

Supporting Information

**A Computational Study of NHC-Catalyzed [3 + 3] annulation of enals with
pyrazol-5-amines: Mechanism, Regio- and Stereoselectivities**

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Contents:

1. Computational Details	S2
2. Test calculations of stereoselective transition states	S3
3. Generation of the active NHC.....	S4
4. Generation of R2.....	S5
5. Other Possible Reaction Pathways	S6
6. Conformational Search	S11
7. RR/RS/SS-Configurational Reaction Pathways.....	S12
8. Transformation Pathways of 1,2-Addition Intermediate.....	S13
9. Possible Reaction Pathways for the Transformation of M3.	S14
10. Reaction Pathways for the Transformation of M4SR→M6S.	S15
11. Cartesian coordinates of all the stationary points	S17

1. Computational Details:

(1) Calculation of enantiomeric excess (ee)

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

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

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

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

(2) Global reactivity indexes (GRI) analysis

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

2. Test calculations of stereoselective transition states.

Table S1. Different computational levels.

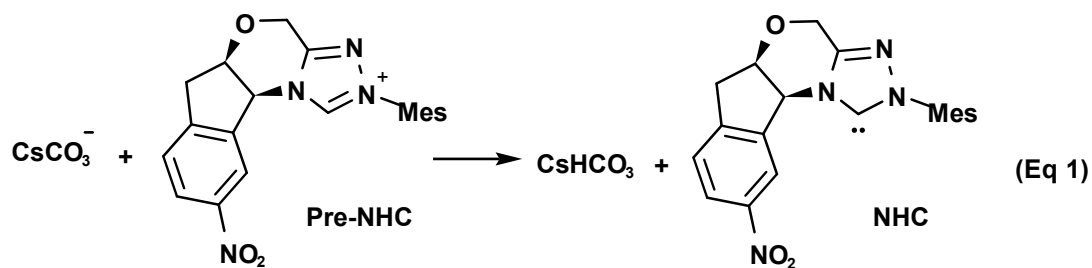
Level	Functional	Basis set	Solvent model
L1	M06-2X-D3	6-311++G(2df,2pd)	IEFPCM
L2	ω B97X-D	6-311++G(2df,2pd)	IEFPCM
L3	M06-2X-D3	6-311++G(2df,2pd)	SMD
L4	M06-2X-D3	def2-TZVP	IEFPCM
L5	M06-2X-D3	def2-QZVP	IEFPCM

Table S2. Comparison of relative energies for stereoselective transition states at different levels. Energies are given in kcal/mol.

species	L1	L2	L3	L4	L5
TS4RR	2.6	3.5	2.6	3.4	3.4
TS4SR	0.0	0.0	0.0	0.0	0.0

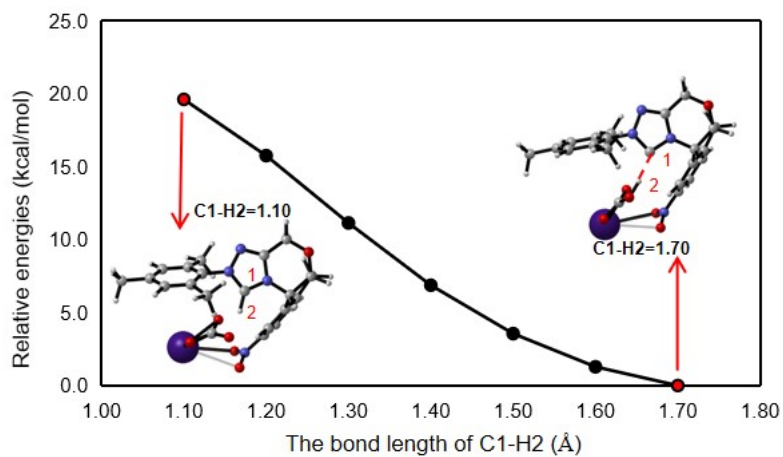
It should be noted that only the transition state associated with the most feasible pathway towards R- and S-configurational product were considered. In addition, the single-point energies of L1/L3/L4/L5 were based on the geometries optimized at IEF-PCM(THF)M06-2X/6-31G(d,p) level, and the single-point energies of L2 were based on the geometries optimized at IEF-PCM(THF) ω B97X-D/6-31G(d,p) level.

3. Generation of the active NHC.



The deprotonation of **Pre-NHC** by CsCO_3^- (derived from Cs_2CO_3) generates the active **NHC** (Eq 1). However, we can not locate the transition state despite of lots of attempts. We scanned the changes of C–H bond. Fig. S1 shows that with the aid of CsCO_3^- , formation of the active catalyst **NHC** is barrierless.

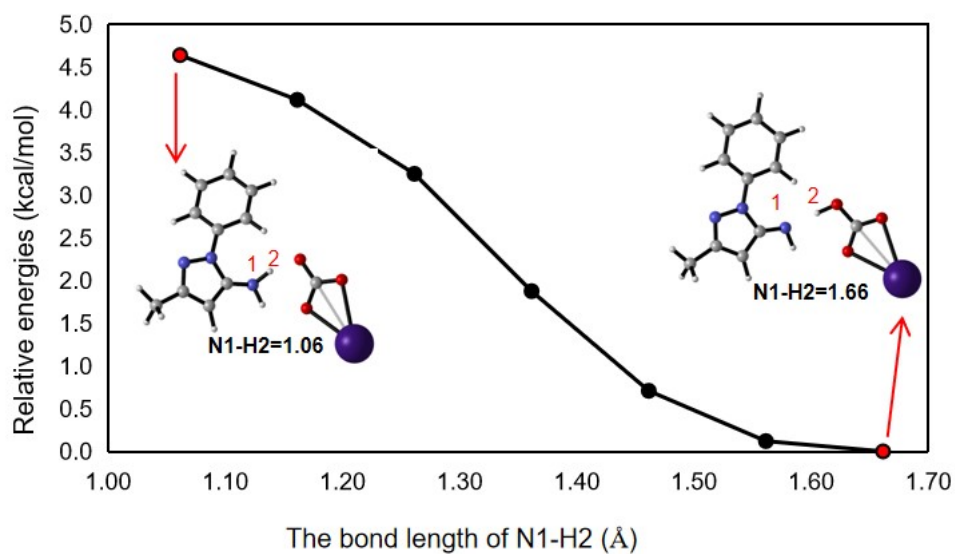
Fig. S1 The deprotonation of NHC precursor by base CsCO_3^- . Bond distances are in Å.



4. Generation of R2.

The **Pre-R2** was deprotonated by the base (CsCO_3^-) to generate the real reactant **R2**. However, we cannot locate the transition state despite lots of attempts. We scanned the changes of N–H bond. Fig.S2 shows that this process has no energy barrier.

Fig. S2 The deprotonation of Pre-R2 by base (CsCO_3^-) generating R2. Distances in Å.



5. Other Possible Reaction Pathways.

Fig. S3 Free energy (kcal/mol) profile of steps 1 and 2. Energies are in kcal/mol.

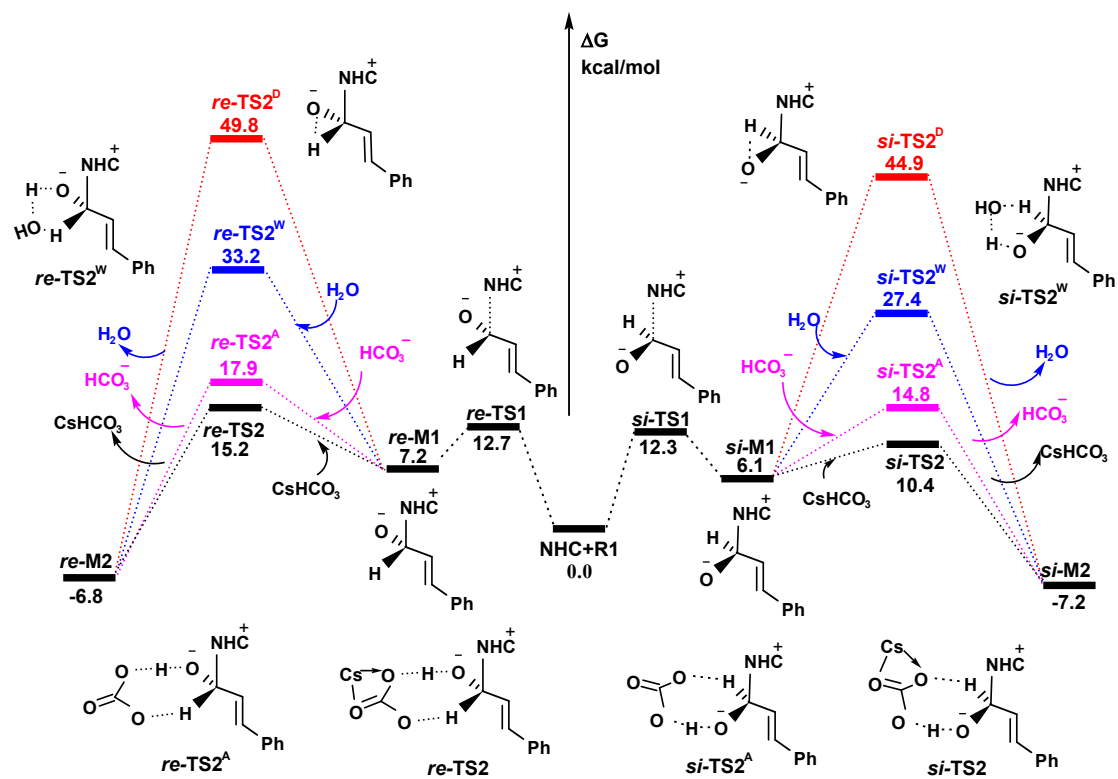


Fig. S4 (a) Optimized geometries of key transition states (distance in Å).

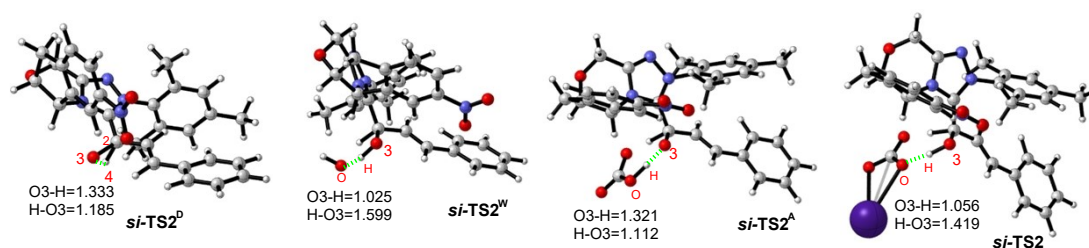
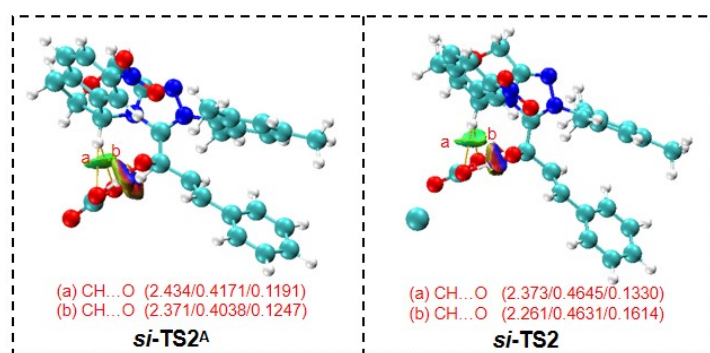


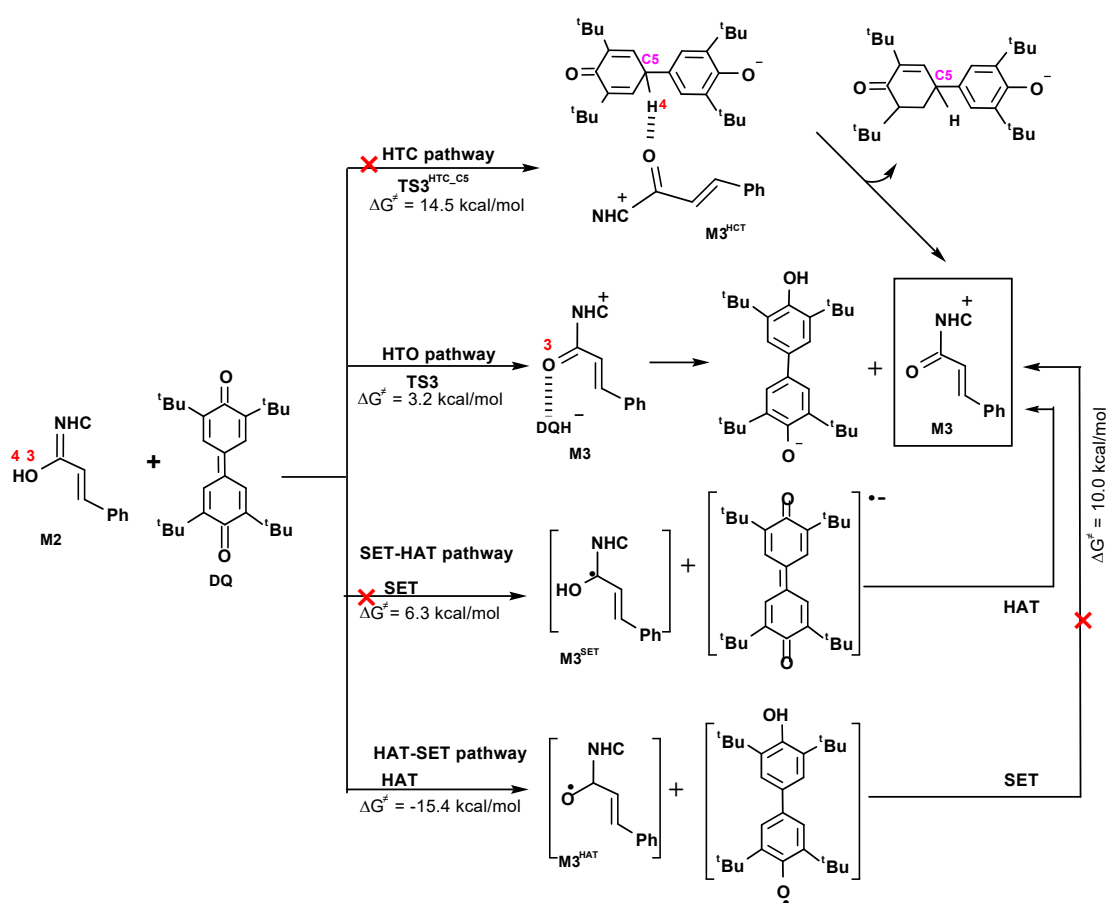
Fig. S4 (b) NCI and AIM analyses for *si-TS2^A* and *si-TS2*. The values in parentheses are distances, Laplacian of electron densities ($\nabla^2\rho$) and electron densities (ρ_{bcp}), which are given in Å, 10^{-1} a.u. and 10^{-1} a.u., respectively.



To better understand how CsHCO_3 facilitates proton transfer, we examined the transition states of the direct, water, HCO_3^- and CsHCO_3 mediated proton transfer mechanisms. As shown in Fig.S4a, *si-TS2^D* features a three-membered ring, and the significant strain account for its high energy barrier. For *si-TS2^W*, *si-TS2^A*, and *si-TS2*, each structure exhibits an hydrogen bond $\text{O3-H}\cdots\text{O}$. The O3-H and H-O distances are 1.025/1.599 Å in *si-TS2^W*, 1.321/1.112 Å in *si-TS2^A*, 1.056/1.419 Å in *si-TS2*. The O3-H-O angles are 143.48, 176.68 and 172.84° in *si-TS2^W*, *si-TS2^A*, and *si-TS2*, respectively. This result indicates that the hydrogen bond in *si-TS2^W* is weaker than those in *si-TS2^A* and *si-TS2*, while the hydrogen bond in *si-TS2^A* and *si-TS2* are comparable. Moreover, NCI and AIM analyses (Fig. S4b) revealed stronger interactions in *si-TS2* than in *si-TS2^A*. Taken together, the stronger hydrogen bond interactions should be the main reason for the lower energy of *si-TS2* compared to *si-TS2^D*, *si-TS2^W* and *si-TS2^A*.

Scheme S1 Possible Oxidation Pathways.

In addition to the HTO pathway (Fig. 1), we also investigated the hydride transfer to the carbon (HTC), hydrogen atom transfer–single electron transfer (HAT–SET) and single electron transfer–hydrogen atom transfer (SET–HAT) pathways (Scheme S1). The calculated energy barriers for HTC, HAT-SET and SET-HAT mechanisms are 14.5, 10.0 and 6.3 kcal/mol, respectively, which are higher the 3.2 kcal/mol for HTO pathway. Obviously, the most energetically favored oxidation pathway is the HTO pathway via **TS3**.



Scheme S2 Possible HTC Reaction Pathways.

As presented in Scheme S2, four possible HTC pathways corresponding to the hydride H4 transfers from the O3 atom to four different types of carbon atoms (C2, C3, C4 and C5) of DQ have been investigated. The energy barriers are calculated to be 26.5 ($\text{TS3}^{\text{HTC-C2}}$), 17.7 ($\text{TS3}^{\text{HTC-C3}}$), 21.8 ($\text{TS3}^{\text{HTC-C4}}$) and 14.5 ($\text{TS3}^{\text{HTC-C5}}$), which are much higher than the HTO pathway (TS3 , 3.2 kcal/mol). Therefore, the HTC pathways can be ruled out.

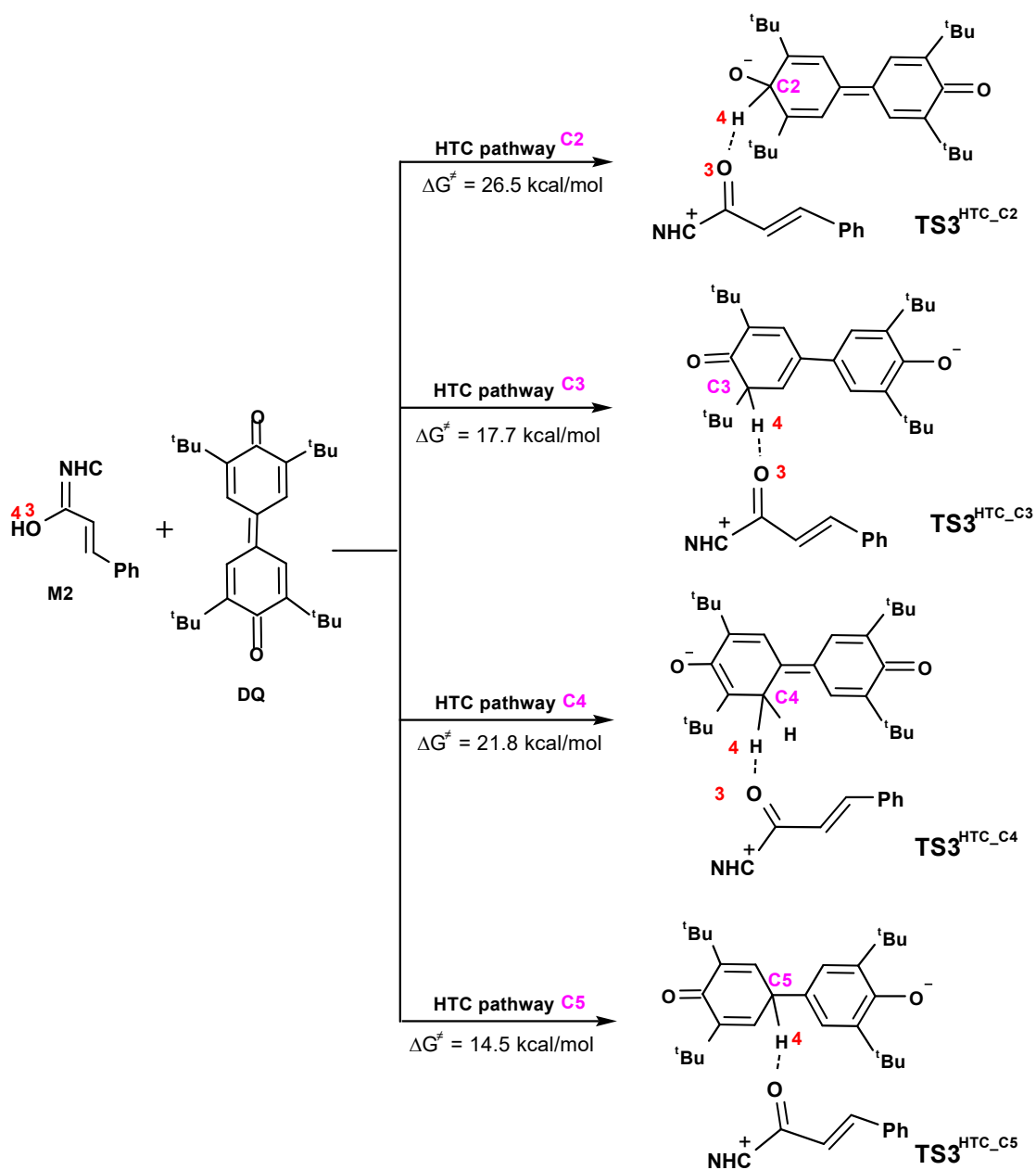
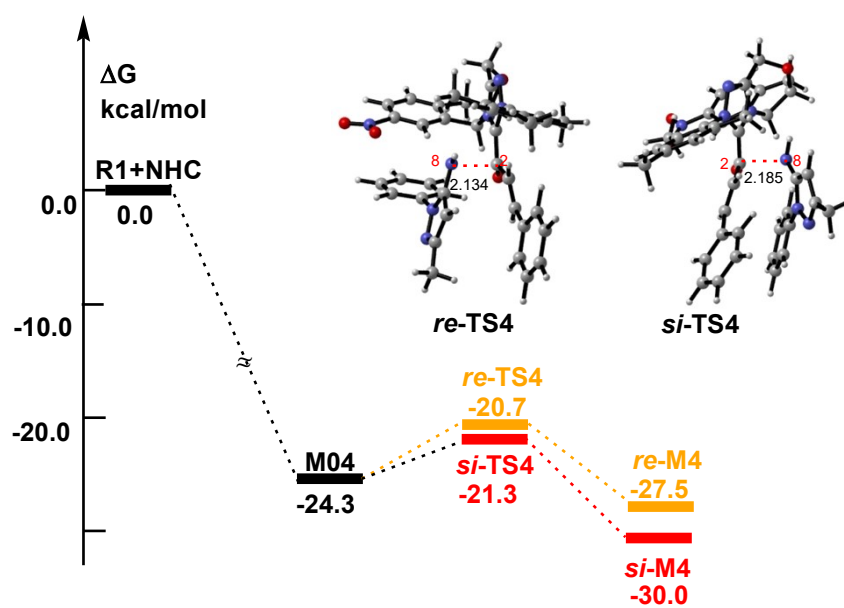
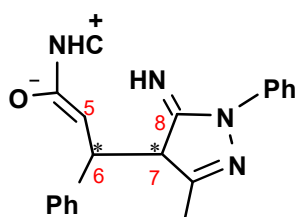


Fig. S5 Free energy profile for 1,2-addition mechanism. Energies and bond distances are in kcal/mol and Å, respectively.



6. Conformational Search.

Table S3. Energies of different conformations of TS4s.

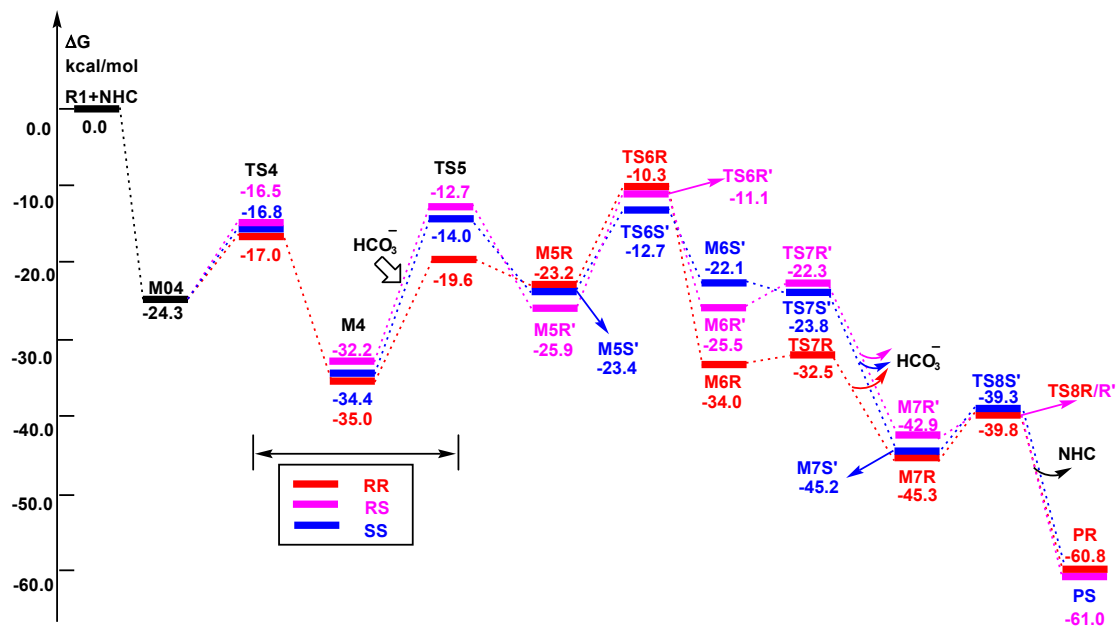


TS4

species	Dihedral angle C5-C6-C7-C8	Free energies (a.u.)	Relative energies (kcal/mol)
TS4RR	23.86	-2229.749814	2.6
TS4RR'	-6.81	-2229.747016	4.3
TS4RR''	-93.48	-2229.749184	3.0
TS4RR'''	170.65	-2229.734722	12.0
TS4RS	-48.65	-2229.749034	3.1
TS4RS'	-158.93	-2229.740718	8.3
TS4RS''	63.01	-2229.745153	5.3
TS4RS'''	175.56	-2229.728919	15.7
TS4SR	127.13	-2229.753939	0.0
TS4SR'	33.01	-2229.75019	2.3
TS4SR''	-68.90	-2229.744921	5.6
TS4SR'''	163.81	-2229.745378	5.4
TS4SS	-81.32	-2229.749388	2.8
TS4SS'	-179.84	-2229.731383	14.1
TS4SS''	88.28	-2229.734993	11.9
TS4SS'''	-21.41	-2229.746111	4.9

7. RR/RS/SS-Configurational Reaction Pathways

Fig. S6 Free energy profiles of RR/RS/SS-configurational pathways. Energies are in kcal/mol.



8. Transformation Pathways of 1,2-Addition Intermediate.

In this work, we investigated the reaction pathways starting from *re/si*-M4. To form the six-membered ring product, *re/si*-M4 should undergo proton transfer (from C7 to C5). However, for both direct and mediator assisted proton transfer, we can not locate the transition state despite of lots of attempts. The flexible potential energy scan shown in Fig. S7 indicates that the energy barrier keeps increasing with the proton transferring to C5. The corresponding energy barrier is estimated to be not lower than 76 kcal/mol for direct mechanism (Figs. S7a and S7b) or 37 kcal/mol for HCO_3^- assisted mechanism (Figs. S7c and S7d). Therefore, the 1,2-addition pathway can be ruled out safely.

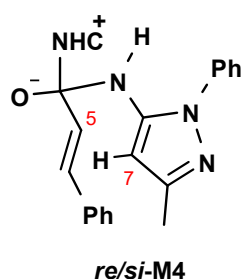
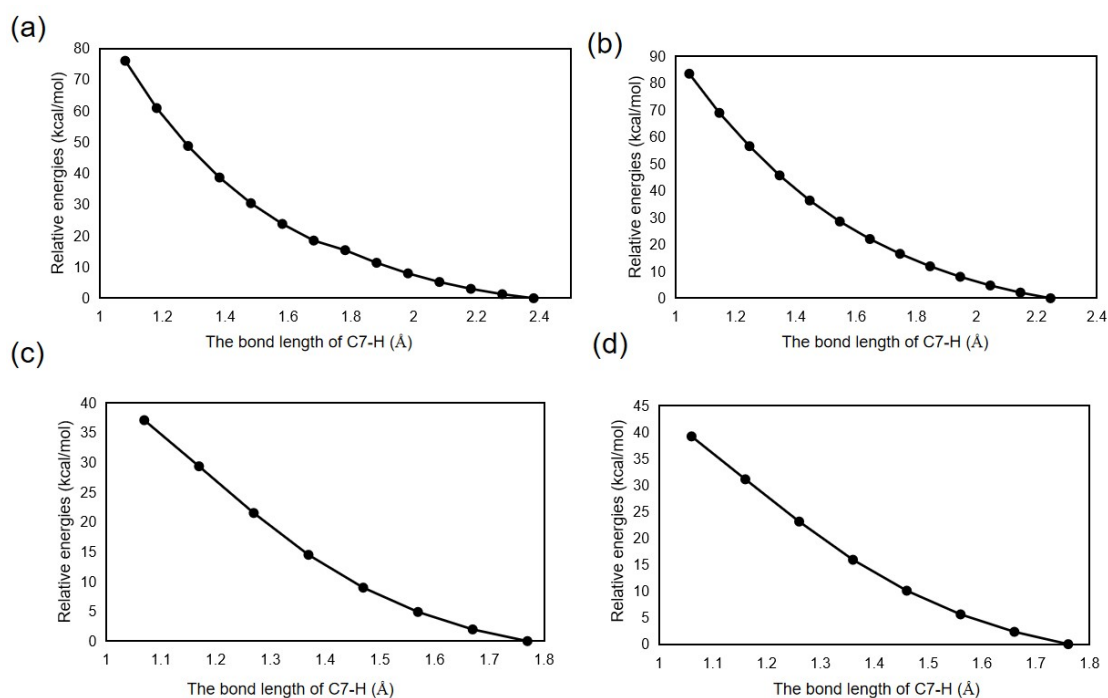
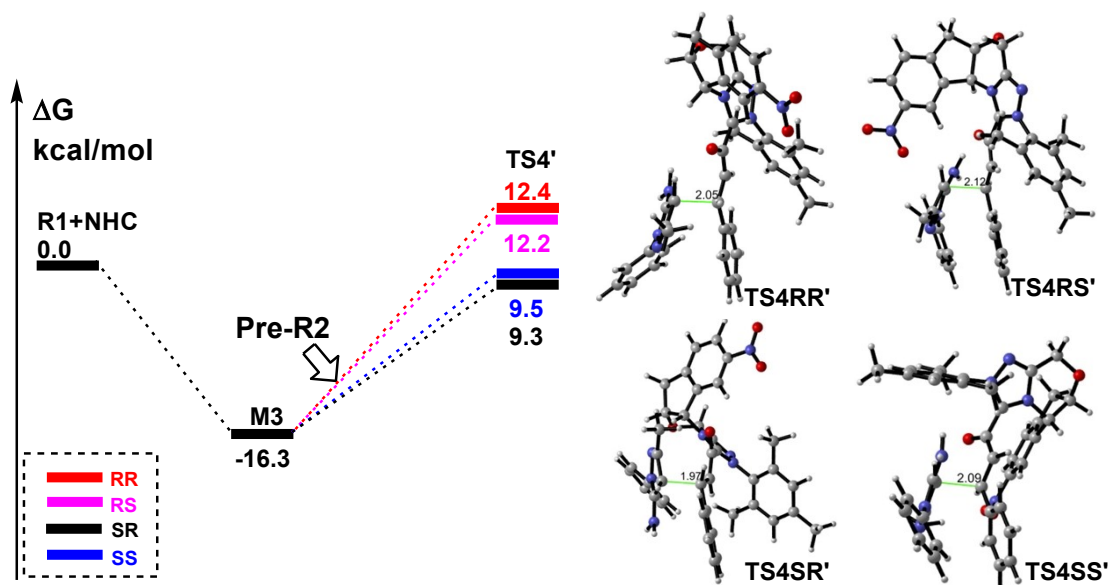


Fig. S7 (a) and (b) Energy change along proton transfer in *re*-M4 and *si*-M4, (c) and (d) Energy change along proton transfer in *re*-M4 and *si*-M4 in the presence of HCO_3^- .



9. Possible Reaction Pathways for the Transformation of M3.

Fig. S8 Free energy profile for the reaction of **M3** and **Pre-R2**. Energies and bond distances are in kcal/mol and Å, respectively.



10. Reaction Pathways for the Transformation of M4SR→M6S.

Scheme S3. Proposed pathways for the transformation of M4SR to M6S.

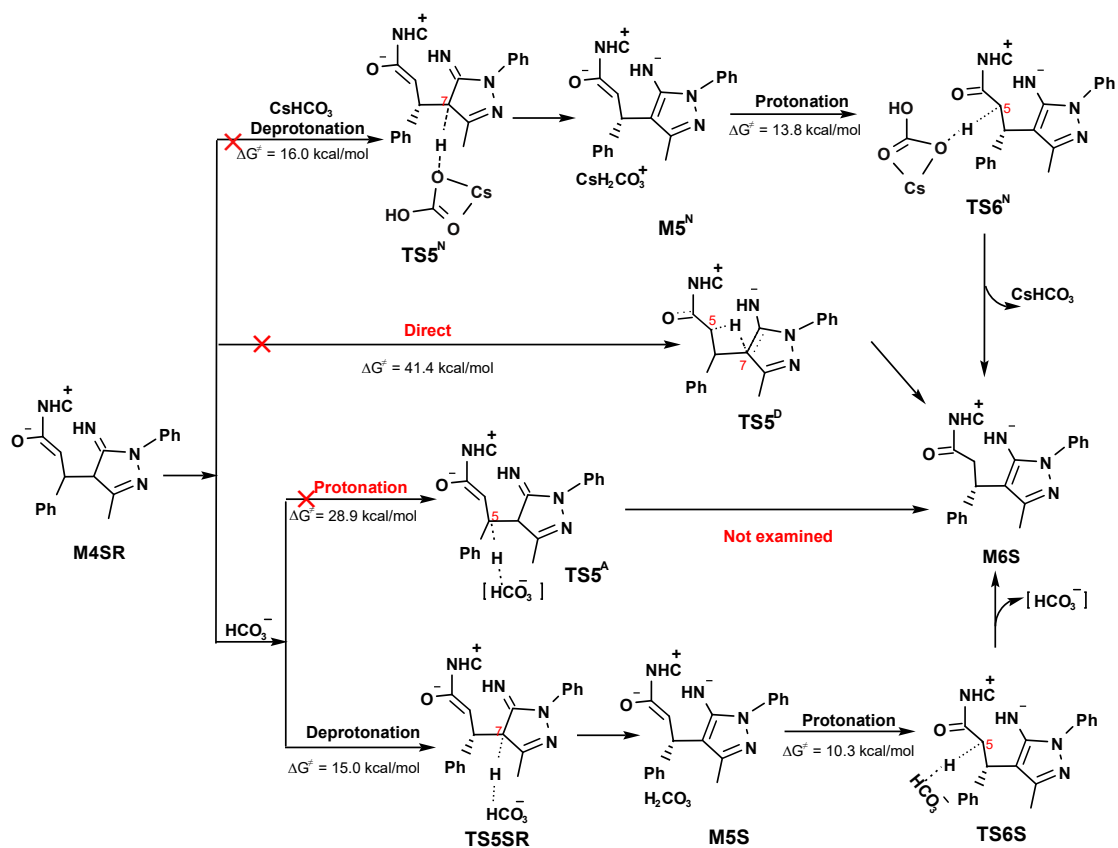
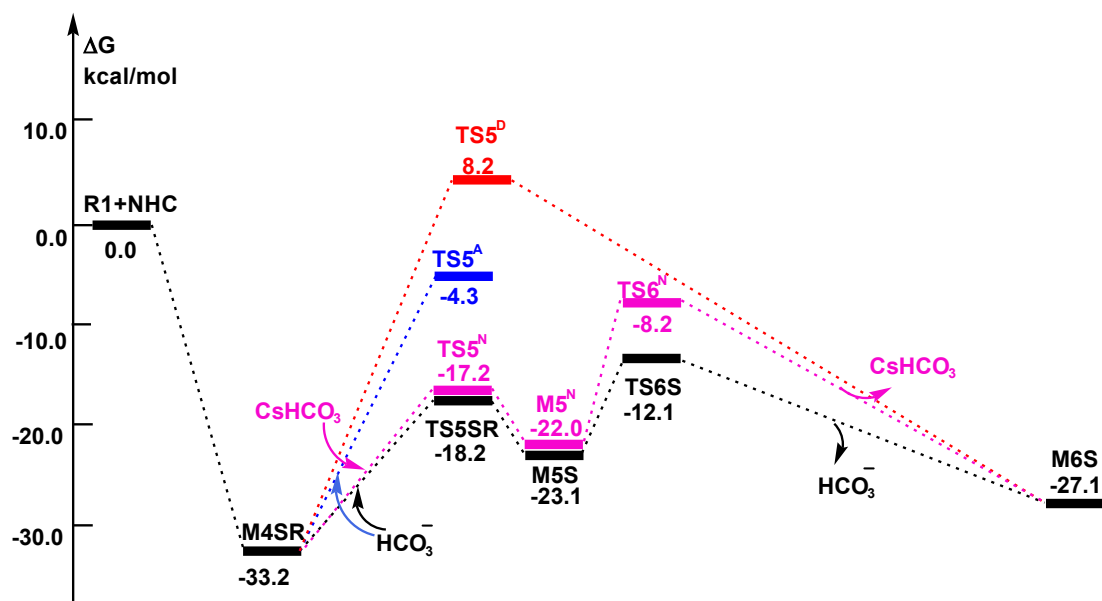


Fig. S9 Free energy (kcal/mol) profile for the transformation of **M4SR**→**M6S**. Energies are in kcal/mol.



11. Cartesian coordinates of all the stationary points

NHC

C	-0.48247100	-0.27936600	-0.65665100
C	-0.34335100	-2.25859500	0.42798900
C	1.67241500	-1.56104700	-0.87828500
H	1.61066800	-1.69464300	-1.96046700
N	-1.54105500	-1.83710200	0.69531100
N	-1.59143100	-0.62978000	0.02452000
N	0.31739200	-1.35633500	-0.36520700
C	0.30917300	-3.52591300	0.88715500
H	-0.39615000	-4.35520200	0.81755700
H	0.62011700	-3.43262800	1.93566800
C	2.30929100	-2.78601000	-0.17123800
O	1.40501100	-3.84473800	0.05034300
C	3.37100600	-0.81768200	0.63319300
C	2.59752600	-0.44126800	-0.46984300
C	2.71707100	0.81490400	-1.04269000
C	3.65120500	1.67458800	-0.47556800
C	4.44226800	1.32827200	0.61679100
C	4.29982700	0.06450100	1.17912900
C	3.02257700	-2.21435600	1.07561800
H	2.11377600	1.12571200	-1.88645900
H	5.15374500	2.04458400	1.00759400
H	4.90765500	-0.22321200	2.03022900
H	2.34991200	-2.16784900	1.94022500
H	3.88976500	-2.81080700	1.36531900
C	-2.80323400	0.13091900	0.08241900
C	-3.11024200	0.81561400	1.26013800
C	-3.64317000	0.14508000	-1.03481300
C	-4.30334400	1.53745700	1.30103800
C	-4.82261600	0.88308600	-0.95021600
C	-5.16756300	1.58466900	0.20688000
H	-4.56056800	2.07809700	2.20878100
H	-5.49122400	0.90584100	-1.80763100
C	-3.27774300	-0.61650700	-2.28092200
H	-3.09169100	-1.67051700	-2.05192700
H	-2.35979600	-0.21801800	-2.72176500
H	-4.07917800	-0.55592700	-3.01913300
C	-2.17260600	0.77110300	2.43692000
H	-1.16031200	1.05676100	2.13445200
H	-2.11154500	-0.23999800	2.84977600
H	-2.50666400	1.44966100	3.22353500

H	3.06538900	-3.19223600	-0.84713200
C	-6.43593900	2.39749100	0.25891200
H	-6.28557300	3.37904600	-0.20223400
H	-7.24499500	1.90130100	-0.28269900
H	-6.75953900	2.56121300	1.28920800
N	3.81569000	3.01035300	-1.06015400
O	4.62309800	3.76496400	-0.54517600
O	3.13718400	3.29461800	-2.03172800
H₂O			
O	0.02432200	0.00000000	0.01729100
H	0.06782100	0.00000000	0.97925400
H	0.94792700	0.00000000	-0.25467000
HCO₃⁻			
H	-8.97724900	6.49895100	-3.08667300
C	-8.26864100	5.05384900	-2.09480900
O	-7.33382700	4.70823500	-1.35643200
O	-9.26098800	4.42181000	-2.51378900
O	-8.19298100	6.39160000	-2.53494200
DQ			
C	2.80615900	1.28442700	-0.00551300
C	1.45878900	1.23643000	-0.08185700
C	0.69369700	0.00067300	-0.09319500
C	1.46107600	-1.23370400	-0.09001300
C	2.80853100	-1.27975200	-0.01413000
C	3.56682400	0.00270400	0.08861200
H	0.91799900	2.16916000	-0.13410600
H	0.92224700	-2.16694400	-0.15253100
C	-0.69365400	-0.00054100	-0.09309500
C	-1.45874500	-1.23629500	-0.08142000
C	-1.46102900	1.23383800	-0.09002500
C	-2.80610800	-1.28427700	-0.00494500
H	-0.91795600	-2.16903600	-0.13350800
C	-2.80847800	1.27990200	-0.01403500
H	-0.92220500	2.16706800	-0.15272000
C	-3.56676800	-0.00253500	0.08896400
O	4.78453300	0.00333600	0.24291600
O	-4.78447200	-0.00313800	0.24331000
C	3.58611400	-2.59579600	-0.01528200
C	4.58459300	-2.61321700	-1.18859600
C	4.33904900	-2.76187700	1.31854900
C	2.65274900	-3.80107900	-0.17948100
H	4.05904700	-2.49999000	-2.14237100
H	5.32250800	-1.81680300	-1.09570100
H	5.10873000	-3.57446600	-1.20329000

H	3.63614500	-2.76074300	2.15785300
H	4.86591700	-3.72193000	1.31928300
H	5.06687200	-1.96477400	1.46656200
H	3.25231200	-4.71541600	-0.19200600
H	1.94115900	-3.88299700	0.64877900
H	2.09216800	-3.75605300	-1.11903900
C	3.58133400	2.60187600	0.00331200
C	4.33310900	2.75996100	1.33873700
C	4.58059300	2.62923200	-1.16919700
C	2.64582900	3.80656700	-0.15308600
H	3.62977400	2.75070900	2.17763500
H	5.06291500	1.96366700	1.48120200
H	4.85750400	3.72133500	1.34702600
H	4.05582900	2.52206800	-2.12410600
H	5.10332600	3.59132800	-1.17658200
H	5.31952500	1.83315900	-1.08138500
H	3.24383100	4.72198200	-0.16021400
H	2.08485700	3.76634600	-1.09262900
H	1.93454800	3.88213500	0.67602800
C	-3.58605300	2.59595000	-0.01533400
C	-4.33893300	2.76222400	1.31850400
C	-2.65269200	3.80120600	-0.17974400
C	-4.58457900	2.61321100	-1.18861100
H	-5.06674300	1.96513700	1.46666700
H	-3.63599200	2.76122100	2.15777900
H	-4.86580800	3.72227300	1.31911600
H	-2.09216900	3.75605500	-1.11933100
H	-3.25225000	4.71554500	-0.19235200
H	-1.94104800	3.88322900	0.64846000
H	-5.10870300	3.57446500	-1.20342600
H	-4.05907200	2.49983700	-2.14239000
H	-5.32250200	1.81682300	-1.09557200
C	-3.58128100	-2.60172600	0.00423700
C	-4.33295300	-2.75950100	1.33975700
C	-4.58062800	-2.62935600	-1.16818900
C	-2.64578500	-3.80645100	-0.15194800
H	-3.62955800	-2.75002000	2.17860100
H	-5.06277200	-1.96319200	1.48207900
H	-4.85732200	-3.72088800	1.34832600
H	-4.05593500	-2.52241700	-2.12316200
H	-5.10336500	-3.59145200	-1.17530600
H	-5.31954900	-1.83325700	-1.08050600
H	-3.24378700	-4.72186800	-0.15883200
H	-2.08486900	-3.76644400	-1.09153300

H	-1.93445400	-3.88183200	0.67714100
[DQH]-			
H	-5.27959300	0.75364900	-0.19655600
C	-2.85518300	1.16459400	-0.31678800
C	-1.45877700	1.13450500	-0.32280200
C	-0.71955700	-0.00762500	-0.00028900
C	-1.44257000	-1.16209700	0.32436900
C	-2.83590300	-1.21310100	0.32775000
C	-3.53093600	-0.02860900	0.00965800
H	-0.91071800	2.02397200	-0.60733000
H	-0.88062300	-2.04461600	0.60415000
C	0.75874000	0.00306900	-0.00062400
C	1.50134200	-1.14471100	-0.31387100
C	1.48409100	1.16095400	0.31543300
C	2.88874700	-1.17444100	-0.31982700
H	0.95152100	-2.04005700	-0.59049800
C	2.87089400	1.20998100	0.32730400
H	0.92095800	2.04829100	0.59128100
C	3.64317500	0.02288800	0.00604700
O	-4.90536100	-0.09984600	0.03577200
O	4.92214200	0.03153700	0.01060700
C	-3.58102400	-2.51189500	0.67795600
C	-4.45387500	-2.31396900	1.93055900
C	-4.45254200	-2.96181800	-0.50970500
C	-2.60806900	-3.65948600	0.98327100
H	-3.83320100	-2.01658100	2.78211900
H	-5.21766700	-1.55269700	1.77455600
H	-4.94998400	-3.25706300	2.18664400
H	-3.82790100	-3.13980300	-1.39135800
H	-4.96057900	-3.90023900	-0.26011600
H	-5.20628900	-2.21597200	-0.76192900
H	-3.18409200	-4.56118200	1.21300700
H	-1.96071300	-3.88393400	0.12960200
H	-1.97537300	-3.43798500	1.84833500
C	-3.61507800	2.45707700	-0.66995600
C	-4.47747000	2.26053600	-1.93572100
C	-4.46498700	2.93262800	0.52909600
C	-2.65633300	3.61359200	-0.99055500
H	-3.83147200	2.02043900	-2.78513200
H	-5.21717900	1.45803000	-1.86896700
H	-5.01649900	3.18522300	-2.16574800
H	-3.80841800	3.17334200	1.37025500
H	-5.01975300	3.83661500	0.25788300

H	-5.18823600	2.20028500	0.89786500
H	-3.24221000	4.50800200	-1.22297400
H	-2.00715600	3.84771900	-0.14189900
H	-2.02828600	3.38907900	-1.85723600
C	3.61382600	2.50199300	0.68975900
C	4.50428800	2.93866600	-0.48781900
C	2.66178000	3.66303200	1.00191400
C	4.48813800	2.27279700	1.93526300
H	5.19714300	2.13666200	-0.74285800
H	3.88699300	3.16951500	-1.36365100
H	5.07044100	3.84119600	-0.22453200
H	2.01948600	3.44322900	1.86154900
H	3.24754700	4.55699600	1.24286200
H	2.01913000	3.90399800	0.14796000
H	5.05327400	3.18131100	2.17914700
H	3.86005500	2.02262000	2.79788900
H	5.18142300	1.45191000	1.75272700
C	3.65132900	-2.45727200	-0.67440000
C	4.53742900	-2.21772900	-1.90953000
C	4.53373200	-2.88182300	0.51366700
C	2.71725600	-3.63015200	-0.99665500
H	3.91700300	-1.96914700	-2.77811800
H	5.22263100	-1.39242100	-1.71642800
H	5.11150500	-3.12150200	-2.15005300
H	3.90934400	-3.12320000	1.38156600
H	5.11705400	-3.77509400	0.25636400
H	5.21076400	-2.06926500	0.77774300
H	3.31675800	-4.51646400	-1.23210000
H	2.06934200	-3.87983200	-0.14926400
H	2.08068100	-3.41816300	-1.86254600
R1			
C	-6.07044700	-0.23417000	-1.58469100
C	-4.68844500	-0.13477700	-1.66528100
C	-4.04379600	1.07678900	-1.37183700
C	-4.82235200	2.18068900	-0.99897700
C	-6.20739800	2.08110200	-0.91754500
C	-6.83421700	0.87294800	-1.21023300
H	-6.55733100	-1.17638700	-1.81387500
H	-4.10723700	-1.00291400	-1.95931500
H	-4.33049100	3.12248200	-0.77197200
H	-6.79569100	2.94509700	-0.62691100
H	-7.91451200	0.79083900	-1.14810700
C	-2.58965300	1.23667800	-1.43947000
H	-2.20633200	2.23071500	-1.20860200

C	-1.67736300	0.30120700	-1.75033200
C	-0.24369000	0.64575900	-1.76820700
H	0.44172700	-0.18165300	-2.03204300
O	0.19979200	1.75004300	-1.51726900
H	-1.94192600	-0.72309600	-1.99438500

Pre-R2

C	4.01729700	-1.31731600	5.67665100
C	2.69138400	-0.97724100	5.31503200
C	2.66304900	-1.08512400	3.93803200
N	3.90938600	-1.48451700	3.55350100
H	1.87797100	-0.67876000	5.95821900
N	4.75465500	-1.61803200	4.62057200
C	4.39529700	-1.68651800	2.23727400
C	3.70541300	-2.51374200	1.35116600
C	5.58151000	-1.06504500	1.84833100
C	4.18600700	-2.68530100	0.05524700
H	2.81959500	-3.04631500	1.68566900
C	6.06516300	-1.26098700	0.55970700
H	6.10643700	-0.44067300	2.56261400
C	5.36444400	-2.06026200	-0.34288300
H	3.64661800	-3.32578500	-0.63463200
H	6.98878400	-0.77932700	0.25580800
H	5.74222700	-2.20205000	-1.34981600
N	1.67612200	-0.73617200	3.03069500
H	0.75314300	-0.72845300	3.44269900
C	4.60581700	-1.36970700	7.05133500
H	4.08510300	-2.10202800	7.67455100
H	5.65938800	-1.64762100	6.99359000
H	4.52613600	-0.39867500	7.54784200
H	1.68375700	-1.24675200	2.15835400

R2

C	3.79547500	-0.96708800	5.94248900
C	2.46242600	-1.17471100	5.56868400
C	2.46925400	-1.43885400	4.17326600
N	3.83994000	-1.36208000	3.83396200
H	1.58326300	-1.14774700	6.19636900
N	4.64482200	-1.07066800	4.93273800
C	4.45559400	-1.54582600	2.59733500
C	3.72565500	-1.82705300	1.42734100
C	5.85800900	-1.44730100	2.50675600
C	4.39297000	-2.00293600	0.21846500
H	2.64931800	-1.90114700	1.50250900
C	6.50100300	-1.62538500	1.28911500
H	6.41823500	-1.23062300	3.40623000

C	5.77925900	-1.90580300	0.12912200
H	3.80934900	-2.22164100	-0.67206200
H	7.58397100	-1.54337900	1.24911600
H	6.28623300	-2.04554200	-0.82021200
N	1.52505000	-1.70412200	3.29005700
H	0.64501100	-1.69896800	3.80663000
C	4.32163100	-0.65709000	7.31216700
H	4.08679400	-1.46075100	8.01732000
H	5.40600800	-0.53176900	7.27787700
H	3.87732900	0.26133100	7.70839800

re-TS1

C	0.46015200	-0.61634800	-0.01933000
C	1.10852600	-2.73878800	-0.15702800
C	2.66884000	-1.07366500	-1.19982800
H	2.35952200	-0.74516800	-2.19192000
N	-0.03980900	-2.79090800	0.44685200
N	-0.41747200	-1.47211400	0.51715800
N	1.45103600	-1.44177800	-0.45068900
C	2.00400600	-3.89399500	-0.48181400
H	1.41361400	-4.70966000	-0.90204800
H	2.48422800	-4.25890100	0.43522500
C	3.61145900	-2.30271100	-1.19741400
O	2.95814600	-3.52403000	-1.45404300
C	4.48105600	-0.70123800	0.30890200
C	3.50552800	-0.05705800	-0.46206600
C	3.43128400	1.32536400	-0.53011200
C	4.34153300	2.03398600	0.24620100
C	5.30742400	1.42590100	1.04290700
C	5.38456500	0.03711200	1.06723200
C	4.39440300	-2.19467500	0.13196300
H	2.70899400	1.81351000	-1.17639300
H	5.98807900	2.04095200	1.61793700
H	6.14686100	-0.45544800	1.66132400
H	3.83968700	-2.64012300	0.96674900
H	5.36844600	-2.68511400	0.08260900
C	-1.68508200	-1.13114500	1.09625000
C	-1.70551300	-0.48403700	2.33404300
C	-2.84048200	-1.40959000	0.36378600
C	-2.94719500	-0.09439600	2.83237300
C	-4.05871200	-0.99999000	0.90372700
C	-4.12921800	-0.33442100	2.12674900
H	-2.99233700	0.41916700	3.79017100
H	-4.96889900	-1.16770700	0.33183800
C	-2.75839000	-2.07681400	-0.98125600

H	-2.32841000	-3.07900800	-0.90056900
H	-2.11530700	-1.49419600	-1.65204200
H	-3.74923400	-2.14954800	-1.43256200
C	-0.42868100	-0.18339100	3.07464500
H	0.14054500	0.60478200	2.56971900
H	0.21598000	-1.06561300	3.12632200
H	-0.64446100	0.15015400	4.09093800
H	4.31219300	-2.16937100	-2.02510800
C	-5.44901700	0.14643400	2.67105900
H	-5.45393000	1.23762300	2.75705900
H	-6.27458800	-0.14236400	2.01725600
H	-5.63656400	-0.26225000	3.66838000
N	4.28429900	3.50016900	0.21737700
O	5.12887900	4.11809100	0.84378900
O	3.39227100	4.02291100	-0.42753100
C	-5.49973500	2.05775300	-0.31178400
C	-4.12013700	2.07455400	-0.48024300
C	-3.51730000	1.35338600	-1.52015900
C	-4.33939100	0.64557500	-2.40570600
C	-5.72037700	0.61712300	-2.23078000
C	-6.30514900	1.31943800	-1.17894400
H	-5.95148400	2.62585900	0.49577000
H	-3.49992700	2.65610300	0.19589100
H	-3.88371300	0.09500300	-3.22504400
H	-6.33998100	0.04947300	-2.91810000
H	-7.38199900	1.30459600	-1.04393800
C	-2.05468700	1.27484400	-1.66975100
H	-1.65509700	1.06959800	-2.66250400
C	-1.18927000	1.35380700	-0.65587700
C	0.29162400	1.20240800	-0.85384300
H	0.86403300	1.70734800	-0.04867500
O	0.79132400	1.09875200	-1.99902300
H	-1.52998200	1.50439300	0.36790500
si-TS1			
C	0.39783000	-0.92494800	-0.49512200
C	1.82209200	-2.11550100	0.73632200
C	2.80622800	-1.13582300	-1.28829300
H	2.42823500	-0.91244200	-2.28829300
N	0.72383200	-2.12197500	1.42692200
N	-0.13214800	-1.37183500	0.64958500
N	1.66357700	-1.40927200	-0.42774100
C	3.12693400	-2.81358900	0.93799000
H	3.01546500	-3.64940800	1.62791300
H	3.88704000	-2.12490100	1.33185400

C	3.78781500	-2.36708700	-1.31889200
O	3.49763700	-3.33886500	-0.32651200
C	4.98789400	-0.37121800	-0.63654400
C	3.64631000	-0.00532400	-0.73005800
C	3.19088300	1.23854000	-0.31230600
C	4.14987500	2.09598800	0.21198500
C	5.50040000	1.76841300	0.31820400
C	5.92582800	0.51845900	-0.11426300
C	5.20451100	-1.76747900	-1.15510300
H	2.14699400	1.53729700	-0.41292900
H	6.19122200	2.48716200	0.74012000
H	6.97126400	0.24061000	-0.03364100
H	5.80436100	-2.38921400	-0.48428900
H	5.72022900	-1.74009300	-2.12028900
C	-1.45424600	-1.07730600	1.12224000
C	-1.67022700	0.15613700	1.73788900
C	-2.47007000	-2.00365100	0.88679700
C	-2.97728700	0.46096100	2.11306300
C	-3.75972900	-1.65632900	1.28486300
C	-4.03182600	-0.42323700	1.87882500
H	-3.18077100	1.42355300	2.57648100
H	-4.57533200	-2.35074700	1.09721800
C	-2.17462700	-3.30713200	0.19437400
H	-1.41770600	-3.88059300	0.73728200
H	-1.78348500	-3.13045400	-0.81363300
H	-3.07771700	-3.91377400	0.11081200
C	-0.54365400	1.13924000	1.90874700
H	-0.25612700	1.55027500	0.93205700
H	0.33952400	0.66029500	2.34348900
H	-0.84728800	1.96078600	2.56013500
H	3.68563400	-2.90439600	-2.26148500
C	-5.44758300	-0.01949400	2.19064100
H	-5.49652100	0.60728700	3.08440400
H	-5.85503200	0.55724500	1.35210200
H	-6.08846000	-0.89152200	2.33974200
N	3.71615600	3.41537800	0.69037100
O	4.57416700	4.19513200	1.07020500
O	2.52295900	3.65900500	0.68709800
C	-6.07051700	-0.24561600	-1.53403200
C	-4.68349500	-0.16805200	-1.54154800
C	-4.03101800	1.04939800	-1.29483400
C	-4.81552200	2.17714300	-1.02090700
C	-6.20665300	2.10381600	-1.01929700
C	-6.84003500	0.89180900	-1.28104000

H	-6.55658900	-1.19743100	-1.72471700
H	-4.09830400	-1.06544900	-1.72032000
H	-4.32319900	3.12449600	-0.81780000
H	-6.79378600	2.99310100	-0.81300000
H	-7.92340600	0.82869200	-1.27958800
C	-2.56698300	1.19013700	-1.31959900
H	-2.16660700	2.14394900	-0.97702300
C	-1.67750200	0.28178400	-1.72936600
C	-0.20921900	0.59226700	-1.73439400
H	0.30965800	0.11021500	-2.58828000
O	0.23148700	1.66747000	-1.27333700
H	-1.96766900	-0.69637900	-2.10997100
re-M1			
C	0.48799900	-0.91286000	-0.17648200
C	1.54481400	-2.83018800	-0.30562700
C	2.86274000	-0.84235200	-1.09965500
H	2.51829900	-0.50442100	-2.07581800
N	0.33627600	-3.14294600	0.05492000
N	-0.30699900	-1.93599600	0.13253600
N	1.68597500	-1.47503400	-0.45605700
C	2.68614500	-3.76681300	-0.54651900
H	2.30938300	-4.68906400	-0.98993200
H	3.17051200	-4.01639200	0.40597500
C	4.00737700	-1.88716900	-1.13434300
O	3.59344100	-3.19366300	-1.46166400
C	4.57459100	-0.23279200	0.45170400
C	3.49188100	0.26058200	-0.28345100
C	3.16054900	1.60881200	-0.28506900
C	3.94324300	2.43358100	0.51388100
C	5.01642200	1.97392100	1.27451700
C	5.34174000	0.62282700	1.23811200
C	4.75372500	-1.70798400	0.20676300
H	2.32422200	1.96283300	-0.88713500
H	5.58642000	2.67613300	1.86971700
H	6.18836500	0.25077500	1.80504600
H	4.28267200	-2.28223500	1.01369000
H	5.79842600	-2.01769500	0.14515300
C	-1.72993400	-1.91408600	0.34065100
C	-2.22372900	-2.07978000	1.63202200
C	-2.53952400	-1.72371900	-0.78346100
C	-3.61037300	-2.03800500	1.79236200
C	-3.91329500	-1.67988500	-0.56886200
C	-4.46316000	-1.83084100	0.70830000
H	-4.02855900	-2.15911600	2.78822900

H	-4.57375700	-1.51377500	-1.41642500
C	-1.93530100	-1.56343800	-2.15323900
H	-1.35944800	-2.45491500	-2.42524000
H	-1.25678800	-0.70195500	-2.19583700
H	-2.71936900	-1.42258500	-2.89883600
C	-1.29061400	-2.27840100	2.79611600
H	-0.57951800	-1.44932500	2.87473900
H	-0.70769800	-3.19658700	2.67815800
H	-1.84903100	-2.34025900	3.73104500
H	4.67498300	-1.58597500	-1.94518400
C	-5.95277700	-1.72698900	0.90007100
H	-6.24241700	-1.97461700	1.92314200
H	-6.28618400	-0.70582800	0.68603300
H	-6.48543500	-2.39474300	0.21742500
N	3.62790800	3.86705700	0.55486400
O	4.31765900	4.58406000	1.26122900
O	2.69350200	4.26411200	-0.11755800
C	-5.39366500	2.11428800	0.78058200
C	-4.10163800	1.64803500	0.56502500
C	-3.34312400	2.11332000	-0.52023900
C	-3.93297100	3.03799100	-1.39142500
C	-5.22830000	3.50202600	-1.18015500
C	-5.96354600	3.04467000	-0.09018300
H	-5.96215400	1.74772100	1.63057600
H	-3.68142600	0.90129300	1.23380300
H	-3.36026700	3.39767000	-2.24226100
H	-5.66202500	4.22146900	-1.86770500
H	-6.97353100	3.40413000	0.07884200
C	-1.96950700	1.65658900	-0.78400100
H	-1.54251100	1.88621400	-1.75944100
C	-1.18160800	0.98111200	0.05297800
C	0.23155900	0.59912600	-0.36525300
H	0.87659300	1.03371000	0.44907800
O	0.60188400	0.90909600	-1.60838400
H	-1.49207800	0.73767100	1.06962600
si-M1			
C	0.36669600	-0.93894200	-0.43697700
C	1.82428500	-2.04126200	0.78193500
C	2.76222600	-1.12085400	-1.29778900
H	2.36422900	-0.91074400	-2.29247800
N	0.74333900	-2.02759500	1.50124600
N	-0.14981700	-1.32725700	0.73079200
N	1.63659700	-1.38967400	-0.40660300
C	3.13994900	-2.72303000	0.97440400

H	3.04770700	-3.53441600	1.69547900
H	3.90266200	-2.01564100	1.32631700
C	3.73891000	-2.35554500	-1.31798900
O	3.47688900	-3.28921500	-0.28062400
C	4.95506000	-0.35141800	-0.70114100
C	3.61208700	0.01366700	-0.76352700
C	3.15975500	1.25827600	-0.34574700
C	4.12828300	2.11929900	0.15154800
C	5.48261800	1.79649200	0.22689700
C	5.90258900	0.54524000	-0.20800500
C	5.15840900	-1.75122400	-1.21652000
H	2.10221800	1.52042400	-0.43677700
H	6.18156200	2.51981000	0.62728400
H	6.95075700	0.27193400	-0.15158500
H	5.78680700	-2.36691500	-0.56691300
H	5.63249900	-1.72921900	-2.20298800
C	-1.45994200	-1.00768300	1.22891400
C	-1.65191700	0.26157300	1.77471600
C	-2.48374400	-1.93776700	1.04888700
C	-2.95784600	0.61010900	2.11317800
C	-3.77052100	-1.54106700	1.40480900
C	-4.02665100	-0.26378300	1.90724100
H	-3.14895500	1.60241900	2.51438300
H	-4.59650500	-2.23148500	1.25258600
C	-2.20412500	-3.29160200	0.45346500
H	-1.44644600	-3.82863700	1.03125700
H	-1.82543100	-3.20086300	-0.57077300
H	-3.11282400	-3.89466900	0.42665000
C	-0.50812800	1.23108200	1.89223500
H	-0.17331300	1.51714500	0.88458500
H	0.34179200	0.77940900	2.41491400
H	-0.81609300	2.12300900	2.44037800
H	3.60583900	-2.92708100	-2.23609200
C	-5.44000900	0.19145000	2.14883700
H	-5.49491400	0.90567700	2.97369200
H	-5.81821000	0.68739800	1.24677700
H	-6.09991200	-0.65069200	2.36922800
N	3.70034800	3.43998000	0.63173400
O	4.56223100	4.21891600	1.00517800
O	2.50757400	3.68574900	0.63658100
C	-6.13523000	-0.18375600	-1.57589400
C	-4.74705000	-0.23881200	-1.56401500
C	-3.98067200	0.92497300	-1.39432100
C	-4.65794900	2.13891900	-1.22156900

C	-6.04997700	2.19813300	-1.23563500
C	-6.79549600	1.03649400	-1.41739100
H	-6.70805500	-1.09660200	-1.70786300
H	-4.25049200	-1.19879900	-1.67275700
H	-4.07898900	3.04770000	-1.07988300
H	-6.55039100	3.15256200	-1.10500600
H	-7.87989500	1.07685300	-1.42902700
C	-2.50844700	0.91956700	-1.37411200
H	-2.01367700	1.86290100	-1.14511000
C	-1.70608500	-0.12371000	-1.58484600
C	-0.18929400	0.02371900	-1.51428100
H	0.18227700	-0.44682700	-2.46511000
O	0.29700900	1.23685200	-1.25242900
H	-2.09384600	-1.11247100	-1.83484200

re-TS2

C	-0.02909500	0.10417100	0.89539800
C	1.39461700	1.38009600	1.99644200
C	2.25476700	-0.86128200	1.61073500
H	1.83833300	-1.85030200	1.42632700
N	0.43004300	2.18175800	1.67789700
N	-0.44731100	1.38070600	0.98588600
N	1.16575300	0.10668600	1.54213300
C	2.62964900	1.59988400	2.81044400
H	2.50510300	2.47109500	3.45343200
H	3.49878300	1.76160200	2.15908100
C	2.97888500	-0.78068100	2.99109400
O	2.79233000	0.46787000	3.64605000
C	4.60314400	-0.69077700	1.20084400
C	3.34580400	-0.53414900	0.61633300
C	3.19433900	-0.12051900	-0.69755900
C	4.36165800	0.05324900	-1.42676500
C	5.63489700	-0.13690200	-0.89576800
C	5.75875400	-0.49654600	0.44504200
C	4.46308100	-1.05617400	2.65853400
H	2.22473500	0.02345300	-1.16881800
H	6.50328600	0.01772100	-1.52509800
H	6.74178200	-0.60847400	0.89049200
H	5.11632800	-0.47302300	3.31289300
H	4.69411500	-2.11514300	2.81890700
C	-1.56409800	1.98420200	0.31714400
C	-1.39003500	2.36718700	-1.01425900
C	-2.76893400	2.12592600	1.00972900
C	-2.49693300	2.91178800	-1.66783400
C	-3.84108700	2.67859800	0.31485200

C	-3.72336400	3.07164100	-1.02255100
H	-2.39645400	3.21170700	-2.70761900
H	-4.79642800	2.79088500	0.82233100
C	-2.90941500	1.62053400	2.41912500
H	-2.09484700	1.97745400	3.05516300
H	-2.88130500	0.52404800	2.42637300
H	-3.85836400	1.94163300	2.85117900
C	-0.07727300	2.15551500	-1.72211100
H	0.06675000	1.10169900	-1.99652600
H	0.76530400	2.45348300	-1.08974400
H	-0.04076800	2.74661900	-2.63870400
H	2.57488800	-1.51881300	3.68449100
C	-4.90398000	3.67081400	-1.74079100
H	-4.75509700	3.66402600	-2.82211500
H	-5.82004500	3.11937400	-1.51322100
H	-5.05934800	4.70824900	-1.42793500
N	4.24316900	0.45626500	-2.83059800
O	3.24307100	1.05933600	-3.16266700
O	5.16945800	0.17665300	-3.57420100
C	-6.49473800	-0.98882800	-0.30748400
C	-5.11912700	-0.90526800	-0.12911200
C	-4.36198900	-2.04913200	0.17093300
C	-5.03754300	-3.26912500	0.30761500
C	-6.41557600	-3.35400000	0.13059900
C	-7.15132600	-2.21359700	-0.18155500
H	-7.06013500	-0.09128100	-0.54029000
H	-4.62902600	0.06171200	-0.21080300
H	-4.46729300	-4.16197800	0.55020000
H	-6.91422600	-4.31246900	0.23727300
H	-8.22599900	-2.27515000	-0.31961300
C	-2.90275700	-2.01231100	0.36194600
H	-2.44453400	-2.89604800	0.79915700
C	-2.10240700	-0.99521600	0.02018300
C	-0.61814800	-1.04205500	0.18327400
H	-0.10985400	-0.99477500	-0.97404600
O	-0.15417400	-2.24792700	0.72139300
H	-2.51869900	-0.12301600	-0.47581800
H	0.53623100	-2.57745800	0.00071100
C	1.54209600	-2.04012500	-2.03908000
O	2.44573200	-2.12683400	-2.90938200
O	0.55588100	-1.18944400	-2.17408900
O	1.59457100	-2.75896700	-0.94522600
Cs	4.44567600	-3.67465800	-1.34490500

si-TS2

C	-0.27850200	-0.90139000	-0.18046400
C	-1.73920100	-1.73943400	-1.59272700
C	-2.73736900	-0.92118000	0.50714100
H	-2.38587100	-0.85025100	1.53862600
N	-0.60792100	-1.81277600	-2.22309100
N	0.29418400	-1.26847900	-1.33879700
N	-1.58827100	-1.19372500	-0.34873000
C	-3.10102300	-2.24551200	-1.93815600
H	-3.04290800	-2.98080400	-2.73996600
H	-3.75562300	-1.42146500	-2.25406100
C	-3.81217400	-2.05395300	0.34379200
O	-3.58882400	-2.89625400	-0.77924200
C	-4.81755700	0.11014300	-0.09537700
C	-3.45109900	0.33701200	0.06422600
C	-2.88198800	1.57792300	-0.18219000
C	-3.74296700	2.57971000	-0.61172200
C	-5.11303400	2.39078400	-0.78303500
C	-5.65797200	1.13961200	-0.51736700
C	-5.16710800	-1.31341500	0.25071300
H	-1.82340200	1.75583500	-0.02228700
H	-5.72640300	3.21518400	-1.12368200
H	-6.72135500	0.97050300	-0.64897600
H	-5.81345600	-1.79371900	-0.48918000
H	-5.68728200	-1.35211600	1.21327700
C	1.62212700	-0.94981600	-1.77872600
C	1.94817900	0.40115600	-1.94639800
C	2.52408400	-1.99045900	-2.00265000
C	3.25334400	0.69471500	-2.33388100
C	3.81566600	-1.64271400	-2.40145800
C	4.19829700	-0.30978700	-2.55821300
H	3.54176100	1.73531900	-2.45973400
H	4.54095900	-2.43278300	-2.57789600
C	2.11630400	-3.42480200	-1.79892300
H	1.34036900	-3.71680100	-2.51187100
H	1.70565300	-3.57619500	-0.79530600
H	2.97306300	-4.08810900	-1.92467000
C	0.93927400	1.49165800	-1.69531200
H	0.76968000	1.62855200	-0.62013700
H	-0.02426200	1.25707300	-2.16032800
H	1.29451400	2.43810600	-2.10575700
H	-3.76886200	-2.72638300	1.20040200
C	5.61478000	0.05402100	-2.91625900
H	5.64135100	0.82061900	-3.69487200

H	6.12873900	0.46020900	-2.03833400
H	6.17454700	-0.81585800	-3.26520900
N	-3.17723800	3.90161700	-0.90420800
O	-3.94463500	4.79341100	-1.22412100
O	-1.96943100	4.03632200	-0.81510200
C	6.12009700	0.25269600	1.02367500
C	4.74159300	0.09683400	0.93289600
C	3.87401600	0.90945200	1.68146300
C	4.43972900	1.89914600	2.49711000
C	5.81989000	2.06025900	2.58391000
C	6.66819300	1.23450600	1.85050000
H	6.77153400	-0.39099500	0.43955400
H	4.33111600	-0.64906700	0.25750300
H	3.78237100	2.54584100	3.07252300
H	6.23274000	2.83243300	3.22571300
H	7.74437500	1.35769200	1.91508300
C	2.41167500	0.77418300	1.61113100
H	1.81954600	1.60547300	1.98797900
C	1.75596900	-0.28476600	1.11775400
C	0.27999200	-0.39392200	1.07868500
H	-0.12241400	-1.31148900	1.88357500
O	-0.42167300	0.75117000	1.48573300
H	2.30894900	-1.15689300	0.77107100
H	-0.90731400	0.44890100	2.37315800
C	-1.37779900	-1.41067300	3.70365800
O	-1.79078800	-1.95270500	4.75758200
O	-0.79047300	-2.10954300	2.76478900
O	-1.54067300	-0.12306800	3.50592600
Cs	-2.13943900	0.54069700	6.38813400

re-TS2^A

C	-0.03547000	0.13367900	0.95511200
C	1.41614700	1.43027800	2.00406900
C	2.24773900	-0.82967200	1.65869400
H	1.80155400	-1.81171300	1.49699500
N	0.45953600	2.23641300	1.67379100
N	-0.43872100	1.42359700	1.01494700
N	1.16670400	0.14726500	1.59407400
C	2.66421600	1.65521100	2.79716700
H	2.55822900	2.54165500	3.42283100
H	3.52623300	1.79207800	2.13085300
C	2.99696200	-0.72626400	3.02259100
O	2.82826400	0.54008600	3.65592800
C	4.58947900	-0.66323600	1.20701200
C	3.32295000	-0.52437700	0.63984400

C	3.15217800	-0.13215800	-0.67754500
C	4.30899400	0.04775100	-1.42251700
C	5.58930300	-0.12889300	-0.90657700
C	5.73219800	-0.47269700	0.43437100
C	4.47359900	-1.01240100	2.67054500
H	2.17573100	0.00366600	-1.13579400
H	6.44799200	0.02402100	-1.54861100
H	6.72132800	-0.58012900	0.86705900
H	5.14074200	-0.42897700	3.31075100
H	4.69953000	-2.07203400	2.83230600
C	-1.54772600	2.02566600	0.33687200
C	-1.36940400	2.39862500	-0.99751600
C	-2.75504400	2.18021800	1.02170900
C	-2.46927500	2.94837800	-1.65766200
C	-3.82269500	2.73484000	0.32018300
C	-3.69708600	3.12153600	-1.01758000
H	-2.36354300	3.24083300	-2.69928300
H	-4.77874900	2.85626800	0.82421700
C	-2.90224700	1.68311900	2.43348400
H	-2.08973600	2.04369900	3.07007600
H	-2.87161600	0.58672900	2.44769400
H	-3.85342900	2.00559800	2.85995600
C	-0.05648100	2.16949000	-1.69944900
H	0.07853100	1.11124200	-1.96055000
H	0.78647200	2.46435900	-1.06631500
H	-0.01104200	2.75020900	-2.62240900
H	2.60158800	-1.44567800	3.74028800
C	-4.86486000	3.73530600	-1.74526000
H	-4.78117200	3.58525800	-2.82359500
H	-5.80972200	3.30336300	-1.40661300
H	-4.90991500	4.81356900	-1.56051900
N	4.17241500	0.46717600	-2.81909500
O	3.13556900	1.01052100	-3.15222300
O	5.11839900	0.27405000	-3.56587400
C	-6.48154600	-1.07457800	-0.31846800
C	-5.11014200	-0.97199000	-0.12018800
C	-4.32936100	-2.11227200	0.13460700
C	-4.98416100	-3.35030500	0.20306700
C	-6.35816900	-3.45429300	0.00721900
C	-7.11538200	-2.31620900	-0.25819000
H	-7.06194900	-0.17800900	-0.51648300
H	-4.64055700	0.00831300	-0.15308400
H	-4.39850800	-4.24260600	0.40840300
H	-6.83755900	-4.42712900	0.06241000

H	-8.18712000	-2.39280500	-0.41141400
C	-2.87523700	-2.05579400	0.34688400
H	-2.39111800	-2.95774900	0.71388600
C	-2.09487300	-0.99286700	0.10744800
C	-0.61483200	-1.03676800	0.28951100
H	-0.13953500	-0.95577800	-0.89735500
O	-0.11516800	-2.22506400	0.77367400
H	-2.52569500	-0.09106800	-0.31926500
H	0.71766100	-2.59084300	-0.15981600
C	1.44826900	-2.07136300	-2.02035900
O	2.30239800	-2.20675600	-2.90727000
O	0.46722700	-1.21037700	-2.10288400
O	1.52925800	-2.79561500	-0.90724000

si-TS2^A

C	-0.27761500	-0.95334700	-0.12612700
C	-1.75566500	-1.83693100	-1.49939800
C	-2.73561500	-0.91710600	0.57025900
H	-2.38191300	-0.84890900	1.59828800
N	-0.63398900	-1.93749800	-2.14106200
N	0.28215800	-1.36361300	-1.28252900
N	-1.59394100	-1.25158100	-0.27514700
C	-3.12368100	-2.33199700	-1.83423000
H	-3.07119500	-3.10799200	-2.59771700
H	-3.75669700	-1.51167400	-2.20190200
C	-3.86769100	-1.99589200	0.41257100
O	-3.64570400	-2.91104600	-0.65289100
C	-4.74166000	0.20720500	-0.12223300
C	-3.37635600	0.36981900	0.10133500
C	-2.73224400	1.57845000	-0.12306100
C	-3.51941100	2.61286800	-0.61073900
C	-4.88768500	2.48977700	-0.84890400
C	-5.50820300	1.27236100	-0.59535100
C	-5.17781700	-1.19279400	0.22211100
H	-1.67663800	1.69429000	0.11436000
H	-5.44051800	3.33943800	-1.22939100
H	-6.57177500	1.15574200	-0.77524900
H	-5.79834700	-1.65563400	-0.55117800
H	-5.76082000	-1.19129500	1.14852000
C	1.58197300	-1.00433100	-1.76712600
C	1.86331500	0.35656200	-1.94278000
C	2.51197800	-2.01422400	-2.01435200
C	3.14851900	0.69005800	-2.36292500
C	3.78223700	-1.62734800	-2.44512900

C	4.11967300	-0.28383600	-2.60943000
H	3.40142200	1.73954900	-2.49397500
H	4.52883400	-2.39461200	-2.63454300
C	2.15630500	-3.46000300	-1.79454800
H	1.39193800	-3.78919900	-2.50414100
H	1.74909200	-3.61218900	-0.78979100
H	3.03661300	-4.09403800	-1.91119800
C	0.83067700	1.41816900	-1.66310300
H	0.68923900	1.55538300	-0.58324800
H	-0.14062200	1.15209700	-2.09517300
H	1.14295900	2.37316700	-2.08937100
H	-3.90009500	-2.62309300	1.30313300
C	5.51721500	0.12526600	-2.99383400
H	5.50532000	0.88773200	-3.77722900
H	6.03170800	0.55381000	-2.12657800
H	6.10023100	-0.72766100	-3.34733300
N	-2.87497000	3.89871200	-0.89997300
O	-3.58423600	4.83274200	-1.23784600
O	-1.66243400	3.96577000	-0.79632600
C	6.11705400	0.38087300	0.94474000
C	4.74258900	0.18180400	0.88302700
C	3.86506100	0.95159000	1.66612500
C	4.42011500	1.94473200	2.48589400
C	5.79560300	2.14994800	2.54273700
C	6.65356300	1.36571100	1.77558200
H	6.77423200	-0.23154400	0.33339600
H	4.33970300	-0.56324000	0.20191800
H	3.75644600	2.55803200	3.08992100
H	6.19779900	2.92325500	3.19036800
H	7.72659600	1.52304100	1.81764400
C	2.40740700	0.77358400	1.62505800
H	1.79343600	1.56800200	2.04380400
C	1.76715900	-0.28502200	1.10763600
C	0.29243100	-0.41151000	1.10297200
H	-0.04911000	-1.38863200	1.88766500
O	-0.43748200	0.65559800	1.59019500
H	2.33260100	-1.13199100	0.71935600
H	-0.93504100	0.20636500	2.72806100
C	-1.26289900	-1.54608000	3.75821900
O	-1.69466800	-2.12110500	4.76512400
O	-0.70859300	-2.18040000	2.76025900
O	-1.38040500	-0.22036800	3.65305800

re-M2

C	0.40336500	0.84127300	0.85148400
C	2.03987200	2.24695400	0.28460700
C	2.81634600	0.34625000	1.63253200
H	2.42362700	-0.18222400	2.49883800
N	1.02533500	2.69611800	-0.36451600
N	-0.01397700	1.83814800	-0.01792800
N	1.74252900	1.15824500	1.07173700
C	3.44206800	2.75875300	0.32219900
H	3.46603900	3.82091800	0.07941400
H	4.06910400	2.21768600	-0.40206900
C	4.04729000	1.24087100	2.03996200
O	3.92078900	2.59503600	1.64338000
C	4.75243200	-0.47696700	0.46438700
C	3.37117700	-0.60787100	0.60044700
C	2.64498000	-1.48764300	-0.18851600
C	3.35803400	-2.22677100	-1.12344800
C	4.73864100	-2.12846800	-1.27914900
C	5.44453200	-1.24275900	-0.47280300
C	5.29183600	0.55307100	1.42053200
H	1.56873400	-1.58808000	-0.10546100
H	5.23511600	-2.73216200	-2.02825700
H	6.51908500	-1.14476600	-0.58602800
H	5.93214900	1.29355400	0.93100300
H	5.89268400	0.07570600	2.20078800
C	-1.17899400	1.82647000	-0.84059500
C	-1.30878400	0.85712200	-1.84419800
C	-2.17474400	2.77594500	-0.58931100
C	-2.49313900	0.83887200	-2.57995300
C	-3.33724700	2.72687500	-1.35751000
C	-3.51660400	1.76097200	-2.34990600
H	-2.61965500	0.08370100	-3.35245500
H	-4.12589200	3.45080500	-1.16760300
C	-1.99209800	3.78796700	0.50925700
H	-1.10285800	4.39963700	0.33221600
H	-1.85114400	3.28766800	1.47274000
H	-2.86158700	4.44344900	0.58072900
C	-0.23713400	-0.17242600	-2.08184000
H	-0.34094100	-1.00454900	-1.37593800
H	0.76341300	0.25108400	-1.94908900
H	-0.31120200	-0.58131000	-3.09129600
H	4.12170100	1.28446800	3.12628600
C	-4.77993300	1.71992600	-3.17061200
H	-5.08942500	0.68930900	-3.36263300
H	-5.59705500	2.23805000	-2.66423200

H	-4.62805200	2.20302900	-4.14126500
N	2.61524100	-3.14326900	-1.99516300
O	1.40220700	-3.18540800	-1.87384700
O	3.24686500	-3.81052500	-2.79549100
C	-5.92703000	-1.21598300	0.32484700
C	-4.57038100	-0.98675400	0.51485200
C	-3.86741400	-1.61899300	1.55790300
C	-4.58129500	-2.50833100	2.37738500
C	-5.93841900	-2.74290100	2.18168600
C	-6.62303300	-2.09382900	1.15652300
H	-6.44363100	-0.71316600	-0.48771300
H	-4.04769800	-0.32241000	-0.16945300
H	-4.05745300	-3.01533900	3.18381900
H	-6.46361500	-3.43425500	2.83396300
H	-7.68156100	-2.27490600	1.00106100
C	-2.44241900	-1.39182100	1.80674400
H	-1.96789400	-2.06083200	2.52178600
C	-1.72172300	-0.39821800	1.23568700
C	-0.32025700	-0.18159100	1.42029600
O	0.37881400	-1.05808100	2.25190300
H	-2.23720200	0.29933300	0.58560400
H	0.22238300	-1.95723100	1.92785900

si-M2

C	0.41196500	-0.89165100	-0.83966300
C	2.03818200	-2.28307700	-0.21531800
C	2.83093900	-0.41744400	-1.61148100
H	2.44481700	0.07886200	-2.49917300
N	1.01467100	-2.71565900	0.43133300
N	-0.01835800	-1.86186600	0.05362700
N	1.75420600	-1.21258400	-1.03189300
C	3.43843900	-2.80041000	-0.22864100
H	3.45784500	-3.85604500	0.04097300
H	4.06189500	-2.24239700	0.48533400
C	4.06567100	-1.32686100	-1.97484700
O	3.92653500	-2.67115600	-1.55034100
C	4.75391300	0.43619600	-0.44313600
C	3.37708300	0.57757000	-0.61135000
C	2.64755400	1.50444400	0.12114500
C	3.35486100	2.27035100	1.03887300
C	4.73063300	2.15855100	1.22931400
C	5.43950000	1.23134200	0.47490500
C	5.30299400	-0.63267100	-1.34947800
H	1.57932400	1.63478800	-0.01040600

H	5.22020100	2.78757000	1.96178400
H	6.51038900	1.12467500	0.61143600
H	5.92183300	-1.36317200	-0.81911800
H	5.92922300	-0.19017900	-2.13003700
C	-1.18645100	-1.80241800	0.86956200
C	-1.32258700	-0.77391000	1.81163300
C	-2.18142700	-2.76537900	0.66969700
C	-2.51586900	-0.70697700	2.53032000
C	-3.35223600	-2.66605600	1.42057900
C	-3.54259500	-1.63421000	2.34232800
H	-2.64532900	0.09071600	3.25829800
H	-4.13778800	-3.40314700	1.27281900
C	-1.98736900	-3.85011800	-0.35523700
H	-1.10616500	-4.45469400	-0.12312700
H	-1.82492800	-3.41648900	-1.34736100
H	-2.86053700	-4.50305800	-0.39900800
C	-0.24544400	0.25734100	2.01570600
H	-0.35381100	1.07519900	1.29446000
H	0.75290200	-0.17080300	1.88205600
H	-0.30850900	0.68503900	3.01823000
H	4.15889200	-1.39506200	-3.05837500
C	-4.83886100	-1.50066500	3.09909300
H	-4.66219700	-1.20477100	4.13611600
H	-5.46997800	-0.73079200	2.64261700
H	-5.39911300	-2.43788100	3.09641100
N	2.61199000	3.23768700	1.85471500
O	3.24521900	3.95314700	2.61183600
O	1.39903100	3.27104700	1.73567600
C	-6.01472100	0.92603500	-0.61709400
C	-4.64206900	0.73541200	-0.71464000
C	-3.84639900	1.59277000	-1.49775800
C	-4.48602300	2.65848100	-2.15136500
C	-5.85981500	2.85188800	-2.04843400
C	-6.63535800	1.98329000	-1.28403100
H	-6.60570000	0.24907700	-0.00706000
H	-4.18094700	-0.07786400	-0.15908900
H	-3.88891600	3.33945900	-2.75252100
H	-6.32569000	3.68362600	-2.56817300
H	-7.70711600	2.13093800	-1.20124000
C	-2.39826500	1.42673900	-1.63889000
H	-1.85969000	2.26213300	-2.08142400
C	-1.71279000	0.32699600	-1.25150500
C	-0.30024900	0.14112600	-1.39681100
O	0.43102500	1.11425400	-2.07857600

H	-2.26449300	-0.50852700	-0.83358100
H	0.07231300	1.18130100	-2.97493300

re-TS2^D

C	0.43988400	-0.95522800	-0.29813300
C	1.56583000	-2.84742900	-0.18820700
C	2.89490700	-0.90035300	-1.08115900
H	2.67873300	-0.61399200	-2.10954900
N	0.38677500	-3.14924600	0.25141500
N	-0.31320600	-1.96919200	0.18091600
N	1.66866900	-1.51622000	-0.52412700
C	2.70121300	-3.80683800	-0.37495100
H	2.32183500	-4.72329300	-0.82908000
H	3.14572000	-4.06503500	0.59382300
C	4.03586800	-1.94593500	-0.93703500
O	3.65244100	-3.25986700	-1.25997600
C	4.41980200	-0.24237500	0.64670800
C	3.45747700	0.24015100	-0.25051200
C	3.22867200	1.60394100	-0.37752900
C	3.93635900	2.44414400	0.47446200
C	4.85957800	1.98764100	1.40923300
C	5.11444300	0.62306000	1.48557200
C	4.60286400	-1.72494600	0.48354500
H	2.54746700	2.00545200	-1.12056500
H	5.37882500	2.69889900	2.03907900
H	5.86001200	0.24510300	2.17661300
H	4.02701600	-2.26267200	1.24532400
H	5.64323800	-2.04430500	0.56830600
C	-1.74426900	-1.99725700	0.27015200
C	-2.33576500	-2.15518300	1.52336800
C	-2.48007900	-1.83549600	-0.91023300
C	-3.72996900	-2.12938300	1.58430800
C	-3.86740300	-1.80475100	-0.79401400
C	-4.50693600	-1.93874900	0.44133900
H	-4.21569900	-2.24427000	2.55008500
H	-4.46580000	-1.66629300	-1.69134400
C	-1.79923100	-1.68224100	-2.24604800
H	-1.02083400	-2.44081100	-2.37883500
H	-1.32685900	-0.69715900	-2.34770800
H	-2.52548500	-1.79550400	-3.05258700
C	-1.49056500	-2.32241000	2.75731400
H	-0.78200400	-1.49393500	2.85967900
H	-0.90383000	-3.24416400	2.70892700
H	-2.11605700	-2.35367500	3.65051300

H	4.80348100	-1.67530200	-1.66580700
C	-6.00573900	-1.82573000	0.53108000
H	-6.37847000	-2.19644600	1.48800100
H	-6.30641700	-0.77672700	0.43213900
H	-6.49397700	-2.38254200	-0.27270900
N	3.71151900	3.89144600	0.36803600
O	4.33755400	4.62143100	1.11745900
O	2.91268400	4.28464400	-0.46299700
C	-5.32679100	2.11616900	0.87800200
C	-4.07933700	1.62125800	0.51754300
C	-3.27751500	2.29527700	-0.41961700
C	-3.78982100	3.46478200	-0.99977900
C	-5.04221000	3.95732800	-0.64386200
C	-5.81669200	3.28837100	0.30065600
H	-5.92490500	1.57929300	1.60901100
H	-3.73016700	0.68808500	0.95199800
H	-3.18984700	3.99415400	-1.73551900
H	-5.41328600	4.86771500	-1.10485400
H	-6.79345900	3.67008400	0.57981300
C	-1.95366500	1.79839000	-0.81825900
H	-1.51840500	2.20116000	-1.72967900
C	-1.24602800	0.88389500	-0.13369100
C	0.06070300	0.39616300	-0.56174000
H	0.96289700	1.15941200	-0.55877000
O	0.62639900	0.93315800	-1.79576600
H	-1.62613700	0.49672300	0.80917500

si-TS2^D

C	0.87771000	-1.17209200	-0.74691200
C	2.64584000	-2.26921200	-0.02220900
C	3.12177600	-0.03368200	-1.07512900
H	2.99869300	0.16701300	-2.13794500
N	1.64004400	-2.94430900	0.43620900
N	0.53874100	-2.25428800	-0.00937500
N	2.24055800	-1.16626800	-0.73551300
C	4.10314100	-2.59541200	0.11195400
H	4.27327000	-3.62916200	-0.19430100
H	4.42091200	-2.49661900	1.15647600
C	4.57714400	-0.39847500	-0.65716400
O	4.85812800	-1.77937300	-0.75670500
C	3.76587800	1.31585800	0.80357500
C	2.81665100	1.17238500	-0.21091900
C	1.75291800	2.05540100	-0.33892100
C	1.67865700	3.07860200	0.59739800

C	2.60513600	3.24900600	1.62362200
C	3.66678500	2.35784500	1.72333100
C	4.80781800	0.23344200	0.73655200
H	1.03325900	1.94562400	-1.14887500
H	2.48846900	4.07013700	2.31955000
H	4.40652900	2.47831900	2.50753400
H	4.64990800	-0.48728100	1.54612400
H	5.82598100	0.61396400	0.84228300
C	-0.78258000	-2.66916500	0.35165300
C	-1.28744800	-2.24094100	1.58471400
C	-1.52522300	-3.42207100	-0.55625500
C	-2.59783400	-2.58903500	1.89702400
C	-2.83601400	-3.74573200	-0.19989200
C	-3.38579900	-3.33672600	1.01454400
H	-3.02006900	-2.26076900	2.84380900
H	-3.43987900	-4.32776500	-0.89121200
C	-0.92754500	-3.83952300	-1.87192700
H	0.01174200	-4.37933200	-1.72021100
H	-0.70564400	-2.95883700	-2.48394600
H	-1.61454200	-4.48108600	-2.42530100
C	-0.44395300	-1.39233400	2.49789100
H	-0.14256500	-0.46554600	1.99506300
H	0.47090600	-1.91689300	2.78868900
H	-0.99732200	-1.12761200	3.39977000
H	5.24476800	0.07781300	-1.37748000
C	-4.80375700	-3.68810700	1.38336500
H	-4.82591500	-4.33264400	2.26707500
H	-5.37654000	-2.78755300	1.62273200
H	-5.30876200	-4.20935400	0.56822300
N	0.57263300	4.03842000	0.49193400
O	0.44945500	4.86770300	1.37878700
O	-0.16318000	3.95859500	-0.47566500
C	-5.19903100	1.56880600	0.25449600
C	-4.01500700	1.02800600	-0.23278000
C	-3.08469000	1.82838000	-0.91599300
C	-3.39820200	3.18095100	-1.11283100
C	-4.58490000	3.72173300	-0.62763700
C	-5.49105300	2.91914300	0.06171500
H	-5.90433300	0.93030400	0.77829800
H	-3.81750400	-0.03251400	-0.09732100
H	-2.68780800	3.81214700	-1.63926300
H	-4.80193300	4.77333100	-0.78852300
H	-6.41870500	3.33736900	0.43898600
C	-1.81356400	1.30081300	-1.42938600

H	-1.29534600	1.88886000	-2.18312800
C	-1.23176600	0.16932500	-1.00039500
C	0.03775000	-0.31941400	-1.54842500
H	0.09531700	-0.66842300	-2.67918800
O	0.71789800	0.49819300	-2.51502000
H	-1.69819200	-0.41597200	-0.21223700

re-TS2^W

C	0.38143400	-0.90180700	-0.32697300
C	1.37648900	-2.84823100	-0.57634600
C	2.80270500	-0.90247900	-1.27602200
H	2.56418000	-0.49850900	-2.25908800
N	0.21010000	-3.13587400	-0.09329200
N	-0.40019900	-1.92408200	0.05733300
N	1.54944600	-1.48933200	-0.71769400
C	2.40739500	-3.85768000	-0.98226600
H	1.92087000	-4.64067200	-1.56595000
H	2.84988300	-4.32063300	-0.09176000
C	3.85935100	-2.03961100	-1.29581800
O	3.38198900	-3.26001600	-1.80256700
C	4.38720900	-0.59664500	0.48872800
C	3.49057000	0.07723500	-0.35384200
C	3.43117700	1.45803100	-0.36580900
C	4.18473300	2.12563400	0.59027400
C	5.01405200	1.48277800	1.49940500
C	5.14478300	0.09777800	1.42383800
C	4.43430700	-2.05945600	0.14049600
H	2.82352600	2.01954900	-1.05599800
H	5.56877500	2.06728500	2.22325400
H	5.84047100	-0.42200100	2.07370900
H	3.80680800	-2.63957600	0.82683200
H	5.44103600	-2.47996100	0.17711900
C	-1.78468800	-1.91552100	0.44679900
C	-2.09478900	-1.93727000	1.80456200
C	-2.74708100	-1.88134700	-0.56646700
C	-3.44712600	-1.89292500	2.14901400
C	-4.08024300	-1.83268600	-0.17219300
C	-4.44621600	-1.83060700	1.17751600
H	-3.72171100	-1.89734600	3.20060000
H	-4.85370400	-1.78122300	-0.93461300
C	-2.33919200	-1.85399000	-2.01346300
H	-1.66840100	-2.68575600	-2.24947600
H	-1.81285100	-0.92016000	-2.24271000
H	-3.21461700	-1.91941600	-2.66088500

C	-1.00700800	-1.96449900	2.84432400
H	-0.33284700	-2.81128100	2.68648900
H	-1.43400900	-2.04262200	3.84496000
H	-0.40187400	-1.05208900	2.80231300
H	4.64491300	-1.71859100	-1.98370700
C	-5.89903400	-1.72737600	1.55880500
H	-6.03231100	-1.76884800	2.64138400
H	-6.31567500	-0.78229400	1.19537200
H	-6.48145100	-2.53533500	1.10713700
N	4.09661400	3.58531600	0.62867700
O	4.41317300	4.14435400	1.66691800
O	3.73136800	4.16204000	-0.37757000
C	-5.57537900	2.12646300	0.53306200
C	-4.27128400	1.67010300	0.38101800
C	-3.49052800	2.07790200	-0.71272700
C	-4.07048200	2.94403900	-1.64912300
C	-5.37807800	3.39750100	-1.50083700
C	-6.13693400	2.99227900	-0.40665300
H	-6.15791200	1.80870200	1.39293000
H	-3.85979900	0.98545500	1.11755300
H	-3.48079600	3.26541600	-2.50364900
H	-5.80199400	4.07062100	-2.23947600
H	-7.15537200	3.34637200	-0.28440100
C	-2.10402700	1.63192600	-0.92561700
H	-1.63200200	1.95254800	-1.85228900
C	-1.38525400	0.86985100	-0.09411800
C	0.05551700	0.53158600	-0.33708900
H	0.64371300	1.26053400	0.47691800
O	0.59055800	1.14096800	-1.49250200
H	-1.79640900	0.56041900	0.86338600
O	1.17233900	2.63180900	0.45796200
H	0.89108700	1.99417600	-1.02230600
H	0.37706700	3.13395700	0.67839100

si-TS2^W

C	-0.21137600	-1.36887900	0.43825900
C	-1.51045600	-2.65310300	-0.77774900
C	-2.73701200	-1.21370300	0.85092900
H	-2.52551500	-1.07426000	1.90816500
N	-0.31601200	-2.89639500	-1.21618300
N	0.48543100	-2.08885500	-0.45236200
N	-1.50022400	-1.73492900	0.24317400
C	-2.81424100	-3.25337400	-1.18291800
H	-2.65460500	-4.23341700	-1.63163100

H	-3.32127900	-2.60885800	-1.91438600
C	-3.93971900	-2.20579200	0.61757900
O	-3.57789700	-3.42316800	-0.00739900
C	-4.44432000	-0.04013200	-0.36566400
C	-3.17539200	0.07754700	0.20081800
C	-2.46488000	1.27051400	0.15180600
C	-3.07901300	2.33258100	-0.49770300
C	-4.34144600	2.24849600	-1.08153000
C	-5.03344400	1.04676900	-1.01110200
C	-5.01922800	-1.41469600	-0.16358100
H	-1.48551200	1.38551400	0.60504300
H	-4.76150100	3.11794600	-1.57115300
H	-6.02051700	0.95990200	-1.45261000
H	-5.25274700	-1.90798900	-1.11306700
H	-5.95259900	-1.37334400	0.40396600
C	1.91275800	-2.14169500	-0.60514100
C	2.48424500	-1.42034500	-1.65708400
C	2.65739000	-2.90626600	0.29777300
C	3.87116700	-1.46424400	-1.78448300
C	4.04107700	-2.91737800	0.12416100
C	4.66228600	-2.20223900	-0.90114900
H	4.34358200	-0.90946800	-2.59080900
H	4.64881000	-3.50505600	0.80797900
C	2.00794200	-3.67858000	1.41570600
H	1.03216100	-4.07056800	1.11498200
H	1.86215600	-3.04777600	2.30140700
H	2.63893700	-4.52187100	1.70278500
C	1.62681100	-0.59909800	-2.58258300
H	1.10774700	0.19359900	-2.02995700
H	0.86276000	-1.21530900	-3.06469900
H	2.23629600	-0.13058800	-3.35631900
H	-4.31986400	-2.50873300	1.59280600
C	6.16166000	-2.23302800	-1.04423800
H	6.52383800	-3.26169300	-1.12432900
H	6.48712500	-1.68397500	-1.92968400
H	6.64161200	-1.78538800	-0.16907900
N	-2.36685900	3.61573100	-0.55540700
O	-2.88431600	4.52667600	-1.17923000
O	-1.29879200	3.70099300	0.02510800
C	4.06592700	3.68581300	-0.45099900
C	3.25312300	2.65511000	0.00502200
C	2.08946000	2.92910700	0.74106300
C	1.77907100	4.26875500	1.01040600
C	2.59364700	5.30135400	0.55598200

C	3.74181400	5.01493800	-0.17782100
H	4.96264500	3.45085400	-1.01617700
H	3.53503400	1.62671500	-0.20564600
H	0.87791900	4.49603000	1.57289500
H	2.33095800	6.33137800	0.77653300
H	4.38143200	5.81742500	-0.53087900
C	1.18841100	1.87639200	1.23960700
H	0.40956800	2.19174400	1.93087700
C	1.24581500	0.58487700	0.89534800
C	0.34398700	-0.46054700	1.45921400
H	0.89472700	-1.16290500	2.32978100
O	-0.65330600	0.03356700	2.31591200
H	2.01002300	0.23874100	0.20490500
O	0.75369000	-1.46914700	3.73242600
H	0.26951600	-2.30536100	3.73280300
H	-0.33048500	-0.43845100	3.16683500

TS3

C	-2.40240000	-0.90492200	0.28185800
C	-3.97532000	-2.05260800	1.30455600
C	-4.57533400	0.31727300	0.97231100
H	-3.99398100	1.23048100	1.06864500
N	-3.05254400	-2.92777300	1.05054100
N	-2.08335900	-2.21580700	0.39841800
N	-3.63428000	-0.80672900	0.85711200
C	-5.24465800	-2.20457100	2.07183600
H	-5.20415800	-3.09932100	2.69186300
H	-6.10544500	-2.27888200	1.39240600
C	-5.52615500	0.13943300	2.21993200
O	-5.33666700	-1.07667500	2.91877600
C	-6.84207500	0.32632500	0.17868700
C	-5.50624000	0.35209100	-0.21719900
C	-5.14200900	0.38414900	-1.55631900
C	-6.17627000	0.38007900	-2.48163700
C	-7.52266600	0.35929100	-2.12337200
C	-7.85907900	0.33481000	-0.77568700
C	-6.96918900	0.29877600	1.67765800
H	-4.10570400	0.42961400	-1.87097800
H	-8.28032500	0.35901000	-2.89702700
H	-8.90145600	0.31570500	-0.47595000
H	-7.60209500	-0.52063000	2.03313500
H	-7.41454900	1.22761600	2.04543100
C	-1.00655600	-2.94562100	-0.21398800
C	-1.09016000	-3.21634900	-1.58320200

C	0.07007000	-3.33844600	0.58249200
C	-0.02300500	-3.90028800	-2.16148200
C	1.10107600	-4.04334900	-0.03944600
C	1.07768800	-4.31700400	-1.40882400
H	-0.05323000	-4.11552000	-3.22658000
H	1.94537300	-4.38018100	0.55654200
C	0.13477200	-2.93711200	2.03049900
H	-0.76976600	-3.22687600	2.57341400
H	0.22853500	-1.84490500	2.10438700
H	0.99736200	-3.38906400	2.52390300
C	-2.25966600	-2.74172300	-2.40306100
H	-2.16977000	-1.67001800	-2.61619200
H	-3.20793200	-2.89997800	-1.88076100
H	-2.29833400	-3.27038000	-3.35630300
H	-5.29168300	0.91093300	2.95337000
C	2.23423900	-5.01521900	-2.07388000
H	1.88657800	-5.72527100	-2.82806300
H	2.87443400	-4.28447600	-2.58027700
H	2.84716200	-5.55096600	-1.34588400
N	-5.83204300	0.39542100	-3.90881600
O	-6.74443900	0.45520200	-4.71456000
O	-4.65246200	0.34305200	-4.21015800
C	3.64430000	-0.96104400	-2.28884800
C	2.40177900	-0.69006800	-1.73396500
C	1.69600600	0.48129300	-2.08302200
C	2.31714900	1.38615900	-2.97212900
C	3.55849800	1.11397100	-3.52056000
C	4.22763100	-0.06760800	-3.18317700
H	4.17572000	-1.86466700	-2.00594500
H	1.97526500	-1.40470800	-1.03511500
H	1.79143900	2.30026100	-3.23876000
H	4.01180800	1.81887300	-4.21119700
H	5.19754100	-0.28942800	-3.61551100
C	0.39513000	0.80082200	-1.55857100
H	-0.05797200	1.73241200	-1.88775700
C	-0.35057800	-0.04960400	-0.77102600
C	-1.65823000	0.18585300	-0.32157600
O	-2.33916800	1.30575200	-0.48921000
H	0.10428700	-0.98447800	-0.47493300
H	-2.19960000	1.99337800	0.45930600
C	1.22856600	0.85007600	2.15852300
H	1.68703700	0.12061000	2.81477500
C	2.00294300	1.36190300	1.07746500
C	1.47156900	2.50406600	0.40325300

H	2.07774300	2.96258500	-0.36751900
C	0.23176900	3.03782700	0.68276600
C	-0.61349300	2.30165000	1.56484400
C	-0.03695700	1.30598400	2.44496400
C	-0.23893200	4.36461100	0.06293300
C	-0.77815600	0.89475800	3.72652100
C	0.89226100	5.02692700	-0.73592200
H	1.79214400	5.16879500	-0.12863100
H	1.16278000	4.44104600	-1.62191000
H	0.55925100	6.01020400	-1.08062300
C	-1.44898800	4.23495200	-0.88065100
H	-2.35017700	3.94292600	-0.34268600
H	-1.63159100	5.20647400	-1.35313800
H	-1.27289300	3.50180300	-1.67223100
C	-0.61767000	5.30805300	1.22007000
H	-0.95218000	6.27216100	0.82172100
H	-1.42627200	4.87824300	1.81575100
H	0.24398000	5.48646000	1.87138700
C	-1.17551400	2.17543900	4.48557700
H	-1.84763400	2.79185100	3.88516200
H	-1.68349500	1.91061000	5.41908100
H	-0.28728900	2.76484200	4.73486400
C	-2.04594200	0.08301100	3.42614500
H	-2.55140800	-0.18476100	4.36043200
H	-2.73103000	0.67272500	2.81751600
H	-1.79981300	-0.84778400	2.90102800
C	0.10992600	0.05774000	4.65598500
H	1.02480900	0.59207100	4.92973000
H	-0.44286200	-0.15848000	5.57509700
H	0.39037100	-0.90193700	4.20874800
O	-1.91016100	2.51340800	1.52825600
C	3.28223000	0.83038800	0.73651600
C	3.68564500	-0.46767000	1.19101200
H	2.95800600	-1.04540600	1.75058800
C	4.24508700	1.58639100	0.00061400
H	3.98880000	2.60243200	-0.27062900
C	4.89791800	-1.01991300	0.90599000
C	5.49661500	1.12685800	-0.29458600
C	5.86314700	-0.25257100	0.08805600
C	5.27627300	-2.42660700	1.37274900
C	6.57047700	2.03494500	-0.90428900
C	6.03097200	3.44193100	-1.18714700
H	5.18773200	3.41155600	-1.88648800
H	5.70692900	3.94911900	-0.27235500

H	6.82314100	4.04513000	-1.64181500
C	7.72625600	2.16537300	0.10758000
H	7.35914200	2.56784000	1.05760000
H	8.18966500	1.19532900	0.29214300
H	8.48623300	2.85129900	-0.28271700
C	7.12088400	1.48408300	-2.23264500
H	7.42304400	0.44176800	-2.13253300
H	6.36578000	1.56834100	-3.01884000
H	7.99004900	2.07792300	-2.53847700
C	6.59334100	-2.39812500	2.17043700
H	7.41658700	-2.03542700	1.55704100
H	6.49205200	-1.74756900	3.04573100
H	6.82925000	-3.40774700	2.52488100
C	4.20327900	-3.02949100	2.28626400
H	4.05317500	-2.42954900	3.19054900
H	3.24264700	-3.11644300	1.76941500
H	4.51041100	-4.03431700	2.59265300
C	5.41885100	-3.34983700	0.14894400
H	4.44897600	-3.45745700	-0.35338400
H	6.14463300	-2.94694000	-0.55936900
H	5.74627800	-4.34750400	0.46337300
O	6.95607700	-0.74728800	-0.24520700

M3

C	-2.49422000	-0.44495100	0.57397700
C	-3.86571500	-0.32888900	2.25537300
C	-4.51997600	1.09958500	0.34113200
H	-3.93021400	1.64415800	-0.40039600
N	-2.96751200	-1.20697300	2.61328800
N	-2.12503600	-1.27373500	1.54949100
N	-3.61635900	0.14806200	1.00002900
C	-4.99260100	0.30101600	3.00765300
H	-4.86576400	0.14807600	4.07854400
H	-5.95544300	-0.12355700	2.69320200
C	-5.14811000	2.07934600	1.40709000
O	-4.90461100	1.68876800	2.74742000
C	-6.90797100	0.95278600	0.17442700
C	-5.71157400	0.37634700	-0.25139100
C	-5.69530000	-0.73186000	-1.08666300
C	-6.92816000	-1.23690700	-1.47432300
C	-8.14175800	-0.68144800	-1.07732700
C	-8.13064900	0.42886700	-0.24198700
C	-6.65619500	2.13086500	1.07413900
H	-4.77507500	-1.18240800	-1.43738100

H	-9.06858100	-1.12513500	-1.41872900
H	-9.06405100	0.87215100	0.08750800
H	-7.24718600	2.10392000	1.99397300
H	-6.89987500	3.06489800	0.55855600
C	-1.09448000	-2.28132400	1.45352300
C	-1.32853900	-3.36164600	0.60036500
C	0.09783500	-2.08862600	2.15650500
C	-0.28179100	-4.26702400	0.42832100
C	1.10416600	-3.02857000	1.95426900
C	0.94094700	-4.10623800	1.07891300
H	-0.42768800	-5.11289900	-0.23796900
H	2.04832300	-2.91130800	2.47922200
C	0.29562600	-0.88356500	3.03327800
H	-0.51532500	-0.77431400	3.75951500
H	0.32482500	0.02839400	2.42316400
H	1.24077500	-0.95139800	3.57562900
C	-2.62974800	-3.53561000	-0.13946300
H	-2.63261500	-2.96712600	-1.07723900
H	-3.48789100	-3.21342300	0.45749100
H	-2.77560200	-4.58480200	-0.39987000
H	-4.67977600	3.06003200	1.32105400
C	2.08585800	-5.04739100	0.82042100
H	1.73731400	-5.99684300	0.40987800
H	2.77645700	-4.59899400	0.09744100
H	2.64940700	-5.24509200	1.73527000
N	-6.94787700	-2.42208700	-2.34197400
O	-8.02921400	-2.82048100	-2.73598100
O	-5.88066300	-2.94312700	-2.61524800
C	3.67994700	-1.87735800	-1.46810100
C	2.37010800	-1.48824700	-1.22374900
C	1.44049300	-1.42677000	-2.27563900
C	1.84924300	-1.77869400	-3.57237300
C	3.15923400	-2.17156200	-3.81454500
C	4.07322900	-2.22384400	-2.76188300
H	4.39431100	-1.88971800	-0.64965500
H	2.07214800	-1.24244300	-0.20886200
H	1.12974100	-1.73958400	-4.38608500
H	3.46725400	-2.44165200	-4.81905400
H	5.09599700	-2.53645500	-2.94712100
C	0.05272300	-1.04870000	-2.05852700
H	-0.63803900	-1.23595700	-2.88159200
C	-0.46393200	-0.53902300	-0.91959900
C	-1.89703800	-0.35209500	-0.81273000
O	-2.69982200	-0.21165800	-1.72245400

H	0.14792400	-0.31141100	-0.04983300
H	-1.83244900	3.58300400	-1.14785600
C	1.47751700	2.07872800	1.18319000
H	1.93312000	1.96907000	2.16033900
C	2.24454200	1.72820500	0.06391600
C	1.68693700	1.98881500	-1.19355900
H	2.27181200	1.72306400	-2.06537500
C	0.41277900	2.53420800	-1.36626800
C	-0.35058100	2.77830600	-0.20529800
C	0.19114200	2.61164600	1.08787900
C	-0.08850000	2.91248100	-2.77502400
C	-0.54354100	3.11532000	2.34293000
C	0.93091400	2.53203200	-3.85892100
H	1.88702200	3.04435800	-3.72000100
H	1.11362200	1.45221100	-3.87233000
H	0.53396300	2.81952600	-4.83705300
C	-1.39620500	2.19671400	-3.16382500
H	-2.21694800	2.31961500	-2.45368600
H	-1.73955800	2.56762300	-4.13499400
H	-1.22559400	1.12143900	-3.25279100
C	-0.25735800	4.44568500	-2.85249400
H	-0.59586600	4.73353700	-3.85288900
H	-0.97479200	4.85952900	-2.13565500
H	0.70088500	4.93522100	-2.65750100
C	-0.82845400	4.62287200	2.19869200
H	-1.48503200	4.82910300	1.35320000
H	-1.30702600	4.99586700	3.11072800
H	0.10772000	5.17186300	2.05713800
C	-1.86124300	2.35899600	2.55618900
H	-2.40299600	2.76556100	3.41646200
H	-2.50273700	2.44414200	1.67976400
H	-1.66639900	1.29790700	2.76044800
C	0.29615100	2.93867200	3.61571100
H	1.23506600	3.49770900	3.56433400
H	-0.27409600	3.31940000	4.46850200
H	0.53047800	1.88837600	3.81743400
O	-1.66361400	3.20859400	-0.27732900
C	3.58993200	1.14380800	0.20660600
C	3.92037800	0.33150400	1.30313000
H	3.14841900	0.15025000	2.04866800
C	4.59424400	1.36615300	-0.74857600
H	4.36824900	2.04075800	-1.56959000
C	5.16121400	-0.26962300	1.45404000
C	5.85376300	0.79541600	-0.67180100

C	6.17766300	-0.10089800	0.42699000
C	5.47830700	-1.14971400	2.66823200
C	6.92957200	1.09378100	-1.72252400
C	6.45608000	2.10069500	-2.77697600
H	5.58613900	1.72972200	-3.33020600
H	6.19068200	3.06413800	-2.32828200
H	7.26142700	2.27637300	-3.49844700
C	8.17532200	1.68693500	-1.03950700
H	7.92684700	2.64089200	-0.56064200
H	8.54794200	0.99662000	-0.28232800
H	8.96202400	1.87408800	-1.78082100
C	7.31475000	-0.20124400	-2.45996300
H	7.62103000	-0.96166400	-1.74038200
H	6.45789900	-0.57132500	-3.03398800
H	8.13645100	-0.01215300	-3.16215700
C	6.74504900	-0.64140100	3.38088000
H	7.58610300	-0.63062700	2.68897100
H	6.58264100	0.37397400	3.75979900
H	6.98243400	-1.28661700	4.23569100
C	4.35031600	-1.14565100	3.70555900
H	4.13625300	-0.13472800	4.07046400
H	3.42429800	-1.55893600	3.29431400
H	4.63794500	-1.76329700	4.56288800
C	5.68881400	-2.60269000	2.20797200
H	4.76266100	-2.99520300	1.76817500
H	6.48092000	-2.64079700	1.45901900
H	5.95938600	-3.24353900	3.05648800
O	7.29782800	-0.70576700	0.49009600

TS3^{HCT-C2}

C	-0.69856500	-0.10723100	-0.84097100
C	-1.40428300	-1.97775300	-1.80281000
C	-2.99783900	-1.02815900	-0.17490200
H	-2.86439600	-0.61871400	0.82339200
N	-0.33629900	-1.68151400	-2.46119900
N	0.10710200	-0.50229700	-1.88724200
N	-1.67674800	-1.08325500	-0.79818900
C	-2.34237500	-3.12390000	-1.98589900
H	-1.81491600	-3.98856500	-2.39207600
H	-3.15188000	-2.84885200	-2.67728000
C	-3.64678900	-2.46265300	-0.12232600
O	-2.84438700	-3.47069000	-0.71033200
C	-5.08682100	-0.94974700	-1.36745900
C	-3.96599700	-0.20649900	-0.99806900

C	-3.80943700	1.11311600	-1.40233800
C	-4.80316600	1.64049600	-2.21569800
C	-5.93281200	0.92478100	-2.60579300
C	-6.07894200	-0.38564300	-2.16869700
C	-5.03921300	-2.33697800	-0.78930100
H	-2.96336000	1.71738000	-1.09868300
H	-6.67213200	1.39762900	-3.23982000
H	-6.95187800	-0.96118100	-2.45747400
H	-5.17586700	-3.11704800	-1.54496300
H	-5.83130200	-2.47285700	-0.04677000
C	1.01215100	0.30425000	-2.65364400
C	0.53878400	1.45557000	-3.29232100
C	2.34907600	-0.10359500	-2.73742500
C	1.47514400	2.25489500	-3.95206500
C	3.24079500	0.71972000	-3.41910300
C	2.82507300	1.91496400	-4.01323600
H	1.13294200	3.16864800	-4.43195700
H	4.28659800	0.42627800	-3.47851300
C	2.77994300	-1.39591400	-2.10756700
H	2.42854000	-2.24929800	-2.69724400
H	2.33997600	-1.49837900	-1.11262300
H	3.86604100	-1.45863200	-2.02464100
C	-0.91217100	1.85399200	-3.26615900
H	-1.13820300	2.45557800	-2.37880200
H	-1.57103600	0.97983100	-3.26022500
H	-1.15383200	2.45729800	-4.14349900
H	-3.74666100	-2.77363000	0.91720100
C	3.81851300	2.80281200	-4.71616700
H	4.16725600	2.34058100	-5.64499200
H	3.37755800	3.77052300	-4.96337700
H	4.69726600	2.97666300	-4.08869300
N	-4.64834900	3.02020200	-2.69135500
O	-5.54399100	3.49470700	-3.36800500
O	-3.62819000	3.61626900	-2.39011400
C	3.73977300	4.82018300	-1.13985800
C	2.75956400	3.86736400	-0.89411200
C	1.51954600	4.23686600	-0.34282700
C	1.30141700	5.59479700	-0.06396200
C	2.28422700	6.54833500	-0.30995400
C	3.51070000	6.16560300	-0.84651400
H	4.68916800	4.51221600	-1.56775000
H	2.95430000	2.83040300	-1.15503000
H	0.34314100	5.90069400	0.34895100
H	2.08977700	7.59198900	-0.08337200

H	4.27968400	6.90652600	-1.03931300
C	0.44561100	3.27324700	-0.08389200
H	-0.51397400	3.68289500	0.22711100
C	0.54165700	1.93917400	-0.24354400
C	-0.55757300	1.02298400	-0.03451100
O	-1.59785700	1.38672800	0.75833800
H	1.47664600	1.50000400	-0.57989800
H	-1.36898300	1.31794500	1.77371700
C	-0.76004900	-1.18775100	2.51027600
H	-0.99767100	-2.24341300	2.45269900
C	0.58364100	-0.78333700	2.14057700
C	0.98728700	0.54629800	2.54124300
H	2.02385200	0.82305300	2.40519400
C	0.13985700	1.46039700	3.08285300
C	-1.30679500	1.11657900	3.14050500
C	-1.64770600	-0.34067800	3.08734800
C	0.61366900	2.76576100	3.72506600
C	-2.93448900	-0.79828900	3.77839000
C	2.12831600	2.93904000	3.56968700
H	2.68785800	2.12445400	4.04148300
H	2.41188600	2.99881900	2.51238900
H	2.43012200	3.87424300	4.05025800
C	-0.05556800	4.03203400	3.16155300
H	-1.13702900	3.92557100	3.09333900
H	0.17402100	4.87218400	3.82598700
H	0.35052100	4.27063600	2.17786700
C	0.28363300	2.64989300	5.22849100
H	0.66809600	3.52880600	5.75600800
H	-0.79604600	2.59673000	5.38582800
H	0.74822200	1.75808400	5.66148600
C	-2.89390900	-0.29590100	5.23849400
H	-2.97097200	0.79016700	5.28867400
H	-3.73196500	-0.73224100	5.79114700
H	-1.96474500	-0.60781800	5.72691600
C	-4.20267800	-0.25067900	3.09444900
H	-5.05979200	-0.40105100	3.75903600
H	-4.11052600	0.81408700	2.87893300
H	-4.42389500	-0.78765500	2.16583500
C	-3.02496100	-2.32704800	3.83130900
H	-2.19340000	-2.75974700	4.39646600
H	-3.95732000	-2.61218500	4.32686100
H	-3.02959100	-2.78041600	2.83566700
O	-2.16621300	1.95440800	3.47397400
C	1.49108300	-1.69265700	1.58584000

C	1.04288100	-2.92223700	0.97868400
H	-0.02366200	-3.11704200	0.96202800
C	2.91652300	-1.46625500	1.63515000
H	3.27109700	-0.61171900	2.19502700
C	1.88284100	-3.80178800	0.37460100
C	3.82616000	-2.31111300	1.09131200
C	3.33301200	-3.47196800	0.30401800
C	1.38904400	-5.08724800	-0.28765400
C	5.33351700	-2.09770200	1.23526000
C	5.65114700	-0.94414900	2.19469000
H	5.27534500	0.01443500	1.82210700
H	5.23246800	-1.11862300	3.19133500
H	6.73652600	-0.85410600	2.29688600
C	5.98764700	-3.37161200	1.80258800
H	5.55667400	-3.62185000	2.77769000
H	5.85413100	-4.21925800	1.13028300
H	7.06027500	-3.20021000	1.94074000
C	5.95663800	-1.75648300	-0.13084100
H	5.77629600	-2.55162900	-0.85462600
H	5.53913900	-0.82000000	-0.51691300
H	7.03790400	-1.62155700	-0.01645300
C	2.18842600	-6.29794600	0.23101000
H	3.24430800	-6.21944400	-0.02418300
H	2.09250800	-6.38290000	1.31868000
H	1.78634500	-7.21377500	-0.21482100
C	-0.08763600	-5.34730500	0.02649800
H	-0.25987400	-5.43755100	1.10471300
H	-0.74110400	-4.55820700	-0.35487600
H	-0.39449700	-6.28653100	-0.44379500
C	1.53935100	-4.96944100	-1.81552700
H	0.94468200	-4.12641100	-2.18707400
H	2.58294700	-4.81422300	-2.09431500
H	1.17891100	-5.88709600	-2.29400600
O	4.10164700	-4.13625500	-0.39643300

TS3^{HCT-C3}

C	-1.49837300	-0.70938000	-0.62220900
C	-2.46904900	-2.58315800	-1.24316900
C	-3.67453700	-1.42653600	0.56203200
H	-3.36899000	-0.87507700	1.44563000
N	-1.55394100	-2.38469100	-2.13805300
N	-0.96634300	-1.20311900	-1.76759500
N	-2.48975800	-1.59292000	-0.29646400
C	-3.43944200	-3.70961300	-1.09575200

H	-3.02419000	-4.62433000	-1.51806900
H	-4.37945100	-3.47505900	-1.61516100
C	-4.28861800	-2.82834700	0.93166100
O	-3.63600100	-3.90831300	0.28917200
C	-5.95191400	-1.46218200	-0.20087100
C	-4.77556300	-0.71326000	-0.18843000
C	-4.68919500	0.51835100	-0.82168700
C	-5.82285400	0.95270300	-1.49476700
C	-7.01357200	0.23043900	-1.53104400
C	-7.08028500	-0.98973300	-0.86969300
C	-5.79344900	-2.73962100	0.57748100
H	-3.79218600	1.12672500	-0.79378100
H	-7.86182700	0.62930400	-2.07304800
H	-7.99821300	-1.56732300	-0.88467800
H	-6.10733100	-3.62460600	0.01530200
H	-6.39778300	-2.71083200	1.48878300
C	-0.11810200	-0.52986400	-2.71438400
C	-0.60869200	0.61941900	-3.34736700
C	1.15187000	-1.05437800	-2.96643200
C	0.26753000	1.30602300	-4.18606800
C	1.97651100	-0.34302100	-3.83596100
C	1.56706900	0.85520800	-4.42288000
H	-0.07950400	2.21508800	-4.67128600
H	2.96677000	-0.73544000	-4.04943700
C	1.60292400	-2.33773700	-2.33109900
H	1.07537800	-3.19103700	-2.76985400
H	1.39254600	-2.34086400	-1.25781600
H	2.67661500	-2.48812000	-2.46726300
C	-2.00961400	1.12790400	-3.13154300
H	-2.05962400	1.79041800	-2.26016300
H	-2.72178800	0.31053300	-2.98008100
H	-2.33793900	1.70506200	-3.99760300
H	-4.14212000	-3.01646100	1.99523000
C	2.51342700	1.65769600	-5.27522700
H	1.99447000	2.12340600	-6.11629700
H	2.96206600	2.46075000	-4.68012100
H	3.32312700	1.03596200	-5.66320900
N	-5.75706500	2.23463400	-2.20687400
O	-6.77033800	2.63764000	-2.74956700
O	-4.68904100	2.82276100	-2.22182000
C	3.24713500	3.88919300	-1.67973700
C	2.24934800	3.02400700	-1.24751200
C	1.06491600	3.52545900	-0.67670200
C	0.92075900	4.91669700	-0.56623200

C	1.92523600	5.78090000	-0.98988100
C	3.09445600	5.27066300	-1.54699600
H	4.15255200	3.48522800	-2.12309500
H	2.39280700	1.95142500	-1.36373500
H	0.00306000	5.32020200	-0.14675800
H	1.79132300	6.85309800	-0.88860000
H	3.88007800	5.94036200	-1.88078100
C	-0.02294800	2.66015900	-0.21840800
H	-0.87237100	3.14488500	0.26133500
C	-0.06692500	1.32501900	-0.39108400
C	-1.17392900	0.51645100	0.07203500
O	-2.01135300	0.92729700	0.96977800
H	0.74951400	0.80761200	-0.88596300
H	-1.46513100	0.64828500	2.11814200
C	0.23015900	-0.55329000	2.30424400
H	-0.01856800	-1.57322500	2.03697500
C	1.47328500	-0.05114200	1.89326500
C	1.78806200	1.32447300	2.24891800
H	2.73016300	1.72445100	1.89743500
C	1.01273300	2.10771900	3.03002700
C	-0.24551600	1.52931900	3.59487100
C	-0.70373400	0.18839000	3.09199100
C	1.43083900	3.51781500	3.44852500
C	-1.66722500	-0.60145600	4.02723000
C	2.70347800	3.96763100	2.71844100
H	3.56862900	3.35459900	2.99207400
H	2.58064200	3.93560000	1.63035100
H	2.92878700	4.99995600	3.00215600
C	0.31566900	4.52472800	3.11450300
H	-0.60617200	4.29128200	3.64637300
H	0.63917100	5.53218600	3.39683800
H	0.11678900	4.52550900	2.03914600
C	1.71965100	3.54415700	4.96195700
H	2.05625800	4.54589600	5.25015400
H	0.82978300	3.29415200	5.53939600
H	2.51478500	2.83404900	5.21167500
C	-1.05741000	-0.68324600	5.43878900
H	-0.98732400	0.30235100	5.90000800
H	-1.68308900	-1.31995700	6.07358100
H	-0.05602200	-1.12481900	5.39473200
C	-3.04433600	0.07639600	4.11529300
H	-3.70978400	-0.51307200	4.75478400
H	-2.94921600	1.07820700	4.53391500
H	-3.51666000	0.17113600	3.13159800

C	-1.84381900	-2.04846000	3.54123800
H	-0.93720500	-2.63904400	3.70668600
H	-2.65438300	-2.52285400	4.10352600
H	-2.08330500	-2.11818400	2.47533300
O	-0.89598000	2.14429000	4.43408400
C	2.42933900	-0.84759300	1.20267000
C	2.36678400	-2.27608500	1.24244300
H	1.61856000	-2.72719800	1.88381000
C	3.52901400	-0.27030100	0.49839400
H	3.62390100	0.80843300	0.49374400
C	3.24011700	-3.08461600	0.57509200
C	4.44312600	-1.00611800	-0.20100900
C	4.26412800	-2.46646600	-0.29277800
C	3.17789400	-4.60990500	0.67569600
C	5.62605400	-0.35348600	-0.91917600
C	5.76577700	1.12931400	-0.55338800
H	4.89522900	1.71565800	-0.86319900
H	5.90444000	1.26830100	0.52432500
H	6.64024700	1.54500200	-1.06373800
C	6.94048500	-1.04671100	-0.51268100
H	7.08473800	-0.98338200	0.57122700
H	6.93940200	-2.09570300	-0.80575700
H	7.78457300	-0.54272000	-0.99600500
C	5.43095600	-0.44783700	-2.44160800
H	5.28571800	-1.48527900	-2.75024000
H	4.55596000	0.14123900	-2.73966400
H	6.30711400	-0.04291800	-2.96113400
C	4.54812500	-5.16155700	1.11015100
H	5.32153000	-4.89837100	0.38880300
H	4.82749000	-4.75991500	2.08997800
H	4.49753500	-6.25276500	1.19295100
C	2.14324200	-5.07310500	1.70828400
H	2.36567400	-4.68402200	2.70760600
H	1.12754800	-4.76660500	1.43583500
H	2.15525500	-6.16609400	1.76217400
C	2.78164900	-5.21068900	-0.68596000
H	1.77004300	-4.89346100	-0.96185600
H	3.47598400	-4.89603200	-1.46538800
H	2.78675600	-6.30501100	-0.62344600
O	4.95159500	-3.15341500	-1.07320300

TS3^{HCT-C4}

C	1.24113000	-1.25978700	0.48617400
C	2.79143300	-2.78290800	0.10538800

C	3.29199700	-0.60684300	-0.93476400
H	2.67821800	0.11535600	-1.47084500
N	1.98234500	-3.35284800	0.93981900
N	1.02483200	-2.40249100	1.18653600
N	2.38761900	-1.51535900	-0.22196500
C	4.02081500	-3.32044800	-0.54943000
H	3.96956300	-4.40732000	-0.60971400
H	4.91541700	-3.03762800	0.02363700
C	4.22474000	-1.40175900	-1.92975200
O	4.05450400	-2.80559000	-1.86436900
C	5.57794500	-0.16691300	-0.33219600
C	4.25056900	0.05227400	0.03595400
C	3.92783800	0.74447400	1.19696000
C	4.98776000	1.19964000	1.96849800
C	6.32373800	1.01011700	1.62327600
C	6.62115000	0.31909800	0.45549200
C	5.67136500	-0.95496400	-1.60892300
H	2.90475000	0.93797400	1.49502400
H	7.10243800	1.39336800	2.27035200
H	7.65414100	0.15035900	0.17122200
H	6.32995800	-1.82487300	-1.52336800
H	6.06637500	-0.33416200	-2.41833400
C	0.10427600	-2.61399300	2.26492100
C	0.31952100	-1.93979700	3.47113900
C	-0.97013500	-3.48216900	2.05232400
C	-0.62344100	-2.13130900	4.48072000
C	-1.88158700	-3.64055100	3.09384200
C	-1.72746500	-2.96792700	4.30912000
H	-0.48960200	-1.61185100	5.42619400
H	-2.73318200	-4.30106700	2.95042800
C	-1.13181200	-4.17936000	0.73172300
H	-0.27072800	-4.81911000	0.51627600
H	-1.19825300	-3.44908100	-0.08237800
H	-2.03506300	-4.78988100	0.71984600
C	1.48827000	-1.01048800	3.66845900
H	1.25782600	-0.00953400	3.28564900
H	2.38437300	-1.36929900	3.15272100
H	1.72094100	-0.91337300	4.73014000
H	3.95466000	-1.14506600	-2.95404200
C	-2.71637100	-3.17013400	5.42722600
H	-2.40804900	-4.00437300	6.06550700
H	-2.78764000	-2.28022400	6.05602900
H	-3.70994800	-3.40135400	5.03740400
N	4.67869300	1.90452900	3.21904000

O	5.60679600	2.37937400	3.84947000
O	3.51062900	1.96989600	3.56158900
C	-4.83549400	0.86930400	2.55344100
C	-3.58619600	0.62539400	1.99528100
C	-2.54117600	1.55491100	2.13725800
C	-2.79123600	2.72886500	2.86481500
C	-4.04089200	2.97141000	3.42499900
C	-5.07055900	2.04486700	3.26802800
H	-5.63262800	0.14313900	2.42446600
H	-3.41792400	-0.28349000	1.42259300
H	-1.98762500	3.44846600	2.99510800
H	-4.21212700	3.88693100	3.98232600
H	-6.04861600	2.23647800	3.69664900
C	-1.22952800	1.33736400	1.53609100
H	-0.61042100	2.21508500	1.35806700
C	-0.72569100	0.11593300	1.22859000
C	0.52547700	-0.02068700	0.54504600
O	1.13531500	1.02988300	0.04836800
H	-1.28954500	-0.78126800	1.46322900
H	0.53866400	1.57288100	-0.88929900
C	0.04988300	1.95131400	-1.93942800
H	0.72640500	1.36469200	-2.55547900
C	-1.27222100	1.37977300	-1.68974200
C	-2.25669500	2.30251000	-1.20409300
H	-3.21514700	1.91095500	-0.89769800
C	-2.08048100	3.65604600	-1.16658800
C	-0.78273600	4.25287200	-1.54862800
C	0.28475800	3.33555000	-1.92171700
C	-3.22696500	4.58888000	-0.76580100
C	1.67094400	3.89681100	-2.22851400
C	-4.48188500	3.81609600	-0.33720100
H	-4.88678300	3.20992500	-1.15489500
H	-4.28846000	3.16314100	0.52141500
H	-5.25478900	4.53326600	-0.04460900
C	-2.80933100	5.49316300	0.40827900
H	-1.95054600	6.10837700	0.14414900
H	-3.64747900	6.14528200	0.67726200
H	-2.56238300	4.88606100	1.28374100
C	-3.60063000	5.45922700	-1.98219300
H	-4.42573400	6.12747700	-1.71259800
H	-2.75026500	6.05892600	-2.30638400
H	-3.93192600	4.83033300	-2.81518100
C	1.60635000	4.80624800	-3.46990200
H	0.90281700	5.62296700	-3.31184500

H	2.59925300	5.22297800	-3.67151100
H	1.29407600	4.23178600	-4.34816200
C	2.17628800	4.69548400	-1.00901000
H	3.17817800	5.08651000	-1.21704400
H	1.50920500	5.52598500	-0.78355900
H	2.24036700	4.04020300	-0.13299900
C	2.70441400	2.79431200	-2.49350300
H	2.45469400	2.17708900	-3.36367400
H	3.67547200	3.25785100	-2.69041600
H	2.81682600	2.15191400	-1.61299200
O	-0.62208700	5.49130800	-1.57434100
C	-1.53042400	0.00596100	-1.83616600
C	-0.58538000	-0.90491200	-2.43283300
H	0.38124800	-0.51214300	-2.72116200
C	-2.82011100	-0.54511700	-1.49547100
H	-3.55042800	0.11330800	-1.04708700
C	-0.86084900	-2.21043700	-2.70050200
C	-3.17499300	-1.83540400	-1.71944200
C	-2.17831900	-2.76389400	-2.31314600
C	0.14054600	-3.12998400	-3.40260400
C	-4.57229800	-2.36329400	-1.38716000
C	-5.49488900	-1.25413200	-0.86560100
H	-5.13111000	-0.81383500	0.06802600
H	-5.61727800	-0.45030800	-1.59917500
H	-6.48306300	-1.67879300	-0.66649900
C	-5.22868800	-2.94477200	-2.65455400
H	-5.31564900	-2.17359000	-3.42695400
H	-4.65236100	-3.77914100	-3.05203700
H	-6.23747300	-3.29599400	-2.41276800
C	-4.47448800	-3.45252900	-0.30372900
H	-3.89323700	-4.30204600	-0.66321100
H	-3.99729100	-3.05406400	0.60029300
H	-5.47879600	-3.79756200	-0.03512000
C	-0.47707900	-3.69918400	-4.69353200
H	-1.36084100	-4.29886000	-4.47745000
H	-0.75775100	-2.88722300	-5.37236300
H	0.25991500	-4.32823700	-5.20418600
C	1.41200900	-2.37087600	-3.78923900
H	1.20358300	-1.55025300	-4.48386200
H	1.90391400	-1.96833700	-2.89981100
H	2.11774300	-3.05606300	-4.26779300
C	0.54772700	-4.27954700	-2.46409200
H	0.99919900	-3.88186400	-1.54742300
H	-0.31566100	-4.88680600	-2.18978400

H	1.29075900	-4.91617100	-2.95701800
O	-2.44059100	-3.96300000	-2.46959900

TS3^{HCT-C5}

C	0.06911600	1.52507800	0.80535000
C	-0.79935300	3.53415000	0.64990400
C	-2.44954100	1.73773500	0.33018000
H	-2.42249600	0.75147900	-0.13239600
N	0.43187700	3.74072300	1.00515700
N	0.96463100	2.48287800	1.11522100
N	-1.07017700	2.20135500	0.50668300
C	-1.90656400	4.49798300	0.37618700
H	-1.50176100	5.47164300	0.10092000
H	-2.53874700	4.61151900	1.26790700
C	-3.27601400	2.75042900	-0.54272200
O	-2.63510000	4.00188800	-0.72855200
C	-4.39508800	2.38171700	1.57617200
C	-3.17341800	1.71560800	1.65933200
C	-2.72462800	1.16101900	2.84829700
C	-3.54928000	1.31029800	3.95434600
C	-4.78072200	1.95890400	3.90711900
C	-5.20998600	2.50007200	2.70066800
C	-4.63585800	2.89014700	0.18018700
H	-1.78543900	0.62631800	2.92354800
H	-5.37632200	2.03743800	4.80791600
H	-6.16150400	3.01755400	2.64408100
H	-4.97527600	3.92910800	0.14841000
H	-5.39733600	2.28232900	-0.31950400
C	2.21583100	2.31079300	1.80747500
C	2.17935700	1.83131000	3.12260300
C	3.39901400	2.62858400	1.13864500
C	3.40421200	1.61916800	3.75211400
C	4.59721900	2.39628300	1.81528700
C	4.61821300	1.88010000	3.11175000
H	3.40919700	1.23834100	4.77036300
H	5.53358200	2.61936900	1.31038200
C	3.36549800	3.18715400	-0.25400700
H	2.91597900	4.18540000	-0.25973900
H	2.76192500	2.55897000	-0.91535600
H	4.37097000	3.25339200	-0.67137200
C	0.88752500	1.53459800	3.83877200
H	0.52953300	0.52482600	3.60567600
H	0.09996700	2.24712300	3.57332300
H	1.03433900	1.58516500	4.91869200

H	-3.39467600	2.35824400	-1.55571500
C	5.91898600	1.57562900	3.80618100
H	5.91391400	1.95069600	4.83272700
H	6.07535900	0.49265400	3.85488500
H	6.76575700	2.01770500	3.27807400
N	-3.08815600	0.76532400	5.23707600
O	-3.85347600	0.80898600	6.18354200
O	-1.96024000	0.30456100	5.28527900
C	5.44731700	-2.16237900	1.95084400
C	4.20032800	-1.55651100	1.87057400
C	3.02744100	-2.33086500	1.84735200
C	3.14342600	-3.72287800	1.95845700
C	4.39376400	-4.32854000	2.04053900
C	5.55003000	-3.55188900	2.02841100
H	6.34304700	-1.54871900	1.95646200
H	4.13170300	-0.47215700	1.83657000
H	2.24468400	-4.33317400	1.96252000
H	4.46471000	-5.40912200	2.11205300
H	6.52500900	-4.02400600	2.09143600
C	1.70680700	-1.71733800	1.67289400
H	0.83313200	-2.28735900	1.98718300
C	1.52339200	-0.50761600	1.11069700
C	0.20930300	0.07831900	0.90928900
O	-0.87982900	-0.58438800	1.05816800
H	2.37449400	0.05527300	0.73853900
H	-1.12819300	-1.11906200	-0.14508400
C	-2.25528400	-1.24189500	-1.98298900
H	-2.53255100	-0.23005500	-2.25655200
C	-0.93404800	-1.42911100	-1.36816700
C	-0.58976600	-2.83069700	-1.08476100
H	0.36809300	-2.99696400	-0.60600100
C	-1.42421000	-3.87569000	-1.26803500
C	-2.75098100	-3.63729700	-1.89507100
C	-3.14307200	-2.23399000	-2.20648300
C	-1.04363700	-5.30382700	-0.86698800
C	-4.52852200	-1.97309300	-2.80469600
C	0.32446900	-5.34263300	-0.17632800
H	1.12874100	-4.98551300	-0.82915400
H	0.32345600	-4.73662300	0.73644400
H	0.55734000	-6.37360100	0.10622800
C	-2.07726400	-5.86946600	0.12468200
H	-3.06904900	-5.92120600	-0.32353800
H	-1.77704000	-6.87771300	0.42976600
H	-2.12693600	-5.24507000	1.02309100

C	-0.97042000	-6.19989500	-2.11630700
H	-0.67228300	-7.21309400	-1.82555700
H	-1.93564300	-6.25102800	-2.62003800
H	-0.22454400	-5.81472600	-2.81915300
C	-4.65987200	-2.68058200	-4.16607700
H	-4.53857100	-3.75845300	-4.06169000
H	-5.64869300	-2.47764600	-4.59151700
H	-3.90601700	-2.30548100	-4.86592800
C	-5.61831800	-2.48105000	-1.84217600
H	-6.60695400	-2.26463600	-2.26125900
H	-5.53421700	-3.55563100	-1.68313400
H	-5.54142700	-1.97341500	-0.87464700
C	-4.77427900	-0.47634200	-3.03119300
H	-4.05696400	-0.04306200	-3.73644600
H	-5.77555800	-0.33607100	-3.44828100
H	-4.72469800	0.08528300	-2.09094300
O	-3.51087000	-4.57472100	-2.14615100
C	0.15012700	-0.48937200	-1.73188200
C	-0.12889300	0.79848000	-2.28867200
H	-1.15371600	1.15578400	-2.27058000
C	1.50759800	-0.92745700	-1.81439900
H	1.74369100	-1.90994800	-1.42797500
C	0.81559800	1.59089900	-2.88256900
C	2.52175900	-0.18705000	-2.35023700
C	2.22203200	1.14303100	-2.90613200
C	0.45527900	2.91165300	-3.56850600
C	3.96199600	-0.70592400	-2.39058600
C	4.07707400	-2.12290400	-1.81541000
H	3.75996300	-2.16754700	-0.76824900
H	3.48321100	-2.84169200	-2.39089300
H	5.12301600	-2.44270000	-1.85730200
C	4.46995300	-0.75118300	-3.84364600
H	3.84697400	-1.42339200	-4.44325200
H	4.45308900	0.24021800	-4.29546300
H	5.49672100	-1.13329300	-3.86394900
C	4.86551200	0.22010800	-1.55501100
H	4.86063700	1.23121200	-1.96377400
H	4.52278700	0.25744200	-0.51262500
H	5.89322500	-0.16132400	-1.55513900
C	0.89767000	2.86885000	-5.04408300
H	1.97546900	2.73632100	-5.12915100
H	0.39704200	2.04639700	-5.56608600
H	0.61445200	3.80479400	-5.53843600
C	-1.05438300	3.16936200	-3.55399100

H	-1.60911600	2.36117700	-4.04451500
H	-1.43392400	3.29652400	-2.53620000
H	-1.26589500	4.09637400	-4.09595200
C	1.14124700	4.08811500	-2.85260700
H	0.81616900	4.14037400	-1.80546600
H	2.22594800	3.97493500	-2.87728400
H	0.86936000	5.03170100	-3.33925900
O	3.12211900	1.87194400	-3.36765900

M3_{SET}

C	0.28860500	-0.74444600	-0.43353100
C	1.80729700	-2.10957200	0.36249700
C	2.71884900	-0.52343500	-1.29170400
H	2.31425100	-0.08826300	-2.20396600
N	0.71830100	-2.42548100	0.99707100
N	-0.21850100	-1.56287000	0.51336200
N	1.59976500	-1.09232600	-0.52817600
C	3.15838700	-2.74401300	0.38156800
H	3.09910600	-3.74197300	0.81434400
H	3.86543000	-2.13985900	0.96617100
C	3.78651400	-1.63580900	-1.62915000
O	3.55045200	-2.86765200	-0.97146800
C	4.83896500	0.20384000	-0.43706500
C	3.47418200	0.48887500	-0.45913900
C	2.94442600	1.56639200	0.23553000
C	3.84123700	2.34690000	0.95186200
C	5.21053200	2.09636600	0.99113800
C	5.71579400	1.01082900	0.28610900
C	5.15512200	-1.01617100	-1.25802700
H	1.88845000	1.80935400	0.22874400
H	5.85371300	2.74368300	1.57382900
H	6.77801100	0.79296300	0.30930900
H	5.76691400	-1.74609400	-0.71943500
H	5.70555200	-0.73896900	-2.16207800
C	-1.54444600	-1.54716600	1.06691700
C	-1.89935700	-0.48794000	1.90825000
C	-2.42391600	-2.56418200	0.68864800
C	-3.21882800	-0.45147000	2.35301600
C	-3.73110900	-2.48235600	1.16796000
C	-4.14713300	-1.42879500	1.98524400
H	-3.53017100	0.36335100	3.00158000
H	-4.44193000	-3.25471500	0.88649400
C	-1.97864400	-3.67884100	-0.21981000
H	-1.21164300	-4.29260800	0.26072800

H	-1.54812600	-3.28556100	-1.14688000
H	-2.82237500	-4.31868100	-0.47998100
C	-0.91824200	0.58989500	2.28572900
H	-0.85321000	1.35173500	1.49998700
H	0.08472000	0.18553500	2.44719700
H	-1.23831300	1.08844400	3.20156400
H	3.73129900	-1.87998900	-2.68924200
C	-5.57690200	-1.32443100	2.44517300
H	-5.63017000	-1.10295500	3.51394800
H	-6.08491900	-0.51124200	1.91668200
H	-6.12468300	-2.24879200	2.25388900
N	3.31386800	3.48948800	1.70894400
O	4.10886200	4.19162900	2.30670800
O	2.10829800	3.67007500	1.69749500
C	-6.14389900	0.86311500	-1.32282300
C	-4.77261800	0.67008000	-1.25397200
C	-3.88908200	1.65742000	-1.73309200
C	-4.42894400	2.83910900	-2.26997500
C	-5.80317000	3.02762100	-2.33830900
C	-6.66499800	2.03978300	-1.86595800
H	-6.81386900	0.09561500	-0.94942200
H	-4.39130000	-0.24685500	-0.81323500
H	-3.75616100	3.60973000	-2.63566400
H	-6.20235200	3.94524900	-2.75685300
H	-7.73892400	2.18545600	-1.91551800
C	-2.44586400	1.51845700	-1.67128000
H	-1.88072000	2.40013100	-1.96899300
C	-1.78391200	0.40304200	-1.22727700
C	-0.38567000	0.29689900	-1.14766400
H	-2.35477000	-0.45789800	-0.90524900
O	0.46456700	1.20208300	-1.68094300
H	0.03556500	1.69808800	-2.39328900

M3_{HAT}

C	0.29702400	-0.87424100	-0.80176400
C	1.80510000	-2.40160400	-0.27066100
C	2.68585200	-0.59899000	-1.71036700
H	2.26154300	-0.07095400	-2.56225000
N	0.75992800	-2.74881600	0.40964100
N	-0.18167200	-1.79166900	0.09497300
N	1.58930700	-1.28712300	-1.03110000
C	3.14209500	-3.05755100	-0.37326000
H	3.06862600	-4.11518300	-0.12084000
H	3.85880400	-2.57901800	0.31001700

C	3.80482500	-1.62046400	-2.14188500
O	3.55498700	-2.95097600	-1.72170100
C	4.74423400	0.06639600	-0.65825200
C	3.38178700	0.34220500	-0.75403800
C	2.78392200	1.33991400	0.00350900
C	3.61061900	2.04123000	0.87021000
C	4.97800600	1.79906500	0.98731300
C	5.55213900	0.80020100	0.21066700
C	5.13561600	-1.05990100	-1.57703900
H	1.72868800	1.57233400	-0.08738200
H	5.56562400	2.38618600	1.68174400
H	6.61383200	0.59216800	0.29129100
H	5.69450400	-1.85026400	-1.06594800
H	5.77173900	-0.69365400	-2.38832100
C	-1.37091400	-1.69946500	0.88319900
C	-1.48590500	-0.66225800	1.81691300
C	-2.38457500	-2.63645900	0.66352200
C	-2.68591100	-0.56401800	2.51898000
C	-3.56236700	-2.50036500	1.39721500
C	-3.73476800	-1.46401400	2.31689900
H	-2.80430400	0.23691000	3.24490500
H	-4.36630300	-3.21452200	1.23789900
C	-2.20800100	-3.72599300	-0.35956900
H	-1.36135300	-4.36917900	-0.10460400
H	-2.00289700	-3.29880900	-1.34692500
H	-3.10746200	-4.33956200	-0.42785100
C	-0.37897700	0.33660200	2.03226700
H	-0.42147700	1.13185000	1.27891600
H	0.60735000	-0.13252700	1.96306900
H	-0.47244800	0.80242200	3.01478600
H	3.83420000	-1.68392100	-3.22916100
C	-5.03498800	-1.29265300	3.05844200
H	-4.85965000	-1.02668000	4.10384000
H	-5.62506200	-0.48607400	2.61048000
H	-5.63424900	-2.20463700	3.02800900
N	3.00980000	3.08358400	1.71033900
O	3.75128700	3.75240400	2.40984000
O	1.79914200	3.22154000	1.66902500
C	-6.02900300	1.25264500	-0.57476600
C	-4.66885000	0.99067400	-0.67782400
C	-3.83251800	1.82742000	-1.43771300
C	-4.40551200	2.94366600	-2.06438300
C	-5.76748600	3.20649300	-1.95863400
C	-6.58681000	2.35955300	-1.21620900

H	-6.65845500	0.59578500	0.01806100
H	-4.24729000	0.14060100	-0.14596600
H	-3.76918100	3.60501500	-2.64646100
H	-6.18964900	4.07438800	-2.45552700
H	-7.64920700	2.56303100	-1.12943100
C	-2.39449200	1.58352900	-1.57916300
H	-1.79139300	2.39553800	-1.98086200
C	-1.76897900	0.43670000	-1.24996600
C	-0.32350100	0.27643300	-1.39336000
O	0.40565100	1.12378900	-1.99325000
H	-2.34502400	-0.40648900	-0.88501700

[DQ]'

C	2.83931700	1.23765300	0.19678900
C	1.46836200	1.19512400	0.18642400
C	0.71867300	-0.00001500	-0.00004800
C	1.46835900	-1.19513400	-0.18666500
C	2.83931400	-1.23762000	-0.19730400
C	3.60176600	0.00002800	-0.00032800
H	0.91880600	2.10955000	0.37298400
H	0.91879100	-2.10957600	-0.37311700
C	-0.71866800	-0.00002600	0.00008400
C	-1.46833600	-1.19512000	0.18693100
C	-1.46837500	1.19506500	-0.18662600
C	-2.83929000	-1.23762700	0.19756000
H	-0.91875200	-2.10951500	0.37356700
C	-2.83933000	1.23757000	-0.19700800
H	-0.91883000	2.10946200	-0.37335900
C	-3.60176100	-0.00003100	0.00033600
O	4.86016100	0.00004500	-0.00044600
O	-4.86015600	-0.00003500	0.00043600
C	3.60014900	-2.54867500	-0.41979200
C	4.48748400	-2.44075600	-1.67336900
C	4.47558900	-2.85642000	0.80911600
C	2.65580900	-3.73940000	-0.62403600
H	3.87204100	-2.24678400	-2.55864800
H	5.21155800	-1.63395900	-1.56364700
H	5.02306000	-3.38387100	-1.83352400
H	3.85044200	-2.97690400	1.70066000
H	5.02456300	-3.79225200	0.65135000
H	5.18785800	-2.05040600	0.98378400
H	3.24999900	-4.64773700	-0.76724300
H	2.00611500	-3.89905400	0.24317600
H	2.02406000	-3.61143300	-1.50943500

C	3.60015000	2.54873700	0.41910600
C	4.48773600	2.44087600	1.67251100
C	4.47533600	2.85648100	-0.80998200
C	2.65581300	3.73943700	0.62351100
H	3.87247600	2.24689900	2.55791600
H	5.21181900	1.63410500	1.56266300
H	5.02330800	3.38401500	1.83254000
H	3.85000500	2.97694000	-1.70140000
H	5.02432900	3.79232300	-0.65234400
H	5.18758000	2.05047200	-0.98478000
H	3.25000400	4.64779800	0.76656600
H	2.00593000	3.89904500	-0.24356700
H	2.02425600	3.61147600	1.50904800
C	-3.60018100	2.54860100	-0.41958000
C	-4.47541700	2.85654800	0.80942300
C	-2.65585800	3.73928300	-0.62416100
C	-4.48771800	2.44050400	-1.67299700
H	-5.18764600	2.05055400	0.98434400
H	-3.85011800	2.97718800	1.70084000
H	-5.02442700	3.79234800	0.65159200
H	-2.02427500	3.61118600	-1.50965900
H	-3.25006200	4.64760900	-0.76738600
H	-2.00600200	3.89905000	0.24290800
H	-5.02328400	3.38361200	-1.83322500
H	-3.87242600	2.24635700	-2.55834100
H	-5.21180800	1.63375700	-1.56302600
C	-3.60010400	-2.54865400	0.42028600
C	-4.48743600	-2.44052600	1.67384700
C	-4.47554400	-2.85663500	-0.80856300
C	-2.65574400	-3.73932800	0.62474000
H	-3.87199700	-2.24635300	2.55908300
H	-5.21154600	-1.63378400	1.56397200
H	-5.02297200	-3.38363200	1.83418900
H	-3.85039800	-2.97728400	-1.70008600
H	-5.02451400	-3.79244000	-0.65062100
H	-5.18781700	-2.05065600	-0.98338000
H	-3.24992000	-4.64765000	0.76810400
H	-2.00604500	-3.89912300	-0.24244100
H	-2.02400100	-3.61119800	1.51011900

[DQH]

C	2.85050400	-1.22809400	-0.31940500
C	1.47883500	-1.17988600	-0.30691100
C	0.75915400	-0.00021100	0.00097800

C	1.48080700	1.17814800	0.30923800
C	2.85251700	1.22436100	0.32136200
C	3.60267200	-0.00238400	0.00079400
H	0.90960600	-2.06091800	-0.57665800
H	0.91294000	2.06015700	0.57837300
C	-0.70844200	0.00236100	-0.00057500
C	-1.42770500	1.16633400	-0.30480400
C	-1.43190100	-1.15667200	0.30259300
C	-2.81659800	1.20660100	-0.31930000
H	-0.87319400	2.05626200	-0.57257800
C	-2.82335700	-1.18912700	0.31282300
H	-0.88216700	-2.04857300	0.57318000
C	-3.50137100	0.00989600	-0.00564700
O	4.85252700	-0.00330400	0.00031600
O	-4.86104700	0.07614000	-0.02799800
C	3.61573600	2.50175700	0.66791900
C	4.49026800	2.27149600	1.91492200
C	4.50004000	2.92025900	-0.52297200
C	2.66451100	3.66557700	0.97399500
H	3.87122400	1.97581800	2.76821400
H	5.23676500	1.49842900	1.73616500
H	5.00311900	3.20347500	2.17566300
H	3.88563800	3.10302500	-1.41072200
H	5.02434100	3.84986900	-0.27694000
H	5.23659300	2.15152200	-0.75492200
H	3.25609400	4.55589600	1.20577600
H	2.02339500	3.90448700	0.11912500
H	2.02784700	3.45477800	1.83930300
C	3.61199900	-2.50605200	-0.66768300
C	4.48481900	-2.27571500	-1.91590400
C	4.49779800	-2.92630500	0.52145400
C	2.65922700	-3.66871400	-0.97322800
H	3.86475800	-1.97859400	-2.76795000
H	5.23240500	-1.50359500	-1.73765500
H	4.99630100	-3.20800100	-2.17825200
H	3.88471200	-3.10912100	1.41011300
H	5.02085800	-3.85620800	0.27389300
H	5.23542400	-2.15841500	0.75273400
H	3.24958400	-4.55954100	-1.20616400
H	2.01890700	-3.90731600	-0.11765600
H	2.02180800	-3.45674400	-1.83769200
C	-3.58080800	-2.48250000	0.66470700
C	-4.43464900	-2.95472300	-0.53290300
C	-2.61595300	-3.63583000	0.97785200

C	-4.43675000	-2.28781400	1.93512300
H	-5.16981500	-2.22901200	-0.89121300
H	-3.78339000	-3.18500200	-1.38079100
H	-4.97856100	-3.86452200	-0.26155600
H	-1.98303700	-3.41094500	1.84115200
H	-3.19847200	-4.53034300	1.21519600
H	-1.97459800	-3.87204700	0.12357900
H	-4.96904400	-3.21560200	2.16551400
H	-3.78847200	-2.04550100	2.78192500
H	-5.18305500	-1.49110900	1.87340100
C	-3.57169400	2.49951500	-0.66718000
C	-4.43881000	2.29543300	-1.92299700
C	-4.44779500	2.94057600	0.52068600
C	-2.60329000	3.65209400	-0.96811100
H	-3.81472500	2.00087600	-2.77277700
H	-5.20284400	1.53370300	-1.77113600
H	-4.93595900	3.23722300	-2.17901400
H	-3.82775400	3.11561200	1.40587400
H	-4.95384100	3.87938500	0.27137700
H	-5.20454100	2.19590900	0.76636300
H	-3.18427400	4.54878200	-1.20174100
H	-1.96370900	3.88433900	-0.11043400
H	-1.96580300	3.43530200	-1.83109100
H	-5.24382400	-0.77611900	0.20025600

M04

C	0.53108400	0.27958800	0.46874800
C	1.82622500	-0.33174900	2.10832900
C	2.38841800	-1.37338800	-0.06494100
H	1.76229500	-1.67288000	-0.90592600
N	1.02252300	0.54805100	2.63364700
N	0.23164800	0.93495700	1.58980700
N	1.57226900	-0.50273300	0.77741700
C	2.84493800	-1.24008000	2.71628100
H	2.69595800	-1.31346600	3.79306000
H	3.86242500	-0.87745900	2.51701800
C	2.87347000	-2.62338800	0.75786600
O	2.61459700	-2.51895700	2.15202000
C	4.78212900	-1.44675000	-0.17706900
C	3.66243100	-0.67180100	-0.47639100
C	3.77435500	0.58254800	-1.05864900
C	5.06128500	1.03041800	-1.32239200
C	6.20323200	0.28241400	-1.04512200
C	6.06127700	-0.97370900	-0.46675800

C	4.38301000	-2.75731500	0.44751000
H	2.90400000	1.17840400	-1.31018500
H	7.17809800	0.69292100	-1.27631600
H	6.93857000	-1.56802700	-0.23520300
H	4.94006100	-2.98637600	1.36073700
H	4.55521000	-3.58178200	-0.25134600
C	-0.62891300	2.08492100	1.70055200
C	-0.23526800	3.25526900	1.04425200
C	-1.79229200	1.98066800	2.46673900
C	-1.08773700	4.35356400	1.14969200
C	-2.60668900	3.10776600	2.53611000
C	-2.27635700	4.29516000	1.87795300
H	-0.81006200	5.27941400	0.65301000
H	-3.52313200	3.05627400	3.11837000
C	-2.13323900	0.70174700	3.17672000
H	-1.47098700	0.54249900	4.03338600
H	-2.01307400	-0.16455400	2.51938200
H	-3.16348800	0.72133300	3.53539300
C	1.05336100	3.34833300	0.26585700
H	0.95937500	2.90024100	-0.72908600
H	1.87492300	2.84467700	0.78551100
H	1.33327400	4.39385300	0.12976800
H	2.30889000	-3.50209800	0.44447200
C	-3.19787100	5.48449000	1.94260000
H	-2.66509400	6.41043400	1.71738000
H	-4.00722400	5.37843500	1.21334600
H	-3.65483500	5.57608300	2.93062600
N	5.22211900	2.36363700	-1.91623500
O	6.34786600	2.72485500	-2.21149100
O	4.22013300	3.03873100	-2.07668300
C	-5.87247000	0.55551000	-1.70035000
C	-4.51591400	0.48570800	-1.39718800
C	-3.55885900	0.50646200	-2.42343100
C	-3.99994300	0.57369000	-3.75573500
C	-5.35268500	0.63301900	-4.05678800
C	-6.29409200	0.62782700	-3.02528900
H	-6.60258800	0.54160600	-0.89765800
H	-4.20233000	0.41520500	-0.36106100
H	-3.26288400	0.57719500	-4.55477800
H	-5.67693700	0.68553100	-5.09097400
H	-7.35345700	0.67718000	-3.25633500
C	-2.12603400	0.45543000	-2.16798300
H	-1.48161400	0.48011600	-3.04485900
C	-1.50675700	0.48544400	-0.95649700

C	-0.07519300	0.43077800	-0.90438400
O	0.72912400	0.54047600	-1.83571200
H	-2.05531500	0.42917800	-0.02117600
C	-0.71224700	-2.36038900	-2.17748100
C	-2.06376000	-2.34595600	-2.50702500
C	-2.78989900	-2.41486900	-1.27284000
N	-1.77537600	-2.43017200	-0.29778600
H	-2.50762900	-2.38607900	-3.49131800
N	-0.50756600	-2.35994800	-0.85985500
C	-1.88460300	-2.49286300	1.09221900
C	-3.12730200	-2.48507400	1.75043600
C	-0.71211900	-2.57651400	1.86600800
C	-3.17167400	-2.55691700	3.14068700
H	-4.02914600	-2.43290700	1.15698800
C	-0.77963700	-2.63401200	3.25203100
H	0.24383500	-2.63455300	1.36625700
C	-2.01023900	-2.62494700	3.90688900
H	-4.14133900	-2.55323900	3.63070600
H	0.14732900	-2.70298600	3.81578700
H	-2.06287700	-2.67514700	4.98938700
N	-4.06297800	-2.44975300	-0.98772600
H	-4.56973900	-2.40541500	-1.87189100
C	0.45325200	-2.32859800	-3.11997700
H	0.85863300	-1.31566100	-3.20646200
H	1.25014400	-2.99034800	-2.76766200
H	0.14812300	-2.66337800	-4.11354100

TS4RR

C	1.14971700	0.28565800	-0.47630100
C	2.44678100	1.75245600	-1.45424200
C	3.06012900	1.31799800	0.89668300
H	2.46881100	1.09663500	1.78277400
N	1.61501500	1.38068900	-2.38090900
N	0.82342700	0.45673500	-1.76262100
N	2.19869800	1.10929900	-0.27382300
C	3.50463600	2.80495700	-1.45999000
H	3.35304000	3.48929600	-2.29403800
H	4.50419700	2.35567800	-1.54142900
C	3.62552500	2.78907400	0.91800800
O	3.34340100	3.53030100	-0.25671900
C	5.45415300	1.18577700	0.95372200
C	4.28622300	0.43801200	0.81706800
C	4.31454300	-0.93590200	0.62434000
C	5.56975700	-1.52536600	0.55892000

C	6.75866700	-0.81032700	0.68949400
C	6.69979300	0.56257000	0.89386400
C	5.14657100	2.64222100	1.17033500
H	3.40556900	-1.52276500	0.54956000
H	7.70431200	-1.33375800	0.62720800
H	7.61425800	1.13694500	0.99659200
H	5.70761300	3.30298600	0.50243100
H	5.39288700	2.93618100	2.19524700
C	-0.22096100	-0.19549300	-2.50704200
C	0.02022200	-1.47351200	-3.00631200
C	-1.44464400	0.46954700	-2.62648000
C	-1.03844700	-2.10733200	-3.65819900
C	-2.46991300	-0.20929200	-3.27873600
C	-2.28626200	-1.49760900	-3.79128300
H	-0.88627800	-3.10695000	-4.05647100
H	-3.44111500	0.27112500	-3.37141900
C	-1.64348400	1.82117900	-1.99930000
H	-1.04756500	2.58536000	-2.50955800
H	-1.33335400	1.81075700	-0.94659100
H	-2.69429800	2.11815400	-2.03467900
C	1.34801700	-2.15169200	-2.79976000
H	1.46647600	-2.45567400	-1.75309900
H	2.17996200	-1.48717100	-3.04997900
H	1.42141100	-3.04722900	-3.41809100
H	3.13855100	3.35052900	1.71450300
C	-3.43613300	-2.22271700	-4.43953900
H	-3.09038200	-3.08008800	-5.01998100
H	-4.12852900	-2.59055000	-3.67529100
H	-3.99883400	-1.55842300	-5.10002800
N	5.64632400	-2.97471200	0.33739400
O	6.75020000	-3.49097600	0.31517600
O	4.60137500	-3.58211300	0.18303300
C	-4.95290300	-2.02601900	0.03573100
C	-3.68428900	-1.52556100	0.30443800
C	-2.79608300	-2.23267300	1.12898000
C	-3.22425300	-3.44109000	1.69248700
C	-4.49442400	-3.94223200	1.42402500
C	-5.36238200	-3.23698200	0.59291500
H	-5.62717700	-1.46333200	-0.60328100
H	-3.38504900	-0.56603500	-0.11161500
H	-2.54635900	-3.99592200	2.33654100
H	-4.80607700	-4.88531800	1.86183200
H	-6.35390600	-3.62630700	0.38487500
C	-1.43627400	-1.73004700	1.39074100

H	-0.85183200	-2.26629900	2.13302700
C	-0.74596700	-1.05905100	0.38327200
C	0.56678800	-0.61409300	0.58328200
O	1.30887200	-0.83928100	1.56955600
H	-1.29351700	-0.72417100	-0.48431400
C	-3.14336900	-0.27322000	3.31393500
C	-1.75011600	-0.13442300	3.02499700
C	-1.65612400	1.02814600	2.18220200
N	-2.98858000	1.33986500	1.89706800
H	-0.93025800	-0.48597900	3.63602500
N	-3.87218000	0.55060000	2.60500300
C	-3.49202100	2.27641000	0.97981500
C	-2.79499700	3.45687900	0.69519600
C	-4.71689700	2.02286600	0.35016600
C	-3.31775500	4.35774700	-0.22735100
H	-1.84518200	3.63842800	1.18054600
C	-5.22927200	2.93813400	-0.56385200
H	-5.25001700	1.11050800	0.59372900
C	-4.53266400	4.10800700	-0.86299200
H	-2.76916700	5.26901700	-0.44556400
H	-6.17959500	2.73209400	-1.04693300
H	-4.93368900	4.81738800	-1.57934200
N	-0.63367500	1.64073700	1.65341200
H	0.19426600	1.21064200	2.06496900
C	-3.77690900	-1.24652100	4.25328100
H	-3.63573300	-0.93415100	5.29301400
H	-4.84733200	-1.31959500	4.05155100
H	-3.32896300	-2.23714400	4.14004100

TS4RR'

C	-0.80194500	-0.12771000	0.35582900
C	-2.13480700	0.95358000	1.70377700
C	-2.63007600	1.29937700	-0.69434900
H	-1.98419100	1.34830700	-1.56871500
N	-1.36536400	0.26125400	2.49119800
N	-0.55011200	-0.42237800	1.63281500
N	-1.83366900	0.72830400	0.39021500
C	-3.16483100	1.99614700	1.98996000
H	-3.03939700	2.38866700	2.99874900
H	-4.17884600	1.58628400	1.88782500
C	-3.15722000	2.72381300	-0.28931500
O	-2.92189200	3.04916700	1.07405200
C	-5.02153000	1.27328200	-0.86296500
C	-3.87829000	0.47796600	-0.91393300

C	-3.94455600	-0.89236300	-1.11999700
C	-5.21493900	-1.43512900	-1.25651900
C	-6.38104200	-0.67311400	-1.21341900
C	-6.28285000	0.69941400	-1.01826800
C	-4.66523700	2.71932100	-0.63952100
H	-3.04820800	-1.50088800	-1.18685300
H	-7.34064000	-1.16120700	-1.32782900
H	-7.17944200	1.30859500	-0.97947200
H	-5.24293600	3.18598300	0.16387700
H	-4.84643200	3.30213000	-1.54789800
C	0.33123000	-1.44737100	2.12390100
C	0.01575900	-2.77695800	1.82881000
C	1.45130200	-1.06272300	2.86400200
C	0.89305800	-3.75223300	2.29964200
C	2.29480500	-2.07851600	3.30836700
C	2.03640800	-3.42245000	3.02977900
H	0.67610700	-4.79636300	2.08954400
H	3.17882900	-1.81129400	3.88160600
C	1.73079200	0.38788700	3.14514100
H	1.00701200	0.79838300	3.85555900
H	1.65659300	0.99406400	2.23536500
H	2.73202300	0.51335200	3.56042400
C	-1.20998100	-3.14872700	1.03322200
H	-1.06951100	-2.94884500	-0.03506000
H	-2.08988100	-2.58724200	1.36414700
H	-1.42489400	-4.21215900	1.14658500
H	-2.60930500	3.48455000	-0.84542400
C	2.98965700	-4.49547100	3.48623100
H	2.47182200	-5.44386300	3.64426000
H	3.76424400	-4.66218800	2.73080100
H	3.48919700	-4.21169700	4.41509900
N	-5.33247200	-2.88571100	-1.44878200
O	-6.44594000	-3.35024700	-1.62292900
O	-4.31000300	-3.54817100	-1.41805300
C	5.62344900	-1.31350300	-0.63461900
C	4.29790600	-0.90126700	-0.70761700
C	3.50095600	-1.26474800	-1.80289200
C	4.06381200	-2.05386800	-2.81303100
C	5.38744500	-2.47730300	-2.73242000
C	6.17317800	-2.10390100	-1.64405600
H	6.23235800	-1.01555600	0.21306600
H	3.88730300	-0.26744700	0.07335400
H	3.45405000	-2.33588600	-3.66732500
H	5.80598500	-3.09456900	-3.52104800

H	7.20759400	-2.42611900	-1.58184800
C	2.09377400	-0.83931800	-1.91742700
H	1.57903400	-1.16378400	-2.81961500
C	1.28369400	-0.66574000	-0.79358600
C	-0.11681800	-0.61573100	-0.90039800
O	-0.86691300	-0.91743400	-1.85331300
H	1.73063500	-0.42431500	0.16499500
C	3.69295900	1.65821500	-2.39935900
C	2.39704000	1.21724500	-2.83645200
C	1.47268100	1.89876700	-1.96765300
N	2.28224300	2.46613000	-0.97774300
H	2.15025000	0.93424200	-3.85122100
N	3.63054200	2.32854700	-1.28161700
C	1.92572700	2.93530000	0.29465600
C	0.58387000	3.10126100	0.67943600
C	2.93982600	3.24153200	1.21797600
C	0.28100900	3.54590800	1.96453500
H	-0.20189000	2.89816600	-0.03445300
C	2.61425300	3.69042000	2.49180400
H	3.97287700	3.11612500	0.92217200
C	1.28450700	3.84274900	2.88181600
H	-0.76480300	3.67661000	2.22857100
H	3.41520600	3.91831700	3.18893000
H	1.03768400	4.19134800	3.87910800
N	0.17449300	1.92264200	-1.94029100
H	-0.14497700	1.37035700	-2.73834700
C	5.01027300	1.39790700	-3.05283300
H	5.04632300	1.86580000	-4.04170100
H	5.81454200	1.80865500	-2.43990900
H	5.17622000	0.32484000	-3.18471300

TS4RR"

C	-0.31560800	-1.27580700	-0.40838100
C	0.81648300	-2.74808200	-1.55337500
C	1.95017100	-0.55411900	-1.29268000
H	1.52879400	0.45202400	-1.23536000
N	-0.29720100	-3.35163600	-1.25267200
N	-0.98828400	-2.41967200	-0.52813100
N	0.84607300	-1.48034100	-1.04465500
C	1.93066400	-3.11835400	-2.47547400
H	1.65979300	-3.98487500	-3.07703900
H	2.85052900	-3.33674500	-1.91665500
C	2.56520000	-0.82418400	-2.71737500
O	2.08245900	-2.00642500	-3.34099900

C	4.30002100	-0.94178700	-1.02129400
C	3.10146700	-0.75103600	-0.33462400
C	3.05463400	-0.69881100	1.05109100
C	4.26144600	-0.87650800	1.71504400
C	5.47280100	-1.09679500	1.06345500
C	5.49311300	-1.12466800	-0.32496000
C	4.09597700	-0.85892400	-2.50846400
H	2.12804400	-0.49447400	1.57791000
H	6.37583000	-1.22760900	1.64640700
H	6.42802000	-1.27742000	-0.85368500
H	4.53713000	-1.69724500	-3.05624900
H	4.55042900	0.05859200	-2.89683500
C	-2.27156300	-2.72754200	0.04305000
C	-2.35021200	-2.91251300	1.42610600
C	-3.37058300	-2.80262400	-0.81279600
C	-3.60864300	-3.18758400	1.95373400
C	-4.60777700	-3.07959200	-0.23205600
C	-4.74411400	-3.27167200	1.14312900
H	-3.70658600	-3.33927400	3.02573500
H	-5.48505800	-3.13910400	-0.87070200
C	-3.22197500	-2.57527500	-2.29378200
H	-2.63666100	-3.37394100	-2.75834200
H	-2.70320200	-1.63224500	-2.50108700
H	-4.20062500	-2.53912000	-2.77424500
C	-1.12713700	-2.81045700	2.29970800
H	-0.75554000	-1.78103100	2.34992000
H	-0.31509200	-3.43610100	1.91582400
H	-1.35836600	-3.13441600	3.31509700
H	2.26575100	-0.02104300	-3.39182300
C	-6.09123000	-3.54881800	1.75737600
H	-6.04535400	-4.41295300	2.42537400
H	-6.42470400	-2.69309800	2.35221300
H	-6.84442100	-3.74329400	0.99174900
N	4.26689900	-0.79257400	3.17844200
O	5.31498000	-1.01741800	3.76169200
O	3.22495600	-0.49712700	3.73733900
C	-6.05188200	2.04418500	-0.37916000
C	-4.73758200	1.58712800	-0.36483200
C	-3.78936300	2.16705500	0.48800200
C	-4.20101900	3.20938000	1.33065200
C	-5.51376100	3.66494000	1.31898700
C	-6.44583400	3.08425700	0.45996100
H	-6.77266500	1.58396200	-1.04764000
H	-4.45634500	0.76685700	-1.01890200

H	-3.47385800	3.66215300	2.00058800
H	-5.81125300	4.47181800	1.98107500
H	-7.47175200	3.43745200	0.44716100
C	-2.37710500	1.72955200	0.52968200
H	-1.80396500	2.10393700	1.37692200
C	-1.96610500	0.48075300	0.02867500
C	-0.68861400	-0.00444500	0.31692900
O	0.19503700	0.45762500	1.06880800
H	-2.58556800	-0.08361600	-0.65860900
C	-1.01062100	2.64219400	-1.84740100
C	-1.48220100	3.34423700	-0.69594000
C	-0.28991200	3.58313500	0.11288400
N	0.70629300	2.86122000	-0.55390700
H	-2.33441000	4.01000800	-0.68097300
N	0.24806600	2.30553900	-1.73508900
C	2.05628400	2.71828600	-0.20269400
C	2.44048400	2.68577700	1.14271100
C	3.02355200	2.57755900	-1.20659600
C	3.78282400	2.52571100	1.46962300
H	1.67964100	2.78220400	1.90499300
C	4.36026600	2.40135200	-0.86068900
H	2.71350600	2.60913500	-2.24610000
C	4.75008800	2.37813700	0.47683200
H	4.07058200	2.49385700	2.51688800
H	5.10416900	2.29266400	-1.64523100
H	5.79316800	2.23736000	0.74119500
N	-0.08906900	4.24472600	1.20320100
H	-0.96194200	4.71156200	1.45015700
C	-1.84262500	2.14489100	-2.97987300
H	-2.38332200	2.96337500	-3.46282500
H	-1.21821600	1.64251100	-3.72097700
H	-2.58899200	1.43293400	-2.60650400

TS4RR'''

C	-1.86919800	0.61166600	-0.74743000
C	-3.95646600	0.73326800	-1.38760600
C	-3.08612200	-1.57778100	-1.27827600
H	-2.10598200	-2.01418500	-1.46753100
N	-3.62737500	1.95912900	-1.10420000
N	-2.32777700	1.86597800	-0.69518900
N	-2.91051100	-0.12283200	-1.18124100
C	-5.20881300	0.15774000	-1.96336100
H	-5.78441500	0.93185400	-2.46972100
H	-5.82857400	-0.29173300	-1.17508300

C	-4.13561900	-1.92895500	-2.39888000
O	-4.80082500	-0.79299000	-2.92807400
C	-4.85577900	-2.84364900	-0.26634400
C	-3.70621400	-2.10179900	-0.00192800
C	-3.26308000	-1.87382100	1.29292200
C	-4.03188600	-2.41458400	2.31369300
C	-5.18190900	-3.16844200	2.08898000
C	-5.59754700	-3.38801400	0.78139700
C	-5.11283300	-2.93608400	-1.74627400
H	-2.35219900	-1.32080200	1.49456100
H	-5.73363800	-3.56264600	2.93318600
H	-6.49421400	-3.96570600	0.58434600
H	-6.14452700	-2.69555700	-2.01965800
H	-4.91083800	-3.94928400	-2.10694600
C	-1.65337100	3.01928400	-0.16092300
C	-1.42102900	3.06521800	1.21391800
C	-1.23748500	4.01331300	-1.05178900
C	-0.71948000	4.16981800	1.69868000
C	-0.54263000	5.09326800	-0.51541100
C	-0.26913000	5.18300900	0.85376100
H	-0.51898200	4.23394500	2.76470900
H	-0.20053800	5.88125900	-1.18188600
C	-1.51219300	3.89477400	-2.52712100
H	-2.58567100	3.93732900	-2.73162900
H	-1.14358200	2.94110400	-2.91986000
H	-1.02235200	4.70216900	-3.07249400
C	-1.87140300	1.96281000	2.13595400
H	-1.16762300	1.12257800	2.10995600
H	-2.86085400	1.58373800	1.86252500
H	-1.91741200	2.32389800	3.16430500
H	-3.62444500	-2.36484800	-3.25659600
C	0.50600600	6.35571400	1.39375200
H	0.56106200	6.32683500	2.48323900
H	1.52760700	6.35378000	1.00211600
H	0.04340300	7.30034500	1.09489900
N	-3.61539800	-2.16739200	3.69974400
O	-4.23263400	-2.72745200	4.58907900
O	-2.67995500	-1.40867300	3.88545800
C	3.71673400	3.69207900	0.58826800
C	2.77390000	2.80551800	0.08456000
C	2.84553300	1.43513800	0.39040700
C	3.89965700	0.98919900	1.19894300
C	4.83101500	1.88185900	1.72254900
C	4.74322000	3.23569400	1.41840000

H	3.64933100	4.74677000	0.33983700
H	1.96976400	3.18788400	-0.53803000
H	3.98229600	-0.07292100	1.41826600
H	5.63120000	1.51347500	2.35648600
H	5.47076700	3.93471300	1.81821300
C	1.85299400	0.46325700	-0.08915100
H	1.88882500	-0.51337600	0.39082300
C	0.56361700	0.88466500	-0.51170800
C	-0.52681300	0.03555900	-0.36979700
O	-0.56576400	-1.15654200	0.02883600
H	0.41353800	1.88327800	-0.89784700
C	2.34852400	-1.64556700	-2.00552200
C	2.89733200	-0.31676800	-1.93557800
C	4.25329200	-0.49954900	-1.45126800
N	4.27486200	-1.84581300	-1.04706600
H	2.61667800	0.51043600	-2.57410700
N	3.12954600	-2.52344700	-1.44475300
C	5.28024700	-2.56043500	-0.37832200
C	6.38638000	-1.91309500	0.19345400
C	5.16245400	-3.95395200	-0.25558200
C	7.34861700	-2.66094600	0.86668900
H	6.47856900	-0.84033900	0.09511700
C	6.13422100	-4.67927700	0.42168600
H	4.30374700	-4.44761400	-0.69079800
C	7.23748100	-4.04298700	0.98785800
H	8.19856800	-2.14572500	1.30470700
H	6.02457600	-5.75651700	0.50534200
H	7.99497700	-4.61403300	1.51427600
N	5.25037100	0.31185900	-1.32656000
H	4.94935300	1.22652100	-1.66425700
C	1.04873000	-2.03849300	-2.62723600
H	1.15752700	-2.11903000	-3.71387000
H	0.71477100	-3.00104900	-2.23619300
H	0.28842500	-1.28221000	-2.42125600

TS4RS

C	-0.12129200	-1.37646500	-0.57775100
C	1.16138600	-2.74836400	-1.69191000
C	2.21474500	-0.57289600	-1.18469100
H	1.77367700	0.42770600	-1.11711600
N	0.04927600	-3.40376300	-1.52431600
N	-0.73614700	-2.53694500	-0.81539600
N	1.09764000	-1.50948800	-1.12155800
C	2.39024100	-3.05262300	-2.48541700

H	2.21410300	-3.89160100	-3.15765400
H	3.23154900	-3.29236300	-1.82079400
C	2.97177100	-0.72234100	-2.54939100
O	2.64283100	-1.90313200	-3.27229800
C	4.53348500	-0.89105000	-0.69787200
C	3.25854000	-0.85611900	-0.13240500
C	3.05932800	-1.02249600	1.23119900
C	4.19649500	-1.22923600	2.00231800
C	5.48508300	-1.26471100	1.47357300
C	5.65523000	-1.09262500	0.10445200
C	4.47205900	-0.65314100	-2.18359500
H	2.07114700	-0.96679700	1.67598600
H	6.32809800	-1.42754800	2.13304500
H	6.64976300	-1.11947600	-0.32799700
H	5.04107600	-1.38536300	-2.76349800
H	4.87275800	0.33778200	-2.42156200
C	-2.03114600	-2.94662400	-0.34371000
C	-2.18392300	-3.20759200	1.01879200
C	-3.06743000	-3.05031900	-1.27490800
C	-3.45569000	-3.58455500	1.44933200
C	-4.31630600	-3.43098300	-0.79182700
C	-4.52844400	-3.69530500	0.56406000
H	-3.60898600	-3.79734000	2.50392400
H	-5.14492000	-3.51878800	-1.49000200
C	-2.83356300	-2.74987000	-2.73132300
H	-2.18839000	-3.50533500	-3.18898000
H	-2.33806400	-1.78131100	-2.86069500
H	-3.77973400	-2.72710200	-3.27337600
C	-1.02945600	-3.08615200	1.97946500
H	-0.75814300	-2.03863700	2.15073300
H	-0.14127400	-3.60047700	1.59867700
H	-1.29134800	-3.52534200	2.94282100
H	2.67718600	0.09171400	-3.21238200
C	-5.90040900	-4.07043200	1.05944700
H	-5.84960000	-4.55624600	2.03572300
H	-6.52601200	-3.17809500	1.16158300
H	-6.40069000	-4.74457300	0.36021300
N	4.03015000	-1.42025500	3.44868200
O	5.03467900	-1.55902300	4.12554200
O	2.89632600	-1.43411100	3.89405300
C	-6.10130900	1.64760900	-0.14254400
C	-4.76128800	1.30323500	-0.27010800
C	-3.81478800	1.75935400	0.65869300
C	-4.25099400	2.56705300	1.71605500

C	-5.59433000	2.90845900	1.84705300
C	-6.52433200	2.45064500	0.91702700
H	-6.82064900	1.29153500	-0.87331400
H	-4.44390400	0.68501300	-1.10598900
H	-3.52419300	2.92609300	2.44024000
H	-5.91356100	3.53212700	2.67611900
H	-7.57160700	2.71761400	1.01471200
C	-2.38890300	1.39495900	0.57692700
H	-1.73494300	1.86811300	1.30702700
C	-1.93599700	0.21287400	0.02089600
C	-0.59656900	-0.19305800	0.23434700
O	0.21934100	0.24109500	1.06757100
H	-2.55484800	-0.36580300	-0.65683500
C	-1.69893700	4.24780500	-0.35439200
C	-1.80287600	2.99848700	-1.03481200
C	-0.45962700	2.52084700	-1.15771800
N	0.28099100	3.40607200	-0.37238500
H	-2.62278500	2.67847600	-1.66197200
N	-0.47031000	4.47655100	0.05264700
C	1.69028200	3.48381000	-0.26922100
C	2.41254700	2.42565900	0.28286100
C	2.35037600	4.63719500	-0.69720000
C	3.80120500	2.50784800	0.36634600
H	1.86576700	1.57074400	0.66988100
C	3.73499300	4.72005400	-0.59043100
H	1.76645500	5.45469900	-1.10664800
C	4.46595500	3.65236200	-0.07016600
H	4.36214800	1.68390600	0.80114200
H	4.24593300	5.61789100	-0.92362200
H	5.54645900	3.71885400	0.00682800
N	0.05360900	1.48473800	-1.77536100
H	-0.68939600	1.06373800	-2.33175900
C	-2.79094900	5.23400900	-0.08549500
H	-3.63177900	4.76491500	0.43282900
H	-2.40923300	6.05436700	0.52518100
H	-3.17491900	5.64806700	-1.02335000

TS4RS'

C	2.63383300	2.20894400	0.87043800
C	2.47091100	4.21210200	1.72738700
C	0.31885900	3.28798100	0.93667500
H	0.05786400	2.67606600	0.07448000
N	3.71528200	3.87484400	1.90618700
N	3.79970000	2.62231100	1.37422300

N	1.77966500	3.22805200	1.08015500
C	1.73756100	5.47521300	2.04369600
H	2.43575200	6.30733600	2.12934100
H	1.18558200	5.37391400	2.98877100
C	-0.15938300	4.77861900	0.77480300
O	0.88062700	5.72675500	0.94845100
C	-1.24315900	3.75407800	2.69762300
C	-0.33495000	2.81361700	2.21365700
C	-0.08290900	1.62635400	2.88527700
C	-0.78380200	1.41929600	4.06561100
C	-1.70859800	2.32906400	4.57226500
C	-1.94143600	3.51120700	3.87942000
C	-1.31157100	4.95613500	1.79444400
H	0.62656000	0.88313700	2.53437500
H	-2.22225100	2.10516300	5.49862100
H	-2.64986000	4.23638300	4.26485200
H	-1.20060800	5.90219600	2.33285300
H	-2.27417900	4.99297500	1.27572900
C	5.05155100	1.91239200	1.41028800
C	5.43223900	1.34298800	2.62657500
C	5.78904700	1.79247100	0.23080700
C	6.62183900	0.61501900	2.63946700
C	6.97233600	1.06086600	0.30121600
C	7.39824000	0.46105200	1.48976100
H	6.94194200	0.15035300	3.56805900
H	7.57080300	0.94640700	-0.59964600
C	5.30174500	2.37861600	-1.06631900
H	4.92684000	3.39734200	-0.93496100
H	4.48802200	1.77023800	-1.48081800
H	6.10730100	2.39773700	-1.80187300
C	4.56669600	1.47571000	3.85091600
H	3.55446800	1.10161900	3.65689700
H	4.47806300	2.52050200	4.16164000
H	4.98593700	0.90251900	4.67834300
H	-0.50144300	4.94096000	-0.24643700
C	8.66673700	-0.35028200	1.51213100
H	8.89259700	-0.70703800	2.51842100
H	8.57692500	-1.21866500	0.85237900
H	9.51424500	0.24276000	1.15767400
N	-0.52444300	0.18693700	4.82061900
O	-1.18063200	-0.01371400	5.82683600
O	0.33886500	-0.56322000	4.40028600
C	5.16939000	-4.04965000	0.78381600
C	4.56904400	-2.80844700	0.61894100

C	3.26514400	-2.71329400	0.10456600
C	2.59433700	-3.88852300	-0.26334200
C	3.19841400	-5.12986700	-0.10162500
C	4.48439800	-5.21285900	0.42905900
H	6.17670600	-4.11339200	1.18290500
H	5.11870700	-1.90751900	0.88128200
H	1.60119100	-3.81037900	-0.70079300
H	2.67017100	-6.02879400	-0.40377500
H	4.95807500	-6.18110800	0.55677400
C	2.60001300	-1.43406400	-0.10266400
H	1.61744200	-1.46752300	-0.56870400
C	2.98919600	-0.24208300	0.48787800
C	2.25826400	0.92339800	0.16831800
O	1.31375300	1.01766900	-0.63333200
H	3.84533300	-0.18862300	1.14692200
C	4.30994200	-1.70361800	-2.65460300
C	3.03474900	-1.09682400	-2.59024100
C	2.09155600	-2.11719000	-2.94126000
N	2.89654000	-3.24296300	-3.18103000
H	2.78606200	-0.05293800	-2.46134800
N	4.24380300	-2.97381600	-2.97729200
C	2.51801800	-4.56659400	-3.43575800
C	1.17343000	-4.93426700	-3.60051300
C	3.51024800	-5.55931700	-3.51325100
C	0.84531100	-6.26781800	-3.83438400
H	0.41255500	-4.16927600	-3.53344500
C	3.16003300	-6.88160900	-3.75129100
H	4.54415000	-5.27436600	-3.37186700
C	1.82546100	-7.25244100	-3.91288800
H	-0.20082800	-6.53358100	-3.95775500
H	3.94341700	-7.63210700	-3.80802500
H	1.55788400	-8.28777200	-4.09715300
N	0.78307300	-2.12657000	-2.96212600
H	0.48370300	-1.17762500	-2.73221500
C	5.61685300	-1.06942400	-2.30727400
H	5.58064700	-0.68776300	-1.27907200
H	6.42597100	-1.79876800	-2.38134100
H	5.83974200	-0.22115700	-2.96306400

TS4RS"

C	1.11256900	0.93530300	-0.68500300
C	0.38656500	2.16226500	-2.33363100
C	-1.36496300	0.80277700	-1.20146100
H	-1.34439900	-0.21853400	-0.81738400

N	1.63774300	2.49528300	-2.19636300
N	2.07001500	1.72944900	-1.15212300
N	0.02814800	1.20588800	-1.42365600
C	-0.64908700	2.57176700	-3.33100000
H	-0.17657100	2.91117100	-4.25241500
H	-1.26812500	3.38507700	-2.92842700
C	-2.19036800	0.94208900	-2.53433600
O	-1.40926500	1.41523700	-3.62184100
C	-3.17061900	2.32686600	-0.79255300
C	-2.03298700	1.74901700	-0.23539600
C	-1.61197900	2.04561400	1.05405400
C	-2.39563400	2.94056200	1.76774700
C	-3.55591500	3.51998000	1.25384000
C	-3.94663300	3.21164300	-0.04199200
C	-3.38289800	1.87485200	-2.21058000
H	-0.72285000	1.60534200	1.49653800
H	-4.12639000	4.20369700	1.86970300
H	-4.83941100	3.66140300	-0.46303300
H	-3.41242800	2.71651100	-2.91081800
H	-4.32624300	1.33559000	-2.32128700
C	3.43248200	1.80117400	-0.69185500
C	3.72696500	2.68467400	0.34516000
C	4.37894800	0.98536000	-1.31512300
C	5.05775400	2.74788500	0.75786900
C	5.69208500	1.08716700	-0.86527400
C	6.04681300	1.96156300	0.16619200
H	5.32431900	3.42604700	1.56403200
H	6.45637800	0.46829500	-1.32852600
C	3.97695900	0.03134600	-2.40795600
H	3.46089500	0.55188200	-3.22005800
H	3.29742900	-0.73578300	-2.01953800
H	4.85300700	-0.46990400	-2.82093600
C	2.64593200	3.50381800	0.99564400
H	1.95798600	2.84208500	1.53302800
H	2.06964400	4.06401700	0.25273500
H	3.07465500	4.21277900	1.70488900
H	-2.53521700	-0.04725400	-2.84204800
C	7.47640900	2.03471100	0.63546700
H	7.62139200	2.85614200	1.33938700
H	7.76516500	1.10498200	1.13501100
H	8.15739400	2.17719800	-0.20786500
N	-1.98104300	3.29654600	3.12909200
O	-2.71266800	4.02347300	3.77793600
O	-0.92136400	2.85107300	3.53705500

C	1.41721000	-5.71746600	-0.99694700
C	1.19736600	-4.37731600	-0.68663500
C	1.63985200	-3.84782700	0.53477700
C	2.27243100	-4.70870200	1.44941800
C	2.47922600	-6.04518100	1.14483600
C	2.05554800	-6.55306400	-0.08684200
H	1.07416000	-6.11010200	-1.94865900
H	0.68690200	-3.74038300	-1.40083200
H	2.60333800	-4.30996200	2.40515300
H	2.97391900	-6.69403800	1.86032500
H	2.22133600	-7.59787800	-0.32937300
C	1.46557900	-2.44634600	0.89228800
H	1.88628600	-2.13965700	1.84787000
C	1.13020600	-1.42470700	0.02411200
C	1.29168900	-0.07656700	0.43544000
O	1.65953600	0.37865900	1.52349700
H	0.78427500	-1.61667500	-0.98699100
C	-0.97202900	-1.56857500	2.44899000
C	-0.65571000	-2.92776900	2.23812800
C	-1.37097900	-3.33263400	1.06101000
N	-1.96057900	-2.13327100	0.61551300
H	-0.16529100	-3.60344000	2.92426500
N	-1.71523500	-1.07504000	1.47842100
C	-2.97060200	-1.99044700	-0.34410600
C	-2.99254300	-2.79438500	-1.49384400
C	-3.95720300	-1.00717300	-0.17019200
C	-4.00115200	-2.62058800	-2.43780900
H	-2.23283200	-3.55527900	-1.61324100
C	-4.96063400	-0.85414100	-1.12113400
H	-3.92839200	-0.38931500	0.71996000
C	-4.99119600	-1.65413600	-2.26314900
H	-4.00969300	-3.25030300	-3.32234900
H	-5.73030300	-0.10391900	-0.96003600
H	-5.77642900	-1.53033200	-3.00139600
N	-1.51039100	-4.46057000	0.42782300
H	-0.99040600	-5.16920500	0.94575100
C	-0.50287800	-0.69249800	3.56720800
H	-0.72099700	-1.15291200	4.53509200
H	0.57537100	-0.52556100	3.49747900
H	-0.99799700	0.28015800	3.52081300

TS4RS'''

C	-1.93239800	0.69434800	-0.67135900
C	-4.07322800	0.57323900	-1.08368600

C	-2.87901700	-1.59536800	-1.22110800
H	-1.88346200	-1.86770300	-1.58056100
N	-3.87111700	1.80946300	-0.73156800
N	-2.53145100	1.86080700	-0.46557800
N	-2.90460200	-0.13936100	-1.07004200
C	-5.29559000	-0.15111100	-1.54792700
H	-6.02810700	0.54856100	-1.94875500
H	-5.75060100	-0.70846300	-0.71724800
C	-4.01223900	-2.05809100	-2.21193900
O	-4.87884700	-1.00349100	-2.59797300
C	-4.28906800	-3.14504000	-0.05425500
C	-3.23014800	-2.25180900	0.09501400
C	-2.64271300	-2.00235200	1.32792600
C	-3.16581800	-2.69877300	2.40850600
C	-4.21287200	-3.61088500	2.29807800
C	-4.78246100	-3.83700900	1.05077000
C	-4.75191600	-3.20738300	-1.48516600
H	-1.81936200	-1.30242700	1.45944900
H	-4.57062300	-4.11907600	3.18470400
H	-5.60710800	-4.53394400	0.94736900
H	-5.83431700	-3.08746900	-1.59019100
H	-4.48975200	-4.17041600	-1.93337600
C	-1.90017800	3.07155700	-0.01029700
C	-1.81698300	3.28239800	1.36765900
C	-1.39040700	3.95082800	-0.96583000
C	-1.17614800	4.44584600	1.78640200
C	-0.76194200	5.10156400	-0.49286300
C	-0.64415500	5.36081700	0.87379800
H	-1.08165000	4.63727900	2.85224900
H	-0.34380900	5.80405100	-1.20899900
C	-1.47767700	3.63661000	-2.43512300
H	-2.50322400	3.40134900	-2.73384700
H	-0.85235300	2.77025100	-2.67999100
H	-1.12950000	4.48233600	-3.02904500
C	-2.37171400	2.27763500	2.34022600
H	-1.83238600	1.32958900	2.24257400
H	-3.43325200	2.09019300	2.14996400
H	-2.26367300	2.63688600	3.36433300
H	-3.56670000	-2.39510600	-3.14680400
C	0.03554000	6.61271000	1.36294800
H	0.62190600	6.41287700	2.26287600
H	0.69930100	7.02528800	0.60053700
H	-0.70466900	7.37908200	1.61427600
N	-2.59447100	-2.44513300	3.73806300

O	-2.99300300	-3.12461600	4.66789900
O	-1.75905400	-1.56449800	3.83613100
C	2.72051800	-1.51038300	-4.79635200
C	2.05618900	-0.83671200	-3.78371300
C	2.28973100	-1.16058300	-2.43376300
C	3.23349700	-2.15353600	-2.13823500
C	3.88150100	-2.84811600	-3.15915500
C	3.62761500	-2.53018400	-4.48694700
H	2.53422100	-1.24653800	-5.83261800
H	1.36253400	-0.03966900	-4.03550900
H	3.44374300	-2.39055000	-1.09922400
H	4.59678900	-3.62500700	-2.90949600
H	4.13795800	-3.06180700	-5.28369300
C	1.58748900	-0.49597900	-1.34003800
H	1.85457300	-0.80791300	-0.33129700
C	0.29884100	0.04973800	-1.48928700
C	-0.48726600	0.32560400	-0.36494600
O	-0.21253600	0.25707500	0.84721300
H	-0.14135700	0.19280000	-2.47090300
C	2.76245200	1.70152400	0.26620300
C	3.18414900	1.27733400	-1.03201900
C	4.33336400	0.43717800	-0.80478000
N	4.34964100	0.27531900	0.59111100
H	2.96884000	1.76442700	-1.97295800
N	3.41465600	1.08675700	1.21810100
C	5.18498500	-0.52252900	1.38568400
C	6.04348700	-1.48198300	0.82545300
C	5.14399700	-0.37403800	2.78169100
C	6.84072600	-2.26299300	1.65802900
H	6.07810700	-1.59143900	-0.24948800
C	5.94766900	-1.16479500	3.59230500
H	4.47356700	0.35909400	3.20970100
C	6.80539800	-2.11585400	3.04154600
H	7.50075100	-2.99961000	1.20889500
H	5.90130100	-1.03265800	4.66931000
H	7.43373800	-2.72863900	3.67948100
N	5.18469800	-0.12521800	-1.60883800
H	4.92345100	0.13466000	-2.56050300
C	1.71449100	2.71864900	0.57777300
H	1.36127700	2.60298700	1.60333000
H	2.11113700	3.73258000	0.45307800
H	0.86252900	2.61752800	-0.09986400

TS4SR

C	1.13512500	2.32904400	-0.40029300
C	1.42648800	4.49762400	-0.36881600
C	-0.94283700	3.75743000	-0.83538900
H	-1.13711500	3.32762200	-1.81600400
N	2.59837200	4.00016600	-0.10201300
N	2.40223800	2.65153600	-0.12180600
N	0.49187300	3.50905800	-0.53885000
C	1.08820900	5.94467400	-0.55261100
H	1.87065200	6.41844400	-1.14706300
H	1.04108100	6.45390200	0.41705800
C	-1.17582000	5.29217200	-0.74866900
O	-0.11712200	6.05948800	-1.27383100
C	-2.20951400	4.28120300	1.12641100
C	-1.87218600	3.24486800	0.24762400
C	-2.43863300	1.98204000	0.37788300
C	-3.30564600	1.79578500	1.45022500
C	-3.62683500	2.79708600	2.36193200
C	-3.07988400	4.06221300	2.18975200
C	-1.55395700	5.57123800	0.72189100
H	-2.22068600	1.19051800	-0.33215300
H	-4.31200400	2.58028500	3.17170800
H	-3.34342200	4.86804800	2.86616700
H	-0.67343200	5.75672700	1.34723200
H	-2.21089900	6.43773700	0.81791700
C	3.52460500	1.77182200	0.07540800
C	3.94441800	1.53041700	1.38598500
C	4.12500400	1.20087300	-1.04539000
C	5.01755800	0.66050300	1.55897700
C	5.19507800	0.33468200	-0.81806100
C	5.65005300	0.05203200	0.46953400
H	5.36673200	0.44894500	2.56676800
H	5.68116500	-0.13147300	-1.67078400
C	3.61618900	1.48347700	-2.43225200
H	3.47785500	2.55658000	-2.59435400
H	2.64960500	0.99366700	-2.59485900
H	4.31639200	1.10884700	-3.17994800
C	3.24013100	2.17278900	2.55123500
H	2.17315300	1.92410900	2.54939800
H	3.32166600	3.26281600	2.50700900
H	3.66817900	1.83094800	3.49428200
H	-2.03757100	5.51328100	-1.38189200
C	6.80051000	-0.89353800	0.69602600
H	7.61560300	-0.39414600	1.22744400
H	6.48680800	-1.74526600	1.30649900

H	7.19055000	-1.27674900	-0.24841000
N	-3.94162500	0.48268200	1.62371600
O	-4.57291600	0.28662800	2.64832600
O	-3.80450900	-0.33812800	0.73396100
C	3.34910400	-3.68605500	0.99835700
C	2.63835100	-2.53708500	0.65278700
C	1.44835700	-2.62837600	-0.07728400
C	1.00106800	-3.89882100	-0.46672500
C	1.70746800	-5.04417400	-0.12085900
C	2.88543900	-4.94189100	0.61900300
H	4.27125400	-3.59562000	1.56448600
H	3.03346500	-1.56754600	0.94228300
H	0.08172400	-3.98205300	-1.04327600
H	1.33975400	-6.01739800	-0.43017600
H	3.43941600	-5.83451100	0.89123900
C	0.64402900	-1.42950600	-0.46844600
H	0.35300800	-1.46113500	-1.52156800
C	1.11016600	-0.09722000	-0.09294500
C	0.54965600	0.98640700	-0.71771500
O	-0.39245600	1.01321600	-1.57963800
H	1.83475200	0.04075700	0.69701900
C	-1.32324700	-2.68921600	1.17935700
C	-1.15334200	-1.58895100	0.21845100
C	-2.01758100	-2.00455500	-0.92464400
N	-2.47846700	-3.27911100	-0.56356900
H	-1.30214600	-0.57737800	0.58242500
N	-2.04669600	-3.64535200	0.70743600
C	-3.23303300	-4.20287100	-1.30463000
C	-3.86140700	-3.83641500	-2.50304600
C	-3.36193200	-5.51796100	-0.83217300
C	-4.59909800	-4.78349300	-3.20829100
H	-3.75856200	-2.82366000	-2.86595900
C	-4.10752100	-6.44439600	-1.55000000
H	-2.87674900	-5.79602200	0.09417100
C	-4.73148500	-6.08896500	-2.74427600
H	-5.08045900	-4.48616800	-4.13528900
H	-4.19704800	-7.45711400	-1.16864800
H	-5.31052400	-6.81740100	-3.30201600
N	-2.25869800	-1.40687500	-2.02783100
H	-1.73406000	-0.52446800	-2.01374700
C	-0.70497200	-2.75693300	2.53253800
H	-1.02459800	-1.90658000	3.14288300
H	-0.98711900	-3.68366900	3.03381300
H	0.38617800	-2.71190300	2.44436200

TS4SR'

C	0.12645900	1.14503500	-1.05857900
C	-1.25248500	2.78825600	-1.49896500
C	-2.36386400	0.61591900	-1.45065400
H	-2.07174800	-0.43433400	-1.54536600
N	-0.12452700	3.37421900	-1.22472100
N	0.72085900	2.33945700	-0.94310300
N	-1.14549700	1.42923500	-1.39656700
C	-2.54226000	3.32694600	-2.03277500
H	-2.37508300	4.29941700	-2.49548700
H	-3.29112300	3.43237100	-1.23836300
C	-3.26827900	1.10578400	-2.63093200
O	-2.95235800	2.42958600	-3.05021500
C	-4.53953800	1.11716600	-0.58674100
C	-3.21447800	0.88251000	-0.22600600
C	-2.79784900	0.88905800	1.09559300
C	-3.77698200	1.15361100	2.04457000
C	-5.11258500	1.39403100	1.72561400
C	-5.50010100	1.37299800	0.39013100
C	-4.70406500	1.00713300	-2.07951200
H	-1.78249900	0.61776900	1.38008300
H	-5.82211500	1.59357100	2.51872800
H	-6.53413300	1.55930900	0.12011500
H	-5.34279100	1.77808600	-2.51751700
H	-5.13092500	0.02896700	-2.32994000
C	2.05531500	2.61571000	-0.48525500
C	2.23108900	2.78633000	0.88935600
C	3.09758600	2.63640600	-1.41058900
C	3.53533000	2.97782000	1.34142800
C	4.38246200	2.83138100	-0.90815600
C	4.61877900	2.99165400	0.45931100
H	3.70965600	3.10851700	2.40621700
H	5.22060100	2.84572000	-1.59999700
C	2.83798800	2.39730300	-2.87254200
H	2.01528200	3.01796400	-3.23796600
H	2.56778800	1.34867700	-3.04136300
H	3.72878700	2.61711500	-3.46220200
C	1.05676100	2.71001200	1.82873100
H	0.56235300	1.73419600	1.75069500
H	0.30960800	3.47389900	1.59204200
H	1.37838700	2.84867600	2.86147900
H	-3.11904100	0.49052400	-3.51848400
C	6.02611200	3.13998300	0.97499600

H	6.04085500	3.61640400	1.95729500
H	6.49802700	2.15661400	1.07165000
H	6.63740000	3.73263400	0.29068600
N	-3.38133400	1.16940400	3.45801700
O	-4.25250800	1.34147400	4.29400700
O	-2.20163000	1.01138800	3.71989800
C	5.91139800	-1.48242800	1.16117600
C	4.57589500	-1.24386100	0.85762400
C	3.92340400	-1.99008700	-0.13448500
C	4.64856100	-2.97863000	-0.81043900
C	5.98682400	-3.21700700	-0.50845300
C	6.62327900	-2.46999600	0.47894300
H	6.39903300	-0.90069200	1.93746300
H	4.02802200	-0.47893600	1.40300500
H	4.15634200	-3.55497700	-1.58968500
H	6.53164700	-3.98598500	-1.04690700
H	7.66508200	-2.65613900	0.71876600
C	2.51478200	-1.73874100	-0.50384700
H	2.07237600	-2.43888600	-1.20894000
C	1.98210300	-0.45742600	-0.48922000
C	0.71608200	-0.24986900	-1.08611200
O	0.04793800	-1.07403500	-1.73185400
H	2.47446000	0.33856400	0.05129700
C	1.26375500	-4.14199000	0.65375200
C	1.49193500	-2.83783600	1.19470200
C	0.22322700	-2.16678000	1.10362600
N	-0.57700600	-3.06397000	0.39675900
H	2.26450500	-2.56988700	1.90204300
N	0.06674200	-4.24680500	0.12755300
C	-1.88086600	-2.86443800	-0.08239600
C	-2.84214000	-2.24796300	0.71965700
C	-2.22186200	-3.31764400	-1.36184100
C	-4.13747900	-2.07926000	0.23699300
H	-2.56144400	-1.89705600	1.70633800
C	-3.51736800	-3.14510100	-1.83288400
H	-1.45524400	-3.78571200	-1.96827600
C	-4.48244400	-2.52194700	-1.03755900
H	-4.87826400	-1.58968800	0.86406900
H	-3.77625900	-3.49450500	-2.82764900
H	-5.49588500	-2.39515200	-1.40601300
N	-0.15064700	-0.95744800	1.43243100
H	0.62584200	-0.53739100	1.94330700
C	2.22275500	-5.28802200	0.61132400
H	2.46248000	-5.63151200	1.62250400

H	1.78685900	-6.11985500	0.05502900
H	3.16477100	-4.99619100	0.13809200

TS4SR"

C	-0.62140900	1.74135400	-0.26177800
C	-2.28275600	2.59993300	0.88124600
C	-2.99842800	1.64188200	-1.25212300
H	-2.50157100	1.42705800	-2.19903500
N	-1.23869500	2.77792400	1.63534000
N	-0.21532300	2.23499100	0.91505300
N	-1.95073800	1.96968400	-0.28495000
C	-3.68381300	3.10355200	1.00050900
H	-3.74201500	3.87648700	1.76608100
H	-4.37774400	2.29239200	1.25383600
C	-3.99195600	2.84668600	-1.38114100
O	-3.98782900	3.70575600	-0.24664300
C	-5.22177600	0.81044800	-0.99888300
C	-3.87654700	0.49472500	-0.78814400
C	-3.49097900	-0.72127400	-0.23774900
C	-4.52176700	-1.60116800	0.08576400
C	-5.86887100	-1.32008900	-0.11986400
C	-6.22468600	-0.09557000	-0.67108700
C	-5.36553100	2.18478100	-1.59599600
H	-2.44971600	-0.99932200	-0.07446800
H	-6.61365900	-2.05438700	0.15949000
H	-7.26920900	0.14911700	-0.83121700
H	-6.15611100	2.78106900	-1.13385800
H	-5.58586700	2.11044900	-2.66641400
C	1.10445000	2.18329800	1.48482100
C	1.35499100	1.15999800	2.40019700
C	2.06411600	3.10327800	1.06268500
C	2.65667800	1.05090600	2.88647900
C	3.34754400	2.95600900	1.58529800
C	3.66243900	1.93217600	2.48322000
H	2.88671500	0.25037900	3.58489800
H	4.12303400	3.65170100	1.27495300
C	1.73585600	4.16601900	0.05015200
H	0.78908200	4.66200400	0.28159700
H	1.64808800	3.72248700	-0.94802500
H	2.52356700	4.91988200	0.01651200
C	0.25920600	0.21912500	2.81677900
H	-0.22525000	-0.22764600	1.94098400
H	-0.50792300	0.74864900	3.39058400
H	0.65927400	-0.59501500	3.42327600

H	-3.70803200	3.48762600	-2.21612400
C	5.07384700	1.76387500	2.98195600
H	5.09445800	1.25078500	3.94563500
H	5.65861700	1.16632800	2.27460900
H	5.57302800	2.72945200	3.08938100
N	-4.18145900	-2.89594100	0.68815300
O	-5.08269500	-3.69460500	0.87458800
O	-3.01531500	-3.10036400	0.97302100
C	5.76325100	-0.22955700	-1.19893400
C	4.38832900	-0.01708100	-1.13725100
C	3.60931000	-0.04390200	-2.30316500
C	4.24458000	-0.32107900	-3.52404300
C	5.61325500	-0.54538300	-3.58452000
C	6.37951900	-0.49517200	-2.41806300
H	6.35302000	-0.19919500	-0.28819600
H	3.92105900	0.18617600	-0.17746000
H	3.64670700	-0.35581800	-4.43173800
H	6.08657100	-0.75225400	-4.53908700
H	7.45051600	-0.66525200	-2.46226500
C	2.16280500	0.18833700	-2.28997500
H	1.70462500	0.34264600	-3.26385300
C	1.46262500	0.72340700	-1.20512300
C	0.15818500	1.18622700	-1.43191200
O	-0.44593000	1.24696600	-2.52547600
H	1.86094400	0.67351400	-0.20175100
C	0.09436900	-1.86618200	-2.04846500
C	1.46291700	-2.03300300	-2.39507000
C	2.13385600	-2.39071700	-1.16339900
N	1.15172700	-2.16327800	-0.18635600
H	1.85226600	-2.26378000	-3.37762600
N	-0.08331900	-1.87760900	-0.74627800
C	1.23445100	-2.51062500	1.17157400
C	2.42875900	-2.32632100	1.87876800
C	0.11416400	-3.03654700	1.82427300
C	2.49273100	-2.68070800	3.22391000
H	3.29158500	-1.92544900	1.36232300
C	0.18971600	-3.36999000	3.17217300
H	-0.80225100	-3.17118600	1.26464100
C	1.37855700	-3.20047100	3.88105400
H	3.42522500	-2.54019900	3.76328800
H	-0.68776800	-3.77639300	3.66647600
H	1.43664900	-3.47186800	4.93014000
N	3.33118700	-2.79070000	-0.88319200
H	3.84734400	-2.86433600	-1.76040300

C	-1.05322100	-1.65788800	-2.98459200
H	-1.27970900	-2.58459100	-3.52157600
H	-1.94361000	-1.35552100	-2.42846700
H	-0.82046900	-0.87747900	-3.71090700
TS4SR'''			
C	2.06719600	-0.81549800	-0.77633400
C	4.18767700	-1.32387200	-0.95675900
C	3.64580100	0.95236900	-1.75441000
H	2.77689800	1.36903600	-2.26070000
N	3.65071500	-2.35483100	-0.37477500
N	2.33150500	-2.01995300	-0.25958500
N	3.25519300	-0.35985800	-1.22056300
C	5.57962600	-1.08507400	-1.44176400
H	6.10990800	-2.02990400	-1.55443000
H	6.13114400	-0.44580100	-0.73865200
C	4.89065500	0.81150000	-2.70922900
O	5.45581500	-0.48957400	-2.71837500
C	5.39865300	2.34851000	-0.89484800
C	4.12844800	1.84052900	-0.63001600
C	3.45720200	2.12491500	0.55047000
C	4.12199900	2.93343500	1.46125600
C	5.38911700	3.46544500	1.22985200
C	6.03430800	3.17140800	0.03475200
C	5.89739300	1.88980800	-2.23863800
H	2.45741000	1.75217500	0.74167200
H	5.84983900	4.09134200	1.98350300
H	7.02316500	3.57108900	-0.16212900
H	6.90879700	1.47407800	-2.20194700
H	5.91821400	2.72506200	-2.94503200
C	1.44472200	-2.89161200	0.46348800
C	1.07739000	-2.52815000	1.75863900
C	1.00154700	-4.05572200	-0.17168700
C	0.21864200	-3.39464400	2.43800300
C	0.13891100	-4.87851000	0.54591800
C	-0.26238100	-4.56340100	1.84904200
H	-0.09024300	-3.13774700	3.44806100
H	-0.23253500	-5.78630900	0.07729500
C	1.42120900	-4.37232000	-1.58190900
H	2.50406100	-4.50944300	-1.64918700
H	1.15076400	-3.55600000	-2.26026600
H	0.93308600	-5.28280300	-1.93077800
C	1.53639800	-1.23442600	2.37655600
H	0.97344700	-0.39011400	1.95787600
H	2.59977000	-1.05045600	2.19503900

H	1.36754200	-1.24364300	3.45428800
H	4.57923800	0.97636800	-3.73989600
C	-1.19994100	-5.47804300	2.59260200
H	-1.46149700	-5.06850100	3.56968900
H	-2.12246900	-5.62963900	2.02530700
H	-0.74391100	-6.46070300	2.74349000
N	3.45627300	3.23367200	2.73510200
O	4.00954600	4.00478300	3.49952100
O	2.38964500	2.68919900	2.96113000
C	-4.40334900	-2.57898500	-0.96486700
C	-3.15584200	-1.98600200	-0.80089900
C	-2.90562800	-0.70171200	-1.30673000
C	-3.94415400	-0.02186700	-1.95906400
C	-5.19358400	-0.61054800	-2.11270900
C	-5.42453400	-1.89515600	-1.62245600
H	-4.58178600	-3.57448200	-0.57081400
H	-2.37415200	-2.52481500	-0.27104800
H	-3.76634700	0.98953700	-2.31766300
H	-5.98985200	-0.06155800	-2.60557900
H	-6.39882300	-2.35775400	-1.74389700
C	-1.61085500	-0.03051900	-1.12771800
H	-1.50412300	0.92227900	-1.64506700
C	-0.40510400	-0.75550900	-0.92216100
C	0.78322200	-0.03789400	-0.87316300
O	0.92366800	1.21345100	-0.92678000
H	-0.41093800	-1.83138600	-0.80788300
C	-2.66182900	0.32586300	1.52934900
C	-1.91388600	1.21393200	0.68603300
C	-2.90014200	2.13025700	0.13623100
N	-4.11958800	1.62958000	0.60727200
H	-0.86516700	1.46945300	0.77700600
N	-3.94351400	0.53051600	1.44226500
C	-5.42457000	1.96736700	0.22001300
C	-5.69498400	3.13315300	-0.51096900
C	-6.48346900	1.11184300	0.56419700
C	-7.00478700	3.42173600	-0.88746700
H	-4.87858100	3.78721700	-0.78131400
C	-7.78252300	1.42281700	0.18442400
H	-6.26739500	0.20618300	1.11513600
C	-8.05748600	2.57817200	-0.54626800
H	-7.19786800	4.32750700	-1.45469600
H	-8.58769400	0.74758700	0.45841600
H	-9.07381600	2.81447600	-0.84348000
N	-2.77606200	3.12553000	-0.68372600

H	-1.77778900	3.25228800	-0.85615000
C	-2.10017800	-0.79780300	2.32990600
H	-1.46588700	-0.42916300	3.14317900
H	-2.90147400	-1.40884800	2.74958400
H	-1.47121700	-1.42398000	1.68637000

TS4SS

C	-1.83320200	0.88478300	-0.80601100
C	-3.69019700	2.03258900	-0.93931200
C	-3.90772300	-0.30298800	-1.72159900
H	-3.22507200	-0.98074100	-2.23221200
N	-2.84298100	2.84220400	-0.37582200
N	-1.69300300	2.10881300	-0.29047100
N	-3.11389600	0.82393500	-1.21680100
C	-5.09592400	2.24075400	-1.39918400
H	-5.30441400	3.30353000	-1.51528000
H	-5.80812900	1.81207900	-0.68085100
C	-5.06120700	0.21596100	-2.65999700
O	-5.18917600	1.62885200	-2.67134100
C	-5.99729300	-1.05878300	-0.81432500
C	-4.62725400	-0.97599400	-0.57404700
C	-4.06047400	-1.43706800	0.60540700
C	-4.93236900	-1.97423100	1.54173900
C	-6.30658300	-2.07975900	1.33584000
C	-6.84543500	-1.61899000	0.14065200
C	-6.34677500	-0.48906700	-2.16274700
H	-2.99028000	-1.39863200	0.77576400
H	-6.92955800	-2.51067800	2.10928000
H	-7.91331800	-1.68626400	-0.03632300
H	-7.17871600	0.22047000	-2.12735900
H	-6.63369300	-1.28797500	-2.85314300
C	-0.56740400	2.61842500	0.44573400
C	-0.38871200	2.16033600	1.75171000
C	0.28727700	3.52616000	-0.18320100
C	0.72460100	2.63854300	2.44201300
C	1.39383100	3.95730300	0.54355400
C	1.63246200	3.51515300	1.84871200
H	0.90585000	2.28512000	3.45330600
H	2.09378800	4.64521700	0.07598300
C	0.02970500	3.97529200	-1.59676600
H	-0.93686000	4.48067900	-1.67795100
H	0.01048200	3.12122300	-2.28277900
H	0.80949400	4.66143500	-1.92882600
C	-1.31977500	1.14656500	2.36511000

H	-1.12536500	0.14369800	1.96356100
H	-2.36879200	1.38593700	2.16554200
H	-1.17706400	1.10128000	3.44535600
H	-4.83598300	-0.04164400	-3.69409800
C	2.85318100	3.98095800	2.59632800
H	3.02258500	3.37481600	3.48796000
H	3.74137600	3.91664900	1.96252000
H	2.74477100	5.02452400	2.90777500
N	-4.37538700	-2.44448600	2.81635300
O	-5.13087300	-2.98860000	3.60267200
O	-3.18849200	-2.25842200	3.02060900
C	4.72389300	0.79772900	-1.90913600
C	3.39791300	0.57174600	-1.56179300
C	2.78468600	-0.65796900	-1.85908800
C	3.54186400	-1.64840700	-2.50251100
C	4.86739200	-1.41581200	-2.85369900
C	5.46181500	-0.19136300	-2.55884700
H	5.19041000	1.74541800	-1.65907700
H	2.84797700	1.33495000	-1.01999600
H	3.07796200	-2.60548300	-2.72707600
H	5.43801600	-2.19338600	-3.35159400
H	6.49938500	-0.01164800	-2.82186100
C	1.40271900	-0.94831000	-1.46625400
H	0.96941600	-1.85606700	-1.88169300
C	0.47367600	0.08855700	-1.16862700
C	-0.85322700	-0.25051300	-0.94084900
O	-1.36243300	-1.40115100	-0.88352800
H	0.78740200	1.12218700	-1.12627200
C	2.41750400	-3.15941000	0.13760300
C	1.64789400	-1.99426200	0.47091800
C	2.60580600	-1.06269900	1.04358900
N	3.84237000	-1.69579200	0.84643000
H	0.58700900	-1.98733500	0.68883000
N	3.69345500	-2.96418400	0.30559800
C	5.13611000	-1.16020900	0.93542300
C	5.36904000	0.11391200	1.47362600
C	6.22202000	-1.91410100	0.46300900
C	6.66639200	0.61839000	1.51185800
H	4.53130900	0.69225400	1.83609200
C	7.50816000	-1.39364700	0.51687800
H	6.03701000	-2.89344300	0.04256700
C	7.74475900	-0.12117500	1.03582700
H	6.82927100	1.60968900	1.92539600
H	8.33436600	-1.99057300	0.14185000

H	8.75153400	0.28186000	1.07202800
N	2.45723600	0.11735500	1.55051600
H	1.46077300	0.33552600	1.53514200
C	1.89817400	-4.43872200	-0.43028800
H	1.35632200	-4.25372700	-1.36437900
H	2.72398500	-5.12296900	-0.63102400
H	1.19738300	-4.91778700	0.25931100

TS4SS'

C	-1.92739400	0.57232300	-0.82478800
C	-4.05152500	0.50776000	-1.33390500
C	-3.05170900	-1.69933200	-0.81478500
H	-2.07795500	-2.14225600	-1.03596600
N	-3.76023200	1.77469900	-1.28067300
N	-2.43394700	1.79320600	-0.94864300
N	-2.94962800	-0.26184300	-1.07405600
C	-5.31899900	-0.21446200	-1.66231600
H	-5.95967000	0.40260400	-2.29126900
H	-5.86335100	-0.47039000	-0.74255600
C	-4.20022800	-2.32997100	-1.68506500
O	-4.95206100	-1.36332100	-2.40160800
C	-4.61773700	-2.73327200	0.67738800
C	-3.48387900	-1.92547900	0.61647500
C	-2.89714400	-1.38867600	1.75505500
C	-3.49990200	-1.70981000	2.96372700
C	-4.62397400	-2.52608000	3.06738300
C	-5.19152300	-3.04376900	1.90927500
C	-5.06158400	-3.15494300	-0.69782100
H	-2.01928200	-0.74495300	1.72426500
H	-5.04202800	-2.73234500	4.04467900
H	-6.07529700	-3.66986500	1.96761200
H	-6.12530100	-2.97194600	-0.87711100
H	-4.88977300	-4.22503500	-0.84748900
C	-1.72902700	3.03294500	-0.75702700
C	-1.75893900	3.60694100	0.51465900
C	-1.04835300	3.58175200	-1.84359400
C	-1.06508100	4.80387000	0.67976300
C	-0.37800600	4.78387800	-1.62747800
C	-0.37163100	5.40163600	-0.37512300
H	-1.06157800	5.27719300	1.65811500
H	0.16396800	5.24006400	-2.45224500
C	-1.00032000	2.86671100	-3.16666900
H	-2.00246300	2.61098000	-3.52333100
H	-0.43194100	1.93308700	-3.07039300

H	-0.51139200	3.48500900	-3.92068800
C	-2.48082600	2.93273200	1.64874100
H	-2.00155800	1.97088000	1.86128500
H	-3.52961000	2.74628500	1.39750500
H	-2.44603800	3.54978500	2.54745800
H	-3.76812500	-2.96071900	-2.46092700
C	0.40588800	6.67297600	-0.15642400
H	1.44783400	6.44238300	0.08886200
H	0.40791000	7.29490500	-1.05431900
H	-0.00883600	7.25374100	0.67003700
N	-2.92937300	-1.14578900	4.19483300
O	-3.40637400	-1.50239800	5.25811300
O	-2.01513100	-0.34922900	4.08260700
C	2.19024600	-3.89425800	-3.27519500
C	1.69925500	-2.71057200	-2.74155100
C	1.96354100	-2.36157600	-1.40604600
C	2.75034700	-3.22550700	-0.63469200
C	3.22700000	-4.42294200	-1.16487300
C	2.94936200	-4.76123700	-2.48433000
H	1.98061800	-4.14604500	-4.31006100
H	1.11795300	-2.04221500	-3.37041900
H	2.98487700	-2.95385300	0.39066600
H	3.82851500	-5.08170900	-0.54705000
H	3.32740400	-5.68883600	-2.90176800
C	1.46236400	-1.11344100	-0.81222600
H	1.69422800	-0.97474200	0.24293900
C	0.20715900	-0.56195200	-1.21546200
C	-0.54080100	0.20308300	-0.33206200
O	-0.28361200	0.59860900	0.83030400
H	-0.21456200	-0.78729900	-2.18995100
C	2.98653100	1.41173300	-0.67276100
C	3.09261300	0.23554100	-1.50674000
C	4.31031900	-0.42640600	-1.04514100
N	4.66258000	0.28691900	0.11162000
H	2.78857800	0.20167400	-2.54567200
N	3.87065800	1.41444500	0.27938600
C	5.69344100	0.05826700	1.03631400
C	6.58706800	-1.01566000	0.90805200
C	5.82459500	0.93046300	2.12951700
C	7.58745100	-1.19563500	1.86101800
H	6.48896700	-1.68796400	0.06809200
C	6.83077100	0.73265900	3.06524000
H	5.12993300	1.75307100	2.22991800
C	7.72337000	-0.33070300	2.94226100

H	8.27217600	-2.03095900	1.74653000
H	6.91338200	1.41985100	3.90201800
H	8.50758800	-0.48134100	3.67662200
N	4.96052500	-1.44730600	-1.49297700
H	4.47488000	-1.78976500	-2.32276200
C	1.98849100	2.51517200	-0.79685000
H	2.31924600	3.38585300	-0.22632100
H	1.85771100	2.80625800	-1.84326200
H	1.01566400	2.20320100	-0.40513600

TS4SS"

C	1.79311700	-4.50048000	-2.60430500
C	1.39973200	-6.63610500	-2.81724000
C	-0.63707300	-5.25875500	-2.55467400
H	-0.85421200	-4.32565800	-2.02955300
N	2.68781700	-6.51735800	-2.95399900
N	2.91567700	-5.17338000	-2.82079500
N	0.81508000	-5.41748000	-2.60719000
C	0.50134400	-7.82781400	-2.73374300
H	1.07513100	-8.72351500	-2.49951400
H	-0.03383300	-7.97959300	-3.68063900
C	-1.28522100	-6.49795600	-1.83144700
O	-0.37880100	-7.57619900	-1.65247900
C	-2.26159900	-6.21586100	-4.03299200
C	-1.22238400	-5.29015400	-3.95053700
C	-0.80430600	-4.55369800	-5.05039300
C	-1.47863400	-4.79207100	-6.24073300
C	-2.53067600	-5.69710300	-6.35876800
C	-2.92827500	-6.41869600	-5.23971200
C	-2.49895000	-6.88488800	-2.70586800
H	-0.00579900	-3.81943000	-4.98739300
H	-3.01112300	-5.83133800	-7.31974800
H	-3.73636400	-7.13826200	-5.31418300
H	-2.58239300	-7.97290300	-2.77951500
H	-3.42476300	-6.51628700	-2.25313900
C	4.20083100	-4.62623000	-3.17641000
C	4.34223000	-4.18344100	-4.49352400
C	5.22928700	-4.62524600	-2.23761200
C	5.60430900	-3.73428200	-4.87132400
C	6.46581000	-4.14514700	-2.66379000
C	6.66712900	-3.69393400	-3.96950200
H	5.75182700	-3.39054700	-5.89181900
H	7.29298900	-4.12700600	-1.95783800
C	5.01228100	-5.09436400	-0.82407000

H	4.40346100	-6.00130300	-0.78558100
H	4.50268800	-4.32144300	-0.23710200
H	5.96812800	-5.29899000	-0.33908600
C	3.17270000	-4.16451800	-5.44172900
H	2.47750900	-3.35985800	-5.16614300
H	2.62627100	-5.11444100	-5.43314600
H	3.50601900	-3.96479800	-6.46074900
H	-1.58315100	-6.22578300	-0.81958800
C	8.00271500	-3.13867100	-4.38838700
H	8.04792800	-2.06585100	-4.17245600
H	8.82168700	-3.61968000	-3.84873000
H	8.16731600	-3.26842100	-5.46033400
N	-1.04697800	-4.06534200	-7.44135000
O	-1.73293900	-4.16330800	-8.44423600
O	-0.02208900	-3.41084500	-7.36943500
C	2.26929700	-0.97415800	3.00288700
C	2.24189600	-1.48784900	1.71091600
C	1.58263200	-0.79857200	0.68220600
C	0.93862100	0.40921800	0.99415100
C	0.96420300	0.92094400	2.28471000
C	1.63313700	0.23103500	3.29589800
H	2.78754000	-1.51796500	3.78628400
H	2.73739200	-2.43209000	1.50490500
H	0.42660300	0.94895700	0.20113300
H	0.46274700	1.85812400	2.50393000
H	1.65624900	0.62834700	4.30534100
C	1.51911900	-1.28940000	-0.69802700
H	0.88885800	-0.72328900	-1.38185000
C	1.93046900	-2.53210100	-1.12027100
C	1.52973700	-3.01969900	-2.39279900
O	0.84347700	-2.48083100	-3.26501600
H	2.50581300	-3.19990500	-0.48759300
C	4.29902500	-0.64623500	-1.67475300
C	3.33839200	0.36498100	-1.47883800
C	2.62034500	0.48689300	-2.71941900
N	3.18198100	-0.52784300	-3.50750300
H	3.24746800	1.03717600	-0.63817200
N	4.20375800	-1.20385700	-2.86579200
C	3.03672800	-0.69212000	-4.89318000
C	1.77802500	-0.60604500	-5.49843300
C	4.16686900	-0.95468700	-5.67467800
C	1.66107300	-0.80260500	-6.87057900
H	0.91872500	-0.40031500	-4.87473700
C	4.03469000	-1.15640700	-7.04478200

H	5.13293400	-1.00951600	-5.18596800
C	2.78179300	-1.08601200	-7.65085200
H	0.67954800	-0.75908100	-7.33208200
H	4.91842800	-1.36588700	-7.64178700
H	2.67767000	-1.24797000	-8.71899000
N	1.65622900	1.26212600	-3.13533900
H	1.47004400	1.93339800	-2.38936400
C	5.24444600	-1.19903400	-0.65780200
H	5.90143500	-1.93925900	-1.12087900
H	5.85263600	-0.40931800	-0.20699300
H	4.68940500	-1.68254000	0.15594700

TS4SS'''

C	0.93376600	-1.77401400	-0.12986500
C	2.74244200	-2.30237300	0.99356300
C	3.23529500	-1.52708600	-1.26404400
H	2.68697100	-1.45397200	-2.20366900
N	1.77373800	-2.44193800	1.84888900
N	0.65719000	-2.10125600	1.14175200
N	2.27462100	-1.88864300	-0.22212800
C	4.19563200	-2.64379000	1.08093200
H	4.36582400	-3.33348900	1.90739200
H	4.80584400	-1.74511200	1.23340000
C	4.37027700	-2.59970400	-1.33450500
O	4.52309600	-3.32493200	-0.11895200
C	5.34305700	-0.40710800	-1.15703300
C	3.97773400	-0.25271500	-0.90419700
C	3.46310400	0.91009400	-0.34847700
C	4.38491500	1.91660500	-0.07709200
C	5.74598600	1.81091800	-0.34526900
C	6.23354400	0.62880300	-0.89188700
C	5.63148000	-1.78741200	-1.68703700
H	2.40291300	1.05755400	-0.14473100
H	6.40149300	2.63837100	-0.10439000
H	7.29483100	0.51233900	-1.08301000
H	6.52140900	-2.24616200	-1.24955300
H	5.76871400	-1.75923100	-2.77358100
C	-0.61799300	-2.05854400	1.80762300
C	-1.00586700	-0.83924300	2.36764000
C	-1.42672900	-3.19373000	1.78010100
C	-2.29004700	-0.77148400	2.90489300
C	-2.69819400	-3.07652000	2.33894700
C	-3.14966900	-1.87315100	2.88634400
H	-2.63129200	0.17267300	3.32355400

H	-3.35863400	-3.93957300	2.32666700
C	-0.95888100	-4.45849200	1.11398100
H	0.03005800	-4.75656100	1.47314000
H	-0.89008600	-4.31202800	0.03016200
H	-1.65861500	-5.27384300	1.30153700
C	-0.10084200	0.35854900	2.30514600
H	0.09352400	0.63970100	1.26084700
H	0.86296300	0.15218200	2.78295200
H	-0.56188700	1.21674900	2.79844600
H	4.14351000	-3.35795700	-2.08447200
C	-4.55847600	-1.75273200	3.40435700
H	-4.63495600	-0.98171500	4.17383500
H	-5.23426400	-1.47800000	2.58719000
H	-4.91099700	-2.69890100	3.82072900
N	3.90180800	3.14787600	0.55831800
O	4.65627500	4.10378300	0.60150600
O	2.77319600	3.14173900	1.01979300
C	-5.35793700	0.09975700	-0.18666200
C	-4.01409400	-0.07301400	-0.49784000
C	-3.63180200	-0.66384000	-1.71213500
C	-4.63265700	-1.06357700	-2.60582200
C	-5.97829300	-0.89653400	-2.29179900
C	-6.34536300	-0.31333000	-1.08083000
H	-5.63559700	0.56999000	0.75246900
H	-3.25261100	0.27207700	0.19802700
H	-4.34792400	-1.51936700	-3.55112600
H	-6.74012500	-1.22225000	-2.99298300
H	-7.39406500	-0.17651800	-0.83726400
C	-2.21125400	-0.87612500	-2.04102600
H	-1.98899000	-1.23045200	-3.04366500
C	-1.31731700	-1.20067600	-1.02442800
C	0.02581300	-1.48757200	-1.30654300
O	0.56423400	-1.56144600	-2.43459000
H	-1.63576100	-1.08314900	-0.00122200
C	-2.72863100	1.94483300	-2.75645500
C	-1.51571500	1.18904800	-2.80413500
C	-0.78162100	1.58341800	-1.63155900
N	-1.68956600	2.36884700	-0.92200100
H	-1.04302100	0.79090900	-3.69114000
N	-2.85680100	2.58751400	-1.62320700
C	-1.54881000	2.90568700	0.36992600
C	-0.30952100	3.37711800	0.81312300
C	-2.66650200	2.97850500	1.20800400
C	-0.19253200	3.90134700	2.09611200

H	0.55233800	3.30554200	0.16283600
C	-2.53640200	3.51174400	2.48739700
H	-3.62317700	2.62436600	0.83815900
C	-1.30026500	3.97216800	2.94012900
H	0.77782200	4.25719900	2.42843000
H	-3.40796100	3.56619500	3.13277600
H	-1.20300300	4.38542800	3.93881000
N	0.39374200	1.23997100	-1.18073600
H	0.82900200	0.67075200	-1.90740100
C	-3.79405100	2.01038000	-3.80175500
H	-3.49959300	2.67707100	-4.61875400
H	-3.97559000	1.02078400	-4.22871500
H	-4.72441500	2.38045400	-3.36628400

M4RR

C	1.54271100	0.54571700	-0.58476100
C	3.20069100	1.54020600	-1.61868700
C	3.44020900	1.51577300	0.84483900
H	2.70432300	1.60433600	1.64159200
N	2.42841600	1.11696100	-2.57372500
N	1.40619200	0.49108500	-1.91698600
N	2.69713700	1.21829700	-0.38883700
C	4.43337900	2.37993800	-1.66487100
H	4.50640400	2.89427600	-2.62258500
H	5.33194600	1.76385700	-1.52007400
C	4.30909700	2.81935000	0.66742200
O	4.28717100	3.35114800	-0.64717100
C	5.73462200	0.93902900	1.25872300
C	4.44620300	0.42405100	1.12913300
C	4.18462800	-0.93414800	1.24690000
C	5.27899800	-1.75590700	1.47744500
C	6.58228900	-1.27865600	1.60648300
C	6.81219000	0.08715800	1.50057500
C	5.73969700	2.43685200	1.12102000
H	3.17133700	-1.31813400	1.19140400
H	7.38932500	-1.97752900	1.78631500
H	7.81851300	0.47963800	1.60026400
H	6.47648400	2.79854500	0.39694300
H	5.97494400	2.90892600	2.07961200
C	0.37148600	-0.16071400	-2.67338200
C	0.44510500	-1.54522200	-2.82760600
C	-0.68035700	0.61650000	-3.16185700
C	-0.60678100	-2.16555700	-3.50002600
C	-1.70618500	-0.05099600	-3.82718500

C	-1.69149200	-1.43839700	-3.99263400
H	-0.58255700	-3.24432100	-3.63037300
H	-2.54510800	0.52464400	-4.21053700
C	-0.74010800	2.09702200	-2.89869500
H	0.21493100	2.58448800	-3.11014700
H	-0.98692700	2.28321300	-1.84627200
H	-1.51372900	2.56406000	-3.50983000
C	1.58483400	-2.33104700	-2.23810900
H	1.48299800	-2.38628900	-1.14777200
H	2.54977500	-1.86609200	-2.46040200
H	1.59220100	-3.34943200	-2.62865800
H	3.89413200	3.61451500	1.28594500
C	-2.84965000	-2.13748200	-4.65471300
H	-2.54875900	-3.10386000	-5.06439600
H	-3.64579400	-2.31651000	-3.92439200
H	-3.26966400	-1.53143300	-5.46070000
N	5.05042200	-3.20144900	1.59509100
O	6.00710800	-3.91182800	1.85350600
O	3.91689800	-3.61473800	1.42499900
C	-4.74100000	-1.20249000	-0.75537700
C	-3.56744800	-0.66408200	-0.23593400
C	-2.81320000	-1.37010000	0.71029100
C	-3.26234200	-2.62976000	1.11209000
C	-4.43658900	-3.17243500	0.59330400
C	-5.18065700	-2.45917600	-0.34183600
H	-5.31312400	-0.63827800	-1.48564200
H	-3.23530400	0.31753500	-0.56621800
H	-2.67708900	-3.20144700	1.82813400
H	-4.76565800	-4.15453800	0.91803100
H	-6.09557100	-2.87874400	-0.74782700
C	-1.53660400	-0.78716900	1.28637800
H	-1.01701600	-1.56750300	1.85903000
C	-0.61238500	-0.28312400	0.21865200
C	0.68812800	0.00105400	0.52825700
O	1.27044500	-0.10067900	1.66087000
H	-1.00808600	-0.14201900	-0.77514700
C	-2.80738000	-0.09269800	3.38485900
C	-1.82563500	0.34663800	2.34145000
C	-2.56393100	1.51588600	1.72662400
N	-3.83769200	1.47511900	2.28759300
H	-0.84909000	0.63850400	2.74391000
N	-3.92707700	0.52608600	3.30642700
C	-4.98807400	2.21482700	1.96331400
C	-4.98566500	3.14940800	0.91807100

C	-6.16766400	1.99881200	2.69178800
C	-6.15303300	3.84727400	0.61887300
H	-4.07669100	3.32345600	0.36104200
C	-7.31944800	2.70808000	2.37593200
H	-6.16865700	1.27457500	3.49512400
C	-7.32520900	3.63792500	1.33800600
H	-6.13593000	4.56738900	-0.19380900
H	-8.22283800	2.52616200	2.95005800
H	-8.22768300	4.18885400	1.09553300
N	-2.16367600	2.36694800	0.86061800
H	-1.19400400	2.13942500	0.63838500
C	-2.56243500	-1.15906500	4.39569700
H	-1.71998100	-0.88649200	5.03857400
H	-3.45188500	-1.30857900	5.00866900
H	-2.30436100	-2.10303100	3.90601000

M4RS

C	-0.02374000	1.23522900	-0.87450400
C	-1.51668600	2.42686200	-1.93903100
C	-2.18460000	0.07638900	-1.55835000
H	-1.60885200	-0.85678100	-1.50868000
N	-0.54012200	3.25544000	-1.71036800
N	0.37990300	2.49514300	-1.03484100
N	-1.24082800	1.18480500	-1.44132300
C	-2.77366900	2.55822500	-2.73506700
H	-2.73989500	3.44665700	-3.36437700
H	-3.64877800	2.61782200	-2.07379000
C	-2.95644100	0.16812700	-2.92318900
O	-2.82271000	1.42259700	-3.58096200
C	-4.53057200	0.01525200	-1.08356700
C	-3.26809200	0.14995100	-0.50687500
C	-3.10140900	0.31075100	0.86214300
C	-4.26157900	0.33659700	1.62573700
C	-5.53939600	0.19857400	1.08612600
C	-5.67507500	0.03321500	-0.28732400
C	-4.42663700	-0.15955300	-2.57544500
H	-2.11135400	0.38073400	1.30338300
H	-6.40125000	0.22622000	1.74070900
H	-6.66030900	-0.07258900	-0.72875600
H	-5.10490100	0.48920900	-3.13698100
H	-4.65867000	-1.19373800	-2.85057800
C	1.56824400	3.09012300	-0.48811900
C	1.63163100	3.26845100	0.89661800
C	2.58651100	3.46796400	-1.36342500

C	2.79123000	3.84884200	1.40555400
C	3.72368900	4.04665800	-0.80239300
C	3.84440000	4.23821100	0.57494700
H	2.87195600	4.00396500	2.47841700
H	4.53565400	4.35104200	-1.45777800
C	2.45395000	3.25767300	-2.84831300
H	1.67988100	3.90621200	-3.26859800
H	2.17206000	2.22509000	-3.07890300
H	3.39759400	3.47525900	-3.35026100
C	0.49350700	2.85638600	1.79426200
H	0.38782700	1.76672200	1.83939400
H	-0.45740100	3.26291000	1.43364800
H	0.65883000	3.22491200	2.80753700
H	-2.53938600	-0.55186000	-3.62766800
C	5.09912900	4.83119800	1.16089100
H	4.87810500	5.41046700	2.06021700
H	5.80070200	4.03903100	1.44177500
H	5.60261100	5.48166500	0.44250500
N	-4.13440100	0.52402500	3.07653200
O	-5.15325000	0.50216000	3.74661700
O	-3.01842700	0.69729100	3.53284600
C	6.21877700	-1.15869500	-0.73219000
C	4.84370400	-1.31353400	-0.88506500
C	3.99672800	-1.33862700	0.22724000
C	4.56047300	-1.19344200	1.49736700
C	5.93596200	-1.03955300	1.65524800
C	6.77053900	-1.02465300	0.54029600
H	6.85995200	-1.14376400	-1.60799900
H	4.42563600	-1.40811000	-1.88453100
H	3.91225600	-1.20537200	2.36980000
H	6.35566100	-0.93266200	2.65065500
H	7.84273400	-0.90823400	0.66156000
C	2.49627400	-1.47787500	0.06493700
H	2.04147400	-1.61536100	1.05329500
C	1.88162900	-0.24292400	-0.52639200
C	0.60924200	0.08109300	-0.15612800
O	-0.17227500	-0.50030500	0.66990000
H	2.43241100	0.36002700	-1.24154800
C	2.27440300	-4.02204900	0.11011800
C	2.13490400	-2.78940600	-0.74731500
C	0.66019300	-2.85550200	-1.08415700
N	0.14481900	-3.80541100	-0.21976400
H	2.74180000	-2.82839400	-1.65629400
N	1.13854400	-4.54329600	0.41097600

C	-1.21503900	-4.11496100	-0.01773800
C	-2.11487100	-3.06449900	0.17836200
C	-1.64871600	-5.43948300	0.01119500
C	-3.46434200	-3.34633700	0.35994600
H	-1.71774700	-2.05382900	0.23208200
C	-2.99951600	-5.70927000	0.21698800
H	-0.92833600	-6.23918300	-0.12350300
C	-3.91179100	-4.66798400	0.37705300
H	-4.16547400	-2.52921800	0.51438300
H	-3.34087400	-6.73930300	0.24264300
H	-4.96393800	-4.88592000	0.52891900
N	-0.02107600	-2.25116300	-1.98018600
H	0.60260900	-1.61115200	-2.47174600
C	3.55559600	-4.57543000	0.63605900
H	4.01596400	-3.88219700	1.34683000
H	3.37038700	-5.52792000	1.13476300
H	4.27273500	-4.72302500	-0.17706900

M4SR

C	1.23453200	2.35868400	-0.23037900
C	1.38234500	4.39923400	0.54149900
C	-0.84159000	3.81324100	-0.50781400
H	-0.83444000	3.84414900	-1.59710600
N	2.54902400	3.87201400	0.77041000
N	2.44245100	2.60205700	0.28007100
N	0.54103300	3.50327400	-0.07052700
C	0.94155300	5.79070000	0.87670900
H	1.72356200	6.49658000	0.59331400
H	0.77631600	5.87844100	1.95770200
C	-1.23142300	5.15144900	0.17279400
O	-0.21380000	6.12360200	0.14077300
C	-2.40111400	3.41003900	1.25487100
C	-1.88630800	2.88107300	0.06506600
C	-2.42518000	1.73882000	-0.51119000
C	-3.45936400	1.11773400	0.18258900
C	-3.95036700	1.58552900	1.39899000
C	-3.41951100	2.75223400	1.93877800
C	-1.76373900	4.73849500	1.56549000
H	-2.04783700	1.36571900	-1.45661500
H	-4.75424700	1.05143100	1.88970700
H	-3.81935600	3.15499400	2.86302900
H	-0.95373600	4.61353300	2.29374500
H	-2.46591900	5.46791400	1.97256500
C	3.58400800	1.72482900	0.26976800

C	3.99290000	1.15722300	1.47506300
C	4.20891400	1.47185700	-0.95544500
C	5.08599600	0.28966600	1.43312800
C	5.29323900	0.59851100	-0.94268000
C	5.74393400	-0.00045800	0.23842100
H	5.42089800	-0.17632800	2.35622900
H	5.79964100	0.37792600	-1.87917200
C	3.72060900	2.10983800	-2.22912500
H	3.65372800	3.19711300	-2.12047800
H	2.72533200	1.74526600	-2.50600200
H	4.40499800	1.88998700	-3.04959600
C	3.26767100	1.45630200	2.76006200
H	2.18462000	1.34312500	2.63880900
H	3.45228700	2.48495700	3.08383000
H	3.59584800	0.78029200	3.55059500
H	-2.05481500	5.57505000	-0.40655700
C	6.92240500	-0.93886300	0.20718500
H	7.07123600	-1.42106800	1.17543800
H	6.78016400	-1.71664600	-0.54843900
H	7.83980300	-0.40009100	-0.04852400
N	-4.08684600	-0.07376200	-0.40474100
O	-4.99337800	-0.60449600	0.21162400
O	-3.67305500	-0.46043400	-1.48492200
C	3.61010900	-3.29618200	0.61530900
C	2.83115800	-2.32085200	0.00480900
C	1.44881100	-2.49214500	-0.15482600
C	0.87015800	-3.67527900	0.30862200
C	1.65115800	-4.65664400	0.92125200
C	3.02038200	-4.47196900	1.07945000
H	4.67806100	-3.13414700	0.73373700
H	3.29490600	-1.40284900	-0.35191700
H	-0.19662100	-3.84888400	0.20453600
H	1.18011300	-5.56683700	1.27919200
H	3.62300800	-5.23540600	1.56112400
C	0.66648500	-1.37609100	-0.82742200
H	0.91015200	-1.38917000	-1.90236700
C	1.08212800	-0.03109500	-0.29472000
C	0.75087400	1.12581500	-0.93326800
O	0.09989600	1.33360100	-2.01345300
H	1.63442500	0.00348800	0.63679600
C	-1.52408600	-1.58276000	0.58422500
C	-0.86808200	-1.48441600	-0.76420400
C	-1.53292500	-2.62931300	-1.50310800
N	-2.50081300	-3.10779300	-0.61981900

H	-1.22624600	-0.56712200	-1.25388200
N	-2.46093100	-2.46101300	0.61045100
C	-3.52381300	-4.04617400	-0.85413500
C	-3.38901800	-5.02561300	-1.84498400
C	-4.68382400	-4.00027000	-0.07088300
C	-4.41609900	-5.94442700	-2.04290400
H	-2.49417700	-5.05053200	-2.45068200
C	-5.69235900	-4.93386700	-0.27672100
H	-4.78370800	-3.22442900	0.67775000
C	-5.56858100	-5.91087100	-1.26327900
H	-4.30325200	-6.70004800	-2.81420900
H	-6.58796200	-4.88942500	0.33529100
H	-6.36118800	-6.63435600	-1.42252700
N	-1.32808500	-3.08615500	-2.67520400
H	-0.58080500	-2.54699900	-3.11370700
C	-1.17124700	-0.79055900	1.79935100
H	-1.07078000	0.27184800	1.56068600
H	-1.93358800	-0.93450300	2.56746600
H	-0.20248000	-1.12627900	2.18780200

M4SS

C	-1.78508100	0.77245300	-0.58602100
C	-3.68727800	1.85711300	-0.61053600
C	-3.87809900	-0.50924600	-1.30216000
H	-3.20570900	-1.18229000	-1.83261000
N	-2.82881400	2.71391300	-0.14458000
N	-1.64935200	2.01760800	-0.12263400
N	-3.09219500	0.65783000	-0.88931300
C	-5.12862200	2.00256000	-0.97250300
H	-5.38308300	3.05361100	-1.10537200
H	-5.77300900	1.57391700	-0.19241700
C	-5.10733200	-0.05897200	-2.17749300
O	-5.29027000	1.34821200	-2.21692900
C	-5.87686400	-1.31020800	-0.24174800
C	-4.49885700	-1.17097100	-0.09235000
C	-3.83921300	-1.58424700	1.05644300
C	-4.62919600	-2.12990900	2.05840300
C	-6.00925700	-2.28959700	1.94504500
C	-6.64072900	-1.87726600	0.77805600
C	-6.33204600	-0.79326000	-1.57991100
H	-2.75989900	-1.50706500	1.14201000
H	-6.56427700	-2.72649600	2.76565800
H	-7.71443200	-1.98907100	0.67107100
H	-7.18536500	-0.11176200	-1.51106900

H	-6.63321800	-1.62227800	-2.22771100
C	-0.49045500	2.59935200	0.49693300
C	-0.14269700	2.15899400	1.77765500
C	0.20819900	3.58685000	-0.19686300
C	0.97669200	2.74409200	2.36411900
C	1.32471000	4.13512300	0.43304300
C	1.72552800	3.72092800	1.70422800
H	1.28573000	2.41050300	3.35131800
H	1.89624800	4.90017900	-0.08582600
C	-0.22701400	4.02174900	-1.57079000
H	-1.21543000	4.48933800	-1.53855000
H	-0.29295600	3.16615800	-2.25138400
H	0.48227200	4.73738600	-1.98826000
C	-0.91228100	1.06286800	2.46863400
H	-0.71140300	0.08826400	2.00530300
H	-1.99256400	1.23377800	2.41998800
H	-0.62187300	0.99655400	3.51786200
H	-4.93942900	-0.33700600	-3.21756400
C	2.96389600	4.28592700	2.34867600
H	2.79811400	4.48674800	3.40993200
H	3.78785600	3.56853900	2.27457500
H	3.27841900	5.21208600	1.86384800
N	-3.97502500	-2.55497700	3.30209400
O	-4.65669400	-3.11468600	4.14384400
O	-2.78615200	-2.31942900	3.42870000
C	4.56476200	0.79347600	-2.60874200
C	3.44983500	0.41842200	-1.86359400
C	2.63702600	-0.64272900	-2.28274200
C	2.96090300	-1.29897600	-3.47276900
C	4.07468000	-0.92448000	-4.22121600
C	4.88342800	0.12179900	-3.78761700
H	5.18645500	1.61543300	-2.26759100
H	3.20888800	0.95071200	-0.94695500
H	2.32331100	-2.10559100	-3.82613400
H	4.30649700	-1.44855200	-5.14309600
H	5.75321000	0.41630000	-4.36611300
C	1.43454400	-1.09071300	-1.47668000
H	0.88773300	-1.84307600	-2.06416500
C	0.46538900	0.01628300	-1.16150800
C	-0.78966000	-0.33655600	-0.75213700
O	-1.26028100	-1.50890200	-0.55412600
H	0.74445300	1.05208100	-1.31808800
C	2.75830900	-3.02637900	-0.43355000
C	1.84695800	-1.86321500	-0.17719600

C	2.68747600	-1.04592400	0.78317700
N	3.89629000	-1.73053700	0.88830000
H	0.90495700	-2.17831200	0.29023300
N	3.88796600	-2.92020600	0.16108200
C	5.06000500	-1.39604200	1.60330400
C	5.14902500	-0.20654800	2.34115700
C	6.15708200	-2.27065000	1.57294300
C	6.32312400	0.08900100	3.02892900
H	4.30245600	0.46341200	2.37230600
C	7.31728800	-1.95499300	2.26861600
H	6.08864000	-3.18733000	1.00282100
C	7.41364900	-0.77404500	3.00236800
H	6.37591600	1.01364300	3.59609900
H	8.15536500	-2.64437100	2.23367300
H	8.32219100	-0.53350800	3.54409600
N	2.40882300	0.04685800	1.38232100
H	1.47397500	0.33552200	1.08984500
C	2.42342600	-4.20280000	-1.28448600
H	2.26821900	-3.89532200	-2.32317300
H	3.23261800	-4.93306400	-1.25017200
H	1.49597300	-4.66939600	-0.93933400

re-TS4

C	-0.09121900	-1.54597200	-0.68586800
C	1.36948300	-3.16080000	-0.42247600
C	2.31816600	-1.22161100	-1.55492500
H	1.92631600	-0.38662600	-2.13687400
N	0.30289500	-3.58803000	0.18049000
N	-0.59651700	-2.57061000	0.01483200
N	1.17389900	-1.91961400	-0.96369900
C	2.66348200	-3.84353100	-0.72851100
H	2.55090600	-4.92144900	-0.61496500
H	3.46333400	-3.49328000	-0.06417400
C	3.15990200	-2.21212800	-2.42871700
O	2.93866500	-3.57724500	-2.09244800
C	4.59957000	-1.08542600	-0.85277700
C	3.29181200	-0.77031000	-0.48707200
C	2.99332300	-0.11152700	0.69619200
C	4.07990000	0.23454200	1.48816000
C	5.40166100	-0.05510300	1.15724400
C	5.66532300	-0.73323800	-0.02688500
C	4.62327500	-1.78800100	-2.18532200
H	1.97045400	0.16136900	0.96329200

H	6.19824800	0.25210600	1.82323300
H	6.68606900	-0.98051400	-0.29875100
H	5.28359300	-2.65860500	-2.21344400
H	4.95003200	-1.09698200	-2.97059900
C	-1.88602000	-2.69384900	0.63818600
C	-1.96794600	-2.43035600	2.00699700
C	-2.98000700	-3.07454100	-0.14396900
C	-3.23558200	-2.49353000	2.58787300
C	-4.21993400	-3.13044500	0.48696300
C	-4.36825600	-2.82404700	1.84347700
H	-3.33672100	-2.28024000	3.64861600
H	-5.09309100	-3.41347100	-0.09601300
C	-2.82641200	-3.35348600	-1.61410200
H	-1.96109500	-3.99254000	-1.81004600
H	-2.68654300	-2.41862200	-2.16972100
H	-3.71815400	-3.84578500	-2.00435100
C	-0.74038300	-2.13414400	2.82948100
H	-1.02306600	-1.72933800	3.80219600
H	-0.07060900	-1.41919900	2.34081800
H	-0.16828700	-3.05276700	2.99313000
H	2.87784500	-2.13842900	-3.47910200
C	-5.73350500	-2.83694900	2.47832900
H	-5.66472000	-2.89806700	3.56601800
H	-6.27762000	-1.92043300	2.22729100
H	-6.32699800	-3.68078600	2.11843400
N	3.82142200	0.99569100	2.71357100
O	4.77471600	1.50351100	3.28282600
O	2.66805800	1.09485600	3.09268500
C	-6.40827800	0.94256100	-0.49726400
C	-5.11036900	0.51551100	-0.75388200
C	-4.16635900	1.39304300	-1.30626700
C	-4.56596500	2.70032700	-1.61350000
C	-5.86347800	3.12912600	-1.35244300
C	-6.78945100	2.25160600	-0.79133700
H	-7.12861200	0.24921400	-0.07400300
H	-4.82873900	-0.51285500	-0.53870200
H	-3.84013500	3.38551100	-2.04431600
H	-6.15205700	4.14859600	-1.58889800
H	-7.80344900	2.58238400	-0.59114400
C	-2.77573600	0.98979300	-1.55536800
H	-2.20035200	1.58546900	-2.26113900
C	-2.15661300	-0.02707300	-0.93982200
C	-0.71569100	-0.24938200	-1.17829600
O	-0.11124900	0.30235500	-2.11540600

H	-2.65952700	-0.57904800	-0.15489800
C	-1.49307100	3.97192700	0.45391000
C	-1.72151200	2.63136900	0.81464500
C	-0.53018100	1.95344200	0.53728500
N	0.30385400	2.90824900	0.00054700
H	-2.62495300	2.19463400	1.21522700
N	-0.26895900	4.14385700	-0.03149600
C	1.69999200	2.81054600	-0.26740900
C	2.15007000	2.31199800	-1.48599100
C	2.60269800	3.28674300	0.68442800
C	3.52029800	2.26710800	-1.74252600
H	1.41707000	1.95791100	-2.20245200
C	3.96790600	3.24899700	0.41755500
H	2.22241000	3.67949700	1.62211000
C	4.42790700	2.73176000	-0.79419400
H	3.87849800	1.87152700	-2.68893400
H	4.67359200	3.60799900	1.16065700
H	5.49372700	2.69236100	-0.99643800
N	-0.15935900	0.64865600	0.67567500
H	-0.86011400	0.22760400	1.28756300
C	-2.43919500	5.12891800	0.55221700
H	-2.67164900	5.36166400	1.59582600
H	-1.99573800	6.01402400	0.09181300
H	-3.38483200	4.90658000	0.04847400

si-TS4

C	-1.85617200	-3.77991200	-1.03868000
C	-0.51868400	-5.48643800	-0.78311700
C	0.40127300	-3.68865700	-2.21554900
H	-0.07895400	-2.96766100	-2.88008600
N	-1.55963700	-5.77560400	-0.05911100
N	-2.38034600	-4.68757500	-0.21644400
N	-0.65685900	-4.26941100	-1.38952600
C	0.68514100	-6.28474300	-1.16444900
H	0.52795500	-7.34092500	-0.95002300
H	1.57502900	-5.93528900	-0.62402500
C	1.13991200	-4.82499300	-3.01425100
O	0.81695000	-6.13487800	-2.56713800
C	2.74085200	-3.54980800	-1.71092200
C	1.48013000	-3.07590300	-1.35057100
C	1.30713400	-2.17780300	-0.30735400
C	2.45579900	-1.78010200	0.36366900
C	3.73225900	-2.22633300	0.02798800
C	3.87661400	-3.12172600	-1.02503300

C	2.64666500	-4.51029600	-2.86646500
H	0.32919700	-1.79376200	-0.04024900
H	4.58549600	-1.87532300	0.59429900
H	4.86075100	-3.48721600	-1.29760800
H	3.21386200	-5.43207800	-2.70940200
H	3.02846300	-4.04495700	-3.78061400
C	-3.59178600	-4.56900700	0.54942400
C	-3.60752700	-3.67091200	1.61815300
C	-4.69312100	-5.33868600	0.16733700
C	-4.80076300	-3.55987900	2.33146300
C	-5.85854300	-5.19130500	0.91411200
C	-5.93022100	-4.30626000	1.99370300
H	-4.84674900	-2.87074000	3.17035600
H	-6.73446400	-5.77391000	0.64109100
C	-4.62204100	-6.24117900	-1.03430100
H	-3.82536400	-6.98263500	-0.93112100
H	-4.41507800	-5.65506000	-1.93805000
H	-5.56895700	-6.76257000	-1.17891300
C	-2.40275800	-2.83569700	1.96498000
H	-2.27071800	-2.02092500	1.24300300
H	-1.48534600	-3.43238600	1.96735800
H	-2.52218000	-2.38793400	2.95224100
H	0.82032800	-4.81007800	-4.05589400
C	-7.21800400	-4.14059700	2.75696500
H	-7.88242500	-3.44501800	2.23458900
H	-7.74544500	-5.09251200	2.85116000
H	-7.03703200	-3.74168300	3.75693300
N	2.31382500	-0.84779900	1.48901200
O	3.32982600	-0.45324600	2.03483300
O	1.18695600	-0.52296900	1.81990800
C	-7.97259500	-1.13081900	-2.15588800
C	-6.63297000	-1.48229400	-2.03642400
C	-5.72297200	-0.61029200	-1.41983300
C	-6.18248200	0.62901400	-0.95572200
C	-7.52380600	0.97769400	-1.07256200
C	-8.42347400	0.09673400	-1.67082500
H	-8.66386300	-1.80911500	-2.64639200
H	-6.27854400	-2.41771800	-2.46150500
H	-5.47716400	1.31886400	-0.50025900
H	-7.86674200	1.93919000	-0.70409400
H	-9.46848700	0.37158700	-1.77207600
C	-4.30060300	-0.95011700	-1.31001400
H	-3.59228100	-0.12893700	-1.20693200
C	-3.81377200	-2.19380500	-1.38121800

C	-2.36099800	-2.42395000	-1.46330600
O	-1.50663400	-1.52804300	-1.44923400
H	-4.46686800	-3.05582700	-1.48118700
C	-5.70863100	-3.45479000	-5.01139900
C	-4.64807300	-4.16459900	-4.41295200
C	-3.68911300	-3.20533600	-4.06783100
N	-4.23518800	-1.99761000	-4.47031500
H	-4.55624300	-5.23231400	-4.27446100
N	-5.47055100	-2.15451000	-5.04094800
C	-3.71170200	-0.68689600	-4.37166900
C	-2.33927700	-0.45788200	-4.24523300
C	-4.59760200	0.39617500	-4.41679500
C	-1.86725300	0.84792900	-4.15140300
H	-1.66422600	-1.30122200	-4.19051300
C	-4.10887900	1.69426100	-4.32559000
H	-5.65883600	0.20123300	-4.50840800
C	-2.74200200	1.93084700	-4.18925200
H	-0.79981600	1.01526600	-4.04477300
H	-4.80634000	2.52587800	-4.35328600
H	-2.36480000	2.94535000	-4.11242400
N	-2.47912600	-3.31839600	-3.45335100
H	-2.32286000	-4.32313500	-3.35072000
C	-6.99052800	-3.99693000	-5.56295400
H	-7.55364000	-4.53286100	-4.79303200
H	-7.60767900	-3.17900700	-5.93894800
H	-6.80486000	-4.69882400	-6.38100600

re-M4

C	-2.30715600	-3.66237200	-1.01379400
C	-0.71910500	-5.17774900	-1.10136800
C	-0.22797500	-3.15962700	-2.41076400
H	-0.85648600	-2.46825500	-2.97379100
N	-1.56825300	-5.65152100	-0.24111500
N	-2.54603500	-4.69384100	-0.19337600
N	-1.13996100	-3.97749000	-1.60489500
C	0.56298100	-5.73849300	-1.62590400
H	0.57709800	-6.82232800	-1.51339000
H	1.41673700	-5.31371500	-1.07898800
C	0.69048200	-4.05229500	-3.31336200
O	0.61508400	-5.43738500	-3.00573300
C	2.04946100	-2.61399200	-1.89682700
C	0.72784900	-2.44837000	-1.48664800
C	0.39009700	-1.73279600	-0.34974200
C	1.44209700	-1.14884600	0.34307000

C	2.77303100	-1.26605100	-0.04685700
C	3.08325000	-2.01825800	-1.17683100
C	2.11836700	-3.47604900	-3.13147800
H	-0.64243700	-1.58493500	-0.03555500
H	3.54367800	-0.77741300	0.53618300
H	4.11706500	-2.13873600	-1.48269300
H	2.84716600	-4.28764700	-3.04663500
H	2.39909400	-2.87883500	-4.00455000
C	-3.62509600	-4.85277400	0.74428100
C	-3.46330600	-4.31172800	2.02281000
C	-4.74848800	-5.58924200	0.35437500
C	-4.53442800	-4.44663200	2.90777200
C	-5.78700100	-5.69496400	1.27635900
C	-5.70454000	-5.11517800	2.54660500
H	-4.44272000	-4.02956100	3.90705000
H	-6.67814700	-6.25337900	1.00022400
C	-4.81387800	-6.24465900	-0.99873500
H	-3.98924100	-6.95333800	-1.12146300
H	-4.73584900	-5.50354300	-1.80127600
H	-5.75576100	-6.78225500	-1.11865300
C	-2.16858500	-3.66072600	2.44225000
H	-2.20552800	-3.39397000	3.49910800
H	-1.95004600	-2.75095000	1.87302000
H	-1.33128800	-4.34888400	2.28963400
H	0.36537800	-3.99205700	-4.35155400
C	-6.86103500	-5.21582400	3.50579700
H	-6.53004500	-5.09094200	4.53861600
H	-7.60053200	-4.43659700	3.29557300
H	-7.36454200	-6.18090900	3.41461900
N	1.11897900	-0.33070900	1.51652400
O	2.00891700	0.34647500	2.00389700
O	-0.02224100	-0.37266500	1.94037000
C	-8.60499600	-4.45291000	-2.58238700
C	-7.33306700	-4.02519600	-2.22127600
C	-6.52490200	-3.32926400	-3.13390200
C	-7.03004700	-3.08703400	-4.41722100
C	-8.30451000	-3.51321300	-4.77972600
C	-9.09736100	-4.19750400	-3.86259400
H	-9.21552800	-4.99061700	-1.86359500
H	-6.96241300	-4.24068900	-1.22164000
H	-6.41201600	-2.55321900	-5.13410500
H	-8.67766900	-3.31148200	-5.77885600
H	-10.09086500	-4.53288800	-4.14202700
C	-5.17053600	-2.85704500	-2.80141000

H	-4.57659000	-2.43350800	-3.60974600
C	-4.59941400	-2.88515600	-1.59703400
C	-3.17233600	-2.36091400	-1.38743400
O	-2.65434400	-1.74428000	-2.40208400
H	-5.13049500	-3.26077200	-0.72336100
C	-5.52193200	1.15397600	0.01375400
C	-5.29949900	-0.23811100	0.00278500
C	-3.93169600	-0.38939400	-0.12710700
N	-3.41414100	0.87485300	-0.19044000
H	-6.02977600	-1.02955300	0.08441900
N	-4.37900100	1.81821600	-0.10154800
C	-2.05966000	1.30361300	-0.26395000
C	-1.20138700	0.76983700	-1.21965200
C	-1.63333600	2.30398900	0.61144100
C	0.10772300	1.24632600	-1.28526400
H	-1.56954400	-0.02133300	-1.87163000
C	-0.32544300	2.76592300	0.53473700
H	-2.33174300	2.70270500	1.33857000
C	0.55056200	2.23803200	-0.41470600
H	0.78961800	0.82732000	-2.02048600
H	0.01383700	3.53555000	1.22039500
H	1.57359400	2.59646600	-0.47021800
N	-3.12637500	-1.55172300	-0.08524500
H	-3.51653300	-2.12930500	0.66022900
C	-6.82115600	1.88877500	0.12050000
H	-7.35589800	1.61320900	1.03365300
H	-6.63776200	2.96444800	0.13525200
H	-7.47408600	1.65923300	-0.72612500

si-M4

C	-2.37652800	-3.96931600	-1.39735600
C	-0.66070700	-5.27513000	-0.98578800
C	-0.23117400	-3.63784200	-2.74887300
H	-0.84644600	-3.10475500	-3.47642200
N	-1.54040900	-5.60378700	-0.08890700
N	-2.60010300	-4.77406100	-0.35433500
N	-1.13250200	-4.28655400	-1.80261100
C	0.68822600	-5.83409300	-1.30890100
H	0.78890500	-6.84006500	-0.90252600
H	1.47995100	-5.19880500	-0.89028700
C	0.69176900	-4.69743200	-3.43586900
O	0.76813200	-5.92577700	-2.72028900
C	2.03517600	-2.92518300	-2.48873100

C	0.73421200	-2.72312300	-2.03050100
C	0.43120600	-1.78527500	-1.05408700
C	1.50231200	-1.05252800	-0.55854300
C	2.81385000	-1.21128500	-1.00230500
C	3.08445600	-2.16181300	-1.98126100
C	2.06236100	-3.99481800	-3.54903300
H	-0.59601900	-1.61396700	-0.73706100
H	3.59900900	-0.60211700	-0.57245200
H	4.10023100	-2.30739400	-2.33303600
H	2.87657900	-4.71444700	-3.43092800
H	2.16324400	-3.53385300	-4.53835100
C	-3.74323000	-4.80242800	0.52020400
C	-3.81880500	-3.83550500	1.52454500
C	-4.72429600	-5.76678600	0.29815800
C	-4.96074700	-3.84159600	2.31990500
C	-5.84916300	-5.73012100	1.12236800
C	-5.98770200	-4.76894000	2.12412100
H	-5.06440300	-3.08825900	3.09703100
H	-6.63905700	-6.46037100	0.96693600
C	-4.57955600	-6.77565700	-0.80963200
H	-3.67030400	-7.37075700	-0.68407400
H	-4.51061100	-6.28253900	-1.78649000
H	-5.43642300	-7.45027100	-0.83012400
C	-2.74090200	-2.79656900	1.67531100
H	-2.70177200	-2.15778800	0.78286200
H	-1.75626200	-3.26184500	1.79292600
H	-2.93195900	-2.17055400	2.54835400
H	0.29586400	-4.97587700	-4.41294900
C	-7.24249600	-4.69007700	2.95211200
H	-7.88738300	-3.89085400	2.57009200
H	-7.80454200	-5.62560300	2.91580200
H	-7.01316100	-4.46133300	3.99592700
N	1.23689100	-0.06192800	0.49286100
O	2.15610300	0.65996600	0.84141400
O	0.11432900	-0.01896200	0.96388600
C	-8.86297300	-2.93548200	-0.19398100
C	-7.58271600	-2.89173300	-0.73266600
C	-6.62520600	-1.99462600	-0.23752400
C	-6.99656600	-1.13779600	0.80602600
C	-8.27874300	-1.17910900	1.34741300
C	-9.21876100	-2.07777900	0.84758400
H	-9.59103200	-3.63459500	-0.59367800
H	-7.32619500	-3.55487500	-1.55397400
H	-6.26458700	-0.43628600	1.19781500

H	-8.54451100	-0.50715300	2.15752400
H	-10.22084900	-2.10981500	1.26329000
C	-5.24743900	-1.93921900	-0.75406700
H	-4.64148500	-1.07621800	-0.48072000
C	-4.64517600	-2.88273300	-1.47575800
C	-3.19584500	-2.73392100	-1.93244100
O	-2.57717100	-1.64848300	-1.54926000
H	-5.16656300	-3.79675900	-1.76612300
C	-5.29714300	-0.74260600	-5.34211900
C	-5.20557900	-1.79746500	-4.41073600
C	-3.85320500	-1.97849400	-4.19307900
N	-3.21687800	-1.05060800	-4.97321500
H	-6.00965500	-2.35355600	-3.95235000
N	-4.09200200	-0.29916400	-5.67760800
C	-1.82609800	-0.82960100	-5.17309100
C	-0.96914400	-0.69001500	-4.08373000
C	-1.35635400	-0.70026500	-6.48092500
C	0.38198500	-0.43377100	-4.31953200
H	-1.37908200	-0.79460800	-3.07905700
C	-0.00824800	-0.44072600	-6.69963500
H	-2.05460000	-0.79821400	-7.30465200
C	0.86501800	-0.30981600	-5.62011000
H	1.05795400	-0.31164400	-3.47750600
H	0.36124900	-0.34079900	-7.71505900
H	1.91592900	-0.10134600	-5.79336500
N	-3.15132500	-2.95546900	-3.45337600
H	-3.58112900	-3.85712900	-3.66150900
C	-6.52508900	-0.11872100	-5.92706500
H	-7.13927100	0.34576900	-5.15069800
H	-6.24019200	0.64849800	-6.64904300
H	-7.14277100	-0.86463600	-6.43483500

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C	-1.91906200	-0.32915700	-0.76629900
C	-3.69979700	-0.72885100	-1.96455000
C	-2.54676300	-2.77964300	-1.20031900
H	-1.49554400	-3.01860600	-1.04940800
N	-3.65936500	0.56747200	-1.85248700
N	-2.55190700	0.80004700	-1.09532200
N	-2.65065200	-1.31628400	-1.31465800
C	-4.61152900	-1.61772600	-2.74474800
H	-5.12466600	-1.04883500	-3.51924800
H	-5.35903400	-2.08347300	-2.08792600
C	-3.14219200	-3.47518800	-2.48309300

O	-3.78063600	-2.57451900	-3.37313300
C	-4.29027000	-4.26642400	-0.49160800
C	-3.40970600	-3.27530200	-0.06205800
C	-3.39294800	-2.83135100	1.25252600
C	-4.30622400	-3.41889500	2.11664800
C	-5.19830600	-4.41465700	1.72517100
C	-5.18789300	-4.84593200	0.40440100
C	-4.10317000	-4.56690000	-1.95370800
H	-2.69439400	-2.07907200	1.60026500
H	-5.88563900	-4.82986900	2.45140300
H	-5.87793300	-5.61637300	0.07769900
H	-5.04096600	-4.55181300	-2.51726400
H	-3.66293700	-5.55924200	-2.08857900
C	-2.21628400	2.14088800	-0.69172700
C	-2.47442500	2.51442400	0.62744300
C	-1.59896100	2.97224900	-1.62914900
C	-2.06434600	3.79056600	1.01137800
C	-1.20781300	4.23558400	-1.19264900
C	-1.41966900	4.65348400	0.12443200
H	-2.24706500	4.11307400	2.03293400
H	-0.71924300	4.90611800	-1.89498500
C	-1.33430100	2.49484800	-3.03148000
H	-2.26471000	2.24092500	-3.54651400
H	-0.70823400	1.59545300	-3.02283200
H	-0.81866800	3.26466600	-3.60638700
C	-3.12085300	1.57085900	1.60629800
H	-2.38750000	0.85332600	1.99311500
H	-3.93812400	1.00663900	1.14812800
H	-3.52170600	2.12347700	2.45704800
H	-2.33215800	-3.90577300	-3.07092800
C	-0.92964600	6.00074500	0.58445000
H	-0.97226900	6.73460100	-0.22322700
H	-1.51983800	6.37060300	1.42512600
H	0.11184000	5.92851200	0.91540100
N	-4.33284900	-2.96133100	3.51191200
O	-5.08179400	-3.53217200	4.28453300
O	-3.60683500	-2.03166900	3.81844300
C	3.00529000	3.75113700	0.99923300
C	2.17575200	2.68942900	0.65749800
C	2.18790300	1.50535700	1.41146100
C	3.04975600	1.41835600	2.51208800
C	3.88524800	2.47900100	2.84820600
C	3.86704000	3.64687900	2.09060300
H	2.98195800	4.66213200	0.40931400

H	1.51523400	2.79232100	-0.19816900
H	3.05991400	0.51330400	3.11304400
H	4.54734300	2.39365000	3.70318500
H	4.51600100	4.47609700	2.35211600
C	1.32349700	0.35401300	1.07003000
H	1.16737300	-0.36113500	1.87666700
C	0.21216200	0.51615100	0.20218100
C	-0.68168500	-0.54528200	0.07193100
O	-0.56197700	-1.69332600	0.55928200
H	0.07470000	1.42405700	-0.36288800
C	3.57171200	-1.36002300	1.06964500
C	2.51864500	-1.01936800	0.13845000
C	3.17582700	-0.16200300	-0.78805100
N	4.40753200	0.07023300	-0.29735000
H	1.68500400	-1.67073000	-0.09714600
N	4.66161600	-0.68352000	0.83999500
C	5.44264000	0.87967300	-0.83957500
C	6.74578100	0.38240700	-0.83858500
C	5.15515900	2.14256700	-1.35433800
C	7.76679500	1.15848300	-1.37240900
H	6.93903100	-0.59703900	-0.41640100
C	6.18679500	2.90184700	-1.90228800
H	4.14837400	2.54166500	-1.28969100
C	7.48972100	2.41366600	-1.91382000
H	8.78242600	0.77765300	-1.37286000
H	5.96880000	3.88541300	-2.30454300
H	8.29013800	3.01154900	-2.33605200
N	2.65551500	0.43025300	-1.87582700
H	3.26864400	0.90651000	-2.52324100
C	3.45442700	-2.29256700	2.22631500
H	3.26529500	-3.31143300	1.87766200
H	4.37231800	-2.27949100	2.81457100
H	2.61389400	-2.01027600	2.86885000
H	1.82729700	0.01162500	-2.27098000

NTS4RS

C	-0.31295400	-0.62872000	0.51727300
C	-1.70911200	-0.67393400	2.19194800
C	-2.62034300	0.38533400	0.14062300
H	-2.15300700	1.00785400	-0.62718300
N	-0.66164100	-1.31789700	2.61789500
N	0.19751600	-1.28942500	1.55536300
N	-1.53839200	-0.24595900	0.90397800
C	-2.96346400	-0.24943800	2.88386400

H	-2.82224900	-0.25434700	3.96410600
H	-3.79564500	-0.91919900	2.62700600
C	-3.53450000	1.23315500	1.10369200
O	-3.20371800	1.08358700	2.47427800
C	-4.86580100	-0.44481300	-0.04259400
C	-3.54403900	-0.67372200	-0.42124400
C	-3.18457200	-1.77324200	-1.18917600
C	-4.20862500	-2.63603300	-1.55297800
C	-5.54186300	-2.43447200	-1.20222500
C	-5.87443200	-1.32229300	-0.43851500
C	-4.98702700	0.80159600	0.79053200
H	-2.15880400	-1.94018500	-1.50170300
H	-6.29135000	-3.14699100	-1.52308600
H	-6.90522700	-1.15004800	-0.14797100
H	-5.54524500	0.64205500	1.71816200
H	-5.50630200	1.58810600	0.23473700
C	1.43377200	-2.02509200	1.58265000
C	1.57439600	-3.10613500	0.70292700
C	2.42452400	-1.63126000	2.48324100
C	2.78939600	-3.78497400	0.72954600
C	3.62197400	-2.34665000	2.46429300
C	3.82274800	-3.41804700	1.59523600
H	2.93080700	-4.62820500	0.05831100
H	4.41556000	-2.05537200	3.14744000
C	2.21297400	-0.49880400	3.45172700
H	1.68516200	-0.84894400	4.34402400
H	1.60390400	0.29738400	3.01683000
H	3.17098200	-0.07944100	3.76430600
C	0.47056500	-3.53715700	-0.22972600
H	0.42101600	-2.90562300	-1.12302800
H	-0.50770200	-3.49854900	0.25979900
H	0.64143400	-4.56307500	-0.55893700
H	-3.37941700	2.29309000	0.90647100
C	5.11590700	-4.18990600	1.60168800
H	5.48276100	-4.34677600	0.58421400
H	5.88695700	-3.66801800	2.17132300
H	4.97109800	-5.17621000	2.05307800
N	-3.86317100	-3.82623800	-2.34091200
O	-4.77411600	-4.53368100	-2.73406500
O	-2.68308700	-4.04473700	-2.55316800
C	5.84714000	1.19314500	-1.00481400
C	4.47256100	1.00307200	-0.88225000
C	3.65922200	0.95812800	-2.02052900
C	4.25644300	1.09974600	-3.28023200

C	5.62759800	1.28411300	-3.40337000
C	6.42764700	1.33524500	-2.26212100
H	6.46566200	1.22120000	-0.11384100
H	4.04277300	0.87561500	0.10579200
H	3.63312700	1.06139600	-4.17064500
H	6.07327900	1.38511700	-4.38732000
H	7.49919900	1.47867200	-2.35424700
C	2.18242900	0.76208200	-1.94491700
H	1.75592700	0.36301800	-2.86601300
C	1.57518300	0.23517500	-0.76673200
C	0.29711700	-0.31133700	-0.83029200
O	-0.43461400	-0.52136200	-1.82216200
H	2.04973700	0.33915000	0.20166500
C	0.09134200	2.37882000	-2.44164100
C	1.52552200	2.58580200	-2.29807200
C	1.63493800	3.15767100	-0.98483800
N	0.43245900	3.02370500	-0.41360500
H	2.16882900	2.88653100	-3.11484100
N	-0.52982400	2.56645800	-1.31641100
C	0.04569700	3.21617100	0.94097100
C	0.85076500	2.74233400	1.97532300
C	-1.17219700	3.84068300	1.20490600
C	0.42694300	2.90322100	3.29292600
H	1.78851600	2.24197900	1.75221300
C	-1.59068500	3.97825100	2.52350600
H	-1.77474600	4.20064800	0.37780600
C	-0.79361200	3.51287300	3.56837000
H	1.05068400	2.53881000	4.10263900
H	-2.54281800	4.45358500	2.73428700
H	-1.12489800	3.62514900	4.59475400
N	2.73035100	3.58894200	-0.35603300
H	3.56489000	3.75836200	-0.89749700
C	-0.61215600	1.90626200	-3.66550500
H	-0.19802000	0.94811500	-3.98923000
H	-1.67188600	1.76564200	-3.45092000
H	-0.49629100	2.63095100	-4.47561600
H	2.66034500	4.04522300	0.54293600

NTS4SR

C	1.09863900	2.04788200	-0.29094100
C	1.47417600	4.18729100	-0.06994000
C	-0.89941900	3.62032400	-0.59677500
H	-1.25919100	2.96836800	-1.38981800
N	2.61926600	3.61931400	0.18058300

N	2.36882700	2.29046100	0.04315100
N	0.51733900	3.26211500	-0.37643800
C	1.11451000	5.63554100	-0.11155600
H	1.99806300	6.23451200	-0.33021900
H	0.70216700	5.95141300	0.85602000
C	-1.04240400	5.14601100	-0.96453400
O	0.19183100	5.80702700	-1.16541800
C	-2.24317600	4.67222800	1.09832000
C	-1.68499400	3.46458500	0.68252100
C	-1.85281500	2.29855400	1.41323000
C	-2.59316500	2.38867200	2.58187600
C	-3.16952100	3.57609100	3.02662400
C	-2.99381300	4.73041700	2.27308200
C	-1.91725900	5.78778800	0.14386900
H	-1.42836300	1.35381600	1.10158500
H	-3.74167000	3.58084900	3.94585500
H	-3.43326300	5.66538700	2.60344800
H	-1.38604200	6.60831600	0.63706300
H	-2.82517100	6.21832000	-0.28636800
C	3.41851900	1.32817100	0.25953700
C	3.72924200	0.99998100	1.58090500
C	4.01074400	0.72660700	-0.85168800
C	4.67112700	-0.00871500	1.77561100
C	4.94552100	-0.27548300	-0.60051900
C	5.27433000	-0.66521400	0.69966900
H	4.93119100	-0.29437600	2.79134800
H	5.42281200	-0.76968000	-1.44255800
C	3.61979300	1.10939100	-2.25324400
H	3.56864500	2.19497300	-2.37379100
H	2.63703500	0.69502700	-2.50605000
H	4.34177500	0.71659300	-2.97001700
C	3.03640600	1.67773100	2.73284800
H	1.95040100	1.54136500	2.67133100
H	3.23265200	2.75341500	2.73382900
H	3.37750400	1.26261300	3.68169100
H	-1.54129800	5.21111700	-1.93074500
C	6.23831800	-1.79750500	0.93470900
H	7.02596700	-1.80913800	0.17819700
H	6.70115300	-1.72647500	1.92086900
H	5.71197800	-2.75621700	0.87818400
N	-2.77262800	1.16991100	3.37939000
O	-3.41348400	1.24980800	4.40959500
O	-2.26248800	0.14046600	2.96395800
C	2.56448200	-4.39925000	0.97070400

C	1.98575800	-3.15115500	0.77199900
C	1.05284100	-2.95920400	-0.25697300
C	0.72075200	-4.04221200	-1.08125700
C	1.30176800	-5.29021800	-0.88279800
C	2.22237100	-5.47138900	0.14645400
H	3.28637800	-4.53664400	1.76899500
H	2.26798900	-2.32494000	1.41878300
H	0.00673400	-3.89905600	-1.88961100
H	1.03911000	-6.11844300	-1.53320800
H	2.67715900	-6.44381000	0.30379000
C	0.41214800	-1.65643700	-0.51400800
H	-0.06139200	-1.58307500	-1.49061900
C	0.97826100	-0.43526400	-0.07188100
C	0.41207200	0.73466400	-0.57129700
O	-0.66143800	0.81991300	-1.22538200
H	1.80385100	-0.41637600	0.62324200
C	-1.51628100	-2.92040600	1.23623900
C	-1.49912500	-1.74884500	0.39174000
C	-2.21729200	-2.16791500	-0.76518900
N	-2.45666300	-3.48523200	-0.61494200
H	-1.51429800	-0.73142900	0.75023800
N	-2.02254800	-3.95327700	0.62308800
C	-3.00257000	-4.39380600	-1.55842600
C	-4.09210500	-4.01712100	-2.34342300
C	-2.43932400	-5.66498800	-1.67267800
C	-4.59610500	-4.91547100	-3.28092100
H	-4.56357000	-3.05015500	-2.19894000
C	-2.96484500	-6.55660100	-2.60066200
H	-1.60746300	-5.93457200	-1.03146800
C	-4.03456600	-6.18220700	-3.41319300
H	-5.44345700	-4.62651600	-3.89312200
H	-2.53186500	-7.54686400	-2.69363900
H	-4.43531500	-6.88084700	-4.13945300
N	-2.48343700	-1.42603000	-1.84691300
H	-2.02029500	-0.51868800	-1.87440700
C	-0.98659500	-3.00705900	2.62535200
H	-1.57378700	-2.36784100	3.29034900
H	-1.02446400	-4.03741400	2.98011700
H	0.04901500	-2.65530300	2.65620500
H	-2.75726100	-1.86075000	-2.71625300

NTS4SS

C	-2.12492100	1.01521600	-0.68715800
C	-3.92365700	1.73991200	-1.67927200

C	-3.63845700	-0.77729100	-1.69200600
H	-2.97193100	-1.12232800	-2.48409500
N	-3.30415000	2.81248900	-1.27334200
N	-2.18703900	2.33709300	-0.65569300
N	-3.22716400	0.60694300	-1.33612700
C	-5.24705600	1.65462500	-2.37697200
H	-5.28873400	2.39317500	-3.17845500
H	-6.04621100	1.87949200	-1.66009100
C	-5.12463000	-0.70871600	-2.12462900
O	-5.40993600	0.38375000	-2.96511700
C	-5.00912200	-1.68781000	0.03055400
C	-3.70767200	-1.67508900	-0.48349300
C	-2.69483700	-2.43111800	0.08266400
C	-3.02031000	-3.15872400	1.21879000
C	-4.29962800	-3.18268300	1.76735700
C	-5.31114800	-2.44681500	1.15786200
C	-5.92171300	-0.82624000	-0.80451700
H	-1.69028600	-2.45443200	-0.32254400
H	-4.48960900	-3.77600100	2.65315600
H	-6.31783400	-2.46987800	1.56017100
H	-6.06325500	0.14768800	-0.32078600
H	-6.90961400	-1.26312900	-0.95849700
C	-1.21673100	3.20972000	-0.04609500
C	-1.39064800	3.53913800	1.30109800
C	-0.15343200	3.66528100	-0.82731300
C	-0.42547700	4.36121100	1.87796800
C	0.78302700	4.48942600	-0.19953000
C	0.66259800	4.84389900	1.14619100
H	-0.52610700	4.63243300	2.92551900
H	1.62301600	4.86368600	-0.77951900
C	0.00156500	3.25096800	-2.26663100
H	-0.95129300	3.28750700	-2.80050900
H	0.38383100	2.22536800	-2.33043000
H	0.70964500	3.90412000	-2.77814100
C	-2.56534000	3.01151600	2.07843300
H	-2.52794300	1.91816600	2.12159900
H	-3.50728200	3.30128800	1.60260600
H	-2.55790600	3.40425100	3.09563000
H	-5.31663900	-1.59734900	-2.72993600
C	1.67141200	5.75210600	1.79732600
H	1.91517000	5.40722800	2.80487100
H	2.59246000	5.80601200	1.21417900
H	1.26861000	6.76573800	1.88544400
N	-1.95513000	-3.92459000	1.87535200

O	-2.24343500	-4.57805400	2.85869200
O	-0.83006900	-3.85959700	1.39979300
C	3.44513800	-2.08529900	-2.64916100
C	2.48359700	-1.38863900	-1.92793900
C	1.87171100	-1.97525800	-0.81013300
C	2.26645700	-3.25894400	-0.41488800
C	3.22670000	-3.95821100	-1.14075200
C	3.81220600	-3.37489600	-2.26215700
H	3.91438200	-1.62229500	-3.51097400
H	2.21044800	-0.37976700	-2.22445600
H	1.79767500	-3.71539700	0.45349400
H	3.51441000	-4.95773200	-0.83263500
H	4.56053600	-3.91919000	-2.82929800
C	0.81175700	-1.28096400	-0.05500400
H	0.33219400	-1.87985400	0.71954900
C	-0.04193500	-0.34644400	-0.69436200
C	-1.10938400	0.16032600	0.04566900
O	-1.35827300	-0.01669300	1.25356400
H	0.10738000	-0.03985100	-1.72193700
C	2.54748900	-1.25831600	2.12559000
C	1.74473500	-0.23937400	1.49403600
C	2.68431300	0.48802700	0.72040600
N	3.86069400	-0.16216300	0.82927100
H	0.80377100	0.14888800	1.86715200
N	3.77563900	-1.24927900	1.68461700
C	5.07235200	0.08657200	0.13081700
C	5.58425400	1.38080400	0.05001300
C	5.73957900	-0.99113400	-0.44775800
C	6.76631000	1.59884400	-0.65387300
H	5.08557300	2.20026200	0.55907800
C	6.92757700	-0.76169000	-1.13186000
H	5.31324100	-1.98435100	-0.35392100
C	7.43749500	0.53159100	-1.24473300
H	7.17068400	2.60303000	-0.72143200
H	7.45238100	-1.59550000	-1.58622300
H	8.36212800	0.70554800	-1.78448400
N	2.44948100	1.51877600	-0.10666000
H	1.61941500	2.07558300	0.03826500
C	2.06447200	-2.28882300	3.08912700
H	1.18138400	-2.80567500	2.69547300
H	2.85007800	-3.02124100	3.27836200
H	1.77309800	-1.82447400	4.03527500
H	3.19791600	1.93056700	-0.64385100

TS5RR

C	1.54071400	0.66283500	0.71499100
C	3.11226600	0.57021800	2.22816400
C	2.87747000	-1.48503300	0.87166200
H	1.99041700	-1.94310500	0.43170200
N	2.59093200	1.75331700	2.37759500
N	1.61676400	1.79915200	1.41357700
N	2.51084900	-0.11522300	1.21521500
C	4.12353300	-0.17484700	3.03329500
H	4.29416000	0.32222900	3.98785200
H	5.07693600	-0.24839500	2.49050500
C	3.35279500	-2.26545000	2.15119300
O	3.56229300	-1.44595700	3.29370600
C	5.07458100	-2.34473300	0.43946600
C	4.07497500	-1.50717800	-0.05305300
C	4.22889600	-0.80957700	-1.24402900
C	5.43655200	-0.97949900	-1.90858100
C	6.45832200	-1.80756600	-1.44575500
C	6.27226600	-2.50187100	-0.25740200
C	4.65117400	-2.99384100	1.72919200
H	3.42433000	-0.19251500	-1.63387600
H	7.37513600	-1.89264100	-2.01519300
H	7.05414100	-3.15140500	0.12194200
H	5.40628100	-2.91318600	2.51691900
H	4.45889400	-4.06015100	1.57228400
C	0.89751900	3.01603600	1.15888500
C	1.23388500	3.74733200	0.01824500
C	-0.11492600	3.39144200	2.04455100
C	0.50823700	4.91360000	-0.22763900
C	-0.81260000	4.56143400	1.75129500
C	-0.51420500	5.33284200	0.62468700
H	0.74528000	5.50186000	-1.11048100
H	-1.61480800	4.87419700	2.41526300
C	-0.44447300	2.53958200	3.24114200
H	0.40813200	2.48299200	3.92435300
H	-0.69172800	1.51275600	2.94503800
H	-1.29503300	2.95730200	3.78221600
C	2.30895000	3.27383500	-0.92418700
H	1.98224300	2.38389400	-1.47476400
H	3.22378000	3.01015100	-0.38376700
H	2.55045300	4.05218500	-1.64962300
H	2.56004400	-2.94640600	2.45166300
C	-1.27758000	6.60340800	0.35233300
H	-1.13820400	6.93658600	-0.67837300

H	-2.34696400	6.46239100	0.52996400
H	-0.93895500	7.40736700	1.01373300
N	5.64999000	-0.24864600	-3.16291600
O	6.69095500	-0.44429200	-3.76952300
O	4.77973000	0.51975100	-3.53303400
C	-4.63165700	2.15401700	-2.82880600
C	-3.79273600	1.12152900	-2.42028300
C	-2.58728900	1.38967400	-1.76150800
C	-2.24923000	2.72518000	-1.52185400
C	-3.08885400	3.76175900	-1.92557300
C	-4.28473700	3.48142800	-2.58041900
H	-5.56299700	1.92155800	-3.33648200
H	-4.08117200	0.08927000	-2.60734600
H	-1.31639200	2.95305500	-1.01281400
H	-2.80300200	4.79094800	-1.72362700
H	-4.94263300	4.28672800	-2.89226700
C	-1.65043400	0.25668300	-1.34319900
H	-1.05911300	-0.02527500	-2.22619500
C	-0.63785100	0.68672800	-0.31955800
C	0.65782900	0.28006800	-0.43077500
O	1.23759900	-0.41264400	-1.33915700
H	-0.96217100	1.23714100	0.55797000
C	-2.65204700	-2.12942700	-1.82559700
C	-2.39704600	-1.01474800	-0.93118100
C	-3.58761300	-0.98812500	-0.08189000
N	-4.26800100	-2.15943400	-0.39840100
H	-1.62477000	-1.63925700	-0.00966700
N	-3.68976600	-2.82766100	-1.48116700
C	-5.42422200	-2.71121500	0.17940700
C	-6.03836500	-2.12961600	1.29839800
C	-5.97325300	-3.87895000	-0.37408100
C	-7.18141200	-2.71327300	1.83800200
H	-5.61660300	-1.23078700	1.72425500
C	-7.11380700	-4.44443900	0.18190200
H	-5.49357000	-4.33021100	-1.23221400
C	-7.73073100	-3.86880600	1.29120200
H	-7.64446200	-2.24992800	2.70429400
H	-7.52252500	-5.34837200	-0.25998100
H	-8.62135000	-4.31496500	1.72126500
N	-3.93809300	-0.15912800	0.86140100
H	-3.31909600	0.65189500	0.79331200
C	-1.77820900	-2.52732100	-2.96822300
H	-0.73127700	-2.52917800	-2.65047400
H	-2.05529300	-3.51530200	-3.33857600

H	-1.86681500	-1.80520700	-3.78732000
C	-0.60026700	-1.56032400	1.92862600
O	-0.92685800	-2.23629100	0.88145500
O	-1.54160700	-0.72925600	2.45490300
H	-2.38693200	-0.78786600	1.96753900
O	0.48025700	-1.60995300	2.51255500

TS5RS

C	1.54287700	-0.34462700	-0.98319900
C	2.99228300	-0.61108400	-2.60491200
C	3.82263800	0.76899600	-0.72840000
H	3.33191800	1.45437800	-0.03757800
N	1.97626800	-1.34034800	-2.95558900
N	1.08660800	-1.17915600	-1.92464500
N	2.77207100	0.00836600	-1.40638100
C	4.25971400	-0.27318500	-3.31812400
H	4.15649200	-0.45615300	-4.38732400
H	5.09771200	-0.87062300	-2.93208200
C	4.73267100	1.49879700	-1.78574900
O	4.46538300	1.11461800	-3.12680100
C	6.08560200	0.03973200	-0.39253500
C	4.76307200	-0.17477300	-0.01141600
C	4.40997200	-1.16634200	0.89372800
C	5.44688900	-1.94831100	1.38365600
C	6.78206300	-1.76426000	1.02734300
C	7.10617300	-0.75409900	0.13048700
C	6.18900400	1.18102200	-1.36827900
H	3.37784500	-1.28477300	1.21360000
H	7.53973700	-2.41217700	1.44964100
H	8.13875500	-0.59613300	-0.16240000
H	6.79201800	0.94243300	-2.24952400
H	6.64692200	2.05213500	-0.88944200
C	-0.10278900	-1.98642100	-1.87465900
C	-0.15800600	-3.02291800	-0.94143300
C	-1.15018000	-1.67866600	-2.74678500
C	-1.32674900	-3.78502800	-0.90813000
C	-2.29099600	-2.47112600	-2.67231300
C	-2.40360600	-3.51405200	-1.74932200
H	-1.40617900	-4.58531400	-0.17669100
H	-3.13004500	-2.23505100	-3.32049900
C	-1.06658100	-0.50098400	-3.67933800
H	-0.32782600	-0.66743000	-4.46919400
H	-0.77251400	0.40012300	-3.13112400
H	-2.04171400	-0.31189400	-4.13054300

C	0.94908000	-3.26176500	0.05012300
H	0.88800300	-2.52758700	0.86395900
H	1.93934100	-3.17263900	-0.40840800
H	0.86149600	-4.25773700	0.48748300
H	4.53286700	2.56961600	-1.76842700
C	-3.70369000	-4.26155500	-1.62144900
H	-3.60539000	-5.13025300	-0.96663600
H	-4.45716900	-3.58866200	-1.19750100
H	-4.06791100	-4.60034300	-2.59542300
N	5.11948400	-3.02927400	2.32130800
O	6.04264700	-3.63956600	2.83497300
O	3.94293800	-3.26476700	2.53203300
C	-2.56504000	-2.90259800	2.20279000
C	-2.28074900	-1.71069000	1.54538000
C	-1.57375800	-0.69207500	2.19439800
C	-1.14194800	-0.90386300	3.50376800
C	-1.42175000	-2.10091700	4.16433900
C	-2.13776800	-3.10346300	3.51643900
H	-3.12622700	-3.67793500	1.68706200
H	-2.63615700	-1.55024700	0.52942500
H	-0.58020300	-0.12164500	4.00823100
H	-1.07680200	-2.24863100	5.18354500
H	-2.35856400	-4.03530000	4.02823300
C	-1.25265100	0.60159600	1.46362300
H	-0.62455600	1.20416900	2.13817200
C	-0.41960800	0.26664300	0.25068400
C	0.93017400	0.08157900	0.31541700
O	1.76534000	0.22773800	1.27602600
H	-0.94625700	0.08119700	-0.67875500
C	-3.76837300	1.47898800	1.77291900
C	-2.49237500	1.41289400	1.07817500
C	-2.25880200	2.80567900	0.67417900
N	-3.46214400	3.46250400	0.96522100
H	-2.94889100	0.91884400	-0.21561300
N	-4.35573600	2.63343900	1.64178200
C	-3.83699500	4.78917900	0.73480200
C	-2.94669600	5.72869700	0.18831100
C	-5.14188400	5.20048000	1.06142400
C	-3.36664700	7.03918500	-0.02119700
H	-1.94359900	5.40982500	-0.05671500
C	-5.53758400	6.51388800	0.84477800
H	-5.82721200	4.47737700	1.48302000
C	-4.65734100	7.44885000	0.30175100
H	-2.66258500	7.75111800	-0.44306200

H	-6.55069900	6.80733800	1.10498600
H	-4.97202500	8.47394000	0.13516000
N	-1.22602800	3.38308200	0.14705100
H	-0.51064000	2.66320400	0.03260800
C	-4.51583100	0.37910600	2.46167000
H	-5.46740800	0.77170700	2.82702100
H	-4.70024400	-0.43710600	1.75753500
H	-3.94561300	-0.02997300	3.30034400
C	-4.12084100	-0.19727600	-1.52078600
O	-4.60316500	-0.96545400	-0.69562100
O	-4.55627800	-0.22531100	-2.81347300
H	-5.24193200	-0.90689500	-2.84226100
O	-3.20998000	0.69396700	-1.35409300

TS5SR

C	-2.30874400	0.16873400	-0.78346900
C	-3.88993500	-1.34297800	-0.87017700
C	-1.63595500	-2.25416200	-1.18100400
H	-0.67407700	-1.86138500	-1.52062100
N	-4.51790500	-0.22411600	-0.65166800
N	-3.51322900	0.70379400	-0.59089000
N	-2.53776400	-1.14379900	-0.94066300
C	-4.36479700	-2.71981400	-1.21040900
H	-5.42341400	-2.70327000	-1.46746300
H	-4.21083500	-3.40498600	-0.36697200
C	-2.22712000	-3.19866600	-2.26790800
O	-3.64943100	-3.12478600	-2.36743900
C	-1.50773600	-4.48882400	-0.35952700
C	-1.46864300	-3.14723200	0.02778900
C	-1.27453900	-2.77800900	1.34822700
C	-1.09683200	-3.80833300	2.26527400
C	-1.11866200	-5.15409900	1.91322400
C	-1.32965700	-5.49888500	0.58166300
C	-1.74647000	-4.60094200	-1.84432200
H	-1.26812300	-1.74541400	1.68050800
H	-0.97653500	-5.90670300	2.67827800
H	-1.35940900	-6.54290600	0.28881200
H	-2.48089800	-5.36383200	-2.11380300
H	-0.80756500	-4.83867900	-2.35643200
C	-3.76412000	2.07427100	-0.24012200
C	-3.54435800	2.45800100	1.08355800
C	-4.17371800	2.95421600	-1.24263700
C	-3.77481200	3.79679900	1.40198400
C	-4.39581000	4.27802400	-0.87206500

C	-4.20556200	4.71331000	0.44209600
H	-3.61297800	4.12835800	2.42473500
H	-4.71063100	4.99020800	-1.63078400
C	-4.30262600	2.47764000	-2.66204900
H	-5.02332700	1.65855300	-2.74386200
H	-3.32608000	2.10981800	-2.99521400
H	-4.62313700	3.29016000	-3.31574000
C	-3.04320500	1.48005000	2.11353100
H	-1.97970300	1.26990900	1.94887600
H	-3.58809000	0.53195100	2.06663500
H	-3.15365300	1.89239600	3.11771700
H	-1.85190200	-2.90465000	-3.24866400
C	-4.47816500	6.14676200	0.81735300
H	-3.91743500	6.43524900	1.70886700
H	-4.20893800	6.82413500	0.00366300
H	-5.54209300	6.29331300	1.03028600
N	-0.87395500	-3.45286500	3.67109000
O	-0.76944600	-4.35816800	4.48009600
O	-0.80330800	-2.26881900	3.95248200
C	0.30801700	3.70137900	2.80755400
C	0.32380300	3.03459000	1.58924100
C	1.33895400	2.11891400	1.27770300
C	2.34193300	1.89234600	2.21889500
C	2.32778500	2.55891600	3.44653900
C	1.31404600	3.46273300	3.74613200
H	-0.48749200	4.40837800	3.02634100
H	-0.46420400	3.21108000	0.85773700
H	3.14108800	1.19062600	1.99330600
H	3.11556900	2.36885400	4.16947700
H	1.30600300	3.97993200	4.70060000
C	1.26430000	1.39350300	-0.06627200
H	1.13971900	2.16478400	-0.83993700
C	-0.02387400	0.61017000	-0.11178600
C	-1.03517700	0.94707700	-0.95483500
O	-1.09565800	1.80877900	-1.90795600
H	-0.19594700	-0.15248300	0.64208300
C	2.90914300	-0.67357100	0.13692500
C	2.49967700	0.59051900	-0.44392600
C	3.76841000	1.29795400	-0.64869100
N	4.75059600	0.33735900	-0.36713100
H	2.11938600	0.30738800	-1.78271200
N	4.19793700	-0.84502400	0.12706300
C	6.14095600	0.41012300	-0.50769300
C	6.78318000	1.58062600	-0.94414300

C	6.91942300	-0.72206600	-0.20892200
C	8.16914200	1.59967900	-1.07515600
H	6.18421300	2.45091100	-1.17159400
C	8.30082000	-0.67789600	-0.34397500
H	6.42264900	-1.62400400	0.12269500
C	8.94234900	0.48091600	-0.77864900
H	8.64743400	2.51379500	-1.41582500
H	8.88083600	-1.56529100	-0.10717200
H	10.02193100	0.50946800	-0.88426400
N	4.02532800	2.50760000	-1.03028500
H	3.13242600	2.98617500	-1.15487300
C	2.02370400	-1.76746600	0.64333800
H	1.29854600	-2.04536000	-0.12813700
H	2.62558700	-2.63985700	0.90520400
H	1.46933700	-1.44523800	1.53298200
C	0.75731500	-0.64622500	-2.99053800
O	1.54926900	0.36461600	-2.83772600
O	-0.48319000	-0.32836200	-3.43463100
H	-0.64729100	0.61320200	-3.17334000
O	1.01768300	-1.82661400	-2.76547200

TS5SS

C	-0.50264000	2.03844500	-0.46364500
C	-1.48598500	3.99866200	-0.37448100
C	-3.05806600	2.09556500	-0.33058300
H	-3.03105200	1.10396000	-0.77964700
N	-0.21632400	4.27297400	-0.36578400
N	0.38436600	3.04287800	-0.40656400
N	-1.70576100	2.65150100	-0.43488600
C	-2.68265200	4.88930600	-0.43393100
H	-2.40138700	5.88204600	-0.78434100
H	-3.15388000	4.97953800	0.55478000
C	-4.10002400	3.05770900	-1.01182700
O	-3.55781800	4.31560300	-1.38762200
C	-4.70999200	2.67974500	1.30889700
C	-3.48833400	2.03751300	1.11849100
C	-2.78965600	1.46025100	2.17088700
C	-3.36736600	1.57738600	3.42823000
C	-4.58825100	2.20998300	3.65726400
C	-5.27142400	2.76403900	2.58239600
C	-5.25615500	3.20227800	0.00731200
H	-1.85822600	0.92612300	2.00328400
H	-4.97959300	2.26287600	4.66525100
H	-6.22226500	3.26218300	2.73916900

H	-5.58295900	4.24497800	0.06418500
H	-6.12021900	2.60980500	-0.30929600
C	1.81070000	2.92380600	-0.28071100
C	2.32776500	2.53334200	0.95790100
C	2.59181100	3.11169600	-1.42026200
C	3.69636600	2.28605200	1.01684400
C	3.95770000	2.85394800	-1.30693400
C	4.51829800	2.41894500	-0.10436800
H	4.12553300	1.93810200	1.95418100
H	4.58995300	2.96656800	-2.18442800
C	1.95699400	3.49751900	-2.72970500
H	1.41998400	4.44689700	-2.64777700
H	1.23026500	2.73878300	-3.04394700
H	2.71231200	3.59117300	-3.51135200
C	1.44246400	2.31581200	2.15381700
H	0.98446200	1.31726100	2.11161300
H	0.64805000	3.06706700	2.21110800
H	2.03243700	2.35812600	3.07225100
H	-4.44466400	2.62360500	-1.95003100
C	5.97564600	2.06013300	-0.00013400
H	6.49461500	2.71840800	0.70370100
H	6.06192900	1.03442600	0.37274400
H	6.47616200	2.12991000	-0.96860700
N	-2.65100600	1.01610900	4.58062900
O	-3.20294100	1.05351300	5.66868800
O	-1.54256700	0.55110800	4.39009900
C	2.10406200	-1.78663800	-4.70883900
C	1.72431400	-1.19928000	-3.50156900
C	1.60446300	-1.96108100	-2.33826800
C	1.85124200	-3.33674200	-2.42137200
C	2.22641800	-3.92774000	-3.62253900
C	2.36156300	-3.15207800	-4.77426500
H	2.19513700	-1.17247000	-5.60020700
H	1.51612600	-0.13412500	-3.46427000
H	1.75443100	-3.94067000	-1.52413200
H	2.41743300	-4.99618300	-3.65988800
H	2.65899000	-3.61026200	-5.71261500
C	1.22031500	-1.35185300	-0.99483700
H	0.33839900	-1.90300800	-0.63804600
C	0.83423600	0.09731100	-1.04782600
C	-0.32634600	0.54953400	-0.49184800
O	-1.31743800	-0.10409900	0.00185500
H	1.59010500	0.79670700	-1.38543300
C	3.70919000	-1.14407300	-0.09787400

C	2.32000600	-1.53875200	0.05791300
C	2.00990900	-1.13487600	1.43610000
N	3.26354500	-0.83662400	1.99582800
H	2.49596500	-2.92645100	0.33971700
N	4.27240600	-0.82134700	1.02948800
C	3.58681900	-0.42851900	3.29117400
C	2.61832200	-0.32879900	4.30596100
C	4.92254700	-0.10407200	3.59494900
C	2.99157300	0.09613900	5.57788300
H	1.59136900	-0.57235900	4.07213300
C	5.27010400	0.31759300	4.87239800
H	5.66917900	-0.19126800	2.81633700
C	4.31131400	0.42404100	5.87837700
H	2.22702300	0.17157200	6.34613400
H	6.30781800	0.56210400	5.08149300
H	4.58831300	0.75392500	6.87427400
N	0.89416500	-1.07720500	2.08467300
H	0.12608500	-1.23942800	1.42999800
C	4.51502600	-1.14486900	-1.35555200
H	4.15003600	-0.36971800	-2.03955600
H	5.56324800	-0.94588800	-1.11945500
H	4.42871000	-2.11211500	-1.85574400
C	3.59852100	-4.66945800	0.27028400
O	4.42558000	-4.24967000	-0.52972700
O	3.72548700	-5.92348200	0.79123000
H	4.53031200	-6.28765700	0.39873000
O	2.55081800	-4.07475300	0.72180800

M5R

C	-1.09441500	0.49694200	-0.84732500
C	-2.40524000	-0.00925500	-2.53155400
C	-2.20079700	-1.81982100	-0.86723400
H	-1.36575200	-2.14533500	-0.25240300
N	-2.01377200	1.20368200	-2.78154700
N	-1.20679200	1.51142400	-1.72000000
N	-1.86589300	-0.48178300	-1.36774200
C	-3.21860500	-0.95702500	-3.34787800
H	-3.28593400	-0.60849100	-4.37813300
H	-4.23283000	-1.05497700	-2.93505600
C	-2.45575300	-2.81165300	-2.06090000
O	-2.52136400	-2.18586400	-3.33640500
C	-4.38894600	-2.75493400	-0.58299100
C	-3.49930200	-1.79820500	-0.09675700
C	-3.82520900	-0.97059500	0.96886700

C	-5.09721700	-1.12559400	1.50584200
C	-6.01616000	-2.06501600	1.04030200
C	-5.65428000	-2.89448500	-0.01352600
C	-3.77488600	-3.54283000	-1.70930200
H	-3.10688600	-0.26572100	1.37563700
H	-6.99096400	-2.13417800	1.50620500
H	-6.35329200	-3.63477900	-0.38809400
H	-4.42126300	-3.60649400	-2.59022200
H	-3.56630900	-4.56751600	-1.38595200
C	-0.61519600	2.81814100	-1.63965900
C	-1.24385100	3.77752300	-0.84859500
C	0.59246700	3.03909300	-2.30849000
C	-0.61936100	5.02113400	-0.73625500
C	1.17684300	4.29415800	-2.16247500
C	0.58939800	5.29148600	-1.37768800
H	-1.08294500	5.78785500	-0.12046300
H	2.12446000	4.49306900	-2.65713400
C	1.27196500	1.92646100	-3.06131100
H	2.08941800	2.31828700	-3.66844000
H	0.57361600	1.39679300	-3.71449800
H	1.69478600	1.19687100	-2.35758200
C	-2.50698200	3.45158000	-0.09849800
H	-2.28944700	2.75272600	0.71825300
H	-3.24942300	2.98172400	-0.75019900
H	-2.94392400	4.35346000	0.33254100
H	-1.60822300	-3.49360400	-2.12308400
C	1.27305300	6.62448400	-1.21907800
H	1.41962300	7.10721700	-2.18956500
H	0.69071500	7.29648300	-0.58547000
H	2.26023900	6.49482100	-0.76522800
N	-5.49461400	-0.25729200	2.61933200
O	-6.60012600	-0.42273500	3.10856800
O	-4.70267500	0.58924000	2.99515100
C	4.38635800	3.52504200	2.83556800
C	3.68910300	2.34545800	2.58114600
C	2.38444000	2.37739700	2.08292900
C	1.79792400	3.62544100	1.84105900
C	2.49120100	4.80618400	2.09282800
C	3.79143100	4.76095100	2.59241000
H	5.40136000	3.47669600	3.21868500
H	4.15775500	1.38169200	2.75940800
H	0.78602400	3.66826000	1.44495300
H	2.01230300	5.76247600	1.89980500
H	4.33660100	5.67932500	2.78723900

C	1.59473700	1.09762100	1.82188300
H	0.95437200	0.91686500	2.69918400
C	0.68898700	1.24597600	0.62554900
C	-0.35226900	0.38445900	0.44618800
O	-0.74751200	-0.56258000	1.22093100
H	0.96549200	1.96212900	-0.13319700
C	2.31385900	-1.34625800	2.30458200
C	2.43256700	-0.13973700	1.64602600
C	3.35553900	-0.34914800	0.55723200
N	3.72590700	-1.69410900	0.68403100
H	1.01460600	-1.79319700	0.42117500
N	3.08383600	-2.31511200	1.76224200
C	4.58398300	-2.46105100	-0.10748800
C	5.14411900	-1.95762000	-1.29393600
C	4.89473000	-3.77420700	0.28849800
C	5.99363300	-2.75940900	-2.05017300
H	4.90235500	-0.94695200	-1.59173600
C	5.74430300	-4.55600400	-0.48399600
H	4.47016000	-4.16572600	1.20383100
C	6.30408000	-4.05932100	-1.65976100
H	6.41596500	-2.35401200	-2.96543000
H	5.97096000	-5.56707000	-0.15805800
H	6.96652800	-4.67473900	-2.25966600
N	3.80685400	0.45192400	-0.37239700
H	3.40068100	1.37094800	-0.19304500
C	1.40264200	-1.68816700	3.44223600
H	0.39219300	-1.34413800	3.20310700
H	1.39072300	-2.76882900	3.60318000
H	1.72790500	-1.20664500	4.36957000
C	0.84259200	-3.65168300	-0.16675300
O	0.86806700	-2.31631500	-0.39199900
O	1.53119000	-4.09850200	0.85024800
H	2.21489500	-3.37266800	1.26619300
O	0.19620900	-4.36389000	-0.91220200

M5R'

C	0.97470400	-0.64551200	0.98140600
C	0.09555400	-1.82395000	2.62552900
C	-1.40688200	-0.11199800	1.71500300
H	-1.31167200	0.86829700	1.25072900
N	1.17788000	-2.48010600	2.30758700
N	1.71287300	-1.73618100	1.26093800
N	-0.06854600	-0.70002200	1.85753100
C	-0.98689300	-2.11906800	3.62026500

H	-0.58186300	-2.64654900	4.48722700
H	-1.75483400	-2.75327100	3.15206600
C	-2.10115400	-0.00699600	3.10556800
O	-1.53144300	-0.89264300	4.09154200
C	-3.54270500	-1.16823200	1.55737200
C	-2.31036100	-1.02986000	0.92005400
C	-2.01260900	-1.68160900	-0.27116600
C	-3.00166200	-2.52497200	-0.78348200
C	-4.25763200	-2.66470600	-0.17713700
C	-4.53400000	-1.98046000	1.00031700
C	-3.58575400	-0.31470100	2.79987900
H	-1.06829900	-1.55981500	-0.78317000
H	-4.99553300	-3.30316700	-0.64547400
H	-5.51177200	-2.06290900	1.46418700
H	-4.07739100	-0.78248800	3.65927600
H	-4.10909400	0.62496200	2.57380200
C	2.90548700	-2.15107900	0.57779500
C	2.78402200	-3.12367400	-0.42346300
C	4.11443400	-1.52018900	0.88783800
C	3.95343400	-3.51380100	-1.07787200
C	5.25316900	-1.93808000	0.19567500
C	5.19308400	-2.93804600	-0.77826900
H	3.88732800	-4.26103700	-1.86580100
H	6.20222800	-1.45051000	0.40576900
C	4.16631100	-0.37509100	1.86687900
H	3.60902200	-0.59608700	2.78437000
H	3.72291900	0.51761400	1.40898200
H	5.19932000	-0.13786800	2.13778300
C	1.43101100	-3.63025500	-0.84694300
H	0.90022300	-2.82660300	-1.37076400
H	0.81610200	-3.93562600	0.00614500
H	1.51848200	-4.48005300	-1.52979100
H	-1.96918900	0.98736400	3.53559100
C	6.44390000	-3.38861200	-1.49601500
H	6.92365400	-4.22662000	-0.97137800
H	6.22000800	-3.72639600	-2.51374600
H	7.17888000	-2.57922300	-1.56211000
N	-2.71726100	-3.28402200	-1.99371300
O	-3.63478400	-3.94894100	-2.49576400
O	-1.57039200	-3.24295100	-2.45174700
C	3.16094600	5.30691900	-0.08559200
C	2.45744000	4.10021700	-0.08614400
C	1.18573500	4.00693200	-0.66138000
C	0.62966500	5.15951500	-1.23321600

C	1.32468100	6.36820100	-1.23107000
C	2.59658900	6.44907700	-0.65597900
H	4.15245700	5.34932500	0.36042900
H	2.90860000	3.20818500	0.33934600
H	-0.36062800	5.09250900	-1.67608100
H	0.87365100	7.25013600	-1.68127000
H	3.13950000	7.39185100	-0.65347000
C	0.45190300	2.67829100	-0.74301700
H	0.64650000	2.28539000	-1.74979500
C	0.87910300	1.61765900	0.24153500
C	1.14474200	0.31861800	-0.10388300
O	1.48570300	-0.18956700	-1.26401700
H	0.69814400	1.84934200	1.28916300
C	-1.75784500	3.37449800	0.53075700
C	-1.03808000	2.72524600	-0.49926300
C	-1.93967400	1.74500200	-1.04569800
N	-3.15743800	1.98064400	-0.35356300
H	4.69009600	3.53699600	-2.30464000
N	-3.01876500	2.96100800	0.63302300
C	-4.40569800	1.37612300	-0.51662700
C	-4.66440700	0.46639200	-1.56226700
C	-5.44836500	1.68693200	0.38359500
C	-5.92471200	-0.11491300	-1.68159700
H	-3.85760400	0.22243200	-2.24139600
C	-6.69795500	1.08623600	0.24889900
H	-5.25665600	2.41209000	1.16464600
C	-6.95333900	0.17843400	-0.78242100
H	-6.09564400	-0.82101500	-2.49179700
H	-7.48394000	1.34161800	0.95787800
H	-7.93075600	-0.28769200	-0.88332700
N	-1.78772400	0.75666500	-1.89393800
H	-0.81272600	0.72125100	-2.19921500
C	-1.26776700	4.42706200	1.48299200
H	-2.02456400	4.60753900	2.25325000
H	-0.33011600	4.12604100	1.96729200
H	-1.05517200	5.37107200	0.96769000
C	3.72020900	1.95825400	-2.15498500
O	2.87596400	2.37938100	-2.92794300
O	3.73664800	0.82258200	-1.50570700
H	2.77138300	0.36673200	-1.55062100
O	4.83828200	2.69091900	-1.84978800

M5S

C	-0.94081500	1.94483800	-0.63958000
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C	-0.69312400	2.61584500	-2.71461800
C	1.39044900	2.63955900	-1.37998400
H	1.65996100	2.75754100	-0.31526400
N	-1.92356200	2.17296600	-2.67133400
N	-2.05597600	1.75043000	-1.35659300
N	-0.06682200	2.50789600	-1.50049100
C	0.12320700	3.19351500	-3.82924600
H	-0.51888200	3.65791400	-4.58092000
H	0.71262100	2.39731300	-4.30937200
C	1.90577600	3.80580200	-2.28451100
O	0.95607800	4.21371200	-3.29216100
C	3.12205600	1.76810700	-2.79433500
C	2.07762700	1.41490600	-1.93907600
C	1.77922700	0.09408300	-1.64887800
C	2.58206000	-0.88480800	-2.22704100
C	3.65193500	-0.56325100	-3.07172900
C	3.91754300	0.77179400	-3.36604900
C	3.22714000	3.27045600	-2.89931200
H	1.00104000	-0.18206900	-0.95301800
H	4.26254900	-1.36351200	-3.47017500
H	4.75752800	1.02980600	-4.00377600
H	3.35087400	3.64648800	-3.92142400
H	4.08402700	3.61950900	-2.30929000
C	-3.21216500	1.10161300	-0.79806900
C	-3.35031100	-0.27875400	-0.98780800
C	-3.99603000	1.84080700	0.09835400
C	-4.29824200	-0.93610700	-0.19762000
C	-4.91559500	1.13386500	0.87106100
C	-5.05179700	-0.25362800	0.76321400
H	-4.40641500	-2.01379800	-0.29764400
H	-5.48356300	1.66851600	1.62685500
C	-3.79287000	3.32603600	0.26442800
H	-3.86382900	3.84336600	-0.70043900
H	-2.80587900	3.53676000	0.69011400
H	-4.54165900	3.74222000	0.94275400
C	-2.46514600	-1.03512500	-1.95039600
H	-1.44402800	-1.15376300	-1.56542000
H	-2.38832600	-0.51990400	-2.91337800
H	-2.85831600	-2.04049700	-2.12740000
H	2.06244100	4.71383400	-1.70026200
C	-5.94558500	-0.99165900	1.72981600
H	-6.01309800	-2.05812800	1.49068900
H	-5.53941000	-0.88883900	2.74377300
H	-6.96168100	-0.57821800	1.74115400

N	2.25380400	-2.28279600	-1.97873300
O	3.09041900	-3.14384900	-2.27461100
O	1.11775900	-2.53942200	-1.55111500
C	-2.38870000	-2.52779500	3.64112800
C	-1.73740200	-1.57613700	2.85095800
C	-0.40935800	-1.21450100	3.10573000
C	0.25533800	-1.84034600	4.16945100
C	-0.38783600	-2.79141600	4.95875800
C	-1.71755200	-3.14081400	4.70018600
H	-3.42261400	-2.78871200	3.42140700
H	-2.27614600	-1.08456900	2.04595700
H	1.28833200	-1.56667600	4.36775800
H	0.14750300	-3.26063100	5.78158600
H	-2.21975700	-3.88468200	5.31514300
C	0.27758200	-0.10676800	2.32090100
H	0.32592600	0.74912400	3.00806700
C	-0.47982300	0.35153400	1.09821200
C	-0.70351400	1.65489200	0.79978500
O	-0.66841200	2.73430500	1.54543400
H	-0.62534700	-0.39517900	0.32186200
C	2.26774400	-1.59188800	1.34897500
C	1.67696200	-0.40344400	1.81922100
C	2.55598200	0.66200400	1.41922200
N	3.63651200	-0.00881100	0.79113900
H	-1.77428100	2.54815100	2.53365900
N	3.44029000	-1.38803300	0.74397200
C	4.74972700	0.51643500	0.13911100
C	4.99418700	1.90451600	0.06457100
C	5.65851100	-0.36504400	-0.48810000
C	6.09506600	2.37928100	-0.64894600
H	4.30837600	2.57061100	0.57309000
C	6.74700000	0.13257000	-1.19449900
H	5.46428500	-1.42823100	-0.42914500
C	6.97540000	1.50956100	-1.29680100
H	6.26574000	3.45448100	-0.69118500
H	7.42412300	-0.56824000	-1.68006500
H	7.82831500	1.89219300	-1.85305200
N	2.47370300	1.97484200	1.50216300
H	1.61289200	2.22505600	1.99215100
C	1.75334600	-2.99989500	1.42871900
H	0.70468000	-3.05639700	1.12057800
H	2.34255300	-3.63994400	0.76603700
H	1.80885300	-3.39430400	2.45080400
C	-2.51510400	1.42854800	3.94381100

O	-1.51816000	1.25578400	4.61924500
O	-3.65956100	0.70081700	4.14505300
H	-3.39619300	0.02672600	4.79520200
O	-2.69407600	2.28590200	2.96638700

M5S'

C	-1.16325800	0.66748600	0.92869200
C	-2.67679900	0.05905400	2.43689800
C	-3.59868300	0.30193700	0.16748700
H	-3.34580100	0.93876400	-0.67974000
N	-1.56300000	0.06263500	3.10521300
N	-0.60662000	0.42870600	2.16050600
N	-2.50460700	0.42207900	1.12736200
C	-4.06979700	-0.24012400	2.88175000
H	-4.16400500	-0.11297300	3.96190400
H	-4.34163300	-1.27575800	2.62427400
C	-4.96612000	0.69195300	0.83230200
O	-4.95225300	0.69557400	2.26578600
C	-5.14163500	-1.49580800	-0.20654400
C	-3.79337700	-1.13293600	-0.27851600
C	-2.80937600	-2.03168500	-0.68481700
C	-3.24032100	-3.31990700	-1.00433900
C	-4.58402800	-3.70482800	-0.96726200
C	-5.54646400	-2.78324800	-0.56146000
C	-5.98338500	-0.33428300	0.26426700
H	-1.76286800	-1.75256100	-0.77087600
H	-4.84708200	-4.71878900	-1.24274100
H	-6.59281400	-3.07284400	-0.51074900
H	-6.72050200	-0.60172700	1.02920000
H	-6.53442600	0.10758400	-0.57702600
C	0.77863400	0.16548700	2.43086700
C	1.30908400	-1.07100900	2.02523400
C	1.55171400	1.16629200	3.02791800
C	2.68191700	-1.25913300	2.19075500
C	2.92139000	0.92759600	3.17289800
C	3.50252600	-0.26827400	2.73685900
H	3.12749900	-2.18514400	1.83884600
H	3.54983200	1.70318900	3.60612700
C	0.92311000	2.47678500	3.43570800
H	0.08665300	2.32045400	4.12672000
H	0.52132900	3.00887500	2.56367800
H	1.65611500	3.12913500	3.92044500
C	0.45403800	-2.12629600	1.37770200
H	0.32057600	-1.91063300	0.30791900

H	-0.53546400	-2.19191200	1.84421100
H	0.93201100	-3.10719100	1.43548800
H	-5.23685100	1.71697000	0.57144800
C	4.99245200	-0.49506300	2.79853500
H	5.24074200	-1.36478300	3.42050800
H	5.36204100	-0.69534400	1.78642300
H	5.52183400	0.37477800	3.20248900
N	-2.24247700	-4.34426200	-1.35468700
O	-2.63680400	-5.33917200	-1.97232300
O	-1.08643500	-4.15869300	-0.98715300
C	2.08342300	5.43034200	-1.91206300
C	1.57573600	4.19808800	-1.49270300
C	2.06745300	3.00127700	-2.02283900
C	3.08207100	3.06561100	-2.98774800
C	3.59674700	4.29158800	-3.40431900
C	3.09991300	5.48347100	-2.86612900
H	1.67603300	6.34869900	-1.49503400
H	0.76085700	4.15893500	-0.77497700
H	3.46179700	2.13579000	-3.40323800
H	4.38506500	4.31928800	-4.15379200
H	3.50029800	6.44151100	-3.19105600
C	1.45129500	1.66683700	-1.65219300
H	0.76906900	1.41445300	-2.47342300
C	0.67808800	1.60329600	-0.36755000
C	-0.59266600	1.06889000	-0.32494700
O	-1.37325600	0.89736500	-1.39466800
H	1.22795000	1.80416800	0.54269900
C	3.64852000	0.43877900	-0.79159400
C	2.37920400	0.50657700	-1.41537800
C	1.92928600	-0.85909200	-1.54498300
N	3.02563300	-1.62019100	-1.06317400
H	-1.55441600	2.14745300	-1.96880400
N	4.05967200	-0.80730200	-0.60205600
C	3.13847700	-3.00180700	-0.88577700
C	2.10385800	-3.88506100	-1.25573100
C	4.30655000	-3.53406600	-0.29802200
C	2.23551600	-5.25069700	-1.01474100
H	1.20866500	-3.47578900	-1.70247800
C	4.41963300	-4.90454700	-0.07543400
H	5.10589100	-2.85633500	-0.02668600
C	3.38688400	-5.77902500	-0.42470300
H	1.40798800	-5.90120000	-1.28925400
H	5.33001800	-5.29034200	0.38074400
H	3.47798400	-6.84704700	-0.23946500

N	0.79619300	-1.38748600	-1.93469900
H	0.15174400	-0.64002100	-2.19926600
C	4.51484400	1.56252200	-0.30364400
H	4.01831000	2.11234100	0.50725700
H	5.45496300	1.15796100	0.08418500
H	4.73705100	2.28818500	-1.09236100
C	-1.07351200	3.53502400	-3.29216900
O	-0.46448500	2.82118100	-4.07454500
O	-1.14337300	4.89258500	-3.47579000
H	-0.56702000	5.05211000	-4.24143900
O	-1.72601500	3.19155100	-2.21573900

TS5^D

C	-1.91209500	-0.41426200	0.15675300
C	-3.60992400	-1.11879400	-1.01571500
C	-2.93614500	-2.61037200	0.88960600
H	-1.93385700	-3.03304500	1.01959100
N	-3.26584300	0.01157300	-1.56364400
N	-2.20582400	0.43407400	-0.81879100
N	-2.80337300	-1.41216700	0.05542000
C	-4.66633900	-2.09467000	-1.43737300
H	-4.29531500	-2.68280800	-2.28802800
H	-5.56845000	-1.56322400	-1.74122600
C	-3.88327700	-3.62140400	0.19358500
O	-4.99490700	-2.92254900	-0.34582500
C	-4.46732500	-3.46016000	2.48890700
C	-3.62313500	-2.37917200	2.21956900
C	-3.49226900	-1.31570800	3.09564500
C	-4.25269600	-1.38234600	4.25925000
C	-5.09576800	-2.44460400	4.56581800
C	-5.20352100	-3.50198600	3.66670400
C	-4.42704500	-4.45653100	1.35516300
H	-2.83229700	-0.47182900	2.91184500
H	-5.66092700	-2.42797800	5.48899700
H	-5.86573700	-4.33381400	3.88058700
H	-5.40280200	-4.87717400	1.10470700
H	-3.74393200	-5.28102600	1.58535200
C	-1.56663600	1.70919500	-1.03500800
C	-1.99962300	2.77690600	-0.23899400
C	-0.54856100	1.81251400	-1.98332900
C	-1.37599600	4.00245200	-0.43772100
C	0.05715000	3.06317000	-2.12614600
C	-0.34951700	4.16428800	-1.37471500
H	-1.69037200	4.85445700	0.15979300

H	0.87379100	3.17259400	-2.83626400
C	-0.11829700	0.65089800	-2.83948100
H	-0.68819300	0.62953100	-3.77382000
H	-0.27097500	-0.30915900	-2.33888100
H	0.94286300	0.74673900	-3.08445900
C	-3.08269900	2.59105300	0.79098800
H	-2.71180600	1.98426400	1.62464200
H	-3.95660800	2.08839000	0.36429000
H	-3.40200400	3.55671600	1.18488100
H	-3.37636600	-4.20193100	-0.58607500
C	0.28533300	5.51607000	-1.56346100
H	-0.44475900	6.22555700	-1.96631900
H	0.64092900	5.90825900	-0.60719100
H	1.13987300	5.46606300	-2.24208500
N	-4.16390300	-0.26417100	5.20703200
O	-4.77460900	-0.35750200	6.25784100
O	-3.48626400	0.69672000	4.88920800
C	3.12602800	-3.75567000	2.12690500
C	2.26123900	-2.71468700	1.79325000
C	2.75497200	-1.44138400	1.50558300
C	4.13608000	-1.22814900	1.56055600
C	5.00206200	-2.26579700	1.89128600
C	4.49948400	-3.53531200	2.17423200
H	2.72456900	-4.74024900	2.34656900
H	1.18921400	-2.89105900	1.75792100
H	4.52938200	-0.24105700	1.32988300
H	6.07172200	-2.08411900	1.92490100
H	5.17465300	-4.34605000	2.42830600
C	1.82013600	-0.29928500	1.17356700
H	1.60897500	0.25846800	2.09649600
C	0.47145600	-0.66761800	0.54511800
C	-0.74465600	-0.24024800	1.12217100
O	-0.94695900	0.40251800	2.16134400
H	0.44513500	-1.49923600	-0.15961200
C	2.98879400	0.43280500	-1.11219700
C	2.28791500	0.69669900	0.11809600
C	2.41024500	2.13433300	0.32560900
N	3.07590200	2.57036800	-0.82908100
H	0.88736100	0.36161400	-0.23836600
N	3.39314400	1.52787500	-1.69276700
C	3.35319300	3.88032400	-1.23735800
C	3.39627700	4.94089500	-0.32080600
C	3.61369400	4.13409800	-2.59411000
C	3.67405500	6.22861800	-0.77059500

H	3.19055800	4.74180000	0.72148800
C	3.89312100	5.42669600	-3.02167900
H	3.59399100	3.30773700	-3.29337100
C	3.92021400	6.48691800	-2.11659200
H	3.70048900	7.04103800	-0.05003500
H	4.08818100	5.60498500	-4.07505700
H	4.13576900	7.49505500	-2.45491000
N	2.00505000	2.92364800	1.26921300
H	1.50079500	2.36654800	1.95991000
C	3.18109800	-0.89464700	-1.77201700
H	2.22113300	-1.41063100	-1.89048400
H	3.62642200	-0.75443200	-2.75862100
H	3.82696900	-1.54416200	-1.17385800

TS5a

C	-2.48097900	0.60630500	-0.56397200
C	-3.98982900	-0.87958900	-1.08148700
C	-1.72688000	-1.83764100	-0.78452000
H	-0.86110500	-1.56911000	-1.40008300
N	-4.64782200	0.23313900	-0.94250400
N	-3.69838500	1.14659900	-0.59873100
N	-2.66504700	-0.70973300	-0.80357000
C	-4.49157900	-2.20278600	-1.56347800
H	-4.40496300	-2.19099200	-2.65845700
H	-5.52860200	-2.35238000	-1.26242800
C	-2.34816600	-3.11030200	-1.40020200
O	-3.70839100	-3.23681300	-1.00561100
C	-1.21656200	-3.66795000	0.63389200
C	-1.36207600	-2.27637200	0.61526400
C	-1.18375700	-1.51761100	1.75970600
C	-0.79821900	-2.19794800	2.91016500
C	-0.58870700	-3.57112600	2.94921900
C	-0.81581700	-4.31920200	1.79522100
C	-1.56329000	-4.23999200	-0.72110300
H	-1.32512500	-0.44156700	1.79433100
H	-0.28216300	-4.03715000	3.87772400
H	-0.69728600	-5.39731600	1.81575500
H	-2.15896300	-5.15402200	-0.66739800
H	-0.65356200	-4.45850700	-1.29157400
C	-4.11948700	2.49474700	-0.32664300
C	-4.05984200	2.96054200	0.99187600
C	-4.63746100	3.24144400	-1.38433800
C	-4.53271500	4.24622500	1.23270900
C	-5.09316400	4.52795300	-1.08526600

C	-5.04911000	5.04422700	0.20746300
H	-4.49616100	4.63712800	2.24697600
H	-5.49156300	5.13869200	-1.89172500
C	-4.71144300	2.68770200	-2.78229700
H	-5.59121500	2.04362700	-2.88604400
H	-3.82526400	2.08694100	-3.02217600
H	-4.80635300	3.50474600	-3.50088000
C	-3.48358800	2.12707200	2.10611600
H	-2.38865600	2.17723500	2.09443100
H	-3.77534500	1.07550700	2.02180600
H	-3.82631300	2.49689500	3.07402400
H	-2.26596100	-3.06739200	-2.48978700
C	-5.55498300	6.43120200	0.50999200
H	-4.79409400	7.01885500	1.03128400
H	-5.82958700	6.96076800	-0.40434200
H	-6.43648300	6.39194000	1.15736000
N	-0.63347600	-1.42371400	4.14230000
O	0.03853700	-1.91105600	5.03656200
O	-1.18066400	-0.33770200	4.20619800
C	1.01953800	2.35623600	3.49714000
C	0.99016600	2.42481700	2.10575400
C	1.46474800	1.36673100	1.32413400
C	1.97473700	0.23717800	1.97537100
C	2.01408300	0.17064000	3.36627300
C	1.53091200	1.22798800	4.13322800
H	0.63994300	3.18682700	4.08445700
H	0.57494500	3.29802900	1.61033000
H	2.34554500	-0.60649900	1.40063800
H	2.40998400	-0.71723500	3.85044400
H	1.54334600	1.16581300	5.21669800
C	1.30217000	1.42580000	-0.18516500
H	1.14994000	2.47682700	-0.45800400
C	0.05179400	0.66430000	-0.60809600
C	-1.18663100	1.39846900	-0.40026200
O	-1.30037500	2.59279000	-0.17564400
H	0.02467700	-0.30260600	-0.10732300
C	2.95800500	-0.49661600	-0.93988900
C	2.52411600	0.94775800	-0.99678000
C	3.81313500	1.65377200	-0.61169300
N	4.75472100	0.64081200	-0.45677700
H	2.29566500	1.16703600	-2.05018600
N	4.20536000	-0.62194000	-0.67313300
C	6.12407000	0.72220900	-0.14212900
C	6.75141600	1.95568600	0.08232300

C	6.87684500	-0.45914800	-0.05533500
C	8.11042700	1.99057800	0.38340300
H	6.17289800	2.86561100	0.02031700
C	8.23115100	-0.39917400	0.24738000
H	6.39279700	-1.41090000	-0.22771600
C	8.86218800	0.82321700	0.46933200
H	8.58171900	2.95400800	0.55312900
H	8.79705100	-1.32382000	0.30868200
H	9.92035400	0.86289900	0.70523300
N	4.03553200	2.89788200	-0.44015200
H	3.17391600	3.41560700	-0.61568800
C	2.10845100	-1.69039200	-1.23581800
H	1.45389400	-1.49666600	-2.09276500
H	2.74814800	-2.55368400	-1.42635600
H	1.46254400	-1.92706600	-0.37922000
C	-1.52003100	-0.08937900	-3.27173300
O	-1.91769200	1.10372000	-3.03246700
O	-0.23880800	-0.36053800	-3.01664000
H	0.00807100	0.32360700	-1.83151400
O	-2.28688900	-1.02583600	-3.64955700

TS6R

C	-1.47278600	0.43857700	-0.77734900
C	-2.75798000	0.10680500	-2.49874400
C	-2.97457400	-1.60509800	-0.72228800
H	-2.26621800	-2.01489600	-0.00059700
N	-2.08853900	1.18805900	-2.78838800
N	-1.28916200	1.37962400	-1.69688000
N	-2.41276700	-0.37262000	-1.26627800
C	-3.65686500	-0.76592800	-3.31365600
H	-3.60840700	-0.48844300	-4.36585500
H	-4.69657300	-0.69271500	-2.96701600
C	-3.20598600	-2.64257600	-1.87545700
O	-3.13641900	-2.07640000	-3.17937100
C	-5.25877400	-2.30317700	-0.62256800
C	-4.34285200	-1.37469300	-0.12828400
C	-4.70325600	-0.40645600	0.79640500
C	-6.03470500	-0.39847700	1.19358200
C	-6.97948900	-1.30640600	0.71951600
C	-6.58573000	-2.27344900	-0.19770200
C	-4.59503900	-3.25500000	-1.58329500
H	-3.98301400	0.29674100	1.20218600
H	-8.00113400	-1.24239100	1.07186800
H	-7.30710100	-2.98859200	-0.57818000

H	-5.15479700	-3.39316500	-2.51270900
H	-4.48177200	-4.23964700	-1.11848100
C	-0.35079900	2.46713400	-1.58538000
C	-0.60698300	3.45309700	-0.62857400
C	0.83143500	2.40034100	-2.32993200
C	0.38041200	4.41579900	-0.42933200
C	1.78012600	3.39388600	-2.09476400
C	1.57692000	4.39835400	-1.14570900
H	0.22191000	5.17955100	0.32694200
H	2.71671700	3.35900400	-2.64587400
C	1.13856700	1.25059100	-3.25376800
H	1.84544600	1.56676900	-4.02313700
H	0.24593800	0.85763100	-3.74245900
H	1.61532500	0.43832800	-2.68909400
C	-1.87132500	3.45379200	0.19131000
H	-1.82195000	2.70600200	0.99112600
H	-2.74977600	3.23209100	-0.42188900
H	-2.01488300	4.42869800	0.65976400
H	-2.40364400	-3.37957000	-1.83670600
C	2.62786500	5.45036900	-0.91130500
H	2.55971600	6.23897600	-1.66788400
H	2.50629800	5.90858600	0.07264300
H	3.63012500	5.01866600	-0.97031400
N	-6.46761400	0.61796000	2.15941500
O	-7.62437100	0.58499800	2.54367700
O	-5.64854000	1.44326100	2.52371100
C	2.98504100	3.72520800	2.04849800
C	2.87733400	2.37067000	1.73246900
C	1.72121200	1.65567700	2.05284200
C	0.67505600	2.32976900	2.69678900
C	0.78057400	3.68124300	3.01233800
C	1.94008300	4.38623700	2.68871200
H	3.89288900	4.26487200	1.79378500
H	3.69415100	1.86217200	1.22852900
H	-0.22875200	1.77797200	2.94665000
H	-0.03977000	4.18365500	3.51746000
H	2.02822500	5.44009900	2.93699400
C	1.53233300	0.19048200	1.65339200
H	0.97926200	-0.29735800	2.46820600
C	0.62380600	0.15658200	0.42878400
C	-0.77973000	0.27293600	0.56389700
O	-1.52892100	0.07353900	1.52564900
H	1.02050100	0.67345200	-0.44103900
C	3.36856400	-1.56367700	2.26390700

C	2.78919800	-0.60105600	1.41134700
C	3.63080200	-0.54664000	0.25758100
N	4.59981800	-1.53669800	0.50850500
H	0.49316100	-1.08492400	-0.11641200
N	4.43732700	-2.14179700	1.74798000
C	5.68541300	-1.93273100	-0.27939400
C	5.88241800	-1.44314200	-1.58189800
C	6.60723200	-2.86026700	0.24046600
C	6.97905400	-1.87033600	-2.32530600
H	5.17155600	-0.73083800	-1.97604500
C	7.69261800	-3.27413800	-0.52071200
H	6.45039500	-3.24437200	1.23946200
C	7.89449200	-2.78422600	-1.81047300
H	7.11293200	-1.47710800	-3.32946100
H	8.39058900	-3.99073400	-0.09664300
H	8.74596200	-3.10893200	-2.39982100
N	3.64547300	0.21232500	-0.82579600
H	2.92852400	0.92681200	-0.70699300
C	2.86947300	-1.98484000	3.61318300
H	1.86873600	-2.42428500	3.54164100
H	3.54510600	-2.72783300	4.04068400
H	2.80716100	-1.13095200	4.29517900
C	-0.02652300	-3.11406600	0.20717100
O	0.13523700	-2.17293100	-0.66855400
O	0.89319100	-3.15902800	1.20312400
H	1.59128900	-2.49246000	1.04502200
O	-0.94113600	-3.92978600	0.21523700

TS6R'

C	1.15660300	-1.03138300	0.64270900
C	0.36566400	-2.22438500	2.28718100
C	-1.20536700	-0.51381500	1.41017500
H	-1.04328000	0.47180600	0.96343700
N	1.56568900	-2.68975200	2.08489000
N	2.03896100	-1.93653900	1.04119900
N	0.08361500	-1.20566500	1.42283100
C	-0.66302500	-2.48439600	3.34144000
H	-0.22823100	-3.03087300	4.17771100
H	-1.50355000	-3.05931400	2.92980100
C	-1.75673800	-0.38955200	2.87093400
O	-1.06774200	-1.21049100	3.81132800
C	-3.40897900	-1.43443000	1.43575900
C	-2.25897600	-1.29398300	0.66256000
C	-2.18552800	-1.76160300	-0.64220000

C	-3.31756900	-2.40837600	-1.12057300
C	-4.47849000	-2.58578100	-0.36964300
C	-4.52806900	-2.08827800	0.92457600
C	-3.25517200	-0.73947500	2.76082500
H	-1.32244600	-1.58915200	-1.27754100
H	-5.33031800	-3.07870200	-0.82018700
H	-5.43313900	-2.18711700	1.51437500
H	-3.57801300	-1.33719000	3.61810100
H	-3.84546200	0.18329600	2.74625800
C	3.37847400	-2.10017200	0.54066100
C	3.57186700	-2.90700700	-0.57687000
C	4.40391800	-1.41222800	1.19436200
C	4.87924000	-3.03053400	-1.04651000
C	5.68838800	-1.56786700	0.68538300
C	5.94081300	-2.36859900	-0.43224900
H	5.06579400	-3.64297200	-1.92486500
H	6.50866200	-1.03100500	1.15484300
C	4.11207200	-0.50764800	2.36016700
H	3.51928100	-1.01501500	3.12663200
H	3.55678300	0.37223500	2.01748400
H	5.04118500	-0.15907700	2.81326000
C	2.40598100	-3.56017600	-1.26744100
H	1.76388100	-2.79346800	-1.71538700
H	1.79839700	-4.13810000	-0.56406800
H	2.75168600	-4.22930600	-2.05649900
H	-1.60802500	0.62888700	3.23135300
C	7.34660400	-2.49541600	-0.95886900
H	7.96893100	-3.08077300	-0.27487700
H	7.36392400	-2.98495200	-1.93466800
H	7.81016900	-1.50927600	-1.05588500
N	-3.31827600	-2.86564200	-2.50949600
O	-4.36418100	-3.29748000	-2.97137600
O	-2.27790100	-2.78948000	-3.13998800
C	2.76842400	5.43389600	0.32294000
C	2.33704400	4.11530500	0.16153500
C	1.21744900	3.81988800	-0.61671200
C	0.54584000	4.88172800	-1.23799300
C	0.97537000	6.19395000	-1.08622500
C	2.09144400	6.47790700	-0.29640800
H	3.63953700	5.64100000	0.93781800
H	2.88689700	3.31523600	0.64500400
H	-0.33859300	4.65997900	-1.83006100
H	0.43842300	6.99900500	-1.57933000
H	2.42699400	7.50253800	-0.16913600

C	0.66795300	2.40926400	-0.79818400
H	0.73285800	2.17822300	-1.87181500
C	1.47337300	1.32328300	-0.06459600
C	1.17622700	-0.00563400	-0.49105100
O	0.87091700	-0.44492300	-1.59521700
H	1.39251900	1.41712800	1.02584900
C	-1.39216800	2.78376800	0.77964400
C	-0.79141700	2.33623500	-0.40823300
C	-1.80400700	1.60682800	-1.11169300
N	-2.93155300	1.70885500	-0.26763600
H	2.86140600	1.37201600	-0.25068400
N	-2.66283700	2.41516100	0.90171700
C	-4.22110600	1.20866600	-0.45791200
C	-4.60317500	0.54565200	-1.63771400
C	-5.17937800	1.37751700	0.56029100
C	-5.89814400	0.05160500	-1.76767300
H	-3.86187900	0.41725300	-2.41542800
C	-6.46482100	0.87224000	0.41013100
H	-4.89509100	1.92140100	1.45187500
C	-6.83929100	0.19835900	-0.75183300
H	-6.16515400	-0.47198800	-2.68230100
H	-7.18434800	1.01462000	1.21203100
H	-7.84421300	-0.19595100	-0.86463100
N	-1.81838200	0.93835200	-2.24389600
H	-0.85860400	0.91657200	-2.58886400
C	-0.76737800	3.58560600	1.88303900
H	-1.47439900	3.68218400	2.71058800
H	0.14964800	3.11456700	2.25376600
H	-0.48802500	4.58575900	1.53588700
C	4.54957300	0.72337700	-1.23126700
O	3.91460300	-0.01275700	-1.97541000
O	5.90700400	0.82341500	-1.35909400
H	6.13704900	0.21198200	-2.07207000
O	4.09816200	1.47655500	-0.29125800

TS6S

C	-0.93592200	1.42553900	-0.66075800
C	-0.67653600	1.90889800	-2.76941700
C	1.45820600	1.48444400	-1.59836000
H	1.75006800	1.68524500	-0.54869300
N	-1.95923900	2.00128400	-2.56446600
N	-2.10060700	1.69114000	-1.24535700
N	-0.00917800	1.55447500	-1.62704600
C	0.16213200	2.29755000	-3.94215000

H	-0.43647500	2.83831400	-4.67401100
H	0.60922000	1.41459400	-4.41786000
C	2.07719700	2.58387500	-2.53768700
O	1.14168800	3.18114200	-3.42873500
C	2.98853200	0.40603900	-3.09398400
C	1.99288300	0.18029500	-2.14087400
C	1.64564600	-1.10833300	-1.76760700
C	2.31657500	-2.15162700	-2.39014800
C	3.31077800	-1.96019200	-3.34525300
C	3.64910300	-0.66009800	-3.70076900
C	3.22708500	1.87631700	-3.28761900
H	0.90918900	-1.32042400	-1.00494100
H	3.79906400	-2.81843800	-3.78910100
H	4.42347500	-0.48044900	-4.43913700
H	3.23920900	2.17999800	-4.33881300
H	4.19230500	2.15210600	-2.84743700
C	-3.38582900	1.68606600	-0.59395600
C	-4.09417900	0.48576200	-0.53466200
C	-3.82689000	2.88091400	-0.02077900
C	-5.29741700	0.50043200	0.16585200
C	-5.03484700	2.83885800	0.66908100
C	-5.76525700	1.65500300	0.79412500
H	-5.85554700	-0.42622700	0.26852700
H	-5.39744300	3.74461600	1.14794200
C	-3.00138900	4.13499800	-0.11579400
H	-2.75086400	4.37031300	-1.15455700
H	-2.06610200	4.00407900	0.43795400
H	-3.54169200	4.98166700	0.30979700
C	-3.55470700	-0.77710100	-1.14811100
H	-2.82768700	-1.23441900	-0.46911300
H	-3.07101300	-0.58981300	-2.11051800
H	-4.35996500	-1.49758900	-1.30020700
H	2.44548200	3.41087200	-1.92879900
C	-6.99196300	1.59114100	1.66046500
H	-7.77679600	0.98788900	1.19684900
H	-6.71127400	1.11039000	2.60361200
H	-7.39004800	2.58597300	1.87083500
N	1.95808000	-3.51972300	-2.01397400
O	2.68839200	-4.42506600	-2.38017200
O	0.94034500	-3.68450300	-1.36103700
C	-0.95027500	-3.98872700	3.43997400
C	-0.76934500	-2.82475200	2.69217300
C	0.07183500	-1.81076700	3.14778800
C	0.72005200	-1.98292500	4.37621000

C	0.53949900	-3.13842800	5.12756600
C	-0.29685100	-4.15166000	4.65708900
H	-1.60672300	-4.76867400	3.06655600
H	-1.29583300	-2.70824000	1.75061500
H	1.38744600	-1.20087800	4.73069800
H	1.05072700	-3.25108600	6.07885700
H	-0.43937200	-5.05732000	5.23827700
C	0.38089300	-0.55836600	2.34545800
H	0.27462500	0.29557400	3.03185300
C	-0.60002300	-0.27925700	1.17570300
C	-0.80584600	1.09165600	0.82313300
O	-1.08673800	2.02112500	1.59397000
H	-0.41561600	-0.92376400	0.31578400
C	2.60997200	-1.63637600	1.36410100
C	1.78638500	-0.57659900	1.81016800
C	2.41389400	0.60729700	1.35636900
N	3.56917000	0.16899900	0.69690200
H	-1.82969100	-0.52339900	1.60189700
N	3.67761800	-1.20772200	0.70711600
C	4.51355700	0.91497700	-0.01800900
C	4.57284400	2.31859000	0.05730000
C	5.43738200	0.24105900	-0.83687700
C	5.54059900	3.01207700	-0.66729100
H	3.85967500	2.83531500	0.68467900
C	6.39007400	0.95252700	-1.55448800
H	5.38327400	-0.83806700	-0.89940800
C	6.45545600	2.34483400	-1.47820400
H	5.57432300	4.09507200	-0.58909800
H	7.09000600	0.40909800	-2.18280900
H	7.20367200	2.89509200	-2.03915700
N	2.04195300	1.88255400	1.38032200
H	1.19637300	1.95453800	1.94223300
C	2.43057500	-3.11735900	1.52470600
H	1.49697600	-3.45621100	1.06746400
H	3.26336700	-3.63123500	1.03759300
H	2.39543300	-3.40751400	2.57947300
C	-3.79750800	-0.14103100	2.73516100
O	-3.35999500	1.11098000	3.04555900
O	-4.89314800	-0.47597900	3.17416200
H	-2.51089500	1.31315100	2.61586400
O	-3.02808200	-0.87660500	2.00793700

TS6S'

C	-1.27119300	0.47856400	0.86159500
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C	-2.72654500	-0.08192500	2.38687800
C	-3.72104000	0.36772300	0.17806800
H	-3.43355400	1.06186300	-0.60968800
N	-1.58157000	-0.08667300	3.00771800
N	-0.68264000	0.25227900	2.03785400
N	-2.57587900	0.24721000	1.07469100
C	-4.12191500	-0.22622500	2.89506200
H	-4.14100500	-0.15917900	3.98212800
H	-4.55668300	-1.18616800	2.58418200
C	-4.98387800	0.88410400	0.95923300
O	-4.84127700	0.87589300	2.37242500
C	-5.49302700	-1.20431800	-0.17435600
C	-4.12960100	-0.98337200	-0.36290500
C	-3.31105500	-1.92820200	-0.96811800
C	-3.92342100	-3.10985500	-1.36588300
C	-5.28262900	-3.36464000	-1.19401100
C	-6.07873300	-2.39786100	-0.59308800
C	-6.14717700	-0.02262300	0.49130500
H	-2.25222600	-1.75340300	-1.13092500
H	-5.69215400	-4.30917700	-1.52865600
H	-7.13859000	-2.57787400	-0.44742300
H	-6.77407500	-0.30246700	1.34308800
H	-6.78534700	0.51067100	-0.22048600
C	0.72594400	0.28139700	2.33574200
C	1.47795900	-0.86460100	2.06642200
C	1.26451600	1.47384700	2.81910800
C	2.85493300	-0.76440500	2.24862600
C	2.64908600	1.52236600	2.97590700
C	3.45515400	0.42184900	2.67293900
H	3.47756000	-1.62252200	2.00695400
H	3.10798400	2.44620900	3.32011300
C	0.38010500	2.66378900	3.08414900
H	-0.34883300	2.44380100	3.87046800
H	-0.19047900	2.94167800	2.18907400
H	0.97624400	3.52300300	3.39571400
C	0.83129600	-2.12929100	1.57628900
H	0.57435000	-2.04090900	0.50967100
H	-0.07621000	-2.35586600	2.14548800
H	1.52397700	-2.96799600	1.67380400
H	-5.14913500	1.93204900	0.71172400
C	4.95466800	0.49425300	2.77428400
H	5.32799900	-0.15998900	3.56872600
H	5.38670800	0.15762800	1.82651400
H	5.29526400	1.51170700	2.98047900

N	-3.09787900	-4.14759900	-1.99826800
O	-3.64674600	-5.18450300	-2.33468400
O	-1.91200300	-3.91957500	-2.15018100
C	2.81721800	5.17272800	-1.62609400
C	2.11982800	4.02667800	-1.24207200
C	2.07831500	2.90439000	-2.06953600
C	2.74415400	2.96296000	-3.29944000
C	3.43805700	4.10259800	-3.68938700
C	3.48136800	5.21534200	-2.84740700
H	2.84038300	6.03424700	-0.96527700
H	1.60478400	4.01050700	-0.28604500
H	2.72918300	2.08571400	-3.94189400
H	3.94850400	4.12489500	-4.64780400
H	4.02549900	6.10635100	-3.14524400
C	1.41387500	1.60053200	-1.66371100
H	0.82931400	1.25566800	-2.53030500
C	0.42960200	1.72524400	-0.49241100
C	-0.69597900	0.86629700	-0.49009400
O	-1.37907200	0.48660600	-1.45764000
H	0.94264700	1.79912400	0.46217800
C	3.73567500	0.63282800	-0.79407900
C	2.43895300	0.54341500	-1.33580400
C	2.11531300	-0.84422500	-1.33874900
N	3.27141600	-1.46756300	-0.83430200
H	-0.32755100	2.91282300	-0.58404400
N	4.25757500	-0.55107300	-0.50232400
C	3.51036300	-2.81712600	-0.58117200
C	2.60028600	-3.82479700	-0.95158400
C	4.70158000	-3.19132300	0.07037800
C	2.88679300	-5.15609200	-0.66481800
H	1.68229100	-3.53148100	-1.44375800
C	4.96537700	-4.52758900	0.34567100
H	5.40402800	-2.41584400	0.34752000
C	4.06348000	-5.52635800	-0.01650300
H	2.16969500	-5.91788800	-0.95926300
H	5.89117900	-4.78786800	0.85159300
H	4.27318500	-6.56862100	0.20152900
N	1.02791000	-1.50569300	-1.68874100
H	0.34696200	-0.82623900	-2.02313000
C	4.55885700	1.85009000	-0.48643400
H	4.10548300	2.42736800	0.32831000
H	5.55878600	1.53688000	-0.17566700
H	4.64373000	2.51908800	-1.34748900
C	-2.03204100	3.92107800	-0.01848100

O	-2.43782500	3.00001700	0.69650500
O	-2.77944000	5.04492400	-0.15797700
H	-3.56773200	4.91123800	0.38586400
O	-0.94168000	3.97508000	-0.68520100

M6R

C	0.54339300	-0.03260300	-0.97285200
C	1.74909800	1.67136200	-1.62468400
C	1.56728900	1.44405700	0.83387800
H	0.76282100	1.04624600	1.45871500
N	1.32850700	1.13224100	-2.72832300
N	0.61106300	0.03698200	-2.30469600
N	1.33363800	0.96907300	-0.52635300
C	2.41209300	2.98251600	-1.36289500
H	2.42460400	3.59186000	-2.26531600
H	3.43999400	2.84553600	-1.00093300
C	1.58542800	3.02079600	0.88003000
O	1.59253700	3.62874600	-0.40191300
C	3.63885500	2.13112000	1.82957400
C	2.93346700	1.03483800	1.33522100
C	3.48345000	-0.23853400	1.32017500
C	4.77176600	-0.36571100	1.82244000
C	5.50307800	0.70520900	2.33121700
C	4.92826800	1.96986900	2.33510800
C	2.82601500	3.39308500	1.72445000
H	2.93871200	-1.09678500	0.94474000
H	6.50369500	0.53617200	2.70838700
H	5.48327300	2.81908100	2.71933900
H	3.37304000	4.21679900	1.25594500
H	2.51172300	3.73379200	2.71673000
C	0.07524400	-0.89812700	-3.25144000
C	0.73637500	-2.11479400	-3.42254200
C	-1.08800400	-0.54641600	-3.94449200
C	0.18298500	-3.01833000	-4.33154500
C	-1.59663400	-1.48132700	-4.84097000
C	-0.97736500	-2.71900600	-5.04437000
H	0.67437500	-3.97519700	-4.48607100
H	-2.50321300	-1.24141300	-5.39100700
C	-1.75956900	0.77628300	-3.69365400
H	-1.12004500	1.60333500	-4.01779800
H	-1.95317800	0.90917700	-2.62170900
H	-2.70251000	0.83443300	-4.23948400
C	1.98876600	-2.44250400	-2.65078200
H	1.76687800	-2.68234600	-1.60417300

H	2.68974800	-1.60254300	-2.65537400
H	2.48739900	-3.30951500	-3.08610100
H	0.66846400	3.38111700	1.34408600
C	-1.56497000	-3.70528600	-6.01971100
H	-0.95679400	-4.60922400	-6.08493400
H	-2.57544200	-3.99357700	-5.71584200
H	-1.63801000	-3.26657100	-7.01889500
N	5.39404100	-1.69500200	1.81186900
O	6.50873600	-1.80782900	2.29168400
O	4.76354500	-2.61448400	1.31957800
C	-5.56799500	-2.15848600	-1.23104800
C	-4.35767700	-1.70842900	-0.71632800
C	-3.56672800	-2.54691800	0.07784200
C	-4.01577700	-3.83806900	0.34991200
C	-5.23305900	-4.29117700	-0.16043200
C	-6.01045900	-3.45324500	-0.95320500
H	-6.17326300	-1.49937700	-1.84593600
H	-4.01187500	-0.69552800	-0.91654400
H	-3.40927800	-4.49289700	0.97114700
H	-5.57180100	-5.29778500	0.06483000
H	-6.95799900	-3.80281800	-1.35074900
C	-2.24105600	-2.04765700	0.62904800
H	-1.84593500	-2.82653900	1.29343800
C	-1.23607700	-1.88881800	-0.55037400
C	-0.02910400	-1.10899000	-0.10730100
O	0.51702100	-1.29967600	0.96683000
H	-1.71563100	-1.39159600	-1.39256500
C	-2.70365400	-0.65945700	2.79608600
C	-2.36889600	-0.78607400	1.43134000
C	-2.01555500	0.50040400	1.00844000
N	-2.17469300	1.30013500	2.13554800
H	-0.91245400	-2.88550600	-0.87568300
N	-2.58715300	0.58358000	3.23500000
C	-1.76250100	2.63499500	2.28751100
C	-2.02164200	3.58109000	1.28930000
C	-1.07265900	3.01480000	3.44512900
C	-1.55461900	4.88580000	1.43398200
H	-2.59936200	3.29367400	0.41704100
C	-0.62950500	4.32537600	3.58699300
H	-0.89861300	2.27031900	4.21355700
C	-0.85453300	5.26318100	2.57790100
H	-1.75152500	5.61182400	0.65188900
H	-0.09422500	4.61317000	4.48648600
H	-0.49517600	6.28071600	2.68777300

N	-1.53088200	0.85525700	-0.19959400
H	-1.17358300	1.81174900	-0.17385100
C	-3.15628900	-1.75608200	3.70716600
H	-3.36328700	-1.35875600	4.70234700
H	-4.06135800	-2.23605000	3.32154500
H	-2.38884300	-2.53260900	3.79577500

M6R'

C	0.30464700	-0.76884500	-0.12333300
C	-0.03138800	-1.73976600	1.80026000
C	-2.01880400	-1.80070600	0.34113700
H	-2.44492600	-1.09362700	-0.38378300
N	1.22357400	-1.39421900	1.81975000
N	1.42107300	-0.80039500	0.61177800
N	-0.63463400	-1.37731100	0.63040800
C	-0.87585300	-2.38438300	2.84889100
H	-0.41322300	-2.26590200	3.82831000
H	-0.99659300	-3.45631400	2.63742200
C	-2.87425900	-1.83090700	1.66529100
O	-2.10577000	-1.69492200	2.85143600
C	-2.93474300	-4.00616400	0.58937600
C	-2.02213400	-3.23908200	-0.13608200
C	-1.23470600	-3.80463600	-1.12870400
C	-1.40001100	-5.16332100	-1.36339800
C	-2.31056500	-5.95409100	-0.66736000
C	-3.08873500	-5.36530800	0.32173200
C	-3.64599600	-3.16907400	1.61597900
H	-0.52598100	-3.22802600	-1.71006300
H	-2.38968000	-7.00839100	-0.90042300
H	-3.79631000	-5.96358200	0.88571000
H	-3.67208300	-3.63249900	2.60664400
H	-4.68287100	-2.99164300	1.31220300
C	2.73641400	-0.37066900	0.23003400
C	3.37179200	-1.03058900	-0.82500400
C	3.30616400	0.69521400	0.93569400
C	4.61410000	-0.53545100	-1.22224100
C	4.54555300	1.14949800	0.49254300
C	5.20422300	0.55887900	-0.59075100
H	5.13163200	-1.02393100	-2.04334000
H	5.01086000	1.98590400	1.00813600
C	2.62299200	1.30267200	2.13217900
H	2.75080800	0.65835500	3.00698900
H	1.54732300	1.42695000	1.96941800
H	3.05382900	2.27967900	2.35671200

C	2.75909000	-2.22159900	-1.51860900
H	2.06993500	-1.92263300	-2.31668900
H	2.21041100	-2.86017600	-0.82030600
H	3.54125700	-2.82407900	-1.98285200
H	-3.55114900	-0.97916200	1.68598700
C	6.53113900	1.09955000	-1.05396000
H	7.22789900	1.19306600	-0.21689500
H	6.98152800	0.45235600	-1.80838200
H	6.40752300	2.09573100	-1.48927300
N	-0.56320300	-5.79420500	-2.39097800
O	-0.75174100	-6.97303000	-2.63568300
O	0.27934600	-5.10571100	-2.94116100
C	2.51718200	4.52138400	-3.59729400
C	1.97898100	3.30419900	-3.17499100
C	0.62375700	3.19534000	-2.86528000
C	-0.18655400	4.32949400	-2.99688000
C	0.34507600	5.54092900	-3.42004900
C	1.70484900	5.64241100	-3.71977100
H	3.57586300	4.58784400	-3.82842400
H	2.63514000	2.44315600	-3.08360300
H	-1.24138500	4.25300200	-2.74395500
H	-0.29907500	6.40993300	-3.51230700
H	2.12328900	6.58916500	-4.04598500
C	-0.01324900	1.90769600	-2.37334500
H	-0.76461200	1.60787400	-3.11749000
C	0.95980600	0.73458300	-2.20635200
C	0.10947100	-0.34044700	-1.55244500
O	-0.77745700	-0.91890400	-2.15465100
H	1.78573200	1.03664500	-1.55873900
C	-0.24186500	2.66499500	0.13670400
C	-0.71617200	2.04316500	-1.04323000
C	-2.01126600	1.52964400	-0.73052200
N	-2.16393400	1.84562100	0.62858000
H	1.36635500	0.34641600	-3.14831600
N	-1.08406000	2.53565200	1.14448800
C	-3.22680200	1.51407200	1.47978700
C	-4.51317300	1.26136600	0.97993500
C	-2.99122100	1.41864100	2.85830500
C	-5.52949400	0.88611100	1.85468100
H	-4.68362900	1.33115200	-0.08542700
C	-4.01903300	1.04595300	3.71591600
H	-1.99428900	1.61803300	3.23139200
C	-5.29303600	0.76738200	3.22285400
H	-6.51970000	0.68654700	1.45563000

H	-3.81685800	0.96035900	4.77928600
H	-6.09001800	0.46771900	3.89535100
N	-2.90588700	0.84566300	-1.41171900
H	-2.54561900	0.71305100	-2.35588300
C	1.00328400	3.48379600	0.30057500
H	1.12714200	3.76163400	1.34923400
H	1.89801600	2.94427000	-0.03121900
H	0.94215000	4.39563300	-0.30240500

M6S

C	1.06848900	-0.54688200	0.11335600
C	0.95775200	-0.71681000	-2.07817500
C	-0.69866000	0.84655200	-1.21797700
H	-1.28538000	0.95377300	-0.30492900
N	1.96268700	-1.46198300	-1.74511100
N	2.05710400	-1.31354000	-0.38390500
N	0.38325300	-0.11482900	-0.98583200
C	0.31130500	-0.51020100	-3.40965600
H	0.61357200	-1.30379900	-4.09301000
H	0.60218700	0.45915000	-3.83697600
C	-1.66320000	0.36287100	-2.36050500
O	-1.08467200	-0.61233400	-3.21387700
C	-0.93099700	2.63101600	-2.79395800
C	-0.16146900	2.16998200	-1.72379200
C	0.94365200	2.87272700	-1.27061200
C	1.23448100	4.06753800	-1.91992800
C	0.47651200	4.56586800	-2.97476600
C	-0.62045900	3.83479600	-3.41941600
C	-2.03503900	1.65887700	-3.11303100
H	1.58006000	2.52698500	-0.46344400
H	0.76108400	5.50122700	-3.43997000
H	-1.21238100	4.19452000	-4.25408200
H	-2.14604100	1.46468300	-4.18292700
H	-2.99369100	2.03977400	-2.74421500
C	3.20224800	-1.89704000	0.26892600
C	4.31549200	-1.07719600	0.47842000
C	3.18964900	-3.25572300	0.57571000
C	5.44815600	-1.66232000	1.03484600
C	4.35253500	-3.79651700	1.12803900
C	5.48340600	-3.01918000	1.36843900
H	6.32694900	-1.04601500	1.20882800
H	4.36983400	-4.85558800	1.37300600
C	1.97125900	-4.11228700	0.36129000
H	1.45469700	-3.85941200	-0.56959700

H	1.26769300	-3.97835900	1.18946900
H	2.24764100	-5.16723900	0.32127400
C	4.27317400	0.38912700	0.14264200
H	3.66741600	0.92805600	0.87976200
H	3.83773700	0.56497100	-0.84626700
H	5.27661100	0.81704500	0.15566600
H	-2.53901200	-0.12034000	-1.92724600
C	6.71580300	-3.62012600	1.99280800
H	6.73630500	-4.70423300	1.86385800
H	7.62460700	-3.20083400	1.55438000
H	6.74238500	-3.41075800	3.06695400
N	2.41115400	4.82624200	-1.47804300
O	2.63895600	5.89175600	-2.02216000
O	3.09690900	4.34542200	-0.59226400
C	-2.63733500	3.82441000	3.83044000
C	-1.88694800	2.88172900	3.12743200
C	-1.97877800	1.52462800	3.43706200
C	-2.82756200	1.13152100	4.47710500
C	-3.57794500	2.06750800	5.17999800
C	-3.48751300	3.42087300	4.85477900
H	-2.55531200	4.87602500	3.57386700
H	-1.23381600	3.21865900	2.32737000
H	-2.90469800	0.07513700	4.72269600
H	-4.23193800	1.74270500	5.98319600
H	-4.07144200	4.15453300	5.40111700
C	-1.25146600	0.44717800	2.65628100
H	-0.91676300	-0.31943200	3.37057000
C	0.06123400	0.97560800	2.00075900
C	1.02618300	-0.10346700	1.55579700
O	1.89592300	-0.51176200	2.29937300
H	-0.17037400	1.66409100	1.18389100
C	-3.37879900	0.08411900	1.05369200
C	-2.13333300	-0.22019500	1.64784600
C	-1.66472200	-1.36575700	0.98619900
N	-2.63421500	-1.66403500	0.04310700
H	0.62105600	1.53743000	2.75447200
N	-3.69770500	-0.79606700	0.10867900
C	-2.70833600	-2.78372000	-0.81256000
C	-1.57428600	-3.24016700	-1.48947300
C	-3.93544000	-3.42515100	-1.00135000
C	-1.66132100	-4.35532400	-2.31748000
H	-0.63683300	-2.70203400	-1.40053500
C	-4.01577400	-4.52550800	-1.84696900
H	-4.80768600	-3.04649800	-0.48156100

C	-2.87964000	-5.00410900	-2.49853900
H	-0.77325800	-4.70201700	-2.83663600
H	-4.97217400	-5.01842500	-1.98928000
H	-2.94579000	-5.86916100	-3.14972300
N	-0.48569900	-1.94814800	1.23439800
H	-0.32371500	-2.74058300	0.61733600
C	-4.32170300	1.21857200	1.32339500
H	-3.85280900	2.18386800	1.11044200
H	-5.20482600	1.10814800	0.69115700
H	-4.63147400	1.24168300	2.37180300

M6S'

C	-1.24607600	0.73914100	0.84670700
C	-2.64106400	-0.06895800	2.32186200
C	-3.67502600	0.24244200	0.12517900
H	-3.52113700	0.92108600	-0.71080000
N	-1.49936700	0.00711200	2.94481500
N	-0.63980000	0.50334300	2.01759300
N	-2.53054300	0.36886200	1.03462300
C	-4.00344500	-0.44297300	2.80796300
H	-4.04075800	-0.39191100	3.89552600
H	-4.26675600	-1.45922400	2.48609800
C	-5.01241300	0.56621100	0.87827300
O	-4.88871300	0.53311000	2.29214800
C	-5.16605600	-1.59106700	-0.20746900
C	-3.83297900	-1.19506300	-0.32932300
C	-2.84411500	-2.06155300	-0.78084000
C	-3.27040100	-3.34286700	-1.11882600
C	-4.59449500	-3.76329400	-1.03564700
C	-5.55712100	-2.87657500	-0.56981500
C	-6.01591100	-0.47873700	0.34637500
H	-1.79128500	-1.78754500	-0.87137000
H	-4.84697300	-4.77779400	-1.31703200
H	-6.59068200	-3.19156400	-0.47557400
H	-6.68549900	-0.80503500	1.14677400
H	-6.63503400	-0.04018900	-0.44302300
C	0.77556600	0.50602800	2.30241200
C	1.46397600	-0.68636100	2.05690600
C	1.36448800	1.66148400	2.81451100
C	2.84178900	-0.65722600	2.24858600
C	2.74993800	1.63770000	2.97487600
C	3.50017200	0.49862200	2.67110700
H	3.41719500	-1.55137900	2.02164300
H	3.25198700	2.53054100	3.33923600

C	0.54060300	2.88049800	3.13658900
H	-0.29763100	2.62580300	3.79156500
H	0.12027500	3.33674900	2.23235700
H	1.15233800	3.63265100	3.63636700
C	0.74377600	-1.93398100	1.62862900
H	0.35772900	-1.83315900	0.60418900
H	-0.08992200	-2.15303900	2.30360600
H	1.42882000	-2.78343800	1.63772300
H	-5.32908900	1.58516200	0.65674600
C	4.99893900	0.48905500	2.79994900
H	5.31126700	-0.07103900	3.68716900
H	5.43450800	0.00117100	1.92327000
H	5.40158300	1.50136500	2.87744300
N	-2.27098600	-4.32466100	-1.56068700
O	-2.67353200	-5.35438300	-2.07536800
O	-1.09844500	-4.05738300	-1.37711200
C	3.35179800	5.19339900	-1.71030600
C	2.53895400	4.15667000	-1.25046500
C	2.27317700	3.04905200	-2.05566100
C	2.83439500	3.00490800	-3.33637300
C	3.64167900	4.03647400	-3.80021900
C	3.90597400	5.13760200	-2.98436500
H	3.55426300	6.04326000	-1.06575200
H	2.13525600	4.21260300	-0.24304600
H	2.64022200	2.13901300	-3.96445100
H	4.06637600	3.98246500	-4.79780200
H	4.53853900	5.94385100	-3.34155800
C	1.45467000	1.85513200	-1.59355400
H	0.79520400	1.58108400	-2.43145200
C	0.48831800	2.24513400	-0.42163500
C	-0.76395700	1.42883700	-0.40877400
O	-1.50139600	1.36069000	-1.37693500
H	1.02970300	2.21509700	0.51983600
C	3.64637700	0.60565400	-0.78318100
C	2.31612200	0.68376500	-1.25334100
C	1.83237900	-0.65217200	-1.27277700
N	2.91725600	-1.41823100	-0.83265800
H	0.13061800	3.26821800	-0.59416800
N	4.01668700	-0.63957800	-0.53778800
C	3.02188800	-2.80716600	-0.66676100
C	2.00319700	-3.67941700	-1.08016400
C	4.17242300	-3.33917700	-0.06135600
C	2.13837700	-5.04807100	-0.87101600
H	1.11158700	-3.26871000	-1.53209400

C	4.28861000	-4.71119700	0.13379700
H	4.96196800	-2.66420500	0.24348400
C	3.27441100	-5.57974800	-0.26478800
H	1.32980800	-5.69980800	-1.19005900
H	5.18635900	-5.10228200	0.60398500
H	3.36946900	-6.64901300	-0.10557700
N	0.64855000	-1.16580900	-1.58906900
H	0.08676200	-0.41218800	-1.98594200
C	4.63722300	1.69924600	-0.51525800
H	4.29035800	2.35546600	0.29153200
H	5.58569500	1.24992200	-0.21215900
H	4.80485600	2.32700500	-1.39526200

TS5^N

C	-2.30542600	0.10389700	-0.80306700
C	-3.90972900	-1.38046200	-0.88785700
C	-1.67796900	-2.32191900	-1.28523600
H	-0.72478400	-1.94001900	-1.66158000
N	-4.51072700	-0.26117200	-0.60616800
N	-3.49224600	0.64830900	-0.54724900
N	-2.55741500	-1.19813200	-1.00709400
C	-4.42280700	-2.73935400	-1.24201700
H	-5.48775800	-2.69611100	-1.46766300
H	-4.25861300	-3.44738700	-0.41944100
C	-2.33143100	-3.26428700	-2.34616800
O	-3.74648400	-3.12767800	-2.42675800
C	-1.58929600	-4.55503600	-0.44144700
C	-1.48360700	-3.21154000	-0.07741600
C	-1.21414500	-2.83188600	1.22682500
C	-1.02310500	-3.85357200	2.14939700
C	-1.11169200	-5.20263700	1.82018700
C	-1.40277900	-5.55812500	0.50671300
C	-1.90563900	-4.68189100	-1.90959700
H	-1.15916100	-1.79628100	1.54348400
H	-0.95874100	-5.94918500	2.58920100
H	-1.48687700	-6.60432700	0.23297200
H	-2.69660800	-5.40508900	-2.12332700
H	-1.01175500	-4.99028500	-2.46239900
C	-3.70883300	2.02307700	-0.18566400
C	-3.47498900	2.39786500	1.13842600
C	-4.09557300	2.91631700	-1.18653300
C	-3.65886900	3.74373100	1.45722800
C	-4.26981200	4.24694900	-0.81498000
C	-4.05781700	4.67555200	0.49808800

H	-3.48494100	4.06845200	2.48019400
H	-4.56559500	4.96904200	-1.57191200
C	-4.26075000	2.44570300	-2.60457300
H	-5.01308700	1.65446300	-2.67590500
H	-3.30480800	2.04352800	-2.95652400
H	-4.56195100	3.27041300	-3.25195400
C	-3.00790200	1.40543600	2.16949100
H	-1.94243100	1.18888300	2.02928200
H	-3.55961100	0.46301100	2.10212600
H	-3.13704200	1.81029800	3.17444400
H	-1.96481900	-3.00778700	-3.34054000
C	-4.27639300	6.11788400	0.87303500
H	-3.69982200	6.38762500	1.76031400
H	-3.98929900	6.78392800	0.05615400
H	-5.33295900	6.30177000	1.09298300
N	-0.70968200	-3.48387300	3.53407100
O	-0.60871400	-4.37837500	4.35394200
O	-0.56270900	-2.29975300	3.78396100
C	0.17365800	3.84820600	2.74918200
C	0.21350400	3.14042000	1.55449200
C	1.25369700	2.24095100	1.28233000
C	2.25258000	2.06751000	2.23883400
C	2.21401100	2.77537500	3.44235200
C	1.17842700	3.66659900	3.70175800
H	-0.63989500	4.54310500	2.93756100
H	-0.57687800	3.27265200	0.81659900
H	3.06974800	1.37681400	2.04700500
H	2.99935000	2.62718400	4.17721800
H	1.15160900	4.21707800	4.63682300
C	1.21310200	1.47279800	-0.03792900
H	1.09828500	2.21201900	-0.84405900
C	-0.05855700	0.66235200	-0.07649100
C	-1.03099300	0.87616000	-0.99460800
O	-1.05465200	1.62586900	-2.04905000
H	-0.25762600	-0.01151600	0.75152900
C	2.85242400	-0.59871400	0.22002300
C	2.46181500	0.66838100	-0.36180600
C	3.73734400	1.35999400	-0.58375600
N	4.70899200	0.38604700	-0.29786700
H	2.10914000	0.37789200	-1.69756900
N	4.14111300	-0.79040100	0.19855000
C	6.09923900	0.42140200	-0.48578200
C	6.74554700	1.54736300	-1.02135900
C	6.86159900	-0.71370100	-0.15664500

C	8.12389400	1.52020200	-1.21943600
H	6.15950800	2.42167900	-1.26559800
C	8.23621500	-0.71582900	-0.36311900
H	6.36516800	-1.57660200	0.26729200
C	8.88166500	0.39796000	-0.89694700
H	8.60774100	2.40032900	-1.63260800
H	8.80650300	-1.60093500	-0.09750200
H	9.95496700	0.39151100	-1.05420400
N	4.01046400	2.54824300	-1.01033400
H	3.13013400	3.04929900	-1.13105500
C	1.95416300	-1.68594100	0.71581800
H	1.22072000	-1.93754800	-0.05653900
H	2.54358600	-2.57163600	0.96128500
H	1.41107700	-1.36883200	1.61343800
C	0.87787100	-0.65773700	-2.96878400
O	1.64045800	0.38544700	-2.80210600
O	-0.35362700	-0.40360600	-3.41882700
H	-0.60375500	0.53128900	-3.09791100
O	1.22466800	-1.82061200	-2.74035300
Cs	4.31751600	-1.35445000	-3.08264800

M5^N

C	2.66148300	0.28820100	-0.80895300
C	3.96407100	2.03262600	-0.94089700
C	1.58227800	2.60099400	-0.77419300
H	0.63655300	2.11047700	-1.03263800
N	4.77325600	1.01145400	-0.96446700
N	3.94372400	-0.06480700	-0.86949700
N	2.66120500	1.62736300	-0.83805600
C	4.18298500	3.49571900	-1.16094400
H	5.17412200	3.67063900	-1.57792300
H	4.08511600	4.05264300	-0.22032000
C	1.85638100	3.77156900	-1.77075300
O	3.22872200	3.89927900	-2.12839300
C	1.34349100	4.65423400	0.42191900
C	1.51785600	3.27794700	0.57566600
C	1.59512200	2.68952700	1.82644000
C	1.45515300	3.53084200	2.92340800
C	1.26756500	4.90487100	2.80832800
C	1.21517800	5.47503100	1.53977700
C	1.32472900	5.02312100	-1.03979300
H	1.76688500	1.62853100	1.97352600
H	1.17103700	5.50460000	3.70452400
H	1.08232000	6.54601300	1.43076900

H	1.93830100	5.89627400	-1.27564000
H	0.30041900	5.23786500	-1.36274700
C	4.43303500	-1.41562200	-0.79271100
C	4.48685100	-2.02617400	0.46125500
C	4.78883800	-2.05507900	-1.98355000
C	4.93459100	-3.34768700	0.50078700
C	5.22386800	-3.37321100	-1.88725400
C	5.30316900	-4.03246900	-0.65654400
H	4.99200900	-3.85049500	1.46299400
H	5.50111300	-3.90201700	-2.79554500
C	4.66966200	-1.34431200	-3.30336600
H	5.28714700	-0.44169700	-3.32547200
H	3.63027400	-1.04559900	-3.47262700
H	4.98111900	-1.99714300	-4.11966500
C	4.04892800	-1.32077000	1.71693200
H	2.96395900	-1.41435900	1.84324600
H	4.30259400	-0.25706400	1.70184300
H	4.52146800	-1.77292000	2.59031200
H	1.33512900	3.57927500	-2.70876100
C	5.80115900	-5.45186900	-0.58451700
H	5.45547500	-5.94691700	0.32548800
H	5.46136400	-6.03121800	-1.44605400
H	6.89559200	-5.47481100	-0.58224900
N	1.50519400	2.93360800	4.26240000
O	1.45460600	3.68096200	5.22204000
O	1.59049600	1.71974600	4.33677200
C	1.78893200	-4.63840700	1.71075400
C	1.28873600	-3.64835600	0.87317300
C	0.11374000	-2.95910000	1.20006500
C	-0.55138000	-3.28140200	2.38053500
C	-0.05080500	-4.27572300	3.22290300
C	1.11828000	-4.95508200	2.89290100
H	2.69973800	-5.16399900	1.43805800
H	1.81489600	-3.40064400	-0.04855400
H	-1.46637100	-2.75203600	2.63112600
H	-0.57907600	-4.51953500	4.13957800
H	1.50426000	-5.72903400	3.54881400
C	-0.37444000	-1.86193400	0.24356600
H	-0.40294400	-2.31576100	-0.75772400
C	0.71262600	-0.82121800	0.19102000
C	1.53065800	-0.66484400	-0.85269600
O	1.47627500	-1.34646200	-2.02476200
H	0.90872800	-0.24694000	1.09276800
C	-2.17277900	-0.10611400	1.14501000

C	-1.73921400	-1.29834200	0.52872300
C	-2.93009100	-2.03855700	0.22002800
N	-3.96943100	-1.19329900	0.65268700
H	-1.74383400	-0.64495600	-1.45948900
N	-3.49108800	-0.01612300	1.22309800
C	-5.35426000	-1.37323400	0.56852400
C	-5.92519200	-2.45349700	-0.12645600
C	-6.20316500	-0.42025500	1.16213600
C	-7.31087200	-2.56123700	-0.21499600
H	-5.26769900	-3.18671100	-0.57269300
C	-7.58330200	-0.54799500	1.05706500
H	-5.76109500	0.40325100	1.70786400
C	-8.15280100	-1.61737000	0.36745900
H	-7.73450100	-3.40379200	-0.75414200
H	-8.21821800	0.19672700	1.52831300
H	-9.23063800	-1.71461100	0.29052100
N	-3.12806400	-3.20537900	-0.34113500
H	-2.21294700	-3.62198200	-0.51341300
C	-1.35947100	1.04474400	1.65511400
H	-0.79863700	1.49850800	0.83179700
H	-2.02529500	1.79940900	2.07976400
H	-0.65239200	0.73628200	2.43322600
C	-0.71272900	0.68314200	-2.36018200
O	-1.31654100	-0.55354700	-2.33644300
O	0.35954400	0.72708400	-3.02304700
H	1.03868400	-0.68633600	-2.66093700
O	-1.25655700	1.60693200	-1.72267300
Cs	-4.29897700	1.15713100	-1.67536800

TS6^N

C	-0.91056700	1.50968600	-0.71449500
C	-0.76159100	2.06194300	-2.81555700
C	1.44610100	1.73508500	-1.72545700
H	1.75142100	1.96850800	-0.68752200
N	-2.03777800	2.07841600	-2.56015900
N	-2.11080900	1.72491000	-1.24842500
N	-0.02842900	1.71604800	-1.71040900
C	-0.00879300	2.52477600	-4.01733400
H	-0.67102600	3.06342200	-4.69411100
H	0.44448200	1.67774100	-4.55027500
C	1.98127600	2.79936600	-2.75960500
O	0.96482000	3.42590100	-3.52754200
C	2.94494600	0.61618800	-3.23548500
C	2.05290600	0.43238500	-2.18011200

C	1.89728200	-0.80726200	-1.58150500
C	2.66693100	-1.84637500	-2.07546700
C	3.55946800	-1.70466800	-3.13460300
C	3.68994500	-0.45518700	-3.72839900
C	3.01039400	2.05909100	-3.64974800
H	1.28025100	-0.96556400	-0.70592700
H	4.14113100	-2.55754400	-3.46334400
H	4.38883900	-0.31175900	-4.54581700
H	2.77471200	2.21144400	-4.70864700
H	4.01665700	2.45247800	-3.47732100
C	-3.36819800	1.68494200	-0.54545300
C	-4.05766000	0.47555700	-0.46261300
C	-3.81723800	2.87595600	0.03316100
C	-5.24880400	0.47843700	0.26153200
C	-5.00972000	2.82125700	0.74708400
C	-5.72353900	1.62905400	0.89031600
H	-5.80268500	-0.45209200	0.36093900
H	-5.37704500	3.72559700	1.22496000
C	-3.01693000	4.14349500	-0.08929800
H	-2.82026500	4.39132600	-1.13679800
H	-2.05419800	4.02188500	0.41785800
H	-3.54887500	4.97793700	0.36939100
C	-3.52509400	-0.78663100	-1.08420400
H	-2.84374800	-1.28492100	-0.38581500
H	-2.98537100	-0.58992000	-2.01390800
H	-4.34331600	-1.47570400	-1.30245800
H	2.45300700	3.61413600	-2.20896500
C	-6.94678700	1.56445300	1.76245400
H	-7.69911200	0.89117100	1.34383500
H	-6.65159200	1.17347000	2.74180100
H	-7.39519800	2.55047300	1.90006100
N	2.53051700	-3.14852000	-1.42744800
O	3.46511700	-3.92576400	-1.49977000
O	1.47318800	-3.39084900	-0.86605400
C	-0.77395600	-4.25869300	2.70372100
C	-0.50801100	-3.01748200	2.12964100
C	-0.15016000	-1.92300300	2.92323100
C	-0.11323200	-2.08895900	4.30927700
C	-0.39287200	-3.32481700	4.89189000
C	-0.71057200	-4.41985700	4.08850200
H	-1.01729800	-5.10570900	2.06857900
H	-0.53112400	-2.91295900	1.04798500
H	0.16048300	-1.24440000	4.93630600
H	-0.34754800	-3.43605700	5.97090200

H	-0.90475100	-5.38954500	4.53687400
C	0.29205100	-0.61318500	2.29985800
H	0.13379600	0.18345700	3.04247400
C	-0.58415300	-0.22591100	1.07424600
C	-0.74574000	1.14987700	0.75762100
O	-1.01214800	2.07674100	1.54873700
H	-0.41567600	-0.85794800	0.20299100
C	2.64351300	-1.73731600	1.66144500
C	1.74070100	-0.66554200	1.88778400
C	2.37689200	0.48414400	1.34963100
N	3.57827900	0.00989400	0.81304500
H	-1.82375600	-0.42172700	1.56755700
N	3.73011700	-1.34525300	1.01337800
C	4.48777200	0.66570200	-0.02751700
C	4.49549100	2.06384600	-0.17701000
C	5.40924200	-0.10089600	-0.75812300
C	5.39447600	2.66096400	-1.05735800
H	3.79618400	2.65361200	0.39957100
C	6.29722400	0.51492300	-1.63086600
H	5.39431600	-1.17674000	-0.63992900
C	6.29724700	1.89945500	-1.79691600
H	5.38624600	3.74303600	-1.15932700
H	6.99260700	-0.09985200	-2.19548700
H	6.99217800	2.37425100	-2.48206800
N	1.99781900	1.75299300	1.26789800
H	1.17387300	1.88189600	1.84721400
C	2.59566700	-3.18140400	2.07575600
H	1.94278000	-3.76847900	1.42622600
H	3.60609100	-3.59014900	2.00264500
H	2.23418900	-3.29585800	3.10141200
C	-3.60251800	0.09268800	2.88966800
O	-3.16862800	1.35381700	3.03342200
O	-4.63747700	-0.23311700	3.47266400
H	-2.34037600	1.53448900	2.54034100
O	-2.90463300	-0.72889900	2.16736100
Cs	-4.05514400	-3.21983400	3.55557300

TS7R

C	-0.37898400	-0.65801300	0.84263700
C	-1.95718900	-0.27741100	2.30506000
C	-2.21475700	0.98497600	0.18709400
H	-1.47978200	1.38164700	-0.51617000
N	-1.16512300	-1.12503800	2.89200800
N	-0.19258200	-1.36723400	1.95087400

N	-1.52422600	0.02082700	1.04324000
C	-3.11163400	0.52198900	2.81434200
H	-3.16473200	0.46910200	3.90091700
H	-4.05830400	0.16398100	2.38772600
C	-2.85765300	2.12944500	1.05515000
O	-2.83660200	1.86427900	2.45018300
C	-4.55221500	1.07829800	-0.33400200
C	-3.38307300	0.34371600	-0.52387000
C	-3.36491100	-0.82510400	-1.27038600
C	-4.57663000	-1.23264000	-1.81178800
C	-5.76474400	-0.52418900	-1.64600200
C	-5.75149900	0.64852100	-0.90033600
C	-4.29311900	2.30138400	0.50465700
H	-2.45058100	-1.38324100	-1.43599900
H	-6.67590200	-0.89969000	-2.09437000
H	-6.66744500	1.21150800	-0.75628600
H	-5.00523700	2.41863400	1.32683600
H	-4.35156200	3.20647000	-0.10901800
C	0.84461400	-2.33194900	2.18843600
C	0.71686500	-3.59090400	1.59599700
C	1.93464300	-1.94985800	2.97073400
C	1.74757300	-4.50085500	1.81573100
C	2.93818800	-2.89907100	3.16215300
C	2.86189500	-4.17135800	2.59292300
H	1.67932900	-5.49031300	1.37056800
H	3.80408000	-2.63252500	3.76217700
C	2.02283300	-0.55744800	3.53421900
H	1.20594200	-0.36783900	4.23731200
H	1.94534200	0.18517400	2.72945000
H	2.96980300	-0.41541900	4.05676600
C	-0.47601400	-3.93059100	0.74051700
H	-0.44893900	-3.38874200	-0.21257000
H	-1.41243100	-3.66777300	1.24189700
H	-0.49314000	-4.99732000	0.51442100
H	-2.27306200	3.04480200	0.94278400
C	3.96808200	-5.17478600	2.78986800
H	3.56423800	-6.15307700	3.06324000
H	4.53848500	-5.30277400	1.86476500
H	4.65950800	-4.85472200	3.57148000
N	-4.60638500	-2.47534800	-2.59251700
O	-5.66315600	-2.80410500	-3.10310400
O	-3.57257300	-3.11403800	-2.68391300
C	6.19464100	-0.11017400	-0.32842300
C	4.83675600	0.14470500	-0.48439900

C	4.09980600	-0.49708400	-1.48523300
C	4.75261100	-1.39675200	-2.32729000
C	6.11559100	-1.65327300	-2.17648200
C	6.83987800	-1.01093000	-1.17669200
H	6.75340800	0.39696300	0.45225700
H	4.32885200	0.85379600	0.16603100
H	4.18984900	-1.89796700	-3.11138900
H	6.61003900	-2.35231400	-2.84415700
H	7.90107600	-1.20644500	-1.05939300
C	2.60980700	-0.23190100	-1.62221200
H	2.28586900	-0.64769300	-2.58531500
C	1.85294100	-1.01443100	-0.50746800
C	0.41728900	-0.53929200	-0.42128700
O	-0.24946200	-0.36323000	-1.44907200
H	2.35648500	-0.89561400	0.45217400
C	2.34993000	2.18493300	-2.64208400
C	2.24969900	1.22636200	-1.60849100
C	1.50552500	1.84544300	-0.61047400
N	1.21704000	3.10947500	-1.08678500
H	1.85939700	-2.08068700	-0.76863300
N	1.73024900	3.31778400	-2.34313300
C	0.29561000	4.01323400	-0.52399800
C	0.33671300	4.30074100	0.84437600
C	-0.68210200	4.59940700	-1.33330800
C	-0.61371800	5.15452600	1.40062200
H	1.12057800	3.86640300	1.45684500
C	-1.61821200	5.45978900	-0.76906400
H	-0.68965800	4.36680500	-2.39221500
C	-1.59424500	5.73495500	0.59895000
H	-0.57760900	5.37311000	2.46291100
H	-2.37552800	5.91276600	-1.40111200
H	-2.32986100	6.40330100	1.03375500
N	1.05253300	1.26088900	0.52543600
H	0.31701100	1.82880900	0.94977900
C	3.06210400	2.01736100	-3.94637100
H	2.64583600	1.17573600	-4.51040500
H	2.96822500	2.92171800	-4.55002900
H	4.12400900	1.80618700	-3.78651900

TS7R'

C	0.76255800	-1.56404500	-0.06508600
C	1.50354400	-3.50175800	0.63599600
C	3.02377400	-2.35099000	-1.01005200
H	2.72123200	-2.29305600	-2.05288500

N	0.41870400	-3.28703900	1.31862800
N	-0.02406700	-2.07514600	0.88443200
N	1.77678300	-2.45222700	-0.20076200
C	2.33791100	-4.74583400	0.65475200
H	1.67767800	-5.61239100	0.59382100
H	2.90425200	-4.81605300	1.59055100
C	3.90745400	-3.58972400	-0.67835100
O	3.17228400	-4.77478400	-0.48050700
C	4.93248600	-1.67555400	0.27775500
C	3.91996100	-1.20812800	-0.56842900
C	3.87012000	0.12911800	-0.94140500
C	4.82854900	0.97250200	-0.39460900
C	5.83283500	0.54058000	0.46584700
C	5.88956900	-0.80771800	0.79767300
C	4.82408200	-3.15902400	0.48696800
H	3.11787200	0.50265500	-1.62462700
H	6.55160900	1.25260500	0.85147000
H	6.67325500	-1.17609400	1.45081000
H	4.37637600	-3.36456800	1.46548900
H	5.78809200	-3.67056300	0.45656400
C	-1.25117000	-1.55719200	1.43629500
C	-1.20048400	-0.56719000	2.41486800
C	-2.44627400	-2.14306300	0.99492400
C	-2.42499400	-0.07265000	2.87981800
C	-3.63160900	-1.62047500	1.49319700
C	-3.63992800	-0.56944500	2.41867500
H	-2.41609300	0.71098600	3.63414500
H	-4.57545100	-2.03020300	1.13773000
C	-2.43041400	-3.29609100	0.03307100
H	-1.90305400	-4.15355500	0.46144300
H	-1.92224600	-2.99071300	-0.88611600
H	-3.44953600	-3.59662200	-0.21287900
C	0.08424100	-0.07018400	3.03230700
H	0.97458900	-0.45823300	2.53342200
H	0.12826500	-0.37942300	4.08058700
H	0.13456200	1.02241100	3.00992300
H	4.52360300	-3.77361900	-1.56109700
C	-4.94763700	-0.00258700	2.90373400
H	-4.80535800	0.64231700	3.77331900
H	-5.42114500	0.58815000	2.11325400
H	-5.64501700	-0.80088800	3.17223500
N	4.77177300	2.39601300	-0.75109100
O	5.65943400	3.12299300	-0.33995900
O	3.83647900	2.77349400	-1.43565000

C	0.01036600	4.76554600	1.83095300
C	-0.26564400	3.62103400	1.09047700
C	0.29145200	3.43977600	-0.18152500
C	1.13486400	4.42617800	-0.69009700
C	1.41177900	5.57690800	0.04785600
C	0.85068700	5.74998300	1.30942000
H	-0.43440600	4.89469800	2.81300600
H	-0.94765900	2.86822300	1.48404100
H	1.58114200	4.29107100	-1.67111300
H	2.06860400	6.33611700	-0.36519300
H	1.06543100	6.64506300	1.88448300
C	0.01365500	2.16815100	-0.96059100
H	0.55259500	2.21917300	-1.91628100
C	0.59953400	0.98593400	-0.16310800
C	0.65808400	-0.30860300	-0.93827500
O	1.25005100	-0.40061700	-2.03475600
H	0.00725300	0.85621500	0.74292200
C	-2.56015700	2.80686700	-1.15669100
C	-1.45440900	1.91779000	-1.16840000
C	-2.00036500	0.64581700	-1.31721300
N	-3.37069500	0.83621200	-1.34518100
H	1.63099300	1.22635000	0.13188700
N	-3.70477000	2.14971800	-1.26015000
C	-4.40733700	-0.12331600	-1.34202100
C	-4.25557000	-1.37108000	-1.94898900
C	-5.61360700	0.20283200	-0.71248100
C	-5.29623700	-2.29494700	-1.88680200
H	-3.32611400	-1.61543700	-2.44530800
C	-6.64635500	-0.72526200	-0.66471100
H	-5.71905200	1.18541200	-0.26864200
C	-6.49133000	-1.98533000	-1.24250900
H	-5.16750200	-3.26623600	-2.35532000
H	-7.57479200	-0.46332200	-0.16658800
H	-7.29627300	-2.71163500	-1.19991500
N	-1.39115000	-0.59525200	-1.37630600
H	-1.07333800	-0.75043700	-2.33515100
C	-2.58648000	4.30512400	-1.09462800
H	-3.56564000	4.65938000	-1.42327800
H	-2.40276600	4.67457500	-0.08153500
H	-1.81719400	4.73970300	-1.73817800

TS7S

C	1.10058600	0.42732900	0.11908600
C	1.22624800	-0.03208400	-2.02736600

C	-1.06126800	-0.18192000	-1.20491900
H	-1.55342500	-0.47729800	-0.27780900
N	2.42280300	0.34445300	-1.70390400
N	2.32712000	0.66466800	-0.37361800
N	0.37178400	0.00674800	-0.95351300
C	0.69814100	-0.54447500	-3.32872000
H	1.52064100	-0.92225800	-3.93636100
H	0.18665600	0.25650600	-3.88085900
C	-1.31596200	-1.30069800	-2.27900800
O	-0.16164600	-1.62558600	-3.03639900
C	-2.44866500	0.74907600	-2.92126700
C	-1.65275000	1.06759800	-1.81989700
C	-1.43261000	2.38091300	-1.43704300
C	-2.06313300	3.36564900	-2.18760400
C	-2.88474300	3.08375100	-3.27471600
C	-3.07737700	1.75712000	-3.64822400
C	-2.46229400	-0.73915500	-3.15248000
H	-0.78844300	2.65865700	-0.60933200
H	-3.34372000	3.89876100	-3.82014200
H	-3.69431900	1.51876600	-4.50784000
H	-2.31434300	-1.01405800	-4.20034100
H	-3.41870700	-1.16589600	-2.83193200
C	3.45448000	1.32980100	0.23160900
C	3.45077800	2.72703500	0.22878700
C	4.51682500	0.56830700	0.71015500
C	4.57551500	3.36982100	0.73687400
C	5.62323400	1.25944300	1.20576500
C	5.66888000	2.65261300	1.22968600
H	4.60033400	4.45667700	0.74721100
H	6.46946500	0.69034400	1.58248300
C	4.45892700	-0.93458100	0.74011300
H	4.03256500	-1.34347300	-0.18115000
H	3.83978000	-1.26655200	1.58036300
H	5.45674000	-1.35639600	0.87025800
C	2.25607900	3.49834400	-0.26529900
H	1.43001800	3.41381400	0.45074000
H	1.90443700	3.12873100	-1.23432700
H	2.49442400	4.55754300	-0.37172800
H	-1.59721300	-2.22985300	-1.78207500
C	6.86122200	3.37567500	1.79995900
H	7.75197300	2.74428100	1.78504000
H	7.07365300	4.28964200	1.24017600
H	6.67330900	3.66284500	2.83954400
N	-1.82495800	4.76827500	-1.82637000

O	-2.42275300	5.62710300	-2.44918800
O	-1.03699800	4.99470200	-0.92375200
C	-4.87783300	0.67661200	3.29836900
C	-3.61585200	0.54389100	2.72116700
C	-2.63895700	-0.25471100	3.31860000
C	-2.95116300	-0.91143800	4.51242800
C	-4.21043400	-0.78461200	5.09077400
C	-5.18031400	0.01096000	4.48271100
H	-5.62560600	1.30089300	2.81922100
H	-3.40584300	1.06231500	1.78931800
H	-2.19691700	-1.53712100	4.98307500
H	-4.43407500	-1.30429800	6.01715300
H	-6.16295900	0.11445300	4.93156800
C	-1.28343900	-0.49749700	2.68582900
H	-0.55708400	-0.67719700	3.49118300
C	-0.74922600	0.76701800	1.94748500
C	0.71680300	0.74545700	1.54760200
O	1.56814000	1.25361500	2.25714200
H	-1.38041300	0.99447700	1.08452000
C	-2.24872700	-2.52122000	1.19012900
C	-1.27290300	-1.69096100	1.78397700
C	-0.04652900	-2.09498700	1.23888800
N	-0.35684600	-3.09884500	0.33668100
H	-0.82156000	1.61790400	2.63100800
N	-1.70046600	-3.38751500	0.34140000
C	0.52234500	-3.91840900	-0.40277700
C	1.65953000	-3.37961800	-1.01142500
C	0.23761400	-5.27887900	-0.54661200
C	2.52364400	-4.20428400	-1.72499000
H	1.85204500	-2.31379800	-0.95965200
C	1.09719200	-6.09002500	-1.27862100
H	-0.65678600	-5.67707900	-0.08243800
C	2.24847800	-5.56203700	-1.86146600
H	3.40479300	-3.77354600	-2.19023300
H	0.86990900	-7.14585700	-1.38608600
H	2.91905200	-6.20184700	-2.42508800
N	1.12087400	-1.52161200	1.55344000
H	1.89660100	-1.91484600	1.02571900
C	-3.73732800	-2.53898700	1.37045100
H	-4.20008200	-1.63998900	0.95185700
H	-4.14937300	-3.41327100	0.86289100
H	-4.01038000	-2.57426200	2.42855900

TS7S'

C	0.66786900	-1.62485500	0.43160900
C	2.23876500	-2.01241000	1.91354600
C	2.95375200	-2.48223500	-0.39256300
H	2.43305700	-2.85199800	-1.27318500
N	1.24042000	-1.55982900	2.60648900
N	0.26769400	-1.31828900	1.67707400
N	1.92934300	-2.08282200	0.58195500
C	3.55869600	-2.55578800	2.35009700
H	3.53082500	-2.80549800	3.41017100
H	4.36160700	-1.82652500	2.17481100
C	3.91795700	-3.56303900	0.22189400
O	3.75396300	-3.75039400	1.61795000
C	5.19523400	-1.65005800	-0.55710100
C	3.85254400	-1.30965500	-0.71812700
C	3.45907300	-0.03878700	-1.11782800
C	4.48343200	0.87852200	-1.32267400
C	5.83317500	0.58297900	-1.14978800
C	6.19554100	-0.70411800	-0.77327000
C	5.34443600	-3.08901800	-0.14339900
H	2.41347300	0.24942500	-1.22655400
H	6.57354900	1.35579200	-1.31598700
H	7.24129400	-0.96075100	-0.64236000
H	6.01954700	-3.22588200	0.70655000
H	5.74165200	-3.68396700	-0.97186900
C	-0.90709900	-0.59345300	2.09490300
C	-0.76746400	0.79704800	2.20845000
C	-2.08763800	-1.26953300	2.39862100
C	-1.91370900	1.52469400	2.50020100
C	-3.21416900	-0.48712000	2.67400000
C	-3.15331800	0.90444400	2.68343600
H	-1.84146600	2.60770300	2.55876700
H	-4.15995500	-0.98631900	2.87472200
C	-2.18647000	-2.77395200	2.41818300
H	-2.50313500	-3.11099400	3.40870900
H	-1.23372900	-3.25404500	2.18786600
H	-2.92974300	-3.13052400	1.69749000
C	0.57459500	1.45648800	2.04004100
H	0.97243500	1.26253300	1.03708000
H	1.28284000	1.07014600	2.77964500
H	0.48634200	2.53689100	2.16918900
H	3.69702300	-4.53902500	-0.20939600
C	-4.38570500	1.74662500	2.86949500
H	-5.25937200	1.13716300	3.10942100
H	-4.24578400	2.48340200	3.66546100

H	-4.58697800	2.29650900	1.94314900
N	4.12792800	2.23554800	-1.74478000
O	4.92383300	3.13202400	-1.52158400
O	3.05513800	2.39196000	-2.30098000
C	-5.83172800	-2.35662500	-0.79732300
C	-4.55010800	-1.82300200	-0.71492500
C	-3.81514200	-1.53983800	-1.87127400
C	-4.39200100	-1.80874800	-3.11225900
C	-5.67866000	-2.33962200	-3.20053100
C	-6.40157200	-2.61569500	-2.04345500
H	-6.38972300	-2.56537800	0.11038800
H	-4.12366600	-1.58744500	0.25883200
H	-3.83069900	-1.59404900	-4.01780300
H	-6.11434300	-2.53732900	-4.17500200
H	-7.40243500	-3.02988200	-2.11115000
C	-2.42227700	-0.95394400	-1.76796600
H	-1.96047500	-0.98614900	-2.76542900
C	-1.55750300	-1.86197400	-0.85126300
C	-0.06262400	-1.63283200	-0.90199700
O	0.60206400	-1.99881200	-1.88693400
H	-1.94036000	-1.76491200	0.15792900
C	-3.39001200	1.39831000	-0.87849400
C	-2.39874400	0.45512600	-1.25236600
C	-1.18026800	1.07672700	-0.99387200
N	-1.49313900	2.33520700	-0.52109700
H	-1.68961600	-2.90285900	-1.16823100
N	-2.83521500	2.52440000	-0.44683900
C	-0.63473100	3.41058800	-0.20121700
C	0.65625000	3.47385900	-0.73024200
C	-1.09487800	4.42651300	0.64149900
C	1.49731300	4.52258500	-0.37423100
H	0.99904200	2.69017800	-1.39011700
C	-0.24569100	5.47532400	0.98232700
H	-2.11191400	4.38224100	1.01262500
C	1.05679200	5.52497900	0.48842400
H	2.50008000	4.54963700	-0.79260000
H	-0.60797500	6.25806100	1.64164700
H	1.71481200	6.34273200	0.76345600
N	0.08452400	0.54113200	-1.06148300
H	0.25211400	0.22908400	-2.01971700
C	-4.88679800	1.31168500	-0.90105300
H	-5.26098400	0.69673300	-0.07568900
H	-5.30131500	2.31700200	-0.79805900
H	-5.25400500	0.86380000	-1.82789400

M7R

C	0.72735200	0.88143400	-0.60557300
C	2.42067300	1.94272900	-1.51107400
C	2.45158900	1.98509700	0.95275000
H	1.67519000	1.98506100	1.71581100
N	1.78318500	1.42920100	-2.51892700
N	0.73514800	0.76818000	-1.93696600
N	1.81022600	1.63584300	-0.32563700
C	3.59784400	2.86067500	-1.46784000
H	3.72882300	3.35277100	-2.43111500
H	4.51637000	2.31090100	-1.21983900
C	3.20918900	3.35956400	0.82780900
O	3.29023600	3.84797900	-0.50303600
C	4.75188900	1.62067300	1.53151300
C	3.53740700	0.98527600	1.28235900
C	3.40506100	-0.39557300	1.34025100
C	4.55831700	-1.11222700	1.62858200
C	5.79303600	-0.51350400	1.87494900
C	5.88969000	0.87163000	1.83208000
C	4.60804100	3.11621600	1.44361900
H	2.43364400	-0.86294400	1.20673500
H	6.65198200	-1.13426400	2.09640300
H	6.84061400	1.35739800	2.02326400
H	5.37980400	3.59056800	0.83005100
H	4.66895300	3.56308200	2.44088100
C	-0.14772300	-0.00918500	-2.76602400
C	0.25329500	-1.30645000	-3.09311900
C	-1.35967500	0.54991700	-3.16860600
C	-0.64603000	-2.08400100	-3.81825400
C	-2.22515800	-0.27008800	-3.89163400
C	-1.89345600	-1.58953700	-4.20631800
H	-0.37157300	-3.10358900	-4.07583800
H	-3.18401800	0.13064600	-4.21032300
C	-1.71902300	1.96323900	-2.79917300
H	-0.95173100	2.66341900	-3.14400000
H	-1.79444100	2.06062600	-1.71013800
H	-2.67276200	2.24614800	-3.24679000
C	1.59522500	-1.83638700	-2.66258300
H	1.71278100	-1.80018200	-1.57342200
H	2.40539100	-1.24245300	-3.09619600
H	1.71748000	-2.87244600	-2.98040900
H	2.66209100	4.13339600	1.36542000
C	-2.87398800	-2.47594400	-4.92789300

H	-2.35962100	-3.19253000	-5.57210000
H	-3.46712200	-3.04654200	-4.20558200
H	-3.56424200	-1.88997700	-5.53833400
N	4.47222800	-2.57682700	1.67673700
O	5.47396800	-3.19872500	1.98890600
O	3.40564900	-3.09472800	1.39582300
C	-4.44203400	-3.55480900	-0.82237000
C	-3.72771700	-2.46967500	-0.32478900
C	-2.69933700	-2.65612600	0.60616200
C	-2.40162800	-3.95374900	1.02245200
C	-3.11338400	-5.04464100	0.52499400
C	-4.13613400	-4.84839800	-0.39831100
H	-5.24066300	-3.39280400	-1.54011900
H	-3.97363200	-1.45986600	-0.64685400
H	-1.60588700	-4.10945700	1.74649700
H	-2.86976400	-6.04723300	0.86283300
H	-4.69450000	-5.69568800	-0.78369500
C	-1.89680400	-1.47669800	1.11792100
H	-1.25498900	-1.81531700	1.94114300
C	-0.97745000	-0.93906200	0.00838500
C	-0.21477400	0.31059100	0.52162000
O	0.49076600	0.10928800	1.60135700
H	-1.59322800	-0.71187100	-0.86658900
C	-3.92186500	-0.22556100	2.34806600
C	-2.73628600	-0.32094200	1.57692200
C	-2.36756600	0.98637300	1.34499700
N	-3.30347200	1.78286800	1.94055000
H	-0.24548100	-1.70420500	-0.27052800
N	-4.25763800	1.03494800	2.57322600
C	-3.33261400	3.19213200	2.04605900
C	-2.85702300	3.99430900	1.00647400
C	-3.86122300	3.77449500	3.20052300
C	-2.89210500	5.38000800	1.13969500
H	-2.48211400	3.53643600	0.09797200
C	-3.90443300	5.15894000	3.31210500
H	-4.23239300	3.13051000	3.98851200
C	-3.41382000	5.96830000	2.28827300
H	-2.52230700	6.00045200	0.32975400
H	-4.31683600	5.60712300	4.21030900
H	-3.44377100	7.04842500	2.38383600
N	-1.25333000	1.42967300	0.63351300
H	-0.81347600	2.21568400	1.11333700
C	-4.75918600	-1.34540700	2.88000700
H	-4.13722500	-2.08178800	3.39730000

H	-5.50284600	-0.95594000	3.57740800
H	-5.27402700	-1.87105200	2.06979100

M7R'

C	0.84903600	1.51312100	-0.21607800
C	2.09495200	3.00122400	-1.23047200
C	3.18369200	1.95349000	0.78760200
H	2.77843500	2.23377300	1.75704600
N	0.99564300	2.96033500	-1.92311800
N	0.23859000	2.02110900	-1.28753300
N	2.06523400	2.10673300	-0.18891700
C	3.23902900	3.94240400	-1.44847500
H	2.84040200	4.92751800	-1.69516600
H	3.86028900	3.60655200	-2.28717200
C	4.36809800	2.83975100	0.30310900
O	3.97949700	4.07237700	-0.25722900
C	4.98290900	0.57365600	-0.00350300
C	3.82864800	0.58142300	0.78668100
C	3.45236900	-0.54231500	1.51103900
C	4.22493800	-1.68219400	1.34173300
C	5.35186900	-1.73787000	0.52503800
C	5.74733200	-0.58386800	-0.14044000
C	5.23610600	1.93118800	-0.59640200
H	2.55785500	-0.51449700	2.12674400
H	5.90588400	-2.66439200	0.43653900
H	6.64213200	-0.58753500	-0.75341300
H	4.91107000	1.95069800	-1.64268200
H	6.28793100	2.22311200	-0.57657900
C	-1.07302500	1.70939100	-1.79818600
C	-1.23048500	0.62465600	-2.65886600
C	-2.13056300	2.53585600	-1.40467400
C	-2.53444000	0.31898400	-3.06047700
C	-3.40611700	2.19207500	-1.83422900
C	-3.62885300	1.07310600	-2.64281900
H	-2.68999300	-0.52953900	-3.72334400
H	-4.25017900	2.79821800	-1.51327400
C	-1.88670600	3.73389000	-0.53124800
H	-1.13487600	4.39675100	-0.96982800
H	-1.52283400	3.41937600	0.45227200
H	-2.81074900	4.29588000	-0.38726400
C	-0.06980000	-0.16905300	-3.20565400
H	0.87433200	0.06754600	-2.71131200
H	0.05050300	0.04157600	-4.27247500
H	-0.24693600	-1.24297000	-3.09914500

H	4.94272200	3.09520400	1.19616300
C	-5.02664500	0.68559800	-3.04925000
H	-5.06539900	0.38868600	-4.10058300
H	-5.37542200	-0.16359100	-2.45248900
H	-5.72642700	1.50910200	-2.89133100
N	3.81203000	-2.89409800	2.05366700
O	4.29342200	-3.95834600	1.70439700
O	2.99327000	-2.77632700	2.95141300
C	-0.47773000	-4.83413100	-1.46030100
C	-0.66199400	-3.62847700	-0.79167500
C	0.03126900	-3.35314100	0.39362800
C	0.90897200	-4.31543700	0.89422000
C	1.09899600	-5.52384200	0.22406900
C	0.40788600	-5.78694400	-0.95445400
H	-1.02615500	-5.03427200	-2.37579700
H	-1.36535300	-2.89210500	-1.17775500
H	1.44660400	-4.11967200	1.81842900
H	1.78931500	-6.25800700	0.62810500
H	0.55340300	-6.72789400	-1.47544900
C	-0.12969800	-2.01201900	1.08176700
H	0.43246100	-2.02851900	2.02574900
C	0.46067400	-0.90092100	0.19732400
C	0.32451900	0.49499400	0.86536000
O	0.96044600	0.68224800	1.99366300
H	-0.07805500	-0.90966400	-0.75638800
C	-2.76218900	-2.32646200	1.53177600
C	-1.55886000	-1.61001700	1.30916900
C	-1.94595000	-0.28691400	1.23938600
N	-3.30355000	-0.25671100	1.40352700
H	1.51834400	-1.08837200	-0.00975200
N	-3.80597500	-1.51340300	1.58510700
C	-4.19798100	0.82022500	1.20126900
C	-3.91498200	2.09888800	1.67912600
C	-5.38586600	0.57901800	0.50612200
C	-4.80685300	3.13999700	1.42975100
H	-3.02501100	2.28192000	2.26994600
C	-6.27662300	1.62075900	0.27819800
H	-5.58897200	-0.42585600	0.15489800
C	-5.98763700	2.90868700	0.72961300
H	-4.57991900	4.13343000	1.80396800
H	-7.19681400	1.42590900	-0.26375200
H	-6.68242100	3.72151900	0.54645300
N	-1.15037700	0.82428600	0.97305600
H	-1.18171700	1.49367800	1.73863000

C	-2.94555000	-3.80020300	1.72036100
H	-3.95325700	-4.00088400	2.08873500
H	-2.79817900	-4.34014600	0.78009900
H	-2.21962400	-4.19557100	2.43601700

M7S

C	-0.82290700	1.04172300	-0.73389600
C	-1.55004300	0.56053400	-2.75175400
C	0.59657600	-0.47995700	-2.23913200
H	1.41776600	-0.26192300	-1.55183600
N	-2.48386900	1.29650400	-2.22970700
N	-2.02142800	1.57580500	-0.96930100
N	-0.52337300	0.37524300	-1.86840400
C	-1.34990300	0.04032900	-4.13890600
H	-2.01620600	0.55229500	-4.83264400
H	-1.54016000	-1.03914400	-4.18942400
C	1.02391300	-0.19852000	-3.71851300
O	-0.01816600	0.36921300	-4.50246400
C	0.72658400	-2.56791400	-3.39528100
C	0.21089700	-1.94698200	-2.25522300
C	-0.56489800	-2.64298400	-1.34161100
C	-0.77456000	-3.99297700	-1.60017000
C	-0.25233100	-4.64809500	-2.71038700
C	0.50557000	-3.92273600	-3.62389400
C	1.46986800	-1.57528500	-4.25032500
H	-1.01270200	-2.18183000	-0.46868400
H	-0.45745000	-5.70143600	-2.85351900
H	0.90257300	-4.40748700	-4.50918000
H	1.24790500	-1.66687000	-5.31621800
H	2.55120100	-1.69599000	-4.12242000
C	-2.88466900	2.35042500	-0.10812200
C	-3.94071500	1.68296700	0.50619700
C	-2.68549400	3.72799100	-0.01784700
C	-4.82668300	2.45136600	1.26377100
C	-3.59736500	4.45010100	0.74478500
C	-4.66987100	3.82999600	1.39369500
H	-5.65767800	1.95666900	1.75984200
H	-3.46527100	5.52527500	0.84065300
C	-1.49857800	4.37642100	-0.66991700
H	-1.41111100	4.09190900	-1.72337900
H	-0.60219300	4.03721700	-0.14013400
H	-1.56569800	5.46379600	-0.60944400
C	-4.11447200	0.19489000	0.35498100
H	-3.21564500	-0.34198800	0.67591500

H	-4.30350300	-0.07583900	-0.68840100
H	-4.95214400	-0.15701500	0.95852000
H	1.83058100	0.53556000	-3.75443300
C	-5.62284400	4.64467700	2.22970200
H	-5.13806900	4.97759000	3.15276600
H	-5.94973700	5.53887900	1.69225400
H	-6.50615500	4.06448600	2.50391100
N	-1.60531700	-4.75691600	-0.66045000
O	-1.74576600	-5.94967800	-0.86499200
O	-2.11094000	-4.15410900	0.26977200
C	2.19379100	-3.70359400	3.07966000
C	2.06569300	-2.43160800	2.53045500
C	1.20474600	-1.48897300	3.10209500
C	0.47134000	-1.85118000	4.23280100
C	0.59457000	-3.12511500	4.78515600
C	1.45738900	-4.05453900	4.21099800
H	2.87173800	-4.42178500	2.62861300
H	2.64963200	-2.15121900	1.65635700
H	-0.20076500	-1.12570100	4.68440100
H	0.01902200	-3.38889200	5.66697900
H	1.55964400	-5.04503100	4.64274600
C	1.03391100	-0.11737800	2.48119700
H	0.50572300	0.53031900	3.19285900
C	0.14975500	-0.19753600	1.22430700
C	0.02463600	1.21760700	0.58255600
O	-0.45879600	2.13231300	1.35116700
H	0.59132600	-0.92547700	0.52972600
C	3.59675900	0.64098100	2.67080300
C	2.31871900	0.53636800	2.06487200
C	2.41394100	1.29925700	0.92069700
N	3.68618800	1.79418700	0.86927800
H	-0.85460900	-0.53899300	1.49822400
N	4.41399300	1.39913400	1.95727100
C	4.26862300	2.65634100	-0.08769700
C	3.87004900	2.61110900	-1.42585700
C	5.26846500	3.54308100	0.31876600
C	4.45925800	3.47322100	-2.34681100
H	3.11611100	1.89831500	-1.73990500
C	5.85891900	4.38575000	-0.61514000
H	5.56838600	3.55251100	1.35949800
C	5.45351800	4.36222700	-1.94903700
H	4.14425800	3.43651900	-3.38481700
H	6.63563900	5.07252800	-0.29451100
H	5.91117200	5.02928200	-2.67170100

N	1.41297200	1.52572900	-0.02208800
H	1.39969300	2.50690700	-0.30334400
C	4.06119500	0.01177800	3.94594000
H	4.21018200	-1.06540800	3.82276300
H	5.00296000	0.46329900	4.26269700
H	3.31695600	0.14537100	4.73604500

M7S'

C	-1.09984900	0.29738200	0.54264200
C	-2.63003700	0.23603500	2.11117100
C	-3.52823000	-0.08970700	-0.18223800
H	-3.26287900	0.39963500	-1.11840600
N	-1.51098400	0.37707300	2.75519100
N	-0.56765000	0.40456500	1.76616800
N	-2.42653200	0.19490500	0.75780700
C	-4.03391500	0.20247500	2.61506400
H	-4.09591800	0.67326100	3.59593300
H	-4.39268300	-0.83325600	2.69490900
C	-4.90860500	0.37765300	0.41941700
O	-4.80845200	0.96063700	1.70778900
C	-4.94194600	-2.02704600	0.03650800
C	-3.67826300	-1.58298000	-0.34258600
C	-2.69300100	-2.45901200	-0.76913700
C	-3.00679100	-3.80871200	-0.74946300
C	-4.25634500	-4.29531700	-0.36717400
C	-5.23903700	-3.39112400	0.01893000
C	-5.83052800	-0.87117200	0.40831900
H	-1.75139000	-2.07278700	-1.14197000
H	-4.44028700	-5.36241900	-0.37484600
H	-6.21920600	-3.74969100	0.31457000
H	-6.31605100	-0.99882800	1.38102000
H	-6.62821700	-0.74876300	-0.33014000
C	0.82215500	0.54110400	2.12385500
C	1.57262600	-0.62568600	2.32071300
C	1.35140700	1.82181500	2.28834300
C	2.92247200	-0.47065200	2.61801800
C	2.71433500	1.91994500	2.58363200
C	3.51525300	0.79091000	2.73013500
H	3.52866200	-1.36188400	2.76079100
H	3.15237400	2.90913800	2.69913500
C	0.52242200	3.07678200	2.17842100
H	0.41941800	3.54254500	3.16281200
H	-0.48014700	2.88861100	1.79039900
H	1.01220200	3.79771000	1.51630300

C	0.94806400	-1.99305600	2.26343200
H	0.28846100	-2.09535000	1.39909000
H	0.35975800	-2.18105900	3.16816700
H	1.72399200	-2.75937400	2.18774400
H	-5.31573100	1.17257600	-0.20460400
C	4.99384600	0.91651600	2.98713600
H	5.24169500	1.88951500	3.41663700
H	5.34397400	0.13613200	3.66702900
H	5.55122500	0.81259900	2.05026200
N	-1.96123400	-4.76232800	-1.13349700
O	-2.25849900	-5.94037500	-1.21285700
O	-0.83975800	-4.32367900	-1.34000700
C	3.24590700	4.87184100	-0.87375300
C	2.69760100	3.59711500	-0.96426000
C	1.90938600	3.23190600	-2.06349000
C	1.68611000	4.17220700	-3.06799700
C	2.23767900	5.45122300	-2.98300700
C	3.01752600	5.80494500	-1.88622300
H	3.85582000	5.13781400	-0.01547500
H	2.89108800	2.86252500	-0.18286500
H	1.07753500	3.89975900	-3.92647400
H	2.05755200	6.17022600	-3.77620900
H	3.44749300	6.79918200	-1.81863300
C	1.28841000	1.84963500	-2.12139400
H	0.78519300	1.72737200	-3.08951100
C	0.23345200	1.72245300	-1.00266100
C	-0.40074900	0.30638500	-0.88582900
O	-1.25122100	-0.00775200	-1.82353900
H	0.73071200	2.00229400	-0.07219700
C	3.66110600	0.56823000	-2.18634900
C	2.28228700	0.74597000	-1.89963400
C	1.90960800	-0.42043100	-1.26778400
N	3.01248400	-1.21772200	-1.20320700
H	-0.59456100	2.41771200	-1.17512800
N	4.09839100	-0.61188100	-1.76693800
C	3.12313700	-2.47386300	-0.56382900
C	2.16709100	-3.46208100	-0.79585100
C	4.18496300	-2.70919800	0.30986800
C	2.24431600	-4.67215400	-0.11207300
H	1.38246300	-3.30465100	-1.52844100
C	4.26756500	-3.93003900	0.97174300
H	4.92227500	-1.92840900	0.46348600
C	3.29203400	-4.90884400	0.77450000
H	1.48596800	-5.42733700	-0.29163700

H	5.09212700	-4.11450500	1.65301900
H	3.35684700	-5.85454700	1.30237000
N	0.69222800	-0.71448700	-0.68229100
H	0.31978000	-1.61772500	-0.95909600
C	4.59312800	1.50915300	-2.88470800
H	4.84358800	2.36396200	-2.24901000
H	5.51384100	0.98596900	-3.14916500
H	4.13656400	1.90844100	-3.79465400

TS8R

C	0.84159100	0.86604000	-0.40824100
C	2.21496300	2.25019200	-1.47619100
C	2.65633200	2.01692900	0.94812000
H	1.98895300	1.96058700	1.80818900
N	1.47511200	1.75136800	-2.41780400
N	0.63717500	0.89798000	-1.73111700
N	1.85543900	1.75375400	-0.25058800
C	3.29963800	3.27412700	-1.52679400
H	3.19136900	3.90861200	-2.40627000
H	4.28639700	2.79015400	-1.55975800
C	3.39357200	3.40489100	0.84325600
O	3.15438500	4.08594900	-0.37696200
C	5.02279600	1.61092000	1.08851100
C	3.77067600	1.00313300	1.05073500
C	3.62372800	-0.37660600	1.06379000
C	4.79309800	-1.12295900	1.09587600
C	6.06426500	-0.55162700	1.13439000
C	6.18022500	0.83272700	1.13572300
C	4.89879300	3.11100200	1.07702000
H	2.64232200	-0.84085600	1.07855800
H	6.93592000	-1.19326200	1.15858100
H	7.16086400	1.29588400	1.16409800
H	5.50527200	3.58124900	0.29625300
H	5.22785600	3.53293100	2.03126100
C	-0.24632700	0.04235300	-2.47239400
C	0.26463700	-1.18583700	-2.90799800
C	-1.56669900	0.43369500	-2.68494900
C	-0.60167200	-2.03981600	-3.58221200
C	-2.39660100	-0.45475700	-3.37431900
C	-1.93421800	-1.69089200	-3.82302200
H	-0.23266700	-3.00386000	-3.92376600
H	-3.43272300	-0.17551600	-3.55066400
C	-2.09608800	1.72718100	-2.12698200

H	-1.36781800	2.53631600	-2.22800600
H	-2.31537600	1.61153200	-1.05835500
H	-3.01774600	2.01811100	-2.63371000
C	1.69104700	-1.56947500	-2.61577800
H	1.85728100	-1.66456400	-1.53629300
H	2.38714500	-0.81104500	-2.98621200
H	1.93564500	-2.52462300	-3.08257300
H	3.00317900	4.07806200	1.60595500
C	-2.84275300	-2.64736900	-4.55025100
H	-2.46590300	-2.85421700	-5.55628200
H	-2.90011900	-3.60187200	-4.01813800
H	-3.85366800	-2.24404100	-4.64059000
N	4.68301500	-2.58603000	1.07996100
O	5.70692900	-3.23769600	1.19686300
O	3.57340300	-3.07208400	0.94340800
C	-3.99781500	-3.44709000	-1.17866200
C	-3.36326500	-2.42719900	-0.47813600
C	-2.67834100	-2.69549000	0.71207600
C	-2.63827700	-4.00690900	1.18309500
C	-3.27193100	-5.03359500	0.48265700
C	-3.95336800	-4.75698300	-0.69900700
H	-4.53386100	-3.21862700	-2.09530500
H	-3.40631900	-1.40439700	-0.84805500
H	-2.10879300	-4.22633400	2.10670700
H	-3.23402700	-6.04916600	0.86418800
H	-4.45145400	-5.55443100	-1.24124200
C	-1.97213000	-1.57196900	1.44749200
H	-1.60595100	-1.95983300	2.40706100
C	-0.76772500	-1.08091300	0.61077900
C	-0.11178900	0.16175400	1.21376200
O	0.74816100	0.06677400	2.11011900
H	-1.14118200	-0.85946400	-0.39132000
C	-4.22014400	-0.20288500	1.99878200
C	-2.85055500	-0.37276300	1.66961100
C	-2.35682400	0.91035400	1.58937300
N	-3.38906100	1.76615100	1.83866000
H	0.00099800	-1.85518900	0.53437900
N	-4.53630400	1.07749000	2.11374100
C	-3.37846400	3.18025200	1.91500500
C	-2.50544500	3.93020600	1.12260600
C	-4.27050500	3.81743400	2.77994000
C	-2.51907600	5.31918700	1.21781700
H	-1.83229000	3.43308600	0.43336400
C	-4.28140500	5.20542600	2.85224800

H	-4.94349200	3.21457100	3.37735100
C	-3.40301700	5.96284900	2.07876800
H	-1.83998600	5.89909300	0.60125600
H	-4.97690100	5.69648900	3.52520000
H	-3.41142200	7.04553200	2.14444200
N	-1.04966900	1.28881700	1.29847600
H	-0.67829600	1.98527900	1.94133500
C	-5.25345200	-1.26302700	2.21407500
H	-4.89033000	-2.02267900	2.91211300
H	-6.16379300	-0.81613800	2.61699300
H	-5.49307800	-1.77425800	1.27665400

TS8R'

C	0.99331500	1.31456700	-0.30196800
C	1.82840300	3.18526700	-1.15600600
C	3.13064400	2.18945900	0.75336100
H	2.70962800	2.28605900	1.75400300
N	0.77756300	2.94040500	-1.87953300
N	0.28806600	1.77881500	-1.33847900
N	2.00560900	2.21313200	-0.20171500
C	2.74449600	4.36483600	-1.26063700
H	2.15289000	5.27363700	-1.38233200
H	3.39790000	4.26677600	-2.13621000
C	4.11903100	3.32717500	0.37073500
O	3.48474500	4.50857300	-0.06634700
C	5.11590400	1.24614000	-0.20242600
C	3.99237900	0.95875600	0.57920800
C	3.78134900	-0.30957900	1.09824600
C	4.71396900	-1.28357700	0.76572800
C	5.84008400	-1.03386700	-0.01388500
C	6.04675600	0.25316800	-0.49816800
C	5.12463300	2.69182000	-0.61685300
H	2.92525100	-0.51307800	1.73257900
H	6.53341000	-1.83799700	-0.22648800
H	6.92272500	0.47527900	-1.09823700
H	4.78724100	2.78079400	-1.65568700
H	6.11072700	3.15611400	-0.55287500
C	-0.91821600	1.19406600	-1.85078900
C	-0.85235700	0.01038000	-2.58840700
C	-2.13015300	1.83515400	-1.55837400
C	-2.06303100	-0.57482300	-2.97524900
C	-3.30269200	1.22240400	-1.98444400
C	-3.29120000	0.00009500	-2.66315600
H	-2.03458500	-1.50839600	-3.53399700

H	-4.25156500	1.70340700	-1.76302800
C	-2.16085800	3.14107300	-0.81316400
H	-1.76923500	3.95237800	-1.43438200
H	-1.54347400	3.08367900	0.08802700
H	-3.18320700	3.38600000	-0.51479400
C	0.44642200	-0.63461000	-3.00430700
H	1.29727800	-0.28542100	-2.41729200
H	0.65019300	-0.41830500	-4.05764400
H	0.38111700	-1.72132700	-2.89400200
H	4.65151100	3.60590300	1.28277900
C	-4.58535500	-0.68670700	-3.01146800
H	-4.44544600	-1.42851800	-3.80054100
H	-4.98247900	-1.20391900	-2.13088000
H	-5.34015100	0.03276600	-3.33887500
N	4.49193700	-2.64641500	1.26198900
O	5.37943000	-3.46643100	1.10025600
O	3.42629100	-2.88894800	1.80428000
C	-0.94777100	-4.71120400	-1.72640800
C	-1.04571800	-3.56485300	-0.94458400
C	-0.46142600	-3.51280700	0.32570600
C	0.22806700	-4.63080500	0.79397200
C	0.32714400	-5.78278700	0.01375700
C	-0.26059000	-5.82673800	-1.24702100
H	-1.41077700	-4.73713700	-2.70856600
H	-1.59146100	-2.69575400	-1.30920900
H	0.69593900	-4.59660200	1.77451700
H	0.86464900	-6.64607500	0.39375900
H	-0.18680400	-6.72396700	-1.85329500
C	-0.51844100	-2.23484200	1.13804000
H	-0.16184100	-2.45468900	2.15355100
C	0.42259600	-1.19456800	0.49185000
C	0.37474400	0.17277200	1.18183400
O	1.11180600	0.44213100	2.15866800
H	0.10200700	-1.08626200	-0.54510800
C	-3.20976700	-2.07420900	1.18193900
C	-1.87628300	-1.59128300	1.19032600
C	-2.00636800	-0.22056500	1.28575200
N	-3.33984300	0.05859600	1.34217200
H	1.45712900	-1.54709200	0.50464500
N	-4.08473300	-1.08356700	1.27757600
C	-3.98585500	1.30952200	1.46799000
C	-3.47275900	2.29599800	2.30980500
C	-5.16648100	1.53699500	0.75804600
C	-4.10611300	3.53337900	2.38915500

H	-2.61324700	2.08835900	2.93759100
C	-5.80260600	2.76877500	0.85926100
H	-5.56266200	0.74306300	0.13494300
C	-5.26682600	3.77745700	1.66079000
H	-3.69924800	4.29841100	3.04201400
H	-6.71852200	2.94426300	0.30427800
H	-5.76161100	4.74032500	1.73010000
N	-0.98232100	0.71794900	1.24119300
H	-0.99719800	1.42497000	1.96673800
C	-3.68730100	-3.49098500	1.10802600
H	-4.74584500	-3.53579300	1.37037400
H	-3.55442400	-3.90189900	0.10290700
H	-3.12263100	-4.12934600	1.79298100

TS8S

C	1.38518300	0.72050900	-0.52778800
C	1.31293200	1.25930500	-2.68896100
C	-0.47429300	-0.24865100	-1.98498700
H	-0.56313600	-0.99788500	-1.19142200
N	2.36894100	1.86551500	-2.24375800
N	2.38664700	1.52272700	-0.90642800
N	0.69512800	0.55893000	-1.68708200
C	0.76985400	1.08177500	-4.06809400
H	1.49025600	1.41803300	-4.81275900
H	-0.16706700	1.63913300	-4.19654300
C	-0.31779100	-0.96737300	-3.36890800
O	0.58496100	-0.31444700	-4.25281900
C	-2.50638400	0.05285300	-3.20871700
C	-1.76315600	0.53965100	-2.13082100
C	-2.24955400	1.56018900	-1.32741300
C	-3.53383000	2.01557300	-1.59708200
C	-4.31101000	1.53256900	-2.64457900
C	-3.77955500	0.55068600	-3.47467800
C	-1.75087400	-1.02679900	-3.93874600
H	-1.68996900	1.98987700	-0.50600600
H	-5.30630200	1.92986000	-2.79850400
H	-4.35743600	0.17478200	-4.31204700
H	-1.73550300	-0.88471100	-5.02233000
H	-2.19891800	-2.00607100	-3.73959000
C	3.49453900	1.97481500	-0.10946200
C	3.29157400	2.94997100	0.86705700
C	4.75278400	1.42831400	-0.38451500
C	4.40981600	3.39178200	1.57527600
C	5.83683800	1.90025200	0.35149000

C	5.68445100	2.88177300	1.33304200
H	4.27634300	4.15498500	2.33806100
H	6.82404100	1.48929400	0.15480500
C	4.92907600	0.36405500	-1.43563500
H	4.81846100	0.78025900	-2.44073500
H	4.17721600	-0.42404700	-1.32649800
H	5.91812400	-0.08953100	-1.35549300
C	1.92155500	3.47607100	1.19041600
H	1.98697100	4.45113200	1.67647300
H	1.43585800	2.77454400	1.87540500
H	1.29598200	3.57093200	0.29862200
H	0.10164200	-1.96498500	-3.23081900
C	6.86945000	3.35477300	2.13480700
H	7.03182700	2.70522200	3.00092700
H	7.78301400	3.33966600	1.53600000
H	6.71506100	4.36990300	2.50690500
N	-4.10726600	3.02436100	-0.69890400
O	-5.29132800	3.28686800	-0.82291300
O	-3.37348200	3.53239300	0.12919500
C	-4.76030300	0.44516300	1.18042900
C	-3.49983400	-0.11731100	1.36231700
C	-2.66740000	0.31292100	2.40125400
C	-3.12950200	1.31145700	3.25964600
C	-4.39089100	1.87730100	3.08078900
C	-5.20820600	1.45002900	2.03764900
H	-5.39028500	0.10630500	0.36278700
H	-3.14730800	-0.89671600	0.68871500
H	-2.48928800	1.65680300	4.06756500
H	-4.73175500	2.65746500	3.75395800
H	-6.18514400	1.89829000	1.88877600
C	-1.24099800	-0.19835300	2.50723600
H	-0.84217400	0.07463800	3.49291700
C	-0.41424200	0.51179400	1.41406100
C	1.00637400	-0.04233500	1.28399300
O	1.90554900	0.29324900	2.06404600
H	-0.95246300	0.34655200	0.48009600
C	-1.78679300	-2.81613300	2.70141200
C	-1.07633000	-1.67004500	2.26166900
C	-0.04053100	-2.17712200	1.50297200
N	-0.16730900	-3.53500000	1.49842800
H	-0.36165100	1.58705900	1.60141000
N	-1.23645800	-3.93238300	2.25250800
C	0.66578300	-4.50590600	0.89312900
C	1.31011500	-4.23633800	-0.31637000

C	0.81593100	-5.74856300	1.51216500
C	2.12379700	-5.20995000	-0.88981100
H	1.16526800	-3.27990500	-0.80565500
C	1.61853700	-6.71586500	0.91916600
H	0.29703600	-5.93607000	2.44430100
C	2.28164200	-6.45038700	-0.27831700
H	2.62493100	-4.99687700	-1.82833600
H	1.73302600	-7.68083000	1.40196300
H	2.91312700	-7.20646400	-0.73216400
N	0.94902900	-1.45607900	0.83499900
H	1.87645600	-1.86582200	0.93116400
C	-3.01200100	-2.85613500	3.55771100
H	-3.87495400	-2.44574200	3.02466300
H	-3.23100900	-3.88531900	3.84638900
H	-2.87402200	-2.25540000	4.46126100

TS8S'

C	-1.15124100	0.35449200	0.64597500
C	-2.57894700	0.32117300	2.34622200
C	-3.59423100	-0.08027100	0.12199700
H	-3.40308800	0.37826700	-0.84916100
N	-1.42129400	0.48921900	2.90911900
N	-0.55777100	0.49873400	1.83699100
N	-2.45832500	0.25187500	0.98254800
C	-3.95302700	0.26231400	2.92603900
H	-3.98361700	0.75199400	3.89922200
H	-4.27841600	-0.78137000	3.04496400
C	-4.95235200	0.38743300	0.76739900
O	-4.80282100	0.97783100	2.04810900
C	-4.98578400	-2.02331700	0.41266900
C	-3.72893700	-1.57876600	0.01206800
C	-2.73572500	-2.45818200	-0.38634200
C	-3.04727900	-3.80886000	-0.35525300
C	-4.29298200	-4.29425700	0.04029700
C	-5.27568900	-3.38883200	0.42311500
C	-5.86905000	-0.86529400	0.79321100
H	-1.76545200	-2.10353000	-0.70939100
H	-4.47336500	-5.36193900	0.04492200
H	-6.25057000	-3.74754900	0.73558100
H	-6.32300500	-0.98505600	1.78194100
H	-6.68887500	-0.75386700	0.07739900
C	0.85634900	0.61928600	2.04955100
C	1.61219700	-0.55528400	2.13497400
C	1.41662400	1.89334000	2.15977200

C	2.98949700	-0.41889200	2.28293100
C	2.80479800	1.97598200	2.29162500
C	3.60482300	0.83446200	2.32986100
H	3.59650500	-1.31699300	2.35331600
H	3.26796100	2.95831800	2.35933700
C	0.56135800	3.13372100	2.15708600
H	0.11897400	3.29461100	3.14537100
H	-0.26222800	3.05977600	1.44169500
H	1.15931600	4.01098200	1.90110700
C	0.94997500	-1.90612600	2.09510700
H	0.39749300	-2.03324700	1.15859400
H	0.24347000	-2.01275200	2.92498000
H	1.69640700	-2.70218300	2.15863100
H	-5.38818800	1.17867600	0.15794100
C	5.10603900	0.93691900	2.38976600
H	5.42802500	1.92948900	2.71137600
H	5.52625300	0.19572400	3.07433900
H	5.53174500	0.74807300	1.39820200
N	-2.00675500	-4.76262700	-0.74915700
O	-2.23520700	-5.95117700	-0.61758600
O	-0.95811300	-4.31199100	-1.18476300
C	3.04498700	4.93959200	-0.89082300
C	2.55225400	3.64318000	-0.99055300
C	1.91520400	3.20668700	-2.15707800
C	1.78042000	4.09781200	-3.22101200
C	2.27468500	5.39886000	-3.12608700
C	2.90704200	5.82357500	-1.96131600
H	3.54088800	5.26000700	0.02099500
H	2.67501800	2.94579300	-0.16388900
H	1.28625100	3.77048300	-4.13224500
H	2.16559000	6.07971300	-3.96450300
H	3.29313700	6.83513300	-1.88690600
C	1.34417400	1.80541400	-2.22957700
H	0.98089400	1.63160900	-3.25143000
C	0.15673500	1.68182500	-1.24714700
C	-0.46298700	0.27530500	-1.21311500
O	-1.44964800	-0.00326900	-1.93057700
H	0.54595500	1.94861500	-0.26331700
C	3.72332700	0.57953700	-1.85717000
C	2.31301700	0.72371600	-1.83879200
C	1.84843200	-0.47405300	-1.33871100
N	2.93459200	-1.26501900	-1.09690500
H	-0.65177500	2.37109200	-1.50581900
N	4.08903300	-0.61674700	-1.41763100

C	2.99415200	-2.55846100	-0.52753400
C	1.99692100	-3.50113200	-0.77300800
C	4.07893100	-2.88356400	0.29109100
C	2.04601800	-4.74044900	-0.14010300
H	1.19170100	-3.29706000	-1.46601900
C	4.13086400	-4.13190700	0.89974600
H	4.85900500	-2.14639800	0.44194400
C	3.10644000	-5.05882600	0.70339100
H	1.24831700	-5.45204000	-0.32732600
H	4.97327600	-4.37844100	1.53804600
H	3.14578500	-6.02666900	1.19200700
N	0.52261700	-0.79615600	-1.05782400
H	0.16274300	-1.60463900	-1.55528400
C	4.76372300	1.55702600	-2.30908300
H	4.92387400	2.33811900	-1.55957700
H	5.70753600	1.03517000	-2.47734000
H	4.45954100	2.05578100	-3.23290900

PR

C	-1.47266600	-2.20791000	2.92221500
C	-0.64497500	-1.13792000	2.59925200
C	-0.41307300	-0.11235300	3.52149100
C	-1.02901000	-0.17731900	4.77059000
C	-1.86045500	-1.24817900	5.09746500
C	-2.08299700	-2.26603500	4.17501000
H	-1.63835600	-2.99929400	2.19807700
H	-0.15632800	-1.10086700	1.62790800
H	-0.85350600	0.61362900	5.49531000
H	-2.32980600	-1.28755400	6.07541600
H	-2.72496300	-3.10290900	4.43017600
C	0.47476300	1.06150500	3.15245700
H	0.66879800	1.63651900	4.06800700
C	-0.25327800	1.98211600	2.14349700
C	0.60484300	3.04808700	1.47531100
O	0.20271300	4.16533300	1.21507700
H	-0.64663300	1.35873500	1.32937600
C	2.70559400	-0.40190200	2.73484800
C	1.78137500	0.65502500	2.53209200
C	2.37645300	1.43757400	1.57340100
N	3.55361500	0.86305700	1.22456900
H	-1.09836400	2.49143400	2.60833700
N	3.76898000	-0.26893400	1.95390100
C	4.52137000	1.31457400	0.29282100
C	4.11925000	1.89268300	-0.91151400

C	5.87398800	1.15534600	0.59278400
C	5.08647600	2.34189100	-1.80719200
H	3.06468600	1.96282000	-1.15777100
C	6.82778400	1.58947200	-0.31996400
H	6.15453700	0.69043000	1.53069900
C	6.43935900	2.19208200	-1.51610000
H	4.77535100	2.79305700	-2.74350200
H	7.88089900	1.46417400	-0.09109400
H	7.18839100	2.53721100	-2.22064000
N	1.86903600	2.63913200	1.09817200
H	2.47159100	3.33027700	0.66766400
C	2.59516800	-1.55917200	3.67588700
H	1.80478900	-2.24682400	3.36140100
H	3.54297000	-2.09869200	3.70800700
H	2.34474600	-1.21809300	4.68423900

PS

C	-4.67654100	-3.76717000	-0.36405300
C	-3.95028500	-2.66803200	0.08213500
C	-2.89190600	-2.83137200	0.98147700
C	-2.57399300	-4.11557600	1.42206000
C	-3.29911000	-5.21966300	0.97615200
C	-4.35213100	-5.04801600	0.08270000
H	-5.49807600	-3.62507200	-1.05905800
H	-4.21395200	-1.66785100	-0.25505900
H	-1.75549400	-4.25192700	2.12415300
H	-3.04157000	-6.21264900	1.33075700
H	-4.92049900	-5.90592600	-0.26182600
C	-2.08455200	-1.63416700	1.44517900
H	-1.44329200	-1.96419700	2.27398500
C	-1.17374500	-1.12829100	0.30100400
C	-0.48521100	0.20700200	0.54825900
O	0.64825300	0.45420200	0.18502800
H	-1.79033800	-0.99119500	-0.59747000
C	-4.14738600	-0.32511200	2.59979800
C	-2.92279000	-0.47296000	1.90011000
C	-2.47818200	0.81562400	1.73197500
N	-3.39280700	1.65613700	2.27467000
H	-0.39543700	-1.85406300	0.06192200
N	-4.42117400	0.95239500	2.82838100
C	-3.35332400	3.06988600	2.36836300
C	-2.86747400	3.82927100	1.30391400
C	-3.81941200	3.68396100	3.53058400
C	-2.82151700	5.21610200	1.42244300

H	-2.55626000	3.34386200	0.38445100
C	-3.78639300	5.07004600	3.62645100
H	-4.20211700	3.06677900	4.33496100
C	-3.27963700	5.83937400	2.57971100
H	-2.44288500	5.80840100	0.59618200
H	-4.15030400	5.55055200	4.52861800
H	-3.24871300	6.92029000	2.66417700
N	-1.26671300	1.17108700	1.15433400
H	-0.83168000	2.06361000	1.35469700
C	-5.08234800	-1.39673700	3.06373200
H	-4.53448000	-2.19872400	3.56578300
H	-5.81202800	-0.97484400	3.75656400
H	-5.61482500	-1.84745500	2.22098100