.42252700	-2.16650800	-0.32096400
H	1.07322700	-0.55215600	0.88386300
H	-0.19009700	-2.39964300	-1.19138400
C	1.11876700	-3.28101200	0.34347300
C	0.79812700	-4.59612500	-0.01517200
C	2.10523300	-3.08163800	1.32255100
C	1.42958600	-5.67998700	0.58892900
H	0.04083000	-4.76371200	-0.77656100
C	2.73851500	-4.16210900	1.92460200
H	2.38596300	-2.07021900	1.60705100
C	2.40256000	-5.46716900	1.56188500
H	1.16308300	-6.69110000	0.29735000
H	3.50148000	-3.98783300	2.67706100
H	2.89991900	-6.30920700	2.03225300
C	4.57888100	-0.56143100	-0.23559300
C	3.98951400	-1.43950900	-1.33727400
C	4.06320300	-0.79002500	-2.72257200
C	3.92175400	0.81122000	-0.08749900
C	4.00026700	1.70681900	-1.33676500
C	2.93491100	1.39429600	-2.36625400
H	5.64898200	-0.41362000	-0.44072700
H	2.94168500	-1.67491300	-1.11842300
H	3.97940800	-1.56026800	-3.49355600

H	4.40832200	1.33965000	0.73979000
H	5.00308000	1.64085300	-1.77831500
C	1.85050100	-0.26308600	-3.77298200
H	1.07622200	-0.68222700	-3.11293400
C	0.93194400	2.00504200	-3.48383500
C	1.27038700	0.93258700	-4.51414100
H	0.37507800	0.63568700	-5.06797700
H	2.00770900	1.30807500	-5.23310600
H	0.04374100	1.67279300	-2.92860200
H	2.18267500	-1.03618200	-4.47200600
H	0.67423100	2.94746300	-3.98160600
N	2.01045000	2.27778800	-2.53768800
N	3.01170700	0.17958400	-3.00152300
H	5.04694100	-0.32238300	-2.85897400
H	4.53562900	-2.38975300	-1.36329300
H	4.51764700	-1.09184300	0.72234000
H	2.86649700	0.70198000	0.20169300
H	3.83286800	2.74786600	-1.05247700
H	0.54576600	0.96794100	-0.97953900

Si-M02^{DH}

C	5.23455600	-1.28598400	-0.85413000
C	4.07810000	-0.73117700	-0.30846100
C	4.13704100	0.12489500	0.78676900
C	5.38334000	0.43125500	1.32682300
C	6.54552700	-0.11602300	0.77905200
C	6.47919200	-0.97925600	-0.31257200
C	4.91319700	-2.17671400	-2.02665500
C	3.38778400	-2.38680700	-1.95802400
C	2.85920200	-1.18929700	-1.08535300
H	3.23519200	0.55039300	1.21422500
H	5.44866300	1.10198400	2.17714500
H	7.50984800	0.12957300	1.21191500
H	7.38349200	-1.41034000	-0.73083700
H	5.42555600	-3.14209500	-1.99566900
H	2.92259100	-2.36895800	-2.94394900
H	5.18435200	-1.69011500	-2.96941900
H	2.43470800	-0.40170500	-1.71359200
N	1.78210400	-1.66460400	-0.21394400
O	3.04409500	-3.66203400	-1.42732800
C	0.61470500	-1.11268500	0.13277600
C	1.84932300	-2.88784300	0.39658800
N	0.02876100	-1.99237400	0.93996200
N	0.78301700	-3.11811200	1.10946700

C	2.98898800	-3.76321400	-0.01395000
H	3.92430500	-3.44783600	0.46480100
H	2.78221300	-4.80197800	0.24017300
C	-1.30607900	-1.87126800	1.46749600
C	-2.36241500	-2.11322100	0.58793800
C	-1.47491200	-1.47173900	2.79510300
C	-3.65444500	-1.91130100	1.07578100
C	-2.78363300	-1.29434000	3.23550000
C	-3.88009700	-1.49983600	2.39096300
H	-4.49825600	-2.08901800	0.41265900
H	-2.95441700	-0.98780700	4.26433300
C	-0.29100600	-1.25876300	3.69903600
H	0.38807200	-0.49971100	3.29765300
H	0.28371000	-2.18279600	3.80997200
C	-2.10195200	-2.56891200	-0.82267100
H	-1.35680500	-3.36933500	-0.84790400
H	-1.72922600	-1.74219600	-1.44026900
H	-3.02018700	-2.94887900	-1.27107500
H	-0.61772600	-0.93353900	4.68709600
C	-5.27776000	-1.27823300	2.90820700
H	-5.43961600	-1.82975600	3.83813200
H	-5.44551900	-0.21796800	3.12587900
H	-6.02666200	-1.60010200	2.18169800
C	0.05624400	0.22482700	-0.29227300
O	-0.05144900	0.25091700	-1.67762400
H	-1.01748800	0.54129300	-1.87488800
C	0.92792200	1.31920800	0.27991400
C	1.58060900	2.19138200	-0.49228400
H	0.99897400	1.33980300	1.36638000
H	1.43744900	2.10822800	-1.56845500
C	2.50161800	3.24412300	-0.03471600
C	3.12236600	4.05330600	-0.99363400
C	2.80787000	3.45473100	1.31807000
C	4.02322700	5.04536200	-0.61804100
H	2.89518900	3.89740100	-2.04468000
C	3.70730000	4.44376600	1.69407200
H	2.34010800	2.84649100	2.08704700
C	4.31906300	5.24292600	0.72751100
H	4.49388200	5.66216000	-1.37666000
H	3.93231100	4.59481100	2.74492600
H	5.02112700	6.01494200	1.02503700
C	-5.22762000	3.02076900	0.74036000
C	-6.23838600	2.20273200	-0.05846000
C	-5.79224100	0.75250100	-0.24923000

C	-3.82892800	3.06141400	0.12790600
C	-3.11514700	1.69876800	0.02873100
C	-3.51149600	0.90466000	-1.19829600
H	-5.15446100	2.59521900	1.75120300
H	-6.41035700	2.65352400	-1.04355500
H	-6.65145100	0.12288200	-0.49172700
H	-3.20122700	3.71685500	0.73899600
H	-3.27414200	1.11129300	0.94444800
C	-5.30740400	0.06248300	-2.61104400
H	-5.57907500	0.91088000	-3.25337900
C	-2.94005600	0.00626300	-3.34128100
C	-4.23693900	-0.78853200	-3.27446000
H	-4.55619000	-1.08631400	-4.27607100
H	-4.09429800	-1.69765800	-2.68377300
H	-3.00956200	0.76610200	-4.13008800
H	-6.21245100	-0.52294300	-2.43470500
H	-2.10243400	-0.64634100	-3.61345200
N	-2.59378700	0.67836700	-2.08935800
N	-4.81882600	0.54793800	-1.32099300
H	-5.37894000	0.36587400	0.69020900
H	-7.19894500	2.20385700	0.46754600
H	-5.59618600	4.04480900	0.85824200
H	-3.86789900	3.51133100	-0.87207900
H	-2.04518800	1.88954400	-0.06380200
H	-0.93304200	0.26721900	0.18560300

Si-TS2

C	-4.31422000	-1.54847400	0.64455200
C	-3.10094600	-1.43470300	-0.02933000
C	-2.03393500	-2.29006700	0.23554700
C	-2.20021700	-3.26308600	1.21862400
C	-3.41094700	-3.37777500	1.90795100
C	-4.47730300	-2.52858900	1.62130100
C	-5.32087800	-0.53876100	0.15836800
C	-4.59049400	0.25726100	-0.95454000
C	-3.12144100	-0.29656900	-1.02125000
H	-1.11874000	-2.21209100	-0.34958100
H	-1.38631100	-3.94438900	1.44539200
H	-3.52471700	-4.14287700	2.66957200
H	-5.42077900	-2.63016800	2.14970500
H	-5.66410900	0.12684000	0.95739700
H	-5.06085500	0.07219900	-1.92052500
H	-6.21477300	-1.02301300	-0.24439600
H	-2.83045900	-0.62294600	-2.01810200

N	-2.15796800	0.75177900	-0.63775000
O	-4.67284100	1.66470900	-0.79557900
C	-0.79678400	0.70414900	-0.67445400
C	-2.50558100	1.85420200	0.10035400
N	-0.40439500	1.78940100	0.03458400
N	-1.47085000	2.51170800	0.51499800
C	-3.95270200	2.15295300	0.31448000
H	-4.29346100	1.70158600	1.25614700
H	-4.10904700	3.23052000	0.37232300
C	0.93278700	2.23475200	0.28042700
C	1.60682900	2.92205800	-0.72901300
C	1.51668700	1.92436500	1.51354700
C	2.92886600	3.29394500	-0.48051800
C	2.83581100	2.31893300	1.71682100
C	3.55791100	2.99623400	0.72791400
H	3.47786700	3.82634600	-1.25291900
H	3.31679000	2.08562400	2.66381200
C	0.74362600	1.14942400	2.54633300
H	0.41162800	0.18712100	2.13900600
H	-0.15186400	1.69493100	2.85767800
C	0.92836100	3.22383600	-2.03740400
H	-0.03273200	3.72069300	-1.87546700
H	0.73119300	2.29609600	-2.58545200
H	1.55346500	3.86621000	-2.65900700
H	1.35906900	0.95591600	3.42589300
C	4.99634100	3.37435500	0.96760600
H	5.35406200	4.07559400	0.21142100
H	5.12290100	3.83202400	1.95211100
H	5.63636100	2.48694200	0.93456400
C	0.00923700	-0.22665200	-1.42324600
O	-0.70836900	-1.15979900	-2.24790000
H	-0.08273900	-0.02867100	-2.58579400
C	1.28889400	-0.66954500	-0.86292000
C	1.84410300	-1.84994400	-1.18721900
H	1.79393200	-0.00090100	-0.17275900
H	1.30624000	-2.48518100	-1.88687700
C	3.12667600	-2.35095800	-0.67579900
C	3.57676900	-3.61627900	-1.08048500
C	3.94024700	-1.61828700	0.20602800
C	4.78641400	-4.13349800	-0.62598200
H	2.96304000	-4.19848000	-1.76297400
C	5.14724800	-2.13364800	0.66026400
H	3.63008700	-0.63156900	0.54031100
C	5.57944400	-3.39494600	0.24808500

H	5.10991900	-5.11557100	-0.95707200
H	5.75788900	-1.54644200	1.33965500
H	6.52349300	-3.79393100	0.60467800

Si-TS2^D

C	-5.30865700	-0.47544000	-1.34758900
C	-3.92412700	-0.37722200	-1.45771000
C	-3.16963500	-1.33256800	-2.13418300
C	-3.83809000	-2.42342200	-2.68566500
C	-5.22666500	-2.54041500	-2.56787500
C	-5.97211200	-1.56530800	-1.90793300
C	-5.89220900	0.70252800	-0.60894200
C	-4.67468600	1.59993800	-0.25824300
C	-3.39138200	0.84333900	-0.74758000
H	-2.09816400	-1.16500500	-2.24562800
H	-3.28065200	-3.18635300	-3.22037900
H	-5.73145700	-3.39647900	-3.00525300
H	-7.05218900	-1.65489000	-1.83318200
H	-6.43567000	0.40275200	0.29344300
H	-4.73622600	2.54258800	-0.80336800
H	-6.60560300	1.25342800	-1.22859100
H	-2.75049000	1.43964300	-1.39381700
N	-2.55537500	0.45049800	0.39957300
O	-4.62830900	1.99394900	1.10546900
C	-1.31620100	-0.14488700	0.37237800
C	-3.03988200	0.34579900	1.67642100
N	-1.15714100	-0.59531400	1.65260200
N	-2.22105000	-0.26249600	2.46954400
C	-4.38023100	0.92324400	1.99160200
H	-5.15276100	0.14627100	1.91635700
H	-4.38975200	1.31886000	3.00790500
C	-0.10361300	-1.40151300	2.16961300
C	0.82005000	-0.82354400	3.04491700
C	-0.01985600	-2.73825600	1.75797700
C	1.88293100	-1.61816000	3.48010400
C	1.05687100	-3.49066400	2.21943700
C	2.02441400	-2.94282900	3.06792200
H	2.61984200	-1.18720600	4.15359800
H	1.14742600	-4.52826000	1.90559500
C	-1.03176100	-3.31387600	0.80460500
H	-0.86757300	-2.92472300	-0.20759100
H	-2.05042100	-3.04092500	1.09561200
C	0.66297100	0.60350000	3.49823300
H	-0.16065200	0.69050900	4.21357500

H	0.43103700	1.26222000	2.65419300
H	1.57786400	0.95579400	3.97949500
H	-0.95384000	-4.40188400	0.77110700
C	3.20508300	-3.77009400	3.50615800
H	3.70602900	-3.32213100	4.36676100
H	2.89843300	-4.78471700	3.77271300
H	3.93803600	-3.85174100	2.69645200
C	-0.36287500	0.05966100	-0.70969700
O	-0.82227800	0.56776200	-1.84713200
C	0.80986400	-0.85122600	-0.76978500
C	1.44848700	-1.07085200	-1.93183200
H	1.22389000	-1.24371500	0.15546600
H	1.02921100	-0.60136100	-2.81887400
C	2.70493700	-1.81313100	-2.08554500
C	3.44651800	-1.66289300	-3.26687200
C	3.22604100	-2.65736800	-1.08887700
C	4.66759600	-2.30675100	-3.44292500
H	3.05598500	-1.01887500	-4.05074300
C	4.44721800	-3.29872000	-1.26300900
H	2.66194100	-2.82240100	-0.17332400
C	5.17833200	-3.12578100	-2.43882500
H	5.22162000	-2.16652200	-4.36634100
H	4.82868300	-3.94656900	-0.47889500
H	6.13049200	-3.62921900	-2.57185100
C	4.84536500	2.10556300	-0.75762200
C	4.48037100	3.54894400	-1.10329100
C	3.70002000	4.25889500	0.00703200
C	3.64605000	1.20364900	-0.47078700
C	2.78644000	1.65036000	0.72595000
C	1.79615500	2.72669600	0.35240200
H	5.50307100	2.11349200	0.12260700
H	3.88881600	3.58574700	-2.02649200
H	3.77657500	5.34082800	-0.11849000
H	3.99867800	0.18523400	-0.27469100
H	3.42473800	1.98713400	1.55221900
C	1.35386000	4.96038900	-0.51682800
H	1.33266400	4.89047500	-1.61251800
C	-0.47518600	3.32336700	-0.15137700
C	-0.04225200	4.76680400	0.05731400
H	-0.73996700	5.45646800	-0.42368300
H	-0.02491700	4.99624400	1.12782100
H	-0.66495800	3.09872200	-1.20808400
H	1.74316000	5.94701000	-0.25282200
H	-1.40592700	3.11336600	0.38833700

N	0.54031000	2.38952000	0.32276900
N	2.26797400	3.95419400	0.02850400
H	4.14103200	4.02497200	0.98342500
H	5.39994600	4.11409000	-1.28988900
H	5.42675400	1.67275800	-1.57853600
H	3.00208700	1.13009500	-1.35512300
H	2.20230600	0.80383800	1.09437500
H	0.15166400	1.08542100	-0.00498100

Si-TS2^{DH}

C	5.61347300	0.43758400	-0.91041100
C	4.22463600	0.52400800	-0.94667100
C	3.56905700	1.75104000	-0.87581600
C	4.33842400	2.90492400	-0.75528000
C	5.73356700	2.82599800	-0.71521600
C	6.37986700	1.59542700	-0.79580300
C	6.08776100	-0.98762900	-1.02265300
C	4.80277300	-1.85298900	-1.03308400
C	3.59244200	-0.84306900	-1.05834600
H	2.48375300	1.80970100	-0.92014700
H	3.85204400	3.87300100	-0.69515600
H	6.31877200	3.73524100	-0.62194000
H	7.46379500	1.53862900	-0.76654600
H	6.73911100	-1.28534200	-0.19401500
H	4.75681400	-2.47339300	-1.92765000
H	6.65836300	-1.14483000	-1.94234900
H	3.00200600	-0.95560800	-1.96446800
N	2.68056600	-1.09124200	0.07575000
O	4.75216600	-2.78334200	0.03544800
C	1.41119400	-0.67205500	0.28950200
C	3.13030300	-1.63289500	1.25595900
N	1.15276700	-1.00143600	1.56757500
N	2.22181800	-1.60418700	2.17802800
C	4.51545900	-2.18607400	1.29240600
H	5.23886600	-1.38806900	1.51064400
H	4.59677900	-2.95475800	2.06056800
C	-0.11744000	-0.92467700	2.23185200
C	-1.01717600	-1.97753400	2.04585600
C	-0.38595300	0.17633700	3.05139300
C	-2.26652500	-1.86587700	2.65623000
C	-1.65121300	0.24515900	3.63202000
C	-2.60639200	-0.75606400	3.43192600
H	-2.98868000	-2.66792000	2.52508100
H	-1.89339300	1.09583600	4.26392900

C	0.66457600	1.22401300	3.31039300
H	1.08389700	1.62323500	2.38093200
H	1.49586800	0.79562600	3.87865000
C	-0.62370100	-3.21117600	1.27810200
H	0.16300700	-3.75408900	1.81130900
H	-0.23880400	-2.96997900	0.28290200
H	-1.48132100	-3.87605800	1.16176000
H	0.24701700	2.05406200	3.88192600
C	-3.98068300	-0.63209700	4.03502500
H	-3.94323600	-0.12322600	5.00070600
H	-4.63341600	-0.04600000	3.37927100
H	-4.44153100	-1.61191300	4.17503700
C	0.46904600	-0.05319500	-0.63780700
O	1.01455300	0.00969500	-1.93969200
H	0.30827700	-0.22892000	-2.55760700
C	-0.13095800	1.22316200	-0.18536400
C	-0.44056700	2.24160600	-1.00042200
H	-0.41859300	1.27133000	0.85956600
H	-0.13445500	2.19209100	-2.04340900
C	-1.15516500	3.45893700	-0.58327100
C	-1.18933100	4.56005600	-1.44843900
C	-1.81875200	3.56535200	0.65028300
C	-1.84784000	5.73378200	-1.09342300
H	-0.68641600	4.49157400	-2.40949500
C	-2.47584100	4.73705800	1.00549800
H	-1.83719900	2.72004600	1.33525400
C	-2.49287000	5.82846300	0.13667400
H	-1.85784100	6.57463600	-1.77966300
H	-2.98442700	4.79810700	1.96263900
H	-3.01052600	6.74028600	0.41559300
C	-5.31195100	0.67083800	-1.40409700
C	-5.61238600	-0.59677500	-2.20560800
C	-5.21725900	-1.89439000	-1.49425500
C	-3.83860300	0.88440000	-1.05654000
C	-3.22361900	-0.27591300	-0.25568000
C	-2.82848400	-1.42624400	-1.14794700
H	-5.88709500	0.63211700	-0.46908400
H	-5.11041200	-0.56653800	-3.18076500
H	-5.76260900	-2.73402600	-1.92874000
H	-3.74171500	1.79836600	-0.46215800
H	-3.92224500	-0.62432200	0.51298100
C	-3.46009100	-3.35005700	-2.51434400
H	-3.59590200	-3.04327500	-3.55932400
C	-1.10500300	-2.61499400	-2.33565100

C	-2.03438100	-3.81754600	-2.26852400
H	-1.75811900	-4.56706100	-3.01291200
H	-1.96512000	-4.27979500	-1.27872100
H	-1.05629600	-2.23618200	-3.36500100
H	-4.16740200	-4.15722800	-2.30864300
H	-0.08228900	-2.88182300	-2.04258800
N	-1.56306800	-1.55455000	-1.44575100
N	-3.79368000	-2.23034900	-1.62720200
H	-5.49423800	-1.85334000	-0.43463100
H	-6.68817600	-0.63712900	-2.40424000
H	-5.67823200	1.54054600	-1.95857800
H	-3.24148000	1.04362900	-1.96398600
H	-2.32316900	0.05859200	0.26302800
H	-0.60894900	-0.86566700	-0.82561400

Re-M2

C	-1.57116400	3.53667000	0.81087600
C	-1.75391200	2.18107000	0.51352700
C	-2.36541300	1.33470300	1.43494300
C	-2.76099400	1.85516500	2.66657500
C	-2.55959300	3.20168900	2.96925200
C	-1.96981100	4.05418100	2.03768200
C	-0.95412100	4.27154400	-0.34851000
C	-1.23885400	3.30853700	-1.51915100
C	-1.25911900	1.88535500	-0.89332500
H	-2.54557600	0.28960900	1.20764500
H	-3.23734100	1.20446900	3.39265100
H	-2.87920000	3.59121600	3.93065400
H	-1.83427700	5.10837000	2.26015900
H	0.12076600	4.40899500	-0.18406100
H	-2.24523000	3.50288800	-1.89734500
H	-1.38839100	5.25907100	-0.51922300
H	-1.91619200	1.22382600	-1.46155600
N	0.11934400	1.35524700	-0.93957100
O	-0.38778800	3.41186100	-2.63688300
C	0.66588500	0.30131600	-0.21048100
C	1.18709300	2.11334400	-1.38608600
N	2.01726500	0.58030700	-0.17353100
N	2.32355500	1.68248500	-0.96609900
C	0.97977800	3.27048300	-2.31977500
H	1.39714000	4.18661800	-1.88565000
H	1.50225600	3.07344000	-3.25851100
C	3.04892800	-0.39405600	0.02283300
C	3.37657800	-1.24684100	-1.03494000

C	3.69750900	-0.45514100	1.25923100
C	4.39509700	-2.17957000	-0.83082700
C	4.70929500	-1.39929900	1.41898500
C	5.07323900	-2.26568600	0.38488000
H	4.66373600	-2.85172900	-1.64241400
H	5.22360100	-1.46487000	2.37519900
C	3.27145700	0.45223200	2.37945200
H	2.24613600	0.21065700	2.67646500
H	3.28250000	1.49884900	2.06314400
C	2.64569100	-1.15635200	-2.34900300
H	2.76472400	-0.16284600	-2.79229800
H	1.57207500	-1.32656300	-2.21359900
H	3.02470000	-1.89818400	-3.05401900
H	3.92689800	0.33838900	3.24486000
C	6.19218100	-3.25718500	0.57756900
H	7.16561700	-2.76936300	0.46318500
H	6.16207000	-3.69578700	1.57819800
H	6.13641600	-4.06450300	-0.15580900
C	0.03981000	-0.79672700	0.33316600
O	0.73821200	-1.50161000	1.30824200
H	1.07329100	-2.32251600	0.92020500
C	-1.24056000	-1.27443200	-0.07795300
C	-1.87231000	-2.35767700	0.43571500
H	-1.70426200	-0.74396300	-0.90627800
H	-1.38320300	-2.91179200	1.23347600
C	-3.16985900	-2.86667800	-0.00903000
C	-3.58984000	-4.14436200	0.39790200
C	-4.04429400	-2.12592200	-0.82513400
C	-4.81306600	-4.66783100	-0.00705800
H	-2.93680400	-4.73282600	1.03738000
C	-5.26309900	-2.65067800	-1.23461500
H	-3.77657000	-1.11715300	-1.12741500
C	-5.65707300	-3.92704700	-0.83155900
H	-5.10759600	-5.65992400	0.32179000
H	-5.91689600	-2.05457800	-1.86425300
H	-6.61167700	-4.33292000	-1.14990300

Si-M2

C	3.80169700	1.06074400	1.29607100
C	2.90001100	1.61220500	0.37943400
C	1.95100300	2.54343500	0.79469100
C	1.89564500	2.88763800	2.14545100
C	2.77721300	2.31597000	3.06364700
C	3.74417700	1.40490000	2.64210900

C	4.76210700	0.11951200	0.61949800
C	4.58955600	0.48579500	-0.87156900
C	3.14644900	1.04585700	-1.00735900
H	1.26991200	2.98908900	0.07942000
H	1.15893400	3.60860100	2.48531700
H	2.72009400	2.59482600	4.11126300
H	4.44767200	0.97816700	3.35094500
H	4.47824700	-0.92086500	0.81684600
H	5.27804000	1.29629400	-1.12173400
H	5.79582200	0.24172000	0.95140000
H	3.04709600	1.78114500	-1.80500200
N	2.25520600	-0.10271900	-1.30887800
O	4.87042400	-0.54708100	-1.79169900
C	0.88651100	-0.15264500	-1.04588100
C	2.71704800	-1.40169000	-1.18849600
N	0.65281400	-1.47667400	-0.70424600
N	1.81045800	-2.23700200	-0.81907500
C	4.13266800	-1.72994800	-1.56313700
H	4.59017900	-2.36036800	-0.79143700
H	4.14053100	-2.28756100	-2.50311800
C	-0.43263700	-1.97162100	0.07541700
C	-1.36443700	-2.81744600	-0.53151500
C	-0.55837300	-1.55122900	1.40712800
C	-2.46497000	-3.22688800	0.22234900
C	-1.67888400	-1.97498500	2.11799900
C	-2.64469800	-2.80411000	1.54017300
H	-3.20504500	-3.87886200	-0.23519800
H	-1.80241700	-1.65078600	3.14906200
C	0.46442700	-0.63653800	2.02553300
H	0.32735500	0.39515300	1.68020900
H	1.48224300	-0.93002700	1.74729800
C	-1.18693600	-3.22757900	-1.96817600
H	-0.22816500	-3.73258000	-2.11439200
H	-1.18817900	-2.34726300	-2.61928600
H	-1.98969600	-3.89572000	-2.28436600
H	0.38339000	-0.64662800	3.11410500
C	-3.85842800	-3.21968700	2.33152600
H	-3.56901200	-3.69996700	3.27064100
H	-4.47024400	-2.34877800	2.58700400
H	-4.48006800	-3.91744900	1.76703000
C	0.00441200	0.88363200	-1.21615300
O	0.53480100	2.06545400	-1.73553100
H	0.21614100	2.15326900	-2.64459300
C	-1.39237900	0.84230700	-0.90229800

C	-2.25209800	1.87607900	-1.04628800
H	-1.77460200	-0.10877400	-0.54638900
H	-1.87583300	2.82748900	-1.41589400
C	-3.68331100	1.82019700	-0.74204900
C	-4.49919300	2.91214300	-1.08115000
C	-4.29725200	0.71857500	-0.11641000
C	-5.86613200	2.90467200	-0.82381500
H	-4.04530800	3.77661200	-1.55916100
C	-5.66271100	0.71074600	0.13779300
H	-3.70191900	-0.13970200	0.18577200
C	-6.45907000	1.80138200	-0.21466800
H	-6.46948200	3.76388500	-1.10093800
H	-6.11034700	-0.15289600	0.62111100
H	-7.52497300	1.79121500	-0.01183300

[3 + 2] annulation

TS3RR'

C	0.22629500	-0.68640600	0.81134900
O	0.71920300	-0.19680700	1.99534300
H	0.21909800	0.68507300	2.10833800
C	-1.09945200	-0.77947900	0.52679500
C	-2.14133500	-0.28283300	1.38875200
H	-1.37968300	-1.15248200	-0.45061800
H	-1.88075500	-0.28664900	2.44681700
C	-3.52345900	-0.74960800	1.12569300
C	-4.42950200	-0.85353500	2.19351400
C	-4.00370300	-1.02727000	-0.16590700
C	-5.75713200	-1.20889200	1.98337200
H	-4.07440300	-0.65208400	3.20147900
C	-5.33191200	-1.38759400	-0.37505100
H	-3.34009700	-0.96777500	-1.02616400
C	-6.21834100	-1.47834500	0.69598200
H	-6.43336700	-1.28146600	2.83010700
H	-5.67496700	-1.59518400	-1.38435600
H	-7.25379800	-1.75601500	0.52926200
C	-0.74450100	2.14366600	1.70918600
C	-1.96209700	1.64543700	1.16600600
H	-0.81440000	2.65305600	2.66308000
N	-2.12650400	1.71753800	-0.27233900
S	-1.92178000	3.16786700	-1.06764900
O	-2.64409200	2.97307000	-2.32717400
O	-2.23576600	4.34634800	-0.26771800
C	-0.17642900	3.19960400	-1.40208200
C	0.51688000	2.02366100	-1.67465100

C	1.86131600	2.09994000	-2.02782100
C	2.51354200	3.33444300	-2.11764800
C	1.79373800	4.49788500	-1.82273800
C	0.45242500	4.44009800	-1.46572100
H	0.01085100	1.06895600	-1.57828900
H	2.42108500	1.19197600	-2.24318000
H	2.29262000	5.46144100	-1.87606900
H	-0.10362300	5.34011000	-1.22667800
C	3.95816600	3.41939500	-2.53715600
H	4.53374300	4.03386300	-1.83840600
H	4.04166400	3.88774100	-3.52276600
H	4.41392900	2.42802600	-2.59104800
C	-3.24335100	2.02577800	1.86713300
O	-4.25625900	2.35662100	1.29261600
O	-3.15284300	1.91041900	3.19713500
C	-4.35124400	2.23116800	3.91080900
H	-5.17217900	1.59635900	3.57021500
H	-4.61686600	3.27783700	3.75118400
H	-4.13069700	2.04765800	4.96048800
H	0.00280200	2.51103300	1.01623500
C	5.37231300	-0.27253900	1.85385300
C	4.01937200	-0.60076400	1.83484200
C	3.47882000	-1.50935700	2.74062600
C	4.32835900	-2.09403100	3.67624400
C	5.68757300	-1.76954500	3.70129800
C	6.21832100	-0.85609300	2.79343800
C	5.71016900	0.73955900	0.79084100
C	4.44147500	0.85219500	-0.08568100
C	3.29611000	0.14400800	0.73412100
H	2.41750100	-1.73774100	2.72164000
H	3.93190100	-2.80544500	4.39308800
H	6.33689600	-2.23504900	4.43589100
H	7.27494700	-0.60684400	2.81450500
H	6.56614100	0.44983700	0.17334400
H	4.16405000	1.89130500	-0.26841000
H	5.94875600	1.71020000	1.23666500
H	2.58488400	0.87357000	1.12063700
N	2.53955100	-0.77732100	-0.12245100
O	4.63750700	0.31291000	-1.38611300
C	1.23394500	-1.14469700	-0.11513000
C	3.14604300	-1.44667900	-1.15151900
N	1.12156800	-2.01565000	-1.14003100
N	2.30679900	-2.19498800	-1.79964600
C	4.56532600	-1.10104800	-1.45097800

H	5.24860700	-1.57733200	-0.73553200
H	4.82616300	-1.41063600	-2.46221300
C	-0.03215600	-2.78800000	-1.50659400
C	-0.36239600	-3.88398300	-0.70201800
C	-0.79805700	-2.38665000	-2.60342100
C	-1.52940200	-4.57661800	-1.01266600
C	-1.95311200	-3.12023200	-2.87675600
C	-2.34256000	-4.20078300	-2.08486400
H	-1.81319100	-5.42819700	-0.39984100
H	-2.56986600	-2.82699000	-3.72286600
C	-0.45717200	-1.16836000	-3.42096200
H	0.60937700	-0.93606000	-3.39780200
H	-1.00695300	-0.29513000	-3.04877600
C	0.49022200	-4.26564300	0.47817200
H	0.33262400	-3.56667800	1.30782800
H	1.55433000	-4.24914700	0.22537400
H	0.23264600	-5.26612500	0.82813300
H	-0.75373900	-1.31479900	-4.46140000
C	-3.63339900	-4.92561900	-2.35930300
H	-4.45330300	-4.45056400	-1.81017900
H	-3.88531300	-4.89872800	-3.42157200
H	-3.57940100	-5.96805300	-2.03854500
H	-3.02962100	1.35031600	-0.57880600

TS3RS'

C	-5.69864400	-2.09220800	0.15781400
C	-4.40178000	-2.03704700	-0.36180300
C	-3.37561900	-2.79481600	0.19685100
C	-3.66317200	-3.59212300	1.30344000
C	-4.95421200	-3.63866900	1.83115800
C	-5.98327100	-2.89468700	1.25687700
C	-6.64089400	-1.21659400	-0.62472000
C	-5.86143700	-0.98403700	-1.93595100
C	-4.35858500	-1.11157500	-1.56131500
H	-2.38036700	-2.77313300	-0.23286500
H	-2.87554600	-4.18858800	1.75222500
H	-5.16228100	-4.26938200	2.68966000
H	-6.99172000	-2.94626100	1.65596000
H	-6.82233500	-0.28001800	-0.08526200
H	-6.08243900	-1.79801500	-2.62946900
H	-7.61337200	-1.67791800	-0.80889900
H	-3.73297600	-1.47193700	-2.37784100
N	-3.87086400	0.24477400	-1.21153800
O	-6.16713500	0.19992900	-2.64311700

C	-2.67975900	0.58946400	-0.66586100
C	-4.62460000	1.38874900	-1.27636900
N	-2.77720100	1.90305800	-0.40699300
N	-3.98850000	2.41019400	-0.78588400
C	-5.98664600	1.38444500	-1.90107900
H	-6.75765100	1.51582400	-1.13321400
H	-6.06067800	2.21827300	-2.60113700
C	-1.73933800	2.75614500	0.09776400
C	-0.69880500	3.10250400	-0.76272300
C	-1.79507400	3.14198000	1.44126900
C	0.34710500	3.85096900	-0.21984100
C	-0.73381800	3.89668800	1.93089400
C	0.35101900	4.24546200	1.11785600
H	1.18160300	4.12128800	-0.86173300
H	-0.74353300	4.20570400	2.97345500
C	-2.94554900	2.71835400	2.31478300
H	-3.02169000	1.62597800	2.35963400
H	-3.89538500	3.09438000	1.92408900
C	-0.70126800	2.66458700	-2.20103100
H	-1.67358500	2.84912700	-2.66749900
H	-0.47082000	1.59675200	-2.26977000
H	0.06419300	3.20337600	-2.76144300
H	-2.81381800	3.09230700	3.33077900
C	1.51352400	5.00931900	1.69703900
H	1.17167700	5.88273000	2.25851300
H	2.07976800	4.37716300	2.39001600
H	2.19630700	5.34662100	0.91440800
C	-1.52490300	-0.27440300	-0.52114700
O	-1.43216400	-1.17183600	-1.53191200
H	-0.47576800	-1.58483800	-1.50548600
C	-0.73856800	-0.16624500	0.58000800
C	0.30658100	-1.06091600	1.03145700
H	-0.96885400	0.67501400	1.22644500
H	0.08227900	-2.11992900	0.90349600
C	0.89912200	-0.71842100	2.33809900
C	1.13192900	0.62250800	2.70153300
C	1.31583200	-1.71770200	3.23373600
C	1.73267600	0.94560700	3.91116600
H	0.85305600	1.42029000	2.01343300
C	1.92746200	-1.39252500	4.44167500
H	1.14988300	-2.76010200	2.97330800
C	2.13534200	-0.06001300	4.79115400
H	1.89721500	1.98928200	4.16481700
H	2.23600800	-2.18585700	5.11578300

H	2.60906500	0.19241800	5.73416000
C	1.18120500	-1.88686300	-1.60630600
C	1.73597900	-1.31945900	-0.44322000
H	1.16962300	-1.26254900	-2.49489600
N	2.59542100	-2.15354200	0.36696700
S	3.99819000	-2.78708700	-0.29270100
O	3.64433400	-3.76807600	-1.30893100
O	4.78014500	-3.20070200	0.86966900
C	4.85698200	-1.45556900	-1.09262900
C	5.83646000	-0.76486600	-0.38285100
C	6.44628200	0.33248300	-0.97578200
C	6.07694200	0.75783300	-2.25799400
C	5.09301800	0.04316300	-2.94638300
C	4.47946300	-1.06794700	-2.37456900
H	6.11072200	-1.09233300	0.61425000
H	7.21997900	0.87213000	-0.43674700
H	4.80480800	0.35655400	-3.94541000
H	3.71386500	-1.62338900	-2.90594600
C	6.71555000	1.97834900	-2.86632400
H	7.78969900	2.00073800	-2.66720900
H	6.56109200	2.01071500	-3.94644500
H	6.28362000	2.88900600	-2.43806300
C	2.10219000	0.13283100	-0.50345100
O	1.60097000	0.93994000	-1.25675000
O	3.03859700	0.45730900	0.40219200
C	3.44858900	1.82340400	0.39691700
H	3.86618600	2.08376600	-0.57951800
H	2.59839100	2.47515900	0.61358700
H	4.20874800	1.91017900	1.17171300
H	1.29047400	-2.95603100	-1.73986200
H	2.83966600	-1.73395400	1.26431900

TS3SR'

C	-5.18083100	-3.24947600	-0.12124500
C	-4.02649600	-2.47400700	-0.17904700
C	-2.90558200	-2.77484800	0.59059900
C	-2.96347800	-3.88012200	1.43560300
C	-4.11882600	-4.66428800	1.49944500
C	-5.23287000	-4.35734200	0.72163900
C	-6.24194200	-2.72743300	-1.05539500
C	-5.70726600	-1.36917500	-1.57116200
C	-4.19024500	-1.32663600	-1.14936500
H	-2.00558300	-2.16812100	0.52463900
H	-2.10369900	-4.13788500	2.04519500

H	-4.14710600	-5.52307200	2.16240600
H	-6.12843700	-4.96912000	0.77408000
H	-7.21320700	-2.58577400	-0.57060900
H	-5.78280600	-1.29421500	-2.65564600
H	-6.39884600	-3.41528100	-1.89187600
H	-3.54044100	-1.42352700	-2.01465600
N	-3.86394100	-0.04599600	-0.49728900
O	-6.46917300	-0.27110600	-1.09376400
C	-2.69529500	0.63436300	-0.36439500
C	-4.79707300	0.59618600	0.27216000
N	-2.99361200	1.65763700	0.46184800
N	-4.30334700	1.64171600	0.85871100
C	-6.19569100	0.07567100	0.24833900
H	-6.30129200	-0.78397800	0.92504200
H	-6.89342000	0.85571000	0.55210800
C	-2.10526100	2.64309000	1.00506700
C	-1.35173200	2.29630100	2.12958300
C	-2.00475300	3.87510700	0.35795900
C	-0.46124600	3.25253600	2.61325600
C	-1.08464200	4.79028800	0.86891400
C	-0.30711100	4.49482500	1.99023400
H	0.13072500	3.02345800	3.49569100
H	-0.96928200	5.75194000	0.37624200
C	-2.81629400	4.15778300	-0.87676600
H	-3.88330300	4.00597000	-0.69147200
H	-2.52343600	3.48269800	-1.68896800
C	-1.46648700	0.92431100	2.73679800
H	-0.92955900	0.19845200	2.11226700
H	-2.50950200	0.60382800	2.81059100
H	-1.03110400	0.90609100	3.73756200
H	-2.66190500	5.18330000	-1.21405800
C	0.68253900	5.49369300	2.53079200
H	0.83655200	6.31637600	1.83008000
H	0.32945200	5.91490800	3.47706700
H	1.64837800	5.01830100	2.72383800
C	-1.43611000	0.28870700	-0.98659000
O	-1.45684000	-0.89992100	-1.66846800
H	-0.60908200	-1.36430900	-1.32255200
C	-0.35200300	1.10832900	-0.98514600
C	0.86102800	0.80017500	-1.70926400
H	-0.39496800	2.03125200	-0.42244600
H	0.67402600	0.20281600	-2.60249300
C	1.78777700	1.93423200	-1.93495200
C	2.53275300	2.01635700	-3.12196300

C	1.99627300	2.92695400	-0.96041700
C	3.44250400	3.04896900	-3.33153300
H	2.38462200	1.26080100	-3.88984400
C	2.89595600	3.96368900	-1.17512200
H	1.45523700	2.88119900	-0.01590200
C	3.62529500	4.03248100	-2.36196900
H	4.00335400	3.08892700	-4.26027400
H	3.03415400	4.71947200	-0.40734100
H	4.33030200	4.84064900	-2.52643600
C	0.86662200	-1.76924400	-0.47844700
C	1.74831000	-0.69867300	-0.80317700
H	0.96589400	-2.67421100	-1.06776600
H	0.61175000	-1.89132600	0.56843300
N	2.73205800	-0.94586700	-1.84239800
S	3.76645200	-2.26015100	-1.75732900
O	4.85316100	-1.90115200	-2.66649100
O	3.00484300	-3.47872100	-2.00055500
C	4.43259000	-2.35826700	-0.11502700
C	5.64038900	-1.72040800	0.15705000
C	6.13636500	-1.74854900	1.45237700
C	5.43617400	-2.39486800	2.47884500
C	4.22886900	-3.02844700	2.17472000
C	3.71854500	-3.01859000	0.87923500
H	6.17339200	-1.21343900	-0.63978800
H	7.08041100	-1.25958400	1.67588600
H	3.68351500	-3.54282800	2.96055600
H	2.78224800	-3.50910300	0.63731000
C	5.98565100	-2.39933800	3.88116500
H	5.36598400	-3.00068800	4.54879700
H	7.00214200	-2.80224700	3.89940800
H	6.03204100	-1.38194100	4.28111900
C	2.35506300	0.09841200	0.32148100
O	3.48089600	0.54599200	0.30242400
O	1.50869100	0.30379100	1.34144800
C	2.08516300	0.99331800	2.45384800
H	3.00894500	0.50060200	2.76329000
H	2.30324600	2.03173700	2.19033200
H	1.34327800	0.94835500	3.24910800
H	3.31358200	-0.12367900	-2.01326700
TS3SS'			
C	5.81983300	-2.64220600	0.46525000
C	4.54179000	-2.09573900	0.38969300
C	3.53777700	-2.69240500	-0.36764500

C	3.83967200	-3.86324300	-1.05859800
C	5.11931200	-4.42041600	-0.98440500
C	6.11651200	-3.81679100	-0.22184700
C	6.71941300	-1.81394900	1.34638500
C	5.93371000	-0.51124100	1.62493700
C	4.44825300	-0.82601600	1.20761000
H	2.54298900	-2.25674600	-0.40591500
H	3.07526200	-4.34709800	-1.65753100
H	5.33908400	-5.33248000	-1.53002900
H	7.11054100	-4.25074600	-0.16936700
H	7.68162500	-1.57708100	0.88201000
H	5.96879800	-0.23580700	2.67882800
H	6.93328300	-2.33428900	2.28534100
H	3.80907000	-0.94674500	2.08089500
N	3.89744700	0.27363400	0.40709300
O	6.49020100	0.60999800	0.95356200
C	2.63350800	0.73850400	0.26977300
C	4.68603100	0.97178700	-0.46774800
N	2.72019600	1.68923500	-0.68110300
N	4.00225600	1.84788700	-1.13769800
C	6.15390100	0.70474500	-0.41812200
H	6.40331300	-0.21309200	-0.96789100
H	6.70566200	1.54042200	-0.84765600
C	1.62100800	2.33636700	-1.34050600
C	0.88971200	1.58164200	-2.26166700
C	1.29422400	3.64437700	-0.98212300
C	-0.24246000	2.17485300	-2.81336500
C	0.15347800	4.19604100	-1.56531900
C	-0.63151000	3.47102300	-2.46620200
H	-0.85079700	1.59741100	-3.50372300
H	-0.13612100	5.20897100	-1.29683900
C	2.11750900	4.39197000	0.03257900
H	3.16682900	4.44377100	-0.27113900
H	2.08540200	3.89077000	1.00696000
C	1.29315500	0.17271000	-2.59758000
H	1.02149200	-0.49645600	-1.77274900
H	2.37251500	0.09598800	-2.76344100
H	0.76490600	-0.17514800	-3.48454800
H	1.74045500	5.40738800	0.16110000
C	-1.88115800	4.06118700	-3.06360100
H	-1.73672200	4.27789900	-4.12675500
H	-2.70446700	3.34697100	-2.97805000
H	-2.16060400	4.99085300	-2.56341500
C	1.46741000	0.27189500	0.98205400

O	1.59587800	-0.98442900	1.53073900
H	0.75139200	-1.44398700	1.20184800
C	0.37601900	1.05431600	1.17519100
C	-0.78330200	0.60036100	1.90326200
H	0.35889900	2.04035400	0.72671500
H	-0.54744500	-0.15756700	2.65099800
C	-1.72641300	1.62946800	2.39726900
C	-2.40187000	1.42125400	3.61027900
C	-2.03894000	2.78822600	1.66427800
C	-3.34818600	2.32698300	4.07506200
H	-2.16703400	0.53362500	4.19361900
C	-2.98744900	3.69419600	2.13047000
H	-1.54211900	2.98430100	0.71491100
C	-3.64802600	3.47081500	3.33699500
H	-3.85080200	2.14159700	5.01966000
H	-3.21229700	4.58049600	1.54481900
H	-4.38605300	4.17945600	3.69795900
C	-0.81071800	-1.73336900	0.30316900
C	-1.64153600	-0.63372300	0.66201800
H	-1.03886200	-2.68575900	0.76945100
N	-1.99821300	0.31313000	-0.37921900
S	-2.66518400	-0.18530300	-1.82772400
O	-1.63884900	-0.84623800	-2.62612600
O	-3.30542700	1.02330200	-2.34984800
C	-3.93940400	-1.38059400	-1.50830400
C	-3.59844800	-2.72004200	-1.34804700
C	-4.60057300	-3.63331500	-1.03560100
C	-5.92924000	-3.22496500	-0.89177600
C	-6.24104300	-1.87179800	-1.06852900
C	-5.25399100	-0.94389300	-1.37186800
H	-2.56572100	-3.03221300	-1.45578500
H	-4.34702500	-4.68128300	-0.90408400
H	-7.27071800	-1.54270200	-0.96123500
H	-5.48879200	0.10721500	-1.49946600
C	-7.01515000	-4.22064100	-0.57994000
H	-7.56640800	-4.48426700	-1.48828500
H	-6.60188800	-5.14037500	-0.16127000
H	-7.73465200	-3.80725300	0.13101000
C	-2.82758600	-0.92336800	1.55242200
O	-3.91719100	-0.41071400	1.41978000
O	-2.53339300	-1.76965900	2.54730200
C	-3.62460100	-2.06394700	3.42473300
H	-4.00635300	-1.14460300	3.87392300
H	-4.42980200	-2.55280300	2.87234700

H	-3.22354900	-2.72957000	4.18630300
H	-0.44398800	-1.76093000	-0.71599800
H	-2.60165200	1.05472300	-0.02056000
TS3RR			
C	0.75420600	0.26242700	-0.38067900
O	-0.03431900	0.97401600	-1.25852900
H	-0.52382000	0.33980900	-1.83175200
C	0.23174200	-0.68364900	0.46843100
C	-1.14089600	-0.98407800	0.55058200
H	0.93148900	-1.23262200	1.09386900
H	-1.81721400	-0.20747600	0.20217800
C	-1.67265400	-1.88110500	1.57116800
C	-2.99452200	-1.71021600	2.02069900
C	-0.93155400	-2.95000400	2.10627600
C	-3.55181700	-2.56731600	2.96238400
H	-3.57993700	-0.88288800	1.62182400
C	-1.48943400	-3.80247200	3.05212400
H	0.08901800	-3.12168300	1.77303100
C	-2.80284000	-3.62090400	3.48458000
H	-4.57435000	-2.41001400	3.29274000
H	-0.89672200	-4.62105800	3.44974100
H	-3.23563100	-4.29284800	4.21841700
C	-3.00668400	-2.68944600	-1.12228700
C	-1.85368600	-1.84822400	-1.58528800
H	-3.76750900	-2.07650500	-0.63337700
H	-2.66531800	-3.45216900	-0.42650100
N	-1.93141500	-0.75773000	-2.33357800
S	-3.36602100	-0.05272600	-2.71693800
O	-3.02190300	1.04384300	-3.61929100
O	-4.35643700	-1.03601400	-3.16541700
C	-3.99376400	0.67940600	-1.21939500
C	-3.31442300	1.75865400	-0.65276000
C	-3.80945600	2.32469100	0.51378100
C	-4.97603000	1.83495600	1.11862500
C	-5.64274900	0.76323100	0.52142600
C	-5.15871100	0.18138500	-0.64885900
H	-2.40538500	2.13491100	-1.11470000
H	-3.28724100	3.16602300	0.96194300
H	-6.55198300	0.37822100	0.97383100
H	-5.67721400	-0.64479900	-1.12450300
C	-5.50030800	2.47633400	2.37578800
H	-6.29204200	1.87623300	2.82769800
H	-5.90858400	3.46835400	2.15905000

H	-4.70106500	2.60573400	3.11063000
C	-0.48328900	-2.45635700	-1.59466000
O	0.46785500	-1.96643400	-2.16765100
O	-0.42946700	-3.60962400	-0.91089000
C	0.88761100	-4.11305900	-0.70269000
H	1.47001200	-3.39380300	-0.11906500
H	1.39499700	-4.28190600	-1.65495200
H	0.77124100	-5.04679800	-0.15383400
H	-3.46879300	-3.15813700	-1.99654400
C	1.49587800	4.64469200	1.13786900
C	0.89502800	3.55418400	0.50392800
C	-0.23058700	2.94482500	1.05896200
C	-0.72890700	3.43390200	2.26596900
C	-0.12884300	4.52446200	2.89777700
C	0.98423900	5.14088800	2.33282600
C	2.69436700	5.14429200	0.37864300
C	2.55742600	4.45058400	-0.99256000
C	1.63403200	3.21124800	-0.77757000
H	-0.71820200	2.11307000	0.56200600
H	-1.59635500	2.96003000	2.71583600
H	-0.53547500	4.89708000	3.83248000
H	1.44844400	5.99521000	2.81614300
H	3.61700500	4.85618000	0.89350400
H	2.03140700	5.11665700	-1.67897400
H	2.71425200	6.23130200	0.27334500
H	0.97483600	3.02665800	-1.62380300
N	2.48718300	2.00931700	-0.62463000
O	3.77419800	4.14313700	-1.64306200
C	2.09929100	0.73801100	-0.31844100
C	3.85375200	2.04412300	-0.53650300
N	3.24364900	0.09174800	-0.01521100
N	4.34215900	0.90312000	-0.16299700
C	4.61577900	3.27664700	-0.91695200
H	5.04144200	3.75352800	-0.02666100
H	5.43928000	2.99779900	-1.57643000
C	3.46557700	-1.31101700	0.19211800
C	3.47964900	-1.80706500	1.50017000
C	3.76540400	-2.09221100	-0.92607600
C	3.77271400	-3.15875200	1.66806800
C	4.08502000	-3.43236800	-0.70177900
C	4.08371600	-3.98181500	0.58021700
H	3.78353200	-3.57427600	2.67280500
H	4.32931500	-4.06191100	-1.55378800
C	3.72587700	-1.50508800	-2.30976700

H	4.35119000	-0.60978200	-2.37583200
H	2.69727000	-1.23118200	-2.56471000
C	3.23271300	-0.89452200	2.67282100
H	2.28998700	-0.34674200	2.57339100
H	4.03019500	-0.14878100	2.74969400
H	3.20174100	-1.46330100	3.60303400
H	4.08037500	-2.23068900	-3.04348500
C	4.39336100	-5.43996900	0.79856800
H	4.79061500	-5.90016900	-0.10796200
H	5.12377500	-5.56978800	1.60138700
H	3.48995800	-5.98627200	1.08774100

TS3RS

C	5.31522900	1.51714800	1.12236000
C	4.22061400	0.66661000	1.26030800
C	4.22782800	-0.38259100	2.17483600
C	5.36449800	-0.57132400	2.95725200
C	6.46540500	0.27886200	2.82517000
C	6.44795300	1.32947300	1.91025700
C	5.05992300	2.56895000	0.07286900
C	3.76623400	2.12390100	-0.64755900
C	3.11603700	1.04795600	0.29840600
H	3.35988200	-1.02757800	2.27576600
H	5.39623900	-1.38431800	3.67537400
H	7.34508100	0.11606500	3.44001600
H	7.30699800	1.98610700	1.80810500
H	5.87611100	2.66618600	-0.64965600
H	3.06056700	2.94096400	-0.78669200
H	4.91785200	3.55180200	0.53393400
H	2.23880100	1.46852000	0.78877800
N	2.65975600	-0.10837400	-0.47251000
O	4.02672400	1.65677800	-1.96461200
C	1.57535300	-0.90669200	-0.32725000
C	3.33050300	-0.52380200	-1.58780900
N	1.66440000	-1.78504800	-1.35061500
N	2.74702500	-1.53500100	-2.15380200
C	4.47665900	0.31740200	-2.03940600
H	5.36349400	0.14528900	-1.41378800
H	4.72070900	0.09697400	-3.07821000
C	0.82343900	-2.91616300	-1.61244900
C	0.85398600	-3.99558900	-0.72401200
C	-0.00514000	-2.87753600	-2.73914400
C	-0.03150700	-5.04560700	-0.96372600
C	-0.86482500	-3.95662600	-2.93582100

C	-0.90730900	-5.03512400	-2.05002200
H	-0.03442000	-5.89373800	-0.28360300
H	-1.52335900	-3.94928000	-3.80071900
C	0.02926300	-1.71315300	-3.69116500
H	1.00162200	-1.64669500	-4.18721700
H	-0.13995900	-0.77251400	-3.15863800
C	1.78290500	-4.01820300	0.46046500
H	1.38121300	-3.41177000	1.27986100
H	2.76823900	-3.61805400	0.20376200
H	1.90873000	-5.03915600	0.82442700
H	-0.74269500	-1.82684100	-4.45430000
C	-1.89455600	-6.15473700	-2.25190800
H	-2.84100300	-5.92044100	-1.75327900
H	-2.10794800	-6.30854700	-3.31205300
H	-1.52247800	-7.09186500	-1.83211000
C	0.60079900	-0.83699500	0.72151600
O	1.07568200	-0.30741300	1.89947800
H	0.50194800	0.43884300	2.16494800
C	-0.66343400	-1.35954200	0.59632900
C	-1.62799100	-1.25384200	1.60700400
H	-0.95233300	-1.72004800	-0.38443300
H	-1.24544600	-1.12535600	2.61705300
C	-2.95330300	-1.86442000	1.50612300
C	-3.72506900	-2.02972400	2.66874300
C	-3.52458700	-2.25646500	0.28162300
C	-5.00723100	-2.56469800	2.61578800
H	-3.30087000	-1.73575600	3.62574500
C	-4.80441500	-2.79570700	0.23088500
H	-2.96859900	-2.13061400	-0.64374600
C	-5.55618800	-2.95263100	1.39512300
H	-5.57806300	-2.68233000	3.53204500
H	-5.22083700	-3.09254500	-0.72721200
H	-6.55607800	-3.37163600	1.34996700
C	-3.27039600	1.05084900	0.59172300
C	-1.92490800	1.08149000	1.26436900
H	-3.19267500	0.60318500	-0.40079300
H	-3.98718400	0.48693400	1.18510400
N	-0.79546600	1.54561500	0.73342900
S	-0.64257100	1.74508400	-0.87963300
O	-1.15299600	0.61432400	-1.67240500
O	0.75252500	2.13879100	-1.11111900
C	-1.66788700	3.14914900	-1.27573000
C	-1.49229300	4.34252000	-0.57597600
C	-2.29718700	5.42942900	-0.88779100

C	-3.27011800	5.34369000	-1.89284000
C	-3.42150900	4.13736300	-2.57850200
C	-2.62488500	3.03551800	-2.27593000
H	-0.74418900	4.41149300	0.20794100
H	-2.17416000	6.36228300	-0.34458800
H	-4.17513800	4.05462300	-3.35629400
H	-2.74498100	2.09079800	-2.79535200
C	-4.12031200	6.54079800	-2.22850400
H	-4.97751800	6.25888900	-2.84275400
H	-4.48880300	7.02638000	-1.32118800
H	-3.53746500	7.28307000	-2.78298300
C	-1.87968700	1.14182600	2.76291700
O	-0.85523800	1.23907700	3.41447300
O	-3.08990000	1.05892900	3.31850700
C	-3.10547000	1.02400200	4.74878300
H	-2.48182700	0.20456800	5.11290700
H	-2.73023900	1.96519500	5.15396500
H	-4.14546000	0.87115500	5.02936500
H	-3.63552100	2.07958200	0.48075700

TS3SR

C	-0.40610200	-1.16061200	1.17629800
O	-1.02317300	-0.57827700	2.25950400
H	-0.72804800	0.35142300	2.33721100
C	0.96302900	-1.26965800	1.11032200
C	1.81837300	-0.67283000	2.04857000
H	1.39024500	-1.71020300	0.21875400
H	1.39475300	-0.48783000	3.03356200
C	3.26923300	-0.85599300	2.00082500
C	4.03824700	-0.61630600	3.15143600
C	3.94694900	-1.21003200	0.81943500
C	5.42339700	-0.73860300	3.13129900
H	3.53229300	-0.33339400	4.07151000
C	5.33092100	-1.33698400	0.80336800
H	3.38732700	-1.36141500	-0.10095900
C	6.07945500	-1.10405000	1.95710700
H	5.99227400	-0.54975400	4.03679600
H	5.83161300	-1.61130400	-0.12062000
H	7.15996700	-1.20195300	1.93934900
C	2.80055500	1.83636500	0.70577500
C	1.44236300	1.52760700	1.27727800
H	3.01787300	1.19733900	-0.15012300
H	2.80308400	2.88155200	0.37171300
N	0.29739000	1.50279500	0.59761300

S	0.30074100	1.21768200	-1.01279500
O	-1.09210100	0.94496900	-1.38580700
O	1.31679000	0.23560300	-1.42222700
C	0.73253600	2.76827700	-1.78112400
C	-0.17478100	3.82592600	-1.72135300
C	0.15833800	5.03300000	-2.31825300
C	1.38355800	5.19828900	-2.97947500
C	2.26904100	4.12084400	-3.03000400
C	1.95090400	2.90218500	-2.43437200
H	-1.13155900	3.69127000	-1.22573300
H	-0.54151000	5.86324200	-2.27925600
H	3.21926500	4.23329800	-3.54388500
H	2.63177700	2.05844700	-2.47835900
C	1.71884200	6.51421300	-3.63080100
H	2.73336500	6.51077900	-4.03347200
H	1.02697100	6.72630800	-4.45145300
H	1.63543800	7.33603900	-2.91418800
C	1.20817400	1.85924500	2.72471700
O	0.13114800	1.76162500	3.28615000
O	2.31537000	2.25689400	3.35097300
C	2.16918400	2.50531500	4.75320500
H	1.43808000	3.29711300	4.92233800
H	1.83897100	1.59737000	5.26265600
H	3.15352800	2.80709100	5.10399400
H	3.57781500	1.70719000	1.45539800
C	-5.38340100	0.58013100	1.03250000
C	-3.99914900	0.42951700	1.01105300
C	-3.15251600	1.52331500	0.85484200
C	-3.72776100	2.78311100	0.70237900
C	-5.11597400	2.94104500	0.70858600
C	-5.95359700	1.84129800	0.87708700
C	-6.08095000	-0.73415300	1.26601400
C	-4.97110800	-1.80999200	1.20505800
C	-3.60667100	-1.01387600	1.23535100
H	-2.07405200	1.40056300	0.83274000
H	-3.08839000	3.65279200	0.58569500
H	-5.54573200	3.93023400	0.58492400
H	-7.03253100	1.96471600	0.88828500
H	-6.85006000	-0.95247500	0.51787400
H	-5.01414500	-2.47815300	2.06546900
H	-6.57227200	-0.74798000	2.24399200
H	-3.12244600	-1.14295500	2.19953900
N	-2.67414700	-1.52947800	0.21831500
O	-5.12709200	-2.66992900	0.08699000

C	-1.31625600	-1.67078400	0.19228100
C	-3.15657200	-2.04889700	-0.95242100
N	-1.07111200	-2.32993300	-0.96822100
N	-2.21874000	-2.55827600	-1.68277600
C	-4.63469500	-2.12091900	-1.12171700
H	-5.06140500	-1.12917000	-1.32387200
H	-4.88931400	-2.79759200	-1.93670200
C	0.15247400	-2.88954400	-1.46488100
C	0.66724900	-2.41307600	-2.67467600
C	0.75353300	-3.93530800	-0.74823600
C	1.88392000	-2.94499700	-3.10462200
C	1.96816000	-4.42636500	-1.22055400
C	2.55969500	-3.92704700	-2.38307100
H	2.31176400	-2.57454700	-4.03302400
H	2.45893200	-5.22603400	-0.67109600
C	0.13080500	-4.50914600	0.49670900
H	-0.95690300	-4.57790900	0.40416200
H	0.35136500	-3.88853500	1.37134500
C	-0.06332700	-1.41113600	-3.52509200
H	-0.67175700	-0.73545300	-2.92518000
H	-0.72047200	-1.93379900	-4.22832500
H	0.65169700	-0.81763300	-4.09838900
H	0.52441200	-5.50948300	0.68426200
C	3.90116400	-4.43942600	-2.83812200
H	3.99852700	-5.51193100	-2.65283600
H	4.05580700	-4.25480000	-3.90316400
H	4.70687900	-3.93789800	-2.29171200

TS3SS

C	-5.00845600	1.29511300	-0.60682100
C	-3.71560400	1.00747300	-0.17424400
C	-3.47102500	0.38460100	1.04251000
C	-4.56765300	0.00157300	1.81398900
C	-5.86883800	0.24840800	1.37146300
C	-6.10043200	0.90296500	0.16107700
C	-4.97226000	2.05714100	-1.91109400
C	-3.51808500	2.55786100	-2.00054500
C	-2.71173500	1.48987200	-1.20363100
H	-2.45472300	0.18885500	1.37604400
H	-4.40693300	-0.49499400	2.76537500
H	-6.71139900	-0.05719400	1.98449100
H	-7.11381000	1.12145900	-0.16332700
H	-5.67070900	2.89682800	-1.95086700
H	-3.16415100	2.63571100	-3.03020100

H	-5.19176900	1.39894300	-2.76034300
H	-2.38111000	0.69042700	-1.86687400
N	-1.53309600	2.09859300	-0.60068000
O	-3.37062700	3.86969200	-1.45822900
C	-0.23895100	1.69486600	-0.42617900
C	-1.70337700	3.27323900	0.08508800
N	0.28202800	2.64664000	0.39792500
N	-0.62564400	3.63604500	0.70021200
C	-3.01446300	3.97247000	-0.08783300
H	-3.77808600	3.54365400	0.57157300
H	-2.89932000	5.03251800	0.13927200
C	1.64943900	2.81640100	0.78923900
C	2.05419800	2.33738400	2.03545600
C	2.52690300	3.40963200	-0.12510900
C	3.40952800	2.44685500	2.35396000
C	3.86918200	3.48693300	0.23338500
C	4.32800300	3.00148300	1.46193500
H	3.75493600	2.07284400	3.31428300
H	4.57690500	3.92851700	-0.46411600
C	2.03209600	3.89191200	-1.46159100
H	1.13735200	4.51168100	-1.35183200
H	1.77041700	3.04146300	-2.10150500
C	1.06737300	1.67921900	2.96016300
H	0.69549500	0.74490200	2.52422700
H	0.20361400	2.32717100	3.13635500
H	1.53467300	1.45277200	3.91985700
H	2.80123500	4.47574000	-1.96926200
C	5.79596100	3.06051200	1.79387000
H	6.36281400	2.40781400	1.12217300
H	6.18697000	4.07414300	1.67029100
H	5.98521200	2.74003500	2.82016300
C	0.42661800	0.62527900	-1.08094800
O	-0.25371300	0.07985800	-2.16385100
H	-0.25845500	-0.87969600	-2.00633100
C	1.73752900	0.26651600	-0.81123900
C	2.49456900	-0.61607200	-1.57309500
H	2.17585800	0.66478200	0.09463900
H	2.12152900	-0.86765100	-2.56252600
C	3.93080600	-0.80257200	-1.36058200
C	4.70946100	-1.40842300	-2.36352100
C	4.58982500	-0.40853000	-0.17896500
C	6.07333800	-1.62201900	-2.19630300
H	4.23103400	-1.69960800	-3.29586900
C	5.95621100	-0.61228500	-0.01985500

H	4.03308600	0.05304100	0.63140200
C	6.70913100	-1.22551800	-1.02143300
H	6.64241600	-2.09367900	-2.99185000
H	6.43515000	-0.29922100	0.90410300
H	7.77391800	-1.38665300	-0.88901100
C	1.69011300	-3.35024800	-2.10944000
C	1.37687000	-2.64436800	-0.81776800
H	1.01541500	-3.00477600	-2.89462700
H	2.72885300	-3.21871800	-2.40846200
N	0.11257300	-2.35567900	-0.60035300
S	-0.55649700	-2.27964300	0.91109300
O	-0.50825900	-0.93306500	1.49644400
O	-0.12112700	-3.39638700	1.75493900
C	-2.25473500	-2.59927000	0.47474300
C	-2.81174300	-2.13514400	-0.71399600
C	-4.17189200	-2.30020200	-0.93797400
C	-4.99070200	-2.91415900	0.01546700
C	-4.40543000	-3.38503000	1.19309600
C	-3.04258100	-3.23242900	1.43020500
H	-2.18493200	-1.65059500	-1.45382600
H	-4.60921000	-1.93559500	-1.86403900
H	-5.02477700	-3.87722900	1.93757600
H	-2.59023200	-3.60462300	2.34361000
C	-6.47123900	-3.04060300	-0.22418800
H	-6.93666500	-3.71074100	0.50130000
H	-6.94916200	-2.05892900	-0.13740400
H	-6.67734000	-3.42014900	-1.22851700
C	2.39715800	-2.72611800	0.29624200
O	2.36077400	-2.07243400	1.31152000
O	3.35522700	-3.60339500	-0.00306000
C	4.37894600	-3.75094900	0.98859100
H	4.85373100	-2.78789800	1.17808100
H	3.94651100	-4.13838900	1.91303900
H	5.09311800	-4.45774200	0.57171300
H	1.51291500	-4.42090500	-1.95288100

M3RR

C	0.88389100	0.49526300	-0.20941500
O	0.21827600	1.55143900	-0.56180400
H	-1.17227800	0.88481900	-0.67621100
C	0.49519100	-0.55193900	0.55966800
C	-0.81721100	-0.61125000	1.30606100
H	1.19629900	-1.35948300	0.72441100
H	-0.97335600	0.35917600	1.80254900

C	-0.75035000	-1.69440100	2.37023600
C	-1.13948000	-1.43728100	3.68496500
C	-0.29416700	-2.97876400	2.04583700
C	-1.08237800	-2.43644100	4.65566200
H	-1.48984600	-0.44313100	3.95151600
C	-0.24065500	-3.97927600	3.01023200
H	0.02472400	-3.19505100	1.02614500
C	-0.63457700	-3.71086200	4.32047700
H	-1.38479500	-2.21562400	5.67449400
H	0.11431100	-4.96904300	2.73844800
H	-0.58681200	-4.48938900	5.07518400
C	-3.36074100	-0.59725100	1.28855600
C	-2.11352800	-0.77311000	0.41792400
H	-3.35513900	0.41119600	1.71288000
H	-3.38286700	-1.33047800	2.09501000
N	-2.03225200	0.25516100	-0.61194900
S	-3.17658800	0.44978200	-1.73418800
O	-2.54223400	1.07775700	-2.89248800
O	-3.91413100	-0.80464200	-1.90297900
C	-4.33480000	1.63050500	-1.06728600
C	-3.84958000	2.81323800	-0.51022100
C	-4.75081400	3.74410000	-0.01408900
C	-6.13206400	3.51079200	-0.06639700
C	-6.58893700	2.31732300	-0.62656400
C	-5.69715100	1.37199100	-1.13068000
H	-2.77887000	2.99067300	-0.45278500
H	-4.38220700	4.66632200	0.42662700
H	-7.65627400	2.12004200	-0.66614000
H	-6.04728100	0.43778100	-1.55664900
C	-7.09432600	4.53888500	0.46851200
H	-8.10858600	4.13960900	0.52781400
H	-7.11493900	5.42150100	-0.17823900
H	-6.79552600	4.87264300	1.46580800
C	-2.06767100	-2.15382800	-0.25432000
O	-1.36063900	-2.43097500	-1.19230100
O	-2.84859900	-3.04823900	0.36262400
C	-2.74862700	-4.38067300	-0.14210600
H	-1.72151800	-4.74380300	-0.04334800
H	-3.03877600	-4.40934200	-1.19391900
H	-3.42512200	-4.98150000	0.46218500
H	-4.26576700	-0.72193300	0.68965000
C	3.88770400	3.52967900	1.50651900
C	2.67260400	3.08817800	0.97372800
C	1.56500800	2.87914000	1.79225100

C	1.70276300	3.09658900	3.16223000
C	2.91843000	3.52402300	3.69865800
C	4.01818800	3.75084400	2.87303900
C	4.92242400	3.71678900	0.42831600
C	4.05641300	3.77588200	-0.84736500
C	2.78061000	2.94846000	-0.53088300
H	0.62343900	2.56345100	1.35517900
H	0.85235800	2.93877900	3.81798800
H	3.00499700	3.69302500	4.76741600
H	4.95834200	4.10208300	3.28747900
H	5.61348400	2.86628600	0.41483100
H	3.72903000	4.80592000	-1.00440500
H	5.52263700	4.62077800	0.55124000
H	1.89261900	3.27171700	-1.07168900
N	3.04136900	1.54812500	-0.95374300
O	4.69076400	3.40102600	-2.05274100
C	2.27245300	0.45940700	-0.74968200
C	4.17226000	1.12482600	-1.59828100
N	2.97013900	-0.56482200	-1.24492700
N	4.15813600	-0.16407400	-1.78176200
C	5.22058100	2.09491900	-2.05013900
H	6.11365800	2.01084400	-1.41987100
H	5.50572500	1.85846900	-3.07640400
C	2.59137000	-1.95253300	-1.26262600
C	3.22499600	-2.80663700	-0.35185700
C	1.57907100	-2.35914200	-2.12832900
C	2.80108100	-4.13026300	-0.32370700
C	1.19293800	-3.70011200	-2.05949300
C	1.78225000	-4.59073900	-1.16670300
H	3.26523400	-4.81734500	0.37996900
H	0.38635600	-4.03891500	-2.70276700
C	0.88714000	-1.39221000	-3.04781900
H	1.58772500	-0.67294700	-3.48141000
H	0.11393000	-0.84580900	-2.49546900
C	4.29370600	-2.29443100	0.57705800
H	3.93916000	-1.42708200	1.14488400
H	5.18189200	-1.97922100	0.02208800
H	4.58588500	-3.06990900	1.28633700
H	0.39338600	-1.92936400	-3.85928900
C	1.33170700	-6.02667500	-1.08884700
H	0.50339500	-6.21921000	-1.77338400
H	2.14985000	-6.70791000	-1.34100600
H	1.00337600	-6.27485600	-0.07467300

M3RS

C	-4.37429700	-2.64761300	1.67803600
C	-3.12498300	-2.49236800	1.07035200
C	-1.95110500	-2.47767800	1.81829800
C	-2.05157200	-2.59806200	3.20344400
C	-3.29760200	-2.74066000	3.81691300
C	-4.46799100	-2.77421700	3.05929500
C	-5.47844900	-2.66377800	0.65147300
C	-4.70461400	-2.98073900	-0.64649400
C	-3.28659100	-2.39448600	-0.42903900
H	-0.99188300	-2.37821600	1.31924300
H	-1.15142200	-2.58425700	3.80950700
H	-3.35559900	-2.83768100	4.89651200
H	-5.43342100	-2.90399500	3.53886200
H	-5.96659000	-1.68307900	0.60309800
H	-4.58890700	-4.06316100	-0.73352700
H	-6.25472700	-3.40483600	0.85255600
H	-2.50121300	-2.89332200	-0.99753300
N	-3.31951400	-0.98902000	-0.90069800
O	-5.30584400	-2.57435400	-1.85896300
C	-2.36712200	-0.05234300	-0.75180300
C	-4.34500100	-0.41065000	-1.59998000
N	-2.84098400	1.03867000	-1.34954400
N	-4.07991100	0.83260200	-1.88579300
C	-5.57185200	-1.19275700	-1.95636100
H	-6.40911800	-0.88791000	-1.31695900
H	-5.84246500	-0.98652700	-2.99297400
C	-2.12480100	2.26688400	-1.57256600
C	-1.09799100	2.25831100	-2.52211500
C	-2.47051700	3.38553800	-0.81634700
C	-0.39311000	3.44641500	-2.69777000
C	-1.73107700	4.54930800	-1.02931500
C	-0.68955900	4.59427600	-1.95707600
H	0.41806900	3.47165200	-3.42120100
H	-1.97361400	5.43781200	-0.45218200
C	-3.58668300	3.32544200	0.19239700
H	-3.40905500	2.53964600	0.93495800
H	-4.54195100	3.10286400	-0.29180300
C	-0.76430900	1.01479100	-3.30320500
H	-1.65228500	0.62406400	-3.81155500
H	-0.37248000	0.22611600	-2.65113500
H	0.00220500	1.22818700	-4.04835900
H	-3.67890900	4.27655100	0.71850500
C	0.13231800	5.84331100	-2.13802800

H	-0.35368100	6.70918500	-1.68431900
H	1.11423800	5.72203000	-1.66883200
H	0.30081400	6.05353900	-3.19714500
C	-1.00814300	-0.27699000	-0.18076600
O	-0.42005400	-1.33080000	-0.64456300
H	1.09975200	-0.49988300	-0.83902300
C	-0.56509400	0.63682500	0.71925800
C	0.78562600	0.48263100	1.36173100
H	-1.19085200	1.48553600	0.96930000
H	0.99644000	-0.59302200	1.44310000
C	0.87022700	1.08310000	2.75251500
C	1.55488100	0.39535400	3.75970600
C	0.30582800	2.32512500	3.06052400
C	1.67838000	0.93380600	5.03872100
H	2.00019900	-0.57055100	3.53336600
C	0.42663700	2.86589300	4.33795200
H	-0.22699200	2.88369300	2.29540100
C	1.11373600	2.17232800	5.33176600
H	2.21177300	0.38200100	5.80654800
H	-0.01767000	3.83196600	4.55628800
H	1.20658200	2.59400600	6.32744400
C	1.78664600	2.51517700	0.13106300
C	1.93794400	1.02658300	0.43068500
H	0.80631900	2.67691300	-0.32622600
H	1.87020900	3.11115800	1.04087100
N	1.82459900	0.24641800	-0.80654500
S	3.04437700	0.07523500	-1.87314300
O	4.07473300	1.05257100	-1.51792500
O	2.46962500	0.08803700	-3.21741700
C	3.71617200	-1.55588500	-1.64829000
C	2.91661100	-2.65696100	-1.95060500
C	3.44271700	-3.93122000	-1.78973600
C	4.75749500	-4.11761800	-1.34409000
C	5.53260400	-2.99430600	-1.04921200
C	5.01858300	-1.70848300	-1.19445200
H	1.89715500	-2.51747300	-2.30020300
H	2.82783500	-4.79782000	-2.01595900
H	6.55117700	-3.12667600	-0.69588800
H	5.60804400	-0.83070900	-0.95378000
C	5.32266400	-5.50721600	-1.20762800
H	6.21982500	-5.51077300	-0.58544400
H	4.59063000	-6.18741000	-0.76497100
H	5.59296000	-5.91080100	-2.18881100
C	3.24122300	0.68213800	1.16068900

O	3.65766500	-0.44828200	1.27799100
O	3.81381100	1.74192700	1.73035400
C	4.95085000	1.45023500	2.54706000
H	4.65234500	0.81923300	3.38772400
H	5.71551300	0.93634300	1.96217600
H	5.31731800	2.41089300	2.90219900
H	2.56250800	2.83081500	-0.56931300

M3SR

C	-4.82454700	-3.30714900	-0.72461300
C	-3.70052300	-2.49151800	-0.62383800
C	-2.60578000	-2.85159900	0.15738700
C	-2.65979500	-4.05343600	0.85636400
C	-3.78919300	-4.87289900	0.77126100
C	-4.87575600	-4.50923000	-0.02196100
C	-5.84947500	-2.71978600	-1.66078700
C	-5.33664300	-1.29773200	-1.99542000
C	-3.85485400	-1.24201500	-1.46180100
H	-1.72099500	-2.22455100	0.18893700
H	-1.80692600	-4.35203000	1.45691400
H	-3.81812800	-5.80665300	1.32418900
H	-5.74850000	-5.15199300	-0.09006700
H	-6.85243200	-2.66060400	-1.22540100
H	-5.34216600	-1.10994100	-3.06891500
H	-5.93283300	-3.31686200	-2.57411300
H	-3.12490300	-1.19637900	-2.26710900
N	-3.65125100	-0.03489000	-0.63850800
O	-6.17828600	-0.28476800	-1.46181100
C	-2.54173400	0.68340800	-0.36601100
C	-4.66420500	0.47166200	0.12635200
N	-2.93425400	1.58284900	0.54842700
N	-4.25988000	1.46814100	0.85568100
C	-6.02975800	-0.09730200	-0.06849200
H	-6.14264900	-1.03832900	0.48759400
H	-6.78684600	0.61040800	0.26814400
C	-2.13106700	2.54675400	1.24932000
C	-1.31826700	2.09180300	2.28931900
C	-2.16890900	3.87373700	0.81953300
C	-0.49890100	3.03447000	2.90825700
C	-1.33427100	4.77798200	1.47439200
C	-0.49287900	4.37517300	2.51434800
H	0.15390000	2.71146500	3.71550400
H	-1.33344600	5.81769100	1.15718600
C	-3.03880700	4.28228700	-0.33852800

H	-4.09085100	4.05926600	-0.14003000
H	-2.75255400	3.73788200	-1.24513600
C	-1.28512200	0.63804800	2.67282000
H	-0.74213700	0.05366800	1.91960300
H	-2.29395800	0.22386800	2.76223900
H	-0.76749100	0.50215100	3.62339600
H	-2.93993200	5.35030600	-0.53589800
C	0.38861500	5.37303600	3.21864500
H	0.63054300	6.21617900	2.56803600
H	-0.11572600	5.77101100	4.10511600
H	1.32072700	4.90984500	3.54993400
C	-1.19080000	0.41011500	-0.94801800
O	-1.07268600	-0.75574500	-1.49177700
H	0.38694500	-1.16003600	-0.75361300
C	-0.22007100	1.35566100	-0.81179800
C	1.15819700	1.08888300	-1.35022700
H	-0.42946200	2.30799600	-0.35036400
H	1.05900900	0.45834600	-2.24345400
C	1.90333300	2.35424300	-1.74154400
C	2.69519900	2.36495400	-2.89472700
C	1.83782100	3.52116100	-0.97055600
C	3.40591000	3.50444800	-3.26603700
H	2.75327400	1.46672500	-3.50318500
C	2.54643200	4.66135400	-1.33950100
H	1.23421600	3.54277800	-0.06606800
C	3.33367100	4.65732000	-2.48914800
H	4.01102300	3.49158000	-4.16715600
H	2.48263900	5.55507600	-0.72632200
H	3.88451100	5.54694600	-2.77723500
C	2.28614900	0.93579700	0.95810200
C	2.01639200	0.21169200	-0.35785300
H	1.33264300	1.17045600	1.43965400
H	2.88029400	0.32317600	1.63719100
N	1.26196800	-1.03575500	-0.18896200
S	1.46424300	-2.10741500	1.01721000
O	0.62412300	-3.25165800	0.65668000
O	1.27998300	-1.53076200	2.35047500
C	3.18260000	-2.54695000	0.89075600
C	3.63640800	-3.14119100	-0.28642400
C	4.98115500	-3.46210100	-0.40046700
C	5.87912700	-3.18940500	0.64113300
C	5.39459900	-2.60180300	1.81116500
C	4.04635800	-2.28031000	1.94599000
H	2.94507700	-3.32741800	-1.10241300

H	5.34733900	-3.92188100	-1.31429700
H	6.07939700	-2.39287900	2.62771200
H	3.66093500	-1.82526300	2.85227700
C	7.34328200	-3.49959700	0.47695000
H	7.86721100	-3.46172400	1.43383400
H	7.48892000	-4.49009200	0.03875600
H	7.81347400	-2.77282400	-0.19406000
C	3.30923400	-0.12824900	-1.12896500
O	3.31402400	-0.71927700	-2.18441400
O	4.41490600	0.32246800	-0.53474300
C	5.63031000	0.08514900	-1.25308800
H	5.75610200	-0.98456400	-1.43188000
H	5.60686700	0.61506100	-2.20810100
H	6.42882100	0.46777300	-0.62050700
H	2.83697000	1.85733000	0.76824700

M3SS

C	-4.79075000	-2.55695300	0.20866500
C	-3.53899300	-1.94871600	0.19962800
C	-3.21552700	-0.95841900	-0.72398600
C	-4.18522200	-0.57105200	-1.64504800
C	-5.44787300	-1.17156700	-1.63816000
C	-5.75891600	-2.16774100	-0.71486400
C	-4.89133000	-3.59137500	1.30093100
C	-3.45648000	-3.73726200	1.86361300
C	-2.65542000	-2.51050400	1.29105800
H	-2.23682100	-0.48835100	-0.72185700
H	-3.94546500	0.20724500	-2.36258000
H	-6.19413300	-0.86031900	-2.36262000
H	-6.73904200	-2.63569400	-0.71734200
H	-5.25201600	-4.56173800	0.94487100
H	-3.44699100	-3.70402600	2.95299200
H	-5.57597800	-3.26442200	2.08979900
H	-2.43352500	-1.76882400	2.05506900
N	-1.36520400	-2.94846900	0.73450300
O	-2.87754100	-4.99716700	1.55113900
C	-0.19925600	-2.29077700	0.55961600
C	-1.25007400	-4.15984700	0.11292200
N	0.56207900	-3.13405700	-0.15288200
N	-0.07846700	-4.30819500	-0.42909500
C	-2.40049000	-5.10449300	0.22441400
H	-3.17634200	-4.85703300	-0.51362200
H	-2.06700100	-6.12911600	0.06169400
C	1.86825100	-2.88843600	-0.69927600

C	1.96471600	-2.05165500	-1.81383600
C	2.96901700	-3.43814700	-0.04205800
C	3.24914200	-1.75325000	-2.26387500
C	4.23107300	-3.11171100	-0.53561600
C	4.38685300	-2.26565600	-1.63565600
H	3.35996500	-1.07785100	-3.10789200
H	5.11038000	-3.51436200	-0.03959600
C	2.78626800	-4.29984300	1.17814900
H	2.18014100	-5.18176800	0.95234700
H	2.27363500	-3.74324700	1.97018700
C	0.74157700	-1.44408400	-2.44335300
H	0.40132300	-0.59185300	-1.84235800
H	-0.07196600	-2.17139400	-2.52665400
H	0.97589000	-1.06595300	-3.43973600
H	3.75162100	-4.63062500	1.56331400
C	5.75833600	-1.89819300	-2.14055500
H	6.53929600	-2.26693300	-1.47259300
H	5.93344600	-2.32042500	-3.13468800
H	5.86126400	-0.81224600	-2.22588900
C	0.05335000	-0.89157600	1.01457600
O	-1.01877300	-0.23606500	1.33946300
H	-0.66592400	1.03115600	0.38315200
C	1.32023400	-0.40041600	0.97323500
C	1.59727700	1.02280200	1.38524500
H	2.15365400	-1.02195100	0.68574300
H	0.93466100	1.26210800	2.22901400
C	3.03903700	1.19312700	1.83177500
C	3.34255400	1.86436800	3.01728000
C	4.09399100	0.67875900	1.06637400
C	4.66405100	2.02700600	3.43017100
H	2.53307100	2.26228800	3.62432700
C	5.41394300	0.84247100	1.47359800
H	3.88045300	0.14950900	0.13850500
C	5.70413600	1.51738500	2.65866700
H	4.87818400	2.54939900	4.35723000
H	6.21728700	0.43642200	0.86572200
H	6.73356000	1.64103400	2.97936200
C	1.17587400	3.49281800	0.92395700
C	1.20374400	2.10056700	0.29091300
H	0.39521800	3.51468700	1.68996500
H	2.13678600	3.73309000	1.38130100
N	-0.10308500	1.69072400	-0.21665200
S	-0.89188800	2.48722300	-1.38599000
O	-1.70283800	1.50859900	-2.11162200

O	0.08259800	3.31005200	-2.10376300
C	-2.04775200	3.58486200	-0.59087800
C	-3.15811800	3.03379800	0.04916700
C	-4.04579700	3.87918700	0.69886500
C	-3.84335900	5.26598500	0.71448700
C	-2.72953600	5.78888700	0.05590400
C	-1.82471000	4.95520800	-0.59813500
H	-3.32563700	1.95946600	0.02730600
H	-4.91543400	3.46145900	1.19853100
H	-2.56754000	6.86277700	0.05025400
H	-0.96159300	5.35775900	-1.11836000
C	-4.81081800	6.16369400	1.44000600
H	-4.62498000	7.21463700	1.21074800
H	-5.84312300	5.92732900	1.16876800
H	-4.71966800	6.03228800	2.52277000
C	2.21924400	1.99743900	-0.85537000
O	2.23813600	1.10921800	-1.67325000
O	3.14449800	2.96035100	-0.79633600
C	4.20062000	2.84068800	-1.75080700
H	4.72884900	1.89454800	-1.60534000
H	3.79956500	2.87764900	-2.76521200
H	4.86614900	3.68162000	-1.56714400
H	0.95588000	4.25189300	0.16971200

TS4RR

C	1.12037000	0.17178200	1.01512800
O	1.04281100	-0.17678300	2.19301000
H	-0.79776600	0.55851500	0.06872600
C	0.27739500	-0.18345300	-0.07826000
C	-0.55088900	-1.44937500	0.08772800
H	0.67131400	0.03476300	-1.06838900
H	-0.62434100	-1.63319400	1.16610400
C	-0.01528600	-2.70262400	-0.57027800
C	-0.13464500	-3.92823400	0.09390000
C	0.57051400	-2.69058500	-1.84137300
C	0.30328700	-5.11257400	-0.49567100
H	-0.58086800	-3.95166700	1.08535300
C	1.01595500	-3.87109000	-2.43069100
H	0.67071200	-1.75192900	-2.37927800
C	0.88202100	-5.08699000	-1.76219900
H	0.19715200	-6.05238600	0.03714700
H	1.46919800	-3.84005600	-3.41681400
H	1.22877600	-6.00606900	-2.22373700
C	-3.02214900	-2.10167500	0.20303400

C	-2.02746400	-1.08189700	-0.34243500
H	-3.01093400	-2.05751700	1.29560500
H	-2.75946900	-3.11002500	-0.12386200
N	-2.15658900	0.25460100	0.22300400
S	-3.49522700	1.08305600	-0.05024700
O	-3.24322100	2.49027200	0.29289900
O	-4.09614800	0.80347400	-1.36808000
C	-4.69035200	0.50264700	1.15186300
C	-4.30586400	0.37038600	2.48519700
C	-5.23835200	-0.05138700	3.42289900
C	-6.55699600	-0.34277200	3.04874300
C	-6.91625800	-0.20529300	1.70733200
C	-5.99036900	0.21739000	0.75498200
H	-3.27839400	0.57646700	2.77056400
H	-4.94265600	-0.16394400	4.46263200
H	-7.93268300	-0.43688500	1.40105700
H	-6.26113900	0.31263200	-0.29115700
C	-7.56104900	-0.78107200	4.08285000
H	-8.44936600	-1.21153400	3.61621500
H	-7.88128900	0.06883000	4.69404800
H	-7.13091800	-1.52476600	4.75878900
C	-2.02824700	-1.01847100	-1.87944700
O	-1.41721900	-0.19391000	-2.52060000
O	-2.69695700	-2.02986500	-2.44380200
C	-2.63831400	-2.07041200	-3.87078500
H	-1.60484500	-2.20343200	-4.19994200
H	-3.03352200	-1.14394000	-4.29112600
H	-3.24640700	-2.92110700	-4.17151000
H	-4.03501100	-1.88517300	-0.14553200
C	5.37342200	-1.34341200	0.82569200
C	4.09757800	-1.23174300	1.38889000
C	3.12991300	-2.20981500	1.16779000
C	3.44626200	-3.28517200	0.33914000
C	4.71281700	-3.38807900	-0.23730400
C	5.68939900	-2.42488100	0.01118100
C	6.25335000	-0.18760800	1.22563200
C	5.49602600	0.39994800	2.43477400
C	4.00411100	0.04184300	2.20404800
H	2.15184300	-2.14328000	1.63134000
H	2.69583200	-4.04533800	0.14491300
H	4.94340800	-4.23381900	-0.87746700
H	6.68038600	-2.51754500	-0.42263700
H	6.32964600	0.53130100	0.40182800
H	5.80860700	-0.12282400	3.34088700

H	7.27007400	-0.48427800	1.49100900
H	3.41932600	-0.03316100	3.11943300
N	3.41687400	1.15022000	1.39761600
O	5.70316600	1.77120400	2.70292200
C	2.23805300	1.16979000	0.75170300
C	4.07992500	2.29123300	1.04044100
N	2.24117800	2.27595100	0.01643500
N	3.38098800	2.99607000	0.19281000
C	5.41827300	2.63023700	1.62301900
H	6.18827000	2.59036300	0.84367500
H	5.38693700	3.64699100	2.01857900
C	1.24779600	2.68563500	-0.94414000
C	1.56961900	2.51819700	-2.29375400
C	0.01697200	3.16143800	-0.48994200
C	0.58187800	2.83756300	-3.22194000
C	-0.93435900	3.46451600	-1.46212100
C	-0.67636000	3.28966200	-2.82210700
H	0.79326300	2.70226200	-4.27941700
H	-1.91359300	3.79866800	-1.13563100
C	-0.29066200	3.30053300	0.97752100
H	0.58629200	3.62428500	1.54516100
H	-0.64591800	2.34939200	1.39234100
C	2.91160200	1.98557000	-2.72384100
H	3.15678800	1.05313300	-2.20253400
H	3.71071900	2.70057900	-2.50838100
H	2.91108400	1.78244000	-3.79542200
H	-1.09483200	4.02178000	1.12303300
C	-1.76923900	3.53707400	-3.82688100
H	-1.38631700	3.52110100	-4.84916800
H	-2.53280600	2.75837300	-3.73291200
H	-2.25763300	4.49908300	-3.65128600

TS4RS

C	-5.54051600	-0.35187600	1.24406700
C	-4.17205800	-0.09711700	1.25448100
C	-3.58189300	0.67208500	2.25369000
C	-4.39755100	1.19914600	3.25072800
C	-5.77330000	0.95154700	3.24462200
C	-6.35297100	0.17258100	2.24660100
C	-5.93336600	-1.22403700	0.08084900
C	-4.65831100	-1.35525700	-0.78671000
C	-3.48706800	-0.75275100	0.07840200
H	-2.50965200	0.84524200	2.25998500
H	-3.96194600	1.80232400	4.04026400

H	-6.39636700	1.37001300	4.02845100
H	-7.42155100	-0.01951300	2.24714200
H	-6.75116800	-0.80566900	-0.51490100
H	-4.43718700	-2.39928400	-1.01009200
H	-6.26062800	-2.21053100	0.42292300
H	-2.76986800	-1.51255700	0.38053700
N	-2.72985500	0.24701200	-0.70007700
O	-4.79662800	-0.74971800	-2.06157900
C	-1.46328800	0.69332500	-0.58838600
C	-3.34629700	1.01507500	-1.64514800
N	-1.37064200	1.69899800	-1.46395200
N	-2.53453900	1.90925700	-2.13364600
C	-4.74471100	0.66224900	-2.02913800
H	-5.46274900	1.08571500	-1.31357800
H	-4.96844400	1.03957400	-3.02650900
C	-0.23372300	2.54487700	-1.72547100
C	0.65661800	2.17832300	-2.73209700
C	-0.04950200	3.64753100	-0.88399800
C	1.80255000	2.96418600	-2.87240400
C	1.10781600	4.39670500	-1.06741200
C	2.04678500	4.06338900	-2.05122600
H	2.52742400	2.69397700	-3.63593700
H	1.28947500	5.25260400	-0.42217800
C	-1.02343100	3.94731300	0.22455500
H	-0.95041700	3.19153500	1.01660800
H	-2.05601600	3.95171100	-0.13572400
C	0.45517200	0.95963300	-3.58981400
H	-0.58859200	0.63997400	-3.61706000
H	1.07249300	0.12973600	-3.22487200
H	0.77214100	1.16821500	-4.61413800
H	-0.80845000	4.91908000	0.67057500
C	3.28925900	4.89524200	-2.22818300
H	4.08113100	4.32232100	-2.71443700
H	3.07737900	5.77068900	-2.85040700
H	3.66014300	5.25628800	-1.26623000
C	-0.41965900	0.09794100	0.35796400
O	-0.84959600	-0.77517200	1.10964400
H	1.51957000	-0.01771400	-0.84450300
C	0.92990600	0.54000600	0.21484800
C	1.95478000	-0.06828700	1.14815900
H	1.06149600	1.58824800	-0.03615500
H	1.58920800	-1.06258500	1.42491200
C	2.22794900	0.69512100	2.42948800
C	2.60709000	-0.00324000	3.58133000

C	2.12844600	2.08955200	2.50495400
C	2.87989000	0.66811100	4.77076300
H	2.68794300	-1.08499300	3.53339000
C	2.40330200	2.76369500	3.69189400
H	1.83362300	2.66253700	1.62898800
C	2.77993100	2.05561100	4.83122600
H	3.16631800	0.10385900	5.65302600
H	2.31944900	3.84568900	3.72718100
H	2.98945900	2.58090900	5.75759300
C	4.08207100	0.96383100	0.12712200
C	3.23436600	-0.30619700	0.24998000
H	3.45471200	1.78411700	-0.23882800
H	4.50838300	1.25333200	1.09092500
N	2.73997400	-0.59322600	-1.11435600
S	2.52992800	-2.07838400	-1.70453000
O	3.57330300	-3.01526800	-1.26268300
O	2.32612800	-1.92342900	-3.15036500
C	0.97981000	-2.72685700	-1.08628800
C	-0.18257800	-2.53218800	-1.82755500
C	-1.38644300	-3.04569000	-1.35216900
C	-1.44173500	-3.74498600	-0.14186200
C	-0.26173000	-3.91158200	0.58971700
C	0.94888200	-3.40972800	0.12727600
H	-0.12901600	-2.02370000	-2.78509800
H	-2.28844400	-2.92355100	-1.94902600
H	-0.29131300	-4.45796500	1.52826100
H	1.86773600	-3.54986900	0.68967100
C	-2.74242900	-4.30767400	0.37290700
H	-3.23108300	-3.61245400	1.06726100
H	-3.43848400	-4.51444100	-0.44405800
H	-2.57608000	-5.23789200	0.92093700
C	4.07231300	-1.44832900	0.83670200
O	3.66508200	-2.26772500	1.63112300
O	5.32101100	-1.43713600	0.37447200
C	6.09535100	-2.59206000	0.70438700
H	6.18737100	-2.69595500	1.78694600
H	5.60908300	-3.47627500	0.28727500
H	7.07166900	-2.43681000	0.24977700
H	4.88507100	0.79619000	-0.59020300
TS4SR			
C	1.23913500	5.03714400	-0.79219500
C	1.08341400	3.65421900	-0.74106100
C	0.05087600	3.06168600	-0.01780000

C	-0.84251100	3.89026500	0.65722100
C	-0.69967600	5.27933800	0.59920400
C	0.33939200	5.86241800	-0.12285500
C	2.43162700	5.42937600	-1.62640000
C	3.17405200	4.10716800	-1.93241100
C	2.16301700	2.96505900	-1.54468000
H	-0.07565100	1.98103400	0.04628800
H	-1.63641000	3.43424100	1.23929100
H	-1.40211700	5.91194500	1.13262300
H	0.45269800	6.94187800	-0.15527300
H	3.10482600	6.12601400	-1.11672600
H	3.43089800	4.02326000	-2.98799100
H	2.11866500	5.90962800	-2.55869200
H	1.77582800	2.45560300	-2.42447000
N	2.83453400	1.94372800	-0.72060300
O	4.42411200	4.01093600	-1.26451600
C	2.53755900	0.65140400	-0.50321900
C	3.80590300	2.28996500	0.17379700
N	3.34049300	0.26653200	0.49007500
N	4.14890900	1.27519800	0.91608100
C	4.33642300	3.68438200	0.10688500
H	3.67734500	4.37041700	0.65690900
H	5.33707900	3.73081000	0.53563800
C	3.40498900	-1.02708900	1.11984700
C	2.70054100	-1.19811100	2.31550400
C	4.09162500	-2.04998800	0.46618500
C	2.70519100	-2.47631700	2.86798900
C	4.06551000	-3.30960600	1.06453200
C	3.37826200	-3.53968100	2.25801300
H	2.15733200	-2.65012200	3.79035900
H	4.58553600	-4.13112300	0.57861600
C	4.77490800	-1.81909900	-0.85515500
H	5.34189300	-0.88438700	-0.85886900
H	4.04029100	-1.77000300	-1.66752300
C	1.91134900	-0.07123800	2.92561400
H	1.04977900	0.19806400	2.30027300
H	2.52496200	0.82560300	3.04822200
H	1.52571200	-0.36394600	3.90291100
H	5.45902900	-2.63891000	-1.07776300
C	3.37321500	-4.90598700	2.89047600
H	4.16502900	-4.98212900	3.64245000
H	2.42238800	-5.10225100	3.39076800
H	3.54333300	-5.68628100	2.14593500
C	1.43863500	-0.10356900	-1.24877100

O	1.12693400	0.37426000	-2.33394300
H	-0.01099500	-0.44988300	0.25506000
C	0.76636400	-1.13142400	-0.51359600
C	-0.40237500	-1.82552000	-1.18257400
H	1.37346500	-1.71500400	0.17041500
H	-0.74320000	-1.17345400	-1.99227500
C	-0.13467000	-3.19927100	-1.76140200
C	-0.96009000	-3.67538400	-2.78686700
C	0.88875500	-4.02974300	-1.29464500
C	-0.77325600	-4.94553800	-3.32564800
H	-1.75275500	-3.03435500	-3.16206700
C	1.07888400	-5.30058100	-1.83333000
H	1.55319100	-3.68823700	-0.50497300
C	0.24779400	-5.76474400	-2.84987400
H	-1.42310500	-5.29275300	-4.12305300
H	1.88134900	-5.92808200	-1.45694500
H	0.39766100	-6.75367200	-3.27128500
C	-1.46726000	-2.99072100	0.85456400
C	-1.57452800	-1.81371500	-0.11639600
H	-0.46806900	-2.98853700	1.30592400
H	-2.20541400	-2.89974900	1.64868200
N	-1.38594700	-0.50619700	0.51342800
S	-2.20296800	0.07316400	1.74883200
O	-1.42948300	1.23112400	2.23470500
O	-2.60730800	-0.90381600	2.77348700
C	-3.72519000	0.71919000	1.06481300
C	-3.69394200	1.39889100	-0.15170300
C	-4.87052600	1.93929900	-0.65829900
C	-6.08157100	1.80642800	0.03172800
C	-6.08625400	1.11794600	1.24763500
C	-4.91558400	0.57231200	1.76823200
H	-2.75710600	1.48257200	-0.69534400
H	-4.85248200	2.46958200	-1.60655700
H	-7.01951800	1.00508500	1.79261300
H	-4.91615600	0.02653200	2.70570700
C	-7.35464000	2.36670300	-0.54766200
H	-7.76502400	1.68853700	-1.30292100
H	-8.11468300	2.50474200	0.22411400
H	-7.17595700	3.32871800	-1.03418900
C	-2.92280900	-1.76788600	-0.84237700
O	-3.10487000	-1.34082100	-1.96129100
O	-3.92115900	-2.16283300	-0.04597900
C	-5.23738900	-1.94654600	-0.56363600
H	-5.37247500	-0.88889000	-0.80433300

H	-5.39404800	-2.54849300	-1.46106400
H	-5.92105200	-2.24914400	0.22715300
H	-1.60719700	-3.93971200	0.33038900
TS4SS			
C	3.08834500	4.36305100	0.21913200
C	2.20905200	3.28623200	0.30154300
C	2.43680200	2.10507500	-0.40100600
C	3.57626200	2.01799800	-1.19838900
C	4.46647600	3.09273600	-1.27786700
C	4.23112500	4.26971100	-0.57135000
C	2.62697100	5.52027400	1.06725000
C	1.19956200	5.14802200	1.52765100
C	1.05170800	3.61133400	1.22050600
H	1.75590900	1.25598900	-0.35291000
H	3.75106800	1.10392300	-1.75639200
H	5.34959500	3.01131400	-1.90359200
H	4.92216900	5.10435000	-0.64144000
H	2.60810800	6.47204800	0.52730000
H	1.05770600	5.32469800	2.59343000
H	3.28002300	5.65484000	1.93516900
H	1.04930300	3.01504000	2.13346500
N	-0.23030000	3.35654800	0.54883900
O	0.19997700	5.94675600	0.90873700
C	-0.98609300	2.25111300	0.50780500
C	-0.76157000	4.24311700	-0.34393500
N	-1.94227400	2.50338000	-0.38543000
N	-1.82460900	3.75375300	-0.91718900
C	-0.11580100	5.58797500	-0.42268000
H	0.77381100	5.55155800	-1.06597500
H	-0.81490800	6.32383000	-0.81829600
C	-3.04809900	1.65446400	-0.75969600
C	-2.94849900	0.93008400	-1.95239800
C	-4.13434400	1.57470800	0.11094000
C	-4.01810500	0.09697600	-2.26993400
C	-5.18138200	0.72987700	-0.25970300
C	-5.13933500	-0.01124700	-1.44046800
H	-3.96760300	-0.49418500	-3.18078200
H	-6.04210200	0.64343600	0.39809500
C	-4.15609500	2.34098000	1.40674800
H	-3.90033100	3.39332900	1.25299600
H	-3.43743200	1.92371500	2.12111100
C	-1.70675800	0.98705000	-2.80113200
H	-1.36623800	2.01486100	-2.94976600

H	-1.89420300	0.53697200	-3.77672500
H	-0.89765300	0.41695900	-2.32686100
H	-5.14523900	2.28941600	1.86306300
C	-6.26905500	-0.93244400	-1.82064500
H	-7.02757100	-0.97673500	-1.03661000
H	-6.75060900	-0.59569400	-2.74341800
H	-5.89636700	-1.94570700	-1.99922100
C	-0.72753700	0.99752000	1.33735900
O	-0.30306200	1.18612100	2.47238800
H	0.25152700	-0.41360800	0.02371200
C	-0.87165900	-0.21634200	0.60337600
C	-0.80212000	-1.54964000	1.32196400
H	-1.56621000	-0.17071600	-0.22653300
H	-0.18828800	-1.41273900	2.22047100
C	-2.13597900	-2.13864300	1.72851500
C	-2.24951900	-2.83634000	2.93416600
C	-3.27394700	-2.00924700	0.92365400
C	-3.46248200	-3.39808200	3.32622900
H	-1.37625200	-2.93196600	3.57491200
C	-4.48782800	-2.56791000	1.31356100
H	-3.21634100	-1.46868200	-0.01802300
C	-4.58704000	-3.26581800	2.51604900
H	-3.52928100	-3.93293000	4.26848300
H	-5.36066700	-2.44864000	0.67687200
H	-5.53482500	-3.69699200	2.82241400
C	0.60863600	-3.69236600	1.12823900
C	0.06205100	-2.48540000	0.37435100
H	1.29582400	-3.33631800	1.90042000
H	-0.19370100	-4.26900700	1.59387500
N	1.09038800	-1.56638900	-0.08083700
S	2.04308100	-1.97196800	-1.29355200
O	2.32337600	-0.76029700	-2.08387600
O	1.57700800	-3.16875500	-2.01765000
C	3.60099800	-2.43003200	-0.54314000
C	4.29021600	-1.47663800	0.20655800
C	5.49006200	-1.82380700	0.80938700
C	6.01474800	-3.11766200	0.68014200
C	5.30781000	-4.05194200	-0.07674100
C	4.10105400	-3.71641600	-0.69057600
H	3.88345400	-0.47445300	0.31209100
H	6.03354500	-1.08444300	1.39175600
H	5.70605100	-5.05631200	-0.19111600
H	3.54787000	-4.43813800	-1.28207900
C	7.30561600	-3.48520200	1.36460300

H	7.70366600	-4.42666800	0.98053800
H	8.06098900	-2.70775700	1.22327900
H	7.15307600	-3.60007300	2.44261800
C	-0.87734900	-2.87605200	-0.78067700
O	-1.25237200	-2.10863600	-1.64096600
O	-1.33366600	-4.12687100	-0.67762400
C	-2.32156000	-4.48926700	-1.64469100
H	-3.19296500	-3.83578300	-1.55063700
H	-1.91261300	-4.40122300	-2.65259100
H	-2.59035400	-5.52064700	-1.42580100
H	1.15421400	-4.34975300	0.44556700

TS4RR^{DH}

C	-1.35469000	0.51021100	0.96550200
O	-1.43618900	0.12563900	2.12854900
H	1.77341100	-0.36696500	-0.80501200
C	-0.22033600	0.90595300	0.20112400
C	1.00406600	1.41077800	0.95305400
H	-0.49550200	1.49127100	-0.67916800
H	1.26618100	0.67194500	1.72112700
C	0.74740700	2.72825200	1.66868000
C	1.22967300	2.90300000	2.96928000
C	0.04727300	3.77954600	1.06894600
C	1.04059300	4.10193200	3.65023600
H	1.75953800	2.08642600	3.45319100
C	-0.13594400	4.98334500	1.74516300
H	-0.36946500	3.66732500	0.06903900
C	0.36189200	5.15072800	3.03492000
H	1.42134500	4.21476200	4.66018700
H	-0.67533300	5.79212100	1.26151700
H	0.21377800	6.08928500	3.55900700
C	3.46536100	2.10307000	0.72665700
C	2.27940700	1.44965100	0.02467200
H	3.69594000	1.55327100	1.64351000
H	3.22251000	3.13380500	0.98118300
N	2.55152200	0.03662100	-0.28026100
S	3.90584300	-0.40645100	-1.14810300
O	3.53300700	-1.70766900	-1.71230400
O	4.36275500	0.64808000	-2.05040400
C	5.14132500	-0.62227300	0.10294100
C	4.81198300	-1.21361800	1.32053100
C	5.81640800	-1.41977900	2.25710600
C	7.14043200	-1.05179400	1.98912100
C	7.43777100	-0.45781100	0.75931000

C	6.44584300	-0.23841500	-0.19054800
H	3.78126400	-1.47197000	1.54073500
H	5.57012100	-1.86648200	3.21581100
H	8.45850000	-0.15574500	0.54463300
H	6.67047700	0.23782300	-1.13884500
C	8.22513500	-1.30457700	3.00166100
H	9.02938100	-0.57201600	2.90869800
H	8.66095600	-2.29758600	2.85198800
H	7.83212500	-1.26541300	4.01970100
C	1.89537100	2.15916500	-1.28074300
O	1.38008000	1.58393600	-2.21725800
O	2.09251600	3.46951900	-1.23163500
C	1.59096000	4.21337400	-2.35041500
H	0.50525400	4.09655700	-2.41238300
H	2.04925100	3.85886300	-3.27422900
H	1.85305900	5.25082100	-2.15706300
H	4.34758200	2.10738800	0.08281100
C	-4.42761100	-3.79589500	1.28470500
C	-3.84763700	-2.55202600	1.51520900
C	-4.17213500	-1.78123600	2.62714000
C	-5.11731200	-2.28309300	3.51769200
C	-5.71082800	-3.52892000	3.29300600
C	-5.36940400	-4.29556400	2.18086200
C	-3.88520800	-4.43173800	0.02915700
C	-3.07144600	-3.31972500	-0.67128500
C	-2.86391900	-2.20815800	0.42380700
H	-3.68844000	-0.82163500	2.79126800
H	-5.39430100	-1.70530400	4.39291500
H	-6.44743800	-3.90444900	3.99576000
H	-5.83342600	-5.26267100	2.01397100
H	-4.66419900	-4.80257900	-0.64374600
H	-2.10191700	-3.67724000	-1.02656400
H	-3.23647600	-5.28041300	0.27002900
H	-1.83187600	-2.18053900	0.77953600
N	-3.14421700	-0.89219400	-0.15315600
O	-3.71022500	-2.83662400	-1.84625600
C	-2.57472300	0.29389400	0.07635800
C	-4.13204000	-0.69463300	-1.07889600
N	-3.22422400	1.16395900	-0.69003100
N	-4.20866800	0.56078200	-1.42036300
C	-4.77657500	-1.92660700	-1.62694800
H	-5.52417300	-2.32505500	-0.92969500
H	-5.24824700	-1.71952500	-2.58647900
C	-3.03830900	2.59296600	-0.71171600

C	-3.41309900	3.31027000	0.42813600
C	-2.50148500	3.18983200	-1.85888900
C	-3.23757800	4.69358500	0.39370000
C	-2.35222500	4.57491100	-1.83661200
C	-2.71371000	5.34072400	-0.72423900
H	-3.51652000	5.27620000	1.26742200
H	-1.94665200	5.06980600	-2.71626000
C	-2.04028800	2.39373300	-3.05168000
H	-2.64536800	1.49975900	-3.21395300
H	-0.99354600	2.08718600	-2.92294300
C	-3.96547500	2.63081800	1.65466500
H	-3.16673800	2.15565000	2.23547900
H	-4.69615000	1.85841600	1.39597500
H	-4.45552000	3.36125100	2.29934600
H	-2.08910200	3.00717900	-3.95336900
C	-2.53903200	6.83627500	-0.74706400
H	-1.51895300	7.10316800	-1.03807800
H	-3.21636000	7.29193300	-1.47530900
H	-2.74633400	7.27540100	0.23077600
C	1.15069900	-5.26274900	0.82270300
C	1.13289800	-5.57591000	-0.67068100
C	1.81382100	-4.52535700	-1.54718100
C	0.43606700	-3.96668300	1.19339400
C	1.05091900	-2.71412000	0.54308400
C	0.62301700	-2.48023900	-0.88417000
H	2.19375200	-5.19809000	1.15895400
H	0.10300400	-5.71264500	-1.02394600
H	2.03648300	-4.96997000	-2.51813600
H	0.47256200	-3.83208600	2.27785100
H	2.14589500	-2.77926800	0.57147000
C	0.83918400	-3.00787000	-3.26629800
H	0.07501300	-3.66285800	-3.69978600
C	-0.58553900	-1.15385500	-2.46873900
C	0.49256300	-1.54313100	-3.46775400
H	0.16012200	-1.38528700	-4.49577000
H	1.37600200	-0.92025000	-3.29139900
H	-1.51377800	-1.71477900	-2.65424100
H	1.79479300	-3.23218900	-3.74721200
H	-0.81853000	-0.08631800	-2.53408400
N	-0.11922800	-1.41536600	-1.11266600
N	0.98949300	-3.34163100	-1.83736200
H	2.77021400	-4.20040100	-1.11826900
H	1.65148500	-6.52538700	-0.83693200
H	0.69490000	-6.09290900	1.37107500

H	-0.62670300	-4.04348800	0.92608000
H	0.76211300	-1.82191600	1.10716100
H	-0.10885000	-0.33061700	-0.37632700

TS4RS^{DH}

C	5.81702600	-1.83205400	-1.33493300
C	4.83202100	-0.85562700	-1.45581600
C	4.90324400	0.14407500	-2.42097400
C	6.00596900	0.15637200	-3.27172100
C	7.00295300	-0.81667200	-3.15435200
C	6.91495200	-1.81867000	-2.19078500
C	5.49162100	-2.81121700	-0.23595700
C	4.30489800	-2.18332700	0.52681800
C	3.74005000	-1.07236100	-0.43471100
H	4.11075200	0.88263000	-2.50899600
H	6.09223100	0.92480600	-4.03254000
H	7.85688200	-0.79065200	-3.82341100
H	7.69149600	-2.57236100	-2.10451500
H	6.32412300	-2.98872800	0.45133600
H	3.52085000	-2.91139600	0.75060500
H	5.20257700	-3.78223200	-0.65189200
H	2.79158500	-1.37653700	-0.88174100
N	3.47157300	0.14760900	0.33034000
O	4.68486600	-1.68257900	1.80263000
C	2.50332700	1.05991000	0.20974500
C	4.28089500	0.55300700	1.35553600
N	2.75566900	1.98441000	1.13113100
N	3.87077900	1.68278200	1.85944200
C	5.32780300	-0.41848600	1.79511100
H	6.19464000	-0.39782500	1.12244800
H	5.65159500	-0.19734400	2.81128500
C	2.06827900	3.24097800	1.29416900
C	1.30631100	3.45110900	2.44838500
C	2.21420200	4.19292500	0.28016600
C	0.67022300	4.68459000	2.56839500
C	1.55429600	5.40901400	0.45380700
C	0.78671000	5.67347100	1.58765600
H	0.07028100	4.87972500	3.45364200
H	1.64795600	6.16831100	-0.31794200
C	3.03782800	3.92772000	-0.95339700
H	2.49841000	3.28793000	-1.66034100
H	3.98470500	3.43600400	-0.70984500
C	1.12778800	2.38694200	3.49970700
H	2.04585300	1.82285000	3.67636800

H	0.34465800	1.67862900	3.20240500
H	0.81404300	2.83769300	4.44234700
H	3.26327300	4.86568200	-1.46179300
C	0.10869300	7.00596000	1.76993100
H	0.04372300	7.55076800	0.82578400
H	-0.89990900	6.88115500	2.17219400
H	0.66936800	7.62573300	2.47658200
C	1.33358000	0.95783400	-0.75850000
O	1.61308800	0.77904700	-1.93958700
H	-2.19756100	-1.44883800	-1.27048500
C	0.07781800	0.82809900	-0.08794600
C	-1.16879700	0.95623000	-0.93904800
H	0.05191200	1.35777600	0.86622600
H	-1.01353100	0.37626500	-1.85843400
C	-1.45283700	2.39055700	-1.37711900
C	-1.97498600	2.62289400	-2.65541200
C	-1.23057300	3.48784800	-0.53958100
C	-2.29601400	3.91033500	-3.07587100
H	-2.13724000	1.78213600	-3.32416800
C	-1.55596300	4.77678200	-0.95785100
H	-0.79077300	3.35255400	0.44624100
C	-2.09519500	4.99285400	-2.22270000
H	-2.69801400	4.06627300	-4.07199000
H	-1.38071400	5.61454700	-0.28961000
H	-2.34612700	5.99807500	-2.54531900
C	-2.56461500	0.80536000	1.20614800
C	-2.41194000	0.31015200	-0.22677100
H	-1.77006400	0.38671200	1.82746500
H	-2.51002100	1.89567600	1.21770500
N	-2.18974600	-1.14826500	-0.29381900
S	-3.12584100	-2.24327800	0.55925900
O	-2.84252200	-2.07510900	1.97824900
O	-2.84490900	-3.51682000	-0.09908300
C	-4.83637200	-1.84510800	0.30075800
C	-5.42584500	-2.15842500	-0.92366200
C	-6.75108900	-1.80774700	-1.13671600
C	-7.49212900	-1.14537600	-0.14858200
C	-6.87922400	-0.85888500	1.07405600
C	-5.55296000	-1.20661300	1.30860300
H	-4.85657500	-2.66957000	-1.69310000
H	-7.22216800	-2.04937200	-2.08490800
H	-7.44739400	-0.36476900	1.85615500
H	-5.08266500	-1.00960000	2.26608300
C	-8.91484900	-0.73360300	-0.41482000

H	-9.45823400	-0.56008200	0.51575800
H	-8.93790100	0.19483200	-0.99505900
H	-9.44336300	-1.49522200	-0.99250500
C	-3.62185800	0.63342400	-1.11842600
O	-3.78376300	0.09265000	-2.19075900
O	-4.41733600	1.56779200	-0.62079700
C	-5.50333900	1.95904400	-1.47386500
H	-5.10576000	2.42400000	-2.37869000
H	-6.09892600	1.08390200	-1.73957300
H	-6.08986700	2.67127300	-0.89835800
H	-3.52405100	0.51594600	1.63424500
C	1.13371300	-5.32396600	-1.48103900
C	1.02085600	-5.78496000	-0.02862800
C	-0.12871500	-5.12952100	0.73958700
C	1.38834000	-3.82722500	-1.65141600
C	0.28786800	-2.93551500	-1.04542000
C	0.44120800	-2.75564000	0.44467800
H	0.20268300	-5.58102900	-2.00306200
H	1.95871300	-5.59566300	0.51016700
H	-0.37540200	-5.73344200	1.61449800
H	1.46075300	-3.59734100	-2.71839000
H	-0.69868400	-3.35460900	-1.27219300
C	0.25154000	-3.65554300	2.71758000
H	1.15605200	-4.15906500	3.08207000
C	1.19404100	-1.41296800	2.27049400
C	0.22491400	-2.19625400	3.14287400
H	0.49037400	-2.12135900	4.19995300
H	-0.78410600	-1.80009900	3.00316200
H	2.23117000	-1.72366600	2.46318300
H	-0.61523300	-4.18062100	3.12873100
H	1.14030000	-0.33857600	2.48907500
N	0.88588900	-1.59108800	0.85766400
N	0.19110300	-3.79200200	1.25545800
H	-1.03504600	-5.07077800	0.12714900
H	0.85995100	-6.86764500	-0.01571000
H	1.93500200	-5.88083000	-1.97709100
H	2.36137900	-3.56724100	-1.21174400
H	0.34034100	-1.93400200	-1.48416800
H	0.37889600	-0.44323900	0.30072200
TS4SR ^{DH}			
C	-5.45336300	2.49453800	1.33940500
C	-4.39395000	1.82501200	0.72990500
C	-3.80577800	2.30139500	-0.43545100

C	-4.26852500	3.50530500	-0.96651100
C	-5.31061400	4.19751000	-0.34453000
C	-5.91590300	3.69291100	0.80588000
C	-5.94492700	1.73641300	2.54759700
C	-5.31671100	0.33668600	2.40151100
C	-4.04332100	0.58452300	1.52618100
H	-3.00905300	1.74564600	-0.92405200
H	-3.82012800	3.90297000	-1.87226100
H	-5.66434800	5.13023700	-0.77148700
H	-6.74205000	4.22128100	1.27132200
H	-7.03350900	1.65869800	2.60332500
H	-5.04456600	-0.10052300	3.36280600
H	-5.59660100	2.20726000	3.47340200
H	-3.15951300	0.71796200	2.15366800
N	-3.79678100	-0.57601400	0.67130700
O	-6.21789500	-0.60059900	1.81875100
C	-2.67467100	-1.22421800	0.31872200
C	-4.84046100	-1.18543500	0.03501900
N	-3.07499400	-2.19029800	-0.50781900
N	-4.42684400	-2.18537000	-0.69000200
C	-6.21206800	-0.71946100	0.40614700
H	-6.45492300	0.22446000	-0.09651100
H	-6.95011200	-1.47383300	0.13525200
C	-2.29723000	-3.25821800	-1.08306500
C	-1.99787800	-3.19261900	-2.44508200
C	-1.93952900	-4.32782600	-0.25870400
C	-1.27446800	-4.25464700	-2.98541300
C	-1.25154100	-5.38030900	-0.85933000
C	-0.90391000	-5.35737200	-2.21171600
H	-1.00791900	-4.22626200	-4.03864900
H	-0.97234900	-6.23546000	-0.24948800
C	-2.24605500	-4.32916900	1.21510300
H	-3.28344700	-4.04354800	1.41376100
H	-1.59071500	-3.63055900	1.74996800
C	-2.46065400	-2.03838400	-3.29262100
H	-2.39805800	-1.08808100	-2.75375000
H	-3.50661500	-2.17446000	-3.58501000
H	-1.85983900	-1.96326000	-4.20031400
H	-2.07630300	-5.32149900	1.63490800
C	-0.16371900	-6.51546800	-2.82697400
H	0.53752200	-6.95661000	-2.11479600
H	-0.86552700	-7.29915200	-3.12932800
H	0.39089100	-6.20414700	-3.71427300
C	-1.29762500	-0.95782200	0.91596100

O	-1.32859700	-0.66671900	2.11683100
H	2.10421900	1.31815700	0.61896800
C	-0.17634500	-0.93552700	0.04332100
C	1.15757900	-1.04322400	0.77313400
H	-0.29052600	-1.53398000	-0.86250300
H	1.12306200	-0.33818600	1.61472500
C	1.38845100	-2.41690500	1.39117100
C	1.85420500	-2.51407600	2.70620000
C	1.16909900	-3.59451300	0.67109700
C	2.11019300	-3.75545800	3.28392000
H	2.02267500	-1.60523500	3.27777200
C	1.43226300	-4.83660800	1.24328800
H	0.77859600	-3.54830100	-0.34230400
C	1.90555000	-4.92157700	2.55066300
H	2.46541800	-3.80994800	4.30809800
H	1.26711100	-5.73993300	0.66366200
H	2.10610600	-5.89027700	2.99682900
C	2.48866200	-1.34553800	-1.41083500
C	2.39082700	-0.59631700	-0.08823100
H	1.63991400	-1.08230300	-2.04628200
H	3.40358000	-1.09988800	-1.94889200
N	2.20297300	0.85021300	-0.28238200
S	3.16531000	1.81225400	-1.24198600
O	2.65453200	3.15970800	-0.99837500
O	3.15826600	1.26339600	-2.59195100
C	4.81712900	1.70436300	-0.61109200
C	5.17732900	2.50603300	0.46966700
C	6.43088600	2.33542200	1.04054300
C	7.32017800	1.36887900	0.55511900
C	6.93333500	0.58523500	-0.53676700
C	5.68283400	0.74343700	-1.12590700
H	4.48584400	3.25109100	0.85026700
H	6.72587100	2.95898700	1.87903900
H	7.62123200	-0.15507800	-0.93470200
H	5.39301200	0.14923700	-1.98620100
C	8.65809300	1.15961600	1.21253100
H	9.38938200	0.76617600	0.50376500
H	9.04294500	2.09151500	1.63178700
H	8.56845900	0.43943800	2.03266100
C	3.61039200	-0.81208400	0.82667500
O	3.81596200	-0.11519500	1.79502200
O	4.35860700	-1.85144000	0.47898400
C	5.43612300	-2.14976300	1.37724700
H	6.08080300	-1.27495100	1.48654500

H	5.03159000	-2.43441200	2.35108000
H	5.97632400	-2.97890200	0.92625200
H	2.48926500	-2.41848400	-1.22009500
C	0.28978100	4.85591000	1.73194100
C	0.24684300	5.53742000	0.36622500
C	-0.92350600	5.06835700	-0.49951800
C	0.43281700	3.33665600	1.65427200
C	-0.74425100	2.61998500	0.96174400
C	-0.64233200	2.62249000	-0.54469000
H	-0.62819400	5.10153900	2.28300900
H	1.17992900	5.35498300	-0.18020300
H	-1.12738300	5.80353500	-1.27996400
H	0.52139300	2.93054700	2.66614000
H	-1.69173600	3.08426600	1.26484400
C	-0.36452700	3.83987000	-2.62403900
H	0.72282900	3.92978600	-2.74122200
C	-0.30586000	1.36888900	-2.58371300
C	-0.87561400	2.57949200	-3.30708000
H	-0.57426300	2.57538300	-4.35676100
H	-1.97070800	2.56158200	-3.27089200
H	0.76866600	1.27478100	-2.78388900
H	-0.83403200	4.72808200	-3.05106000
H	-0.78036900	0.44396300	-2.92812500
N	-0.51089200	1.47180100	-1.14594700
N	-0.68939700	3.79848900	-1.19392500
H	-1.83886800	4.98613000	0.10003300
H	0.15480400	6.61924200	0.50767700
H	1.12355200	5.26129000	2.31400700
H	1.36417900	3.10662200	1.12358900
H	-0.78208300	1.57708700	1.28648400
H	-0.34925500	0.35144400	-0.49709500

TS4SS^{DH}

C	-6.39748200	0.24572500	0.51756800
C	-5.01768400	0.17541000	0.35018300
C	-4.31449000	1.15291500	-0.34365800
C	-5.01917300	2.24131500	-0.85342700
C	-6.40188700	2.33157200	-0.67097800
C	-7.10026400	1.33497000	0.00872700
C	-6.91387800	-0.95801600	1.26470400
C	-5.72835200	-1.95070200	1.30264900
C	-4.46201300	-1.07337700	0.99674600
H	-3.24091500	1.06130000	-0.49930300
H	-4.49232900	3.01858300	-1.39908500

H	-6.93996000	3.18192300	-1.07691300
H	-8.17702300	1.40238700	0.12880100
H	-7.77980600	-1.42656800	0.78805700
H	-5.62727600	-2.42604800	2.27785500
H	-7.20896000	-0.68811100	2.28366500
H	-3.89222700	-0.86612000	1.90084200
N	-3.56312800	-1.76833100	0.06315800
O	-5.89067200	-3.03441500	0.39927800
C	-2.23057700	-1.70512900	-0.12864500
C	-4.08818100	-2.49008800	-0.96942600
N	-2.01155000	-2.39616000	-1.24934000
N	-3.15487800	-2.89826500	-1.78264600
C	-5.55869300	-2.75556000	-0.94634000
H	-6.11304700	-1.89419900	-1.34273500
H	-5.79188000	-3.63654000	-1.54341400
C	-0.74831500	-2.58410400	-1.90789200
C	-0.42213900	-1.68661400	-2.92668300
C	0.10168600	-3.58547900	-1.44277900
C	0.86634300	-1.76613900	-3.44301800
C	1.37923900	-3.62510300	-1.99827000
C	1.78584100	-2.70455300	-2.96462600
H	1.17549300	-1.05667200	-4.20609900
H	2.08594800	-4.36725000	-1.63624300
C	-0.34645800	-4.55233300	-0.37855800
H	-1.25196900	-5.08238400	-0.68866900
H	-0.56965600	-4.04218600	0.56505600
C	-1.43038300	-0.67944900	-3.41281000
H	-1.83444000	-0.08807000	-2.58159800
H	-2.27594600	-1.17780100	-3.89624000
H	-0.97757100	0.00725000	-4.13019600
H	0.43369700	-5.28977500	-0.18142400
C	3.20438400	-2.66858000	-3.45858100
H	3.63347400	-1.69221900	-3.21221000
H	3.80980700	-3.44731700	-2.99074900
H	3.25119800	-2.79413900	-4.54418400
C	-1.25445300	-1.03886000	0.84503500
O	-1.71985800	-0.88643800	1.97552100
H	1.68693200	2.06393600	0.18258300
C	0.00446400	-0.52890600	0.38553100
C	0.97665700	-0.20277800	1.52301900
H	0.45252400	-0.99319700	-0.49155900
H	0.57223200	0.65174400	2.08615200
C	1.13332800	-1.34789800	2.51708500
C	1.05985400	-1.11753000	3.89073200

C	1.34950600	-2.65515100	2.06880400
C	1.21422700	-2.16281900	4.79937800
H	0.87115500	-0.10924400	4.25217000
C	1.50580600	-3.70234500	2.97219700
H	1.40195900	-2.85157800	0.99933400
C	1.44050100	-3.45852500	4.34304200
H	1.15037700	-1.96414700	5.86447700
H	1.67452100	-4.70975500	2.60280900
H	1.55825700	-4.27334600	5.04982100
C	3.10792500	0.99924500	2.16953000
C	2.38747000	0.29128300	1.01762900
H	2.55553400	1.90905400	2.42512100
H	3.15121100	0.35662200	3.04963400
N	2.15841800	1.21054100	-0.11152200
S	3.21652700	1.60904000	-1.34307600
O	2.96997000	3.03720300	-1.55334100
O	3.04444300	0.69653000	-2.46436900
C	4.87412400	1.40780600	-0.74308800
C	5.45735900	2.44982200	-0.02251100
C	6.75067600	2.29092700	0.45542600
C	7.46862200	1.11173900	0.21716700
C	6.86314400	0.09209700	-0.52203000
C	5.56894100	0.23274100	-1.01282600
H	4.90320700	3.36614000	0.15451300
H	7.21625000	3.09464100	1.01826400
H	7.41397400	-0.82214500	-0.72333100
H	5.09454200	-0.55427700	-1.59092800
C	8.87955300	0.96773000	0.72062200
H	9.57167800	1.51102800	0.06943000
H	8.98213700	1.38220100	1.72618500
H	9.18890100	-0.07878800	0.74028200
C	3.16291000	-0.93050000	0.51874000
O	2.94464400	-1.48546900	-0.53257700
O	4.06980600	-1.34403400	1.40093900
C	4.72928300	-2.56971900	1.06711000
H	3.99823100	-3.38066400	1.01851900
H	5.23525100	-2.47736900	0.10406900
H	5.44692400	-2.74608600	1.86480800
H	4.12812500	1.26815900	1.89243400
C	-1.69767000	4.80625300	2.64543900
C	-1.87664600	5.58789600	1.34355300
C	-2.74871900	4.88207100	0.30091800
C	-1.04247800	3.43436800	2.48472200
C	-1.81628600	2.49479400	1.54201000

C	-1.50032700	2.77067800	0.09375600
H	-2.68453600	4.66672700	3.10631300
H	-0.90297100	5.80871400	0.88881400
H	-3.11541100	5.61271900	-0.42251800
H	-0.97501800	2.95499200	3.46599400
H	-2.89452000	2.59006300	1.71479500
C	-1.81008100	4.16153300	-1.90355700
H	-1.03816000	4.93484500	-1.99933500
C	-0.27657400	2.23152100	-1.88565300
C	-1.40590000	2.90135700	-2.65496900
H	-1.09516900	3.16292200	-3.66878800
H	-2.26571000	2.22458200	-2.72949600
H	0.59799200	2.89302800	-1.86671500
H	-2.74107300	4.56989200	-2.30828000
H	0.05193600	1.29076800	-2.34064100
N	-0.70101400	1.94267800	-0.52114700
N	-2.03494600	3.86606800	-0.48182000
H	-3.63388800	4.43477700	0.77181500
H	-2.34491500	6.54977700	1.57545200
H	-1.10810500	5.40697900	3.34505300
H	-0.01325500	3.54179700	2.11580800
H	-1.55070000	1.45494000	1.74314400
H	-0.39489200	0.68303000	-0.06277400

M04RR^{DH}

C	-1.13332700	0.73639900	0.80523400
O	-1.11355200	0.17117300	1.87153700
H	1.51531600	-0.52002000	-0.58610400
C	-0.01711100	1.48209300	0.14468600
C	1.28330800	1.53013500	0.95915600
H	-0.35918300	2.49822400	-0.06722700
H	1.27217600	0.70640900	1.68187900
C	1.37644700	2.82747700	1.74198000
C	1.65539200	2.78552900	3.10951400
C	1.17612400	4.07297900	1.13584500
C	1.73724300	3.95709600	3.85836700
H	1.80152400	1.82326100	3.59322000
C	1.25783300	5.24540000	1.88122500
H	0.94736300	4.14005700	0.07354500
C	1.53904900	5.19079900	3.24495300
H	1.95020000	3.90382100	4.92102400
H	1.09991900	6.20348100	1.39563000
H	1.59898200	6.10535400	3.82575300
C	3.82339300	1.51102500	0.84821200

C	2.54125200	1.21697300	0.07342000
H	3.82950000	0.92787400	1.77299700
H	3.87072700	2.57102800	1.09480000
N	2.42988200	-0.21992800	-0.22214100
S	3.61970600	-0.96502100	-1.10947700
O	2.96786500	-2.11900300	-1.72940800
O	4.32936900	-0.00925300	-1.95758100
C	4.76797500	-1.53882900	0.11676400
C	4.32844900	-1.93532700	1.37807300
C	5.25415900	-2.44463800	2.27978600
C	6.60516000	-2.57133100	1.93561000
C	7.01538800	-2.16191600	0.66392800
C	6.10540400	-1.64490200	-0.25207300
H	3.28497700	-1.81802000	1.65215900
H	4.92532900	-2.74386400	3.27070400
H	8.06276200	-2.24147800	0.38876700
H	6.42821700	-1.31055200	-1.23234900
C	7.58978500	-3.15352500	2.91425900
H	8.61282300	-2.86485000	2.66602900
H	7.53793100	-4.24690000	2.90056900
H	7.37224100	-2.82684700	3.93375300
C	2.45065700	2.01495900	-1.24035900
O	1.78757000	1.65971400	-2.19105500
O	3.11061600	3.16615600	-1.18925500
C	2.96569300	4.00952800	-2.34069400
H	1.90722000	4.20269700	-2.52997400
H	3.40752400	3.52605700	-3.21305500
H	3.49141100	4.93034600	-2.09983300
H	4.70648300	1.25772600	0.25800900
C	-4.82445200	-3.07362300	1.49286400
C	-4.10128100	-1.89178600	1.63401400
C	-4.30445900	-1.02966200	2.70562300
C	-5.26688200	-1.37281200	3.65192800
C	-5.99735700	-2.55683000	3.51968500
C	-5.78152900	-3.41598500	2.44378100
C	-4.40467000	-3.82430300	0.25306900
C	-3.55246300	-2.82004900	-0.55252900
C	-3.11887200	-1.73457200	0.49752200
H	-3.72723800	-0.11378300	2.80004900
H	-5.45110400	-0.71797600	4.49683000
H	-6.74551600	-2.80871200	4.26423800
H	-6.35541900	-4.33218400	2.34533400
H	-5.24429600	-4.17408300	-0.35396300
H	-2.66909300	-3.28289500	-1.00068500

H	-3.80402100	-4.70260500	0.51521700
H	-2.08124400	-1.87454900	0.80399900
N	-3.20567500	-0.40072800	-0.10265000
O	-4.26132300	-2.27919300	-1.66223700
C	-2.41921600	0.67270900	0.00414800
C	-4.21730300	-0.07126700	-0.95882500
N	-2.97888500	1.61652300	-0.75274400
N	-4.10690900	1.16530500	-1.36467000
C	-5.11861200	-1.18607200	-1.38137800
H	-5.84777500	-1.41981400	-0.59560000
H	-5.64347100	-0.92334600	-2.29888400
C	-2.57309000	3.00027500	-0.82927100
C	-2.74900800	3.78229700	0.31748200
C	-1.94190700	3.46074700	-1.98966200
C	-2.23790900	5.07965500	0.28695200
C	-1.45854700	4.76682700	-1.96493400
C	-1.58281300	5.58260900	-0.83690900
H	-2.35053500	5.70636500	1.16737100
H	-0.96176500	5.15409500	-2.85143600
C	-1.70568800	2.58856700	-3.19368400
H	-2.45443100	1.80076800	-3.29181400
H	-0.71266700	2.12599500	-3.13051300
C	-3.41998100	3.24914100	1.55788600
H	-2.71274900	2.69259800	2.18431100
H	-4.25637300	2.58591900	1.31984600
H	-3.80182300	4.07495000	2.15933700
H	-1.72725900	3.19313100	-4.10225700
C	-1.00572200	6.97290600	-0.84526300
H	0.07643100	6.93693200	-1.00644500
H	-1.43498900	7.56599600	-1.65743500
H	-1.19688100	7.48929600	0.09702200
C	0.62146347	-5.71643157	0.50215696
C	-0.42370501	-5.89396254	-0.59518154
C	-0.05970489	-5.25392565	-1.93566735
C	0.90204226	-4.26032532	0.85853215
C	1.44661666	-3.43130205	-0.31696873
C	0.39744337	-2.91831633	-1.27564070
H	1.55935094	-6.18413261	0.17426577
H	-1.39350156	-5.49437975	-0.27066998
H	-0.68652242	-5.70390314	-2.70869835
H	1.63241427	-4.22285526	1.67219385
H	2.18010283	-4.02563627	-0.87769885
C	-0.92446644	-3.39433567	-3.29426839
H	-1.98078637	-3.68545459	-3.27836821

C	-0.85269154	-1.18630843	-2.20362930
C	-0.77127854	-1.90186162	-3.54432673
H	-1.55152263	-1.56064081	-4.22921764
H	0.20125740	-1.68613884	-3.99706602
H	-1.83737722	-1.37938043	-1.74517984
H	-0.42829176	-3.95504189	-4.09351624
H	-0.76910630	-0.10142487	-2.33587690
N	0.21222134	-1.62984065	-1.31413512
N	-0.31194286	-3.81206006	-2.01696103
H	0.98315327	-5.47175104	-2.20793891
H	-0.56495317	-6.96552698	-0.77110132
H	0.30003886	-6.25391264	1.40027164
H	-0.01471874	-3.79558764	1.24731540
H	1.96008371	-2.54252125	0.06116437
H	0.09898000	1.01180500	-0.83967100

M04RS^{DH}

C	5.81702600	-1.83205400	-1.33493300
C	4.83202100	-0.85562700	-1.45581600
C	4.90324400	0.14407500	-2.42097400
C	6.00596900	0.15637200	-3.27172100
C	7.00295300	-0.81667200	-3.15435200
C	6.91495200	-1.81867000	-2.19078500
C	5.49162100	-2.81121700	-0.23595700
C	4.30489800	-2.18332700	0.52681800
C	3.74005000	-1.07236100	-0.43471100
H	4.11395200	0.88583000	-2.50899600
H	6.09223100	0.92480600	-4.03254000
H	7.85688200	-0.79065200	-3.82341100
H	7.69149600	-2.57236100	-2.10451500
H	6.32412300	-2.98872800	0.45133600
H	3.51765000	-2.90819600	0.75060500
H	5.20257700	-3.78223200	-0.65189200
H	2.78838500	-1.37973700	-0.87534100
N	3.47157300	0.14760900	0.33034000
O	4.68486600	-1.68257900	1.80263000
C	2.50652700	1.05991000	0.20974500
C	4.28089500	0.55300700	1.35553600
N	2.75566900	1.98441000	1.13113100
N	3.87077900	1.68278200	1.85944200
C	5.32780300	-0.41848600	1.79511100
H	6.19464000	-0.39782500	1.12244800
H	5.65159500	-0.19734400	2.81128500
C	2.06827900	3.24097800	1.29416900

C	1.30631100	3.45110900	2.44838500
C	2.21420200	4.19292500	0.28016600
C	0.67022300	4.68459000	2.56839500
C	1.55429600	5.40901400	0.45380700
C	0.78671000	5.67347100	1.58765600
H	0.07028100	4.87972500	3.45364200
H	1.64795600	6.16831100	-0.31794200
C	3.03782800	3.92772000	-0.95339700
H	2.49841000	3.29113000	-1.66354100
H	3.98470500	3.43600400	-0.70984500
C	1.12778800	2.38694200	3.49970700
H	2.04585300	1.82285000	3.67636800
H	0.34465800	1.67862900	3.20240500
H	0.81404300	2.83769300	4.44234700
H	3.26327300	4.86568200	-1.46179300
C	0.10869300	7.00596000	1.76993100
H	0.04372300	7.55076800	0.82578400
H	-0.89990900	6.88115500	2.17219400
H	0.66936800	7.62573300	2.47658200
C	1.34638000	0.96103400	-0.76490000
O	1.60988800	0.77904700	-1.93638700
H	-2.19436100	-1.44883800	-1.27048500
C	0.07141800	0.81529900	-0.08154600
C	-1.17199700	0.95623000	-0.94224800
H	0.05191200	1.38977600	0.85022600
H	-1.01353100	0.37626500	-1.85843400
C	-1.45283700	2.39055700	-1.37711900
C	-1.97498600	2.62289400	-2.65541200
C	-1.23057300	3.48784800	-0.53958100
C	-2.29601400	3.91033500	-3.07587100
H	-2.13724000	1.78213600	-3.32416800
C	-1.55596300	4.77678200	-0.95785100
H	-0.79397300	3.35575400	0.44944100
C	-2.09519500	4.99285400	-2.22270000
H	-2.69801400	4.06627300	-4.07199000
H	-1.38071400	5.61454700	-0.28961000
H	-2.34612700	5.99807500	-2.54531900
C	-2.56461500	0.80536000	1.20614800
C	-2.41194000	0.31015200	-0.22677100
H	-1.77006400	0.38671200	1.82746500
H	-2.51002100	1.89567600	1.21770500
N	-2.18974600	-1.14826500	-0.29381900
S	-3.12584100	-2.24327800	0.55925900
O	-2.84252200	-2.07510900	1.97824900

O	-2.84490900	-3.51682000	-0.09908300
C	-4.83637200	-1.84510800	0.30075800
C	-5.42584500	-2.15842500	-0.92366200
C	-6.75108900	-1.80774700	-1.13671600
C	-7.49212900	-1.14537600	-0.14858200
C	-6.87922400	-0.85888500	1.07405600
C	-5.55296000	-1.20661300	1.30860300
H	-4.85657500	-2.66957000	-1.69310000
H	-7.22216800	-2.04937200	-2.08490800
H	-7.44739400	-0.36476900	1.85615500
H	-5.08266500	-1.00960000	2.26608300
C	-8.91484900	-0.73360300	-0.41482000
H	-9.45823400	-0.56008200	0.51575800
H	-8.93790100	0.19483200	-0.99505900
H	-9.44336300	-1.49522200	-0.99250500
C	-3.62185800	0.63342400	-1.11842600
O	-3.78376300	0.09265000	-2.19075900
O	-4.41733600	1.56779200	-0.62079700
C	-5.50333900	1.95904400	-1.47386500
H	-5.10576000	2.42400000	-2.37869000
H	-6.09892600	1.08390200	-1.73957300
H	-6.08986700	2.67127300	-0.89835800
H	-3.52405100	0.51594600	1.63424500
C	1.13371300	-5.32396600	-1.48103900
C	1.02085600	-5.78496000	-0.02862800
C	-0.12871500	-5.12952100	0.73958700
C	1.38834000	-3.82722500	-1.65141600
C	0.28786800	-2.93551500	-1.04542000
C	0.44760800	-2.74924000	0.44787800
H	0.20268300	-5.58102900	-2.00306200
H	1.95871300	-5.59566300	0.51016700
H	-0.37540200	-5.73664200	1.61449800
H	1.46395300	-3.60054100	-2.71839000
H	-0.69868400	-3.35460900	-1.27219300
C	0.25154000	-3.65554300	2.71758000
H	1.15605200	-4.15906500	3.08527000
C	1.19404100	-1.41616800	2.26729400
C	0.22491400	-2.19625400	3.14287400
H	0.48717400	-2.12135900	4.20315300
H	-0.78410600	-1.80009900	3.00316200
H	2.23117000	-1.72366600	2.46958300
H	-0.61523300	-4.18062100	3.13513100
H	1.14030000	-0.33857600	2.48907500
N	0.89548900	-1.60068800	0.85766400

N	0.18790300	-3.79840200	1.25865800
H	-1.03504600	-5.07717800	0.12394900
H	0.85995100	-6.86764500	-0.01571000
H	1.93500200	-5.88083000	-1.97709100
H	2.36137900	-3.56724100	-1.21174400
H	0.34034100	-1.93400200	-1.48416800
H	0.23809600	-0.17123900	0.21752200

M04SR^{DH}

C	-5.46805800	-2.46304500	-1.35444800
C	-4.40134600	-1.80020300	-0.75075200
C	-3.80564600	-2.28083100	0.40882800
C	-4.26928300	-3.48439400	0.93970000
C	-5.31972500	-4.17008700	0.32450700
C	-5.93210200	-3.66039700	-0.81988400
C	-5.96398100	-1.70102000	-2.55828800
C	-5.32562400	-0.30525200	-2.41751200
C	-4.04987700	-0.55953000	-1.54589600
H	-2.99189400	-1.73572900	0.88635700
H	-3.81320800	-3.88687400	1.83928100
H	-5.67389500	-5.10253500	0.75177000
H	-6.76397100	-4.18425500	-1.28017700
H	-7.05244000	-1.61557600	-2.60532900
H	-5.05433500	0.12829000	-3.38062000
H	-5.62672500	-2.17390400	-3.48708400
H	-3.17266300	-0.69962700	-2.18008300
N	-3.80007500	0.59770400	-0.68569100
O	-6.21674700	0.63996300	-1.83316000
C	-2.68198700	1.23829000	-0.32192100
C	-4.84203700	1.20253200	-0.04221800
N	-3.07437300	2.19417600	0.51714900
N	-4.42514000	2.19202000	0.69624100
C	-6.21543100	0.74667600	-0.41979800
H	-6.46440700	-0.19993400	0.07463000
H	-6.94963000	1.50312400	-0.14430600
C	-2.28984700	3.24774600	1.11028600
C	-1.96505700	3.14187000	2.46257000
C	-1.95335600	4.34404500	0.31024300
C	-1.23262400	4.19046200	3.01997700
C	-1.25896500	5.38032500	0.92825600
C	-0.88112700	5.31579300	2.27261000
H	-0.94622200	4.13193700	4.06651200
H	-0.99699100	6.25681200	0.34110800
C	-2.29003800	4.38460300	-1.15641300

H	-3.33150000	4.10495300	-1.34180400
H	-1.64583600	3.70378400	-1.72596900
C	-2.41073100	1.96310000	3.28498300
H	-2.37681600	1.03127200	2.71207000
H	-3.44422600	2.09978900	3.61856500
H	-1.78012300	1.85089400	4.16843300
H	-2.12723700	5.38717100	-1.55391200
C	-0.11040300	6.45100800	2.89282700
H	0.15971400	6.22999200	3.92668600
H	0.80703600	6.64876600	2.33104600
H	-0.70402400	7.36962600	2.88236100
C	-1.31038300	0.98016700	-0.92805800
O	-1.31638300	0.71288500	-2.10985500
H	2.06458800	-1.31987000	-0.58575500
C	-0.15394300	0.91670600	-0.02077500
C	1.16619200	1.05341900	-0.77442000
H	-0.27325400	1.60205300	0.82649100
H	1.13095500	0.33934500	-1.60704700
C	1.37539000	2.42555800	-1.38660600
C	1.83554300	2.52896100	-2.70326300
C	1.14236200	3.60011900	-0.66581400
C	2.07208800	3.77356000	-3.28194500
H	2.01465500	1.62253000	-3.27541600
C	1.38461000	4.84582700	-1.23985800
H	0.76407900	3.55465200	0.35064100
C	1.85196900	4.93703900	-2.54876400
H	2.42375100	3.83268900	-4.30705400
H	1.20723300	5.74660300	-0.65995500
H	2.03647900	5.90831200	-2.99616500
C	2.50266200	1.36667000	1.40632000
C	2.39806900	0.60834000	0.08914500
H	1.65952000	1.10318100	2.04936200
H	3.42214500	1.12550300	1.93866000
N	2.20785500	-0.83445800	0.29900600
S	3.17898500	-1.79413100	1.25015300
O	2.66605900	-3.14219800	1.01657500
O	3.19004700	-1.23953800	2.59766300
C	4.82369200	-1.68727900	0.59970400
C	5.17018900	-2.48371000	-0.48869900
C	6.41226000	-2.30216800	-1.08253300
C	7.30325800	-1.33188500	-0.60986600
C	6.92894300	-0.55077800	0.48889600
C	5.69185300	-0.72058100	1.10080500
H	4.47419300	-3.22752300	-0.86356300

H	6.69361700	-2.91620300	-1.93262700
H	7.61488100	0.20051600	0.86958400
H	5.40977100	-0.12539800	1.96296400
C	8.65018400	-1.14261600	-1.25472600
H	8.64691800	-1.49487800	-2.28788200
H	8.94445900	-0.09043800	-1.24526900
H	9.41664500	-1.70461900	-0.71167100
C	3.61024200	0.82075100	-0.83688600
O	3.80612000	0.12289000	-1.80625100
O	4.35968400	1.86286600	-0.49932400
C	5.42634700	2.16301100	-1.40999800
H	6.07813800	1.29329100	-1.51791500
H	5.01058800	2.43608000	-2.38245800
H	5.96312600	3.00072800	-0.97077400
H	2.49990100	2.43870600	1.21042100
C	0.32771200	-4.89028300	-1.72211600
C	0.28051900	-5.57636000	-0.35855000
C	-0.90729000	-5.12819000	0.49543600
C	0.44255200	-3.36853300	-1.64050100
C	-0.75216100	-2.67525600	-0.95508600
C	-0.65270900	-2.67065900	0.56094500
H	-0.57960300	-5.15061200	-2.28409400
H	1.20415000	-5.37871600	0.19882800
H	-1.10955800	-5.87563900	1.26487500
H	0.53491200	-2.96022700	-2.65134100
H	-1.68962500	-3.15243900	-1.27260400
C	-0.37880100	-3.90789900	2.62642800
H	0.70739500	-4.00678600	2.75428100
C	-0.31242500	-1.44157100	2.57865600
C	-0.88153600	-2.64475700	3.31454600
H	-0.58378000	-2.65026300	4.36444900
H	-1.97685900	-2.62206000	3.27508100
H	0.76789300	-1.35157300	2.77885100
H	-0.85236300	-4.79317000	3.05605400
H	-0.76953800	-0.50948000	2.93821900
N	-0.52287100	-1.53669800	1.14909100
N	-0.70179000	-3.86828300	1.19790900
H	-1.81558900	-5.06388400	-0.11681100
H	0.21393000	-6.65933900	-0.50853400
H	1.17492500	-5.27973100	-2.29586900
H	1.36439000	-3.12314200	-1.09950200
H	-0.79882900	-1.63469100	-1.26969900
H	-0.24096400	0.06668500	0.32370200

M04SS^{DH}

C	-6.39745100	0.24609800	0.51792700
C	-5.01766300	0.17573700	0.35047900
C	-4.31446400	1.15323900	-0.34335800
C	-5.01913600	2.24165200	-0.85311600
C	-6.40184400	2.33193100	-0.67064400
C	-7.10022300	1.33535500	0.00909900
C	-6.91383200	-0.95759900	1.26514500
C	-5.72838000	-1.95037800	1.30289800
C	-4.46201200	-1.07311500	0.99693700
H	-3.24089400	1.06481300	-0.49901000
H	-4.48908200	3.01890000	-1.39879100
H	-6.93991300	3.18228300	-1.07658300
H	-8.17697600	1.40280100	0.12921100
H	-7.77989800	-1.42608000	0.78868400
H	-5.62724800	-2.42579900	2.27806000
H	-7.20867700	-0.68764900	2.28416500
H	-3.89853200	-0.86594400	1.90419300
N	-3.56324500	-1.76806500	0.06322700
O	-5.89087600	-3.03401700	0.39947000
C	-2.23389900	-1.70818400	-0.12866000
C	-4.08842700	-2.48977900	-0.96931900
N	-2.01180300	-2.39602500	-1.24937300
N	-3.15521300	-2.89804400	-1.78259500
C	-5.55895700	-2.75512200	-0.94615600
H	-6.11325900	-1.89369100	-1.34247300
H	-5.79225800	-3.63604900	-1.54326100
C	-0.74867800	-2.58406100	-1.90811600
C	-0.42270200	-1.68677200	-2.92714900
C	0.10134300	-3.58544900	-1.44308100
C	0.86556700	-1.76663600	-3.44396500
C	1.37872400	-3.62532100	-1.99894800
C	1.78509700	-2.70510300	-2.96571500
H	1.17449600	-1.05746300	-4.20741100
H	2.08543700	-4.36751000	-1.63702000
C	-0.34663600	-4.55209000	-0.37860000
H	-1.25246200	-5.08185900	-0.68827400
H	-0.56924000	-4.04500700	0.56508000
C	-1.43093500	-0.67949300	-3.41305400
H	-1.83429200	-0.08448300	-2.58181300
H	-2.27695800	-1.17775600	-3.89576700
H	-0.97834800	0.00680100	-4.13097000
H	0.43336100	-5.28978100	-0.18177700
C	3.20342500	-2.66963900	-3.46033900

H	3.63338100	-1.69380000	-3.21340100
H	3.80854700	-3.44922800	-2.99354700
H	3.24959100	-2.79425200	-4.54607700
C	-1.26407700	-1.04517500	0.85135600
O	-1.71662100	-0.88625700	1.97225200
H	1.67128700	2.05733500	0.17593700
C	0.01087400	-0.51296200	0.37898200
C	0.97991500	-0.20282300	1.52603300
H	0.46205300	-1.03175200	-0.46929700
H	0.56918100	0.65182400	2.07944400
C	1.13324000	-1.34781500	2.51706800
C	1.05965400	-1.11723500	3.89067400
C	1.34938400	-2.65514700	2.06900700
C	1.21388600	-2.16239200	4.79949500
H	0.87097200	-0.10888300	4.25193700
C	1.50553900	-3.70221500	2.97257400
H	1.40513800	-2.85173800	0.99957500
C	1.44012300	-3.45818100	4.34337500
H	1.14995400	-1.96355500	5.86455700
H	1.67423500	-4.70969000	2.60335500
H	1.55777200	-4.27290100	5.05028900
C	3.10811300	0.99898700	2.16928500
C	2.38758800	0.29102800	1.01741900
H	2.55594900	1.90899900	2.42464900
H	3.15111300	0.35651100	3.04950900
N	2.15862700	1.21026100	-0.11178500
S	3.21688800	1.60866300	-1.34325300
O	2.97024200	3.03677400	-1.55375500
O	3.04505100	0.69595800	-2.46441700
C	4.87438500	1.40764700	-0.74295200
C	5.45746600	2.44987400	-0.02250000
C	6.75061900	2.29106700	0.45580500
C	7.46859600	1.11173800	0.21812000
C	6.86331400	0.09193800	-0.52094900
C	5.56922000	0.23250900	-1.01216300
H	4.90328600	3.36625300	0.15411500
H	7.21608700	3.09494100	1.01851700
H	7.41415900	-0.82237700	-0.72186300
H	5.09496900	-0.55463400	-1.59022500
C	8.87926700	0.96804100	0.72241500
H	9.57077200	1.51781900	0.07602300
H	8.97925700	1.37609100	1.73088600
H	9.19149700	-0.07769900	0.73551000
C	3.16288500	-0.93089000	0.51863800

O	2.94450700	-1.48600100	-0.53257500
O	4.06979500	-1.34438800	1.40084700
C	4.72913600	-2.57017800	1.06714500
H	3.99800200	-3.38105400	1.01865700
H	5.23509500	-2.47799800	0.10407900
H	5.44677700	-2.74653100	1.86484600
H	4.12842300	1.26756400	1.89227000
C	-1.69678800	4.80636800	2.64525900
C	-1.87597800	5.58795900	1.34336700
C	-2.74828900	4.88210000	0.30095100
C	-1.04173400	3.43441800	2.48449800
C	-1.81574900	2.49485200	1.54194700
C	-1.49677900	2.77069000	0.08724100
H	-2.68357100	4.66694700	3.10634000
H	-0.90238000	5.80870400	0.88842900
H	-3.11836600	5.61590500	-0.41923400
H	-0.97416100	2.95828500	3.46898400
H	-2.89395100	2.59016000	1.71810800
C	-1.80975000	4.16162300	-1.90359300
H	-1.03772000	4.93483600	-2.00249900
C	-0.27957700	2.23469400	-1.88267000
C	-1.40571400	2.90144200	-2.65507700
H	-1.09823900	3.16621300	-3.67211100
H	-2.26558700	2.22474300	-2.72955600
H	0.59826800	2.89289500	-1.87022800
H	-2.74068200	4.57333500	-2.31150000
H	0.05198000	1.29389900	-2.34089300
N	-0.70389100	1.95230400	-0.52130900
N	-2.03788400	3.87246300	-0.48189100
H	-3.63333800	4.43800800	0.77527300
H	-2.34415400	6.54987400	1.57851000
H	-1.10703300	5.40708600	3.34471900
H	-0.01255600	3.54173100	2.11541900
H	-1.54696500	1.45820000	1.73987600
H	-0.30514000	0.39177400	0.01383700

TS5RR^{DH}

C	-1.13248400	0.76487700	0.44838200
O	-1.26046700	0.11481900	1.45960900
H	1.45781500	-0.88261400	-0.59328100
C	0.12998500	1.38821700	-0.04531700
C	1.25607000	1.24794900	0.98144700
H	-0.05404400	2.43252400	-0.30823100
H	1.09507800	0.30982300	1.52499600

C	1.19891000	2.37647600	1.99425200
C	1.16356300	2.08455400	3.35980800
C	1.16231000	3.71720000	1.59360800
C	1.09917600	3.10376400	4.30656000
H	1.18180700	1.04617700	3.68141600
C	1.09858500	4.73805400	2.53785900
H	1.17249000	3.97373700	0.53527100
C	1.06687700	4.43434900	3.89743400
H	1.07008100	2.85746300	5.36303300
H	1.06923900	5.77262400	2.20849600
H	1.01289600	5.23049300	4.63278200
C	3.72204300	0.87176100	1.36586100
C	2.64342600	1.06047800	0.29765200
H	3.49910400	-0.03610900	1.93516500
H	3.75687300	1.72413600	2.04607000
N	2.48169900	-0.11398700	-0.55688000
S	3.70004000	-0.58958700	-1.49070700
O	3.11417100	-1.33531500	-2.61151700
O	4.60194400	0.53484300	-1.77086000
C	4.65168000	-1.78893900	-0.56948200
C	4.04161200	-2.99360500	-0.22317700
C	4.75005200	-3.92562600	0.52127700
C	6.07003600	-3.67463700	0.91972700
C	6.66150900	-2.46540200	0.55039600
C	5.96017500	-1.51833900	-0.19360600
H	3.02468100	-3.19895900	-0.54919600
H	4.27851400	-4.86512800	0.79761200
H	7.68572100	-2.25952800	0.84797700
H	6.41676200	-0.57753700	-0.48353700
C	6.83816000	-4.70531600	1.70484200
H	7.68729000	-4.25536900	2.22310800
H	7.22638400	-5.48365000	1.04007500
H	6.19910400	-5.19405400	2.44430500
C	2.89757100	2.30248800	-0.58124200
O	2.22441500	2.58929200	-1.54727900
O	3.87771100	3.07614400	-0.11869800
C	4.12296800	4.26280500	-0.87905200
H	3.23323800	4.89725300	-0.88737300
H	4.38671500	4.00017700	-1.90487200
H	4.94914900	4.76819700	-0.38432100
H	4.70323100	0.76558300	0.89963200
C	-5.13564900	-2.63723000	0.67757100
C	-4.17150600	-1.66388000	0.93338700
C	-4.13398400	-0.97926200	2.14686500

C	-5.08795500	-1.28963800	3.11051100
C	-6.05459900	-2.26832100	2.86269900
C	-6.08469700	-2.94825300	1.64847100
C	-4.98284900	-3.23433700	-0.69551700
C	-3.85085100	-2.42727300	-1.37201300
C	-3.24338000	-1.49924300	-0.24949400
H	-3.37818900	-0.22454600	2.33472700
H	-5.07994300	-0.76833200	4.06165800
H	-6.79198700	-2.49736500	3.62508800
H	-6.83976300	-3.70447300	1.45808800
H	-5.89817500	-3.16805000	-1.29262600
H	-3.06284900	-3.08194100	-1.74458100
H	-4.71697900	-4.29482100	-0.64340800
H	-2.20959900	-1.77786700	-0.02392300
N	-3.20059000	-0.10620200	-0.72649700
O	-4.28643500	-1.71175000	-2.51374900
C	-2.35025100	0.88674300	-0.44103400
C	-4.12263800	0.40552600	-1.59696100
N	-2.78745400	1.95316500	-1.10238800
N	-3.89565600	1.66970300	-1.83380600
C	-5.06987100	-0.56819100	-2.21961000
H	-5.90207400	-0.79736900	-1.54153900
H	-5.46360400	-0.17154400	-3.15419900
C	-2.24738900	3.28631800	-0.99315600
C	-2.39503700	3.94753800	0.22749600
C	-1.51402900	3.79088100	-2.07320600
C	-1.76371600	5.18647800	0.35053400
C	-0.90322700	5.02739700	-1.89138200
C	-1.01038900	5.73246000	-0.68699000
H	-1.85082300	5.72375300	1.29101600
H	-0.31239100	5.44359300	-2.70307700
C	-1.32869000	2.99171100	-3.33441100
H	-2.28261200	2.64216700	-3.73607700
H	-0.70148700	2.11360900	-3.14085100
C	-3.14750400	3.34981700	1.38926400
H	-2.49472100	2.70404600	1.98921000
H	-4.01077300	2.76086100	1.06761500
H	-3.50582100	4.14244900	2.04755400
H	-0.82942500	3.59326900	-4.09421600
C	-0.28826800	7.04169800	-0.51161000
H	0.79181300	6.87247700	-0.44525000
H	-0.46252200	7.70340600	-1.36367300
H	-0.60824000	7.55363900	0.39767100
C	-1.16207500	-4.31878600	2.28712100

C	-1.76302000	-4.82889100	0.97921100
C	-0.75275700	-5.06048800	-0.14550600
C	-0.47859900	-2.95886400	2.17730400
C	0.67902400	-2.92638400	1.16296200
C	0.24116500	-2.80492200	-0.27498500
H	-0.43377600	-5.05661600	2.64832700
H	-2.53885300	-4.13759700	0.62125300
H	-1.20112000	-5.71947800	-0.89162200
H	-0.07129000	-2.68407400	3.15477000
H	1.29042400	-3.83047900	1.27827200
C	-0.41579900	-3.95771500	-2.35061600
H	-1.46319100	-3.98990500	-2.67123600
C	0.03418700	-1.52768100	-2.26967600
C	0.32851600	-2.81782400	-3.02258900
H	0.02308600	-2.74873900	-4.06846400
H	1.40900100	-2.98050900	-2.98889500
H	-1.04426300	-1.29880600	-2.31489300
H	0.03436100	-4.91924300	-2.61687000
H	0.58702000	-0.68872800	-2.70129200
N	0.45798600	-1.66334900	-0.88025800
N	-0.36788300	-3.84573900	-0.87802200
H	0.14008500	-5.57328600	0.23635200
H	-2.26416900	-5.78282200	1.17092200
H	-1.95209500	-4.25938400	3.04251300
H	-1.21289400	-2.18447900	1.92704600
H	1.32987300	-2.06954800	1.35810900
H	0.37945400	0.90253700	-0.99762200

TS5RS^{DH}

C	-5.35930500	-2.93493500	0.38211900
C	-4.39784300	-1.96057700	0.63897200
C	-4.26426400	-1.37671100	1.89572200
C	-5.12955800	-1.78544200	2.90649800
C	-6.09937100	-2.76050300	2.65712500
C	-6.21932200	-3.34407000	1.39799000
C	-5.28408000	-3.42177800	-1.04223400
C	-4.33272900	-2.43844500	-1.75967900
C	-3.57967200	-1.67956000	-0.60104500
H	-3.50077700	-0.62829600	2.08341100
H	-5.04904500	-1.34495000	3.89439200
H	-6.76742800	-3.06639300	3.45554000
H	-6.97452900	-4.10091900	1.21054900
H	-6.25321500	-3.44103900	-1.54933700
H	-3.61350900	-2.95655000	-2.39574500

H	-4.87610600	-4.43687400	-1.08493100
H	-2.54628900	-2.02155100	-0.49831000
N	-3.54035400	-0.23658300	-0.89470800
O	-5.01236200	-1.57081200	-2.65235100
C	-2.63746700	0.71483000	-0.61128800
C	-4.59490100	0.38866500	-1.49662600
N	-3.17038600	1.86301900	-1.02270600
N	-4.39343900	1.67480300	-1.58097800
C	-5.67886500	-0.48094400	-2.04475900
H	-6.36647700	-0.79817000	-1.25019500
H	-6.23669800	0.05051300	-2.81458800
C	-2.66296900	3.20221800	-0.84295100
C	-2.25360600	3.90239900	-1.98394400
C	-2.63283900	3.73038400	0.44937400
C	-1.78543200	5.19796900	-1.78987200
C	-2.17531500	5.04265900	0.57770600
C	-1.74759900	5.78598500	-0.52116900
H	-1.44729700	5.76585800	-2.65242500
H	-2.14752000	5.48639200	1.56905100
C	-3.03148500	2.93319800	1.66412500
H	-2.21935300	2.26523900	1.98101800
H	-3.92898700	2.33243800	1.48904200
C	-2.30381100	3.27529800	-3.35143700
H	-3.33468700	3.05997600	-3.64553000
H	-1.74869600	2.33182800	-3.37860700
H	-1.86680300	3.94688700	-4.09072200
H	-3.23122500	3.60447300	2.50054800
C	-1.27038600	7.20368300	-0.35412200
H	-1.01057600	7.41402900	0.68515800
H	-0.39613200	7.39912200	-0.97928100
H	-2.05349700	7.90660900	-0.65500900
C	-1.31795700	0.44906000	0.08120900
O	-1.33438600	-0.44411700	0.89748600
H	1.68345100	-0.88300900	-0.90027800
C	-0.10698000	1.22011200	-0.34918100
C	1.03780000	1.07502600	0.65662800
H	-0.37871700	2.26191400	-0.54179500
H	1.01346500	0.04666800	1.02837700
C	0.83449600	1.98461300	1.85616300
C	0.91985100	1.44916800	3.14536600
C	0.52740100	3.34374500	1.71896900
C	0.70767800	2.24611500	4.26704800
H	1.16466300	0.39734000	3.26105300
C	0.32442700	4.14531900	2.83956000

H	0.44052700	3.79279400	0.73254100
C	0.41059500	3.59849900	4.11751000
H	0.77581300	1.80931500	5.25820600
H	0.10108000	5.20012400	2.71002600
H	0.24728300	4.22240300	4.99030300
C	2.65367200	2.61183300	-0.62102400
C	2.42424700	1.21551300	-0.04492200
H	1.86961500	2.84343100	-1.34855700
H	2.63983000	3.35572800	0.17777600
N	2.42753800	0.15082000	-1.05645400
S	3.57182900	-0.08038700	-2.16391700
O	3.96432200	1.14921600	-2.86084200
O	3.07455200	-1.19493400	-2.98190400
C	5.04247000	-0.67215900	-1.33841900
C	4.96220700	-1.83311500	-0.57280700
C	6.11026000	-2.32733200	0.03500000
C	7.33994200	-1.67349700	-0.11186200
C	7.39225100	-0.50931700	-0.88384200
C	6.24992800	-0.00111200	-1.49602700
H	4.01246600	-2.35219500	-0.47326100
H	6.05622700	-3.23598500	0.62788700
H	8.34097600	0.00518800	-1.00845400
H	6.28326500	0.90025200	-2.09822100
C	8.57354000	-2.19506000	0.57680200
H	9.47538700	-1.94314500	0.01471300
H	8.67086500	-1.75317000	1.57407200
H	8.53052600	-3.27953100	0.69905800
C	3.48745300	0.84254600	1.00574100
O	3.34973300	-0.04276200	1.82287000
O	4.61108600	1.54087700	0.86892000
C	5.69652100	1.11949800	1.70527700
H	5.45130500	1.30116600	2.75319500
H	5.88796200	0.05563400	1.54965800
H	6.55471100	1.71392700	1.39945000
H	3.61252800	2.66894700	-1.13088900
C	0.08888900	-3.66877400	3.05309800
C	-0.94301000	-4.27209700	2.10211000
C	-0.34441600	-4.85460200	0.81940100
C	0.81825100	-2.45465400	2.48462300
C	1.56867000	-2.73013900	1.17239900
C	0.70845500	-2.80713100	-0.06415200
H	0.82472900	-4.44357800	3.30701400
H	-1.69886400	-3.52332800	1.82833400
H	-1.04465700	-5.57567300	0.39362100

H	1.55903400	-2.10320500	3.21036400
H	2.13630900	-3.66582700	1.25914100
C	-0.70779900	-4.16451500	-1.54540100
H	-1.79256400	-4.00008700	-1.48840300
C	0.05162100	-1.88996600	-2.17174800
C	-0.07758500	-3.32914900	-2.64769900
H	-0.68307700	-3.39720300	-3.55388600
H	0.92386800	-3.70604200	-2.87633300
H	-0.95078900	-1.45284500	-2.02033800
H	-0.55652200	-5.22973900	-1.74337100
H	0.57968200	-1.27244200	-2.90278500
N	0.81540200	-1.84158200	-0.93615700
N	-0.10630500	-3.86596200	-0.23897200
H	0.58039800	-5.40328800	1.04106400
H	-1.46784600	-5.08185200	2.61883100
H	-0.40434200	-3.38667700	3.98874100
H	0.11013000	-1.63469000	2.32546000
H	2.28567200	-1.92256000	1.00794800
H	0.18205500	0.80094800	-1.32716600

TS5SR^{DH}

C	-5.48680400	-2.35834000	-1.22678800
C	-4.34419000	-1.68688300	-0.79612000
C	-3.60576600	-2.12877900	0.29649600
C	-4.03562200	-3.27580800	0.96065200
C	-5.17231100	-3.96229600	0.52816100
C	-5.90524700	-3.51048700	-0.56732700
C	-6.10849900	-1.66664800	-2.41308500
C	-5.41504600	-0.28933300	-2.48248100
C	-4.08655600	-0.47056300	-1.65909300
H	-2.72081900	-1.59349000	0.63995800
H	-3.48524000	-3.63785600	1.82278700
H	-5.49223600	-4.85258700	1.05945500
H	-6.79461400	-4.04080400	-0.89273000
H	-7.19064600	-1.53687800	-2.32508800
H	-5.18582200	0.00697500	-3.50558200
H	-5.91964400	-2.22827800	-3.33362000
H	-3.22527800	-0.58307200	-2.31856400
N	-3.85516800	0.71695600	-0.82260000
O	-6.23580000	0.75834300	-1.98598600
C	-2.73350000	1.32305200	-0.40671300
C	-4.89729400	1.32232500	-0.18061200
N	-3.12469900	2.25922400	0.45757800
N	-4.47532500	2.27986100	0.59915800

C	-6.27423100	0.89618200	-0.57817300
H	-6.55922400	-0.03422900	-0.07062200
H	-6.99417900	1.67648100	-0.33376100
C	-2.32328400	3.25564000	1.13007800
C	-1.86099800	2.96430100	2.41514000
C	-2.08830800	4.46337600	0.46790400
C	-1.08493200	3.93993200	3.03926100
C	-1.34100500	5.41715900	1.15497600
C	-0.82124200	5.16875800	2.42784700
H	-0.69075600	3.74057200	4.03183900
H	-1.15005500	6.37495300	0.67756400
C	-2.58171000	4.70448600	-0.93292300
H	-3.63828200	4.44363400	-1.04044000
H	-2.00818600	4.10922900	-1.65292800
C	-2.18445900	1.65318600	3.08166600
H	-1.83257600	0.79876200	2.49063600
H	-3.26533700	1.53773500	3.20715200
H	-1.71502200	1.59778300	4.06422100
H	-2.45679800	5.75371500	-1.20255900
C	0.00868500	6.21611700	3.12091000
H	0.38744100	5.85343000	4.07764000
H	0.86098200	6.50507000	2.49937300
H	-0.58339200	7.11720600	3.30456800
C	-1.34331400	1.00610200	-0.93042700
O	-1.27863100	0.69680900	-2.09630600
H	1.08575300	-1.31467300	0.78827700
C	-0.19832800	0.99553500	0.03492000
C	1.14290600	1.07893500	-0.69382300
H	-0.31818300	1.79106700	0.77243400
H	1.14112000	0.34931700	-1.50981900
C	1.31229100	2.45935700	-1.31680800
C	1.74710800	2.56854800	-2.64200000
C	1.03021100	3.63379800	-0.61074900
C	1.90777400	3.81475700	-3.24203900
H	1.96785700	1.66383200	-3.20060800
C	1.18901800	4.88176600	-1.20922600
H	0.68228000	3.59396400	0.41880500
C	1.63017300	4.97720500	-2.52628400
H	2.24377500	3.87577900	-4.27220800
H	0.96601000	5.77906800	-0.63953100
H	1.75278700	5.94936700	-2.99246600
C	2.40097400	1.43481100	1.52113500
C	2.34734700	0.64098000	0.21269900
H	1.53194300	1.17878700	2.13616100

H	3.29326100	1.17973600	2.09206500
N	2.20240800	-0.81270800	0.39688800
S	3.30549800	-1.66082800	1.24276100
O	2.88297200	-3.06524800	1.13085600
O	3.52086900	-1.15418800	2.60882200
C	4.86988100	-1.50033400	0.41187000
C	5.10928700	-2.24599700	-0.73930400
C	6.32017700	-2.09308300	-1.39958000
C	7.29416700	-1.20459500	-0.92532800
C	7.02787000	-0.47099900	0.23369800
C	5.81820600	-0.61315700	0.90832800
H	4.35077400	-2.92964500	-1.10740600
H	6.51890700	-2.66780900	-2.29966700
H	7.77478000	0.22104400	0.61279200
H	5.60889500	-0.05164600	1.81278900
C	8.61374600	-1.06386500	-1.63725800
H	8.50122100	-1.22492100	-2.71169400
H	9.04563400	-0.07352400	-1.47684000
H	9.33099200	-1.80263900	-1.26525400
C	3.55446200	0.92912900	-0.70676900
O	3.74004800	0.36480900	-1.75854400
O	4.31285600	1.93358400	-0.26456600
C	5.35595100	2.33725600	-1.15864200
H	6.00794200	1.48933000	-1.37784300
H	4.91973200	2.71392500	-2.08685600
H	5.90161100	3.12458200	-0.64289600
H	2.40829400	2.50873900	1.33005700
C	0.29753700	-5.15325600	-1.76844000
C	-0.15088200	-5.88126900	-0.50062400
C	-1.31857100	-5.19874400	0.21612000
C	0.77639800	-3.71819300	-1.54709800
C	-0.28833000	-2.79697800	-0.92302400
C	-0.37613400	-2.95932700	0.57311200
H	-0.54217900	-5.14101000	-2.47692000
H	0.68403000	-5.97711000	0.20418200
H	-1.82612100	-5.91142700	0.86946700
H	1.06512600	-3.28907000	-2.51128400
H	-1.27256700	-2.97465400	-1.37518700
C	-0.90586200	-4.31735100	2.52564200
H	-0.01327500	-4.89132000	2.80240800
C	0.16681100	-2.09922100	2.75403900
C	-0.94675600	-2.99315000	3.27367000
H	-0.83375800	-3.17187900	4.34491300
H	-1.91723200	-2.50701700	3.11576200

H	1.14741900	-2.50663800	3.02839900
H	-1.78130700	-4.92654600	2.76800100
H	0.10108300	-1.09328600	3.18106100
N	0.09901200	-1.98049600	1.30025200
N	-0.90932800	-4.08326400	1.07701500
H	-2.06648700	-4.84775500	-0.50549500
H	-0.46333000	-6.89601300	-0.76755700
H	1.09920700	-5.72582000	-2.24562800
H	1.66644300	-3.69787900	-0.90672800
H	-0.02660200	-1.75326100	-1.11284200
H	-0.31174100	0.04780100	0.58590200

TS5SS^{DH}

C	-6.42401100	0.27358500	0.40835200
C	-5.03186500	0.26158700	0.38217000
C	-4.30975600	1.30115100	-0.20206400
C	-5.01461600	2.34872900	-0.78559600
C	-6.41213400	2.36319900	-0.77134800
C	-7.12450500	1.33130700	-0.16850000
C	-6.98311100	-0.92851900	1.12047600
C	-5.76422100	-1.82270200	1.44728100
C	-4.48782600	-0.98293100	1.04786000
H	-3.22365000	1.30911800	-0.19537300
H	-4.47269300	3.16272800	-1.25572500
H	-6.94472200	3.18822600	-1.23268000
H	-8.20974300	1.34614300	-0.15129500
H	-7.70835800	-1.48391800	0.51681700
H	-5.70979200	-2.04909300	2.51146000
H	-7.49686400	-0.63669700	2.04066900
H	-3.87176800	-0.76253300	1.91708100
N	-3.63974300	-1.75122200	0.10595000
O	-5.83310800	-3.09284200	0.82416900
C	-2.32530900	-1.67436600	-0.17868100
C	-4.16736800	-2.68545500	-0.73478400
N	-2.11770600	-2.55046800	-1.16388500
N	-3.25191000	-3.19045500	-1.51983400
C	-5.60400300	-3.05296200	-0.56859400
H	-6.25021700	-2.32430200	-1.07663600
H	-5.78812300	-4.04433700	-0.98096200
C	-0.87094600	-2.79091700	-1.84566300
C	-0.51021300	-1.89675200	-2.85647800
C	-0.05146100	-3.81800500	-1.37808500
C	0.78181300	-2.00600200	-3.35707600
C	1.22859000	-3.89027800	-1.92455200

C	1.67206700	-2.97081700	-2.87559500
H	1.12005600	-1.29666200	-4.10703600
H	1.91144300	-4.65212300	-1.55889500
C	-0.49886000	-4.73697200	-0.27211500
H	-1.48816400	-5.15687900	-0.47239500
H	-0.55172900	-4.20725800	0.68764800
C	-1.48238400	-0.86055200	-3.35498900
H	-1.84213900	-0.21904400	-2.54224300
H	-2.36014800	-1.33371600	-3.80560800
H	-1.01338700	-0.22067900	-4.10416600
H	0.20837700	-5.55898600	-0.15497300
C	3.09820100	-2.95821200	-3.34427100
H	3.54688500	-2.01299700	-3.02251100
H	3.66752900	-3.78833900	-2.92199000
H	3.15935700	-3.00864800	-4.43497500
C	-1.34076700	-0.75560400	0.52133300
O	-1.83217200	0.05449100	1.27675700
H	1.06839900	1.80274600	-0.24824000
C	0.13623600	-0.87497600	0.26790000
C	0.91266900	-0.28074000	1.44481300
H	0.42147500	-1.90839700	0.07282300
H	0.38713200	0.62936800	1.74276400
C	0.88362800	-1.21840600	2.63969800
C	0.42713700	-0.75234500	3.87510200
C	1.28705500	-2.55603200	2.53700300
C	0.38666600	-1.59146100	4.98619400
H	0.09710600	0.28020000	3.96231200
C	1.24985900	-3.39628100	3.64676900
H	1.63443700	-2.95034100	1.58416800
C	0.80103900	-2.91602400	4.87539400
H	0.02797100	-1.21014300	5.93682100
H	1.57048900	-4.42876100	3.54932300
H	0.77089800	-3.57167400	5.73935400
C	2.95632500	0.94306200	2.25641000
C	2.34624600	0.21348800	1.05283500
H	2.33931400	1.81709600	2.48529800
H	3.00764400	0.30140200	3.13775700
N	2.17906600	1.16252400	-0.05339200
S	3.12075500	1.27816800	-1.35673800
O	2.96449200	2.66259000	-1.83157000
O	2.89739200	0.23714000	-2.37249200
C	4.79998000	1.07638400	-0.79152900
C	5.38472800	2.09349500	-0.03793800
C	6.68655400	1.93436900	0.41745600

C	7.41752600	0.77624900	0.12156000
C	6.81336300	-0.22000900	-0.64821300
C	5.50810000	-0.07573200	-1.11155500
H	4.82026600	2.99351800	0.18715100
H	7.14872200	2.71965300	1.00905000
H	7.37109400	-1.12082900	-0.88917600
H	5.02578800	-0.84895200	-1.70143500
C	8.83802500	0.63014200	0.59945100
H	9.51987900	1.18334100	-0.05446200
H	8.95687500	1.02993900	1.60927300
H	9.15086600	-0.41589900	0.59956500
C	3.16052300	-1.03785000	0.68001600
O	2.88800200	-1.77141000	-0.24374700
O	4.15794500	-1.27712600	1.53265400
C	4.87231500	-2.49663500	1.31322800
H	4.21852700	-3.34978000	1.51208700
H	5.23251400	-2.54681400	0.28448600
H	5.70512700	-2.48263700	2.01301600
H	3.96352100	1.28630800	2.01621300
C	-1.03822500	5.78583900	2.00270500
C	-1.85391900	6.06112300	0.74099100
C	-2.59557600	4.82781300	0.22147000
C	0.03355000	4.71000800	1.83929200
C	-0.50841200	3.31788500	1.46586900
C	-0.77750900	3.17428700	-0.01052100
H	-1.72421200	5.47902300	2.80375300
H	-1.21068000	6.44927500	-0.05829000
H	-3.41054400	5.13819900	-0.43599800
H	0.57761100	4.60993600	2.78331900
H	-1.41052800	3.08145000	2.04233700
C	-1.84775800	3.99521500	-2.02873900
H	-1.16346000	4.77150400	-2.39401500
C	-0.12114600	2.23694000	-2.13878300
C	-1.49848200	2.64420900	-2.63445100
H	-1.50893700	2.70379100	-3.72518800
H	-2.25982700	1.91620400	-2.33105800
H	0.65660300	2.84758600	-2.60818800
H	-2.86260300	4.29588900	-2.29804400
H	0.11683700	1.19617700	-2.39400200
N	0.00107600	2.37906600	-0.68847700
N	-1.76810500	3.90744700	-0.56673600
H	-3.05705500	4.27984700	1.05145700
H	-2.59609200	6.83619700	0.95777800
H	-0.56344500	6.71388500	2.33627100

H	0.76926100	5.01593600	1.08544300
H	0.24277700	2.56963200	1.71874400
H	0.36598800	-0.33072300	-0.66147600

M4RR

C	0.93095100	-1.17514600	0.98279500
O	1.60194100	-1.04412700	1.98807900
H	-0.92196500	-1.73128200	0.00887900
C	-0.46712000	-1.74051600	1.00000100
C	-1.29088800	-0.89263400	1.98211300
H	-0.39890700	-2.77230600	1.36487000
H	-0.65050600	-0.70750900	2.85187400
C	-2.54094800	-1.58859900	2.48122200
C	-2.92590800	-1.44234200	3.81728900
C	-3.33253300	-2.38355100	1.64297100
C	-4.07900500	-2.05271800	4.30402700
H	-2.30609300	-0.84922000	4.48503500
C	-4.48495500	-2.99704400	2.12763700
H	-3.04925800	-2.51910300	0.60333000
C	-4.86495500	-2.83021700	3.45755200
H	-4.35792600	-1.92578300	5.34525300
H	-5.08606800	-3.61124100	1.46431100
H	-5.76333600	-3.30946400	3.83326500
C	-1.73919800	1.53290600	2.48561700
C	-1.55354600	0.52645600	1.34450300
H	-0.78473900	1.64554600	3.00466000
H	-2.50066700	1.18162200	3.18624000
N	-0.42206400	0.77071100	0.46083900
S	-0.07517800	2.21721400	-0.07360100
O	0.44802400	3.15086700	0.95122500
O	0.80672300	2.03484300	-1.24558500
C	-1.57846100	2.99184100	-0.68189700
C	-2.15889200	4.05663900	-0.00115300
C	-3.35536400	4.59816500	-0.46742200
C	-3.97709300	4.09186500	-1.61042300
C	-3.35999100	3.03847600	-2.29652200
C	-2.17084400	2.48704600	-1.83836300
H	-1.66533000	4.45583600	0.87903000
H	-3.81146800	5.42896000	0.06372200
H	-3.82090500	2.64620900	-3.19947800
H	-1.69850900	1.67057700	-2.37269400
C	-5.29411500	4.64510200	-2.08824200
H	-5.32050600	4.71719300	-3.17838000
H	-5.48323700	5.63606300	-1.67021700

H	-6.11805200	3.99102500	-1.78296700
C	-2.81996700	0.38860400	0.47605300
O	-2.87294300	-0.26992700	-0.54046800
O	-3.87640000	1.03836700	0.97233300
C	-5.08411200	0.89882700	0.21956500
H	-5.38525000	-0.15082500	0.18699100
H	-4.93342700	1.26855900	-0.79693300
H	-5.83026500	1.49670100	0.73967600
H	-2.05012700	2.51032500	2.11598900
C	5.44604600	1.50634400	1.11135900
C	4.47982800	0.50268700	1.14324800
C	4.76127800	-0.75836100	1.65841200
C	6.04182300	-1.00227700	2.15070300
C	7.01307500	0.00111400	2.12809500
C	6.72197600	1.26174400	1.61021700
C	4.89073500	2.76926700	0.50372700
C	3.58053900	2.33622500	-0.18783100
C	3.18328500	1.00089400	0.53808100
H	3.99752900	-1.52986300	1.67765600
H	6.28629100	-1.97947400	2.55421700
H	8.00670400	-0.20512900	2.51318300
H	7.48153900	2.03756100	1.58561500
H	5.56205300	3.23896200	-0.22010900
H	2.77428900	3.05861200	-0.06881000
H	4.67669300	3.50865700	1.28326600
H	2.40678700	1.19570900	1.28320900
N	2.63746300	0.03211800	-0.41276500
O	3.75313600	2.21254000	-1.59565900
C	1.64024400	-0.85284800	-0.30748900
C	3.09170500	-0.02769000	-1.69455800
N	1.54944100	-1.43909900	-1.49656000
N	2.44637600	-0.92536300	-2.38624300
C	4.14891600	0.95087600	-2.08582900
H	5.12077600	0.63169400	-1.68341000
H	4.21685500	1.01815600	-3.17141300
C	0.67604400	-2.51913000	-1.86997800
C	-0.48963400	-2.19344800	-2.56797500
C	1.02319100	-3.81606600	-1.49511400
C	-1.34393000	-3.24316700	-2.89108100
C	0.13375800	-4.83253000	-1.84613100
C	-1.04874200	-4.56374200	-2.53613700
H	-2.26454100	-3.02516500	-3.42635500
H	0.37381200	-5.85690200	-1.57385200
C	2.29247000	-4.09905000	-0.73423800

H	2.21810700	-3.76484700	0.30725500
H	3.14815300	-3.58824600	-1.18531800
C	-0.80069300	-0.75758800	-2.88024700
H	-0.03988600	-0.31913700	-3.53328400
H	-0.82092400	-0.18129300	-1.94738900
H	-1.77665300	-0.67377800	-3.36149100
H	2.49813200	-5.17007700	-0.72179100
C	-2.01012500	-5.67139300	-2.87924400
H	-1.53909700	-6.65115300	-2.78064000
H	-2.87742900	-5.64571700	-2.21203500
H	-2.38124600	-5.56508300	-3.90153000

M4RS

C	4.88005400	-2.01329400	-1.19526800
C	3.64296000	-1.40153900	-1.01828000
C	3.52766200	-0.11398100	-0.51813800
C	4.68841200	0.57118100	-0.17199200
C	5.93665100	-0.03518700	-0.33981900
C	6.04298300	-1.32712500	-0.85512800
C	4.72379300	-3.39034900	-1.78643200
C	3.21023000	-3.69829200	-1.70616000
C	2.51916500	-2.29765900	-1.47408500
H	2.54847900	0.32146600	-0.38169800
H	4.61429900	1.57754900	0.23179900
H	6.83655500	0.50542500	-0.06370000
H	7.01652000	-1.79055400	-0.98386200
H	5.28530400	-4.16305900	-1.25300800
H	2.83664200	-4.14381000	-2.62854300
H	5.05735400	-3.40670800	-2.82908100
H	2.06222700	-1.93627100	-2.39315200
N	1.43594500	-2.41269900	-0.47567400
O	2.91875000	-4.66150400	-0.70479200
C	0.19033700	-1.90218400	-0.39976500
C	1.56970800	-3.28934800	0.56172000
N	-0.38952800	-2.53620700	0.62525900
N	0.46244700	-3.39931700	1.23660100
C	2.80035500	-4.12973700	0.60404200
H	3.67957200	-3.54252800	0.89589400
H	2.66653900	-4.95796900	1.29863200
C	-1.78877100	-2.60982400	0.97106800
C	-2.24902200	-2.03868300	2.15353100
C	-2.61494900	-3.32992100	0.09235800
C	-3.62412100	-2.12390500	2.40207900
C	-3.97132200	-3.38117300	0.38680100

C	-4.49750900	-2.76245000	1.52799200
H	-4.01164800	-1.67175600	3.31197100
H	-4.63433800	-3.92397200	-0.28211500
C	-2.05970400	-4.00955200	-1.13256300
H	-1.16361400	-4.59105400	-0.89460300
H	-1.79171200	-3.28786400	-1.91220700
C	-1.34538300	-1.36297800	3.14275900
H	-1.61722800	-0.31052800	3.25106400
H	-0.29988000	-1.39097300	2.83670700
H	-1.44653700	-1.84528300	4.11950800
H	-2.80223000	-4.68686300	-1.55603200
C	-5.97974800	-2.78857300	1.79200200
H	-6.42091200	-3.73445600	1.46920700
H	-6.19632400	-2.64512400	2.85233400
H	-6.47787900	-1.98588900	1.23825600
C	-0.33087000	-0.81199600	-1.33414700
O	0.46655800	-0.40531100	-2.15989400
H	-2.35587000	-0.97852300	-0.60180600
C	-1.80789900	-0.50125600	-1.41067300
C	-2.03629200	1.01202700	-1.38698600
H	-2.16860500	-0.90774800	-2.36334100
H	-1.34648600	1.45699100	-2.10986600
C	-3.45023700	1.39062900	-1.78145200
C	-3.68666700	2.60020200	-2.44256600
C	-4.54515100	0.56956600	-1.48557700
C	-4.97920100	2.98257800	-2.79379000
H	-2.84237100	3.24161800	-2.67573300
C	-5.83801900	0.94995600	-1.83556800
H	-4.39549700	-0.37934000	-0.97575100
C	-6.06042600	2.15883800	-2.49056000
H	-5.14027300	3.92474300	-3.30851400
H	-6.67317400	0.29852500	-1.59682100
H	-7.06802900	2.45405900	-2.76543300
C	-2.72725200	1.43387300	1.06365000
C	-1.61272600	1.55246700	0.01816800
H	-3.07725100	0.39680400	1.10580500
H	-2.32968300	1.70897800	2.04085500
N	-0.44787700	0.73759100	0.36935300
S	0.53888500	1.03698400	1.56216700
O	1.40831400	-0.15615400	1.68725200
O	-0.06272600	1.50145600	2.82737500
C	1.62084100	2.38911200	1.06337100
C	1.83809800	2.66442700	-0.28534400
C	2.71020600	3.68665100	-0.64571300

C	3.37451800	4.44404300	0.32542100
C	3.13779200	4.15481700	1.67292100
C	2.26334100	3.13756300	2.04574000
H	1.31490700	2.08663400	-1.04351100
H	2.87643200	3.90303700	-1.69778200
H	3.64037100	4.73763600	2.43992100
H	2.06550000	2.92743500	3.09188100
C	4.30979000	5.55261700	-0.08351100
H	3.76698900	6.34785600	-0.60329400
H	4.80712200	5.99252900	0.78312400
H	5.07755600	5.18233200	-0.76878100
C	-1.21170600	3.03146700	-0.16341900
O	-0.92040100	3.56080600	-1.21400500
O	-1.15332300	3.67540700	1.00459500
C	-0.60507500	4.99558300	0.95277900
H	0.40951200	4.96079900	0.54670300
H	-1.22659500	5.63889900	0.32711000
H	-0.59455200	5.35145500	1.98098400
H	-3.57670700	2.07905000	0.82238400

M4SR

C	4.88005400	-2.01329400	-1.19526800
C	3.64296000	-1.40153900	-1.01828000
C	3.52766200	-0.11398100	-0.51813800
C	4.68841200	0.57118100	-0.17199200
C	5.93665100	-0.03518700	-0.33981900
C	6.04298300	-1.32712500	-0.85512800
C	4.72379300	-3.39034900	-1.78643200
C	3.21023000	-3.69829200	-1.70616000
C	2.51916500	-2.29765900	-1.47408500
H	2.54847900	0.32146600	-0.38169800
H	4.61429900	1.57754900	0.23179900
H	6.83655500	0.50542500	-0.06370000
H	7.01652000	-1.79055400	-0.98386200
H	5.28530400	-4.16305900	-1.25300800
H	2.83664200	-4.14381000	-2.62854300
H	5.05735400	-3.40670800	-2.82908100
H	2.06222700	-1.93627100	-2.39315200
N	1.43594500	-2.41269900	-0.47567400
O	2.91875000	-4.66150400	-0.70479200
C	0.19033700	-1.90218400	-0.39976500
C	1.56970800	-3.28934800	0.56172000
N	-0.38952800	-2.53620700	0.62525900
N	0.46244700	-3.39931700	1.23660100

C	2.80035500	-4.12973700	0.60404200
H	3.67957200	-3.54252800	0.89589400
H	2.66653900	-4.95796900	1.29863200
C	-1.78877100	-2.60982400	0.97106800
C	-2.24902200	-2.03868300	2.15353100
C	-2.61494900	-3.32992100	0.09235800
C	-3.62412100	-2.12390500	2.40207900
C	-3.97132200	-3.38117300	0.38680100
C	-4.49750900	-2.76245000	1.52799200
H	-4.01164800	-1.67175600	3.31197100
H	-4.63433800	-3.92397200	-0.28211500
C	-2.05970400	-4.00955200	-1.13256300
H	-1.16361400	-4.59105400	-0.89460300
H	-1.79171200	-3.28786400	-1.91220700
C	-1.34538300	-1.36297800	3.14275900
H	-1.61722800	-0.31052800	3.25106400
H	-0.29988000	-1.39097300	2.83670700
H	-1.44653700	-1.84528300	4.11950800
H	-2.80223000	-4.68686300	-1.55603200
C	-5.97974800	-2.78857300	1.79200200
H	-6.42091200	-3.73445600	1.46920700
H	-6.19632400	-2.64512400	2.85233400
H	-6.47787900	-1.98588900	1.23825600
C	-0.33087000	-0.81199600	-1.33414700
O	0.46655800	-0.40531100	-2.15989400
H	-2.35587000	-0.97852300	-0.60180600
C	-1.80789900	-0.50125600	-1.41067300
C	-2.03629200	1.01202700	-1.38698600
H	-2.16860500	-0.90774800	-2.36334100
H	-1.34648600	1.45699100	-2.10986600
C	-3.45023700	1.39062900	-1.78145200
C	-3.68666700	2.60020200	-2.44256600
C	-4.54515100	0.56956600	-1.48557700
C	-4.97920100	2.98257800	-2.79379000
H	-2.84237100	3.24161800	-2.67573300
C	-5.83801900	0.94995600	-1.83556800
H	-4.39549700	-0.37934000	-0.97575100
C	-6.06042600	2.15883800	-2.49056000
H	-5.14027300	3.92474300	-3.30851400
H	-6.67317400	0.29852500	-1.59682100
H	-7.06802900	2.45405900	-2.76543300
C	-2.72725200	1.43387300	1.06365000
C	-1.61272600	1.55246700	0.01816800
H	-3.07725100	0.39680400	1.10580500

H	-2.32968300	1.70897800	2.04085500
N	-0.44787700	0.73759100	0.36935300
S	0.53888500	1.03698400	1.56216700
O	1.40831400	-0.15615400	1.68725200
O	-0.06272600	1.50145600	2.82737500
C	1.62084100	2.38911200	1.06337100
C	1.83809800	2.66442700	-0.28534400
C	2.71020600	3.68665100	-0.64571300
C	3.37451800	4.44404300	0.32542100
C	3.13779200	4.15481700	1.67292100
C	2.26334100	3.13756200	2.04574000
H	1.31490700	2.08663400	-1.04351100
H	2.87643200	3.90303700	-1.69778200
H	3.64037100	4.73763600	2.43992100
H	2.06550000	2.92743500	3.09188100
C	4.30979000	5.55261700	-0.08351100
H	3.76698900	6.34785600	-0.60329400
H	4.80712200	5.99252900	0.78312400
H	5.07755600	5.18233100	-0.76878100
C	-1.21170600	3.03146700	-0.16341900
O	-0.92040100	3.56080600	-1.21400500
O	-1.15332300	3.67540700	1.00459500
C	-0.60507500	4.99558300	0.95277900
H	0.40951200	4.96079900	0.54670300
H	-1.22659500	5.63889900	0.32711000
H	-0.59455200	5.35145500	1.98098400
H	-3.57670700	2.07905000	0.82238400

M4SS

C	-1.47807200	4.50965600	-0.51931000
C	-1.25433400	3.60006600	0.51940000
C	0.00959500	3.05823600	0.74148100
C	1.03999800	3.38763500	-0.13707000
C	0.81205100	4.27620200	-1.18829400
C	-0.43995800	4.86127400	-1.37420800
C	-2.91316900	4.97053400	-0.54527200
C	-3.42169100	4.54684200	0.84948700
C	-2.55084500	3.32735400	1.24544300
H	0.19871800	2.38283400	1.57029300
H	2.01106400	2.91794700	-0.03339100
H	1.62523800	4.50481800	-1.86893100
H	-0.60665400	5.56800600	-2.18133300
H	-3.45980900	4.46525900	-1.35000000
H	-3.20219800	5.33785400	1.56917400

H	-3.02411800	6.04501400	-0.70437900
H	-2.47221800	3.17092900	2.32181200
N	-3.23010600	2.12273200	0.67698600
O	-4.80732400	4.30116400	0.97532900
C	-2.73528500	0.88667600	0.52861600
C	-4.46546300	2.11737900	0.08807900
N	-3.64456100	0.19188800	-0.13960600
N	-4.74177200	0.94390000	-0.41642200
C	-5.32541600	3.34525400	0.07989400
H	-5.40845800	3.73211000	-0.94239200
H	-6.32594400	3.08280500	0.42796100
C	-3.57593400	-1.20192700	-0.51249600
C	-3.14938400	-1.51393200	-1.80826300
C	-3.92395500	-2.15481200	0.44399100
C	-3.07397200	-2.86484600	-2.13429300
C	-3.84787900	-3.49270700	0.05596000
C	-3.42017100	-3.86356700	-1.21800000
H	-2.73305900	-3.14453200	-3.12778000
H	-4.10982400	-4.26079700	0.77870600
C	-4.32587000	-1.75965800	1.84005400
H	-5.06314900	-0.95187200	1.83378900
H	-3.45655700	-1.41805600	2.41364400
C	-2.73827300	-0.44207000	-2.78150700
H	-2.65605500	-0.85653700	-3.78672600
H	-1.75739000	-0.03230800	-2.51361000
H	-3.45770400	0.38052500	-2.80292200
H	-4.75515500	-2.61251900	2.36672900
C	-3.29945100	-5.31410500	-1.60428100
H	-3.65867900	-5.96955800	-0.80846400
H	-3.87171100	-5.52678900	-2.51141100
H	-2.25478100	-5.56762200	-1.81241500
C	-1.45203300	0.36601300	1.15765600
O	-1.34208200	0.55621500	2.34722800
H	-0.01580500	0.58821900	-0.33664500
C	-0.46269500	-0.24288300	0.23746300
C	0.66256900	-0.97948500	0.95708700
H	-0.97404400	-0.87054000	-0.49599100
H	1.00096800	-0.33787500	1.77925600
C	0.19202400	-2.29378100	1.54872800
C	0.46179400	-2.59147000	2.88821500
C	-0.51032100	-3.23381700	0.78653100
C	0.05678100	-3.79826800	3.45148800
H	0.99759600	-1.86386600	3.49265500
C	-0.91062500	-4.44521000	1.34553600

H	-0.75542900	-3.02341900	-0.25372100
C	-0.62860800	-4.73283400	2.67850000
H	0.27538100	-4.00776200	4.49390500
H	-1.45307200	-5.16258800	0.73586300
H	-0.94530100	-5.67577800	3.11275100
C	3.06719200	-1.73188700	0.81824100
C	1.92022000	-1.08989200	0.02845900
H	3.32730400	-1.07301000	1.65226500
H	2.79331500	-2.71493900	1.20676100
N	2.18188000	0.28293200	-0.37986700
S	3.37725200	0.52095300	-1.36959100
O	3.21426900	1.83748100	-2.02076300
O	3.65411500	-0.61975000	-2.27734200
C	4.89173500	0.69924600	-0.40610600
C	4.85069100	1.34764500	0.82608300
C	6.02490500	1.53476900	1.54603400
C	7.25235400	1.07712200	1.05337100
C	7.27204000	0.42715500	-0.18275100
C	6.10113800	0.23689600	-0.91304200
H	3.89377400	1.68040400	1.21856400
H	5.99268100	2.04081200	2.50772200
H	8.21712100	0.06384900	-0.57817400
H	6.11270400	-0.27751300	-1.86836700
C	8.51540800	1.25483000	1.85609100
H	8.50723800	2.20268500	2.40009600
H	8.62307200	0.45392500	2.59506300
H	9.39880800	1.23346000	1.21406600
C	1.51128700	-1.95755800	-1.18045600
O	0.67329700	-1.64072300	-1.99860500
O	2.10504000	-3.15658000	-1.19716100
C	1.70794700	-4.01171300	-2.26833200
H	0.63701800	-4.22470300	-2.20682600
H	1.92265100	-3.53819600	-3.22823200
H	2.28552600	-4.92684400	-2.15250000
H	3.94635900	-1.84788000	0.18023600

TS6RR

C	0.70881300	-0.72472700	0.89002000
O	1.36556400	-0.49304900	1.92573900
H	-0.97209300	-1.78689500	-0.01265300
C	-0.50658800	-1.64755100	0.96194800
C	-1.45658900	-0.91562800	1.89755900
H	-0.20227500	-2.61487300	1.37506200
H	-0.92410500	-0.76166600	2.84135700

C	-2.75506300	-1.63038900	2.20115800
C	-3.33224200	-1.50122300	3.46868400
C	-3.41169500	-2.41823200	1.24796000
C	-4.53993900	-2.12308500	3.77475500
H	-2.82077700	-0.91420600	4.22746600
C	-4.61692500	-3.04546300	1.55316300
H	-2.98296500	-2.53962300	0.25750700
C	-5.18794400	-2.89671400	2.81544700
H	-4.96961000	-2.00880900	4.76493800
H	-5.10899400	-3.65574900	0.80191900
H	-6.12673000	-3.38756400	3.05139200
C	-1.76474700	1.52881000	2.42169100
C	-1.62737500	0.52727100	1.27183300
H	-0.81823800	1.56120600	2.96486700
H	-2.56233700	1.20067200	3.09270800
N	-0.45805400	0.68520800	0.39648000
S	0.09871200	2.14836800	0.00791500
O	0.70663200	2.88640900	1.12977800
O	0.96618100	1.96314300	-1.16876800
C	-1.32215000	3.10900600	-0.49961700
C	-1.64826500	4.26039200	0.20955100
C	-2.76215000	5.00305700	-0.17143900
C	-3.55051200	4.61034400	-1.25499500
C	-3.18528300	3.46242800	-1.96954100
C	-2.07659000	2.71015400	-1.60244500
H	-1.03430700	4.55815000	1.05317100
H	-3.02293300	5.89933000	0.38369700
H	-3.78005900	3.15559500	-2.82586800
H	-1.81037900	1.81376700	-2.15171300
C	-4.78222000	5.38488700	-1.64263400
H	-4.84580500	5.50624800	-2.72696800
H	-4.79132900	6.37422700	-1.18131800
H	-5.68387900	4.85436900	-1.31921300
C	-2.86675000	0.47531600	0.36515400
O	-2.90679800	-0.11176000	-0.69308900
O	-3.92058500	1.10250400	0.89288800
C	-5.12636000	1.00273200	0.13040400
H	-5.41664400	-0.04552300	0.02858400
H	-4.97776300	1.43721900	-0.86060900
H	-5.87841700	1.55922800	0.68595900
H	-2.01248900	2.53331900	2.07789000
C	5.65647000	1.09208500	1.05191900
C	4.51909300	0.29565800	1.15760100
C	4.52161500	-0.88854800	1.88702800

C	5.70466900	-1.27513500	2.51261000
C	6.85144100	-0.48329700	2.41094000
C	6.83517200	0.70655000	1.68504800
C	5.38012600	2.32353300	0.22542700
C	4.01311400	2.06080800	-0.44813400
C	3.36438900	0.90915700	0.39887500
H	3.61146100	-1.47535800	1.96858500
H	5.73597500	-2.19547500	3.08665100
H	7.76585700	-0.79866900	2.90359100
H	7.72931200	1.31833600	1.61015200
H	6.14182300	2.51841600	-0.53530100
H	3.35615200	2.92966200	-0.42984100
H	5.32199900	3.21153900	0.86358700
H	2.59922300	1.30441800	1.06701100
N	2.72749200	-0.07681600	-0.47877900
O	4.15723300	1.75370100	-1.82987100
C	1.58167600	-0.76235300	-0.36602400
C	3.26925800	-0.38380300	-1.69010300
N	1.49685100	-1.48800900	-1.48071000
N	2.54007300	-1.25302700	-2.33015400
C	4.46189400	0.40380500	-2.12016600
H	5.36696400	0.06135900	-1.60056800
H	4.60717800	0.31168800	-3.19612600
C	0.50468100	-2.47264400	-1.81858000
C	-0.61311900	-2.05747200	-2.54348800
C	0.69160700	-3.77405600	-1.35410400
C	-1.60026300	-3.01147400	-2.78005000
C	-0.32305200	-4.69221700	-1.61965200
C	-1.47679900	-4.32434700	-2.31545100
H	-2.49143600	-2.71955800	-3.32979400
H	-0.21367300	-5.71389200	-1.26544700
C	1.92291900	-4.14768100	-0.57147300
H	1.94082300	-3.64467200	0.40257300
H	2.83276900	-3.85763700	-1.10525600
C	-0.73895000	-0.62640400	-2.98215700
H	0.08052400	-0.34636200	-3.65107600
H	-0.69764400	0.02462600	-2.10257600
H	-1.68937000	-0.46458900	-3.49324400
H	1.95305000	-5.22322000	-0.39339200
C	-2.58791600	-5.31719100	-2.53732200
H	-2.22053400	-6.34356500	-2.47688200
H	-3.36428900	-5.19479000	-1.77472900
H	-3.05846400	-5.17180800	-3.51241100

TS6RS

C	4.96836100	-1.71704000	1.17465600
C	3.59513000	-1.68744100	1.40499700
C	3.03480100	-2.24429900	2.54953800
C	3.88363800	-2.85076200	3.47263600
C	5.26241600	-2.88756300	3.24826700
C	5.81473700	-2.31914800	2.10197500
C	5.31600300	-1.03221300	-0.12355900
C	3.96652600	-0.82906100	-0.85100000
C	2.87851400	-0.99041200	0.27211100
H	1.96227800	-2.19508400	2.71294700
H	3.47281800	-3.29542000	4.37307300
H	5.91104300	-3.36552100	3.97556400
H	6.88669400	-2.35200400	1.93178600
H	5.99610200	-1.61323600	-0.75330600
H	3.86881000	0.15975700	-1.29819700
H	5.79289300	-0.06471700	0.06506800
H	2.48861200	-0.01745600	0.56566000
N	1.74301800	-1.78239000	-0.20938000
O	3.81838100	-1.72549600	-1.94321600
C	0.41914100	-1.63362500	-0.05379700
C	1.93562100	-2.78480100	-1.11098000
N	-0.13174300	-2.56851000	-0.82923500
N	0.80315700	-3.29309900	-1.50580500
C	3.32531800	-3.00675500	-1.60531300
H	3.94168100	-3.50086000	-0.84232300
H	3.31100300	-3.61531200	-2.50871500
C	-1.52748600	-2.86846100	-1.00130300
C	-2.21337200	-2.27722200	-2.06024800
C	-2.13024300	-3.70546900	-0.05479900
C	-3.59192900	-2.50867900	-2.12065500
C	-3.50127900	-3.90343500	-0.16233900
C	-4.24990200	-3.29729400	-1.17938600
H	-4.15946900	-2.05255100	-2.92819400
H	-4.00128900	-4.53985300	0.56346900
C	-1.32021000	-4.32778800	1.05166100
H	-0.97130800	-3.57189300	1.76467600
H	-0.43604800	-4.83525200	0.65491000
C	-1.53669800	-1.39998500	-3.07828600
H	-0.45486700	-1.53924500	-3.09298000
H	-1.72096200	-0.34376000	-2.86040600
H	-1.93303800	-1.61360000	-4.07382000
H	-1.91944900	-5.05373900	1.60250700
C	-5.74172700	-3.49616700	-1.23913400

H	-6.15574100	-3.11461600	-2.17406000
H	-5.99949100	-4.55483400	-1.15110200
H	-6.23075700	-2.97083000	-0.41248700
C	-0.19898800	-0.63644500	0.92205400
O	0.57720200	-0.23536800	1.79372100
H	-2.24123800	-1.10085000	0.33915800
C	-1.69858100	-0.63827100	1.16096200
C	-2.11692400	0.81748200	1.32309700
H	-1.89436200	-1.19998700	2.08108600
H	-1.46823700	1.25648200	2.08552200
C	-3.55445000	1.00813600	1.75526100
C	-3.90445400	2.15004600	2.48440100
C	-4.55928900	0.09004400	1.43239500
C	-5.22254600	2.37380200	2.87262500
H	-3.12819500	2.86388700	2.74515100
C	-5.87815400	0.31055400	1.82260500
H	-4.31751400	-0.80966900	0.87102400
C	-6.21535100	1.45476100	2.54165000
H	-5.47338300	3.26474600	3.43989400
H	-6.64382400	-0.41489000	1.56434700
H	-7.24301000	1.62584500	2.84610200
C	-2.89962300	1.46366600	-1.04474200
C	-1.76052400	1.52979100	-0.02272200
H	-3.21063600	0.41999300	-1.16986000
H	-3.76524000	2.04255600	-0.71138200
N	-0.56747400	0.80491000	-0.49155500
S	0.37299800	1.30998100	-1.67436900
O	-0.33874800	1.85105800	-2.84299700
O	1.31978700	0.21345600	-1.96355700
C	1.37244100	2.65127400	-1.03340400
C	1.71024000	2.67263500	0.31566300
C	2.54411300	3.68431000	0.78988700
C	3.04070900	4.67009200	-0.06559500
C	2.67891300	4.62833400	-1.41872500
C	1.84845000	3.62779100	-1.90700500
H	1.29846800	1.92519500	0.99284800
H	2.80407300	3.71178800	1.84427500
H	3.05086500	5.39483300	-2.09352600
H	1.55205300	3.60215600	-2.95062800
C	3.94097500	5.76494600	0.44519600
H	3.50780600	6.75003100	0.24884200
H	4.10569400	5.67266700	1.52042100
H	4.91418800	5.73215400	-0.05358500
C	-1.41254700	2.99543900	0.31226200

O	-1.09905100	3.40890100	1.40661900
O	-1.43973800	3.77460800	-0.77021900
C	-0.96683700	5.11084700	-0.57211100
H	-1.64890400	5.65836100	0.08152500
H	0.02999900	5.08997700	-0.12414100
H	-0.93411300	5.56302100	-1.56135900
H	-2.55295300	1.84871200	-2.00363400

TS6SR

C	4.91332300	-1.97006500	-1.17801000
C	3.67405900	-1.36289400	-1.00108300
C	3.55474200	-0.07706100	-0.49726200
C	4.71261500	0.61099900	-0.14780100
C	5.96304900	0.00873500	-0.31467300
C	6.07365700	-1.28151700	-0.83320000
C	4.76365900	-3.34447700	-1.77667700
C	3.24929500	-3.65423800	-1.71459500
C	2.55322000	-2.25824600	-1.46524600
H	2.57456800	0.35584800	-0.36309800
H	4.63423700	1.61681200	0.25679300
H	6.86105000	0.55129000	-0.03616600
H	7.04874700	-1.74168700	-0.96199300
H	5.31975600	-4.11902600	-1.24006500
H	2.88440000	-4.08356500	-2.64799900
H	5.10931500	-3.35686100	-2.81534500
H	2.09409100	-1.88747800	-2.37947300
N	1.46986500	-2.38860400	-0.46869400
O	2.94982100	-4.63557800	-0.73376300
C	0.22483400	-1.87741300	-0.38600900
C	1.60056300	-3.28395600	0.55320400
N	-0.35800700	-2.52941200	0.62607000
N	0.49209200	-3.40450900	1.22391800
C	2.82997400	-4.12632500	0.58381600
H	3.70957900	-3.54484000	0.88629100
H	2.69450600	-4.96595600	1.26428100
C	-1.75813000	-2.61302700	0.96630300
C	-2.22700300	-2.05652700	2.15219700
C	-2.57542000	-3.33483200	0.08040300
C	-3.60198200	-2.15650100	2.39638900
C	-3.93213400	-3.40048700	0.37015200
C	-4.46719200	-2.79536600	1.51460200
H	-3.99589700	-1.71599300	3.30923400
H	-4.58819400	-3.94460400	-0.30454600
C	-2.00970900	-4.00174300	-1.14667000

H	-1.11192000	-4.58039200	-0.90796600
H	-1.74078600	-3.27230500	-1.91873100
C	-1.33294400	-1.38249300	3.15117600
H	-1.60393300	-0.32935800	3.25612400
H	-0.28408800	-1.41351800	2.85685300
H	-1.44614900	-1.86419400	4.12681600
H	-2.74615900	-4.67969300	-1.57966500
C	-5.94989000	-2.83703800	1.77392000
H	-6.38110600	-3.78530900	1.44471300
H	-6.17109500	-2.70136800	2.83432700
H	-6.45391400	-2.03615000	1.22290100
C	-0.28993000	-0.76569000	-1.30082800
O	0.52073500	-0.33485700	-2.10447600
H	-2.33113000	-1.00457700	-0.63806900
C	-1.77381800	-0.50139100	-1.42461600
C	-2.04427400	1.00315500	-1.38730400
H	-2.09157300	-0.90580800	-2.39313700
H	-1.36202700	1.47389500	-2.10086900
C	-3.46467900	1.35131600	-1.78564500
C	-3.72627400	2.56221900	-2.43479500
C	-4.54126800	0.50121400	-1.50535500
C	-5.02551300	2.91776800	-2.78942000
H	-2.89621800	3.22630500	-2.65563000
C	-5.84084000	0.85479900	-1.85876500
H	-4.37272900	-0.44970300	-1.00528700
C	-6.08849900	2.06532600	-2.50147400
H	-5.20584300	3.86143100	-3.29493100
H	-6.66142700	0.18072800	-1.63261600
H	-7.10137200	2.33958000	-2.77875600
C	-2.76275700	1.40019500	1.06197300
C	-1.64094500	1.53614700	0.02684900
H	-3.10430700	0.36009800	1.09148300
H	-2.37347500	1.66919200	2.04442200
N	-0.47680700	0.72323800	0.38674600
S	0.52082100	1.03831600	1.56847900
O	1.40463200	-0.14427800	1.68580900
O	-0.07721100	1.49714000	2.83669600
C	1.58103100	2.39987800	1.05444800
C	1.79123500	2.66140500	-0.29807900
C	2.65248200	3.68796300	-0.67175200
C	3.31153500	4.46274700	0.28930300
C	3.08197900	4.18618700	1.64067800
C	2.21879800	3.16442700	2.02727200
H	1.27404600	2.06693700	-1.04820600

H	2.81432600	3.89430900	-1.72648600
H	3.58109600	4.78239200	2.39960500
H	2.02663000	2.96289700	3.07615400
C	4.23428200	5.57614100	-0.13463100
H	3.68091300	6.36244900	-0.65691300
H	4.73347100	6.02730500	0.72507900
H	5.00056600	5.20711100	-0.82223400
C	-1.25480000	3.02129000	-0.14094200
O	-0.97583200	3.56470400	-1.18752800
O	-1.20144000	3.65551700	1.03236100
C	-0.67115200	4.98332300	0.98876300
H	0.33944400	4.96623000	0.57161900
H	-1.30736900	5.62463700	0.37592800
H	-0.65452500	5.32879200	2.02040200
H	-3.61534500	2.04126700	0.82073200

TS6SS

C	0.87640500	-1.58351100	-0.74406900
O	1.60269500	-1.64038700	-1.72432700
H	-1.04461900	-2.03145700	0.15945100
C	-0.50919700	-2.18117100	-0.77492700
C	-1.27504100	-1.51580600	-1.92236700
H	-0.38973000	-3.25249700	-0.97328800
H	-0.61151500	-1.50332100	-2.79432300
C	-2.54556000	-2.24320900	-2.31011400
C	-2.92505800	-2.30297600	-3.65490200
C	-3.36723800	-2.86134000	-1.35924700
C	-4.09856200	-2.94415100	-4.04286100
H	-2.28579800	-1.84527000	-4.40586700
C	-4.54040000	-3.50548300	-1.74487500
H	-3.09347800	-2.83159700	-0.30809400
C	-4.91210300	-3.54662200	-3.08676700
H	-4.37256400	-2.97818300	-5.09262800
H	-5.16391500	-3.98025600	-0.99352400
H	-5.82551000	-4.05105200	-3.38543400
C	-1.72942200	0.80606100	-2.81043700
C	-1.48931100	-0.00573300	-1.53339600
H	-0.83405100	0.76616200	-3.43256900
H	-2.57941600	0.39237600	-3.35717900
N	-0.31478300	0.34211300	-0.73905800
S	0.33896200	1.78080600	-0.76313200
O	0.73419900	2.30074600	-2.08926500
O	1.43413900	1.75423000	0.23195800
C	-0.90948600	2.94012700	-0.19038800

C	-0.98495500	4.21337600	-0.75170100
C	-1.94137400	5.10889200	-0.28583400
C	-2.83105100	4.75170600	0.73358500
C	-2.74096900	3.46779400	1.27684700
C	-1.78835800	2.56070600	0.81959100
H	-0.30359900	4.48290700	-1.55162300
H	-2.00378700	6.10271400	-0.72154700
H	-3.42499300	3.17114700	2.06870300
H	-1.73478000	1.55714800	1.23093400
C	-3.87460100	5.72854600	1.20989400
H	-4.34214300	5.38898600	2.13633400
H	-3.43704000	6.71491600	1.38540900
H	-4.66209500	5.85070000	0.45948800
C	-2.71642500	0.02798200	-0.60197700
O	-2.74839800	-0.47819400	0.49861000
O	-3.77276700	0.65150500	-1.13500300
C	-4.93923500	0.67234400	-0.31005000
H	-5.27245100	-0.34782700	-0.10560400
H	-4.72130900	1.17663700	0.63451900
H	-5.69410400	1.21854300	-0.87192700
H	-1.94622900	1.85276100	-2.58609400
C	5.77167800	0.20228100	-1.02188900
C	4.40421100	-0.03978500	-1.12719400
C	3.57537800	0.79897800	-1.86461700
C	4.13787200	1.91459900	-2.47680000
C	5.50690500	2.17096100	-2.36656800
C	6.33449800	1.31295200	-1.64610300
C	6.46706000	-0.86356000	-0.21892100
C	5.34140900	-1.77275200	0.32906400
C	4.01196800	-1.29695500	-0.38787600
H	2.51701600	0.59611200	-1.96453400
H	3.49599900	2.58731600	-3.03582300
H	5.93155300	3.04618100	-2.84848500
H	7.39999600	1.50788900	-1.56783700
H	7.05476700	-0.46033300	0.61268000
H	5.51702200	-2.81951900	0.08063100
H	7.15460500	-1.44305600	-0.84223900
H	3.64557200	-2.06594300	-1.06305200
N	2.93449800	-1.06533300	0.60527200
O	5.28606000	-1.75437200	1.74556100
C	1.59219800	-1.21759900	0.55518200
C	3.24293000	-0.69215800	1.87968300
N	1.16332400	-0.99044300	1.80318800
N	2.18619200	-0.66087700	2.63430100

C	4.67867500	-0.58459500	2.26010900
H	5.13067900	0.32923900	1.85201900
H	4.78215400	-0.58740400	3.34453600
C	-0.14680200	-1.11162500	2.39646200
C	-0.69536600	0.02477200	3.01027200
C	-0.75101900	-2.37013800	2.46934700
C	-1.96368100	-0.10509500	3.56823800
C	-2.02508900	-2.43778900	3.03614900
C	-2.65964600	-1.31473100	3.55626900
H	-2.42008000	0.76984400	4.02608400
H	-2.52301800	-3.40405400	3.07786000
C	-0.09260500	-3.65438500	2.02718600
H	0.06576700	-4.29648600	2.89817700
H	0.87671300	-3.50748400	1.54874400
C	0.06112600	1.31989800	3.14428400
H	0.60220700	1.57550700	2.23028300
H	0.79221800	1.23633100	3.95423400
H	-0.62880000	2.13039600	3.38808900
H	-0.73583900	-4.19908800	1.33085400
C	-4.06698300	-1.39578100	4.08255600
H	-4.77584300	-1.15853500	3.28183300
H	-4.30058300	-2.39854200	4.44723300
H	-4.23107200	-0.68138900	4.89247800

M5RR

C	-0.60620100	-0.43938500	-0.79663800
O	-1.29906600	-0.14723800	-1.84051800
H	0.93235200	-1.81879000	-0.02776500
C	0.44622900	-1.56048900	-0.96812400
C	1.43093800	-0.88593600	-1.90816200
H	-0.01325100	-2.44719500	-1.41316800
H	0.90482900	-0.71621000	-2.85143100
C	2.71673500	-1.62473400	-2.20558600
C	3.29774200	-1.50148000	-3.47213800
C	3.36070500	-2.42318800	-1.25292800
C	4.49627500	-2.14056500	-3.77850100
H	2.79614300	-0.90515800	-4.23029000
C	4.55634000	-3.06837000	-1.55856900
H	2.93110400	-2.53817200	-0.26238500
C	5.13094800	-2.92613400	-2.82002500
H	4.92894700	-2.03016900	-4.76781700
H	5.03835400	-3.68739600	-0.80801200
H	6.06231300	-3.43095400	-3.05590000
C	1.68497600	1.56650000	-2.42840000

C	1.62495800	0.55540500	-1.28286200
H	0.70818600	1.58002600	-2.91548500
H	2.45033800	1.24703000	-3.13990600
N	0.47532600	0.68128500	-0.35561600
S	-0.05644300	2.17526500	0.09728600
O	-0.64306000	2.96164900	-0.99403200
O	-0.90556800	1.95376000	1.27479000
C	1.41752000	3.03669400	0.60732800
C	1.82000600	4.15288000	-0.11918600
C	2.96951500	4.83506300	0.26566600
C	3.71361900	4.41836200	1.37166200
C	3.26453400	3.31428200	2.10793600
C	2.11919500	2.62170200	1.73821000
H	1.23387900	4.47478800	-0.97339500
H	3.29098700	5.70337300	-0.30154000
H	3.82291000	2.99511900	2.98365400
H	1.78178000	1.76433500	2.30968100
C	4.98498000	5.12258100	1.76326700
H	5.04703000	5.24878200	2.84698500
H	5.05698900	6.10503300	1.29326100
H	5.85537900	4.53570000	1.45150800
C	2.89267100	0.51907000	-0.42138300
O	2.97965500	-0.07308200	0.63055500
O	3.91310400	1.16339900	-0.98794700
C	5.15217300	1.07957000	-0.27646900
H	5.46830500	0.03665000	-0.20275000
H	5.03443400	1.49765800	0.72563500
H	5.86732800	1.66023800	-0.85536500
H	1.93959800	2.57281000	-2.09712900
C	-5.62654600	1.18689900	-1.06694400
C	-4.45146000	0.44862000	-1.18207200
C	-4.35821000	-0.65210100	-2.02733500
C	-5.48860600	-1.01936300	-2.75465000
C	-6.67486500	-0.28934500	-2.64047900
C	-6.75174900	0.82083700	-1.80120600
C	-5.44714800	2.34508500	-0.11693900
C	-4.11001300	2.06708200	0.60808300
C	-3.36604300	1.02936300	-0.30442900
H	-3.40974600	-1.17408600	-2.11749000
H	-5.44784700	-1.87564900	-3.42022100
H	-7.54622800	-0.58862100	-3.21455600
H	-7.67475200	1.38731900	-1.71943300
H	-6.25579500	2.44382000	0.61331900
H	-3.49710900	2.96182700	0.71777800

H	-5.38829700	3.28974900	-0.66782900
H	-2.58439300	1.50145700	-0.89742600
N	-2.73720300	-0.00914400	0.51764700
O	-4.32049200	1.61551200	1.94148900
C	-1.55636400	-0.64082600	0.41585500
C	-3.36072900	-0.47239400	1.63588600
N	-1.53720400	-1.49344800	1.44428100
N	-2.65429900	-1.39125400	2.22767300
C	-4.60355500	0.23436900	2.06638300
H	-5.46473000	-0.06881600	1.45672200
H	-4.81257500	0.02388100	3.11494100
C	-0.57022300	-2.51231000	1.75408900
C	0.55856500	-2.16052100	2.49222200
C	-0.81131800	-3.80102000	1.27428100
C	1.50081500	-3.16193900	2.72525500
C	0.15807800	-4.76662900	1.53494100
C	1.32211500	-4.46128600	2.24563100
H	2.39817800	-2.91620700	3.28719400
H	0.00554700	-5.77798000	1.16684700
C	-2.05984500	-4.11292300	0.49282100
H	-2.14147000	-3.47449100	-0.39422200
H	-2.95395200	-3.94011600	1.09934600
C	0.76550100	-0.74046000	2.93507600
H	-0.12823200	-0.33592300	3.41808200
H	0.98576900	-0.12937200	2.05299200
H	1.60832900	-0.67116700	3.62531400
H	-2.05875300	-5.15304000	0.16468500
C	2.38024100	-5.51167600	2.46268000
H	1.93612900	-6.50339600	2.57353100
H	3.06107800	-5.54798500	1.60573100
H	2.97608700	-5.29475200	3.35166800

M5RS

C	5.10649200	-1.55798200	1.25868200
C	3.72741700	-1.41722900	1.39021600
C	3.06888400	-1.75096300	2.56926300
C	3.82429200	-2.25465300	3.62566900
C	5.20780700	-2.40818100	3.49942600
C	5.85941100	-2.05598900	2.31886000
C	5.57217500	-1.09007800	-0.09754900
C	4.28194100	-0.92391700	-0.93387800
C	3.11962400	-0.86307800	0.12250300
H	1.99780400	-1.58892900	2.64825700
H	3.33666200	-2.52547400	4.55668900

H	5.78144100	-2.80366800	4.33189400
H	6.93520800	-2.17299100	2.22636300
H	6.25103100	-1.79031100	-0.59352700
H	4.28372100	-0.00801500	-1.52454900
H	6.09605600	-0.13192500	-0.01589800
H	2.74965000	0.15070600	0.25477900
N	1.97701200	-1.67219600	-0.32071000
O	4.14395300	-1.96232000	-1.89657100
C	0.65010300	-1.46638500	-0.24790500
C	2.18265700	-2.82300200	-1.02100800
N	0.11268300	-2.51284300	-0.88731600
N	1.05851000	-3.36553200	-1.38518500
C	3.58604700	-3.16223700	-1.39562700
H	4.14587300	-3.55110200	-0.53462500
H	3.59403500	-3.90167100	-2.19594300
C	-1.27127700	-2.84450500	-1.10028000
C	-1.95222400	-2.27942900	-2.17377000
C	-1.86145800	-3.74560800	-0.20112300
C	-3.31267900	-2.59103600	-2.29539600
C	-3.21193700	-4.02193700	-0.36702300
C	-3.95816200	-3.43673500	-1.39982700
H	-3.87304100	-2.15130800	-3.11718600
H	-3.69932000	-4.70474100	0.32458600
C	-1.05593900	-4.35720600	0.91317900
H	-0.61024300	-3.58540700	1.55017300
H	-0.23540700	-4.96132500	0.51472300
C	-1.29454700	-1.36920200	-3.17373700
H	-0.21396400	-1.30387200	-3.03550800
H	-1.69367500	-0.35472400	-3.09339600
H	-1.49307400	-1.72978300	-4.18670300
H	-1.68509200	-4.99292400	1.53721100
C	-5.43299900	-3.71765500	-1.51926900
H	-5.82477300	-3.38007600	-2.48048300
H	-5.63948500	-4.78583400	-1.41435900
H	-5.98462100	-3.19807100	-0.72904100
C	0.01377200	-0.30237900	0.58515900
O	0.88704400	0.18275000	1.40381000
H	-1.91900000	-1.36957800	0.57045500
C	-1.32840300	-0.72921900	1.22384600
C	-2.03222000	0.59868700	1.43419700
H	-1.12638400	-1.24533500	2.16527800
H	-1.44113800	1.16730400	2.15498500
C	-3.46216100	0.53353300	1.92092700
C	-3.97442700	1.59617100	2.67302500

C	-4.30568400	-0.54375900	1.62825600
C	-5.29396500	1.58790400	3.11720500
H	-3.32387100	2.43412900	2.90776400
C	-5.62536700	-0.55491300	2.07414600
H	-3.93819400	-1.38714900	1.04813500
C	-6.12521700	0.51065600	2.81837400
H	-5.67082500	2.42142300	3.70186900
H	-6.26352400	-1.40163200	1.83996400
H	-7.15312300	0.49944200	3.16652900
C	-3.01153900	1.08185500	-0.90958100
C	-1.86076700	1.32755700	0.06437000
H	-3.16775100	0.00334900	-1.01810600
H	-3.93529100	1.53074900	-0.53504500
N	-0.59894800	0.72478800	-0.45978700
S	0.29565100	1.42185600	-1.64528300
O	-0.56511300	1.80686500	-2.76262900
O	1.39059200	0.48425500	-1.92405700
C	1.03216500	2.92493500	-1.03105200
C	1.45322200	3.01196700	0.29226100
C	2.09070700	4.17814600	0.70842600
C	2.31511700	5.23963900	-0.17346800
C	1.88199400	5.11582200	-1.49860200
C	1.23468600	3.96607500	-1.93481800
H	1.26986700	2.17856900	0.97227900
H	2.41983900	4.26548800	1.74014700
H	2.04929500	5.93268900	-2.19495300
H	0.88125600	3.87440000	-2.95638900
C	2.97992400	6.50508000	0.30128000
H	2.23690400	7.20106700	0.70393600
H	3.70122800	6.29832800	1.09493800
H	3.49755300	7.01048700	-0.51685500
C	-1.70481400	2.83686300	0.35332500
O	-1.42625800	3.31134600	1.43035300
O	-1.90803600	3.57947200	-0.73407700
C	-1.68393400	4.98329700	-0.55948500
H	-2.42632700	5.39713100	0.12551700
H	-0.68209400	5.15134000	-0.15696500
H	-1.78189100	5.42476300	-1.54901200
H	-2.77029600	1.51086200	-1.88221500

M5SR

C	5.32680400	-1.10156100	-1.20410400
C	4.04241400	-0.63957500	-0.92901000
C	3.83064100	0.58168100	-0.29670500

C	4.94143400	1.32388200	0.09562800
C	6.23443400	0.85688800	-0.15654400
C	6.43624500	-0.35384300	-0.81515900
C	5.29705000	-2.40158200	-1.96300500
C	3.81032500	-2.82917300	-1.99446400
C	2.99219500	-1.58478200	-1.46443400
H	2.81828500	0.92623300	-0.12662900
H	4.79900600	2.27795500	0.59384500
H	7.09052800	1.44732100	0.15514700
H	7.44138600	-0.70856300	-1.02379900
H	5.89827400	-3.18905600	-1.49630400
H	3.48296000	-3.06764200	-3.00668100
H	5.67888600	-2.26999600	-2.98007000
H	2.40460800	-1.11434600	-2.24989000
N	2.01361200	-2.00881300	-0.43775700
O	3.59503200	-4.02953200	-1.26613200
C	0.76790500	-1.58486000	-0.14153200
C	2.28405200	-3.07674400	0.37388600
N	0.32919300	-2.43966000	0.79397600
N	1.26991800	-3.37258700	1.12802600
C	3.54520500	-3.83270800	0.13457900
H	4.42070000	-3.28242500	0.50442900
H	3.49891600	-4.80753200	0.61910600
C	-0.98962100	-2.58031300	1.36117300
C	-1.23703600	-2.10322700	2.65206600
C	-1.94325200	-3.30406500	0.63076800
C	-2.54274400	-2.21359900	3.13237600
C	-3.23141100	-3.38709200	1.15829700
C	-3.55685100	-2.81753800	2.39094600
H	-2.76366900	-1.82595500	4.12402500
H	-3.99282600	-3.92530200	0.59794600
C	-1.60749500	-4.05492800	-0.63547100
H	-0.67934700	-3.71930900	-1.10070700
H	-2.41013300	-3.95813400	-1.37144500
C	-0.14341400	-1.61399000	3.56322300
H	-0.49236600	-0.77056300	4.16028800
H	0.74400000	-1.29729700	3.01843600
H	0.13538700	-2.42888100	4.24006200
H	-1.49516800	-5.11885300	-0.40544400
C	-4.97049500	-2.85905000	2.90764500
H	-5.50303200	-3.73793600	2.53741700
H	-4.99280000	-2.87135000	3.99945600
H	-5.52071200	-1.97264400	2.57479800
C	0.08464900	-0.38170200	-0.88142600

O	0.94362600	0.27077500	-1.59345300
H	-1.69812200	-1.65523400	-1.06134300
C	-1.17898600	-0.88128800	-1.62375900
C	-2.03716900	0.36894200	-1.70814100
H	-0.89202300	-1.26802200	-2.60399200
H	-1.50326000	1.08490800	-2.33705700
C	-3.43308900	0.18782400	-2.25834500
C	-4.00552100	1.20686000	-3.02598600
C	-4.18540900	-0.96718900	-2.01669400
C	-5.29326000	1.07714300	-3.54104400
H	-3.42848900	2.10754600	-3.21566800
C	-5.47287300	-1.09937600	-2.52995900
H	-3.77087400	-1.77214900	-1.41422900
C	-6.03094500	-0.07803300	-3.29558500
H	-5.71817500	1.87788600	-4.13837600
H	-6.03998600	-2.00365600	-2.33198200
H	-7.03260600	-0.18361300	-3.69982700
C	-3.08823800	0.43076200	0.66254500
C	-1.98444200	0.94490600	-0.26024200
H	-3.10101600	-0.66270800	0.63864800
H	-2.89083400	0.75600500	1.68415000
N	-0.65622500	0.46457800	0.21541600
S	0.16399100	1.14366400	1.45865400
O	1.38319000	0.34007300	1.60140600
O	-0.70842000	1.27893700	2.62354000
C	0.67609100	2.79074200	1.00666700
C	1.05477000	3.06995100	-0.30241900
C	1.52408400	4.34812000	-0.59647800
C	1.62373800	5.33180000	0.39211400
C	1.23765500	5.01372200	1.69987400
C	0.75667800	3.74906500	2.01512000
H	0.97708100	2.28875000	-1.06055800
H	1.81828200	4.58574400	-1.61492400
H	1.31160300	5.76893400	2.47742700
H	0.43989800	3.50242300	3.02297500
C	2.10577500	6.71816400	0.05400500
H	1.25834200	7.37595900	-0.16511300
H	2.65733300	7.15865300	0.88781000
H	2.75289000	6.70808400	-0.82546300
C	-2.04658300	2.48406100	-0.36807100
O	-1.86983500	3.11524500	-1.38429500
O	-2.32069600	3.05747300	0.80322200
C	-2.30137300	4.48937100	0.79768500
H	-1.35295200	4.84680900	0.38980000

H	-3.12658600	4.87084000	0.19315000
H	-2.41207800	4.79087900	1.83727800
H	-4.06544200	0.80322300	0.34279500

M5SS

C	5.30837800	-1.40593900	-1.28412900
C	4.13467300	-0.90868900	-0.71756400
C	4.16318100	0.02688100	0.30896500
C	5.40629600	0.46927700	0.76230000
C	6.58558300	-0.01759200	0.19612800
C	6.54533900	-0.96037500	-0.83133300
C	4.99522700	-2.39875200	-2.37665700
C	3.51208300	-2.75467200	-2.15460900
C	2.93226800	-1.50538400	-1.41444700
H	3.24187700	0.38266100	0.75856700
H	5.45550400	1.19673300	1.56639100
H	7.54379800	0.33538800	0.56419200
H	7.46413000	-1.34601400	-1.26327000
H	5.60998900	-3.30198900	-2.34543700
H	2.98369100	-2.92398500	-3.09465200
H	5.12608200	-1.94081400	-3.36361500
H	2.48255700	-0.79917700	-2.11132300
N	1.85619200	-1.90829300	-0.49670700
O	3.37098500	-3.97731200	-1.43313900
C	0.61917000	-1.43007800	-0.23816100
C	2.01218700	-3.06176800	0.21808300
N	0.07699100	-2.33236000	0.59196200
N	0.93754300	-3.35464000	0.88399700
C	3.24599600	-3.86407400	-0.02587400
H	4.12314600	-3.39145900	0.43237900
H	3.12339100	-4.86833700	0.37887900
C	-1.28024400	-2.48929300	1.05836000
C	-1.59508100	-2.18142900	2.38409500
C	-2.19207300	-3.09973400	0.18881800
C	-2.90246500	-2.42345700	2.80226900
C	-3.49436700	-3.28472500	0.64723400
C	-3.87081000	-2.93927000	1.94490800
H	-3.16935600	-2.18697000	3.82992800
H	-4.22332600	-3.73723300	-0.02164500
C	-1.81027800	-3.62275900	-1.17476000
H	-0.85299500	-3.23974400	-1.53242800
H	-2.57322100	-3.36058400	-1.91291200
C	-0.59646800	-1.61647200	3.35648300
H	-0.75123900	-0.53911100	3.46809300

H	0.43173800	-1.76429500	3.02802400
H	-0.73176300	-2.08359300	4.33523500
H	-1.73822100	-4.71421200	-1.14425400
C	-5.29489400	-3.10624800	2.40418700
H	-5.79587100	-3.91476900	1.86698300
H	-5.34455200	-3.31573900	3.47520100
H	-5.85875800	-2.18528800	2.22096000
C	0.06957500	-0.12551800	-0.91900500
O	0.98946400	0.43360200	-1.64181500
H	-1.92249300	-1.05482400	-1.07658900
C	-1.26885300	-0.40040000	-1.65373900
C	-1.87008200	0.99673000	-1.73110000
H	-1.06564800	-0.82896500	-2.63738600
H	-1.20660900	1.60184000	-2.35708800
C	-3.27857700	1.10802500	-2.26791300
C	-3.62571800	2.21192500	-3.05263600
C	-4.26145700	0.15057400	-1.98915200
C	-4.92115600	2.36795900	-3.53872000
H	-2.86656300	2.95413000	-3.28746400
C	-5.55753500	0.30399900	-2.47590700
H	-4.01923100	-0.71300300	-1.37519000
C	-5.89254900	1.41357200	-3.24973200
H	-5.16960100	3.23254600	-4.14599400
H	-6.30739700	-0.44888400	-2.25287900
H	-6.90231300	1.52931500	-3.63014000
C	-1.49606900	3.06753000	-0.31311900
C	-1.68404100	1.55185200	-0.27326400
H	-0.59565000	3.30684400	-0.88313900
H	-2.36107400	3.51656800	-0.80510300
N	-0.52237400	0.77556400	0.20500800
S	0.34159600	1.30220400	1.48677300
O	1.30485600	0.23706000	1.78459900
O	-0.60965500	1.71667300	2.52114000
C	1.30060900	2.75433700	1.08471300
C	2.06253900	2.78039000	-0.08082000
C	2.86235700	3.89116100	-0.32464100
C	2.91012300	4.96497300	0.57112500
C	2.13153000	4.90577800	1.73070600
C	1.32179300	3.80573700	1.99565000
H	1.98838100	1.94915500	-0.78364600
H	3.46058900	3.92741800	-1.23103800
H	2.15873000	5.73194200	2.43557300
H	0.71083800	3.75917000	2.89044300
C	3.75710200	6.17466600	0.27491500

H	4.63898400	5.90498900	-0.31031600
H	3.18767700	6.90894200	-0.30434500
H	4.08567900	6.66271400	1.19516100
C	-2.91593300	1.13963900	0.54131800
O	-3.12321000	0.01984100	0.93990000
O	-3.79421800	2.13997300	0.66886500
C	-5.04777600	1.76916300	1.24788700
H	-5.54082500	1.02697800	0.61485300
H	-4.89752500	1.35210200	2.24496200
H	-5.63621100	2.68299800	1.29582900
H	-1.41361700	3.49546100	0.68843200

TS7RR

C	-0.56629600	-0.17391400	-1.47097500
O	-1.53735800	-0.01482300	-2.21343100
H	0.61791200	-1.72201300	-0.51979000
C	0.35741400	-1.39233500	-1.52377900
C	1.59340800	-0.86383100	-2.24229700
H	-0.13342000	-2.19615900	-2.07461400
H	1.34068200	-0.71117700	-3.29808500
C	2.83477900	-1.72642800	-2.17115900
C	3.67953500	-1.79835600	-3.28273200
C	3.18391400	-2.44062500	-1.01719000
C	4.85284700	-2.54760100	-3.24588200
H	3.40873300	-1.26392800	-4.18990800
C	4.35739400	-3.18998900	-0.97972700
H	2.54889600	-2.40870500	-0.13580200
C	5.19686600	-3.24420900	-2.09058800
H	5.49348300	-2.58878700	-4.12091600
H	4.61321600	-3.73650400	-0.07683900
H	6.10896300	-3.83136900	-2.05820500
C	2.43223300	1.47310400	-2.71812700
C	1.78212900	0.58375000	-1.66010600
H	1.75740700	1.57770600	-3.56878800
H	3.36059100	0.99592700	-3.04091800
N	0.40385700	0.94345100	-1.27036100
S	-0.08839900	2.52204600	-1.19090500
O	0.02287400	3.20915100	-2.47510100
O	-1.38193200	2.52838800	-0.51398300
C	1.12019200	3.22221000	-0.09468500
C	1.96424400	4.23441800	-0.53411600
C	2.90589800	4.75398600	0.35063500
C	3.00130600	4.27765800	1.65995600
C	2.11762900	3.27367700	2.08113800

C	1.17494800	2.74293400	1.21299300
H	1.88120200	4.60070100	-1.55228300
H	3.57529600	5.54106700	0.01714600
H	2.17426500	2.90552500	3.10243400
H	0.50434100	1.94817900	1.52690800
C	4.04414100	4.81058400	2.60596100
H	3.61122100	5.02253400	3.58684000
H	4.49908600	5.72506500	2.22140300
H	4.83939500	4.07226800	2.75179300
C	2.61433800	0.47635700	-0.37718300
O	2.19923300	-0.03764100	0.63512900
O	3.84888800	0.95808300	-0.50818800
C	4.68372300	0.79185700	0.64338300
H	4.82016000	-0.27209000	0.85037900
H	4.22519900	1.27652900	1.50823900
H	5.63236800	1.26208800	0.39363100
H	2.68085600	2.46354800	-2.33723100
C	-5.90102900	0.19830100	-0.73778400
C	-4.59736200	-0.27835500	-0.84948900
C	-4.32393500	-1.53097400	-1.38582600
C	-5.39294400	-2.32201400	-1.80190100
C	-6.70480200	-1.85461000	-1.68560900
C	-6.96833300	-0.59106200	-1.15865300
C	-5.91405800	1.59078600	-0.15519300
C	-4.48124600	1.81334900	0.38483800
C	-3.60212800	0.73825800	-0.33967000
H	-3.29406600	-1.86163100	-1.48892700
H	-5.20822700	-3.30533700	-2.22246800
H	-7.52846000	-2.48265500	-2.01039000
H	-7.98981600	-0.23209600	-1.07280500
H	-6.64492500	1.72309000	0.64828900
H	-4.10352600	2.81142200	0.16093700
H	-6.14422600	2.33009600	-0.92983700
H	-3.02882300	1.17966800	-1.14934600
N	-2.65546100	0.12609700	0.59394400
O	-4.43168800	1.72677100	1.80485000
C	-1.41127300	-0.38124200	0.39698000
C	-3.07576700	-0.16967700	1.86206400
N	-1.16431500	-0.97616900	1.58222200
N	-2.18050200	-0.85140400	2.50683500
C	-4.37780200	0.40649200	2.31378100
H	-5.22139000	-0.20242700	1.96023900
H	-4.41221400	0.46288900	3.40187300
C	-0.11218300	-1.90536500	1.89356400

C	0.92512200	-1.54059100	2.74831800
C	-0.22975400	-3.19927900	1.36186800
C	1.92119600	-2.49092400	2.99396600
C	0.78811400	-4.10808200	1.62988900
C	1.88042900	-3.76492400	2.43460700
H	2.75071200	-2.21912200	3.64300600
H	0.72323400	-5.11069700	1.21397400
C	-1.42996900	-3.59121000	0.53969000
H	-1.42852300	-3.09552500	-0.43582400
H	-2.35912700	-3.30698600	1.04438500
C	1.00942900	-0.18089600	3.38585400
H	1.30040300	-0.27419300	4.43521000
H	0.05662100	0.34990300	3.34094600
H	1.76849000	0.41285100	2.86847100
H	-1.44221300	-4.66925100	0.37195300
C	2.96141700	-4.77571200	2.71961000
H	2.63773000	-5.48274400	3.49031500
H	3.20109400	-5.35577800	1.82461600
H	3.87403900	-4.29097500	3.07322900

TS7RS

C	5.51358600	0.36113000	1.16300100
C	4.17359700	-0.01020800	1.23719600
C	3.65513800	-0.63968300	2.36326600
C	4.51270300	-0.90458700	3.42895200
C	5.85973900	-0.53891700	3.36016400
C	6.36896300	0.09887800	2.23024300
C	5.81119100	1.03977900	-0.15143100
C	4.56932200	0.76930300	-1.03323500
C	3.43513500	0.36013700	-0.02933500
H	2.60105800	-0.90140800	2.40144200
H	4.13404700	-1.39675000	4.31905400
H	6.51687200	-0.75597500	4.19650600
H	7.41718000	0.37923500	2.18162500
H	6.71165400	0.66176000	-0.64489100
H	4.26551800	1.65213600	-1.59659000
H	5.94676700	2.11711600	-0.00779800
H	2.73520900	1.17873400	0.12942600
N	2.66813600	-0.76887700	-0.54675300
O	4.83445100	-0.20998100	-2.03158600
C	1.35504100	-1.07608300	-0.39604000
C	3.30363300	-1.77147100	-1.22677800
N	1.28777600	-2.27322700	-1.00411200
N	2.47826700	-2.72389600	-1.53683900

C	4.73390000	-1.55425700	-1.59469100
H	5.39599500	-1.75651500	-0.74141500
H	5.01791400	-2.19878700	-2.42655800
C	0.14017700	-3.12801400	-1.08963500
C	-0.77044600	-2.94191100	-2.13273700
C	-0.00528600	-4.13079100	-0.12721400
C	-1.87900000	-3.78680800	-2.17632700
C	-1.12561900	-4.95844200	-0.21636400
C	-2.07358300	-4.79510000	-1.22807600
H	-2.61009500	-3.65352500	-2.97039200
H	-1.26386500	-5.73972300	0.52675300
C	1.00997300	-4.28375500	0.97328400
H	1.07404100	-3.36863900	1.57301900
H	2.00629900	-4.46751800	0.56070000
C	-0.55256400	-1.85645800	-3.15151700
H	0.42789300	-1.96237900	-3.62556400
H	-0.58430800	-0.86563200	-2.68620700
H	-1.32183200	-1.89407700	-3.92496700
H	0.74516100	-5.11126900	1.63288900
C	-3.29041700	-5.68063900	-1.30563000
H	-3.29587900	-6.25541800	-2.23638700
H	-3.32325100	-6.38383700	-0.47088900
H	-4.20580900	-5.08177500	-1.28665700
C	0.10473700	0.18885900	0.81580500
O	0.92358900	0.87298100	1.42034600
H	-0.78380000	-1.77470300	0.81175300
C	-0.77117000	-0.88654300	1.44273100
C	-2.13990600	-0.21376600	1.47732900
H	-0.39432800	-1.14191200	2.43458900
H	-2.11090600	0.56810700	2.24108600
C	-3.32615000	-1.10749900	1.75755500
C	-4.46187500	-0.55979900	2.36260100
C	-3.34283400	-2.45843900	1.39892000
C	-5.58921100	-1.34170800	2.60024600
H	-4.45435700	0.48957700	2.64616600
C	-4.46784800	-3.24303000	1.64007100
H	-2.47763200	-2.91305700	0.92423900
C	-5.59549400	-2.68762600	2.24018800
H	-6.46123100	-0.90019300	3.07235200
H	-4.45789800	-4.29269500	1.36051600
H	-6.47136900	-3.29945500	2.43108400
C	-2.91409000	-0.27843000	-0.99128300
C	-2.23178300	0.53353800	0.10482200
H	-2.46556300	-1.27474700	-1.03644500

H	-3.97786100	-0.39224900	-0.76721300
N	-0.79387100	0.78924800	-0.19752700
S	-0.25323000	1.82468500	-1.37228200
O	-1.06448200	1.64027200	-2.57115900
O	1.18777600	1.62838500	-1.48232000
C	-0.54920300	3.47272400	-0.77597900
C	-0.34517600	3.77219100	0.56867000
C	-0.51947000	5.08568800	0.98903200
C	-0.87291900	6.09572400	0.08628100
C	-1.06540800	5.76059500	-1.25777400
C	-0.91041000	4.45043000	-1.69770600
H	-0.06045400	2.98435600	1.26217300
H	-0.37748400	5.33316700	2.03714400
H	-1.35065200	6.53293200	-1.96612300
H	-1.08197100	4.18157700	-2.73464700
C	-1.02462500	7.51746400	0.55888000
H	-1.58050000	8.11869900	-0.16307600
H	-1.54378800	7.55828600	1.51949500
H	-0.04257000	7.98074400	0.69702300
C	-2.96143200	1.87439200	0.34361600
O	-3.09930800	2.40140000	1.42366600
O	-3.40827700	2.40690500	-0.79040600
C	-4.00595700	3.70333000	-0.66029600
H	-4.93734200	3.62844300	-0.09604300
H	-3.31776000	4.37835200	-0.14626900
H	-4.19487300	4.04490100	-1.67580500
H	-2.79845700	0.21551600	-1.95514200

TS7SR

C	5.64013000	-0.05490100	-1.32077400
C	4.34524900	0.12451900	-0.83763600
C	4.00008500	1.23933000	-0.08196000
C	4.99459400	2.17429000	0.20264400
C	6.29700700	1.99755200	-0.26986900
C	6.62841500	0.88322200	-1.03952800
C	5.73863000	-1.31326700	-2.14570000
C	4.44547800	-2.09173400	-1.82671500
C	3.44485000	-1.00597600	-1.28974300
H	2.98310100	1.36465300	0.27567400
H	4.75292200	3.04977500	0.79702700
H	7.05871500	2.73531500	-0.03705000
H	7.64051200	0.74798500	-1.40968500
H	6.61311000	-1.92700900	-1.91256500
H	4.03490000	-2.58238600	-2.71105300

H	5.78102200	-1.07095000	-3.21348400
H	2.77144800	-0.66921500	-2.08031400
N	2.60813700	-1.56431800	-0.23112400
O	4.69291900	-3.15508800	-0.91062700
C	1.26829400	-1.46658700	-0.02520400
C	3.14798900	-2.44513400	0.66977300
N	1.08988900	-2.31327100	1.00119100
N	2.23444500	-2.93992000	1.44764900
C	4.57443800	-2.82950800	0.46750800
H	5.25409000	-2.01702800	0.75466100
H	4.81840500	-3.72389600	1.04012700
C	-0.18677000	-2.72003000	1.51110200
C	-0.63687400	-2.21702800	2.73295000
C	-0.91966800	-3.65252400	0.76233700
C	-1.91092700	-2.60244400	3.15659300
C	-2.18658800	-4.00254100	1.22499100
C	-2.70583300	-3.46955300	2.40890300
H	-2.28940300	-2.20897600	4.09705800
H	-2.77857600	-4.71424100	0.65364400
C	-0.32669900	-4.32288900	-0.45207200
H	0.11151100	-3.61048600	-1.15573100
H	-1.08479900	-4.90783300	-0.97684100
C	0.24512100	-1.36086400	3.60039300
H	-0.35840200	-0.73215400	4.25654500
H	0.89035700	-0.71456800	3.00389800
H	0.88277700	-2.00089300	4.21988100
H	0.47664100	-5.00212500	-0.14767400
C	-4.10419900	-3.81128000	2.85245800
H	-4.37684600	-4.82765000	2.55870200
H	-4.20978100	-3.72186000	3.93587200
H	-4.82625100	-3.12897400	2.39111000
C	0.12707800	0.04917100	-1.09234600
O	1.02569800	0.72782700	-1.57421000
H	-0.92036700	-1.80985600	-1.28929800
C	-0.80520500	-0.88419800	-1.85142000
C	-2.11062000	-0.09789200	-1.86077900
H	-0.41178100	-1.09414800	-2.84705200
H	-1.98444800	0.76285500	-2.52272800
C	-3.35233700	-0.84521300	-2.28868100
C	-4.39714800	-0.13096500	-2.88377300
C	-3.51428600	-2.21744800	-2.07512300
C	-5.57705900	-0.76980800	-3.25543300
H	-4.27578400	0.93624800	-3.05011800
C	-4.69354100	-2.85827400	-2.44659100

H	-2.72228600	-2.79615800	-1.60643800
C	-5.72847400	-2.13721200	-3.03749400
H	-6.37646400	-0.20037200	-3.71907800
H	-4.80300900	-3.92442100	-2.27337900
H	-6.64581500	-2.63896900	-3.32828600
C	-2.97251600	-0.40338800	0.56156300
C	-2.19970300	0.48219100	-0.40897500
H	-2.56083600	-1.41621100	0.53192200
H	-2.88715600	-0.01702400	1.57543200
N	-0.75819500	0.58536600	-0.03819600
S	-0.19782000	1.41504700	1.28120400
O	1.20642700	1.04831300	1.43634200
O	-1.09476500	1.19007100	2.40788300
C	-0.29065400	3.14241400	0.86730800
C	0.00895800	3.56680300	-0.42383800
C	-0.02723800	4.92958400	-0.70001700
C	-0.34048800	5.86294300	0.29376800
C	-0.63361200	5.40233100	1.58201500
C	-0.61582500	4.04400400	1.87745700
H	0.25700300	2.83747600	-1.19126100
H	0.19049500	5.27534900	-1.70638800
H	-0.88970000	6.11607300	2.35971900
H	-0.86670000	3.68008200	2.86822900
C	-0.34178700	7.33712000	-0.01345700
H	-0.62825300	7.52356000	-1.05071600
H	-1.02868800	7.87784900	0.64111900
H	0.65787500	7.75830800	0.13429100
C	-2.80988000	1.89844500	-0.50318000
O	-2.85463900	2.56196100	-1.51392300
O	-3.26210300	2.32874100	0.67115100
C	-3.74906700	3.67676400	0.67642200
H	-2.99056300	4.34644800	0.26511100
H	-4.66048500	3.74465500	0.07953400
H	-3.95074700	3.91413400	1.71874300
H	-4.02676100	-0.44383500	0.27474100
TS7SS			
C	-5.31793800	-1.38356000	1.37772900
C	-4.12040700	-0.92516000	0.83155900
C	-4.09207100	0.10428100	-0.10068200
C	-5.30276900	0.68596100	-0.47625500
C	-6.50703000	0.23917500	0.07230800
C	-6.52385700	-0.80032200	1.00224300
C	-5.06235000	-2.50486500	2.35548500

C	-3.61388400	-2.94746100	2.06203000
C	-2.94935300	-1.68820500	1.41066100
H	-3.14870100	0.42576300	-0.53192400
H	-5.30829400	1.49149000	-1.20421900
H	-7.44090100	0.69961600	-0.23512800
H	-7.46307200	-1.15424200	1.41743600
H	-5.74635100	-3.35077500	2.24724400
H	-3.08196800	-3.23381300	2.97140100
H	-5.14262600	-2.14345500	3.38712700
H	-2.44015700	-1.09222200	2.16759600
N	-1.95290100	-2.07779200	0.41673600
O	-3.57860700	-4.11180200	1.24078000
C	-0.69493500	-1.61513900	0.16819000
C	-2.21603100	-3.15131800	-0.39083900
N	-0.27660600	-2.46929900	-0.78115300
N	-1.19591000	-3.43370200	-1.13948400
C	-3.48964300	-3.89173700	-0.15924500
H	-4.35148400	-3.32849400	-0.53899600
H	-3.45622200	-4.86787000	-0.64315400
C	1.05858300	-2.60592200	-1.29177900
C	1.36840100	-2.16736700	-2.57643100
C	1.98537300	-3.27244800	-0.47784000
C	2.67873700	-2.36154300	-3.02351700
C	3.27894200	-3.42953400	-0.96186200
C	3.64625100	-2.96656400	-2.22907800
H	2.94264000	-2.02429300	-4.02375400
H	4.01492700	-3.94187400	-0.34594000
C	1.57539900	-3.85623700	0.85048400
H	1.22931500	-3.09019800	1.55058500
H	2.41257800	-4.38498700	1.30968500
C	0.35812200	-1.50394200	-3.47355700
H	0.54440300	-0.42669400	-3.51396400
H	-0.66209200	-1.64619000	-3.11674700
H	0.44052700	-1.90300800	-4.48810700
H	0.75025400	-4.56458400	0.72100400
C	5.06602300	-3.11491400	-2.71159500
H	5.49500000	-4.06922200	-2.39511900
H	5.12519500	-3.05242300	-3.80049200
H	5.69548900	-2.31972500	-2.29767600
C	-0.18727400	0.25955600	1.08390500
O	-1.28508600	0.61324800	1.51161800
H	1.52020900	-0.99005500	1.42421300
C	0.99851400	-0.17924700	1.93374300
C	1.86183200	1.08404800	1.93377000

H	0.67291600	-0.48771800	2.92810700
H	1.34765400	1.85179000	2.52438300
C	3.27123600	0.94591500	2.46362000
C	3.83184400	1.99409800	3.19900600
C	4.04835000	-0.19312400	2.22098200
C	5.13873600	1.91726900	3.67393600
H	3.23306000	2.87759000	3.40645300
C	5.35539300	-0.27094800	2.69515000
H	3.64178800	-1.02029000	1.64589900
C	5.90557000	0.78327300	3.42116500
H	5.55476600	2.74189600	4.24393300
H	5.94389200	-1.16146200	2.49731400
H	6.92339000	0.71818500	3.79185700
C	1.85125700	3.10486200	0.38405600
C	1.77552600	1.58150700	0.44218900
H	0.99122100	3.53248000	0.90604500
H	2.76982900	3.43182100	0.87602900
N	0.47803800	1.02258600	0.01666400
S	-0.24307500	1.51703900	-1.37894900
O	-1.28399200	0.54520000	-1.69098900
O	0.83867200	1.75954000	-2.33215600
C	-1.04286800	3.08216400	-1.09303800
C	-2.01447300	3.18690500	-0.09804300
C	-2.66746000	4.40129400	0.06411000
C	-2.36709500	5.50305100	-0.74826500
C	-1.38922400	5.36291900	-1.73512900
C	-0.72065800	4.15487200	-1.91568800
H	-2.22887500	2.33395300	0.54068100
H	-3.42640600	4.50087800	0.83522400
H	-1.14696200	6.20799600	-2.37268500
H	0.03972600	4.03895100	-2.68046400
C	-3.07976500	6.81314100	-0.53987600
H	-4.15967400	6.66181600	-0.46331600
H	-2.74983600	7.28638400	0.39020200
H	-2.88451300	7.50681500	-1.35965100
C	2.89522800	0.90178300	-0.34866500
O	2.87292200	-0.25750600	-0.67713000
O	3.94222100	1.70862400	-0.54120600
C	5.08477500	1.07109800	-1.12168800
H	5.45355800	0.29438400	-0.44681300
H	4.82009400	0.62132800	-2.08058900
H	5.82988300	1.85292100	-1.25140000
H	1.86757100	3.46823100	-0.64528700

PRR

C	-0.36204100	1.13607900	-1.55255100
O	-1.37290000	1.36893900	-2.17321700
H	0.83122400	-0.46938400	-2.20593000
C	0.95746100	0.60963700	-2.06911900
C	1.95290100	0.94755800	-0.95952700
H	1.20620800	1.05389400	-3.03291600
H	2.24901800	1.99517900	-1.08337500
C	3.21020800	0.11106500	-0.88088600
C	4.42155900	0.72934900	-0.56112800
C	3.19541900	-1.27420600	-1.07839700
C	5.59129800	-0.01475200	-0.42987800
H	4.44744900	1.80656000	-0.41726900
C	4.36355800	-2.01991900	-0.94657200
H	2.26755500	-1.78441200	-1.32030700
C	5.56453500	-1.39337500	-0.62022500
H	6.52241100	0.48468500	-0.18264400
H	4.33422200	-3.09365300	-1.10269700
H	6.47454500	-1.97612000	-0.52119800
C	1.63954800	1.93197500	1.37080700
C	1.09164100	0.93109700	0.36063500
H	1.51817200	2.94066100	0.96861100
H	2.70296300	1.73502900	1.52439400
N	-0.23338400	1.28680000	-0.17132900
S	-1.60125500	1.47647700	0.82018800
O	-1.12548400	1.10295100	2.14709300
O	-2.14336100	2.80213500	0.57748900
C	-2.78353300	0.27323800	0.28783000
C	-2.72176200	-1.00830500	0.82650200
C	-3.68988400	-1.93280400	0.45163600
C	-4.70938500	-1.58826600	-0.44023600
C	-4.74810000	-0.28604700	-0.95358100
C	-3.79023100	0.65226600	-0.59762500
H	-1.93306500	-1.27197100	1.52129700
H	-3.65666200	-2.93635000	0.86460400
H	-5.54239200	-0.00575800	-1.63920200
H	-3.81117800	1.66122200	-0.99197900
C	-5.74565500	-2.59631100	-0.85902500
H	-6.74682600	-2.15838000	-0.83993800
H	-5.73590900	-3.47168800	-0.20728100
H	-5.55612100	-2.93459200	-1.88264000
C	1.04049300	-0.50528300	0.88401600
O	0.31129700	-1.35219800	0.41754700
O	1.94105200	-0.72794400	1.83152400

C	2.07507000	-2.09483300	2.24273800
H	2.39926800	-2.70122900	1.39397600
H	1.12310100	-2.46930100	2.62108700
H	2.82998500	-2.09454300	3.02544000
H	1.12636700	1.85885700	2.32831000

PRS

C	0.21082300	1.98280700	-0.22680900
O	1.15745700	2.73065000	-0.29951400
H	-1.72502600	2.83151400	-0.19675000
C	-1.16903500	2.13657000	-0.83552700
C	-1.73153000	0.71489700	-0.80726800
H	-1.10677200	2.56749700	-1.83497100
H	-1.26473100	0.16980100	-1.63509800
C	-3.22475000	0.51977700	-0.88599200
C	-3.70564300	-0.71142500	-1.34563500
C	-4.14167600	1.48727300	-0.47138800
C	-5.07105200	-0.97379400	-1.38420000
H	-2.99836400	-1.46463700	-1.68750700
C	-5.51017700	1.22828300	-0.51345600
H	-3.79774400	2.45256300	-0.11308300
C	-5.97822500	-0.00213600	-0.96632400
H	-5.42691400	-1.93282600	-1.74635100
H	-6.21053800	1.99172600	-0.19036100
H	-7.04431700	-0.20151700	-0.99849000
C	-1.88171900	0.40663200	1.76427100
C	-1.10121900	0.09883600	0.49224900
H	-2.02406300	1.48679600	1.85958300
H	-2.85880700	-0.07696900	1.73811900
N	0.20441000	0.78241300	0.48222600
S	1.48514100	0.33406200	1.49634500
O	1.04818100	-0.93895300	2.05756300
O	1.79991500	1.44662200	2.37495100
C	2.83495500	0.06128700	0.39206500
C	3.75542900	1.08263900	0.17434600
C	4.81383200	0.84273800	-0.69257400
C	4.95577800	-0.39226600	-1.33517400
C	4.00855400	-1.39368300	-1.09532400
C	2.94215300	-1.17945300	-0.23130300
H	3.63116600	2.03908500	0.66856000
H	5.54257300	1.62669600	-0.87549100
H	4.10913600	-2.35424500	-1.59150200
H	2.19990700	-1.94857400	-0.04720100
C	6.12489500	-0.64505800	-2.24902300

H	5.90099300	-1.43366600	-2.97005000
H	6.40058200	0.25991700	-2.79485400
H	6.99876800	-0.96046500	-1.66986000
C	-0.88851400	-1.39949500	0.24610400
O	-0.16491000	-1.82757200	-0.62350800
O	-1.63416500	-2.15522700	1.04029400
C	-1.48733700	-3.56859300	0.85242400
H	-1.74198100	-3.84069500	-0.17324600
H	-0.45723400	-3.86196400	1.06230400
H	-2.17241700	-4.03263200	1.55768700
H	-1.33243200	0.04151800	2.63438600
PSR			
C	-0.21105200	1.98274600	-0.22661800
O	-1.15778200	2.73048300	-0.29930600
H	1.72473800	2.83160800	-0.19656900
C	1.16875500	2.13671000	-0.83538600
C	1.73132900	0.71504900	-0.80735600
H	1.10636100	2.56771200	-1.83478800
H	1.26450100	0.17003900	-1.63522400
C	3.22456400	0.51994100	-0.88611100
C	3.70543000	-0.71144400	-1.34532600
C	4.14150800	1.48757400	-0.47190300
C	5.07082400	-0.97386900	-1.38376000
H	2.99812500	-1.46471800	-1.68700900
C	5.51001100	1.22852500	-0.51385400
H	3.79760500	2.45301800	-0.11399800
C	5.97802100	-0.00208500	-0.96621100
H	5.42667600	-1.93303200	-1.74557200
H	6.21038800	1.99207900	-0.19106200
H	7.04410300	-0.20153600	-0.99826600
C	1.88188000	0.40661100	1.76411900
C	1.10120700	0.09884800	0.49219400
H	2.02442700	1.48676300	1.85931000
H	1.33257600	0.04166200	2.63429500
N	-0.20444300	0.78239000	0.48246500
S	-1.48512000	0.33395300	1.49658800
O	-1.79990100	1.44644000	2.37528000
O	-1.04807500	-0.93904300	2.05778300
C	-2.83491500	0.06119500	0.39228100
C	-3.75515800	1.08264500	0.17426500
C	-4.81348200	0.84283600	-0.69283400
C	-4.95554400	-0.39218600	-1.33528900
C	-4.00856800	-1.39379600	-1.09505600

C	-2.94227800	-1.17965600	-0.23092600
H	-3.63092100	2.03914700	0.66837600
H	-5.54199100	1.62696300	-0.87594800
H	-4.10934600	-2.35443300	-1.59104700
H	-2.20018700	-1.94886900	-0.04660500
C	-6.12437500	-0.64494000	-2.24952300
H	-6.39960400	0.25995300	-2.79573100
H	-5.90030700	-1.43378400	-2.97024800
H	-6.99859400	-0.95999500	-1.67069200
C	0.88851200	-1.39949600	0.24601200
O	0.16475100	-1.82758400	-0.62346500
O	1.63440800	-2.15526100	1.03991800
C	1.48763000	-3.56860400	0.85187700
H	0.45742900	-3.86201000	1.06119900
H	1.74279200	-3.84062400	-0.17369400
H	2.17237100	-4.03269100	1.55743500
H	2.85888500	-0.07714600	1.73792500
PSS			
C	-0.25339900	0.21203100	1.86829100
O	-1.12034500	0.10655000	2.70256000
H	1.75187200	-0.00737700	2.46710900
C	1.13662400	0.78461300	2.02712000
C	1.56078200	1.12345400	0.59801000
H	1.13543700	1.64121400	2.70091800
H	1.10354100	2.08332800	0.33217600
C	3.04473200	1.21980000	0.32536500
C	3.52235300	2.23475800	-0.50704300
C	3.95824400	0.30254000	0.85786000
C	4.87838600	2.33225500	-0.80969100
H	2.82328300	2.95896100	-0.91772600
C	5.31341300	0.39703500	0.55477000
H	3.61495600	-0.50195200	1.50224800
C	5.77794700	1.41136100	-0.28003600
H	5.22994400	3.12962900	-1.45634400
H	6.00837300	-0.32280500	0.97538800
H	6.83537500	1.48539800	-0.51186100
C	0.49164700	0.64484500	-1.66441500
C	0.81058500	0.06462400	-0.29247600
H	-0.22102500	1.46512400	-1.54485300
H	1.41153100	1.03412300	-2.10686300
N	-0.37848900	-0.19789700	0.53518700
S	-1.54624100	-1.34894600	0.08816700
O	-1.75294700	-2.26074000	1.19645700

O	-1.08589900	-1.85000700	-1.19948500
C	-3.00837200	-0.38332900	-0.14595700
C	-3.78888100	-0.06181900	0.96378100
C	-4.92636200	0.70821000	0.76807400
C	-5.28992900	1.15278100	-0.50992900
C	-4.48584300	0.80738500	-1.59948200
C	-3.33846600	0.03949900	-1.42853200
H	-3.49448400	-0.40506900	1.94944000
H	-5.54825100	0.96811400	1.61980000
H	-4.76306800	1.13881900	-2.59542700
H	-2.71774400	-0.24012300	-2.27337100
C	-6.52706000	1.99067700	-0.69218000
H	-7.40051600	1.49020500	-0.26539800
H	-6.41933800	2.95135900	-0.17982000
H	-6.72307900	2.18688700	-1.74757800
C	1.65229300	-1.21349900	-0.34336800
O	1.68540300	-2.01683500	0.56054300
O	2.38979800	-1.28531300	-1.44397000
C	3.32194000	-2.37354700	-1.48723600
H	4.05280900	-2.26120400	-0.68316500
H	2.79676100	-3.32298100	-1.37721800
H	3.80720900	-2.30753400	-2.45818700
H	0.07378500	-0.10698500	-2.33265200

[3 + 3] annulation

TS3^{SI}

C	-4.41277000	-3.03622200	1.18246200
C	-3.17290100	-2.50195400	1.54807700
C	-3.08461300	-1.53167900	2.54507300
C	-4.25989500	-1.08295700	3.14642800
C	-5.49894500	-1.59951600	2.76542100
C	-5.58233500	-2.58808900	1.78699600
C	-4.26825000	-4.08911200	0.11602200
C	-2.75637200	-4.40061200	0.15487000
C	-2.06954900	-3.12354000	0.71178000
H	-2.12124800	-1.14221400	2.85144000
H	-4.20699400	-0.32688600	3.92310000
H	-6.40355500	-1.23837000	3.24437000
H	-6.54361900	-3.00643300	1.50388300
H	-4.58174100	-3.69194100	-0.85597500
H	-2.57457000	-5.19959900	0.87663200
H	-4.86816800	-4.98171700	0.30703900
H	-1.15274700	-3.33778700	1.25618400

N	-1.73971600	-2.25933900	-0.45731600
O	-2.18404600	-4.84801300	-1.05541600
C	-1.49516600	-0.91051300	-0.43279200
C	-2.17463900	-2.55829900	-1.72888800
N	-1.87145600	-0.46965700	-1.66070700
N	-2.28300100	-1.50322500	-2.46934100
C	-2.39985500	-3.98123700	-2.14666800
H	-3.40011600	-4.09471300	-2.57969900
H	-1.66751500	-4.24879100	-2.91192700
C	-2.16648400	0.87811900	-2.04494700
C	-1.33671800	1.53056400	-2.95786100
C	-3.29456400	1.47842200	-1.46869900
C	-1.64139400	2.85882700	-3.25897000
C	-3.55132100	2.80699500	-1.79710000
C	-2.72908800	3.51391100	-2.67941400
H	-1.00776900	3.39499600	-3.96077100
H	-4.41378300	3.30113600	-1.35663400
C	-4.16670000	0.72426800	-0.49866700
H	-3.68385900	0.63566000	0.48245800
H	-4.37200700	-0.29215600	-0.85167700
C	-0.16169400	0.82487000	-3.57378000
H	0.37119700	1.48764500	-4.25749800
H	-0.48632000	-0.06081200	-4.12792200
H	0.53948000	0.49368700	-2.80292000
H	-5.11831600	1.23967900	-0.36028700
C	-3.00215900	4.96466000	-2.97965100
H	-2.54359800	5.60434300	-2.21813000
H	-2.58869700	5.25383100	-3.94803200
H	-4.07453100	5.17276200	-2.98170300
C	-0.84178900	-0.23114800	0.63209000
O	-0.32596100	-1.06026500	1.61626300
H	0.50894000	-1.47092400	1.31601900
C	-0.79845900	1.14742800	0.75639800
C	-0.05125100	1.84431900	1.71526400
H	-1.32709000	1.72312800	0.00577600
H	0.27591800	1.26518800	2.57730100
C	-0.26856500	3.28281200	1.96329200
C	0.07848500	3.82337800	3.20965000
C	-0.74089800	4.16247400	0.97438600
C	-0.06415400	5.18238500	3.47272200
H	0.45946300	3.15957000	3.98203200
C	-0.88756600	5.51941400	1.23937100
H	-0.98831400	3.78938600	-0.01745600
C	-0.55335200	6.03909900	2.48967500

H	0.20754700	5.57195500	4.44918800
H	-1.25767500	6.17932600	0.46034100
H	-0.66664700	7.09932500	2.69078200
C	1.83781300	1.86611400	0.87549600
C	2.23811900	0.59417200	0.47516900
H	2.23608600	2.26433400	1.80311100
H	1.65524300	2.60260900	0.09806200
N	2.06313300	0.17770600	-0.88439400
H	1.77697200	-0.80117800	-0.94920400
S	3.41430500	0.36012700	-1.87164900
O	3.72646200	1.78410200	-1.90962400
O	3.09589600	-0.35832800	-3.10392600
C	4.75227800	-0.47087100	-1.05939000
C	5.45393700	0.19517300	-0.05768700
C	6.43320900	-0.49610100	0.64801200
C	6.72016800	-1.83345900	0.35977000
C	6.00184000	-2.47419200	-0.65646200
C	5.01351300	-1.80402300	-1.36589800
H	5.23290300	1.23479300	0.15797500
H	6.98390600	0.01100100	1.43478900
H	6.21948800	-3.51236400	-0.89068000
H	4.45205400	-2.29877200	-2.15138700
C	7.80178100	-2.56797800	1.10697400
H	8.73324900	-2.56631600	0.53178700
H	8.00447000	-2.09868600	2.07177000
H	7.52329100	-3.61045000	1.27825800
C	2.47307000	-0.45692800	1.41256600
O	2.40406900	-1.66422700	1.13403100
O	2.64974500	-0.03886600	2.68387700
C	2.65454000	-1.07214800	3.66615000
H	2.80977500	-0.57408600	4.62168900
H	1.69700500	-1.60019000	3.66745200
H	3.45713800	-1.78656100	3.47406700

TS3A^{S1}

C	3.15492400	3.93669400	-1.37228900
C	1.94012800	3.26888200	-1.50818900
C	1.01774100	3.62519400	-2.48551900
C	1.33017600	4.68482200	-3.33485800
C	2.54609300	5.36070400	-3.20403600
C	3.46776800	4.99043400	-2.22609400
C	3.97525900	3.34575100	-0.25184800
C	3.00673000	2.41325500	0.51139800
C	1.82590700	2.15971500	-0.48874700

H	0.07852800	3.08650800	-2.58294600
H	0.62670800	4.98721200	-4.10366700
H	2.77413100	6.18578300	-3.87127300
H	4.41045700	5.52052400	-2.12788800
H	4.38879800	4.09628000	0.42836600
H	3.45824700	1.45863700	0.78089300
H	4.81653300	2.76970500	-0.65152700
H	1.94762700	1.17652400	-0.92688500
N	0.53801400	2.19821900	0.21148300
O	2.59251000	2.97571600	1.75093200
C	-0.63379700	1.51760900	0.06400800
C	0.34448200	3.13949700	1.19076600
N	-1.47193000	2.10601900	0.95595700
N	-0.85656500	3.10262000	1.67193700
C	1.53791200	3.91332700	1.64329100
H	1.77570000	4.72212100	0.93957000
H	1.35575000	4.33801000	2.63017500
C	-2.89016400	1.93764100	1.08385600
C	-3.38298000	1.18214400	2.15105700
C	-3.71272000	2.51422900	0.11342100
C	-4.76210800	0.99835300	2.22415800
C	-5.08532600	2.29639000	0.22570000
C	-5.62432700	1.53643300	1.26459600
H	-5.17185400	0.41061700	3.04208800
H	-5.74831100	2.72850500	-0.51945900
C	-3.12873600	3.29728100	-1.03121700
H	-2.66040500	2.62009400	-1.75471400
H	-2.36227300	3.99854700	-0.68730800
C	-2.43901200	0.53740500	3.12737300
H	-1.74463200	1.26947300	3.55038100
H	-1.83864700	-0.22886700	2.62043000
H	-2.98800000	0.06268600	3.94198900
H	-3.90714100	3.85905500	-1.54931400
C	-7.10476700	1.26836900	1.33382400
H	-7.67346800	2.05222800	0.82941100
H	-7.33993100	0.31786100	0.84326200
H	-7.44657600	1.19997900	2.36900600
C	-0.88231000	0.40842100	-0.80270400
O	0.03679000	0.23167400	-1.82478400
H	0.74131200	-0.37578800	-1.53411300
C	-1.99309100	-0.39859100	-0.66716400
C	-2.15731900	-1.64018000	-1.30040300
H	-2.70588200	-0.13413300	0.10455500
H	-1.58535200	-1.78938100	-2.21572800

C	-3.43180300	-2.38139000	-1.25141800
C	-3.68445100	-3.36171000	-2.22242900
C	-4.38378100	-2.20669700	-0.23309400
C	-4.84746200	-4.12415400	-2.19526700
H	-2.95385100	-3.51922700	-3.01210000
C	-5.54803200	-2.96740600	-0.20774900
H	-4.22173800	-1.47024100	0.55088700
C	-5.78957400	-3.92970800	-1.18791600
H	-5.01717400	-4.87198900	-2.96380500
H	-6.27121800	-2.81008100	0.58714000
H	-6.69837400	-4.52190400	-1.16361600
C	-0.92854900	-2.76620400	-0.06532200
C	0.37248600	-2.27851700	-0.12636100
H	-1.16782100	-3.67439000	-0.61388800
H	-1.48647900	-2.63228700	0.85675300
N	1.12885200	-2.46241300	-1.33792800
H	0.55955800	-2.55913200	-2.18181700
S	2.21621600	-3.75066400	-1.32752600
O	2.86874000	-3.72864000	-2.63516000
O	1.57053600	-4.98759600	-0.88880800
C	3.35221900	-3.25003300	-0.06902900
C	4.40774100	-2.40929800	-0.40737700
C	5.26247400	-1.97533700	0.59640500
C	5.06436200	-2.36063600	1.92790500
C	3.99293300	-3.20433300	2.23490200
C	3.13305100	-3.66005000	1.24098700
H	4.55017900	-2.10652400	-1.43960000
H	6.09549300	-1.32373000	0.34811900
H	3.83162500	-3.51051900	3.26440200
H	2.30127900	-4.31707000	1.47139800
C	6.00931800	-1.89181200	3.00260300
H	6.29256700	-0.84787600	2.84778600
H	5.56105400	-1.98760700	3.99346000
H	6.92816300	-2.48676400	2.99126900
C	0.91654400	-1.27197200	0.74921500
O	1.90005900	-0.57083700	0.50539900
O	0.27789900	-1.18633300	1.95003200
C	0.86462800	-0.26479300	2.86425000
H	0.32399700	-0.38606800	3.80245300
H	1.92559200	-0.48480900	3.00253900
H	0.77010400	0.76730600	2.50858500
TS3B ^{S1}			
C	-5.17850600	2.51923000	0.38547700

C	-3.98157200	1.82276400	0.52190300
C	-2.76219100	2.39579300	0.18159700
C	-2.75083600	3.70361200	-0.29601000
C	-3.94812100	4.41238700	-0.43178000
C	-5.16753800	3.82708500	-0.09426900
C	-6.35181200	1.67375600	0.81172200
C	-5.77887900	0.25042500	1.02980500
C	-4.21271500	0.42313700	1.03772400
H	-1.83280000	1.84148200	0.27842500
H	-1.79991400	4.15994800	-0.55087100
H	-3.92865600	5.43016300	-0.80840000
H	-6.09491900	4.38040400	-0.20929400
H	-7.15359500	1.64181700	0.06699500
H	-6.10290600	-0.16728100	1.98300700
H	-6.79113000	2.05095300	1.74041700
H	-3.81361300	0.28291100	2.03917400
N	-3.56459500	-0.55995100	0.16045400
O	-6.24896900	-0.67827800	0.06602100
C	-2.29933400	-1.07875000	0.15007300
C	-4.18945100	-0.97792000	-0.98649300
N	-2.25963800	-1.81558800	-0.99234000
N	-3.43625400	-1.74985300	-1.69864000
C	-5.61046700	-0.57174900	-1.19110800
H	-5.66878900	0.44971500	-1.59335900
H	-6.10075900	-1.25504800	-1.88413000
C	-1.11232000	-2.42995800	-1.59096000
C	-0.82124400	-3.76122600	-1.28784300
C	-0.30317400	-1.63726500	-2.40889100
C	0.37335100	-4.28374000	-1.78279800
C	0.88450100	-2.19785400	-2.87346200
C	1.24582800	-3.50871400	-2.55094300
H	0.63871100	-5.30988700	-1.54090900
H	1.55346300	-1.58416900	-3.47161500
C	-0.71912400	-0.23964900	-2.77917300
H	-1.02996600	0.33129200	-1.89659000
H	-1.57327700	-0.26356600	-3.46345300
C	-1.73066700	-4.55786600	-0.39196900
H	-2.76829000	-4.50347900	-0.73231100
H	-1.69984500	-4.16765900	0.63256300
H	-1.42469600	-5.60466400	-0.36440800
H	0.10650300	0.28405500	-3.26501600
C	2.57381200	-4.05512300	-3.00584900
H	3.38912300	-3.52654500	-2.50141700
H	2.66569100	-5.11988300	-2.78244800

H	2.71034100	-3.91313700	-4.08133300
C	-1.29216400	-0.90187400	1.14537100
O	-1.63058500	-0.02116100	2.16046300
H	-0.90848600	0.62205700	2.28437400
C	-0.17505800	-1.70752900	1.25404700
C	0.76700400	-1.59830200	2.28666100
H	0.03690700	-2.40238700	0.45187400
H	0.42065200	-1.12258100	3.20273500
C	1.77530200	-2.66143400	2.46328100
C	2.17038500	-3.06656300	3.74467900
C	2.40035600	-3.26332000	1.35734700
C	3.12914900	-4.06145500	3.91876900
H	1.70815600	-2.60215100	4.61208700
C	3.34994300	-4.26332200	1.53174100
H	2.15674500	-2.92229900	0.35226500
C	3.71836100	-4.67175900	2.81385900
H	3.41394700	-4.36257000	4.92246300
H	3.81632800	-4.71554000	0.66127600
H	4.46519200	-5.44726200	2.94897200
C	1.96192700	0.00261500	1.62882400
C	1.43163300	0.86064000	0.67274900
H	2.73119900	-0.68740200	1.29790500
H	2.09017600	0.40552800	2.62747900
N	1.50632500	0.55443800	-0.72340700
H	0.90298200	1.17815200	-1.25992200
S	2.99439800	0.52113900	-1.47970100
O	2.69858000	0.60182800	-2.91047800
O	3.72552900	-0.62635600	-0.95064000
C	3.87277600	1.98636100	-1.00085600
C	3.70195600	3.15082900	-1.74524800
C	4.34321800	4.31127500	-1.33097600
C	5.13990100	4.32371800	-0.18022300
C	5.28313700	3.14217700	0.55295100
C	4.65360400	1.96905800	0.15169200
H	3.08574300	3.13850000	-2.63823600
H	4.22496800	5.22418600	-1.90752600
H	5.89671200	3.14061600	1.44907200
H	4.77513200	1.04658000	0.70977700
C	5.85253200	5.58146400	0.24108100
H	6.82692700	5.65274100	-0.25311100
H	5.27842100	6.46968400	-0.03160700
H	6.02612100	5.59546500	1.31906000
C	0.68977000	2.04700800	0.96127800
O	0.34850600	2.90092300	0.14509200

O	0.30611300	2.12222800	2.27673000
C	-0.29072200	3.36235100	2.66664800
H	0.40155900	4.18664700	2.48401300
H	-1.21482800	3.53844400	2.11272600
H	-0.49516100	3.26926500	3.73196800

TS3C^{SI}

C	-3.69400700	-3.88649100	-0.28152300
C	-2.80664500	-2.81772100	-0.38013500
C	-1.61139500	-2.79568800	0.33091700
C	-1.31273600	-3.87333500	1.16052700
C	-2.19830000	-4.94852600	1.26624700
C	-3.39218300	-4.96458000	0.54616000
C	-4.90823000	-3.67446100	-1.14909900
C	-4.80313100	-2.21590000	-1.65907100
C	-3.34027900	-1.74890100	-1.30531900
H	-0.90894500	-1.96700800	0.27612000
H	-0.37546100	-3.86147100	1.70485700
H	-1.95491500	-5.78268400	1.91697100
H	-4.07882700	-5.80148500	0.63414200
H	-5.85245000	-3.81324100	-0.61234000
H	-4.94983800	-2.15748700	-2.73753200
H	-4.91556400	-4.37058900	-1.99358200
H	-2.74549600	-1.64112100	-2.20822900
N	-3.34887400	-0.44344200	-0.62603700
O	-5.81864600	-1.38064700	-1.12507700
C	-2.38666200	0.51740400	-0.48320400
C	-4.38570100	-0.11172800	0.20627800
N	-2.92748700	1.39010300	0.40418100
N	-4.17275500	0.99912300	0.83239900
C	-5.58755000	-0.99574300	0.21462100
H	-5.42252800	-1.86487800	0.86734500
H	-6.45777500	-0.44394000	0.56952900
C	-2.31151300	2.51836200	1.03546000
C	-2.40006600	3.77152900	0.42163400
C	-1.64837800	2.29935600	2.24275300
C	-1.74394000	4.83180100	1.03975200
C	-1.01676600	3.39687300	2.83094400
C	-1.04333300	4.65952300	2.23874500
H	-1.77809600	5.81524900	0.57709400
H	-0.50088900	3.26242900	3.77842600
C	-1.63912000	0.93183100	2.86995600
H	-1.19397100	0.97213000	3.86532300
H	-1.06292500	0.21900100	2.26653800

C	-3.13331400	3.93201100	-0.88215400
H	-4.14824100	3.53058400	-0.81310900
H	-2.61879100	3.38945100	-1.68381700
H	-3.19057100	4.98368000	-1.16598100
H	-2.65674400	0.54236400	2.96339800
C	-0.34620500	5.83248700	2.87767900
H	0.32470600	6.31961900	2.16422700
H	-1.07169400	6.58235200	3.20714800
H	0.24035900	5.52251100	3.74435900
C	-1.13195100	0.57592400	-1.17041700
O	-0.90860400	-0.47011000	-2.05005900
H	-0.28107500	-1.10485000	-1.65030800
C	-0.32480100	1.69725100	-1.20011700
C	0.83785600	1.80754400	-1.97755900
H	-0.56074500	2.50770700	-0.52160500
H	0.88095100	1.16281500	-2.85347600
C	1.51476900	3.11038800	-2.10821700
C	2.18611800	3.44646900	-3.29207900
C	1.56635400	4.02399200	-1.04111200
C	2.85444000	4.66101100	-3.42040600
H	2.16987300	2.74743400	-4.12463500
C	2.22580900	5.24059700	-1.17308200
H	1.09905600	3.77058900	-0.09121400
C	2.87192700	5.56947100	-2.36467900
H	3.36018300	4.89933800	-4.35131000
H	2.24627800	5.93154500	-0.33533500
H	3.38936300	6.51799400	-2.46463200
C	2.26884100	0.72875600	-0.89653300
C	1.77380300	-0.42232500	-0.30158800
H	2.52805200	1.55359500	-0.24500300
H	2.88660700	0.63487900	-1.78706600
N	1.52725000	-1.57975200	-1.12953700
H	1.75632300	-1.35527900	-2.09889900
S	2.36842700	-3.04411200	-0.85498500
O	2.63108300	-3.55057300	-2.20255200
O	1.62190800	-3.87261600	0.07545000
C	3.90392100	-2.58928900	-0.09298800
C	5.00863500	-2.34630000	-0.90117800
C	6.20463300	-1.96463200	-0.30134600
C	6.29928700	-1.81885700	1.08516800
C	5.16463600	-2.06208400	1.86948900
C	3.96207500	-2.44775700	1.29213400
H	4.93335900	-2.46770400	-1.97690900
H	7.07794000	-1.77756200	-0.91911100

H	5.22790200	-1.94582500	2.94795900
H	3.07190800	-2.62353900	1.88888300
C	7.60010600	-1.42777200	1.73473400
H	8.30339300	-1.02426200	1.00396400
H	7.43940800	-0.67789900	2.51329200
H	8.06787000	-2.29665300	2.20836000
C	1.32148100	-0.46184500	1.05710300
O	0.92888400	-1.45621300	1.66439400
O	1.44543700	0.75055200	1.67900200
C	1.61565700	0.69124000	3.09153900
H	0.92846800	-0.02415400	3.54221700
H	2.64507400	0.40180800	3.32904500
H	1.42134300	1.69567000	3.46815200

M3^{S1}

C	5.70282000	-1.78725600	0.73483500
C	4.38145400	-1.63215900	1.16321800
C	3.39878800	-2.56329200	0.83860200
C	3.76173200	-3.65421900	0.05011500
C	5.07786800	-3.80933500	-0.38893800
C	6.06031000	-2.88179100	-0.04504600
C	6.57198600	-0.66171100	1.23689300
C	5.72101200	-0.08592400	2.38941100
C	4.24950100	-0.38248700	2.00302300
H	2.38525000	-2.42540200	1.20326000
H	3.01403200	-4.39180800	-0.22377800
H	5.34225400	-4.66808800	-0.99800100
H	7.08585900	-3.01477600	-0.37602600
H	6.73343800	0.07587900	0.44196400
H	5.93011800	-0.65385400	3.29856600
H	7.55518400	-0.98767100	1.58265900
H	3.57191300	-0.48606100	2.85082100
N	3.75999100	0.77287500	1.21580700
O	5.95480400	1.26440500	2.73641900
C	2.59717200	0.87065500	0.54674100
C	4.42348300	1.95829800	1.04922800
N	2.60374200	2.08764500	0.00329400
N	3.73981500	2.78305500	0.30764900
C	5.75867700	2.18792800	1.68824600
H	6.55106100	2.12699800	0.93238400
H	5.78394800	3.18667800	2.12688600
C	1.52877700	2.68431500	-0.74389800
C	1.65719400	2.78149300	-2.12851000
C	0.38160400	3.07089400	-0.04519500

C	0.56301000	3.28147600	-2.83506700
C	-0.68352900	3.55982500	-0.79635300
C	-0.61337800	3.66343900	-2.18840400
H	0.62911700	3.36024800	-3.91728300
H	-1.59948700	3.84565600	-0.28413100
C	0.30894300	2.95576600	1.45446000
H	1.14027200	3.49124800	1.92520800
H	0.36680400	1.91184800	1.78470600
C	2.91572000	2.33263400	-2.82235900
H	3.14493500	1.28764700	-2.58553700
H	3.77499900	2.93192600	-2.50787200
H	2.80901500	2.42144500	-3.90439100
H	-0.62696600	3.38087900	1.82008200
C	-1.80242300	4.17140400	-2.96018000
H	-2.68464800	3.56962600	-2.72330500
H	-2.02599600	5.20831100	-2.69139200
H	-1.62598300	4.12884600	-4.03689100
C	1.48611400	-0.13539700	0.59220200
O	1.23030900	-0.56076600	1.77704100
H	-0.88051100	-0.01434700	1.23138500
C	0.93041200	-0.44224000	-0.60944900
C	-0.24094900	-1.37793800	-0.74173600
H	1.27076400	0.06909900	-1.50569700
H	-0.24821600	-2.03995900	0.13343600
C	-0.12570400	-2.23539400	-1.98397400
C	0.10163400	-3.60902100	-1.88217500
C	-0.22085800	-1.66744600	-3.25932300
C	0.23316300	-4.40015000	-3.02194300
H	0.17541400	-4.06112500	-0.89590100
C	-0.09219800	-2.45365700	-4.40054000
H	-0.39346800	-0.59778300	-3.35913700
C	0.13609100	-3.82428700	-4.28586200
H	0.40938200	-5.46688800	-2.92148800
H	-0.17117500	-1.99651100	-5.38224600
H	0.23531000	-4.43746100	-5.17598100
C	-1.54867100	-0.54905000	-0.72799600
C	-1.84282400	-0.07761300	0.70106700
H	-2.38707300	-1.12848400	-1.12817900
H	-1.42042300	0.33437200	-1.35888700
N	-2.40855000	1.27437500	0.80347700
H	-2.51382800	1.55959600	1.77641900
S	-3.78811800	1.71010500	-0.01694000
O	-3.54414100	1.52848600	-1.44241500
O	-4.11753300	3.03091800	0.51015500

C	-5.07351000	0.58124800	0.45432500
C	-5.26147300	-0.58775000	-0.27644000
C	-6.19150000	-1.51899200	0.17750400
C	-6.92374300	-1.29444500	1.34718100
C	-6.72193800	-0.10091400	2.05084400
C	-5.79692600	0.83763500	1.61638700
H	-4.70611700	-0.75249600	-1.19427600
H	-6.35304600	-2.43257500	-0.38743500
H	-7.29649700	0.09150900	2.95218300
H	-5.63453800	1.76022100	2.16385700
C	-7.89457400	-2.32633100	1.85692900
H	-8.75942300	-1.85483900	2.32892300
H	-8.24580800	-2.97335200	1.05066800
H	-7.41402400	-2.96067600	2.60927400
C	-2.66030200	-1.05504100	1.55105300
O	-3.20192600	-0.73093400	2.58298400
O	-2.66364000	-2.29786900	1.06966200
C	-3.38187300	-3.25362400	1.85883900
H	-3.27144000	-4.20569600	1.34437600
H	-2.96089500	-3.30571700	2.86412300
H	-4.43416700	-2.96499500	1.91904100

M3A^{SI}

C	4.89628200	-1.09996600	-0.14248900
C	3.65312100	-1.03091000	0.49376600
C	2.66285900	-1.98130300	0.25577700
C	2.93598100	-3.00363600	-0.65122800
C	4.17078800	-3.07029900	-1.29967300
C	5.16196400	-2.12243200	-1.04706200
C	5.80304300	0.01353400	0.32075400
C	5.14227700	0.42093600	1.65507700
C	3.63294800	0.13078200	1.46139500
H	1.70849500	-1.91531400	0.77180900
H	2.17951900	-3.75826300	-0.84989400
H	4.36641300	-3.87571100	-2.00058200
H	6.12760000	-2.18924500	-1.53895300
H	5.79503900	0.83721000	-0.40330400
H	5.49416400	-0.25158300	2.44049300
H	6.84192700	-0.29342100	0.45728700
H	3.09466700	-0.07360100	2.38730600
N	3.02446400	1.35716900	0.88938300
O	5.41520100	1.72185900	2.13418400
C	1.77759400	1.50432900	0.41421900
C	3.62639900	2.58592900	0.82039900

N	1.66619900	2.79012500	0.08659800
N	2.81739800	3.48304900	0.33087500
C	5.04484300	2.76869700	1.26478900
H	5.70225300	2.82679300	0.38855500
H	5.13489100	3.70260400	1.82136100
C	0.45868300	3.42993700	-0.36438800
C	-0.58299300	3.58279800	0.55571400
C	0.35667000	3.78604700	-1.70958000
C	-1.79059700	4.08225200	0.06747000
C	-0.86927600	4.28811700	-2.14414500
C	-1.95606000	4.42022000	-1.27735500
H	-2.62582600	4.19274300	0.75635200
H	-0.98223100	4.56356900	-3.18950200
C	1.51775300	3.59978600	-2.64939600
H	1.84904800	2.55562000	-2.66493000
H	2.37396000	4.20607100	-2.34097200
C	-0.42574600	3.19439600	2.00386500
H	0.39912300	3.74465200	2.46779200
H	-0.21434400	2.12515900	2.12251700
H	-1.34270800	3.41343300	2.55359700
H	1.23835300	3.88353900	-3.66475200
C	-3.29611700	4.87975400	-1.78793000
H	-3.18994200	5.53470100	-2.65530500
H	-3.89536800	4.01542400	-2.09350000
H	-3.85286600	5.41284500	-1.01377900
C	0.72686700	0.44722400	0.40483100
O	0.60304700	-0.15033900	1.55046500
H	-1.77619900	1.39333000	0.49161400
C	0.07993900	0.25978100	-0.77214800
C	-0.98583800	-0.78952800	-0.94108000
H	0.32136900	0.89892200	-1.61741600
H	-0.79230100	-1.56166800	-0.18676200
C	-0.87979100	-1.44083300	-2.30764100
C	-0.46366700	-2.76742900	-2.43016600
C	-1.15684400	-0.71996800	-3.47428700
C	-0.33599500	-3.36714800	-3.68166800
H	-0.23913400	-3.33007400	-1.52762300
C	-1.03157300	-1.31392700	-4.72672500
H	-1.46748900	0.32028100	-3.40471100
C	-0.62245000	-2.64222500	-4.83526400
H	-0.01060800	-4.40074000	-3.75518700
H	-1.25343100	-0.73914900	-5.62064200
H	-0.52487800	-3.10584800	-5.81171300
C	-2.41362900	-0.23415600	-0.70106300

C	-2.50220200	0.57760000	0.59328400
H	-3.13572200	-1.05917900	-0.69135000
H	-2.69257700	0.42872100	-1.52508500
N	-2.09184500	-0.10324500	1.81858200
H	-1.04927800	-0.19981400	1.89222300
S	-2.91389900	-1.43109400	2.32614800
O	-4.25783700	-1.36227300	1.75338800
O	-2.73670400	-1.52758800	3.77120400
C	-2.09335400	-2.84787100	1.62232600
C	-2.76035400	-3.63469400	0.68904100
C	-2.09230400	-4.71071500	0.11451300
C	-0.76517200	-4.99786500	0.45161400
C	-0.11920100	-4.18808900	1.39197000
C	-0.77581200	-3.11548400	1.98736800
H	-3.78626800	-3.39995100	0.42472100
H	-2.60394500	-5.33126400	-0.61595000
H	0.91223500	-4.39989800	1.66142400
H	-0.26108800	-2.48487600	2.70611600
C	-0.04017900	-6.13498100	-0.21946100
H	0.91432200	-6.34121100	0.26896500
H	-0.64150500	-7.04759100	-0.20628400
H	0.16228800	-5.89522600	-1.26953300
C	-3.81466500	1.31834900	0.82434700
O	-4.18581300	1.74119200	1.89182700
O	-4.46411700	1.55242400	-0.32376400
C	-5.65786400	2.32995700	-0.19167500
H	-6.06943900	2.41792000	-1.19518700
H	-6.36370400	1.82754800	0.47174000
H	-5.42413300	3.31635000	0.21560900

M3B^{S1}

C	4.70380300	-1.79724600	-0.21863800
C	3.87419200	-1.26477000	0.77184700
C	2.82866500	-2.01020300	1.31255300
C	2.60913500	-3.29884100	0.81960900
C	3.42380300	-3.82253800	-0.18857100
C	4.48287000	-3.08073700	-0.70670400
C	5.77941600	-0.82069400	-0.61473500
C	5.76313100	0.17900100	0.56174800
C	4.32004100	0.13691500	1.13197200
H	2.22365600	-1.57385200	2.10382400
H	1.79832600	-3.90658400	1.21472000
H	3.23583000	-4.82471800	-0.56054500
H	5.12741500	-3.49810200	-1.47430700

H	5.52284300	-0.33977300	-1.56569000
H	6.42344900	-0.19150000	1.34866200
H	6.76124300	-1.28189300	-0.74037400
H	4.24143400	0.36667200	2.19333200
N	3.52966100	1.16855400	0.41636600
O	6.22093100	1.48541900	0.27755600
C	2.19665500	1.37152400	0.46747200
C	4.04182500	2.04953600	-0.49602100
N	1.95884500	2.33724700	-0.42505500
N	3.10275100	2.77192100	-1.03418700
C	5.51514900	2.13747900	-0.75358600
H	5.75063500	1.72519900	-1.74198500
H	5.81905200	3.18532300	-0.74260400
C	0.69716600	2.88955800	-0.84037300
C	0.19479800	2.46073100	-2.07054400
C	0.04704400	3.81810400	-0.02522300
C	-1.01403600	3.01294300	-2.49494100
C	-1.15719300	4.34078900	-0.49585500
C	-1.70006900	3.95258500	-1.72277300
H	-1.43163500	2.69202100	-3.44686400
H	-1.68989600	5.06199800	0.11975000
C	0.58810900	4.18670000	1.32738600
H	1.66941700	4.34717200	1.29998900
H	0.38635100	3.37659800	2.03778700
C	0.91357600	1.41145700	-2.87769100
H	1.06628100	0.49836700	-2.28824500
H	1.89785100	1.76411800	-3.19847800
H	0.33515100	1.14373000	-3.76373800
H	0.10995200	5.09459600	1.69786700
C	-3.01019000	4.53235100	-2.19195000
H	-3.79849900	4.36881900	-1.44997000
H	-2.92604900	5.61258600	-2.34236500
H	-3.32877200	4.08160000	-3.13435700
C	1.29212700	0.74966200	1.49734900
O	1.86594200	0.56176400	2.62261300
H	0.14079100	-2.37215400	1.58389300
C	0.02286400	0.47328000	1.07951700
C	-0.99581000	-0.08417100	2.02899100
H	-0.26276500	0.66792100	0.05154300
H	-0.44682900	-0.38210800	2.93240500
C	-2.04465300	0.93990700	2.44253500
C	-2.57916100	0.92368100	3.73237400
C	-2.53613200	1.87774700	1.52846700
C	-3.57888700	1.81979800	4.10552800

H	-2.20183400	0.20157500	4.45299200
C	-3.53578400	2.77484300	1.89618800
H	-2.12036700	1.91533400	0.52501600
C	-4.06296900	2.74840500	3.18672500
H	-3.97663600	1.79524900	5.11551700
H	-3.89892500	3.50137900	1.17361500
H	-4.83940800	3.44958200	3.47612300
C	-1.72938500	-1.33273100	1.49125900
C	-0.75747500	-2.39025600	0.96045600
H	-2.44480900	-1.04352900	0.71644600
H	-2.31719200	-1.77091500	2.30505100
N	-0.26136900	-2.09839500	-0.39787700
H	0.74631100	-2.19730600	-0.51445100
S	-1.03954000	-2.56575700	-1.78428300
O	-1.46945600	-3.96309100	-1.74741600
O	-0.14531200	-2.13351700	-2.85606400
C	-2.49276700	-1.55873000	-1.74786700
C	-3.72619100	-2.13684200	-1.48009300
C	-4.82988200	-1.30484000	-1.30094900
C	-4.70445900	0.08321900	-1.37994200
C	-3.45194200	0.63260700	-1.68861100
C	-2.34349300	-0.17787900	-1.87093000
H	-3.80771200	-3.21442100	-1.38982800
H	-5.79864600	-1.74269800	-1.07985800
H	-3.34400700	1.71168800	-1.76463700
H	-1.36840700	0.25043200	-2.08277300
C	-5.87158600	0.99354700	-1.11010500
H	-5.94847600	1.77080500	-1.87532300
H	-6.81234900	0.44136000	-1.07774900
H	-5.73629200	1.49402900	-0.14524600
C	-1.26950500	-3.82951100	1.03914600
O	-0.54488500	-4.78946300	1.15681700
O	-2.59564400	-3.90180500	0.93022300
C	-3.12152700	-5.22578900	0.78695200
H	-2.71879700	-5.67163700	-0.12505200
H	-2.85297000	-5.83749100	1.64925600
H	-4.20155000	-5.11065900	0.71878200

M3C^{S1}

C	-0.06051800	4.51705900	-0.85777400
C	0.57254700	3.45620400	-1.51327500
C	-0.13380200	2.60508600	-2.35820800
C	-1.50049500	2.82609500	-2.52260900
C	-2.14030500	3.87243300	-1.85712300

C	-1.42450400	4.72925200	-1.02260100
C	0.93070900	5.33020300	-0.06527600
C	2.25976500	4.94857600	-0.75017100
C	2.05954300	3.49117400	-1.24276900
H	0.39035300	1.80022900	-2.86645500
H	-2.07587000	2.18250200	-3.18203500
H	-3.20460000	4.02995200	-2.00261700
H	-1.91966600	5.55652500	-0.52325400
H	0.91500600	5.02894200	0.98891400
H	2.38166700	5.56519700	-1.64374200
H	0.74689500	6.40588600	-0.10265200
H	2.66519600	3.22469600	-2.10860800
N	2.49486900	2.58881400	-0.14749800
O	3.44022600	5.14667900	-0.00030200
C	2.40632100	1.24608800	-0.09640700
C	3.18652900	2.98911300	0.96512100
N	3.03554800	0.89262900	1.02450100
N	3.52717900	1.97243100	1.70311400
C	3.48695500	4.43384900	1.21503800
H	2.78858900	4.83950500	1.95694800
H	4.49831100	4.52847700	1.61251300
C	3.35734400	-0.43817900	1.46674200
C	2.70038700	-0.94027500	2.59152500
C	4.32772300	-1.15049100	0.75965000
C	3.04225100	-2.22398100	3.01068300
C	4.63930300	-2.42828200	1.22476500
C	4.01104100	-2.97825300	2.34220100
H	2.54129400	-2.64528900	3.87905300
H	5.38654900	-3.01014400	0.69139600
C	4.99450700	-0.57090000	-0.45912000
H	5.39626200	0.42627300	-0.25050500
H	4.28836700	-0.47301800	-1.29129800
C	1.67111400	-0.11336400	3.31354600
H	1.02084900	0.40932500	2.60453400
H	2.15014900	0.65124000	3.93297700
H	1.05343200	-0.74191400	3.95731100
H	5.81787500	-1.21054300	-0.78009800
C	4.36011900	-4.36172600	2.82733900
H	5.07892200	-4.84474100	2.16214000
H	4.79612700	-4.32376900	3.83008600
H	3.46685500	-4.99093700	2.88425600
C	1.86901500	0.36540700	-1.18923600
O	2.26689400	0.70865800	-2.35210500
H	-1.30691100	0.16227800	-1.96318600

C	1.05778400	-0.65001100	-0.77219000
C	0.50997300	-1.64311900	-1.75597000
H	0.86897600	-0.78472700	0.29045400
H	0.61742700	-1.18289900	-2.74784600
C	1.28060700	-2.95785100	-1.78100400
C	1.30190000	-3.73816600	-2.94119500
C	1.95396300	-3.42785000	-0.65105200
C	1.97935700	-4.95424900	-2.97442400
H	0.78821500	-3.38077200	-3.83127400
C	2.63416300	-4.64295800	-0.67980700
H	1.96315100	-2.82774900	0.25494100
C	2.64931400	-5.41201400	-1.84117300
H	1.99058800	-5.54182200	-3.88743400
H	3.16179800	-4.98180800	0.20809400
H	3.18385500	-6.35643400	-1.86645500
C	-0.98965400	-1.92972500	-1.53095100
C	-1.77511200	-0.62308000	-1.36340100
H	-1.13280400	-2.57082700	-0.65764500
H	-1.39175700	-2.47603400	-2.39088800
N	-3.17855400	-0.64416800	-1.81892600
H	-3.28886600	-0.62099200	-2.82957000
S	-4.30437600	-1.69250400	-1.19488300
O	-3.73021500	-2.97717200	-0.80806700
O	-5.38456500	-1.67763300	-2.18008500
C	-4.83402500	-0.87872200	0.29081700
C	-5.17490500	-1.67154700	1.38336600
C	-5.68516900	-1.06051900	2.52315900
C	-5.85013600	0.32710300	2.58457700
C	-5.48990700	1.09791300	1.47315800
C	-4.98561100	0.50540800	0.32100200
H	-5.03262200	-2.74580000	1.33628600
H	-5.95697500	-1.66930600	3.38036000
H	-5.60618400	2.17700200	1.51132500
H	-4.68686300	1.10423900	-0.53311300
C	-6.37071300	0.98548600	3.83455800
H	-6.94378300	1.88423300	3.59660600
H	-7.00793700	0.30559300	4.40365600
H	-5.54030000	1.28455800	4.48245500
C	-1.78810700	-0.05015400	0.05583700
O	-1.83126900	1.12824800	0.31021900
O	-1.84431900	-1.01021200	0.98659300
C	-2.06110700	-0.54680000	2.32260800
H	-1.23283000	0.08746800	2.64193600
H	-2.99229300	0.02343900	2.37114400

H	-2.12272700	-1.43984200	2.94131800
TS4 ^{SI}			
C	-2.93878000	4.35914300	0.18881800
C	-1.91155800	3.51818700	0.61008600
C	-1.32746000	3.65006500	1.86616100
C	-1.79282200	4.65882000	2.70645500
C	-2.82389200	5.50620700	2.29281200
C	-3.40569100	5.36140900	1.03492200
C	-3.40101000	4.00361900	-1.20148600
C	-2.34253200	3.01699700	-1.74243500
C	-1.56971500	2.51475300	-0.46770400
H	-0.53565800	2.97476300	2.17788000
H	-1.35284300	4.78676700	3.68994100
H	-3.17424500	6.28797800	2.95913800
H	-4.20478100	6.02409200	0.71680100
H	-3.48243900	4.86803400	-1.86724400
H	-2.78099400	2.15719800	-2.24755100
H	-4.38362000	3.52186300	-1.17200400
H	-1.87095700	1.49018100	-0.23436800
N	-0.12726200	2.50093000	-0.73692500
O	-1.49905200	3.61942300	-2.71856600
C	0.83580800	1.66625300	-0.33555400
C	0.46909700	3.45714400	-1.51038500
N	1.96666500	2.13610200	-0.85268500
N	1.75476900	3.25975500	-1.59688300
C	-0.44484300	4.41207200	-2.20704900
H	-0.80152100	5.18567400	-1.51411600
H	0.06537200	4.88460900	-3.04553900
C	3.29259100	1.61157500	-0.65523500
C	3.91824800	0.99237900	-1.74428400
C	3.88001600	1.74447400	0.60334500
C	5.19811900	0.48923000	-1.53309900
C	5.16928400	1.22981800	0.75556500
C	5.83909500	0.60386200	-0.29411700
H	5.70952000	-0.00494100	-2.35521100
H	5.65367200	1.31674900	1.72453300
C	3.15891000	2.38877900	1.75871300
H	2.44012300	1.69509800	2.20895700
H	2.61125700	3.28326700	1.44779100
C	3.22614500	0.87158700	-3.07585400
H	3.08966300	1.85399600	-3.53631200
H	2.23312800	0.42158900	-2.97029300
H	3.81215300	0.24944900	-3.75294100

H	3.87104000	2.67607900	2.53329800
C	7.22821800	0.05088200	-0.11090100
H	7.56908000	0.16587800	0.91996000
H	7.25889800	-1.01198100	-0.36871700
H	7.93862400	0.56483900	-0.76498600
C	0.62698900	0.45736700	0.55719800
O	-0.01800800	0.66119800	1.58171500
H	-1.38050800	-3.46304200	0.30758000
C	1.03199900	-0.79344800	-0.01361400
C	1.02123600	-2.02943200	0.87943500
H	1.85458800	-0.72079400	-0.72682100
H	0.17481300	-1.91702400	1.57198200
C	2.27704000	-2.20042400	1.71636900
C	2.19288000	-2.85292000	2.95139400
C	3.52915200	-1.76032100	1.28129600
C	3.32493600	-3.05845700	3.73284200
H	1.22308600	-3.19770900	3.30295300
C	4.66582300	-1.96380600	2.06215200
H	3.63150200	-1.24781300	0.32805200
C	4.56949300	-2.61315500	3.28922700
H	3.23545000	-3.56057000	4.69117600
H	5.62856000	-1.60756100	1.70650600
H	5.45474700	-2.76911700	3.89750300
C	0.74630000	-3.27911100	0.01289000
C	-0.69551600	-3.29667300	-0.53892300
H	0.90067800	-4.18369100	0.60978900
H	1.45820100	-3.30626700	-0.82119900
N	-0.94252200	-2.03635200	-1.21207600
H	0.04367900	-1.06532600	-0.71420700
S	-2.43728100	-1.59254300	-1.49848000
O	-3.13624500	-2.44498500	-2.47591600
O	-2.38803600	-0.14728900	-1.80901000
C	-3.35960500	-1.76701100	0.02724900
C	-4.50407100	-2.55244100	0.06433200
C	-5.21144800	-2.67344300	1.25963100
C	-4.78192100	-2.02616500	2.41832900
C	-3.61833600	-1.24714400	2.35892000
C	-2.90545000	-1.11564400	1.17519700
H	-4.82872500	-3.05901900	-0.83793200
H	-6.10954900	-3.28383400	1.29002600
H	-3.26925000	-0.73977800	3.25443200
H	-1.99565500	-0.52072200	1.15091700
C	-5.53082400	-2.17185400	3.71731900
H	-6.50402300	-2.64206400	3.56381900

H	-4.96464100	-2.78923100	4.42184900
H	-5.68777700	-1.19858500	4.18995400
C	-0.89733100	-4.50685800	-1.44540300
O	-1.56523400	-5.47243500	-1.15010400
O	-0.23277600	-4.39663600	-2.59937700
C	-0.41067400	-5.48506600	-3.50798600
H	0.17562000	-5.23680000	-4.39023400
H	-0.05767900	-6.41728000	-3.06233500
H	-1.46623400	-5.58902300	-3.76686800

TS4A^{S1}

C	-3.48046000	-3.87453800	1.09079700
C	-2.29594000	-3.23692500	0.71000700
C	-1.14800900	-3.33872100	1.48723400
C	-1.22450700	-4.02326300	2.69801500
C	-2.42149600	-4.61339200	3.10784200
C	-3.55535300	-4.55848000	2.29885900
C	-4.51915100	-3.76589200	0.00710300
C	-3.63711200	-3.46161800	-1.22323900
C	-2.44300500	-2.63389800	-0.66999000
H	-0.21880800	-2.91260200	1.13178200
H	-0.33984500	-4.11086100	3.32044700
H	-2.46162400	-5.14738600	4.05215200
H	-4.47181500	-5.05995100	2.59448700
H	-5.22062900	-2.95158300	0.22192600
H	-3.21246200	-4.39841700	-1.58989500
H	-5.10434500	-4.67751100	-0.12972800
H	-1.53341300	-2.69578300	-1.27069400
N	-2.86429500	-1.19161100	-0.69449300
O	-4.28514900	-2.88189100	-2.33214800
C	-2.20630900	-0.08472700	-0.29575000
C	-4.00036800	-0.74919700	-1.33029200
N	-2.97131100	0.94643300	-0.64309700
N	-4.09439700	0.54873400	-1.29283000
C	-4.94462800	-1.67650900	-2.03052800
H	-5.84305400	-1.83557200	-1.42226700
H	-5.24715100	-1.21930700	-2.97371800
C	-2.72096000	2.34814700	-0.42255300
C	-2.45157500	3.13589200	-1.54643500
C	-2.74909300	2.84406600	0.88247800
C	-2.19779500	4.48679800	-1.32570300
C	-2.48945600	4.20430900	1.04293800
C	-2.21549700	5.03606200	-0.04182500
H	-1.97214400	5.12333100	-2.17744200

H	-2.49052500	4.62006100	2.04685900
C	-3.04683100	1.96480100	2.06861500
H	-2.18549500	1.34266100	2.32982100
H	-3.89262300	1.29933900	1.87050100
C	-2.41154600	2.54341400	-2.93048600
H	-3.41197000	2.25516200	-3.26457700
H	-1.78785300	1.64316500	-2.96098900
H	-2.00376000	3.26472900	-3.63961200
H	-3.29124800	2.57962700	2.93609500
C	-1.96403000	6.50540700	0.16780600
H	-1.55428000	6.69129200	1.16327600
H	-1.26420400	6.89611900	-0.57483900
H	-2.89669500	7.07151600	0.07570800
C	-0.86012400	0.05025900	0.40762500
O	-0.73730000	-0.53302800	1.48071200
H	2.23049100	1.37814700	-2.36196300
C	0.11860800	0.80502800	-0.31763700
C	1.34604100	1.22441500	0.50069600
H	-0.29321800	1.57662600	-0.97099200
H	1.42507500	0.47397700	1.29162800
C	1.06673200	2.54727900	1.19282600
C	0.59371600	2.55416600	2.50895100
C	1.21424800	3.77119000	0.53233500
C	0.30220100	3.75166200	3.15912800
H	0.46096500	1.60560900	3.02392800
C	0.93325500	4.97014700	1.18140200
H	1.55713800	3.78881900	-0.49990100
C	0.48247300	4.96548300	2.50008400
H	-0.05457800	3.73561700	4.18473900
H	1.06430200	5.91197700	0.65620000
H	0.27043000	5.90148600	3.00853700
C	2.69285600	1.19575100	-0.27701500
C	2.64345100	0.59393100	-1.70804600
H	3.42414500	0.64383600	0.32049600
H	3.09678000	2.20612700	-0.37386800
N	1.72590600	-0.52555600	-1.88701800
H	0.64442800	-0.03038300	-1.13822600
S	2.01505000	-2.03130300	-1.42502900
O	2.65874700	-2.86564300	-2.44684300
O	0.72061000	-2.54210800	-0.91809100
C	3.13974900	-1.99617600	-0.04002700
C	4.51245900	-2.02682400	-0.27674200
C	5.38856600	-1.86515800	0.79140600
C	4.91088000	-1.68565300	2.09423500

C	3.52812700	-1.67857000	2.30677000
C	2.63867300	-1.83172100	1.24837900
H	4.87608800	-2.17493900	-1.28931700
H	6.46064500	-1.88114200	0.61389100
H	3.14395200	-1.54549100	3.31439200
H	1.56485300	-1.79401500	1.41280800
C	5.86890300	-1.53758300	3.24697000
H	6.76325500	-0.98618400	2.94765500
H	5.40216100	-1.01474600	4.08439400
H	6.19244900	-2.51986800	3.60623200
C	4.04270000	0.35702200	-2.27759500
O	4.30671300	-0.39246100	-3.18605900
O	4.96359800	1.12062800	-1.67159600
C	6.30056400	0.95207000	-2.14901500
H	6.91238600	1.64252900	-1.57220900
H	6.62855900	-0.07738500	-1.98625200
H	6.35800900	1.18149800	-3.21447500

TS4B^{SI}

C	-3.16400300	2.96531300	-0.77262600
C	-2.08357600	2.39621200	-1.45937000
C	-2.28787400	1.28898000	-2.28163000
C	-3.56996200	0.74870400	-2.38523800
C	-4.64222800	1.32215700	-1.70180000
C	-4.44418200	2.43390700	-0.88500100
C	-2.74833400	4.22483300	-0.06692100
C	-1.54448900	4.64490500	-0.93034400
C	-0.86922700	3.30937200	-1.37162300
H	-1.46791200	0.86708500	-2.84867200
H	-3.72671000	-0.12580600	-3.00631500
H	-5.63868700	0.90650100	-1.81717800
H	-5.27802200	2.89975600	-0.36856500
H	-2.45907700	4.00412800	0.96690100
H	-1.92389900	5.10267500	-1.84698100
H	-3.52197300	4.99474600	-0.04433200
H	-0.35187700	3.39293200	-2.32674700
N	0.20597100	2.98879000	-0.37457300
O	-0.67276100	5.59832100	-0.37047000
C	1.10502600	1.98066900	-0.34971100
C	0.59295100	3.86357400	0.60988500
N	1.96625700	2.27765700	0.62018200
N	1.66108000	3.45070900	1.22850900
C	-0.09055700	5.17233800	0.83870400
H	-0.82632200	5.08975400	1.64679300

H	0.65761100	5.91115800	1.12829700
C	3.16137300	1.56890400	0.99615600
C	3.17775600	0.92680900	2.23550100
C	4.22761500	1.53714700	0.09231500
C	4.31166500	0.17435100	2.54035700
C	5.33475100	0.77090800	0.44848800
C	5.38487100	0.06854000	1.65466400
H	4.34788600	-0.35244000	3.49024000
H	6.17477600	0.71395900	-0.23895900
C	4.17359200	2.25132000	-1.23240800
H	3.70418900	3.23519000	-1.14441000
H	3.60558300	1.67124500	-1.96920100
C	2.02528100	1.04701900	3.19409700
H	1.06483300	0.93187800	2.68540500
H	2.03667900	2.02867900	3.67852000
H	2.09124600	0.27764500	3.96430000
H	5.18134400	2.38767800	-1.62740900
C	6.56456100	-0.81066300	1.97559600
H	6.42860000	-1.79960200	1.52549300
H	7.49099200	-0.39089500	1.57713600
H	6.67742500	-0.94691000	3.05308100
C	1.13474500	0.81709100	-1.31767500
O	0.59852000	1.05506600	-2.40652700
H	-1.08491500	-0.72953000	-1.28859600
C	1.67103600	-0.42612100	-0.87812500
C	1.65451800	-1.54145600	-1.92651400
H	2.54517900	-0.38401000	-0.23522200
H	1.80621100	-1.08610000	-2.91141400
C	2.80734400	-2.48763100	-1.66049700
C	3.89075000	-2.56264500	-2.53612600
C	2.83037100	-3.26141700	-0.49349900
C	4.97589500	-3.39385500	-2.25935000
H	3.88506300	-1.96341300	-3.44312900
C	3.91327700	-4.08820300	-0.21274000
H	1.98784100	-3.20354800	0.19363800
C	4.99090500	-4.15812200	-1.09616800
H	5.80873700	-3.44335800	-2.95418000
H	3.91731000	-4.68128900	0.69668300
H	5.83424200	-4.80591200	-0.87833600
C	0.27671000	-2.28576200	-1.96455500
C	-0.79455000	-1.74637900	-0.98777700
H	0.42590300	-3.34260200	-1.71835000
H	-0.14196200	-2.24063700	-2.97373300
N	-0.21217800	-1.78511100	0.35717100

H	0.80697600	-0.97820100	-0.00962400
S	-0.92466600	-0.86011300	1.48540100
O	-0.91268100	0.56657100	1.08447500
O	-0.30263400	-1.18404900	2.77378500
C	-2.63379000	-1.33586100	1.58658600
C	-3.57219300	-0.64468700	0.83415700
C	-4.90412800	-1.05465600	0.87666700
C	-5.29776400	-2.13651200	1.66540800
C	-4.32649800	-2.81064800	2.42093700
C	-2.99588700	-2.42171100	2.38306100
H	-3.26218600	0.20817400	0.23825300
H	-5.64642700	-0.51780900	0.29261800
H	-4.62435000	-3.65101900	3.04228300
H	-2.23866800	-2.93981300	2.96232200
C	-6.73239300	-2.59359100	1.70173600
H	-6.83231000	-3.58532400	1.24901900
H	-7.09409100	-2.66813700	2.73095700
H	-7.38217100	-1.90623100	1.15679000
C	-2.03781700	-2.59772300	-1.19687900
O	-2.83693300	-2.38665700	-2.08315800
O	-2.11647200	-3.63714400	-0.36625000
C	-3.28113200	-4.45103600	-0.52327500
H	-4.17979700	-3.83347800	-0.45969000
H	-3.25936900	-4.96258000	-1.48801800
H	-3.25391000	-5.17013800	0.29327700

TS4C^{S1}

C	1.82061200	4.01705100	0.55924800
C	1.04834600	3.01636300	1.15717500
C	1.60651100	1.78472600	1.49021200
C	2.95226600	1.56347800	1.20291200
C	3.72864300	2.56713800	0.62211400
C	3.16937700	3.80253900	0.29904300
C	1.00275600	5.24632200	0.26384900
C	-0.25498700	5.03296500	1.12978500
C	-0.37296600	3.49721600	1.35552500
H	1.03071800	0.99847900	1.96490200
H	3.37539300	0.58798600	1.42038400
H	4.77830600	2.38002200	0.41402500
H	3.77372400	4.58301500	-0.15341400
H	0.76283600	5.29116000	-0.80414300
H	-0.08760100	5.47670000	2.11298400
H	1.50933500	6.17923300	0.51976800
H	-0.80154600	3.23556000	2.32237900

N	-1.30454400	2.94786000	0.33355000
O	-1.44575300	5.63119100	0.65730300
C	-1.64874900	1.66495800	0.12434100
C	-1.96501000	3.69145000	-0.60234700
N	-2.46840300	1.67292500	-0.92235500
N	-2.68506100	2.93422200	-1.38357200
C	-1.86220600	5.18470500	-0.61298600
H	-1.19032000	5.51317700	-1.41423400
H	-2.84956000	5.60863400	-0.80090700
C	-3.14424500	0.56235600	-1.54752500
C	-2.66264700	0.13375200	-2.79126900
C	-4.23465600	-0.01424500	-0.89864600
C	-3.33426800	-0.92354100	-3.39552200
C	-4.88095600	-1.05974500	-1.56150000
C	-4.44618300	-1.52767000	-2.79857100
H	-2.97905100	-1.28739200	-4.35620500
H	-5.73611700	-1.52696700	-1.08112100
C	-4.67451800	0.41621900	0.47455500
H	-4.58294400	1.49665900	0.61752100
H	-4.06931300	-0.08459600	1.24122500
C	-1.44413000	0.75902500	-3.41520900
H	-0.54963400	0.55693500	-2.81364000
H	-1.55670800	1.84268000	-3.50776600
H	-1.27741900	0.34355600	-4.41006600
H	-5.71474500	0.13393500	0.64511300
C	-5.14500000	-2.67245400	-3.48405700
H	-5.98659100	-3.03495600	-2.89041700
H	-5.52256100	-2.36743000	-4.46428500
H	-4.45381100	-3.50479400	-3.64514300
C	-1.32724600	0.52375100	1.07608700
O	-1.34297500	0.84397500	2.26445100
H	2.03572100	-3.37679100	0.48909800
C	-0.95470000	-0.72954200	0.50502000
C	-0.98463300	-1.93020800	1.45451100
H	-1.36538700	-0.92078900	-0.48907400
H	-0.61503700	-1.57508500	2.42514000
C	-2.40625200	-2.41303600	1.66105300
C	-3.04301100	-2.23808600	2.89320000
C	-3.12718200	-2.99076500	0.61151400
C	-4.36639300	-2.63439300	3.07609300
H	-2.49566100	-1.77694800	3.71110000
C	-4.44560800	-3.39776500	0.79413400
H	-2.66100500	-3.11062000	-0.36430900
C	-5.07170300	-3.21876300	2.02671500

H	-4.84499400	-2.48754600	4.03943300
H	-4.98729200	-3.84967700	-0.03211700
H	-6.10106400	-3.53286100	2.16762600
C	-0.03764300	-3.02966700	0.94711600
C	1.43694400	-2.55434400	0.90082300
H	-0.30913600	-3.32883700	-0.07155600
H	-0.10953800	-3.91228100	1.59061000
N	1.58037800	-1.32062000	0.14052700
H	0.30501600	-0.68325800	0.25564100
S	1.99801300	-1.46525900	-1.39541500
O	1.53542700	-0.24928000	-2.08431200
O	1.61644100	-2.76479300	-1.97977900
C	3.78366400	-1.42427000	-1.45309700
C	4.43542700	-0.19238100	-1.46482200
C	5.82363000	-0.15761600	-1.44539700
C	6.57534800	-1.33913500	-1.40977800
C	5.89933600	-2.56062800	-1.40804600
C	4.50717300	-2.61176700	-1.43108600
H	3.84986300	0.72021400	-1.50511500
H	6.33820100	0.79997400	-1.46866400
H	6.46932500	-3.48543000	-1.39770700
H	3.98364000	-3.56203200	-1.45516000
C	8.08038400	-1.28377900	-1.36906300
H	8.42960500	-0.96378300	-0.38217600
H	8.51863400	-2.26162100	-1.57862500
H	8.46736600	-0.56843000	-2.09949500
C	1.91564900	-2.38581300	2.33689400
O	2.14320800	-3.32066200	3.07170800
O	1.99361400	-1.11078800	2.73321000
C	2.37841500	-0.91217500	4.09586500
H	1.63822900	-1.35133300	4.76763800
H	3.35158800	-1.36853600	4.28462000
H	2.42749500	0.16703600	4.23187100

M4^{S1}

C	-2.81197200	3.56339600	-0.21321700
C	-1.74461700	2.81216000	0.27053800
C	-1.42368100	2.77773700	1.62379300
C	-2.20579500	3.51778000	2.50659400
C	-3.28188800	4.27197600	2.03162800
C	-3.59232200	4.30079100	0.67350200
C	-2.95414300	3.41718200	-1.70629500
C	-1.68279200	2.67291300	-2.16909100
C	-1.05775300	2.08084400	-0.85668300

H	-0.58489800	2.18603800	1.98571500
H	-1.98000100	3.50700800	3.56780300
H	-3.88309700	4.84494500	2.73028900
H	-4.42919400	4.89125900	0.31331900
H	-3.04862800	4.37339100	-2.22971000
H	-1.92368200	1.85466900	-2.84478900
H	-3.82945800	2.80682200	-1.94599400
H	-1.21933500	0.99796900	-0.82819900
N	0.39047000	2.31862300	-0.84348000
O	-0.78321000	3.50441300	-2.90004600
C	1.37027800	1.57646500	-0.33782200
C	0.97715200	3.42693100	-1.39159400
N	2.50053100	2.22026000	-0.58458700
N	2.27581500	3.38672300	-1.25589600
C	0.05438200	4.34475000	-2.13020600
H	-0.51302000	4.96649700	-1.42449000
H	0.61444800	4.98667300	-2.80919500
C	3.80399800	1.67551400	-0.29918200
C	4.47400700	1.02790900	-1.34435300
C	4.27462800	1.73062800	1.01376400
C	5.67002800	0.39176300	-1.02533500
C	5.47761300	1.07353300	1.27647100
C	6.18105900	0.40004400	0.27688400
H	6.21263600	-0.12870200	-1.80996600
H	5.87158800	1.09069000	2.28894600
C	3.51567100	2.45583100	2.09347900
H	2.63124700	1.88912500	2.40158000
H	3.18017400	3.43756400	1.74779500
C	3.91880300	1.02418700	-2.74386900
H	3.90486600	2.03602300	-3.15884900
H	2.88966900	0.64961100	-2.77221500
H	4.52563400	0.39204100	-3.39234400
H	4.14933400	2.59644500	2.96982100
C	7.48526300	-0.28849000	0.58263600
H	7.59017100	-0.48112400	1.65233600
H	7.56203300	-1.23775200	0.04666000
H	8.32854200	0.33501800	0.26969500
C	1.20445200	0.24446300	0.37509600
O	1.02409800	0.26179300	1.56969000
H	-1.77545100	-3.15060200	0.17786400
C	1.16553700	-0.93339500	-0.52829400
C	0.88989400	-2.24981600	0.19087400
H	2.07719200	-0.95631200	-1.14142900
H	0.19754200	-2.02687700	1.01587000

C	2.13680700	-2.85815900	0.82355900
C	2.03428900	-4.09268400	1.47763400
C	3.37670200	-2.21266900	0.83797000
C	3.13332900	-4.67387100	2.09935900
H	1.07482500	-4.60221200	1.51056900
C	4.48189700	-2.79152500	1.46181300
H	3.51304100	-1.24076300	0.37048600
C	4.36812100	-4.02652200	2.08955600
H	3.02427500	-5.63309400	2.59554800
H	5.43127500	-2.26340600	1.45484600
H	5.22793200	-4.47887800	2.57285400
C	0.14193700	-3.18837700	-0.77643100
C	-1.37176200	-2.89295600	-0.81797300
H	0.26760200	-4.23227000	-0.47481400
H	0.56008500	-3.09170800	-1.78592600
N	-1.62250600	-1.50979800	-1.18551600
H	0.32910500	-0.73670200	-1.21920500
S	-3.13153300	-1.08433000	-1.04471700
O	-4.11059100	-2.07063200	-1.55327400
O	-3.28073800	0.29208100	-1.57461200
C	-3.49931700	-0.95933700	0.71372900
C	-4.76474000	-1.28271200	1.18878100
C	-5.05697300	-1.10835800	2.53988700
C	-4.09810200	-0.61364200	3.42683700
C	-2.82649100	-0.30403200	2.93108100
C	-2.52539400	-0.47691800	1.58630400
H	-5.50529800	-1.67493300	0.49985600
H	-6.04584600	-1.36196400	2.91218900
H	-2.06495600	0.07685100	3.60770400
H	-1.53067600	-0.25543300	1.20940100
C	-4.40941800	-0.42284600	4.88885800
H	-5.45499600	-0.65067600	5.10505000
H	-3.78470100	-1.07237700	5.50940100
H	-4.21289900	0.60836100	5.19719600
C	-1.99887800	-3.92524600	-1.75490300
O	-2.45855300	-4.98249100	-1.38280900
O	-1.90285100	-3.58005500	-3.04248600
C	-2.50241900	-4.49638000	-3.95705000
H	-2.34543100	-4.07687100	-4.94901000
H	-2.03647500	-5.48097100	-3.87855800
H	-3.57040900	-4.58878300	-3.74793600
M4A ^{SI}			
C	2.62524900	-3.85344300	0.31242600

C	2.17745800	-2.54466900	0.10283200
C	2.47638100	-1.52703000	1.00164300
C	3.19359200	-1.85143200	2.15225200
C	3.61755900	-3.16149700	2.38008100
C	3.34588900	-4.17153400	1.45731400
C	2.26524800	-4.74003400	-0.85169600
C	2.02274600	-3.69856700	-1.96512000
C	1.48705600	-2.43826100	-1.23657700
H	2.16569100	-0.50807900	0.79966900
H	3.43399600	-1.07026800	2.86634000
H	4.18180500	-3.39462400	3.27780900
H	3.70434200	-5.18300300	1.62220500
H	1.36315700	-5.32179000	-0.62779100
H	2.98564900	-3.41330100	-2.39425100
H	3.05188300	-5.44696500	-1.12282500
H	1.68031900	-1.49732800	-1.75491900
N	-0.00616900	-2.57623900	-1.15800100
O	1.23351400	-4.10974800	-3.05998100
C	-0.91496600	-1.80423200	-0.54277000
C	-0.72218000	-3.53296200	-1.83763300
N	-2.10496700	-2.31946100	-0.82772800
N	-2.00421500	-3.40207500	-1.63770600
C	-0.05454400	-4.55172500	-2.70954100
H	-0.03878000	-5.52368400	-2.20180300
H	-0.62906600	-4.65702400	-3.63107500
C	-3.37753500	-1.85467900	-0.33588700
C	-4.21173200	-1.16519900	-1.22451900
C	-3.70426600	-2.11331500	0.99611900
C	-5.41608500	-0.68995700	-0.71554500
C	-4.92886500	-1.61843600	1.45072300
C	-5.78707600	-0.90322100	0.61769100
H	-6.08221000	-0.13768300	-1.37349200
H	-5.21157800	-1.79830300	2.48443500
C	-2.79218400	-2.89846100	1.90147100
H	-1.92733800	-2.30399400	2.21208100
H	-2.41917800	-3.79730700	1.40155800
C	-3.81583000	-0.95336000	-2.66134100
H	-3.80082600	-1.90345800	-3.20299700
H	-2.81481000	-0.51706000	-2.74454700
H	-4.52074600	-0.28409500	-3.15534000
H	-3.32956400	-3.20391700	2.79987700
C	-7.09629000	-0.36359100	1.13025800
H	-7.21705500	-0.56248900	2.19688600
H	-7.15680400	0.71701500	0.97084300

H	-7.93717700	-0.81931500	0.59951000
C	-0.74740200	-0.54517300	0.30758500
O	-0.29394000	-0.66416900	1.41673700
H	-0.02785200	2.56471200	-2.07419700
C	-1.19106100	0.72396300	-0.35145300
C	-0.96790200	1.93381900	0.54974900
H	-2.23179300	0.61772300	-0.68030900
H	0.04120200	1.83396100	0.96410400
C	-1.94016700	2.00278900	1.71440900
C	-1.54408900	2.67430800	2.87716800
C	-3.22463100	1.45545100	1.67454400
C	-2.40167300	2.80010700	3.96430500
H	-0.54395200	3.10000400	2.92465600
C	-4.08623300	1.57420300	2.76487500
H	-3.57805900	0.92373500	0.79448000
C	-3.68095400	2.24752600	3.91239100
H	-2.07014900	3.32350400	4.85580000
H	-5.07773100	1.13280400	2.71061800
H	-4.35190900	2.33811700	4.76056000
C	-0.96804400	3.24076100	-0.25683400
C	0.19522000	3.29278700	-1.27588100
H	-0.84613200	4.07320200	0.44687500
H	-1.92727600	3.37931000	-0.76732600
N	1.45938400	3.06560800	-0.61378700
H	-0.57818600	0.78927000	-1.25722000
S	2.31223000	1.90251300	-1.21096600
O	3.02923500	2.16851900	-2.48232400
O	1.57962800	0.58688300	-1.28975600
C	3.56141400	1.66666500	0.03826800
C	3.30237200	1.93821100	1.37874400
C	4.24795800	1.59370600	2.33961200
C	5.44408300	0.96350000	1.98204900
C	5.68877500	0.71615500	0.62836700
C	4.75655300	1.06413500	-0.34329200
H	2.37273500	2.42796800	1.64782200
H	4.05190400	1.81027800	3.38671100
H	6.62132600	0.24268100	0.33301000
H	4.94724400	0.87867900	-1.39556200
C	6.42819500	0.52379800	3.03412600
H	6.37362300	1.15844500	3.92152000
H	6.21453200	-0.50456500	3.34747500
H	7.45222100	0.54502800	2.65422200
C	0.17757300	4.64166500	-1.99354600
O	1.08282000	5.43477100	-2.05817400

O	-1.01592200	4.84965900	-2.58586700
C	-1.13035800	6.07834300	-3.30501000
H	-2.13795800	6.09372900	-3.71635300
H	-0.97790900	6.92766000	-2.63594300
H	-0.38969900	6.12137700	-4.10632300

M4B^{S1}

C	-3.40514800	2.59763100	-0.81087500
C	-2.27321000	2.11142600	-1.47919100
C	-2.36404600	0.95794000	-2.25729800
C	-3.58559200	0.28727100	-2.33084100
C	-4.70456100	0.76850100	-1.65249400
C	-4.62240100	1.93118400	-0.88905300
C	-3.11967500	3.91492500	-0.14652400
C	-1.92984100	4.41250600	-0.98684400
C	-1.14756100	3.12861900	-1.40271400
H	-1.51658000	0.59456400	-2.82686700
H	-3.65621700	-0.61104700	-2.93353000
H	-5.65079400	0.24195000	-1.73408700
H	-5.49774600	2.32688000	-0.38258100
H	-2.85164000	3.76151400	0.90475800
H	-2.31721700	4.83671600	-1.91584200
H	-3.95817400	4.61311800	-0.17939400
H	-0.62500800	3.24732200	-2.35184900
N	-0.06603500	2.90149200	-0.38585300
O	-1.13864900	5.42622500	-0.41383500
C	0.91260200	1.97500500	-0.34656800
C	0.22794700	3.79927200	0.60838300
N	1.73274400	2.33494700	0.63601700
N	1.31858700	3.47158400	1.24235500
C	-0.55971400	5.05254400	0.81434300
H	-1.30603300	4.91943300	1.60493700
H	0.12382300	5.84673200	1.11642200
C	3.00586600	1.76202700	0.99746700
C	3.09027200	1.03584500	2.18574400
C	4.08535200	1.97569900	0.13506800
C	4.31519900	0.42904400	2.46136100
C	5.28513900	1.34873700	0.46133000
C	5.40889900	0.55328900	1.60392400
H	4.40977000	-0.16281900	3.36780700
H	6.14176600	1.48122200	-0.19434700
C	3.95313100	2.81280300	-1.11152900
H	3.39428300	3.73350800	-0.92038700
H	3.44025400	2.27159500	-1.91602700

C	1.92027800	0.93662500	3.12306400
H	1.00490500	0.67522500	2.58776200
H	1.76465100	1.89544100	3.62859800
H	2.09884800	0.16866700	3.87622900
H	4.94041100	3.08549500	-1.48652400
C	6.69480900	-0.17530900	1.89033100
H	6.68799300	-1.15264100	1.39639700
H	7.55763400	0.38037300	1.51643900
H	6.82425700	-0.34484600	2.96118500
C	1.10775000	0.84993400	-1.34359900
O	0.61132700	1.01980900	-2.43551000
H	-0.79639000	-0.82453000	-1.18966800
C	1.94505500	-0.32960000	-0.95304000
C	1.91266100	-1.49818600	-1.95021700
H	2.98190000	0.02456400	-0.89906800
H	2.18300900	-1.07660600	-2.92517300
C	3.03782100	-2.43696800	-1.54691500
C	4.24251600	-2.43396600	-2.25195700
C	2.91034600	-3.26276400	-0.42481700
C	5.30431900	-3.24399800	-1.85280500
H	4.34970400	-1.79156300	-3.12310600
C	3.97094400	-4.07142700	-0.02521300
H	1.97077700	-3.25019800	0.12602300
C	5.17061500	-4.06548100	-0.73693000
H	6.23254500	-3.23450800	-2.41593900
H	3.86267900	-4.70853300	0.84745600
H	5.99493000	-4.69881400	-0.42413000
C	0.54777200	-2.21715000	-2.12667800
C	-0.56362300	-1.89997900	-1.11235300
H	0.71998100	-3.29878900	-2.10383100
H	0.14873900	-1.98318300	-3.11645600
N	-0.19997900	-2.27397000	0.23490100
H	1.67783100	-0.64719600	0.05812000
S	-0.65428300	-1.27573900	1.35863300
O	-0.55166000	0.16003400	0.93974900
O	0.03934200	-1.61734500	2.61360800
C	-2.39746500	-1.48388200	1.72797300
C	-3.34283400	-0.65362900	1.14081300
C	-4.69806300	-0.91254600	1.34296100
C	-5.11875300	-1.99499400	2.11710500
C	-4.14561200	-2.81500900	2.70325600
C	-2.79293400	-2.56761000	2.50993700
H	-3.01587600	0.18830000	0.53682700
H	-5.44037700	-0.25868000	0.89235800

H	-4.45727400	-3.65589800	3.31788100
H	-2.03855400	-3.20300600	2.96355100
C	-6.58349600	-2.29628400	2.30541400
H	-6.88334400	-3.15775300	1.69918500
H	-6.80638300	-2.53980900	3.34766100
H	-7.20423300	-1.44760600	2.01006300
C	-1.85342700	-2.54480000	-1.63607900
O	-2.20951800	-2.48795900	-2.79733800
O	-2.57929500	-3.12537600	-0.68486200
C	-3.88464000	-3.55403900	-1.06774000
H	-4.46389000	-2.70436700	-1.44021000
H	-3.82734100	-4.32108800	-1.84284300
H	-4.33884700	-3.94803700	-0.15957700

M4C^{S1}

C	0.15405900	4.51009900	0.15656800
C	-0.29720200	3.42638700	0.91669600
C	0.59921400	2.49087800	1.42991200
C	1.95586700	2.63398600	1.14170000
C	2.40519000	3.71712500	0.38575700
C	1.51030300	4.66823400	-0.10257200
C	-0.98686100	5.37731500	-0.30600200
C	-2.15297300	4.91431100	0.59095300
C	-1.80659800	3.46224000	1.02493500
H	0.27921300	1.65513000	2.04390900
H	2.63993100	1.86730300	1.48770600
H	3.46516300	3.82272100	0.17596000
H	1.86322200	5.51339800	-0.68574000
H	-1.19046900	5.19770800	-1.36722900
H	-2.16706600	5.51672600	1.50095400
H	-0.79605800	6.44631400	-0.19108300
H	-2.20877700	3.19554300	2.00242300
N	-2.44266300	2.54057300	0.03902400
O	-3.45127300	5.03944500	0.04550400
C	-2.28764000	1.21282800	-0.06991800
C	-3.22522200	2.92636800	-1.01228200
N	-2.93745000	0.84627800	-1.16565700
N	-3.54281500	1.90459900	-1.76324200
C	-3.65138800	4.35385800	-1.16915700
H	-3.11813000	4.81682600	-2.00707000
H	-4.71996200	4.38351300	-1.38763800
C	-3.06543000	-0.48349700	-1.71327000
C	-2.25065800	-0.81171000	-2.80256200
C	-3.97321400	-1.36553100	-1.12472800

C	-2.38826400	-2.09642200	-3.32262700
C	-4.08317100	-2.62938900	-1.70238100
C	-3.29884900	-3.01292500	-2.78998800
H	-1.76534700	-2.38783200	-4.16379200
H	-4.78934700	-3.33585000	-1.27441300
C	-4.75524100	-1.00905900	0.11124700
H	-5.09287100	0.03093100	0.10202000
H	-4.14150000	-1.16651500	1.00865100
C	-1.22793300	0.15231600	-3.34195900
H	-0.36506100	0.22816600	-2.66710000
H	-1.64757700	1.15261300	-3.47554000
H	-0.85654000	-0.19655400	-4.30637200
H	-5.63099700	-1.65355500	0.20177300
C	-3.40185500	-4.40769400	-3.34790700
H	-4.42332100	-4.78767500	-3.27492800
H	-3.08926600	-4.44142700	-4.39339300
H	-2.75399000	-5.08771300	-2.78460500
C	-1.66866900	0.32393500	0.99213600
O	-1.97721500	0.59983000	2.13216100
H	3.01967900	-2.40242600	1.11424100
C	-0.68962600	-0.69339400	0.56069100
C	-0.37520200	-1.72575000	1.64840000
H	-0.99048500	-1.16510300	-0.38202500
H	-0.19629600	-1.17343300	2.57942900
C	-1.58699000	-2.61098400	1.87282000
C	-2.31374200	-2.53336300	3.06430300
C	-2.02866200	-3.48691700	0.87601100
C	-3.45130200	-3.31346100	3.26009200
H	-1.98571700	-1.84553400	3.83908600
C	-3.15971700	-4.27505300	1.07245300
H	-1.48958700	-3.55115700	-0.06740700
C	-3.87697200	-4.18934000	2.26402200
H	-4.00370900	-3.23762500	4.19155900
H	-3.48202200	-4.95588800	0.28977400
H	-4.76048000	-4.80141500	2.41554900
C	0.88952700	-2.52759600	1.29696800
C	2.19952600	-1.68999600	1.29853100
H	0.79728200	-2.96983700	0.30043700
H	0.99958900	-3.34318700	2.02065600
N	2.19008600	-0.56288500	0.38837800
H	0.24371900	-0.13150800	0.32806500
S	2.56530800	-0.87271500	-1.10493400
O	2.04338200	0.21651000	-1.95713300
O	2.24770400	-2.25003500	-1.55327000

C	4.35224500	-0.75490800	-1.24363900
C	4.95355400	0.50171700	-1.15011200
C	6.33614900	0.60470900	-1.18463100
C	7.14255500	-0.53668100	-1.30195600
C	6.52264600	-1.78233600	-1.38900800
C	5.13197100	-1.89800200	-1.36093600
H	4.32888100	1.38651300	-1.06453600
H	6.80628200	1.58297400	-1.11985400
H	7.13316100	-2.67653600	-1.48302800
H	4.64691200	-2.86494000	-1.44341200
C	8.64349400	-0.40475500	-1.33435600
H	9.01550800	0.05901000	-0.41575700
H	9.12426700	-1.37924800	-1.44155900
H	8.96284000	0.22623700	-2.16920700
C	2.41676500	-1.22248900	2.73118000
O	2.82539300	-1.94162800	3.61603100
O	2.03282500	0.04362300	2.95142200
C	2.14738500	0.49114300	4.30371500
H	1.51316500	-0.11005600	4.95870400
H	3.18218500	0.41793000	4.64297000
H	1.81958700	1.52978900	4.29893400

TS5^{SI}

C	4.93147300	-2.28553900	0.89956000
C	3.56319300	-2.11884500	1.09702800
C	2.87875400	-2.81886800	2.08513700
C	3.59426300	-3.70894400	2.88217700
C	4.96734400	-3.88331600	2.68960700
C	5.64552200	-3.17215200	1.70162900
C	5.43064100	-1.40736200	-0.22013000
C	4.15916200	-0.86100200	-0.91223200
C	2.99723500	-1.11853200	0.11656400
H	1.81274700	-2.66698500	2.22921100
H	3.08375000	-4.26928300	3.65847100
H	5.51173700	-4.58251900	3.31630700
H	6.71202900	-3.31394800	1.55441200
H	6.05095800	-1.94162000	-0.94601600
H	4.21477500	0.20713600	-1.11663100
H	6.03130400	-0.58116000	0.17406900
H	2.69853300	-0.18527900	0.58984500
N	1.80838200	-1.65560800	-0.55616700
O	3.95779300	-1.45159900	-2.18855500
C	0.49812200	-1.43023900	-0.37597700
C	1.93520700	-2.44898700	-1.65615700

N	-0.11108300	-2.11293200	-1.34923000
N	0.77336500	-2.74861000	-2.16395200
C	3.31236600	-2.70846400	-2.16596700
H	3.83708000	-3.43338600	-1.52850400
H	3.26997100	-3.08946400	-3.18577000
C	-1.52678500	-2.23240900	-1.57005500
C	-2.19835600	-3.23942200	-0.86393200
C	-2.16694900	-1.30162300	-2.38692600
C	-3.58610000	-3.23926500	-0.92093300
C	-3.56599500	-1.34105800	-2.39910500
C	-4.28579000	-2.27745000	-1.65993100
H	-4.13779900	-3.99185100	-0.36351900
H	-4.09950400	-0.60806600	-3.00000000
C	-1.42946400	-0.30012300	-3.23502300
H	-1.66361000	-0.48372600	-4.28816100
H	-0.34821200	-0.35979100	-3.10559600
C	-1.43672200	-4.25025300	-0.04744600
H	-0.90881800	-3.78163000	0.79089500
H	-0.68525100	-4.75918400	-0.65800200
H	-2.11617100	-4.99849600	0.36224900
H	-1.73670000	0.72155000	-2.99503800
C	-5.79170700	-2.28017400	-1.67424200
H	-6.18483400	-1.29830400	-1.94718200
H	-6.16993500	-3.00642900	-2.40073600
H	-6.18965400	-2.55546300	-0.69430000
C	-0.07329300	-0.63001300	0.79408400
O	0.73747300	-0.33252000	1.66731700
H	-2.54207600	0.98090100	-0.71681800
C	-1.54727200	-0.76089400	1.11605800
C	-2.08453200	0.39809600	1.96955000
H	-1.65606900	-1.69538200	1.68302000
H	-1.47657300	0.45117700	2.87737900
C	-3.50682600	0.05914200	2.37736000
C	-3.83334100	-0.14820800	3.71797300
C	-4.51747200	-0.07303700	1.41606300
C	-5.13457600	-0.47661200	4.09646600
H	-3.05933600	-0.04882100	4.47459400
C	-5.81780400	-0.39779900	1.78982800
H	-4.28968700	0.07721300	0.36221400
C	-6.13106700	-0.60210000	3.13321900
H	-5.36744100	-0.63271700	5.14520200
H	-6.58910000	-0.48949000	1.03099000
H	-7.14518100	-0.85590200	3.42463100
C	-1.99027200	1.76383100	1.23877500

C	-1.77412800	1.63413300	-0.27870300
H	-1.14635800	2.34243000	1.62476000
H	-2.89981700	2.34111300	1.43813500
N	-0.46376300	1.03322700	-0.53554000
H	-2.15223400	-0.85952200	0.21834000
S	0.67076000	1.78860300	-1.34734300
O	0.15203300	2.57688000	-2.48145200
O	1.70458600	0.78756500	-1.68214500
C	1.49641100	2.97753900	-0.28629900
C	1.97192900	4.16448500	-0.83736400
C	2.64930000	5.06756000	-0.02619800
C	2.86171300	4.79968000	1.33113400
C	2.37276600	3.60242200	1.85899200
C	1.68937300	2.68845800	1.05948000
H	1.79124300	4.37442100	-1.88661400
H	3.01710400	5.99922300	-0.44863800
H	2.52179900	3.38550100	2.91325700
H	1.29494500	1.76546500	1.47891300
C	3.60693100	5.78552800	2.19350100
H	3.19123600	6.79143400	2.08810500
H	3.56150600	5.50405100	3.24749500
H	4.66086600	5.83671500	1.90270400
C	-2.03122900	2.97609000	-0.95538000
O	-2.82614100	3.14784400	-1.84898100
O	-1.30415200	3.95219200	-0.40407100
C	-1.29838700	5.18967300	-1.11750300
H	-0.63342200	5.84872300	-0.56176300
H	-0.91368400	5.01667600	-2.12558800
H	-2.30515100	5.60792900	-1.16960800

TS5A^{S1}

C	-4.84469300	-2.27843400	0.95479200
C	-3.69849800	-1.49914700	0.82455600
C	-3.78024600	-0.14539200	0.51757700
C	-5.03404000	0.41457100	0.29433800
C	-6.18713000	-0.36921700	0.39420100
C	-6.10061800	-1.71724700	0.73370900
C	-4.51869700	-3.68030100	1.39341500
C	-2.97505800	-3.77091100	1.38028600
C	-2.45439100	-2.29048700	1.15828600
H	-2.87879300	0.44545000	0.46105700
H	-5.10957500	1.46969800	0.04709800
H	-7.16016700	0.07853900	0.21726700
H	-6.99829900	-2.32093200	0.82974500

H	-4.93869100	-4.44832400	0.73549100
H	-2.58562200	-4.14551500	2.32691100
H	-4.90527800	-3.87521800	2.39829800
H	-1.97452000	-1.90674000	2.05715700
N	-1.41424000	-2.27111500	0.10377200
O	-2.51722500	-4.70731400	0.41759500
C	-0.25851700	-1.58615200	-0.02061300
C	-1.44683800	-3.17718300	-0.91721600
N	0.37863800	-2.14531000	-1.05369200
N	-0.36029900	-3.13427000	-1.62993300
C	-2.52899800	-4.20020900	-0.90552200
H	-3.50131900	-3.76680700	-1.17367200
H	-2.28996200	-5.01301900	-1.59009200
C	1.76396200	-2.02739000	-1.44878900
C	2.12203400	-1.26914200	-2.55737300
C	2.68425400	-2.80086500	-0.71910500
C	3.48780600	-1.19236600	-2.85717600
C	4.02546300	-2.69161900	-1.06112900
C	4.44752600	-1.86888400	-2.11462800
H	3.79344000	-0.58061100	-3.70192000
H	4.75931000	-3.27236800	-0.50752400
C	2.23008800	-3.73518400	0.37272500
H	1.48009500	-4.43801800	-0.00415300
H	1.78195900	-3.19956400	1.21573700
C	1.11971400	-0.59982200	-3.44854700
H	1.30721200	0.47468500	-3.47777900
H	0.09630900	-0.75565200	-3.10697400
H	1.21602500	-1.00099400	-4.46247100
H	3.07531000	-4.30903700	0.75511700
C	5.91407000	-1.73890300	-2.43247400
H	6.40607500	-1.08282300	-1.70733800
H	6.41388200	-2.71001700	-2.38721300
H	6.06774900	-1.31406000	-3.42622300
C	0.13116500	-0.43163000	0.92411100
O	-0.79483800	-0.05351100	1.65630200
H	0.87692000	2.87866100	0.23846800
C	1.54551800	-0.50392900	1.47871900
C	2.10114100	0.85692100	1.89966600
H	1.47000100	-1.16473000	2.35168700
H	1.29887500	1.42202000	2.39259300
C	3.25044700	0.71423100	2.87617400
C	3.32678200	1.54492800	3.99605200
C	4.27389300	-0.21499500	2.66033500
C	4.39398900	1.44949800	4.88577400

H	2.53795900	2.27182100	4.17211900
C	5.34193600	-0.31381500	3.54829500
H	4.23933100	-0.86866200	1.79090100
C	5.40514600	0.51788400	4.66453800
H	4.43274000	2.10035000	5.75363500
H	6.12629600	-1.04249900	3.36880300
H	6.23640600	0.43893400	5.35770000
C	2.56075800	1.61377900	0.64967300
C	1.40047000	2.04302000	-0.24859700
H	3.24234100	0.97525900	0.07305700
H	3.11554600	2.51419200	0.93521200
N	0.49087700	0.92299400	-0.51745900
H	2.22734600	-0.96065300	0.76099100
S	-0.78059000	1.34008500	-1.41685100
O	-1.61267600	0.13496400	-1.57436900
O	-0.38708500	2.02503300	-2.66037200
C	-1.75619800	2.57282900	-0.54676400
C	-1.72235700	2.68873400	0.83938000
C	-2.54767200	3.62062400	1.46337600
C	-3.40564800	4.43823800	0.72390700
C	-3.41951800	4.30410900	-0.66929400
C	-2.59673400	3.38455800	-1.30812000
H	-1.08336000	2.03286600	1.42338800
H	-2.52531500	3.71248100	2.54575600
H	-4.07981300	4.93318300	-1.26007100
H	-2.59534600	3.29503400	-2.38935500
C	-4.27300600	5.46441500	1.40434500
H	-3.77473600	6.43932300	1.41977100
H	-5.22298800	5.58932900	0.87940900
H	-4.48208800	5.18282100	2.43863900
C	2.01232200	2.58699400	-1.54322600
O	2.71389500	1.95010900	-2.29353000
O	1.72226100	3.88044700	-1.71463900
C	2.16608600	4.43695100	-2.95327600
H	3.24820000	4.33622300	-3.05432500
H	1.67399700	3.91967200	-3.77983300
H	1.87821200	5.48607000	-2.93241900

TS5B^{SI}

C	-3.86565100	2.28796700	-0.92333300
C	-2.75887800	1.57460800	-1.39682700
C	-2.88293100	0.24115500	-1.77215700
C	-4.12713100	-0.37222300	-1.63580800
C	-5.22747500	0.33463200	-1.15071000

C	-5.10596800	1.67359700	-0.78918900
C	-3.52637500	3.73483400	-0.71183700
C	-2.29509100	3.88885300	-1.62442500
C	-1.58058000	2.49823700	-1.62174700
H	-2.02182700	-0.28230800	-2.17077800
H	-4.24634200	-1.41385900	-1.90357900
H	-6.18836200	-0.16335300	-1.06239400
H	-5.96528400	2.23681700	-0.43787600
H	-3.29069800	3.92412700	0.34069000
H	-2.64348000	4.03692600	-2.64931800
H	-4.32777400	4.41830500	-1.00013300
H	-1.06487500	2.28498500	-2.55748300
N	-0.49726200	2.51588700	-0.58855800
O	-1.46469500	4.99159500	-1.34771700
C	0.47987200	1.61652400	-0.32305400
C	-0.17283200	3.65685800	0.09987000
N	1.34154000	2.25176900	0.48079600
N	0.93661700	3.51920800	0.75857400
C	-0.91810700	4.94288300	-0.05026900
H	-1.68066600	5.05571500	0.72747900
H	-0.20651700	5.76359700	0.04423100
C	2.70860900	1.95019100	0.84936700
C	3.68861800	2.23731600	-0.10992200
C	2.99939200	1.48471900	2.12811400
C	5.00916800	1.95781900	0.22321200
C	4.34453000	1.22721200	2.41377500
C	5.35342100	1.44153000	1.47719000
H	5.78867800	2.14851000	-0.50993800
H	4.60239800	0.85107600	3.40064700
C	1.92798900	1.24692100	3.15515100
H	1.11178100	1.96476200	3.05320900
H	2.35111100	1.32682200	4.15851900
C	3.31819200	2.81345600	-1.45256000
H	2.78031500	3.75969100	-1.33399100
H	2.67152200	2.13936800	-2.02682100
H	4.21406900	3.00190100	-2.04522100
H	1.49101400	0.25001800	3.04010600
C	6.79469300	1.15591700	1.80944800
H	6.87829000	0.53083900	2.70078500
H	7.29214300	0.64688800	0.97982900
H	7.33962600	2.08643300	1.99731700
C	0.67882600	0.25975200	-1.04785200
O	0.29092000	0.27578900	-2.22657000
H	-0.93591200	-2.94971200	0.25223700

C	1.96591900	-0.44914300	-0.64039100
C	2.06903400	-1.88109600	-1.14698500
H	2.79767200	0.12564400	-1.06119700
H	1.77663700	-1.89556100	-2.20040700
C	3.48400800	-2.41672800	-1.03238700
C	3.88122300	-3.46996300	-1.86309600
C	4.40012500	-1.92825500	-0.09571600
C	5.15516300	-4.02069100	-1.76549300
H	3.17656900	-3.85575400	-2.59665300
C	5.67789700	-2.47697800	0.00465600
H	4.12842600	-1.10771500	0.56379800
C	6.06045700	-3.52438200	-0.82815500
H	5.44399100	-4.83507900	-2.42275800
H	6.37417700	-2.08218300	0.73886900
H	7.05549900	-3.95070900	-0.74959300
C	1.11095000	-2.77901100	-0.35848800
C	-0.34688300	-2.31624200	-0.42557400
H	1.41354300	-2.78053700	0.69426500
H	1.17570000	-3.80836200	-0.72792300
N	-0.56080600	-0.90168600	-0.06409400
H	2.06034400	-0.43354700	0.44983800
S	-0.84662600	-0.68836100	1.51011600
O	-0.96402300	0.76058100	1.73872400
O	0.09918000	-1.42668600	2.37095600
C	-2.44735300	-1.39309500	1.86274500
C	-3.58501500	-0.64377000	1.57894300
C	-4.83357900	-1.17673300	1.87347100
C	-4.96133300	-2.45167100	2.43670200
C	-3.80239900	-3.18247600	2.71174100
C	-2.54342200	-2.65930400	2.43264500
H	-3.48324600	0.34637500	1.14293900
H	-5.72552200	-0.59321800	1.66028400
H	-3.88659100	-4.16806400	3.16074500
H	-1.64077500	-3.20990400	2.67678500
C	-6.32373600	-3.02782800	2.72176900
H	-6.76045000	-3.45069900	1.81111000
H	-6.26878100	-3.82517400	3.46584800
H	-7.00851400	-2.25880000	3.08723300
C	-0.92748400	-2.62638800	-1.80683200
O	-0.29445400	-2.77584400	-2.82522400
O	-2.25429800	-2.81899100	-1.75249500
C	-2.85099600	-3.20571700	-2.99463700
H	-2.80176400	-2.38230100	-3.71198600
H	-2.33431700	-4.07252200	-3.40923000

H	-3.88665300	-3.45319100	-2.76786600
TS5C ^{S1}			
C	-3.86565100	2.28796700	-0.92333300
C	-2.75887800	1.57460800	-1.39682700
C	-2.88293100	0.24115500	-1.77215700
C	-4.12713100	-0.37222300	-1.63580800
C	-5.22747500	0.33463200	-1.15071000
C	-5.10596800	1.67359700	-0.78918900
C	-3.52637500	3.73483400	-0.71183700
C	-2.29509100	3.88885300	-1.62442500
C	-1.58058000	2.49823700	-1.62174700
H	-2.02182700	-0.28230800	-2.17077800
H	-4.24634200	-1.41385900	-1.90357900
H	-6.18836200	-0.16335300	-1.06239400
H	-5.96528400	2.23681700	-0.43787600
H	-3.29069800	3.92412700	0.34069000
H	-2.64348000	4.03692600	-2.64931800
H	-4.32777400	4.41830500	-1.00013300
H	-1.06487500	2.28498500	-2.55748300
N	-0.49726200	2.51588700	-0.58855800
O	-1.46469500	4.99159500	-1.34771700
C	0.47987200	1.61652400	-0.32305400
C	-0.17283200	3.65685800	0.09987000
N	1.34154000	2.25176900	0.48079600
N	0.93661700	3.51920800	0.75857400
C	-0.91810700	4.94288300	-0.05026900
H	-1.68066600	5.05571500	0.72747900
H	-0.20651700	5.76359700	0.04423100
C	2.70860900	1.95019100	0.84936700
C	3.68861800	2.23731600	-0.10992200
C	2.99939200	1.48471900	2.12811400
C	5.00916800	1.95781900	0.22321200
C	4.34453000	1.22721200	2.41377500
C	5.35342100	1.44153000	1.47719000
H	5.78867800	2.14851000	-0.50993800
H	4.60239800	0.85107600	3.40064700
C	1.92798900	1.24692100	3.15515100
H	1.11178100	1.96476200	3.05320900
H	2.35111100	1.32682200	4.15851900
C	3.31819200	2.81345600	-1.45256000
H	2.78031500	3.75969100	-1.33399100
H	2.67152200	2.13936800	-2.02682100
H	4.21406900	3.00190100	-2.04522100

H	1.49101400	0.25001800	3.04010600
C	6.79469300	1.15591700	1.80944800
H	6.87829000	0.53083900	2.70078500
H	7.29214300	0.64688800	0.97982900
H	7.33962600	2.08643300	1.99731700
C	0.67882600	0.25975200	-1.04785200
O	0.29092000	0.27578900	-2.22657000
H	-0.93591200	-2.94971200	0.25223700
C	1.96591900	-0.44914300	-0.64039100
C	2.06903400	-1.88109600	-1.14698500
H	2.79767200	0.12564400	-1.06119700
H	1.77663700	-1.89556100	-2.20040700
C	3.48400800	-2.41672800	-1.03238700
C	3.88122300	-3.46996300	-1.86309600
C	4.40012500	-1.92825500	-0.09571600
C	5.15516300	-4.02069100	-1.76549300
H	3.17656900	-3.85575400	-2.59665300
C	5.67789700	-2.47697800	0.00465600
H	4.12842600	-1.10771500	0.56379800
C	6.06045700	-3.52438200	-0.82815500
H	5.44399100	-4.83507900	-2.42275800
H	6.37417700	-2.08218300	0.73886900
H	7.05549900	-3.95070900	-0.74959300
C	1.11095000	-2.77901100	-0.35848800
C	-0.34688300	-2.31624200	-0.42557400
H	1.41354300	-2.78053700	0.69426500
H	1.17570000	-3.80836200	-0.72792300
N	-0.56080600	-0.90168600	-0.06409400
H	2.06034400	-0.43354700	0.44983800
S	-0.84662600	-0.68836100	1.51011600
O	-0.96402300	0.76058100	1.73872400
O	0.09918000	-1.42668600	2.37095600
C	-2.44735300	-1.39309500	1.86274500
C	-3.58501500	-0.64377000	1.57894300
C	-4.83357900	-1.17673300	1.87347100
C	-4.96133300	-2.45167100	2.43670200
C	-3.80239900	-3.18247600	2.71174100
C	-2.54342200	-2.65930400	2.43264500
H	-3.48324600	0.34637500	1.14293900
H	-5.72552200	-0.59321800	1.66028400
H	-3.88659100	-4.16806400	3.16074500
H	-1.64077500	-3.20990400	2.67678500
C	-6.32373600	-3.02782800	2.72176900
H	-6.76045000	-3.45069900	1.81111000

H	-6.26878100	-3.82517400	3.46584800
H	-7.00851400	-2.25880000	3.08723300
C	-0.92748400	-2.62638800	-1.80683200
O	-0.29445400	-2.77584400	-2.82522400
O	-2.25429800	-2.81899100	-1.75249500
C	-2.85099600	-3.20571700	-2.99463700
H	-2.80176400	-2.38230100	-3.71198600
H	-2.33431700	-4.07252200	-3.40923000
H	-3.88665300	-3.45319100	-2.76786600

M5^{S1}

C	4.87388500	-2.35880000	0.43338200
C	3.60208400	-1.84688000	0.67312200
C	2.91330400	-2.13047200	1.84888500
C	3.50869500	-2.98112700	2.77602600
C	4.77446900	-3.52151300	2.53085400
C	5.46972300	-3.20629700	1.36547300
C	5.43802300	-1.84063900	-0.86409600
C	4.27328300	-1.08455100	-1.55097100
C	3.13875900	-0.96434500	-0.46195600
H	1.95523900	-1.65347300	2.03185200
H	2.99145500	-3.22006900	3.69963700
H	5.22474800	-4.18591700	3.26169500
H	6.46016900	-3.61489300	1.18772300
H	5.80787800	-2.63215900	-1.52407600
H	4.56909600	-0.08439100	-1.86787300
H	6.27663000	-1.16211500	-0.67968200
H	2.97377000	0.06039800	-0.14162300
N	1.84720100	-1.41727300	-1.00601900
O	3.86786500	-1.72467200	-2.75185900
C	0.58823800	-1.01120800	-0.76028700
C	1.79104700	-2.38140800	-1.97155100
N	-0.17260900	-1.75941200	-1.57096800
N	0.56841000	-2.61101100	-2.34436600
C	3.07747900	-2.87781100	-2.53743600
H	3.56368500	-3.58882800	-1.85526100
H	2.90579300	-3.36139600	-3.49854300
C	-1.60539200	-1.79545100	-1.73272000
C	-2.32477700	-2.78014500	-1.03904000
C	-2.20559800	-0.91089600	-2.62975900
C	-3.70635700	-2.80589700	-1.20876400
C	-3.59401200	-0.98705500	-2.76690800
C	-4.35981100	-1.90781300	-2.05723900
H	-4.28457900	-3.55486900	-0.67150200

H	-4.08222000	-0.31334200	-3.46719800
C	-1.42737800	0.08161300	-3.44637800
H	-1.76325500	0.04958400	-4.48628700
H	-0.35248300	-0.10784000	-3.42418900
C	-1.66851100	-3.77560000	-0.11475900
H	-1.98585000	-3.60216400	0.91936600
H	-0.57892900	-3.72421100	-0.14529900
H	-1.96744000	-4.79097600	-0.38635400
H	-1.59382300	1.08966300	-3.05877200
C	-5.85906400	-1.94438400	-2.19806800
H	-6.18695500	-1.38930700	-3.07924800
H	-6.22178100	-2.97204000	-2.27998300
H	-6.33760200	-1.49652000	-1.32139300
C	0.18403700	0.00453100	0.38750700
O	1.20834800	0.43333500	1.05297400
H	-0.98560500	2.63776200	1.07152500
C	-0.84540100	-0.77522000	1.24644000
C	-1.60284900	0.14184500	2.19614200
H	-0.26640600	-1.52615600	1.79378600
H	-0.87546400	0.73017900	2.76833900
C	-2.47163800	-0.64309500	3.15428900
C	-2.32157200	-0.49636300	4.53417400
C	-3.44318200	-1.53284900	2.67824200
C	-3.11779600	-1.21805500	5.42145300
H	-1.57148800	0.19095200	4.91626700
C	-4.23991300	-2.25555700	3.56134500
H	-3.58250000	-1.66311800	1.60578500
C	-4.07963400	-2.10049600	4.93753200
H	-2.98465600	-1.09019000	6.49125800
H	-4.98731300	-2.94142900	3.17451000
H	-4.70038600	-2.66491500	5.62590900
C	-2.42999800	1.07569600	1.31497300
C	-1.52857300	1.93602000	0.42407100
H	-3.04572200	1.75253500	1.91598600
H	-3.09938600	0.48353000	0.67827700
N	-0.59226100	1.12283600	-0.38326700
H	-1.58399000	-1.29254900	0.63495700
S	0.44954100	2.12364800	-1.25472000
O	-0.40680600	2.92635800	-2.13111700
O	1.47137500	1.26859200	-1.85792700
C	1.24460900	3.30734600	-0.17932300
C	0.63213700	4.54658800	-0.00440400
C	1.25840500	5.50202300	0.79050700
C	2.48795500	5.23928200	1.39765400

C	3.08500200	3.98926100	1.19208900
C	2.46938100	3.01760100	0.41575700
H	-0.31775100	4.75653200	-0.48518700
H	0.78622600	6.46964800	0.93272200
H	4.04631900	3.77655800	1.65116200
H	2.92008700	2.04516100	0.27260100
C	3.15349500	6.26685900	2.27408600
H	2.80262100	7.27413600	2.04079900
H	2.93110000	6.07104200	3.32805800
H	4.23945000	6.23994500	2.15744600
C	-2.44615000	2.78183000	-0.45252700
O	-2.65916800	3.95608800	-0.25554200
O	-3.05799700	2.05794700	-1.38853300
C	-3.86294800	2.80870200	-2.29973800
H	-4.27301000	2.08414600	-3.00064600
H	-4.66392300	3.32613700	-1.76913300
H	-3.23927800	3.53778800	-2.82199900

M5A^{S1}

C	5.31433300	1.33984500	-0.90016400
C	3.93397600	1.22454700	-1.03937700
C	3.26631500	1.75133400	-2.14050200
C	4.01118600	2.42954900	-3.10212200
C	5.39571000	2.56288400	-2.96249200
C	6.05755000	2.01377500	-1.86631700
C	5.79719200	0.64123000	0.34534200
C	4.51635900	0.27757200	1.13515100
C	3.33303300	0.45828500	0.11503200
H	2.19524200	1.59963800	-2.24110600
H	3.51617100	2.85333100	-3.96999700
H	5.96151800	3.09558200	-3.72034600
H	7.13453700	2.11214500	-1.76610900
H	6.45285500	1.26065800	0.96538600
H	4.52941400	-0.75262600	1.49040700
H	6.35654500	-0.26426000	0.08956300
H	2.90965200	-0.49434600	-0.19371900
N	2.23035300	1.20999100	0.73444500
O	4.39243100	1.05394900	2.32014700
C	0.89702600	1.11903900	0.59406600
C	2.48370400	2.18419900	1.65702900
N	0.40490100	2.04438400	1.42801600
N	1.38447000	2.71379300	2.10582500
C	3.89559600	2.36091400	2.10467900
H	4.48406200	2.90786800	1.35518200

H	3.92687100	2.90058500	3.05076900
C	-0.97146000	2.38805800	1.66883600
C	-1.48656700	3.50268800	0.98762900
C	-1.72725600	1.61405000	2.54477300
C	-2.83767000	3.77826500	1.14148700
C	-3.08903300	1.92863100	2.65542000
C	-3.65977800	2.98521200	1.95519300
H	-3.26872300	4.62175100	0.60769500
H	-3.70827200	1.31818800	3.30803500
C	-1.15003300	0.50029600	3.37370800
H	-1.24811300	0.75266700	4.43410400
H	-0.09492100	0.32060000	3.16115200
C	-0.60271700	4.34370100	0.10610200
H	-0.12241700	3.73960500	-0.67072300
H	0.19449000	4.81329300	0.68977500
H	-1.18348100	5.12701100	-0.38242200
H	-1.69282600	-0.43122000	3.19620700
C	-5.13140500	3.28833100	2.05957100
H	-5.62379900	2.62549800	2.77321100
H	-5.29519900	4.32182900	2.37756100
H	-5.61831900	3.16584300	1.08699000
C	0.17310100	0.16509500	-0.42537600
O	1.03243400	-0.37218800	-1.23152200
H	-2.52625100	-0.05563700	0.62865700
C	-0.93535900	0.95913000	-1.15726300
C	-1.76878600	0.03355200	-2.05555900
H	-0.42080100	1.69991100	-1.77752300
H	-1.10130100	-0.35720800	-2.82774300
C	-2.86421200	0.84114400	-2.72143700
C	-2.85955300	1.06527400	-4.09836300
C	-3.89313500	1.40468700	-1.95632700
C	-3.85762100	1.83006600	-4.70170600
H	-2.06624900	0.63439100	-4.70384900
C	-4.89078600	2.16777100	-2.55331700
H	-3.91265900	1.24803100	-0.87840800
C	-4.87611000	2.38281900	-3.93138300
H	-3.83834900	1.99125200	-5.77508500
H	-5.68136900	2.59523500	-1.94402800
H	-5.65458400	2.97670700	-4.39951100
C	-2.32116900	-1.16176400	-1.23197300
C	-2.05632300	-0.97618700	0.26558900
H	-1.84379300	-2.09541500	-1.54180200
H	-3.39825300	-1.27577300	-1.39354800
N	-0.60491800	-0.83881800	0.51740400

H	-1.60202800	1.49625700	-0.48112900
S	0.26719100	-2.01143600	1.28052200
O	-0.50269200	-2.47742000	2.43624900
O	1.58378400	-1.42612400	1.54000600
C	0.46418700	-3.44749000	0.23167700
C	0.35590300	-4.69780400	0.83768400
C	0.53151300	-5.83847800	0.06406200
C	0.80916500	-5.74585500	-1.30419400
C	0.90491500	-4.47721600	-1.88166500
C	0.73934500	-3.31976600	-1.12537900
H	0.11903400	-4.76773500	1.89389600
H	0.44275200	-6.81758900	0.52691000
H	1.10974600	-4.39179300	-2.94535800
H	0.81191500	-2.32351500	-1.55945100
C	1.01797800	-6.98998900	-2.12678600
H	0.35422300	-7.79433000	-1.80066300
H	0.83784200	-6.79888700	-3.18665700
H	2.04649500	-7.35072000	-2.02296000
C	-2.73867800	-2.06584400	1.08706100
O	-3.45545900	-1.84201100	2.03284800
O	-2.50815000	-3.28125100	0.59135900
C	-2.97454900	-4.36605400	1.39830100
H	-2.66299400	-5.27337400	0.88404200
H	-2.51073800	-4.30140600	2.38526900
H	-4.06072000	-4.32715200	1.49630500

M5B^{S1}

C	-4.43447600	-3.03112000	0.72403400
C	-3.46393100	-2.03937100	0.60646500
C	-3.81645400	-0.71525300	0.36700900
C	-5.16040800	-0.40376500	0.18695600
C	-6.13629100	-1.40134000	0.26607000
C	-5.78071600	-2.71820700	0.54735400
C	-3.83388900	-4.35638000	1.10516800
C	-2.30284500	-4.13354600	1.10931700
C	-2.08004000	-2.58002900	0.88416600
H	-3.04226900	0.03699900	0.33511800
H	-5.44936800	0.62498900	-0.00735200
H	-7.18167800	-1.14614100	0.12220500
H	-6.54107200	-3.48859800	0.63665400
H	-4.08920400	-5.16200800	0.40825200
H	-1.86042700	-4.41542800	2.06509700
H	-4.17829900	-4.67365400	2.09395600
H	-1.64561500	-2.09849100	1.75879600

N	-1.09586700	-2.35737700	-0.20408100
O	-1.65596700	-4.97048100	0.16301300
C	-0.10787000	-1.45061200	-0.35605200
C	-0.95419900	-3.27314800	-1.21262100
N	0.60946200	-1.88458100	-1.40204200
N	0.08283500	-3.02058300	-1.95025900
C	-1.79456600	-4.50084100	-1.16650000
H	-2.84139700	-4.28912400	-1.42019600
H	-1.40006300	-5.25532400	-1.84580100
C	1.96632300	-1.54022100	-1.76499400
C	2.23610700	-0.57429500	-2.72645300
C	2.97778900	-2.28155200	-1.12602500
C	3.58253300	-0.27152200	-2.96727700
C	4.29611400	-1.94445200	-1.40351100
C	4.61679400	-0.92233900	-2.30672600
H	3.81190100	0.50101700	-3.69691000
H	5.09488800	-2.49163200	-0.90839000
C	2.64996100	-3.41796400	-0.19238600
H	1.88000900	-3.14671100	0.53656500
H	3.53981300	-3.72788500	0.35784500
C	1.16741800	0.11068300	-3.52407800
H	1.20488500	1.18668600	-3.34666100
H	0.16758200	-0.24061100	-3.26486600
H	1.33616600	-0.07477300	-4.58925400
H	2.27368600	-4.27830700	-0.75480500
C	6.05567100	-0.54799400	-2.54732700
H	6.45011600	0.02052700	-1.69895100
H	6.67960500	-1.43814900	-2.66293600
H	6.16031100	0.06849600	-3.44220800
C	0.11442800	-0.23357500	0.61141600
O	-0.88732400	-0.10399000	1.42619600
H	0.41334600	2.75803800	0.84937000
C	1.46412300	-0.50675700	1.32298400
C	1.99018700	0.72413300	2.04954200
H	1.25219100	-1.31643400	2.02903400
H	1.19637600	1.11161100	2.70031400
C	3.20204100	0.39639300	2.89542100
C	3.21368500	0.68027400	4.26212200
C	4.33551000	-0.19614700	2.32543300
C	4.32670200	0.38102600	5.04588300
H	2.33913800	1.13860000	4.71649400
C	5.44906200	-0.49500700	3.10478500
H	4.34950700	-0.43112300	1.26241600
C	5.44831400	-0.20793900	4.46904600

H	4.31529400	0.60776200	6.10744900
H	6.31922500	-0.95504800	2.64669000
H	6.31603300	-0.44404100	5.07658600
C	2.31348800	1.75743900	0.97411900
C	1.06505500	2.16671900	0.19332900
H	3.04316900	1.34330100	0.26735800
H	2.74576600	2.66411300	1.41036000
N	0.33878200	0.99747900	-0.35470000
H	2.23653900	-0.84212500	0.62860200
S	-1.01423600	1.46191100	-1.22964200
O	-1.70977500	0.22601600	-1.59238900
O	-0.56837000	2.32814200	-2.32281000
C	-2.09102500	2.52879300	-0.26245500
C	-2.27002400	2.40598100	1.11342100
C	-3.17151800	3.25528600	1.74905200
C	-3.89731400	4.21462400	1.03917900
C	-3.69488700	4.31602700	-0.34113200
C	-2.79022200	3.49019800	-0.99532000
H	-1.72038900	1.63796700	1.65280100
H	-3.31541000	3.16580100	2.82230800
H	-4.24847700	5.05757300	-0.91013900
H	-2.62101200	3.58862000	-2.06155200
C	-4.84972900	5.14270300	1.74501600
H	-4.34454900	6.07608900	2.01415600
H	-5.69759200	5.40012200	1.10614100
H	-5.23005700	4.69466300	2.66543200
C	1.54188600	3.06797500	-0.94845900
O	2.34898200	2.74158500	-1.78443100
O	1.00980800	4.28761700	-0.85196200
C	1.34944700	5.17672500	-1.91912100
H	2.43025300	5.32005700	-1.96794800
H	0.99368600	4.76097400	-2.86414000
H	0.84645400	6.11570900	-1.69810000

M5C^{S1}

C	-3.90314300	2.34679000	-0.74326100
C	-2.84186000	1.60742800	-1.27604400
C	-3.01438300	0.28953500	-1.67147700
C	-4.26442200	-0.29942900	-1.48782500
C	-5.32183800	0.42773700	-0.93999500
C	-5.15072800	1.75877700	-0.56233600
C	-3.50458300	3.78325600	-0.55513700
C	-2.33858100	3.89048600	-1.55986700
C	-1.64855500	2.49090500	-1.55229200

H	-2.17773800	-0.23450300	-2.11264500
H	-4.41776500	-1.33616800	-1.76309900
H	-6.29120500	-0.04568200	-0.81492900
H	-5.98142700	2.33489600	-0.16587900
H	-3.17898700	3.96241300	0.47550400
H	-2.76088200	4.00342700	-2.56120900
H	-4.30151500	4.49447100	-0.78188700
H	-1.15868500	2.23936800	-2.49233100
N	-0.54532500	2.50179900	-0.54248000
O	-1.47643000	4.98942200	-1.38854400
C	0.39246400	1.56382700	-0.24696500
C	-0.13912600	3.67223000	0.04739000
N	1.31369600	2.21703100	0.48131800
N	0.98267100	3.52447400	0.67703000
C	-0.84024200	4.97985800	-0.13298000
H	-1.54248900	5.16585600	0.68757400
H	-0.09202000	5.77332300	-0.13017100
C	2.68191500	1.91064300	0.84812200
C	3.65675800	2.20315800	-0.11458700
C	2.98440700	1.46569300	2.13146000
C	4.98306800	1.95168100	0.22001300
C	4.33383100	1.23523000	2.41889500
C	5.33881400	1.46023000	1.48018000
H	5.75769300	2.14543500	-0.51751100
H	4.59920300	0.87575000	3.41011700
C	1.92087200	1.22762000	3.16697700
H	1.08676400	1.92208400	3.04854500
H	2.34281500	1.34396100	4.16728000
C	3.27391900	2.76308700	-1.46044800
H	2.85513500	3.76893800	-1.35206900
H	2.51663500	2.14832400	-1.96142200
H	4.14688100	2.82309800	-2.11155100
H	1.51099400	0.21688400	3.07963600
C	6.78565800	1.21636500	1.82251200
H	6.88448100	0.47098700	2.61463900
H	7.34235700	0.87103000	0.94791400
H	7.25996800	2.13922400	2.17199300
C	0.48460600	0.12645300	-0.90897200
O	0.13698300	0.19854100	-2.14343100
H	-0.99721800	-2.89913600	0.09619800
C	1.88459000	-0.45326500	-0.60983600
C	2.05883600	-1.85808300	-1.15921500
H	2.63209100	0.19416600	-1.07141900
H	1.78951600	-1.84050800	-2.21914600

C	3.48178000	-2.36658700	-1.03365100
C	3.87483400	-3.46251200	-1.81078400
C	4.41303600	-1.80926000	-0.15316500
C	5.15772200	-3.99029500	-1.71195800
H	3.15865800	-3.89707200	-2.50518200
C	5.70113400	-2.33477900	-0.05236300
H	4.14689700	-0.95190500	0.45946300
C	6.07822500	-3.42648800	-0.82852600
H	5.44235300	-4.83894800	-2.32634800
H	6.40959000	-1.88612500	0.63830500
H	7.08069000	-3.83495900	-0.74898300
C	1.09010800	-2.78797300	-0.42593800
C	-0.34924000	-2.28489500	-0.54060300
H	1.36193600	-2.82807700	0.63352500
H	1.14396200	-3.80236000	-0.83204500
N	-0.54354400	-0.87311100	-0.11984300
H	2.05683500	-0.46408700	0.47259200
S	-0.81174500	-0.72775400	1.50575900
O	-0.96463300	0.70376700	1.78287000
O	0.17243300	-1.47832600	2.29951100
C	-2.38303100	-1.49888100	1.81044800
C	-3.54106500	-0.75708500	1.60356100
C	-4.76698800	-1.33316500	1.91354900
C	-4.84818100	-2.63391400	2.42117900
C	-3.66552100	-3.35238200	2.62481700
C	-2.42903400	-2.79079300	2.32880900
H	-3.47694000	0.25691600	1.21855700
H	-5.67726300	-0.75996700	1.76034900
H	-3.71370800	-4.35770900	3.03282600
H	-1.50649200	-3.33006400	2.51851400
C	-6.18621200	-3.25362300	2.72642300
H	-6.60762700	-3.71499400	1.82737500
H	-6.09774200	-4.03078100	3.48832500
H	-6.89792900	-2.50233600	3.07595200
C	-0.87145900	-2.56634300	-1.95466000
O	-0.18965700	-2.92452800	-2.88456600
O	-2.20923300	-2.52982800	-2.01175300
C	-2.76029000	-2.85001600	-3.29414500
H	-2.52865200	-2.05723500	-4.00942900
H	-2.35199400	-3.79385100	-3.65695300
H	-3.83602600	-2.93109800	-3.15179400
TS5 ^{S1}			
C	4.76969900	-2.55309500	0.80697700

C	3.46135400	-2.08851700	0.90546000
C	2.67780900	-2.35444200	2.02278100
C	3.22620600	-3.11499100	3.05268700
C	4.53713200	-3.59086600	2.95803900
C	5.31844400	-3.31117800	1.83848800
C	5.40675400	-2.10739800	-0.48539400
C	4.24923400	-1.52164000	-1.33008900
C	3.06651500	-1.29681600	-0.31979800
H	1.66492700	-1.96513800	2.08101800
H	2.63500300	-3.34034800	3.93433900
H	4.95084300	-4.18552300	3.76646300
H	6.33623700	-3.68397900	1.77016800
H	5.89495200	-2.92024100	-1.03183300
H	4.52212500	-0.57304200	-1.79403000
H	6.16723400	-1.34180100	-0.29950200
H	2.93059000	-0.23859300	-0.09613400
N	1.80773900	-1.76580500	-0.88428600
O	3.91622400	-2.36296900	-2.42787500
C	0.55496400	-1.28373400	-0.69581400
C	1.76575900	-2.86897700	-1.69207400
N	-0.17647200	-2.14926700	-1.41566000
N	0.54735800	-3.13750400	-2.05225400
C	3.07263800	-3.45694600	-2.10887300
H	3.49943200	-4.07817100	-1.30879300
H	2.95593900	-4.06371100	-3.00669800
C	-1.60294700	-2.12246400	-1.54555200
C	-2.35376100	-2.97572500	-0.72623700
C	-2.18463500	-1.24130400	-2.45651800
C	-3.74045400	-2.90572200	-0.81874600
C	-3.58162500	-1.19783700	-2.50257400
C	-4.37039400	-2.00930800	-1.68902500
H	-4.34633300	-3.55106100	-0.18601700
H	-4.06151700	-0.51726000	-3.20199400
C	-1.34201300	-0.37268300	-3.34979900
H	-1.91073800	-0.07472900	-4.23394700
H	-0.44108200	-0.89841000	-3.67621300
C	-1.66855900	-3.90586700	0.23838100
H	-1.01706400	-3.34764900	0.92058000
H	-1.03644400	-4.62380100	-0.29226600
H	-2.40091700	-4.45470400	0.83254600
H	-1.03795800	0.53492800	-2.82035400
C	-5.87447600	-1.92447400	-1.72493000
H	-6.21726300	-1.28716300	-2.54236500
H	-6.32129100	-2.91469500	-1.84853600

H	-6.25752600	-1.50805000	-0.78742200
C	0.13494300	0.37659300	0.65393400
O	1.21318200	0.61114000	1.19245500
H	-1.01353800	3.01984100	0.75788700
C	-0.98533500	-0.34000400	1.39088200
C	-1.94753600	0.66851900	2.03112000
H	-0.51401600	-0.97478600	2.14564500
H	-1.38600100	1.33071600	2.70272000
C	-3.02453500	-0.03278300	2.83076000
C	-3.17311800	0.20671300	4.19752600
C	-3.88823700	-0.94227700	2.21027800
C	-4.16105100	-0.44716400	4.93233900
H	-2.50768100	0.91093700	4.69017600
C	-4.87449300	-1.59718900	2.94094200
H	-3.78944000	-1.14733000	1.14644400
C	-5.01437800	-1.35124500	4.30615300
H	-4.26243800	-0.24887100	5.99473700
H	-5.53486200	-2.30130300	2.44312300
H	-5.78388600	-1.86159700	4.87636600
C	-2.53448400	1.49530600	0.88821600
C	-1.44512400	2.24343400	0.11086400
H	-3.24667300	2.23766700	1.26202800
H	-3.06442900	0.83483200	0.19128000
N	-0.38773500	1.31778100	-0.36913300
H	-1.55730400	-0.96489900	0.70217800
S	0.81426200	2.10024200	-1.27400700
O	0.08482300	2.81474500	-2.31954300
O	1.81061700	1.11015900	-1.65606500
C	1.58211100	3.34045600	-0.25760000
C	0.99522500	4.60151200	-0.18638400
C	1.60715100	5.58033400	0.59180400
C	2.79631300	5.31836600	1.27569000
C	3.36515900	4.04204800	1.17566000
C	2.76452600	3.04726800	0.41816500
H	0.07840100	4.81137800	-0.72977100
H	1.15576600	6.56553600	0.66146600
H	4.29055800	3.82772000	1.70250400
H	3.19395300	2.05528800	0.34695500
C	3.47461500	6.38892700	2.08838900
H	2.79971100	7.22345200	2.28713800
H	3.82806200	5.99154000	3.04306700
H	4.34621900	6.77991300	1.55385700
C	-2.14146900	2.97822300	-1.03087900
O	-2.29728100	4.17697500	-1.04760900

O	-2.64479700	2.14063400	-1.93284600
C	-3.20781300	2.76613500	-3.08892400
H	-3.54035700	1.95511900	-3.73390000
H	-4.04755900	3.40397900	-2.80851500
H	-2.44090100	3.36311300	-3.58701900

TS5A^{S1}

C	4.86315000	-2.58909100	0.86914600
C	3.53856300	-2.17295800	0.97126400
C	2.73927700	-2.54892000	2.04498500
C	3.28846800	-3.37367000	3.02408900
C	4.61466500	-3.80303400	2.92388100
C	5.41240600	-3.41053200	1.85045300
C	5.51355100	-2.01932100	-0.36697300
C	4.35065600	-1.43291900	-1.20260100
C	3.14815600	-1.30091300	-0.19989000
H	1.71661500	-2.18822200	2.11108200
H	2.68535200	-3.68372100	3.87133500
H	5.02808400	-4.44952900	3.69161000
H	6.44284800	-3.74612700	1.77857700
H	6.06012500	-2.76267100	-0.95532800
H	4.59483200	-0.45366300	-1.61593200
H	6.22442500	-1.23007800	-0.10017600
H	2.98941500	-0.26403300	0.09463000
N	1.90761700	-1.75996000	-0.81968900
O	4.06595800	-2.23341800	-2.34445700
C	0.63797200	-1.32426300	-0.64692300
C	1.91372000	-2.82139800	-1.68359600
N	-0.05460200	-2.16646100	-1.43163700
N	0.71353100	-3.09895700	-2.09406900
C	3.24325000	-3.35970300	-2.09499600
H	3.66600600	-4.00837100	-1.31513700
H	3.15895000	-3.92594100	-3.02248100
C	-1.47547700	-2.16273800	-1.62274200
C	-2.22796600	-3.12254100	-0.93328200
C	-2.05799900	-1.19599500	-2.44540100
C	-3.61259000	-3.08667300	-1.07359700
C	-3.45347100	-1.18900000	-2.53775600
C	-4.24204300	-2.11990100	-1.86285900
H	-4.21534100	-3.81336900	-0.53432200
H	-3.92941300	-0.42836900	-3.15317800
C	-1.24689500	-0.19251200	-3.22177100
H	-1.26725900	-0.44346000	-4.28710800
H	-0.20405400	-0.16226100	-2.90227000

C	-1.54834500	-4.12804600	-0.04368100
H	-0.90814700	-3.62498700	0.68979600
H	-0.90634100	-4.79540700	-0.62581000
H	-2.28432900	-4.72825500	0.49305400
H	-1.66505800	0.81114800	-3.10668900
C	-5.74502400	-2.05433200	-1.95278000
H	-6.07373000	-1.93169500	-2.98801600
H	-6.20619500	-2.95821100	-1.54870500
H	-6.12602800	-1.19687900	-1.38736200
C	0.17351200	0.16002400	0.73678400
O	1.22104400	0.31814000	1.37724000
H	-2.24293100	0.66853400	-0.70331500
C	-1.02180100	-0.56010200	1.35194300
C	-1.94749900	0.39924900	2.12306900
H	-0.62103700	-1.32685700	2.01966200
H	-1.43036700	0.72825600	3.02948600
C	-3.19611600	-0.35665100	2.53155300
C	-3.46683100	-0.64251700	3.86949300
C	-4.08516300	-0.81730100	1.55323400
C	-4.60274100	-1.36923300	4.22656900
H	-2.78306300	-0.29198900	4.63830100
C	-5.21573900	-1.54674400	1.90424600
H	-3.88774700	-0.61276800	0.50139100
C	-5.47910100	-1.82412700	3.24569700
H	-4.80041500	-1.58017100	5.27289800
H	-5.89024800	-1.90178100	1.13006800
H	-6.36113700	-2.39250100	3.52249200
C	-2.25582500	1.64569300	1.25464500
C	-1.74631600	1.49794800	-0.18888600
H	-1.76764400	2.52934200	1.67402700
H	-3.33250500	1.84193700	1.22885700
N	-0.29025300	1.24428900	-0.14711700
H	-1.61021200	-1.05737100	0.57922400
S	0.79875100	2.06989500	-1.09850500
O	0.06968000	2.57650600	-2.26004200
O	1.93920200	1.19301900	-1.33787600
C	1.34028800	3.48851000	-0.16824500
C	1.50647700	4.68621500	-0.85747200
C	1.95410400	5.80336400	-0.16126600
C	2.23319900	5.73501000	1.20742000
C	2.05092000	4.51664100	1.86928500
C	1.60768800	3.38520200	1.19288800
H	1.27090300	4.74115800	-1.91519000
H	2.08173400	6.74564700	-0.68664300

H	2.25522900	4.45437000	2.93439000
H	1.46369700	2.43491100	1.69906700
C	2.74070000	6.94444800	1.94721200
H	2.31923600	7.86483000	1.53682600
H	2.49271900	6.89108000	3.00936600
H	3.83009300	7.01461200	1.86346100
C	-2.15628000	2.74151500	-0.96641300
O	-2.93608800	2.72580500	-1.88701600
O	-1.63446200	3.84726300	-0.43548300
C	-1.85349100	5.04563900	-1.18536800
H	-1.31098100	5.82776900	-0.65780100
H	-1.45750100	4.91560800	-2.19518500
H	-2.91939500	5.27432900	-1.23235900

TS5B^{SI}

C	-5.23983100	-1.91290600	0.69951000
C	-4.11103600	-1.47936800	0.00203600
C	-4.18550200	-1.13505300	-1.34243400
C	-5.42479200	-1.20983000	-1.97875300
C	-6.56067000	-1.62097200	-1.28002900
C	-6.47527000	-1.97823100	0.06566300
C	-4.87602100	-2.28852200	2.11560400
C	-3.34951800	-2.47002700	2.05828600
C	-2.89417800	-1.51429800	0.91298700
H	-3.29851200	-0.81620700	-1.87898900
H	-5.50460100	-0.94959700	-3.02932600
H	-7.51620000	-1.67692800	-1.79202700
H	-7.35495800	-2.31943900	0.60363100
H	-5.36011800	-3.20246600	2.46850900
H	-2.86030000	-2.21561600	3.00076500
H	-5.13149100	-1.48196700	2.81301800
H	-2.63380200	-0.52479200	1.29710300
N	-1.70947000	-2.05262300	0.26753200
O	-2.99630000	-3.83338700	1.81538800
C	-0.55161000	-1.45393000	-0.10301300
C	-1.67732200	-3.38166100	-0.06493700
N	0.10196200	-2.47532600	-0.68593200
N	-0.56745600	-3.68281600	-0.66549700
C	-2.78783300	-4.22970500	0.46471100
H	-3.69627200	-4.12089400	-0.13958900
H	-2.49079800	-5.27841900	0.47927100
C	1.40179300	-2.39411800	-1.28177400
C	1.59917100	-1.58048800	-2.39791000
C	2.44888200	-3.11134900	-0.67534400

C	2.90464100	-1.47976000	-2.89665300
C	3.72017000	-2.99151500	-1.22355900
C	3.96888800	-2.17034400	-2.33065000
H	3.08013300	-0.82899900	-3.74935900
H	4.54492300	-3.53090500	-0.76150400
C	2.21375600	-3.94399500	0.55765300
H	1.66505900	-3.37548100	1.31685600
H	3.16560900	-4.26071600	0.98849000
C	0.49518800	-0.83346300	-3.09695100
H	0.71242200	0.23759300	-3.07850200
H	-0.48045900	-0.99019700	-2.63665900
H	0.44377300	-1.15076400	-4.14314100
H	1.61708000	-4.83094600	0.32972700
C	5.36634600	-2.04604400	-2.88024700
H	5.40698200	-1.32437100	-3.69826200
H	6.06270400	-1.72056500	-2.10161000
H	5.72534400	-3.00883500	-3.25622400
C	0.14391100	0.34128700	0.85059000
O	-0.78761700	0.69874900	1.57035300
H	1.37001700	2.93776100	0.30881100
C	1.37533300	-0.32555800	1.44324500
C	2.45980000	0.71890700	1.73648300
H	1.04685200	-0.83631100	2.35185300
H	2.04980100	1.49258900	2.39850500
C	3.66006100	0.08947900	2.41075500
C	4.10241300	0.53815200	3.65612600
C	4.34650800	-0.96259500	1.79378200
C	5.20423800	-0.05013700	4.27531400
H	3.57778000	1.35415300	4.14622300
C	5.44478700	-1.55330400	2.41009400
H	4.02181300	-1.32799500	0.82175200
C	5.87759300	-1.09894400	3.65507200
H	5.53453900	0.31132700	5.24406000
H	5.96287800	-2.37038400	1.91672400
H	6.73350500	-1.55983000	4.13745000
C	2.82723000	1.34778700	0.39320300
C	1.63024300	2.03901800	-0.26729600
H	3.19007500	0.57195000	-0.29276800
H	3.61979000	2.09411700	0.50952000
N	0.46187500	1.13031200	-0.36459100
H	1.79538100	-1.05548500	0.74979300
S	-0.89058100	1.85686400	-1.07103700
O	-1.95140900	0.86194000	-1.12483700
O	-0.39547900	2.45382900	-2.31071400

C	-1.43366900	3.21445000	-0.05678300
C	-2.46368700	3.02423100	0.86236000
C	-2.90319000	4.10899300	1.60619800
C	-2.32160200	5.37541100	1.45453400
C	-1.29226500	5.53519200	0.52546000
C	-0.84671500	4.46279700	-0.24340400
H	-2.90118200	2.03993800	0.97884100
H	-3.71070600	3.97659000	2.32069300
H	-0.83893500	6.51276000	0.39122000
H	-0.06321000	4.59186800	-0.98357100
C	-2.81365400	6.53548600	2.27856100
H	-2.25868100	7.44749500	2.05177900
H	-3.87426900	6.72301900	2.08774200
H	-2.70724900	6.32454500	3.34654000
C	2.10368700	2.46690900	-1.65714600
O	2.49747800	1.70954000	-2.50850100
O	2.12872600	3.79825000	-1.76616700
C	2.53678800	4.28971000	-3.04757700
H	3.54771000	3.95090100	-3.27970100
H	1.84640400	3.92889900	-3.81237600
H	2.50053200	5.37443900	-2.97605800

TS5C^{S1}

C	4.51934000	1.92564500	-0.15006800
C	3.48739400	1.37358700	0.61710300
C	3.46503100	0.01521300	0.90890300
C	4.47256400	-0.79396700	0.38330900
C	5.47952500	-0.25398000	-0.41782600
C	5.51497400	1.11500300	-0.68258800
C	4.39797800	3.42631000	-0.20165000
C	3.53545400	3.69277900	1.05146900
C	2.58394400	2.47015100	1.14146900
H	2.68630400	-0.40487200	1.53347200
H	4.47765400	-1.85563900	0.61600800
H	6.25643700	-0.89927300	-0.81635600
H	6.31948900	1.54328600	-1.27318000
H	3.88577600	3.74109400	-1.11866300
H	4.18338200	3.65379800	1.93060700
H	5.35714000	3.94716500	-0.16011600
H	2.22739800	2.27956900	2.15556900
N	1.39579500	2.75402600	0.30389200
O	2.88842600	4.94319900	1.11913400
C	0.36623200	1.90548700	-0.00478900
C	1.11093800	4.01252900	-0.17234800

N	-0.46105300	2.72814300	-0.67664300
N	-0.02828500	4.02932200	-0.79124500
C	2.01489700	5.18665300	0.03799800
H	2.56761000	5.41067900	-0.88331600
H	1.41698500	6.06251000	0.29426400
C	-1.73879500	2.40219900	-1.24709600
C	-2.89621300	2.60127900	-0.49431400
C	-1.77611000	1.93258200	-2.56671000
C	-4.11763300	2.23442900	-1.06847400
C	-3.01380700	1.58665200	-3.09727200
C	-4.19341600	1.71322900	-2.35595200
H	-5.02712800	2.35652300	-0.48410200
H	-3.06228500	1.20984300	-4.11641700
C	-0.51650000	1.84323700	-3.38196200
H	0.21417100	1.18634100	-2.90447600
H	-0.05743600	2.83250200	-3.48169300
C	-2.87821200	3.21326200	0.88219500
H	-3.29306300	4.22541200	0.84666600
H	-1.87016600	3.28072800	1.29447200
H	-3.49793900	2.62588200	1.56643600
H	-0.73422500	1.46191500	-4.38148400
C	-5.51315900	1.29008600	-2.94810500
H	-5.55353400	0.20224300	-3.06748500
H	-6.34852300	1.59237000	-2.31245300
H	-5.65947900	1.72948500	-3.93886400
C	0.03231000	0.01306700	1.42836400
O	0.72409500	0.29127400	2.38598000
H	0.26565200	-3.22451500	0.65353500
C	-1.45961700	0.19888100	1.39993900
C	-2.12476300	-1.05942700	2.00251300
H	-1.71040100	1.07481000	2.00035200
H	-1.86782600	-1.10467800	3.06635400
C	-3.63011800	-0.96203600	1.86663900
C	-4.45915000	-1.09369600	2.98182500
C	-4.21664700	-0.73440700	0.61561600
C	-5.84417400	-1.00118600	2.85637000
H	-4.01339300	-1.26744300	3.95782900
C	-5.59893600	-0.63622000	0.48863900
H	-3.58909100	-0.62049800	-0.26729800
C	-6.41790300	-0.77044300	1.60889600
H	-6.47351700	-1.10411500	3.73492900
H	-6.03645700	-0.45078500	-0.48841200
H	-7.49595700	-0.69269900	1.50952600
C	-1.58279500	-2.33444000	1.33396000

C	-0.05634200	-2.35536100	1.23325800
H	-1.98293100	-2.40920800	0.31640600
H	-1.91819400	-3.21459400	1.88986900
N	0.50405000	-1.13781300	0.58736600
H	-1.79154200	0.34759100	0.37316000
S	0.40042000	-1.07355200	-1.09879400
O	1.47318400	-0.21864000	-1.59093900
O	-0.97247700	-0.82243600	-1.54782800
C	0.82442600	-2.73611000	-1.55347600
C	2.15519100	-3.13390900	-1.44162300
C	2.49616600	-4.42657500	-1.81388700
C	1.52941200	-5.31491400	-2.30442200
C	0.20590800	-4.88068200	-2.41312500
C	-0.15854400	-3.59015200	-2.03928600
H	2.89708700	-2.43206600	-1.07244700
H	3.52803000	-4.75539300	-1.73015400
H	-0.54894700	-5.56039000	-2.79667300
H	-1.18274800	-3.24226000	-2.12566900
C	1.92356200	-6.70305100	-2.73403600
H	2.65425300	-7.13414600	-2.04570100
H	1.05646100	-7.36452600	-2.78173800
H	2.38247400	-6.67800400	-3.72760200
C	0.63141800	-2.51531100	2.58953500
O	0.05035400	-2.67616800	3.63555200
O	1.95797200	-2.51029800	2.46196100
C	2.68881500	-2.55158700	3.69191000
H	2.42542500	-1.68672400	4.30392800
H	2.46456200	-3.46882900	4.23900200
H	3.73991700	-2.51628600	3.41272800

PS1

C	0.06262000	-0.29627200	1.25933800
O	-0.74636600	-0.65507900	2.09170400
H	0.23184800	0.75303300	-1.73352300
C	1.46121500	-0.87110500	1.20587900
C	2.14707600	-0.72890000	-0.15269700
H	1.37678100	-1.91359800	1.52058700
H	1.59676700	-1.32893800	-0.88906900
C	3.57628200	-1.22720900	-0.11361800
C	3.96982100	-2.30635400	-0.90627100
C	4.52488100	-0.62241200	0.71745400
C	5.28091900	-2.77652400	-0.87051300
H	3.24111600	-2.78327400	-1.55644100
C	5.83544700	-1.08841500	0.75459500

H	4.24255600	0.22055600	1.34365300
C	6.21736000	-2.16840800	-0.03951400
H	5.56851000	-3.61889800	-1.49145000
H	6.55948900	-0.60896500	1.40565000
H	7.23888300	-2.53313500	-0.00857700
C	2.04716800	0.73962100	-0.55964800
C	0.58688300	1.15161800	-0.77860500
H	2.58460800	0.93794200	-1.49029800
H	2.48646000	1.36969000	0.22340900
N	-0.27827200	0.66295100	0.30787000
H	2.04396500	-0.35109500	1.97634900
S	-1.91212500	1.19882800	0.29385700
O	-1.98608800	2.00563500	-0.91967000
O	-2.24449300	1.78467100	1.57806300
C	-2.87791100	-0.26200900	0.03255800
C	-3.01691000	-0.73440800	-1.26956600
C	-3.79518600	-1.86532500	-1.48686300
C	-4.43773800	-2.51088600	-0.42563200
C	-4.28246200	-2.00329500	0.86990500
C	-3.50283300	-0.88040900	1.11163900
H	-2.53631100	-0.21902900	-2.09464800
H	-3.91186200	-2.24852500	-2.49595400
H	-4.77802600	-2.49880800	1.69949500
H	-3.36402600	-0.48599700	2.11112800
C	-5.30643600	-3.71578500	-0.66861000
H	-5.09128000	-4.17269000	-1.63633600
H	-5.16282000	-4.46652300	0.11198700
H	-6.36322000	-3.43047900	-0.65953400
C	0.56333000	2.66862900	-0.91037200
O	0.78239800	3.23077400	-1.95469500
O	0.38025800	3.27700600	0.25955000
C	0.31475100	4.70682100	0.19620900
H	0.15024000	5.04084800	1.21782200
H	1.24807300	5.11037600	-0.19901200
H	-0.51517200	5.00770300	-0.44567400
PA ^{S1}			
C	0.50201900	-1.56494900	0.45150500
O	-0.19207100	-2.55603300	0.50296700
H	1.42578800	1.12260800	1.24215000
C	2.00522500	-1.59185300	0.31876600
C	2.54068800	-0.68765400	-0.80735900
H	2.31397200	-2.62847400	0.18156400
H	2.39195500	-1.21824900	-1.75209000

C	4.03105000	-0.47323000	-0.63626300
C	4.93729800	-1.16947800	-1.43650800
C	4.52714300	0.39280100	0.34359400
C	6.31080500	-1.00461900	-1.26720300
H	4.56326700	-1.84557100	-2.20107900
C	5.89743700	0.56100800	0.51510800
H	3.83988000	0.94699200	0.97941500
C	6.79423700	-0.13837800	-0.29089600
H	7.00110800	-1.55242700	-1.90080700
H	6.26584600	1.24006900	1.27731000
H	7.86317500	-0.00642500	-0.15838000
C	1.71894800	0.61908900	-0.87856400
C	0.83206100	0.89386600	0.35175100
H	1.04623800	0.57605900	-1.73977200
H	2.37348700	1.48450700	-1.01433000
N	-0.03731600	-0.27387300	0.58177700
H	2.40435500	-1.24149200	1.27997600
S	-1.44078900	-0.09354700	1.55348200
O	-1.42006400	1.31007900	1.94425800
O	-1.41146200	-1.12202700	2.57697400
C	-2.82726500	-0.37387500	0.48915900
C	-3.61843800	0.71513600	0.13832500
C	-4.73243500	0.49934000	-0.66447200
C	-5.06152800	-0.78474900	-1.10819600
C	-4.24971100	-1.85945100	-0.72556800
C	-3.13374700	-1.66963500	0.07881500
H	-3.36455200	1.70564400	0.49874600
H	-5.35781600	1.34122800	-0.94661000
H	-4.49939000	-2.86155100	-1.06153800
H	-2.49990400	-2.49826200	0.37413200
C	-6.28476800	-1.01575400	-1.95416000
H	-6.56628100	-0.11180100	-2.49788300
H	-6.11968900	-1.81973800	-2.67474800
H	-7.13295300	-1.30494000	-1.32545300
C	0.06366900	2.16228100	0.00624200
O	0.43363800	3.26041100	0.33601300
O	-0.96101500	1.91854500	-0.81246900
C	-1.68803300	3.07892800	-1.23294900
H	-2.51871600	2.70778000	-1.83014500
H	-2.05167700	3.62699400	-0.36089900
H	-1.04438800	3.73016200	-1.82641900
PB ^{S1}			
C	-0.02242400	-0.45802400	1.34899900

O	0.79973800	-0.91548600	2.11760500
H	-0.19960200	1.02264800	-1.46797200
C	-1.41086200	-1.04365500	1.22136700
C	-2.08565400	-0.75698700	-0.12031600
H	-1.31089000	-2.11380500	1.41466500
H	-1.51063300	-1.24808400	-0.91593900
C	-3.50085500	-1.29400600	-0.15998300
C	-3.85312800	-2.29800800	-1.06282400
C	-4.47825500	-0.79994300	0.71044400
C	-5.15229600	-2.80052800	-1.09864200
H	-3.10271700	-2.69047800	-1.74398800
C	-5.77711000	-1.29757500	0.67553200
H	-4.22755400	-0.01989900	1.42561100
C	-6.11828500	-2.30074700	-0.22974000
H	-5.40785500	-3.58282700	-1.80636700
H	-6.52307300	-0.90239200	1.35760500
H	-7.13078100	-2.69013700	-0.25655300
C	-2.02889500	0.75324100	-0.34101400
C	-0.58228500	1.24678500	-0.46824700
H	-2.50670000	1.26231200	0.50431800
H	-2.55834300	1.04649100	-1.25112500
N	0.29406300	0.62944000	0.53789100
H	-2.00993100	-0.62311800	2.03875600
S	1.92317100	1.17945400	0.56799900
O	2.27854600	1.57446900	1.91635800
O	1.96326600	2.15215200	-0.51904800
C	2.89378800	-0.21693200	0.07861600
C	3.52830100	-0.99330400	1.04539500
C	4.32346000	-2.05095800	0.62774200
C	4.48535700	-2.34247500	-0.73259100
C	3.83590100	-1.54256000	-1.67665100
C	3.04117000	-0.47187900	-1.28155700
H	3.38812300	-0.76511400	2.09513300
H	4.82966200	-2.66337000	1.36828600
H	3.96273500	-1.75175800	-2.73434600
H	2.56127100	0.16762300	-2.01497700
C	5.35051400	-3.49891700	-1.15710100
H	5.42532000	-3.56296100	-2.24392000
H	6.35901100	-3.39724300	-0.74691100
H	4.94125100	-4.44258300	-0.78472700
C	-0.60628300	2.75987600	-0.28211800
O	-0.52930000	3.32059900	0.78258200
O	-0.81741200	3.36302600	-1.44943400
C	-0.92665200	4.79091600	-1.38589300

H	-1.76374100	5.07708400	-0.74718700
H	-0.00368600	5.21518200	-0.98790500
H	-1.09278700	5.12110900	-2.40869100
PC ^{S1}			
C	0.25654300	-1.22497800	0.77878900
O	-0.51911200	-1.68596700	1.59229500
H	0.51064400	-0.84879600	-2.52862200
C	1.68392800	-0.88199400	1.15378700
C	2.40756800	0.07443700	0.20453200
H	1.65371400	-0.50164300	2.17703800
H	1.95889400	1.07055300	0.31181200
C	3.88086600	0.19475200	0.53194200
C	4.43055200	1.43452600	0.86095900
C	4.72052000	-0.92357000	0.49608000
C	5.78786300	1.55966900	1.14926200
H	3.78884700	2.31116700	0.88982200
C	6.07678700	-0.80234800	0.78278600
H	4.31717200	-1.90083100	0.24089200
C	6.61488500	0.44062300	1.11101800
H	6.19744800	2.53215200	1.40353200
H	6.71421800	-1.68014300	0.75086700
H	7.67237000	0.53494000	1.33549200
C	2.16679700	-0.41180400	-1.22569200
C	0.67566200	-0.36148000	-1.56748500
H	2.52310300	-1.44076900	-1.34162900
H	2.69438300	0.21115100	-1.95251300
N	-0.12388600	-1.05278600	-0.54906000
H	2.21237500	-1.84315800	1.18902800
S	-1.72636700	-1.49260700	-0.98855900
O	-1.90071600	-2.90306900	-0.69276600
O	-1.82960100	-1.01484100	-2.36326500
C	-2.85343500	-0.54443100	-0.00368300
C	-3.30968700	-1.04554400	1.21359100
C	-4.24391700	-0.30698000	1.92713100
C	-4.72972100	0.91255800	1.44059600
C	-4.26633900	1.37760000	0.20614900
C	-3.33558500	0.65202100	-0.52791600
H	-2.92629600	-1.98668900	1.58678800
H	-4.60541200	-0.68342200	2.87951200
H	-4.64586900	2.31437900	-0.19103700
H	-2.99678400	0.99682500	-1.49837200
C	-5.75841700	1.68650600	2.22058000
H	-5.52710700	1.68002400	3.28837900

H	-5.81610400	2.72264800	1.88206100
H	-6.74830900	1.23621000	2.09614800
C	0.25299400	1.09339100	-1.75324800
O	0.59090500	1.75164300	-2.70630500
O	-0.47111700	1.55714300	-0.73363200
C	-0.87641500	2.92853400	-0.84125800
H	0.00022500	3.57811900	-0.82467400
H	-1.42493400	3.08511900	-1.77189100
H	-1.51507600	3.11517500	0.01958000

Stetter reaction

TS3^{S2}

C	3.35900900	3.72285100	-1.14771200
C	2.11972200	3.08816400	-1.15240400
C	0.96250500	3.75047300	-1.54829300
C	1.06323200	5.08599400	-1.93150600
C	2.30223400	5.73191500	-1.92378500
C	3.45833300	5.05583000	-1.53835600
C	4.44955900	2.77999500	-0.70280700
C	3.71292800	1.54420500	-0.13768900
C	2.24389100	1.65720600	-0.68170500
H	0.00962900	3.22830600	-1.56547600
H	0.17546700	5.62814300	-2.24020400
H	2.36425800	6.77366500	-2.22206400
H	4.41848900	5.56316300	-1.53563000
H	5.11083900	3.20375000	0.05899300
H	4.15652400	0.60467500	-0.47408700
H	5.07778500	2.48854500	-1.55079300
H	2.09688300	0.94189300	-1.48491900
N	1.26800800	1.35592800	0.37233100
O	3.79803600	1.47941400	1.28271600
C	-0.03494100	0.93703700	0.31682800
C	1.50533000	1.77678800	1.65634800
N	-0.49010400	1.10707300	1.58447200
N	0.47633400	1.62540500	2.42348100
C	2.87022700	2.29279400	1.97243400
H	2.95784600	3.34797800	1.67751800
H	3.06911800	2.20542800	3.04080200
C	-1.85490400	1.10712000	2.02212700
C	-2.70011800	2.12361300	1.55846000
C	-2.28876700	0.08387600	2.86334200
C	-4.03568200	2.07040600	1.94572700
C	-3.63650300	0.07684800	3.22933700

C	-4.52199200	1.05290900	2.77212200
H	-4.71704900	2.83996500	1.59020900
H	-3.99943800	-0.71351500	3.88128000
C	-1.33528300	-0.98542400	3.32141600
H	-1.79284900	-1.60734300	4.09271600
H	-0.41746700	-0.54591700	3.72117100
C	-2.19960600	3.20032700	0.63370200
H	-2.16264400	2.82478200	-0.39641500
H	-1.19503100	3.53614400	0.90876600
H	-2.86879200	4.06194100	0.65262200
H	-1.04046600	-1.63557000	2.48820600
C	-5.98438900	1.01403600	3.13162700
H	-6.33691300	2.00073900	3.44312100
H	-6.58058200	0.71917800	2.26141900
H	-6.18166500	0.30361000	3.93599800
C	-0.68641000	0.32379700	-0.79309500
O	-0.16423500	0.71579900	-2.01048700
H	0.26548700	-0.08353300	-2.39234100
C	-2.11421600	0.01252200	-0.76116900
C	-2.91164700	0.04520100	-1.84082300
H	-2.50467900	-0.35202600	0.18420300
H	-2.48461900	0.36919300	-2.78751200
C	-4.32906700	-0.33885700	-1.86016200
C	-4.97900600	-0.46965200	-3.09560500
C	-5.07691300	-0.57249900	-0.69363200
C	-6.31972100	-0.83418200	-3.17187100
H	-4.41728000	-0.28544300	-4.00792600
C	-6.41452700	-0.94086000	-0.77020700
H	-4.61463100	-0.45304400	0.28341400
C	-7.04481100	-1.07508500	-2.00826500
H	-6.79639200	-0.93289500	-4.14217300
H	-6.97223200	-1.12257100	0.14388700
H	-8.09037800	-1.36063900	-2.06129600
C	0.14353700	-1.63940300	-0.57861600
C	1.07737100	-1.81975400	-1.59073500
H	-0.81064700	-2.14352400	-0.68825500
H	0.49269000	-1.50645000	0.44184400
N	2.45186300	-1.45754400	-1.37665100
H	2.91391600	-1.22134900	-2.25892600
S	3.43846200	-2.62826100	-0.65739700
O	4.76797800	-2.01803900	-0.63498500
O	3.27870500	-3.95120600	-1.25507800
C	2.76003400	-2.70014200	0.97703000
C	2.88278600	-1.59592300	1.81656400

C	2.29910400	-1.65009200	3.07714800
C	1.61065400	-2.79241100	3.50618700
C	1.49797900	-3.87906900	2.63315500
C	2.06967600	-3.84254500	1.36593100
H	3.41670100	-0.70586400	1.49567100
H	2.38365900	-0.79546600	3.74351200
H	0.95682400	-4.76561100	2.95095500
H	1.98204200	-4.67629100	0.67825200
C	1.02759300	-2.87027100	4.89217300
H	1.69443100	-3.43630100	5.55068500
H	0.89423500	-1.87755700	5.32754000
H	0.06164100	-3.38122200	4.88417900
C	0.78702900	-2.41665400	-2.88492800
O	1.62300100	-2.62008000	-3.75228400
O	-0.52670600	-2.68139100	-3.06226100
C	-0.86686000	-3.22850400	-4.33391500
H	-0.57045400	-2.54901100	-5.13594600
H	-0.37250900	-4.19058100	-4.48444700
H	-1.94827100	-3.35469000	-4.32285100

TS3A^{S2}

C	5.55449500	0.97608000	-1.31084700
C	4.17326100	0.81410100	-1.37948300
C	3.39713700	1.56414600	-2.26072700
C	4.03247800	2.50465100	-3.06673800
C	5.41761700	2.68009300	-2.99499300
C	6.18744700	1.91443600	-2.12297700
C	6.17823100	0.03064500	-0.31788600
C	4.99069400	-0.72019800	0.33597100
C	3.68983000	-0.22963600	-0.39988700
H	2.32533400	1.39572100	-2.32456700
H	3.44982100	3.10168800	-3.76071100
H	5.89790000	3.41760900	-3.63017700
H	7.26416500	2.04802200	-2.07606500
H	6.77467400	0.54471300	0.44327400
H	5.08455900	-1.79542700	0.18618000
H	6.84856100	-0.67783900	-0.81291500
H	3.17748700	-1.05396800	-0.88479400
N	2.73981500	0.36307800	0.56117100
O	4.94368100	-0.56655000	1.74487300
C	1.42062100	0.66462100	0.41941600
C	3.16810200	0.95859200	1.71964000
N	1.13666400	1.44783700	1.48120100
N	2.22351500	1.61850100	2.30867700

C	4.58058600	0.73733600	2.14851900
H	5.23786400	1.49839300	1.70609300
H	4.65796800	0.79599500	3.23406100
C	-0.08679100	2.13963900	1.76143700
C	-0.34612500	3.30992500	1.03301800
C	-0.97436800	1.62166200	2.70524400
C	-1.55840100	3.95270100	1.25602400
C	-2.18496700	2.29928000	2.88440200
C	-2.49464000	3.45493100	2.17090800
H	-1.78534800	4.85922000	0.69961400
H	-2.89740600	1.91134200	3.60927500
C	-0.68135400	0.37474100	3.49672800
H	-1.10024600	0.46312400	4.50140800
H	0.39053700	0.18896800	3.58533400
C	0.63216800	3.80867000	0.00338300
H	0.60237100	3.17510400	-0.89173800
H	1.65735200	3.79547900	0.38445800
H	0.38493100	4.82756300	-0.29804900
H	-1.14205000	-0.49912300	3.02397400
C	-3.79788300	4.17954700	2.38520200
H	-4.46770000	3.60966100	3.03228400
H	-3.62514900	5.15617500	2.84726400
H	-4.30602200	4.35576600	1.43204200
C	0.53712400	0.11903000	-0.59981600
O	1.10736700	-0.60133600	-1.54297200
H	0.87900600	-1.71914600	-1.08254700
C	-0.79223500	0.70334800	-0.86911100
C	-1.36775400	0.60585800	-2.07652300
H	-1.34259000	1.15346600	-0.04813600
H	-0.82613600	0.09039100	-2.86725100
C	-2.71172400	1.10757000	-2.39750500
C	-3.42317600	0.53179800	-3.45840400
C	-3.32655700	2.13233200	-1.66156900
C	-4.72363700	0.93313400	-3.75093400
H	-2.95332300	-0.25395100	-4.04466300
C	-4.62367400	2.53779100	-1.95649900
H	-2.78002300	2.61847100	-0.85614500
C	-5.33244100	1.93467000	-2.99687200
H	-5.26143400	0.46306600	-4.56827900
H	-5.08423600	3.33190200	-1.37565700
H	-6.34504900	2.25131800	-3.22459000
C	0.03765800	-1.52717400	0.71726400
C	0.39448700	-2.51335500	-0.28392800
H	-1.00415700	-1.27973800	0.87431500

H	0.67672200	-1.44236000	1.59051800
N	-0.66923200	-3.14863900	-1.03195700
H	-0.88609500	-2.76815500	-1.94745300
S	-1.96998600	-3.86292100	-0.31371800
O	-1.49138200	-4.53493200	0.88684700
O	-2.64768600	-4.60081100	-1.37484400
C	-3.07134800	-2.56304000	0.20755200
C	-3.15116000	-2.22195400	1.55400800
C	-3.87859300	-1.09244700	1.92166900
C	-4.53783000	-0.31768800	0.96262400
C	-4.48690300	-0.71780400	-0.37779000
C	-3.74624700	-1.82679500	-0.76329200
H	-2.62209900	-2.81768500	2.29110900
H	-3.92884800	-0.80573200	2.96898400
H	-5.01061900	-0.13649000	-1.13231100
H	-3.68799600	-2.11001800	-1.81055500
C	-5.25768900	0.94805100	1.33999600
H	-6.22936100	1.01482300	0.84324600
H	-5.40885400	1.01870400	2.41982200
H	-4.66798300	1.81471200	1.01946600
C	1.48587400	-3.46370500	0.08540800
O	1.58517000	-4.61966100	-0.25109300
O	2.43240400	-2.83737900	0.82641200
C	3.48838900	-3.67685600	1.29698000
H	3.08319200	-4.50649600	1.87956300
H	4.06005000	-4.08171800	0.45822100
H	4.11403200	-3.03927600	1.92047700

M3^{S2}

C	3.37832700	3.71519800	-1.11840600
C	2.13528900	3.08829700	-1.13136700
C	0.98448400	3.75900800	-1.53687700
C	1.09606200	5.09431300	-1.91803200
C	2.33925600	5.73211400	-1.90300400
C	3.48846500	5.04812000	-1.51133000
C	4.46105300	2.76681200	-0.67178000
C	3.71552700	1.52803800	-0.12422300
C	2.25249900	1.65040100	-0.67433000
H	0.02827000	3.24315500	-1.56922600
H	0.21339600	5.64260400	-2.23057100
H	2.40981800	6.77350800	-2.20056500
H	4.45187200	5.54918900	-1.50235300
H	5.11171500	3.18464700	0.10250200
H	4.15364100	0.59006300	-0.46769800

H	5.09678100	2.48094700	-1.51231900
H	2.10166300	0.93356100	-1.46995800
N	1.25887400	1.36703800	0.38182900
O	3.79260200	1.44968500	1.29529300
C	-0.01023900	0.92490800	0.34820700
C	1.50928600	1.77776900	1.66517000
N	-0.48267900	1.11764100	1.57506100
N	0.46215200	1.62529200	2.42276800
C	2.87867900	2.27393200	1.99051400
H	2.97797400	3.32953900	1.70591000
H	3.07154200	2.17351900	3.05829800
C	-1.85558700	1.08658200	2.02655500
C	-2.69986200	2.10921700	1.58008000
C	-2.27385200	0.06041700	2.86777400
C	-4.02982900	2.05441500	1.97688100
C	-3.61877800	0.05367400	3.24051500
C	-4.50966300	1.03039100	2.79770300
H	-4.71440700	2.82937000	1.63432200
H	-3.97791300	-0.74200700	3.89294900
C	-1.31722700	-1.01187900	3.31670700
H	-1.78577900	-1.66040200	4.05471100
H	-0.41361400	-0.57158200	3.75293100
C	-2.19926100	3.19522300	0.65868200
H	-2.14355000	2.82328700	-0.36928000
H	-1.21088100	3.55751000	0.95172900
H	-2.88696100	4.04389000	0.66914500
H	-0.98996700	-1.63338200	2.46882500
C	-5.96952400	0.97807100	3.16527500
H	-6.30955900	1.93801000	3.56287100
H	-6.57665900	0.75854100	2.28101900
H	-6.16414200	0.20599700	3.91199500
C	-0.59511600	0.08527000	-0.79049400
O	-0.15741100	0.68414700	-1.98648200
H	0.45064100	-0.04830900	-2.36750200
C	-2.11069500	-0.02343800	-0.75357900
C	-2.89782300	0.08169600	-1.82787700
H	-2.51273000	-0.42129000	0.17510900
H	-2.45080900	0.40500400	-2.76732800
C	-4.32663200	-0.29095300	-1.86751800
C	-4.96079000	-0.43364300	-3.10529500
C	-5.08171600	-0.51553700	-0.70282600
C	-6.30272800	-0.80247600	-3.18991400
H	-4.39298300	-0.25944000	-4.01569300
C	-6.42069300	-0.88783200	-0.78759600

H	-4.62344200	-0.38798300	0.27506000
C	-7.03972700	-1.03004000	-2.02775900
H	-6.77564400	-0.91116300	-4.16156900
H	-6.98473100	-1.05817100	0.12473900
H	-8.08157400	-1.31573600	-2.08907900
C	0.03348700	-1.37258700	-0.61185400
C	1.04527200	-1.73841900	-1.64048400
H	-0.82852000	-2.07573800	-0.67304100
H	0.44503400	-1.51124600	0.42689500
N	2.43650900	-1.43436300	-1.38603000
H	2.92523800	-1.17267100	-2.24508900
S	3.41757200	-2.62636600	-0.69098700
O	4.75710400	-2.02716500	-0.64997900
O	3.27061500	-3.95364500	-1.28529900
C	2.74034100	-2.71043100	0.94852300
C	2.86511000	-1.61545400	1.79881400
C	2.28852700	-1.67899800	3.06016500
C	1.60590300	-2.82620300	3.48406500
C	1.49801600	-3.90941200	2.60596800
C	2.06156300	-3.85848300	1.33785900
H	3.40781500	-0.72765800	1.48376300
H	2.38138800	-0.83315600	3.73661200
H	0.96236200	-4.80046700	2.92057000
H	1.97763200	-4.69018800	0.64227000
C	1.02008800	-2.91400700	4.86830400
H	1.65809900	-3.52922100	5.51055500
H	0.93080000	-1.92825800	5.33422000
H	0.03138900	-3.37988600	4.85091100
C	0.77348700	-2.37642700	-2.86866900
O	1.59193800	-2.61166400	-3.77381800
O	-0.56031600	-2.66359100	-3.05890500
C	-0.89217000	-3.19805900	-4.32825300
H	-0.59287600	-2.52027400	-5.13128100
H	-0.40759900	-4.16368600	-4.49283400
H	-1.97458200	-3.32429800	-4.33276400

M3A^{S2}

C	5.64916400	-0.81588700	1.26058400
C	4.26697000	-0.67369200	1.35698000
C	3.52174400	-1.44652400	2.24084200
C	4.18841200	-2.38014400	3.03471900
C	5.57474600	-2.52992600	2.93842000
C	6.31364600	-1.74705300	2.05550400
C	6.24083100	0.13514200	0.25434600

C	5.03203100	0.87535300	-0.37066100
C	3.74949000	0.37018000	0.39267500
H	2.44732500	-1.30463600	2.32536500
H	3.62798500	-2.99229900	3.73375900
H	6.07986900	-3.26207600	3.56032500
H	7.39126100	-1.86751000	1.98545400
H	6.82817300	-0.37491600	-0.52038500
H	5.11339000	1.94991300	-0.22299900
H	6.91714400	0.84957200	0.73229700
H	3.23703700	1.19708900	0.86974100
N	2.78663600	-0.25916500	-0.54943500
O	4.95737000	0.72430300	-1.77887400
C	1.48787900	-0.58875700	-0.40078000
C	3.21375700	-0.84046600	-1.71270300
N	1.20593000	-1.37259000	-1.43684700
N	2.27017200	-1.52790500	-2.27636600
C	4.61090600	-0.58037500	-2.18007700
H	5.29120500	-1.33552900	-1.76826600
H	4.65069200	-0.62751200	-3.26779700
C	0.00260000	-2.12532800	-1.70536900
C	-0.19972500	-3.30567100	-0.97587900
C	-0.89067500	-1.66289400	-2.67656100
C	-1.36591300	-4.01627300	-1.22071300
C	-2.05396000	-2.41671800	-2.87837500
C	-2.30691700	-3.58355200	-2.16231000
H	-1.55147000	-4.93663200	-0.66280400
H	-2.76413400	-2.07816400	-3.62481900
C	-0.65103300	-0.41062300	-3.46966000
H	-1.11176800	-0.49871600	-4.45830600
H	0.41374200	-0.20603000	-3.60630300
C	0.78994900	-3.74795000	0.06833500
H	0.70738800	-3.11771100	0.96826200
H	1.81784200	-3.67815100	-0.28808700
H	0.59366500	-4.78012200	0.36556700
H	-1.09742200	0.45264500	-2.96828900
C	-3.55812800	-4.39271400	-2.40215600
H	-3.31458400	-5.35561600	-2.85024300
H	-4.08005500	-4.59154600	-1.46102600
H	-4.24430400	-3.87056500	-3.07200000
C	0.48758000	0.15965500	0.47476100
O	1.17677000	0.67225200	1.57671100
H	1.04694700	1.68217000	1.43978200
C	-0.71231900	-0.65585500	0.91671500
C	-1.27663100	-0.56238900	2.12740500

H	-1.24957900	-1.17278800	0.12607600
H	-0.78858300	0.03076000	2.89860600
C	-2.60094400	-1.14339800	2.45562900
C	-3.38751800	-0.56342300	3.45735400
C	-3.11713700	-2.24663100	1.75500600
C	-4.66723200	-1.04139000	3.72686400
H	-2.99648300	0.28612300	4.01035000
C	-4.38893300	-2.73076400	2.02980400
H	-2.50887000	-2.73536700	0.99703200
C	-5.17279100	-2.12415100	3.01457000
H	-5.26628100	-0.56968300	4.50278800
H	-4.76950200	-3.58290400	1.47793200
H	-6.17015700	-2.50293800	3.22819400
C	-0.00165600	1.35679100	-0.45575800
C	0.14373000	2.67568800	0.20089000
H	-1.07406400	1.13260300	-0.72863900
H	0.56567300	1.33912500	-1.42093000
N	-0.94156000	3.25368900	0.94370300
H	-1.13056600	2.95242400	1.89978800
S	-2.32706800	3.84617000	0.27499200
O	-1.99488800	4.62473000	-0.90821800
O	-3.07301900	4.45220100	1.38419000
C	-3.27387200	2.43746100	-0.26629300
C	-3.26151300	2.05544500	-1.60538500
C	-3.86800600	0.85733100	-1.96962000
C	-4.48434400	0.04237600	-1.01523800
C	-4.51566700	0.46819500	0.31806900
C	-3.90611500	1.65408800	0.69524800
H	-2.77290700	2.68852700	-2.33943800
H	-3.85737500	0.54749600	-3.01149900
H	-5.00422100	-0.14857300	1.06796400
H	-3.91452300	1.97273800	1.73509100
C	-5.08137300	-1.28762700	-1.38476600
H	-6.07565700	-1.40851500	-0.94612000
H	-5.15838900	-1.40834200	-2.46795600
H	-4.45634900	-2.09953800	-0.99329700
C	1.22609700	3.55562600	-0.08780200
O	1.38220500	4.72713400	0.25403300
O	2.22873000	2.91822400	-0.80730900
C	3.30442800	3.75255400	-1.20548300
H	2.94587200	4.62044200	-1.76877600
H	3.86412600	4.12103200	-0.33931500
H	3.94845800	3.13658500	-1.83818300

TS4^{S2}

C	3.31143400	2.49795200	-2.21900900
C	2.04695300	1.93449200	-2.05697900
C	1.05551100	2.07139800	-3.02353900
C	1.35351700	2.80596300	-4.16975300
C	2.61707800	3.37817000	-4.33941100
C	3.60579500	3.22505500	-3.36895900
C	4.20170200	2.18580000	-1.04203600
C	3.25203000	1.62976200	0.03902900
C	1.96045200	1.19575400	-0.73819900
H	0.09106800	1.59348100	-2.87622100
H	0.59919700	2.93279900	-4.93944000
H	2.83183700	3.94822600	-5.23777000
H	4.58639100	3.67131500	-3.50492700
H	4.74361900	3.05524000	-0.65752800
H	3.67860200	0.77169400	0.55349400
H	4.94651400	1.42643800	-1.30634700
H	1.94367600	0.11242500	-0.87442700
N	0.77126900	1.58982700	0.02371600
O	3.00386500	2.57323800	1.07597600
C	-0.43554000	1.01086900	0.16938200
C	0.73276600	2.79627400	0.66483800
N	-1.15376700	1.89390600	0.87114100
N	-0.43165700	3.01128600	1.19890100
C	2.02010800	3.54689100	0.77359100
H	2.24398200	4.08919500	-0.15422500
H	1.97454700	4.25391200	1.60154600
C	-2.54052400	1.82597000	1.25538000
C	-3.50103500	2.17171900	0.30372600
C	-2.84993100	1.40174500	2.54727400
C	-4.83683900	2.05025500	0.67871000
C	-4.20109300	1.30774200	2.87696400
C	-5.20317600	1.61698200	1.95473600
H	-5.61023900	2.28394600	-0.04869300
H	-4.47627600	0.97779800	3.87548500
C	-1.76431900	1.02719000	3.52040100
H	-1.04109500	1.83870900	3.63972800
H	-1.21256700	0.14553400	3.17358000
C	-3.09541000	2.61321500	-1.07544400
H	-2.43163200	3.48272500	-1.03272500
H	-3.97321000	2.87641300	-1.66740900
H	-2.55884200	1.80935900	-1.59340200
H	-2.18931300	0.79415500	4.49756800
C	-6.65503300	1.44844200	2.31646400

H	-7.28559100	2.13777300	1.75051600
H	-6.98246100	0.43057900	2.07953200
H	-6.82136800	1.61681900	3.38282300
C	-0.78976600	-0.35464200	-0.40010900
O	-0.43578000	-0.34274700	-1.71955400
H	0.22582900	-1.38632600	-1.64141200
C	-2.24446800	-0.68573200	-0.14583200
C	-3.12799300	-0.80411800	-1.13572600
H	-2.55027000	-0.80868300	0.89275100
H	-2.77135600	-0.64217400	-2.15138100
C	-4.56987900	-1.02523800	-0.94078300
C	-5.46895700	-0.51583800	-1.88610400
C	-5.08364400	-1.67763200	0.18834100
C	-6.84374900	-0.62148900	-1.69373500
H	-5.07945200	-0.01756000	-2.77035900
C	-6.45638000	-1.79226900	0.37658800
H	-4.39953900	-2.10816000	0.91403700
C	-7.34268600	-1.25707000	-0.55948100
H	-7.52593500	-0.21134200	-2.43181900
H	-6.83858000	-2.30573700	1.25389700
H	-8.41384300	-1.34657500	-0.40916200
C	0.14231800	-1.46108700	0.32716500
C	0.72743300	-2.25262900	-0.82049600
H	-0.45665500	-2.05884100	1.01607800
H	0.93768300	-0.97496900	0.90207600
N	2.17654000	-2.21585700	-0.92350200
H	2.50534800	-2.50195300	-1.84439500
S	3.07357800	-3.11258600	0.18977100
O	4.06149600	-3.88618500	-0.56172200
O	2.16774900	-3.75966600	1.13384200
C	3.97078800	-1.87140000	1.09926400
C	5.19624000	-1.42496000	0.61221700
C	5.87252700	-0.42409700	1.30368100
C	5.33547600	0.13928300	2.46655000
C	4.11434200	-0.34785300	2.94632700
C	3.42769900	-1.35221500	2.27176900
H	5.61419500	-1.86375300	-0.28776200
H	6.82905800	-0.06931700	0.93067600
H	3.69676000	0.06566800	3.85966900
H	2.48855900	-1.74228100	2.65106200
C	6.03009200	1.27857800	3.16271700
H	5.62434200	2.23140500	2.80620000
H	5.87595500	1.23645600	4.24313900
H	7.10307500	1.27347200	2.96119200

C	0.16491900	-3.58554600	-1.08064200
O	0.75806500	-4.51080200	-1.60742100
O	-1.14419700	-3.65545200	-0.75960000
C	-1.79734900	-4.87269900	-1.10866000
H	-1.70925500	-5.06217300	-2.18062700
H	-1.36221000	-5.71400800	-0.56463200
H	-2.84251600	-4.73945900	-0.83201500

TS4A^{S2}

C	5.68803800	-0.81740600	0.84814600
C	4.30982500	-0.80359100	1.05076300
C	3.73741800	-1.27846100	2.22612900
C	4.58375500	-1.78994100	3.20782400
C	5.96721300	-1.81227900	3.01222100
C	6.53010700	-1.32257000	1.83494100
C	6.04558600	-0.22502100	-0.49265200
C	4.70888500	-0.14428700	-1.26140700
C	3.60339400	-0.21388100	-0.14950600
H	2.66129600	-1.22385900	2.36299800
H	4.16672400	-2.17122700	4.13423400
H	6.61183500	-2.21548800	3.78679500
H	7.60571200	-1.34153400	1.68750100
H	6.76668900	-0.82155500	-1.05894900
H	4.60704700	0.78560000	-1.82310000
H	6.47285300	0.77627500	-0.37139800
H	3.20281800	0.77858300	0.05351900
N	2.49839100	-1.07000100	-0.59743200
O	4.59838600	-1.16558400	-2.24633700
C	1.16741700	-1.00051800	-0.40481600
C	2.75485200	-2.20976700	-1.30584100
N	0.67765000	-2.09200600	-0.99900700
N	1.66077100	-2.85561900	-1.57527000
C	4.16022900	-2.42285900	-1.76398300
H	4.79081400	-2.79624700	-0.94678400
H	4.18423500	-3.13078200	-2.59186400
C	-0.68123000	-2.55682500	-1.12262800
C	-1.13254800	-3.50275600	-0.19950700
C	-1.44831000	-2.09690800	-2.19311800
C	-2.41627100	-4.01112400	-0.38680100
C	-2.73838700	-2.61289400	-2.31821400
C	-3.23045000	-3.57878600	-1.43746100
H	-2.79776300	-4.74638800	0.31730500
H	-3.36625200	-2.26520500	-3.13530000
C	-0.90804500	-1.07375900	-3.15489100

H	-0.78686100	-0.09980200	-2.66720600
H	-1.58927200	-0.94180500	-3.99675500
C	-0.27493000	-3.90316600	0.96870800
H	-0.10939300	-3.03867100	1.62333200
H	0.70359200	-4.26498700	0.63975100
H	-0.75841900	-4.68806200	1.55132800
H	0.06971500	-1.37316500	-3.54366300
C	-4.60947000	-4.15778500	-1.62010900
H	-5.11722200	-4.27456100	-0.65894200
H	-5.22385600	-3.52385100	-2.26321200
H	-4.55047300	-5.14828300	-2.08232600
C	0.49206600	0.14632400	0.32073700
O	1.25950600	0.44371500	1.41612000
H	1.25950600	1.67749500	1.19488600
C	-0.95653000	-0.16328200	0.66334100
C	-1.36410000	-0.21543100	1.93341200
H	-1.67155800	-0.26246200	-0.15521900
H	-0.62595800	-0.00886100	2.70585300
C	-2.74740000	-0.49216000	2.35876800
C	-3.27270500	0.12986700	3.49770800
C	-3.56354700	-1.37490500	1.64124400
C	-4.58985900	-0.09733300	3.88773700
H	-2.64599900	0.80925000	4.06930800
C	-4.87272900	-1.62012200	2.04173100
H	-3.15996000	-1.87260700	0.76432100
C	-5.39462000	-0.97550000	3.16251300
H	-4.98709900	0.40447100	4.76451500
H	-5.48814800	-2.31480600	1.47666000
H	-6.41690600	-1.16324200	3.47494900
C	0.56762600	1.41645900	-0.65816000
C	0.83016200	2.58345300	0.25453800
H	-0.34906600	1.49738800	-1.24503900
H	1.40004300	1.30661100	-1.35873700
N	-0.36883000	3.22684800	0.76381600
H	-0.15890800	3.92029400	1.47996300
S	-1.38774000	3.97736500	-0.33511300
O	-0.72405100	4.22437400	-1.61434000
O	-2.01039400	5.08485500	0.39125800
C	-2.62388600	2.73133900	-0.62717500
C	-2.72032200	2.12554800	-1.87484600
C	-3.65058100	1.10453100	-2.05747300
C	-4.49214100	0.70273200	-1.01609400
C	-4.39364300	1.35492300	0.21971600
C	-3.45803300	2.35974200	0.42334700

H	-2.06803000	2.44701800	-2.68095900
H	-3.73294100	0.62203900	-3.02824800
H	-5.03932400	1.05236800	1.04018800
H	-3.36481600	2.84007600	1.39268000
C	-5.46101800	-0.43249000	-1.20653800
H	-5.74824700	-0.53941200	-2.25574800
H	-4.99804000	-1.37403800	-0.88838700
H	-6.36293400	-0.29116700	-0.60607300
C	1.88865800	3.53741900	-0.07769900
O	1.90726400	4.70899500	0.25753900
O	2.95187100	2.96246500	-0.70605700
C	4.06863700	3.82866800	-0.90161600
H	3.78776900	4.68360400	-1.51933700
H	4.44556300	4.19312400	0.05616100
H	4.82987600	3.23372500	-1.40531300

M4^{S2}

C	2.27492100	4.24134600	1.50999700
C	1.25030500	3.47248100	0.96332000
C	-0.05630200	3.94473900	0.89238800
C	-0.32667800	5.21667900	1.39139100
C	0.69572500	5.99395800	1.94145500
C	2.00275700	5.51472400	2.00178800
C	3.59139300	3.50815000	1.46041600
C	3.22375900	2.04926200	1.11286500
C	1.77956500	2.13168900	0.50222600
H	-0.83654200	3.33662800	0.44393600
H	-1.33772800	5.60806200	1.35026200
H	0.46844200	6.98220300	2.32829200
H	2.79356900	6.12085200	2.43325000
H	4.14570300	3.53879200	2.40280800
H	3.90847000	1.60770800	0.38736100
H	4.24119900	3.92777900	0.68563300
H	1.82812100	2.04317500	-0.57870500
N	0.93490000	1.03577200	1.00690900
O	3.31891300	1.19425200	2.24750300
C	-0.12180600	0.37515700	0.49133600
C	1.05256000	0.65399700	2.31633200
N	-0.58521100	-0.37351900	1.49957200
N	0.14534600	-0.21525300	2.64310400
C	2.19424800	1.20625100	3.10428100
H	1.96325900	2.21718700	3.46573800
H	2.40965300	0.56316200	3.95745000
C	-1.80705200	-1.13793000	1.57119100

C	-2.95243200	-0.44931100	1.99883300
C	-1.80701700	-2.48509600	1.22517800
C	-4.14216600	-1.16252400	2.04557900
C	-3.03382100	-3.15607600	1.28736200
C	-4.20244900	-2.51521600	1.68672900
H	-5.05082800	-0.65089700	2.35306200
H	-3.06536300	-4.20737200	1.01205200
C	-0.56788500	-3.20341600	0.76703700
H	-0.61653000	-3.41601000	-0.30645600
H	-0.47319000	-4.16313300	1.28219900
C	-2.89346300	1.01187800	2.34880700
H	-2.64650500	1.60563400	1.46094400
H	-2.13289700	1.21101000	3.10976500
H	-3.85827200	1.35405900	2.72475000
H	0.34035100	-2.62842900	0.95959900
C	-5.51948000	-3.24293000	1.72825700
H	-5.88256900	-3.33097900	2.75656400
H	-6.27699700	-2.69258000	1.16205200
H	-5.43354400	-4.24671200	1.30854000
C	-0.62741900	0.45731700	-0.94744000
O	-0.43494200	1.76278482	-1.35099190
H	0.80075257	1.07601735	-2.16910532
C	-2.09888300	0.12525800	-1.02890100
C	-3.03740200	1.04971200	-1.24220200
H	-2.35024200	-0.92917400	-0.94889500
H	-2.71762700	2.08477800	-1.34930100
C	-4.48669100	0.80682500	-1.33994500
C	-5.33142000	1.89445400	-1.59204700
C	-5.06354300	-0.46199400	-1.17419300
C	-6.71054000	1.72787300	-1.67884400
H	-4.89614900	2.88165500	-1.72222900
C	-6.43982300	-0.62981700	-1.26483400
H	-4.43580700	-1.32402700	-0.96655900
C	-7.26985600	0.46378400	-1.51560100
H	-7.34645300	2.58478800	-1.87688800
H	-6.86919200	-1.61980500	-1.14451000
H	-8.34424600	0.32778800	-1.58501300
C	0.20507000	-0.56324100	-1.84244700
C	1.34560798	0.21388187	-2.35678589
H	-0.45758600	-0.83103600	-2.66892000
H	0.39418800	-1.47537100	-1.26010900
N	2.63865400	-0.02498100	-1.59301400
H	3.31437800	0.68153400	-1.89189800
S	3.53668300	-1.46370200	-1.72643300

O	4.93669000	-1.05820400	-1.55940700
O	3.14721000	-2.26688900	-2.88208900
C	3.05626100	-2.38950600	-0.28351000
C	3.11208800	-1.78630400	0.97181000
C	2.85361700	-2.55424400	2.10028700
C	2.55122600	-3.91809400	1.99267700
C	2.50885600	-4.49619100	0.72217000
C	2.75503200	-3.73958500	-0.42129300
H	3.36640400	-0.73554100	1.07116900
H	2.89687600	-2.09316800	3.08392700
H	2.27707000	-5.55294500	0.62363500
H	2.72230800	-4.18386900	-1.41024400
C	2.23596000	-4.72748000	3.22201600
H	2.86827700	-4.43185400	4.06245700
H	1.19467100	-4.56947400	3.52379800
H	2.37352800	-5.79518700	3.04047200
C	1.66354100	0.26363600	-3.77835000
O	2.75153600	0.52717100	-4.29623200
O	0.51829900	0.22555000	-4.53462100
C	0.70774700	0.50422600	-5.91355900
H	1.11118800	1.50950300	-6.06055100
H	1.39535100	-0.21274700	-6.36881200
H	-0.27605900	0.42494900	-6.37620800

M4A^{S2}

C	5.75116000	-0.70937100	0.77224000
C	4.37825600	-0.73341100	1.00937700
C	3.85141400	-1.22575600	2.19840700
C	4.73655300	-1.70778000	3.16094700
C	6.11437800	-1.68718000	2.93181900
C	6.63214800	-1.18559300	1.73873300
C	6.05632600	-0.11879500	-0.58220100
C	4.70151000	-0.10433200	-1.32109300
C	3.63033800	-0.16652400	-0.17719000
H	2.77891300	-1.22023800	2.36773100
H	4.35282900	-2.10076900	4.09665600
H	6.78986200	-2.06880500	3.69067300
H	7.70353800	-1.17499500	1.56311300
H	6.79107900	-0.68991800	-1.15657100
H	4.55520200	0.80141400	-1.91218600
H	6.44123200	0.90182200	-0.47977300
H	3.23652300	0.83265600	0.01201700
N	2.52017400	-1.03758500	-0.58099500
O	4.59586300	-1.16552300	-2.26375700

C	1.19169900	-0.97288300	-0.37127100
C	2.77283100	-2.19338000	-1.26436800
N	0.69851400	-2.08174200	-0.92854500
N	1.67774400	-2.85098000	-1.50022500
C	4.17289400	-2.41005000	-1.73791200
H	4.81691900	-2.75866000	-0.92062100
H	4.18723300	-3.14058300	-2.54621300
C	-0.65653200	-2.56622000	-1.02485500
C	-1.08967300	-3.48681900	-0.06751700
C	-1.42467400	-2.16924900	-2.11970100
C	-2.35848800	-4.03459600	-0.24385600
C	-2.69943100	-2.72478100	-2.23384600
C	-3.17363100	-3.66713400	-1.31893100
H	-2.72599400	-4.75382700	0.48396200
H	-3.32587800	-2.43100100	-3.07269500
C	-0.89828600	-1.18018300	-3.12385500
H	-1.57369200	-1.10443600	-3.97731000
H	0.08924200	-1.47524700	-3.49051800
C	-0.22936700	-3.82469200	1.11869300
H	-0.09844300	-2.93780300	1.75058400
H	0.76378100	-4.16366600	0.80971200
H	-0.69243700	-4.60763800	1.72006300
H	-0.80345300	-0.18170000	-2.68194600
C	-4.53502900	-4.29081300	-1.48530400
H	-4.44228200	-5.34678200	-1.75684100
H	-5.10503500	-4.24372600	-0.55301500
H	-5.10835000	-3.78874600	-2.26722400
C	0.51210400	0.19520000	0.30039000
O	1.28838181	0.34012556	1.43064259
H	1.18020854	1.94868336	0.98946801
C	-0.92674900	-0.09508000	0.67217100
C	-1.34060400	-0.11552600	1.94226700
H	-1.63946500	-0.22052500	-0.14422900
H	-0.61460200	0.10073400	2.72371500
C	-2.72376400	-0.40527700	2.36219700
C	-3.26577100	0.22088300	3.49035600
C	-3.51380500	-1.31975700	1.65560500
C	-4.57607900	-0.03789900	3.88380000
H	-2.65820100	0.92413700	4.05381600
C	-4.81417000	-1.59827600	2.06203100
H	-3.09659800	-1.81776600	0.78520200
C	-5.35328400	-0.95214900	3.17379100
H	-4.98812200	0.46596500	4.75232000
H	-5.40958700	-2.32014500	1.51007900

H	-6.36893100	-1.16614100	3.49072400
C	0.59921200	1.44270500	-0.69322700
C	0.81790371	2.59747505	0.21959494
H	-0.30306700	1.43715600	-1.31334200
H	1.45471900	1.31268400	-1.36141000
N	-0.41397000	3.33485000	0.60566300
H	-0.77133500	3.10442700	1.52708000
S	-1.58691300	3.97225100	-0.35887100
O	-0.97362100	4.34168400	-1.62957400
O	-2.30687700	4.95928000	0.44503900
C	-2.76005800	2.67013900	-0.69538200
C	-2.75112300	2.00744300	-1.91828100
C	-3.62932000	0.94368300	-2.11680500
C	-4.51775100	0.54497000	-1.11324400
C	-4.52074800	1.24676000	0.09817000
C	-3.64572500	2.30200600	0.31420900
H	-2.07141400	2.33160600	-2.70071400
H	-3.63615700	0.42671900	-3.07330700
H	-5.20635000	0.95064700	0.88785500
H	-3.65519300	2.84225500	1.25608300
C	-5.43902600	-0.62758000	-1.31315700
H	-6.39513800	-0.47036600	-0.80787100
H	-5.62840300	-0.81251200	-2.37360400
H	-4.98865500	-1.53341700	-0.89110900
C	1.88309800	3.56341000	-0.07240200
O	2.01029400	4.72445000	0.29927400
O	2.95707100	2.92371300	-0.68405100
C	4.11905800	3.73027300	-0.81154400
H	3.90956300	4.63016200	-1.39397800
H	4.49993400	4.03277900	0.16717200
H	4.86196100	3.11980600	-1.32752800

TS5^{S2}

C	1.99226000	4.62422900	0.25264600
C	1.10423900	3.62993000	-0.14964500
C	-0.15019200	3.94063800	-0.66512200
C	-0.50736500	5.28336200	-0.76671600
C	0.37791100	6.28690500	-0.36389300
C	1.63454100	5.96560100	0.14497900
C	3.28052600	4.02799700	0.76100800
C	2.98076500	2.52282400	0.93158400
C	1.69519500	2.25210200	0.06909700
H	-0.80821000	3.14404000	-1.00285500
H	-1.47998900	5.55435000	-1.16484200

H	0.08257300	7.32809500	-0.44725700
H	2.31938800	6.74742300	0.45989700
H	3.61758900	4.45345800	1.71092600
H	3.81088100	1.90261900	0.58725200
H	4.08775800	4.17233600	0.03525500
H	1.93594100	1.76051700	-0.87311400
N	0.76803400	1.38613100	0.79308700
O	2.81769400	2.16281700	2.30090900
C	-0.10146800	0.44979800	0.33674600
C	0.56825500	1.58205700	2.13399800
N	-0.79693800	0.15197400	1.44893400
N	-0.39030600	0.82953300	2.57823800
C	1.54096300	2.46333900	2.84659600
H	1.28700900	3.52423700	2.72222200
H	1.56699600	2.22578100	3.91040300
C	-2.00060600	-0.63063100	1.51903100
C	-3.21537500	0.07206400	1.53033200
C	-1.93950600	-2.02149600	1.53448500
C	-4.39134200	-0.66678300	1.56232500
C	-3.15094900	-2.72107300	1.56953600
C	-4.37790700	-2.06559700	1.58751600
H	-5.34422700	-0.14178700	1.53377100
H	-3.12402800	-3.80834400	1.58224400
C	-0.63272400	-2.76235900	1.48410300
H	-0.45378500	-3.17440800	0.48386500
H	-0.64000900	-3.60394300	2.18206400
C	-3.23480400	1.57533200	1.47520800
H	-2.64593900	1.93720700	0.62360600
H	-2.80080900	2.00960800	2.38090100
H	-4.25771700	1.93877800	1.36387900
H	0.20891900	-2.11609500	1.73537900
C	-5.67347500	-2.83144900	1.64173200
H	-6.11815000	-2.76948300	2.64023200
H	-6.39502400	-2.41412000	0.93402200
H	-5.52270300	-3.88689100	1.40512000
C	-0.37044300	0.18682900	-1.69878800
O	-0.06766800	1.28720000	-2.20792200
H	1.82700700	0.44847100	-2.70659400
C	-1.81373400	-0.20912500	-1.55579400
C	-2.80926700	0.61896300	-1.88066000
H	-2.01413000	-1.20169300	-1.15428400
H	-2.54583300	1.61676500	-2.23104900
C	-4.23858200	0.30222300	-1.72607300
C	-5.15104800	1.32978300	-1.45744100

C	-4.71515800	-1.01299500	-1.80453300
C	-6.49586600	1.04868400	-1.23141400
H	-4.79306000	2.35505900	-1.40685300
C	-6.06026500	-1.29348500	-1.59540800
H	-4.02525500	-1.81799000	-2.04060500
C	-6.95464700	-0.26536100	-1.29685900
H	-7.18692400	1.85644000	-1.01147900
H	-6.41482800	-2.31728900	-1.66898400
H	-8.00438000	-0.48605400	-1.13095800
C	0.54537600	-1.03378800	-1.96275600
C	1.94178900	-0.60215000	-2.39817400
H	0.07719900	-1.58386800	-2.78477000
H	0.57459100	-1.70280900	-1.09948800
N	2.93139100	-0.58721600	-1.31170100
H	3.77854100	-0.10128900	-1.60663100
S	3.46220500	-2.08788800	-0.75899800
O	4.92113900	-2.01713700	-0.72658000
O	2.79755400	-3.15346400	-1.50452100
C	2.88170500	-2.17583300	0.91409600
C	2.80117100	-1.02994800	1.69910100
C	2.46019200	-1.15490200	3.04034500
C	2.21827600	-2.41135100	3.60790500
C	2.33224500	-3.54679600	2.79961500
C	2.65595100	-3.44018400	1.45137200
H	2.99922300	-0.05601100	1.27053400
H	2.39340200	-0.26086800	3.65444500
H	2.15112400	-4.52780900	3.22924500
H	2.72445300	-4.32070000	0.82110000
C	1.79843400	-2.53080000	5.04785300
H	2.28023000	-1.76901300	5.66476300
H	0.71568800	-2.39028900	5.13541000
H	2.04152400	-3.51535300	5.45237200
C	2.51741700	-1.29971200	-3.62822400
O	3.70473700	-1.43557200	-3.81365400
O	1.58323900	-1.64488100	-4.51153100
C	2.07513100	-2.21944800	-5.72889900
H	2.71720200	-1.50624700	-6.24837100
H	2.64303800	-3.12512000	-5.51083900
H	1.19492600	-2.45051800	-6.32434300

TS5A^{S2}

C	5.54803100	-1.35003500	0.84301100
C	4.16417800	-1.22843700	0.93946600
C	3.43966200	-1.89079400	1.92479200

C	4.13583300	-2.69515300	2.82462100
C	5.52460800	-2.82367900	2.73490000
C	6.24128600	-2.15034600	1.74710300
C	6.08282500	-0.53020600	-0.30504700
C	4.83603300	-0.14721900	-1.13312200
C	3.62384100	-0.33063700	-0.15396100
H	2.36387500	-1.75163700	1.99128500
H	3.59731800	-3.22485000	3.60379000
H	6.05122800	-3.45653300	3.44236900
H	7.31996500	-2.25633600	1.67869900
H	6.79867600	-1.06913200	-0.93269500
H	4.88333300	0.88233900	-1.49138700
H	6.58432100	0.37152600	0.06249800
H	3.28188100	0.62185400	0.25325800
N	2.50065000	-0.96070200	-0.84591200
O	4.72349100	-0.92727400	-2.31809700
C	1.16352600	-0.81700600	-0.66755400
C	2.73657100	-1.98766200	-1.72095500
N	0.66946400	-1.78835600	-1.44707900
N	1.62535900	-2.52288400	-2.12205800
C	4.15172600	-2.21373300	-2.14199700
H	4.69724000	-2.80465600	-1.39413000
H	4.18863200	-2.72987000	-3.10122500
C	-0.70143500	-2.18775300	-1.60188800
C	-1.14627100	-3.28709900	-0.86033500
C	-1.50776500	-1.51708300	-2.52096000
C	-2.43912200	-3.74681000	-1.10032700
C	-2.80600000	-1.99782200	-2.70825600
C	-3.27685300	-3.12248900	-2.02795900
H	-2.80649700	-4.60201100	-0.53780700
H	-3.45419900	-1.49731800	-3.42466700
C	-0.98285400	-0.32784800	-3.27825400
H	-1.70962000	0.01495000	-4.01711400
H	-0.05008600	-0.57347600	-3.79470400
C	-0.26306900	-3.90556100	0.18789600
H	-0.04419300	-3.16604300	0.96750800
H	0.69126300	-4.23283600	-0.23492900
H	-0.75433200	-4.76161600	0.65260400
H	-0.76899500	0.50342300	-2.59753700
C	-4.65744900	-3.66716100	-2.29285400
H	-4.60032400	-4.59005200	-2.87849500
H	-5.17343200	-3.90840200	-1.35893100
H	-5.26779200	-2.95361500	-2.85116500
C	0.57967700	0.52832900	0.79330100

O	1.40449700	0.39636100	1.72325400
H	1.39772800	2.66804600	1.70231500
C	-0.81186600	-0.02351800	0.94096400
C	-1.17487900	-0.61348400	2.08458400
H	-1.49050100	0.07833400	0.09190400
H	-0.43815500	-0.61736900	2.88739300
C	-2.46380500	-1.25910400	2.36717800
C	-2.83900200	-1.49538000	3.69617300
C	-3.32605100	-1.67773200	1.34416400
C	-4.04878600	-2.11191300	3.99966800
H	-2.17232600	-1.18509800	4.49647100
C	-4.52845000	-2.30760300	1.64638900
H	-3.04023100	-1.52141100	0.30707400
C	-4.89811000	-2.52199400	2.97415800
H	-4.32492000	-2.27978500	5.03586400
H	-5.17932000	-2.63993500	0.84253200
H	-5.83675500	-3.01493700	3.20601300
C	0.73891300	1.78553000	-0.09361900
C	0.87137000	3.01891200	0.80401100
H	-0.07881100	1.88826900	-0.81239500
H	1.66116100	1.70169100	-0.66855600
N	-0.41431800	3.53804600	1.26898800
H	-0.29979200	4.26691100	1.97202900
S	-1.45477100	4.15638700	0.11072000
O	-0.75131700	4.39823200	-1.14665600
O	-2.16376300	5.24467400	0.77665900
C	-2.58960100	2.82580700	-0.17901600
C	-2.76677800	2.36270500	-1.47802800
C	-3.70470500	1.36068700	-1.70801100
C	-4.46777000	0.83498000	-0.66138900
C	-4.25847300	1.31687500	0.63681600
C	-3.32112200	2.31003000	0.88727700
H	-2.18264400	2.78844600	-2.28746000
H	-3.86227100	0.99651400	-2.71969000
H	-4.83463200	0.90103000	1.45818000
H	-3.15459000	2.67759400	1.89491000
C	-5.48332400	-0.24087500	-0.93211100
H	-6.16812300	-0.36293900	-0.09063700
H	-6.06410000	-0.01276800	-1.83001100
H	-4.98004800	-1.19935200	-1.10148100
C	1.74979000	4.14618600	0.26543200
O	1.56537200	5.31335200	0.51562800
O	2.80743600	3.68730500	-0.40830300
C	3.74382300	4.68809000	-0.82766000

H	3.25799000	5.39835000	-1.49824700
H	4.13718500	5.22072500	0.03978700
H	4.53849300	4.15387000	-1.34380700
p ^{s2}			
C	-0.37044300	0.18682900	-1.69878800
O	-0.06766800	1.28720000	-2.20792200
H	1.82700700	0.44847100	-2.70659400
C	-1.81373400	-0.20912500	-1.55579400
C	-2.80926700	0.61896300	-1.88066000
H	-2.01413000	-1.20169300	-1.15428400
H	-2.54583300	1.61676500	-2.23104900
C	-4.23858200	0.30222300	-1.72607300
C	-5.15104800	1.32978300	-1.45744100
C	-4.71515800	-1.01299500	-1.80453300
C	-6.49586600	1.04868400	-1.23141400
H	-4.79306000	2.35505900	-1.40685300
C	-6.06026500	-1.29348500	-1.59540800
H	-4.02525500	-1.81799000	-2.04060500
C	-6.95464700	-0.26536100	-1.29685900
H	-7.18692400	1.85644000	-1.01147900
H	-6.41482800	-2.31728900	-1.66898400
H	-8.00438000	-0.48605400	-1.13095800
C	0.54537600	-1.03378800	-1.96275600
C	1.94178900	-0.60215000	-2.39817400
H	0.07719900	-1.58386800	-2.78477000
H	0.57459100	-1.70280900	-1.09948800
N	2.93139100	-0.58721600	-1.31170100
H	3.77854100	-0.10128900	-1.60663100
S	3.46220500	-2.08788800	-0.75899800
O	4.92113900	-2.01713700	-0.72658000
O	2.79755400	-3.15346400	-1.50452100
C	2.88170500	-2.17583300	0.91409600
C	2.80117100	-1.02994800	1.69910100
C	2.46019200	-1.15490200	3.04034500
C	2.21827600	-2.41135100	3.60790500
C	2.33224500	-3.54679600	2.79961500
C	2.65595100	-3.44018400	1.45137200
H	2.99922300	-0.05601100	1.27053400
H	2.39340200	-0.26086800	3.65444500
H	2.15112400	-4.52780900	3.22924500
H	2.72445300	-4.32070000	0.82110000
C	1.79843400	-2.53080000	5.04785300
H	2.28023000	-1.76901300	5.66476300

H	0.71568800	-2.39028900	5.13541000
H	2.04152400	-3.51535300	5.45237200
C	2.51741700	-1.29971200	-3.62822400
O	3.70473700	-1.43557200	-3.81365400
O	1.58323900	-1.64488100	-4.51153100
C	2.07513100	-2.21944800	-5.72889900
H	2.71720200	-1.50624700	-6.24837100
H	2.64303800	-3.12512000	-5.51083900
H	1.19492600	-2.45051800	-6.32434300

PA^{S2}

C	0.48084400	0.77542000	1.12673600
O	1.33379300	0.51427200	1.93115300
H	1.42091100	2.90102300	1.80348700
C	-0.82494600	0.04240600	1.07779100
C	-1.21942300	-0.60427200	2.18252400
H	-1.42522600	0.12833000	0.17044700
H	-0.53055300	-0.58244200	3.03335700
C	-2.49181600	-1.28159800	2.40867600
C	-2.88389300	-1.52747500	3.72861800
C	-3.34063400	-1.68292500	1.35823200
C	-4.10663300	-2.12643200	4.01559000
H	-2.22229200	-1.22287900	4.53698200
C	-4.54643900	-2.30467100	1.64383100
H	-3.03719000	-1.51721700	0.33040900
C	-4.94263100	-2.51878100	2.96260400
H	-4.40000900	-2.30423300	5.04252800
H	-5.19295500	-2.62074500	0.83202800
H	-5.88386600	-3.00553000	3.17708000
C	0.75795000	1.84919600	0.07715200
C	0.88442800	3.14815400	0.88184000
H	-0.02832800	1.90301000	-0.68316900
H	1.70181500	1.64194600	-0.43621900
N	-0.42394500	3.62979400	1.30633100
H	-0.36384600	4.38763800	1.99111900
S	-1.46392200	4.18083000	0.10047700
O	-0.73117200	4.38982500	-1.14220000
O	-2.20465100	5.27162900	0.73052600
C	-2.57073400	2.82323300	-0.18561700
C	-2.74167900	2.35926000	-1.48509800
C	-3.68101600	1.35941800	-1.71947200
C	-4.46147400	0.83688900	-0.67674000
C	-4.25889700	1.33024800	0.62205000
C	-3.32016100	2.32082800	0.87689500

H	-2.14179600	2.77264600	-2.29160100
H	-3.82390200	0.99470800	-2.73167900
H	-4.85154600	0.91759200	1.44038200
H	-3.16856900	2.68914700	1.88505200
C	-5.47743300	-0.22767600	-0.95124400
H	-6.17387100	-0.33950400	-0.12793400
H	-6.04560900	-0.00582300	-1.86871300
H	-4.97597000	-1.18963700	-1.11557700
C	1.75147800	4.23477900	0.27652300
O	1.58485500	5.41229100	0.49362800
O	2.79825400	3.72467900	-0.37206800
C	3.77187000	4.69414600	-0.80777400
H	3.31600200	5.40690100	-1.49277900
H	4.17571100	5.23413700	0.05555100
H	4.56162900	4.12921800	-1.30527800

Cross-coupling reaction

TS3^{S2}

C	-4.93363300	-2.53603400	-1.05856600
C	-3.54632500	-2.42716200	-1.10205600
C	-2.73849700	-3.52967200	-1.36666700
C	-3.34914900	-4.76381000	-1.57554100
C	-4.74102300	-4.88185400	-1.52717400
C	-5.54216200	-3.77057800	-1.27404600
C	-5.57901600	-1.20176500	-0.78112300
C	-4.41520800	-0.24986000	-0.41333800
C	-3.10168700	-1.00880000	-0.82672300
H	-1.65920400	-3.41695100	-1.42219500
H	-2.74177800	-5.63887700	-1.78272600
H	-5.20252500	-5.85068300	-1.68989300
H	-6.62330700	-3.86720700	-1.23962600
H	-6.30917500	-1.23676100	0.03389900
H	-4.46050500	0.69508000	-0.95104400
H	-6.10540000	-0.83213100	-1.66677000
H	-2.64250500	-0.53500300	-1.69074500
N	-2.12121900	-0.97270500	0.26722400
O	-4.45212300	0.12929900	0.95731700
C	-0.76427500	-1.10731500	0.26265000
C	-2.53340500	-1.04748800	1.57177700
N	-0.43967300	-1.26359600	1.57267800
N	-1.54502800	-1.20805400	2.39141800
C	-3.99031200	-0.86888800	1.84465400
H	-4.52880500	-1.81779500	1.70915500

H	-4.14240200	-0.51743600	2.86541600
C	0.79616200	-1.75362600	2.10988600
C	1.19169400	-3.05638500	1.78049400
C	1.56284700	-0.91174500	2.91883100
C	2.43714800	-3.48267800	2.23538300
C	2.79966900	-1.38872300	3.35539000
C	3.25981200	-2.65921300	3.00793900
H	2.77496200	-4.48362700	1.97759700
H	3.42044500	-0.74600900	3.97417000
C	1.07060000	0.45790800	3.29963800
H	0.21946000	0.38229200	3.98411600
H	0.72216300	1.01154800	2.42291200
C	0.33251500	-3.95833400	0.93404300
H	0.51187800	-3.77052100	-0.13107600
H	-0.73294900	-3.80370800	1.12926000
H	0.57039100	-5.00418800	1.13564500
H	1.86068600	1.02788500	3.79061000
C	4.62298300	-3.13705900	3.43509600
H	5.29217400	-3.19769200	2.57051100
H	5.07139800	-2.45985500	4.16430600
H	4.56875900	-4.13594000	3.87607300
C	0.09267900	-1.11577800	-0.88982000
O	-0.46481200	-1.30875800	-2.05609300
H	-0.30965800	-0.19895900	-2.61900800
C	1.53928600	-1.22666600	-0.76108700
C	2.31805400	-1.58850200	-1.79584400
H	1.99569100	-0.94182700	0.18065800
H	1.83427300	-1.83347200	-2.73916800
C	3.78192200	-1.68083700	-1.76037600
C	4.48327700	-1.83952800	-2.96365000
C	4.51906400	-1.63367700	-0.56490500
C	5.87173700	-1.92892700	-2.98105100
H	3.92582900	-1.88512200	-3.89546100
C	5.90532900	-1.72143000	-0.58270500
H	4.00478100	-1.54272600	0.38873600
C	6.58998500	-1.86738100	-1.78990800
H	6.39191800	-2.04625400	-3.92651900
H	6.45729700	-1.67992000	0.35150900
H	7.67283600	-1.93738100	-1.79881600
C	-0.07559300	1.12544700	-2.66579400
C	0.11783800	1.36199400	-1.28756200
H	-1.01501300	1.48733600	-3.08028100
H	0.79827300	1.25705900	-3.29763100
N	1.41473200	1.67295600	-0.77930400

H	1.52506400	1.47765000	0.21432500
S	1.99868400	3.22786700	-1.06020500
O	2.07282100	3.41210000	-2.50200600
O	3.19365800	3.33707100	-0.23196100
C	0.77441500	4.34632600	-0.42901100
C	0.90536600	4.82748800	0.87123800
C	-0.09011300	5.64811800	1.38623300
C	-1.21994900	5.97531600	0.62678400
C	-1.32783700	5.46978600	-0.67258200
C	-0.33473000	4.65770800	-1.21146700
H	1.78172200	4.57029300	1.45667400
H	0.00884900	6.04342100	2.39304100
H	-2.19697800	5.72069400	-1.27323000
H	-0.41146100	4.27624500	-2.22490100
C	-2.31400900	6.82692900	1.21385000
H	-1.90866500	7.56881300	1.90533600
H	-2.87428900	7.34558200	0.43349300
H	-3.02055100	6.20485800	1.77371200
C	-1.04849900	1.68390000	-0.45937400
O	-2.19892400	1.72099500	-0.85986500
O	-0.72826000	1.89452100	0.83689000
C	-1.80467500	2.33557600	1.67011800
H	-2.07928700	3.35917700	1.39998900
H	-2.67383800	1.68501100	1.55075200
H	-1.42380000	2.30252700	2.69030400

TS3A^{S2}

C	3.28038600	3.78853500	-1.06299800
C	2.05205700	3.15365200	-1.21955300
C	0.96102800	3.79821700	-1.79442200
C	1.11884500	5.11767000	-2.20937600
C	2.34771100	5.76584500	-2.05159400
C	3.43586100	5.10784100	-1.48266100
C	4.30087200	2.86816500	-0.44142300
C	3.51362500	1.60046800	-0.02882400
C	2.09333600	1.74130300	-0.69072700
H	0.01769900	3.27309200	-1.92192400
H	0.28581000	5.64573900	-2.66142000
H	2.45495400	6.79503600	-2.37888300
H	4.38786400	5.61668200	-1.36509000
H	4.80164700	3.30305300	0.42979800
H	3.99866500	0.69135600	-0.38868200
H	5.08358900	2.60849900	-1.16056300
H	1.95401400	1.00774600	-1.47857000

N	1.03971200	1.52463500	0.31529000
O	3.44754400	1.42430900	1.37958200
C	-0.25646400	1.09599600	0.20305000
C	1.20387100	1.99203600	1.59887300
N	-0.79472500	1.35751600	1.41862100
N	0.12048400	1.89341400	2.29388700
C	2.58947200	2.35617500	2.02020300
H	2.83642600	3.38959300	1.74395400
H	2.69789200	2.23546500	3.09744300
C	-2.16820100	1.27469700	1.81688300
C	-3.08353100	2.15562100	1.22657900
C	-2.52817900	0.32004400	2.77007100
C	-4.42246800	2.01646900	1.58067900
C	-3.88383400	0.22490600	3.09118700
C	-4.84090200	1.04947400	2.49967400
H	-5.15779200	2.67812900	1.12873700
H	-4.19741100	-0.52003900	3.81799100
C	-1.49433500	-0.56303500	3.41350500
H	-0.83604300	0.02502900	4.05990100
H	-0.88000700	-1.05488600	2.65320700
C	-2.64761700	3.18911700	0.22142500
H	-2.50759700	2.73471800	-0.76631100
H	-1.70242600	3.65812400	0.51140500
H	-3.40507700	3.96890500	0.12691500
H	-1.97875200	-1.33166900	4.01827800
C	-6.30336700	0.91033800	2.83431500
H	-6.70781300	1.85187400	3.21683800
H	-6.87948200	0.64806800	1.94149900
H	-6.46652300	0.13587800	3.58592900
C	-0.83069400	0.47521300	-0.95713100
O	-0.15285600	0.58922900	-2.06870300
H	0.52501500	-0.46276800	-2.11618000
C	-2.21417100	0.01196800	-0.97345800
C	-2.88307700	-0.19758000	-2.12066000
H	-2.67611400	-0.22976100	-0.02144000
H	-2.36794200	-0.00285200	-3.05922100
C	-4.25894500	-0.69981000	-2.21116600
C	-4.73262300	-1.18699600	-3.43739300
C	-5.12756200	-0.72334500	-1.10656200
C	-6.01933600	-1.70438600	-3.55510200
H	-4.07500200	-1.16768800	-4.30244300
C	-6.41081400	-1.24252300	-1.22421100
H	-4.79895700	-0.32082000	-0.15124200
C	-6.86305100	-1.73889900	-2.44779800

H	-6.36289700	-2.08234200	-4.51295200
H	-7.06521300	-1.25541000	-0.35795700
H	-7.86628900	-2.14269000	-2.53690700
C	1.06424800	-1.60001600	-1.64289700
C	0.42672300	-1.66763000	-0.38249200
H	2.14139800	-1.43272200	-1.63359100
H	0.72090500	-2.30060600	-2.39993700
N	1.09154100	-1.35587800	0.84387500
H	1.61183200	-0.47960100	0.87196500
S	2.03152400	-2.54002600	1.57102200
O	1.31792000	-3.80068100	1.43478500
O	2.37553300	-1.99964200	2.88022200
C	3.52688000	-2.64438100	0.62057900
C	3.64026000	-3.60642900	-0.37757400
C	4.78936200	-3.62587100	-1.16253300
C	5.81249100	-2.69373500	-0.96722100
C	5.67005400	-1.73947000	0.04815700
C	4.53368900	-1.70645000	0.84722900
H	2.84326100	-4.32736800	-0.52520300
H	4.89385600	-4.37862900	-1.93816300
H	6.46421300	-1.01789000	0.21896200
H	4.42476000	-0.96572800	1.63453100
C	7.03855400	-2.69832000	-1.84132000
H	7.93280700	-2.44861400	-1.26581400
H	7.18665000	-3.67279800	-2.31041900
H	6.94148100	-1.95437600	-2.63854000
C	-0.85119600	-2.37877100	-0.18084300
O	-1.45024600	-2.47555200	0.87250000
O	-1.31138500	-2.90497000	-1.32958000
C	-2.59010600	-3.53169400	-1.23542400
H	-2.52258200	-4.44254400	-0.63588800
H	-3.31619000	-2.85321300	-0.78325500
H	-2.88329300	-3.76736300	-2.25754000
M3 ^{S2}			
C	0.09795100	-5.48670300	-0.32441500
C	0.56383600	-4.18801800	-0.51089300
C	1.90373600	-3.92151300	-0.77249500
C	2.79048600	-4.99481600	-0.81805800
C	2.33465400	-6.30126500	-0.61855200
C	0.98595800	-6.55801800	-0.37860200
C	-1.39483400	-5.50074500	-0.10793600
C	-1.77696900	-4.02365400	0.13904000
C	-0.56513400	-3.18895600	-0.40288900

H	2.21299400	-2.89738600	-0.96609700
H	3.84255900	-4.81777900	-1.01698900
H	3.03899100	-7.12633600	-0.65639900
H	0.63513200	-7.57533200	-0.23253500
H	-1.71109600	-6.11567000	0.74004200
H	-2.68677000	-3.73383800	-0.38906300
H	-1.91042500	-5.88073700	-0.99591400
H	-0.77690400	-2.71191200	-1.35685600
N	-0.21173000	-2.11551100	0.54885300
O	-2.07475700	-3.78117300	1.51235900
C	0.34635100	-0.89744200	0.37899300
C	-0.26747500	-2.36016000	1.89271700
N	0.61483400	-0.47741600	1.62262100
N	0.22766900	-1.37490400	2.58040300
C	-0.93962000	-3.61570900	2.34103600
H	-0.25399800	-4.47083100	2.27184000
H	-1.28192000	-3.51342100	3.37063700
C	1.38062500	0.67965900	2.00611800
C	2.77627400	0.57481600	1.90588000
C	0.72840100	1.83462500	2.43154500
C	3.51624900	1.72639900	2.13851600
C	1.52012300	2.96888800	2.64184200
C	2.90201600	2.93831400	2.47781100
H	4.59804200	1.68646300	2.03636700
H	1.03425200	3.89525500	2.93760100
C	-0.75411700	1.88245800	2.70898800
H	-0.92736800	1.79671800	3.78601000
H	-1.30251400	1.06740400	2.22776200
C	3.43625800	-0.73109400	1.55401900
H	3.22424100	-1.00958200	0.51681400
H	3.07769800	-1.53846400	2.20031000
H	4.51833900	-0.64961400	1.66717400
H	-1.17037700	2.83675500	2.37453800
C	3.74066100	4.17259800	2.67445600
H	4.41570900	4.31265600	1.82485100
H	3.11978900	5.06453900	2.77541800
H	4.36026600	4.08303200	3.57202200
C	0.56694000	-0.27402600	-1.05739100
O	0.72446000	-1.26751400	-1.89234900
H	-0.62013200	-0.16454500	-3.34775700
C	1.72287400	0.73172900	-0.99557100
C	2.85893000	0.46941600	-1.64341700
H	1.60743900	1.63994400	-0.41402900
H	2.90316500	-0.46414500	-2.20360100

C	4.07733100	1.29570900	-1.60133600
C	5.28382600	0.74873300	-2.05654000
C	4.09126100	2.60472100	-1.09415400
C	6.47093600	1.47379900	-1.99511300
H	5.28583500	-0.26163500	-2.45721000
C	5.27451500	3.33206500	-1.03889900
H	3.16797500	3.06171800	-0.74938800
C	6.47094100	2.76872200	-1.48429500
H	7.39479700	1.02811700	-2.35039000
H	5.26279300	4.34870900	-0.65744100
H	7.39272100	3.33986200	-1.44109600
C	-0.79139200	0.81176200	-2.89786700
C	-0.81361700	0.60726900	-1.39315100
H	-1.72354700	1.23641400	-3.27084300
H	0.03001100	1.48313500	-3.15532100
N	-0.76475200	1.86609600	-0.64410100
H	-0.66480600	1.73688200	0.36018400
S	-1.80158000	3.14675300	-0.88129800
O	-1.67532200	3.57836400	-2.26529200
O	-1.48235500	4.06031100	0.21278500
C	-3.47415700	2.59278500	-0.64572000
C	-4.04544200	2.68551000	0.62144200
C	-5.33667700	2.21050000	0.81310100
C	-6.05703000	1.63117500	-0.23814700
C	-5.46038500	1.55720000	-1.50035500
C	-4.17227900	2.03808300	-1.71443600
H	-3.48979500	3.14205500	1.43392800
H	-5.79578800	2.29142300	1.79422800
H	-6.01268000	1.12539300	-2.32974700
H	-3.72743700	2.00645100	-2.70366000
C	-7.43528800	1.07268700	-0.00573300
H	-7.95918400	1.62500400	0.77726000
H	-8.03474200	1.10408700	-0.91766700
H	-7.37107400	0.02678900	0.31323200
C	-2.00485300	-0.24461000	-0.97697300
O	-2.54203300	-1.08060000	-1.66624000
O	-2.35101300	-0.01611300	0.30314600
C	-3.46971200	-0.75767400	0.80295100
H	-4.28608700	-0.73092400	0.07853600
H	-3.17511900	-1.79057700	1.00507500
H	-3.76260100	-0.25946700	1.72613300
M3A ^{S2}			
C	2.96423800	4.04375500	-0.49982700

C	1.83103200	3.26483200	-0.71605800
C	0.66125700	3.80179200	-1.24571900
C	0.63996500	5.16285200	-1.53947800
C	1.76898900	5.95655700	-1.31556500
C	2.93960600	5.40358100	-0.80096900
C	4.10273700	3.21809200	0.04242600
C	3.47719200	1.85020100	0.40041300
C	2.07064200	1.83052200	-0.30249100
H	-0.18209000	3.14394900	-1.43998600
H	-0.25807300	5.61136500	-1.95187800
H	1.73446500	7.01600700	-1.54923200
H	3.81575300	6.02287200	-0.63309100
H	4.57791500	3.65583400	0.92619700
H	4.08292800	1.01729000	0.04204500
H	4.88502400	3.08940800	-0.71227100
H	2.01913900	1.15585600	-1.15502200
N	1.03775700	1.39770400	0.65741400
O	3.39825500	1.64375600	1.80604900
C	-0.13399300	0.74866900	0.48181000
C	1.08987100	1.81534600	1.96000600
N	-0.74409300	0.83317200	1.66722100
N	0.01150600	1.48750900	2.60440700
C	2.37931600	2.40069400	2.43739300
H	2.44900900	3.46860600	2.19254300
H	2.47517800	2.27208300	3.51514800
C	-2.08896000	0.44920100	2.01216500
C	-3.11278900	1.33706800	1.66286400
C	-2.30077200	-0.76515300	2.66061500
C	-4.41548300	0.93930900	1.94062800
C	-3.62953900	-1.11409500	2.91881600
C	-4.69085600	-0.28568200	2.55700200
H	-5.23772400	1.59342000	1.66091600
H	-3.83293700	-2.06103600	3.41186900
C	-1.15593200	-1.66785700	3.02992200
H	-0.35622400	-1.10945200	3.52514900
H	-0.73444400	-2.13351600	2.13357800
C	-2.81067200	2.64784300	0.98828100
H	-2.46399400	2.47950100	-0.03776600
H	-2.02950200	3.19921600	1.52081500
H	-3.70588500	3.27005500	0.94700900
H	-1.49786500	-2.45445000	3.70477100
C	-6.11868000	-0.68691900	2.81743900
H	-6.58958800	-0.00678600	3.53359100
H	-6.70147800	-0.64024900	1.89240700

H	-6.18244200	-1.70090400	3.21635300
C	-0.52590200	0.10302200	-0.88739900
O	-0.10360900	0.88739900	-1.84173100
H	0.59526100	-1.04905000	-2.99823200
C	-2.03056500	-0.17735400	-0.87524600
C	-2.82966000	0.39597900	-1.77512800
H	-2.42175700	-0.85859900	-0.12574100
H	-2.35946900	1.06462600	-2.49502900
C	-4.28938900	0.22561100	-1.86738600
C	-4.99670600	0.96703400	-2.82175000
C	-5.01168900	-0.64615100	-1.03592200
C	-6.37817400	0.84821200	-2.94794100
H	-4.44938500	1.64423600	-3.47221500
C	-6.38959500	-0.77222400	-1.16682000
H	-4.49484400	-1.22981800	-0.27833600
C	-7.08021100	-0.02425100	-2.12160100
H	-6.90437000	1.43329500	-3.69558400
H	-6.92916600	-1.46276700	-0.52545400
H	-8.15619300	-0.12577200	-2.22055600
C	1.15840100	-1.44223300	-2.15437300
C	0.28337500	-1.43084700	-0.90794900
H	2.03139100	-0.80200700	-2.00263500
H	1.49839000	-2.45792800	-2.37118300
N	1.01954600	-1.63498000	0.34454400
H	1.53395300	-0.82718500	0.68365300
S	1.96926500	-2.99007600	0.59104900
O	1.47330700	-4.04677000	-0.28116900
O	2.03070000	-3.17946400	2.03481800
C	3.60496200	-2.53867200	0.05535700
C	4.11211600	-3.06971800	-1.12438500
C	5.38312100	-2.68610000	-1.54211800
C	6.14431600	-1.78059100	-0.79883200
C	5.61116500	-1.27168600	0.39267600
C	4.34682300	-1.64651500	0.82950800
H	3.52039800	-3.77730000	-1.69557300
H	5.79061200	-3.09967200	-2.45967900
H	6.19811700	-0.57891400	0.98974300
H	3.94743600	-1.25358300	1.76071000
C	7.50571800	-1.34355100	-1.27014400
H	8.20474000	-1.26693600	-0.43406200
H	7.91376900	-2.04224200	-2.00269700
H	7.44798800	-0.35760400	-1.74240300
C	-0.79562200	-2.50043400	-0.95639100
O	-1.30828500	-3.02617800	0.00610200

O	-1.19317500	-2.72333000	-2.21190200
C	-2.36291300	-3.53418300	-2.34242700
H	-2.20480000	-4.51046200	-1.88197000
H	-3.21066200	-3.03802200	-1.86207600
H	-2.53783500	-3.63500900	-3.41145400

TS4^{S2}

C	-1.54453400	5.17949000	-0.13912200
C	-1.56536800	3.80734800	-0.37228000
C	-2.73813000	3.14613400	-0.72314900
C	-3.91004100	3.89059900	-0.83012300
C	-3.89811300	5.26865600	-0.59562100
C	-2.71684600	5.92316300	-0.25266600
C	-0.15488200	5.65080100	0.20795100
C	0.66441900	4.35931400	0.43913600
C	-0.19374700	3.19892400	-0.18059900
H	-2.71636400	2.07890500	-0.92835300
H	-4.83903200	3.39892500	-1.10067400
H	-4.82030000	5.83481800	-0.68108700
H	-2.71246400	6.99373000	-0.07048600
H	-0.11900400	6.28239200	1.10116200
H	1.63726100	4.40334500	-0.05336000
H	0.27738400	6.22957400	-0.61460500
H	0.22521900	2.84166100	-1.12035600
N	-0.26483200	2.05444100	0.73991800
O	0.97576000	4.15961200	1.81369000
C	-0.42998800	0.73133300	0.49599500
C	-0.36504700	2.27189700	2.08963600
N	-0.63399300	0.23086400	1.72394300
N	-0.58655900	1.16590300	2.73152000
C	-0.10053500	3.65501700	2.58654900
H	-0.99572000	4.28463300	2.49333400
H	0.21301400	3.63316300	3.62993600
C	-0.98554600	-1.12781100	2.02861300
C	-2.33209900	-1.49726200	1.90476600
C	0.01340000	-2.01961200	2.41973100
C	-2.64732900	-2.83639000	2.11063100
C	-0.35248500	-3.35668300	2.59818700
C	-1.66837100	-3.78204700	2.43370300
H	-3.68174800	-3.15401300	2.00082400
H	0.41601100	-4.07634600	2.86701200
C	1.42270100	-1.56020200	2.69710700
H	1.46787400	-1.06447900	3.67229400
H	1.78845400	-0.83735200	1.95920800

C	-3.39797200	-0.47895600	1.59969900
H	-3.13567900	0.12660300	0.72810700
H	-3.53012100	0.19960600	2.44900500
H	-4.34987300	-0.97393100	1.39659300
H	2.09676200	-2.41793400	2.70915000
C	-2.04771500	-5.23039300	2.59922700
H	-2.44820000	-5.63128400	1.66283400
H	-1.18727000	-5.83645700	2.88820300
H	-2.82324400	-5.34631700	3.36165700
C	-0.50073600	0.12487000	-1.41097400
O	-0.78419600	1.14097700	-2.07672000
H	0.85798700	0.23371000	-3.61551400
C	-1.52333200	-0.97292100	-1.24704000
C	-2.72853100	-0.84143800	-1.80837100
H	-1.26216400	-1.83575700	-0.64328100
H	-2.91203900	0.06116800	-2.39070600
C	-3.85919500	-1.76889100	-1.64937000
C	-5.13639100	-1.34836100	-2.04221200
C	-3.72142500	-3.04577100	-1.08410700
C	-6.24772400	-2.16570500	-1.86107800
H	-5.25433000	-0.36346400	-2.48661600
C	-4.83109300	-3.86244600	-0.90196000
H	-2.74014200	-3.40541700	-0.78906800
C	-6.09929100	-3.42545200	-1.28581800
H	-7.22892200	-1.81906900	-2.16933000
H	-4.70557400	-4.84758600	-0.46256900
H	-6.96322500	-4.06661300	-1.14315400
C	1.10649300	-0.69158800	-3.09854000
C	0.99314800	-0.41944600	-1.60000400
H	2.10470000	-1.01506200	-3.38980400
H	0.39482500	-1.47288400	-3.37461600
N	1.16335200	-1.62241700	-0.78920200
H	0.94685400	-1.48051800	0.19547300
S	2.44252700	-2.67980100	-0.90135900
O	2.44729400	-3.23668800	-2.24673800
O	2.27849300	-3.54591900	0.26184700
C	3.95867900	-1.77487000	-0.69817800
C	4.50368400	-1.64864000	0.57789300
C	5.63965100	-0.86933300	0.74998800
C	6.22676700	-0.19922800	-0.33065600
C	5.66991400	-0.35959400	-1.60210600
C	4.54090300	-1.15023300	-1.79652100
H	4.04535800	-2.16523400	1.41395600
H	6.07775300	-0.77221500	1.73945200

H	6.12932400	0.13299800	-2.45369500
H	4.13664000	-1.29836000	-2.79201800
C	7.42056600	0.69170600	-0.11585900
H	8.11914900	0.25048400	0.59889500
H	7.95004700	0.87856900	-1.05185100
H	7.10284100	1.65858700	0.28868100
C	1.93707600	0.71216900	-1.18725000
O	2.22494900	1.65187700	-1.88992900
O	2.35473200	0.58029600	0.08060100
C	3.18027500	1.62527100	0.60390100
H	3.88938500	1.96288800	-0.15356100
H	2.55361800	2.45798300	0.93751700
H	3.70524300	1.19010300	1.45323200

TS4A^{S2}

C	-2.64286800	4.18876700	0.15399000
C	-1.64364200	3.25434300	0.41850300
C	-0.73476400	3.43119600	1.45526900
C	-0.83775800	4.58289800	2.23256600
C	-1.83613800	5.52571700	1.97480000
C	-2.74818000	5.33478500	0.93736100
C	-3.48752100	3.74756600	-1.01763800
C	-2.65992600	2.63323500	-1.69404900
C	-1.71260000	2.10572000	-0.56445300
H	0.01321000	2.66858600	1.65344000
H	-0.13822500	4.74974600	3.04531900
H	-1.89977600	6.41948100	2.58755700
H	-3.51937700	6.07323200	0.73896300
H	-3.70155400	4.54529100	-1.73426400
H	-3.28572200	1.82547300	-2.07952500
H	-4.44774900	3.34725100	-0.67303500
H	-2.09712400	1.19864100	-0.09738400
N	-0.39450600	1.79066400	-1.11675700
O	-1.96129000	3.11735300	-2.83724800
C	0.48244700	0.79506900	-0.83551500
C	0.16955600	2.64765500	-2.02362500
N	1.54494900	1.13232400	-1.58692200
N	1.36994600	2.26863900	-2.33980800
C	-0.70448900	3.72305600	-2.58058600
H	-0.78885000	4.56707000	-1.88417200
H	-0.30805400	4.08045700	-3.53074000
C	2.79916800	0.43742700	-1.66506400
C	3.78677500	0.73696800	-0.71788900
C	2.99706100	-0.47679400	-2.70169500

C	4.96155400	-0.01054900	-0.75801500
C	4.19563300	-1.19533300	-2.70195600
C	5.17050700	-0.99865000	-1.72430600
H	5.72983100	0.18214300	-0.01279600
H	4.36488000	-1.92780700	-3.48775600
C	2.00902700	-0.62730900	-3.82628700
H	2.24287400	0.09307400	-4.61728800
H	0.98601600	-0.45279400	-3.49476100
C	3.62579200	1.86915900	0.26196900
H	2.60356500	1.94382200	0.63859400
H	3.87294600	2.81773100	-0.22683600
H	4.29671300	1.73489400	1.11352700
H	2.06099600	-1.63207000	-4.24889300
C	6.42281300	-1.83577400	-1.69575500
H	6.33399800	-2.62776800	-0.94419600
H	6.60625200	-2.31101500	-2.66152600
H	7.29533400	-1.23265700	-1.43308300
C	0.08314900	-0.32152200	0.78450500
O	-0.67679700	0.37788500	1.48409100
H	-0.25651300	-2.58624800	2.02707600
C	1.50606200	-0.54983500	1.22381900
C	1.92106600	-0.12247500	2.41886200
H	2.18358200	-1.04095300	0.53093400
H	1.19656600	0.40129300	3.04128200
C	3.29512700	-0.23519000	2.93084900
C	3.69810500	0.58861000	3.98966600
C	4.23598100	-1.11130800	2.36961200
C	5.00830800	0.56188600	4.45788300
H	2.97509600	1.26567900	4.43680000
C	5.54478200	-1.13891000	2.83708900
H	3.93851100	-1.78130300	1.56749200
C	5.93802700	-0.29891400	3.87906700
H	5.30327400	1.21250600	5.27494100
H	6.26057700	-1.82279900	2.39092600
H	6.96010900	-0.32335700	4.24282300
C	-1.08864500	-2.42141200	1.34018900
C	-0.58915000	-1.61148700	0.14165800
H	-1.85899900	-1.84200500	1.85068700
H	-1.48327000	-3.39224200	1.03559100
N	-1.68489300	-1.14858300	-0.71617400
H	-1.30523300	-0.72354800	-1.56547500
S	-2.82399700	-2.24736000	-1.26128100
O	-2.28227300	-3.60122700	-1.36401200
O	-3.38354400	-1.61250900	-2.45318600

C	-4.03099000	-2.24470400	0.03680600
C	-4.47084900	-3.45847600	0.54799000
C	-5.44747300	-3.45280100	1.54039300
C	-5.97847500	-2.25410900	2.02019200
C	-5.51633200	-1.04565000	1.47992500
C	-4.54720800	-1.03095900	0.48847000
H	-4.04633700	-4.38554800	0.17790300
H	-5.79929200	-4.39520400	1.94902500
H	-5.92204800	-0.10752400	1.84733400
H	-4.18447100	-0.09486500	0.07608600
C	-7.01699400	-2.24470300	3.10979200
H	-7.86250500	-1.60791800	2.83668300
H	-7.39161400	-3.25007100	3.31004000
H	-6.59539800	-1.84777200	4.03826800
C	0.40310800	-2.38730200	-0.71725000
O	0.52297000	-2.21519700	-1.90944300
O	1.15834800	-3.23075600	-0.01414300
C	2.20573500	-3.87042600	-0.75527500
H	1.78571900	-4.43396600	-1.58965500
H	2.90034800	-3.11769200	-1.14022300
H	2.70320100	-4.53398500	-0.05124800
pS2			
C	1.27502600	1.22565200	0.39409400
O	1.25453500	2.43797700	0.30007900
H	0.24323600	1.04881000	2.78170400
C	2.49154500	0.40371500	0.26459300
C	3.66370000	1.00412600	-0.00352000
H	2.38735600	-0.66875200	0.38574300
H	3.64502100	2.08776800	-0.11808100
C	4.96884000	0.36199400	-0.16327700
C	6.07878100	1.16514800	-0.45844600
C	5.15144200	-1.02367800	-0.03436900
C	7.34026800	0.60237500	-0.62287700
H	5.94423400	2.23857300	-0.55949700
C	6.41008900	-1.58459700	-0.19850300
H	4.30734000	-1.66550000	0.19633900
C	7.50767300	-0.77365500	-0.49337900
H	8.19009200	1.23642400	-0.85261600
H	6.53954700	-2.65697500	-0.09630500
H	8.49010500	-1.21643300	-0.62116400
C	0.02559800	0.13448100	2.22755400
C	-0.03904100	0.47693800	0.73704600
H	-0.92226000	-0.26652600	2.58506700

H	0.80816100	-0.60430400	2.40685500
N	-0.09867500	-0.70569300	-0.13048100
H	-0.03150600	-0.46689200	-1.11934500
S	-1.25659900	-1.90089400	0.03651200
O	-1.14095700	-2.43965700	1.38271300
O	-1.04892000	-2.74927500	-1.12892400
C	-2.85517700	-1.14508500	-0.11396100
C	-3.38216600	-0.93530000	-1.38890600
C	-4.62525100	-0.33121900	-1.50772000
C	-5.34346800	0.07416300	-0.37404100
C	-4.78891700	-0.14714400	0.88861900
C	-3.54522000	-0.75775600	1.02944900
H	-2.83037800	-1.25856900	-2.26563600
H	-5.05194800	-0.17352500	-2.49409000
H	-5.33930000	0.15214800	1.77520100
H	-3.12933800	-0.95335200	2.01233700
C	-6.67543800	0.75851100	-0.52570600
H	-7.27082700	0.28816200	-1.31177000
H	-7.24344800	0.73319300	0.40583600
H	-6.53277000	1.80790900	-0.80410400
C	-1.18355200	1.46466500	0.46858400
O	-1.77382400	2.07524800	1.32309600
O	-1.42733600	1.56257300	-0.83869300
C	-2.48839600	2.45780800	-1.19439500
H	-3.39055700	2.19977500	-0.63648900
H	-2.19734700	3.48533100	-0.96923300
H	-2.64508700	2.32512200	-2.26277300

PA^{S2}

C	1.14983300	0.02719900	-1.02166100
O	1.04747900	0.27936700	-2.20535500
H	0.46105700	0.52053800	1.60192100
C	2.40224300	0.17004200	-0.25568000
C	3.48053000	0.70887200	-0.84900400
H	2.41271700	-0.17850000	0.77205700
H	3.36230200	1.02170700	-1.88616900
C	4.80136600	0.92715600	-0.25899700
C	5.80027100	1.49838100	-1.05868100
C	5.10804500	0.58961300	1.06873100
C	7.07464600	1.72707500	-0.55096100
H	5.56907600	1.76185900	-2.08699700
C	6.37960600	0.81829500	1.57495700
H	4.35059600	0.14836000	1.70882000
C	7.36632200	1.38700000	0.76727500

H	7.83754300	2.16925200	-1.18291500
H	6.60583300	0.55436200	2.60277500
H	8.35908200	1.56319800	1.16847800
C	-0.40105500	0.40354000	0.94605600
C	-0.07471100	-0.51071200	-0.23700700
H	-0.70469100	1.38166400	0.56672400
H	-1.21465400	-0.02266200	1.53654400
N	-1.17816200	-0.55367300	-1.18564800
H	-0.90641800	-0.88423400	-2.10992900
S	-2.61590000	-1.24186000	-0.71382200
O	-2.40707400	-2.11657000	0.43886900
O	-3.20929000	-1.77135400	-1.93659700
C	-3.56920900	0.14453700	-0.15200900
C	-4.20340100	0.07246200	1.08148400
C	-4.99054800	1.14493800	1.49368800
C	-5.14638000	2.27447900	0.68870700
C	-4.49663900	2.31409500	-0.55288400
C	-3.70951500	1.25606500	-0.98202900
H	-4.07505200	-0.80551600	1.70539700
H	-5.49082500	1.10069200	2.45638400
H	-4.61122000	3.18827900	-1.18740100
H	-3.19982700	1.29223200	-1.93977900
C	-5.98065900	3.44222000	1.14364100
H	-6.65088900	3.77686500	0.34776300
H	-6.58155100	3.18321300	2.01718700
H	-5.34180700	4.28961400	1.41096800
C	0.32615100	-1.94417200	0.17068800
O	0.36606900	-2.85146300	-0.62330000
O	0.68277300	-2.03704500	1.44819400
C	1.09752200	-3.34559700	1.86833000
H	0.28486400	-4.05680800	1.71462000
H	1.97184200	-3.66083600	1.29694900
H	1.33740900	-3.25421600	2.92492800

