

Unveiling the Dual Activation Effect of NHC-Catalyst in One Asymmetric Reaction System

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Part 1. Method

1 Calculation details

To explore the reaction mechanism in more detail, we performed density functional theory (DFT) calculations using Gaussian 16 B.01.¹ Geometry optimizations were performed using the M06-2X functional² with the dispersion correction D3³, and basis set 6-31G(d, p)⁴⁻⁷ was employed. The solvent module IEF-PCM (THF) was employed for simulating solvent condition.⁸ Minima and transition structures on the potential energy surface were confirmed using frequency analysis at the same level of theory, showing respectively zero and only one imaginary frequency. Gibbs energies were evaluated at the room temperature (298.15 K). Single point corrections were through the high-level basis set 6-311++G (3d2f, 3p2d)⁹⁻¹¹.

2 Calculating analyses methods

In the main text, we mainly employed reactive index, non-covalent interaction, and distortion energy analyses to explain the phenomena in the reaction:

- (1) Non-covalent interaction (NCI) analysis and quantitative atom-in-molecule (AIM)¹² analysis were plotted by using Multiwfn 3.8(dev)¹³ and VMD 1.9.3¹⁴.
- (2) Reactive index analysis is including global reactive index and local reactive index. For the global reactive index, it can be parted global electrophilic index (ω) and global nucleophilic index (N). Global electrophilic index (ω) can be calculated by the equation $\omega = \mu^2 / 2\eta$.¹⁵ Here, μ is electronic chemical potential and can be obtained by the equation $\mu = (E_{\text{HOMO}} + E_{\text{LUMO}}) / 2$, η is chemical hardness and can be gotten by the equation $\eta = E_{\text{HOMO}} - E_{\text{LUMO}}$.¹⁶⁻¹⁸ Global nucleophilic index (N) can be calculated by the equation $N = E_{\text{HOMO}} - E_{\text{HOMO}}(\text{TCE})$. Here, global nucleophilic index is referred to tetracyanoethylene (TCE).¹⁹ For the local reactive index, it can be parted local electrophilic index (ω_k) and local nucleophilic index (N_k). First, the nucleophilic (P_k^-) and electrophilic (P_k^+) Parr functions should be obtained. Parr functions allow for the characterization of the nucleophilic and electrophilic sites of a molecule, can be obtained through the analysis of Mulliken atomic spin density (ASD) $\rho_s(r)$ of the corresponding radical cations (rc) or anions (ra) of the studies molecules, separately. That is said that $P_k^+ = \rho_s^{\text{rc}}(r)$ and $P_k^- = \rho_s^{\text{ra}}(r)$. Then, local electrophilic index can be

calculated by the equation $\omega_k = \omega \times P_k^+$, local nucleophilic index can be calculated by the equation $N_k = N \times P_k^-$.^{20, 21}

(3) Distortion energy analysis is based on the equation $E_{\text{inter}} = E_{\text{act}} - E_{\text{dist}}$. When the activation energy is a constant, high distortion energy means a low interaction energy. The low interaction energy goes against the generation of transition state and subsequent intermediates.

(4) The extent of enantioselectivity, in terms of enantiomeric excess (*e.e.*), was also calculated by using the Boltzmann distribution of diastereomeric transition states with the equation $e.e. = (A-1)/(A+1) \times 100\%$ (Here, $A = R/S$, $R/S = \exp(-\Delta\Delta G^\ddagger/RT)$, and $-\Delta\Delta G^\ddagger = -\Delta G_{\text{R}}^\ddagger - (-\Delta G_{\text{S}}^\ddagger)$)

3 Comparison among different methods

To prove rationality of the density functional M06-2X in the reaction system, we added calculations for the four key transition states **TS4C-RR**, **TS4C-RS**, **TS4C-SR**, and **TS4C-SS** with other density functionals ω B97X-D²² and B3LYP²³. For geometries optimization, the basis set 6-31G(d,p) was employed. For single point corrections, we used the high-level basis set 6-311++G(3d2f, 3p2d). Furthermore, the situations of the dispersion correction D3 and D3(BJ)²⁴ used in B3LYP and M06-2X without D3 were also calculated.

Table S1. Comparisons of relative Gibbs free energies for key transition states ($\Delta\Delta G^\ddagger$) with different methods (unit: kcal/mol)

	M06-2X- D3	M06-2X	ω B97X-D	B3LYP	B3LYP-D3	B3LYP- D3(BJ)
TS4C-RR	10.0	9.9	9.5	15.8	10.7	10.9
TS4C-RS	9.7	10.4	14.0	17.4	10.5	10.8
TS4C-SR	0	0	0	0	0	0
TS4C-SS	7.1	6.0	4.6	2.0	6.9	6.3

As shown in **Table S1**, besides the results from B3LYP, there are little differences between the results calculated by those methods and the results calculated by the selected method and the various levels lead to the same conclusion. For the strange

results from B3LYP, the main reason is that B3LYP is not good at processing the long-range interactions among reaction fragments. When B3LYP with D3 and D3(BJ) were employed, they got much better results (**Table S1**). Therefore, we obtained three results: (1) the selected method M06-2X-D3 is reliable for the reaction systems in our work; (2) although ω B97X-D has dispersion correction D2 to process the long-range interactions among reaction fragments, D2 brings still more obvious errors for the results; and (3) B3LYP-D3(BJ) and B3LYP-D3 have also good performance to process the long-range interactions among reaction fragments in this reaction system, which are like M06-2X-D3.

4 Analysis and discussion of different basis sets

To correct the energy error from overlap integral (S integral) of double ζ basis set 6-31G(d,p), the calculations of single point by higher level triple ζ basis set are necessary. Here, we chose two high-level triple ζ basis sets 6-311++G(2d,2p)^{9, 10} and 6-311++G(3d2f, 3p2d) to execute single point corrections for the four key transition states **TS4C-RR**, **TS4C-RS**, **TS4C-SR**, and **TS4C-SS**.

Table S2. Comparisons of relative Gibbs free energies for key transition states ($\Delta\Delta G^\ddagger$) with corrections by two different high level basis sets (unit: kcal/mol)

	M06-2X-D3/ 6-311++G(2d,2p)	M06-2X-D3/ 6-311++G(3d2f, 3p2d)
TS4C-RR	11.3	10.0
TS4C-RS	10.7	9.7
TS4C-SR	0	0
TS4C-SS	6.7	7.1

As shown in **Table S2**, there are no obvious differences between the results from the two high level triple ζ basis sets 6-311++G(2d,2p) and 6-311++G(3d2f, 3p2d). it is suitable that we chose 6-311++G(3d2f, 3p2d) to correct the energy error, with comparing with the more commonly used basis set 6-311++G(2d,2p).

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Part 2. Discussion of NHC-catalyzed homo-coupling

In the main text, we discussed NHC-catalyzed cross-coupling between **R1** and **R2**. Here, we will examine two NHC-catalyzed homo-couplings. As illustrated in **Fig. 2b**, **M3** can bond with **R1** to form **P3** and **M3'** can bond with **R2** to form **P4**. Given that Michael addition is the chemoselective determining step in the reaction, we calculated the key step and generated the Gibbs free energy profiles for the two homo-couplings.

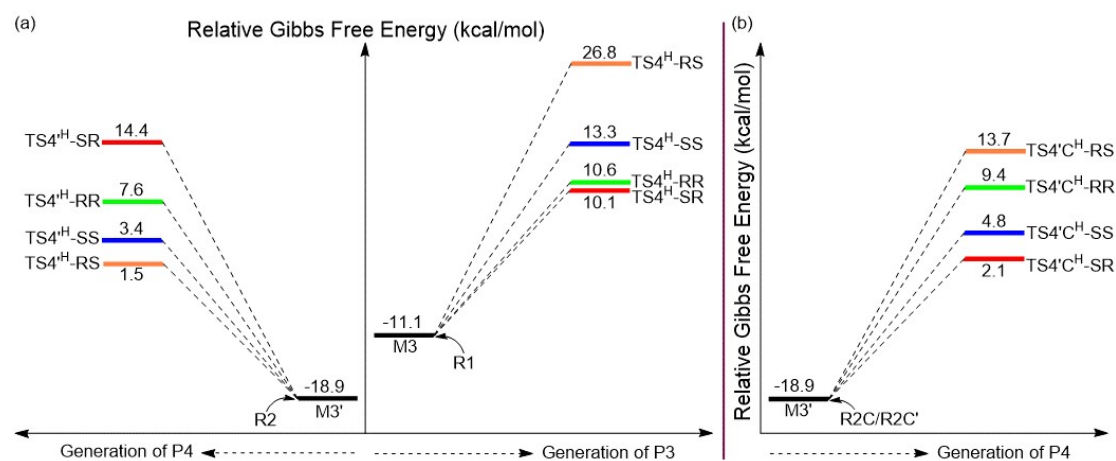


Fig. S1 Gibbs free energy profile of key transition states in two NHC-catalyzed homo-couplings: high energy barriers make the two homo-couplings impossible to process under the room temperature

Fig. S1a presents the Gibbs free energies of two homo-couplings. The pathway to generate **P3** (**M3** bonding with **R1**) has energy barriers ranging from 21.2 to 37.9 kcal/mol, while the pathway to generate **P4** (**M3'** bonding with **R2**) has energy barriers ranging from 20.4 to 33.3 kcal/mol. Furthermore, because the main existing state of **R2** is the complex **R2C/R2C'**, we also discussed the other pathway to generate **P4** (**M3'** bonding with **R2C/R2C'**). As shown in **Fig. S1b**, the energy barriers ranging from 21.0 to 32.6 kcal/mol. However, the high energy barriers for both pathways prevent them from being processed at room temperature, making it impossible to generate homo-coupling products **P3** and **P4** in the reaction system.

Part 3. Discussion of the chemoselectivity for proton transfer

Proton transfer is generally a complex process in a reaction, as it has multiple possible pathways. In the main text, we pointed out that there is no generation of the Breslow intermediate in the proton transfer process in **Pathway R1**. To explain this interesting phenomenon, we have some hypotheses below.

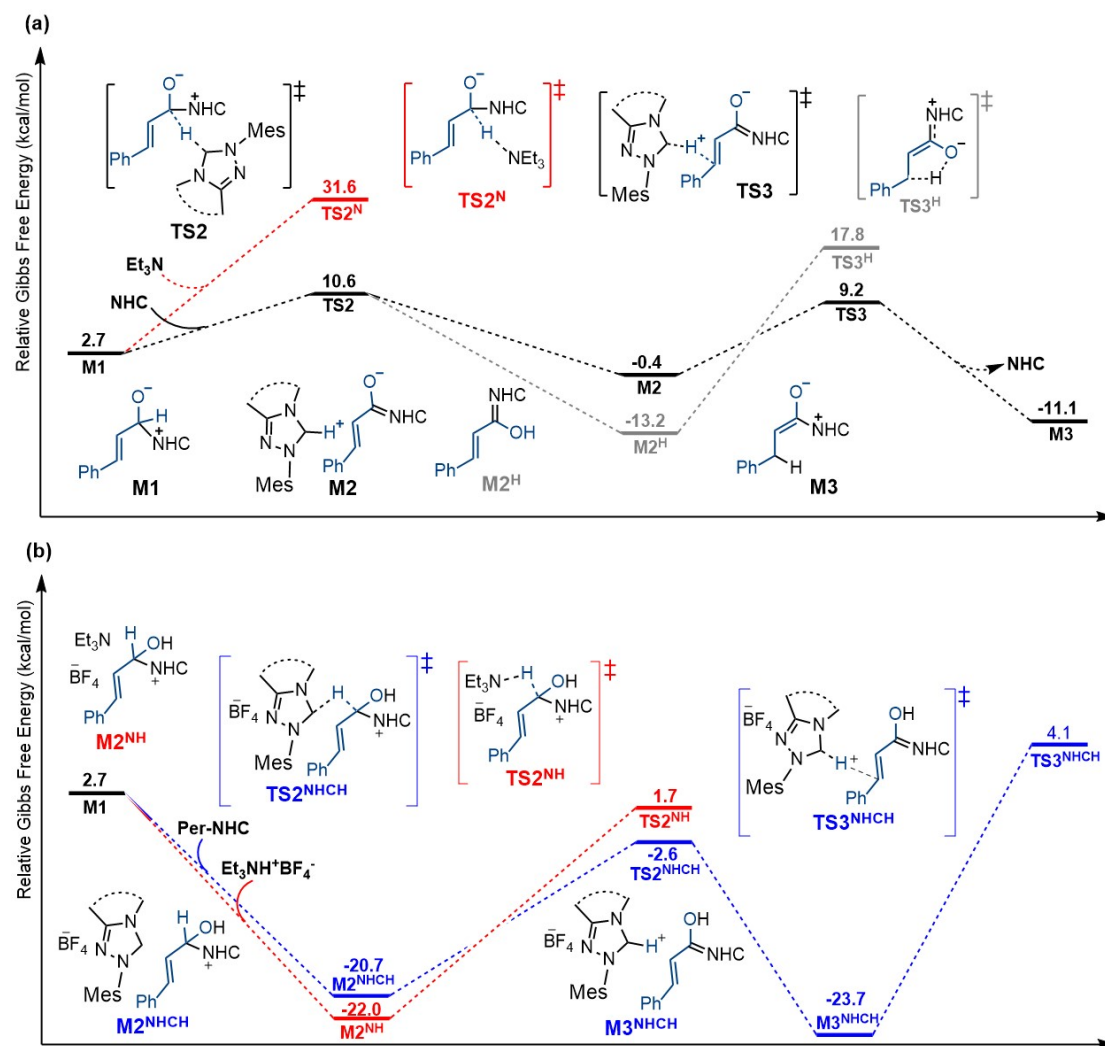


Fig. S2 Possible proton transfer processes and Gibbs free energy profile in Pathway R1 (a) base-assist proton transfer and (b) acid-assist proton transfer: the optimal process of proton transfer is that NHC as base makes proton to shift directly

We have first designed **Et₃N** or **NHC** as base to assist possible proton transfer pathways. As shown in **Fig. S2a**, quite high energy barrier (28.84 kcal/mol) from **Et₃N** assisting proton transfer (via **TS2^N**) makes that the process of proton transfer can be only assisted by **NHC** via **TS2** with lower energy barrier (7.84 kcal/mol). Then, **NHC** assisted proton transfer also has two possible pathways. One is that the

intermediate **M2^H** directly generates **M3** via a five-member ring transition state and jump over an energy barrier 31.00 kcal/mol. The barrier is so high that **M2^H** cannot generate **M3** under room temperature. The other one is that **NHC** keeps on assisting proton transfer and makes **M2** to generate **M3**. Its energy barrier is only 9.65 kcal/mol, so that **M2** can generate **M3** easily under room temperature. Comparing with the traditional pathway of generating enol intermediate **M2^H**, the proton transfer process in this reaction favors to choose the kinetic controlled pathway. As shown in **Fig. S2b**, we also designed **Et₃NH** and **Pre-NHC** as acid to assist proton transfer. Whether **Et₃NH** or **Pre-NHC**, the energy barriers are quite high (23.7 and 27.8 kcal/mol). The high energy barriers make the process of proton transfer impossible to be happened smoothly. Therefore, the chemoselectivity of proton transfer is also controlled by reaction kinetic effectors. Lower energy barrier determines that proton transfer rather processes via the direct shift than the generation of Breslow intermediate.

Part 4. Active effect of Brønsted acid Pre-NHC on substrate R2

In the main text, we discussed the primary state of the substrate **R2**. We found that the complex **R2C/R2C'** is the main form of **R2**. Upon comparing the energy barriers in the stereo-determining step (Michael addition), we observed that the energy barriers for Michael donor **M3** bonding with **R2C/R2C'** were lower than those for **M3** bonding with **R2**. Therefore, we proposed a hypothesis that the **Pre-NHC-Et₃N** complex activates the substrate **R2**.

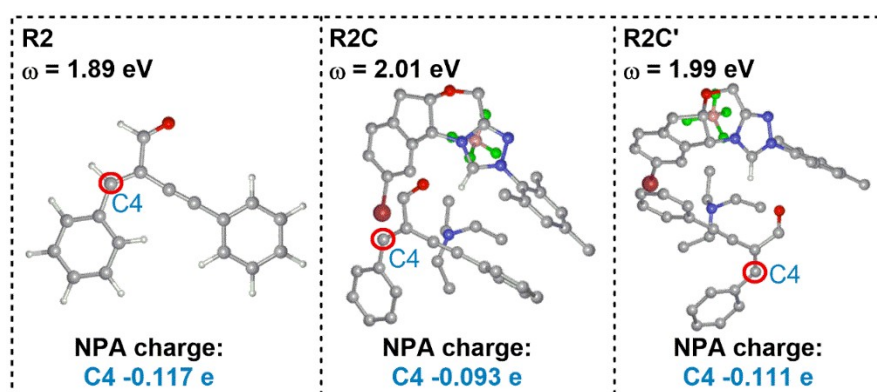


Fig. S3 3D structures of **R2**, **R2C**, and **R2C'** with their electrophilic reactive index and the NPA charge value of **C4** in different existing state of **R2**: the complex **Pre-NHC-Et₃N** can enhance the electrophile of **R2** and decrease the electronic density of the active atom **C4**

Due to **R2** and **R2C/R2C'** playing the role of Michael acceptor, we calculated the electrophilic reactive index (ω) and performed natural population analysis (NPA) of the active atom **C4** in different existing states of **R2** since both **R2** and **R2C/R2C'** play the role of Michael acceptor. **Figure S3** shows that the electrophilic reactive indexes (ω) of the **R2C** and **R2C'** conformations are 2.01 eV and 1.99 eV, respectively, which are much higher than the electrophilic reactive index of **R2** (1.89 eV). Additionally, NPA charge values of the active atom **C4** in **R2**, **R2C**, and **R2C'** are -0.117 e, -0.096 e, and -0.111 e, respectively. Thus, the complex **Pre-NHC-Et₃N** significantly increases the electrophilicity of the substrate **R2** and slightly decreases the negative electronic density of the active atom **C4**. Both high electrophilicity and low negative electronic density assist the **R2C/R2C'** complex as a Michael acceptor to bond with Michael donor **M3**. Moreover, the effect of the complex **Pre-NHC-Et₃N** is stronger in **R2C** than in **R2C'**. As a result, **R2C** can bond with **M3**, leading to the

generation of the main product **P1** with *SR*-configuration. Hence, the effect of **Pre-NHC-Et₃N** also assists in the generation of the main product **P1** with *SR*-configuration.

Part 5. NHC cycle of the optimal pathway

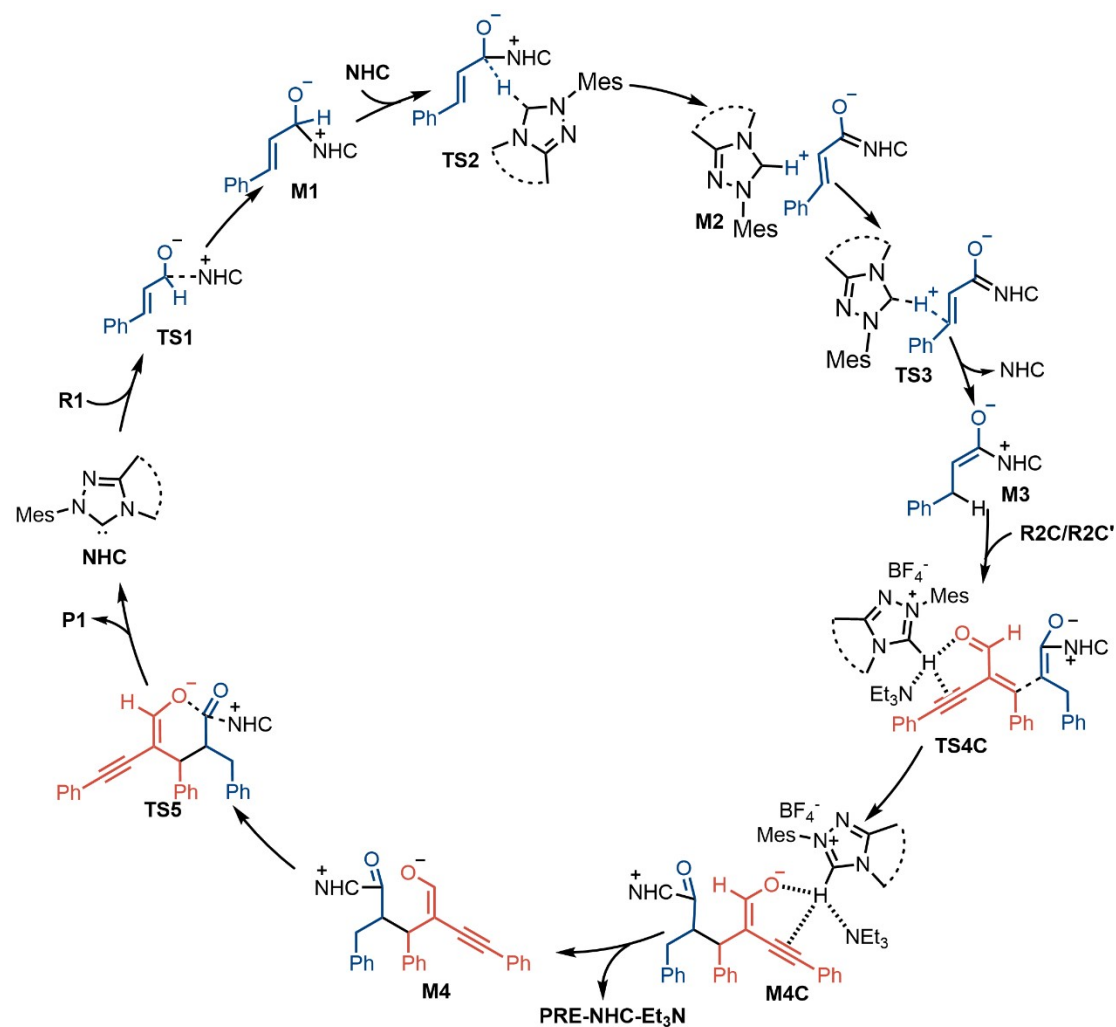


Fig. S4 The optimal pathway of the reaction

The optimal pathway can be divided into four steps: (1) NHC nucleophilically attacks R1 to generate M1 via TS1; (2) NHC assists proton transfer to generate Michael donor M3 via TS2 and TS3, respectively; (3) M3 couples with Michael acceptor R2C/R2C' to generate M4 via four transition states, this step is the stereoselectivity determining step; (4) Self-cyclization and NHC dissociation together in M4 generate the product P1 (*SR*-configuration) via TS5.

Part 6. Discussion of self-cyclization

In the main text, we used Frontier Molecular Orbital (FMO) theory to discuss why the Michael addition and self-cyclization are not a simple one-step [4+2] cyclization in the reaction. After the generation of **M4** through Michael addition, we found that self-cyclization and **NHC** dissociation occur collaboratively via **TS5**.

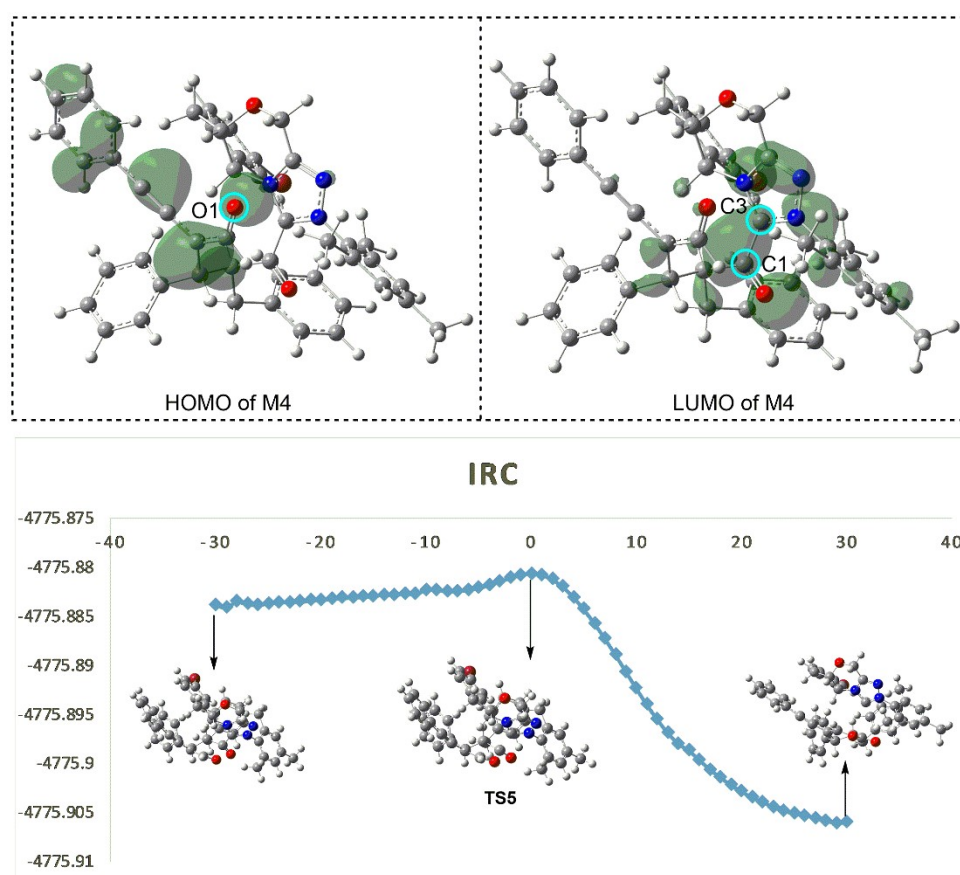


Fig. S5 FMO distribution of the intermediate **M4** and IRC analysis of **TS5**: FMO symmetry matching of atoms **O1** (HOMO), **C1** (LUMO), and **C3** (LUMO) in **M4** is in favor of the process of self-cyclization; and IRC analysis of **TS5** proved that the synergistic process including self-cyclization and dissociation of **NHC** is reasonable

To explain this interesting discovery, we have analyzed the FMO of **M4**. As shown in **Fig. S5**, electrons in HOMO occupy in atom **O1** (green area). Atoms **C1** and **C3** share an empty molecular orbit in LUMO (green area). They are symmetry matching. Hence, the electrons can flux from the occupied orbit in **O1** to the empty orbit between **C1** and **C3**. **C1** and **C3** should be electrophilic in this collaborative process. Due to **C1** and **C3** existing in the same molecule **M4**, comparing the

difference between two electrophilic *Parr* functions (P_k^+) of **C1** and **C3** is enough. By calculation, the electrophilic *Parr* functions (P_k^+) of **C1** and **C3** are 0.003 and -0.002, respectively. The atom **C1** has stronger electrophilicity and more favors to bond with **O1**. Because of symmetry matching of FOM among atoms **O1** (HOMO), **C1** (LUMO), and **C3** (LUMO), the electrons fluxing direction should be from **O1** to **C1** firstly and then to **C3**, so that **O1** bonding with **C1** and breaking of the bond between **C1** and **C3** can happen in the same time. In addition, we employed intrinsic reaction coordinate (IRC) analysis to explore **TS5** more deeply. As shown in **Fig. S5**, the trend in back- and forward processes of **TS5** is consistent with our explain from FMO analysis, that **O1** bonds with **C1** to assist the breaking of the bond between **C1** and **C3**.

Part 7. Discussion about the effect of substituents of R2

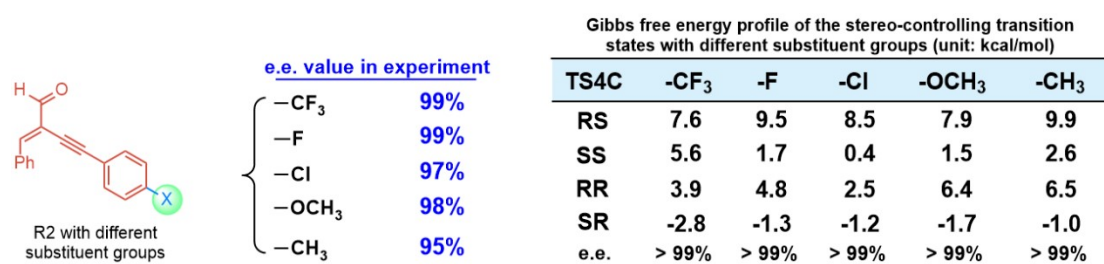


Fig. S6 The effect of different substituents on stereoselectivity: experimental proofs accord to calculating predictions within the allowed error range

We investigated the effect of substituents on the stereoselectivity using five derivatives of **R2** with different electronic substituents (**Fig. S6**). Complexes of these derivatives with **Pre-NHC-Et₃N** were used to couple with **M3**, and the energy barriers of the stereo-controlled transition states were calculated and compared. We found that all substrates with different substituents can provide a quite good stereoselectivity (all *e.e.* > 99%). Synthesizing the derivatives with different electronic effect substituents yielded the *e.e.* values (all *e.e.* > 95%) consistent with our calculating results within the allowed error range. We also compared the energy differences between transition states with *SR*- and *RS*-configurations. It observed that the effect of stereoselectivity with electron-withdrawing groups (-CF₃, -F, -Cl) was stronger than with electron-donating groups (-OCH₃ and -CH₃). Analysis of the *e.e.* values of synthesizing derivatives confirmed that the stereoselectivity with electron-withdrawing group (-CF₃, -F, -Cl) was indeed better, with *e.e.* value of 99%, 99%, and 97%, respectively. Our prediction that electron-withdrawing group enhance stereoselectivity was accurate, and should be helpful in following experiments that aimed to find new reaction model.

Part 8. Thermodynamics parameters of stationary points

Table S3 The single point energies (E) under M06-2X-D3/6-311++G(3d2f, 3p2d)/IEF-PCM, Gibbs free energy corrections (GFEC) under M06-2X-D3/6-31G(d, p)/IEF-PCM, and Gibbs free energy (GFE = E + GFEC) energies of the stationary points (SP) involved in the reaction (unit: a.u.)

SP	E	GFEC	GFE	Imaginary Frequency
R1	-422.81924	0.109827	-422.709413	
R2	-729.925012	0.191964	-729.733048	
NHC	-3625.460306	0.319295	-3625.141011	
Et ₃ N	-292.292044	0.174385	-292.117659	
NHCH-BF ₄	-4050.505488	0.34298	-4050.162508	
PRE-NHC-Et ₃ N	-4342.827499	0.540076	-4342.287423	
TS0	-4342.822162	0.540117	-4342.282045	-1008.03
NHC-Et ₃ NH ⁺ ·BF ₄ ⁻	-4342.825765	0.543352	-4342.282413	
R2C	-5072.78013	0.76443	-5072.0157	
R2C'	-5072.779553	0.761616	-5072.017937	
TS1	-4048.289463	0.454748	-4047.834715	-203.46
M1	-4048.302177	0.4561	-4047.846077	
TS2	-7673.775958	0.801362	-7672.974596	-1293.09
TS2 ^N	-4340.572617	0.654805	-4339.917812	-1280.97
TS2 ^{NH}	-4765.658874	0.679657	-4764.979217	-1179.00
TS2 ^{NHCH}	-8098.846172	0.829024	-8098.017148	-1310.27
M2	-7673.798081	0.805987	-7672.992094	
M2 ^{NH}	-4765.694018	0.677022	-4765.016996	
M2 ^{NHCH}	-8098.878714	0.832894	-8098.04582	
M2 ^H	-4048.327479	0.456088	-4047.871391	
TS3	-7673.778121	0.801396	-7672.976725	-1395.71
TS3 ^H	-4048.271411	0.449386	-4047.822025	-1698.40
TS3 ^{NHCH}	-8098.839431	0.832961	-8098.00247	-1340.17

M3	-4048.326447	0.458285	-4047.868162	
M3 ^{NHCH}	-8098.88159	0.830914	-8098.050676	
TS4C-RS	-9121.102286	1.254084	-9119.848202	-354.33
TS4C-SS	-9121.110289	1.258011	-9119.852278	-264.96
TS4C-RR	-9121.110301	1.262632	-9119.847669	-332.53
TS4C-SR	-9121.116854	1.253273	-9119.863581	-240.93
TS4-RS	-4778.229329	0.67768	-4777.551649	-363.17
TS4-RR	-4778.250725	0.679707	-4777.571018	-259.99
TS4-SS	-4778.246157	0.680704	-4777.565453	-309.55
TS4-SR	-4778.256169	0.67982	-4777.576349	-306.85
M4C	-9121.141591	1.257354	-9119.884237	
M4	-4778.272954	0.681645	-4777.591309	
TS5	-4778.267912	0.683762	-4777.58415	-184.59
P	-1152.797123	0.33378	-1152.463343	
R2C-NHC	-8698.281159	1.110703	-8697.170456	
R2C'-NHC	-8698.271754	1.112379	-8697.159375	
TS1'	-4355.403737	0.541899	-4354.861838	-160.64
TS1'C	-8698.276074	1.110947	-8697.165127	-108.37
TS1'C'	-8698.266174	1.113322	-8697.152852	-129.62
M1'C	-8698.299922	1.116653	-8697.183269	
M1'C'	-8698.292664	1.112452	-8697.180212	
M1'	-4355.419021	0.543972	-4354.875049	
TS2'	-7980.888138	0.884897	-7980.003241	-1523.91
TS2' ^N	-4647.699808	0.737395	-4646.962413	-1270.34
M2'	-7980.911771	0.888354	-7980.023417	
M2' ^H	-4355.429722	0.541128	-4354.888594	
TS3'	-7980.899335	0.884727	-7980.014608	-1431.04
TS3' ^H	-4355.384442	0.538874	-4354.845568	-827.51
M3'	-4355.44664	0.542482	-4354.904158	

TS4'-RS	-4778.255899	0.684272	-4777.571627	-364.25
TS4'-RR	-4778.230962	0.681463	-4777.549499	-465.80
TS4'-SS	-4778.246044	0.683016	-4777.563028	-338.97
TS4'-SR	-4778.231183	0.680593	-4777.55059	-387.55
TS4 ^H -RS	-4471.113563	0.596454	-4470.517109	-381.76
TS4 ^H -RR	-4471.137771	0.594746	-4470.543025	-310.08
TS4 ^H -SS	-4471.134517	0.59584	-4470.538677	-330.03
TS4 ^H -SR	-4471.141562	0.597739	-4470.543823	-308.01
TS4 ^H -RS	-5085.369184	0.764525	-5084.604659	-336.38
TS4 ^H -RR	-5085.359286	0.764292	-5084.594994	-443.49
TS4 ^H -SS	-5085.364935	0.763308	-5084.601627	-387.55
TS4 ^H -SR	-5085.347485	0.763227	-5084.584258	-363.40
R2CF	-1066.893029	0.189966	-1066.703063	
TS4CCF-RS	-9458.073475	1.251942	-9456.821533	-335.45
TS4CCF-SS	-9458.082854	1.258078	-9456.824776	-252.50
TS4CCF-RR	-9458.082623	1.255193	-9456.82743	-318.35
TS4CCF-SR	-9458.088158	1.25004	-9456.838118	-226.64
R2Cl	-1189.504355	0.179344	-1189.325011	
TS4CCI-RS	-9580.683789	1.241697	-9579.442092	-337.64
TS4CCI-SS	-9580.693326	1.23836	-9579.454966	-249.57
TS4CCI-RR	-9580.692266	1.240629	-9579.451637	-322.66
TS4CCI-SR	-9580.698494	1.24096	-9579.457534	-231.25
R2F	-829.143028	0.181985	-828.961043	
TS4CF-RS	-9220.321789	1.245259	-9219.07653	-339.79
TS4CF-SS	-9220.330271	1.241306	-9219.088965	-266.58
TS4CF-RR	-9220.33034	1.246355	-9219.083985	-326.44
TS4CF-SR	-9220.336305	1.242568	-9219.093737	-239.35
R2Me	-769.228828	0.217889	-769.014239	
TS4CMe-RS	-9160.404405	1.278649	-9159.125756	-342.74

TS4CMe-SS	-9160.414097	1.276648	-9159.137449	-258.82
TS4CMe-RR	-9160.412867	1.281612	-9159.131255	-333.42
TS4CMe-SR	-9160.42019	1.277135	-9159.143055	-245.22
R2CNH	-785.272667	0.206593	-785.066074	
TS4CNH-RS	-9176.449881	1.273836	-9175.176045	-354.36
TS4CNH-SS	-9176.458992	1.27099	-9175.188002	-302.62
TS4CNH-RR	-9176.457988	1.272149	-9175.185839	-339.20
TS4CNH-SR	-9176.465321	1.268461	-9175.19686	-258.84
R2NO	-934.330007	0.190253	-934.139754	
TS4CNO-RS	-9325.510776	1.253763	-9324.257013	-333.11
TS4CNO-SS	-9325.521949	1.250357	-9324.271592	-262.12
TS4CNO-RR	-9325.520668	1.255604	-9324.265064	-309.48
TS4CNO-SR	-9325.525534	1.251651	-9324.273883	-222.49
R2OMe	-844.40589	0.221621	-844.184269	
TS4COMe-RS	-9235.585289	1.283065	-9234.302224	-343.34
TS4COMe-SS	-9235.5928	1.280336	-9234.312464	-313.86
TS4COMe-RR	-9235.593039	1.288441	-9234.304598	-329.00
TS4COMe-SR	-9235.599372	1.281806	-9234.317566	-250.10

Part 9. Cartesian coordinates of stationary points

R1

C	-0.93657900	-0.58545300	-0.00000400
C	-1.98451700	0.25444000	-0.00000200
H	-1.15135900	-1.65527000	-0.00000800
H	-1.88818500	1.33627000	0.00000200
C	-3.34478600	-0.29083300	-0.00000500
H	-3.40470700	-1.39904100	-0.00000900
O	-4.35301100	0.38681000	0.00000900
C	0.48680000	-0.23880900	-0.00000200
C	1.43024800	-1.27477900	0.00000100
C	0.94118500	1.08885500	-0.00000300
C	2.79315400	-0.99661400	0.00000300
H	1.08610200	-2.30537200	0.00000200
C	2.30130100	1.36617400	-0.00000100
H	0.22907300	1.90769200	-0.00000600
C	3.23121600	0.32501600	0.00000300
H	3.51117500	-1.80982100	0.00000600
H	2.64042200	2.39669900	-0.00000200
H	4.29342900	0.54636700	0.00000400

R2

C	-2.26604300	1.41108000	0.00732300
C	-1.00086900	1.90026400	0.00719100
H	-3.05249100	2.16493600	-0.03011800
C	-0.86158500	3.38000400	-0.01844000
H	-1.82581500	3.92535000	-0.03447900
O	0.19534500	3.96829200	-0.02103100
C	-2.75562900	0.03714900	0.03329800
C	-4.12925600	-0.16369100	-0.18471600
C	-1.94139500	-1.08289100	0.27344800
C	-4.67325400	-1.44151900	-0.18463800
H	-4.76852100	0.69692900	-0.36088900
C	-2.49037900	-2.35894000	0.28032000
H	-0.88462900	-0.95009500	0.46714200
C	-3.85291300	-2.54409500	0.04701900
H	-5.73493200	-1.57763800	-0.36071400
H	-1.85185400	-3.21509200	0.47180500
H	-4.27409400	-3.54409200	0.05160100
C	0.21137000	1.15201000	0.00652500
C	1.28160800	0.58180700	-0.00763800
C	2.52784200	-0.12219700	-0.02368600
C	2.54858800	-1.51555500	-0.18899200
C	3.73533500	0.57623800	0.12616000

C	3.76014200	-2.19568900	-0.20193000
H	1.61266600	-2.05150300	-0.30983600
C	4.94203900	-0.11270800	0.11155800
H	3.71251500	1.65327500	0.25263700
C	4.95751100	-1.49727200	-0.05169200
H	3.77081600	-3.27287400	-0.33040000
H	5.87309300	0.43190000	0.22767200
H	5.90181300	-2.03139800	-0.06284500

NHC

C	-3.59970900	-1.35176900	-0.20486400
C	-2.37712800	-0.77681100	-0.54945400
C	-2.17209900	0.59352100	-0.50869000
C	-3.24301000	1.38377100	-0.10329600
C	-4.47716500	0.83924900	0.24200300
C	-4.65887100	-0.54346600	0.18918100
C	-3.52276300	-2.85648900	-0.32901400
C	-2.01326300	-3.12721700	-0.31132000
C	-1.39503400	-1.85650600	-0.94982400
H	-1.21128600	1.02304600	-0.77215100
H	-5.28439300	1.48993300	0.55806600
H	-5.61561500	-0.97285900	0.46931600
H	-4.01776000	-3.39282200	0.48357300
H	-1.72082200	-4.04136600	-0.84383800
H	-1.36060000	-1.96128800	-2.03924600
H	-3.95691400	-3.19467200	-1.27616900
Br	-3.00298800	3.26519100	-0.00834700
O	-1.63301900	-3.22037300	1.05389400
C	-0.24653800	-3.43982800	1.21924500
H	-0.03956600	-3.47819100	2.28909100
H	0.05135700	-4.39690600	0.76708900
N	-0.04125300	-1.62958300	-0.47202200
C	0.81052800	-0.65041000	-0.91787600
C	0.50786500	-2.31680000	0.57940700
N	1.68698600	-1.85667800	0.85856700
N	1.84327400	-0.84501500	-0.07138300
C	3.04370200	-0.06785000	-0.03928100
C	2.96882900	1.27805000	0.33338400
C	4.25429800	-0.68683100	-0.36818800
C	4.15713600	2.00895100	0.36499100
C	5.41492800	0.08326600	-0.31732600
C	5.38544700	1.43145100	0.04349500
H	4.12037100	3.05583800	0.65688800
H	6.36501000	-0.38142000	-0.57043900

C	6.65009600	2.25141600	0.05865800
H	7.51463700	1.63985100	0.32701400
H	6.84429700	2.68143900	-0.92933900
H	6.57658100	3.07755000	0.76946800
C	4.29675900	-2.13727400	-0.77024500
H	4.10813900	-2.78756300	0.08825500
H	3.52564300	-2.35665600	-1.51490900
H	5.27140100	-2.38967500	-1.19140400
C	1.65504500	1.92641300	0.68445900
H	1.06631000	2.12280800	-0.21642800
H	1.05097500	1.28028800	1.32781900
H	1.82357900	2.87386000	1.19952400
Et ₃ N			
N	-0.08833500	-0.01272400	-0.39270600
C	0.45709800	-1.04744400	0.49350000
C	1.68280500	-1.73156700	-0.10622000
H	-0.31204700	-1.80659100	0.67858200
H	0.70381500	-0.62397400	1.47941000
H	2.06563600	-2.50737900	0.56387800
H	1.42002500	-2.19682500	-1.06018300
H	2.48339900	-1.01216900	-0.29480900
C	0.19486700	1.34404400	0.06078900
C	1.68318800	1.66970000	0.03625600
H	-0.19410300	1.52981300	1.07903800
H	-0.33533700	2.03160600	-0.60917800
H	1.84659900	2.71816800	0.29910100
H	2.23772500	1.05814100	0.75409300
H	2.09651700	1.48784100	-0.95952800
C	-1.49970900	-0.21226600	-0.71459600
C	-2.48607500	-0.01316300	0.44076300
H	-1.60508600	-1.22683500	-1.11528000
H	-1.75634800	0.47358400	-1.53102500
H	-3.50333300	-0.25268300	0.11924000
H	-2.23991400	-0.66092200	1.28816800
H	-2.48224700	1.02146900	0.79449300
NHCH-BF ₄			
C	3.28138200	1.86075200	-0.85548700
C	2.17384100	1.02003700	-0.98196900
C	2.28573900	-0.35808100	-0.92348900
C	3.56050000	-0.87989500	-0.72664400
C	4.68526500	-0.06940100	-0.61517000
C	4.54588200	1.31764200	-0.67969800

C	2.85781300	3.31119300	-0.91740100
C	1.36081700	3.23300900	-0.60174000
C	0.94793900	1.87311500	-1.21709900
H	1.42134700	-1.01065900	-0.94672000
H	5.65876300	-0.51894900	-0.45743600
H	5.41705100	1.95553000	-0.57053300
H	3.36772100	3.94829600	-0.19209800
H	0.76577500	4.06584400	-0.99751900
H	0.74237900	1.98801200	-2.28643200
H	3.01346600	3.73220900	-1.91658600
Br	3.75726500	-2.75563200	-0.57485200
O	1.25895300	3.16207200	0.80793900
C	-0.04760700	3.00943200	1.30598200
H	0.03244000	2.77104100	2.36510600
H	-0.63286600	3.93062200	1.17405300
N	-0.29110200	1.41494400	-0.58761100
C	-1.20166800	0.54655300	-1.03467800
C	-0.76188900	1.89702700	0.60102200
N	-1.92003700	1.37196500	0.88822900
N	-2.18159300	0.53051800	-0.14804100
C	-3.46840500	-0.11190400	-0.26503400
C	-3.55681000	-1.50593900	-0.27672600
C	-4.58471100	0.72981200	-0.37755700
C	-4.83540800	-2.05644600	-0.39131200
C	-5.83204800	0.12337600	-0.48594400
C	-5.97804400	-1.26609700	-0.48747300
H	-4.93273500	-3.13881500	-0.39836200
H	-6.71296200	0.75333800	-0.57784800
C	-7.34626500	-1.88952700	-0.57166900
H	-7.82659300	-1.88989200	0.41182200
H	-7.99225200	-1.33009400	-1.25240000
H	-7.28948200	-2.92388000	-0.91596100
C	-4.45738700	2.23098800	-0.39865700
H	-4.24306500	2.62215400	0.59888500
H	-3.64558100	2.55502200	-1.05724100
H	-5.38570700	2.67948900	-0.75473900
C	-2.35026400	-2.40093800	-0.18651100
H	-1.87429300	-2.51522500	-1.16715400
H	-1.60067800	-2.00812200	0.50003700
H	-2.65296700	-3.39619200	0.14260400
H	-1.16578800	-0.00914400	-1.95977400
B	0.91706500	-0.68804900	2.05112800
F	0.25112200	-1.11142400	3.19704500
F	1.17999000	0.68788400	2.12503200

F	0.07544100	-0.90690700	0.92444800
F	2.09921500	-1.40066900	1.87730200

PRE-NHC-Et₃N

C	3.66203300	-1.21480900	1.35022300
C	2.41947500	-0.65360100	1.06142300
C	2.28353300	0.48024000	0.28166200
C	3.44774100	1.04567500	-0.22281000
C	4.70498500	0.51677600	0.05159900
C	4.81495500	-0.62443600	0.84864900
C	3.49729500	-2.44260600	2.21792400
C	2.01958700	-2.80846800	2.02572800
C	1.34183000	-1.43912700	1.76233600
H	1.31230100	0.88172700	0.01746700
H	5.58923100	0.98329500	-0.36708100
H	5.79330900	-1.04734400	1.05319200
H	4.13466700	-3.27906600	1.92368300
H	1.57198600	-3.33092300	2.88106700
H	1.06472500	-0.96841800	2.71267700
H	3.69649300	-2.21305400	3.27024600
Br	3.28281000	2.55725800	-1.34803500
O	1.95068000	-3.60785000	0.86134300
C	0.64928300	-4.00468500	0.50085900
H	0.71098600	-4.46672400	-0.48402500
H	0.24001400	-4.72708500	1.22074800
N	0.10651100	-1.63389500	1.00436700
C	-0.89171900	-0.77099600	0.78926300
C	-0.25972700	-2.81673100	0.42554900
N	-1.45636800	-2.73585700	-0.08588400
N	-1.83247500	-1.44844600	0.15627600
C	-3.15047400	-0.95530500	-0.13766100
C	-3.52842500	-0.76010800	-1.46892500
C	-3.98942700	-0.68494100	0.95057900
C	-4.79249600	-0.21106700	-1.68761400
C	-5.24114500	-0.14125100	0.67191400
C	-5.64993400	0.11934400	-0.63740400
H	-5.11175200	-0.03655400	-2.71172600
H	-5.91324800	0.08027000	1.49697400
C	-6.98503300	0.76155100	-0.90723900
H	-7.35718900	0.50014100	-1.89981500
H	-7.72678700	0.45861700	-0.16491500
H	-6.89724700	1.85206900	-0.86151600
C	-3.57745300	-0.99203000	2.36902600
H	-3.13511800	-1.98965300	2.44464500

H	-2.84140100	-0.27630000	2.75018300
H	-4.44553000	-0.95153900	3.02816500
C	-2.62613400	-1.13492700	-2.61105500
H	-1.62042600	-0.73430800	-2.48008800
H	-2.52603100	-2.22267000	-2.67826300
H	-3.04126400	-0.77147700	-3.55241000
H	-0.91950600	0.31019800	1.00943200
B	1.13201300	-1.13426900	-2.31967600
F	0.21295600	-0.35979900	-1.55235800
F	0.48156600	-1.56966600	-3.47226300
F	1.52153400	-2.23236900	-1.53994700
F	2.22693200	-0.33916700	-2.63806800
N	-0.84487000	2.27971100	1.34543200
C	-0.06710700	2.07945000	2.57839600
C	0.17790800	3.31692800	3.44352300
H	0.90052400	1.65091400	2.28700300
H	-0.58875900	1.31803800	3.17606700
H	0.81508000	3.05306000	4.29119900
H	0.68531600	4.10055400	2.87409600
H	-0.75311000	3.72748500	3.84090800
C	-0.16112200	3.19210000	0.40774200
C	-0.35463800	2.84433000	-1.06680700
H	0.91432400	3.13965500	0.61978000
H	-0.46295900	4.23499800	0.59843900
H	0.30028900	3.47731300	-1.67201300
H	-0.09058800	1.80239400	-1.26524300
H	-1.37917100	3.00048500	-1.40449900
C	-2.21923800	2.69128200	1.66330900
C	-3.15986400	2.74594700	0.46554500
H	-2.23012500	3.67339400	2.16401000
H	-2.60751100	1.96552800	2.38920700
H	-4.19099500	2.82722000	0.82030600
H	-2.95806900	3.61406100	-0.16570500
H	-3.08093700	1.84103000	-0.14533700
TS0			
C	3.66086000	-1.08916000	1.45471800
C	2.41141100	-0.55439200	1.14722600
C	2.26583800	0.56096200	0.34735800
C	3.42094200	1.15356800	-0.14249700
C	4.68532200	0.66076700	0.15977800
C	4.80722000	-0.47440300	0.96680700
C	3.49551200	-2.33699800	2.29476600
C	2.03159300	-2.72759900	2.04168700

C	1.32997900	-1.36582400	1.81176500
H	1.29072900	0.91583400	0.04456000
H	5.56603200	1.14224100	-0.24934200
H	5.79191800	-0.87656100	1.18288400
H	4.16188100	-3.15243100	2.00575800
H	1.57285700	-3.29740700	2.86052100
H	1.04589900	-0.92772000	2.77587400
H	3.65239000	-2.12539800	3.35819800
Br	3.21278900	2.63947000	-1.29678900
O	2.01509600	-3.47708000	0.84268000
C	0.72568600	-3.87216500	0.43157300
H	0.82087500	-4.30431600	-0.56328100
H	0.30661400	-4.61787600	1.12238600
N	0.11293700	-1.53287100	1.02953500
C	-0.88773100	-0.63937200	0.83910700
C	-0.19199600	-2.68964600	0.36759600
N	-1.36035300	-2.60251700	-0.19709400
N	-1.76426500	-1.33133600	0.10832400
C	-3.09199400	-0.89057200	-0.21034800
C	-3.41548500	-0.54924600	-1.52604500
C	-4.01857300	-0.83734200	0.84016900
C	-4.70466900	-0.06172900	-1.75678200
C	-5.28950800	-0.34427000	0.55552100
C	-5.64229200	0.06663400	-0.73266900
H	-4.97814800	0.22460100	-2.76923500
H	-6.02430600	-0.28767900	1.35489900
C	-7.00498600	0.64967900	-1.00107800
H	-7.27871400	0.54987900	-2.05328800
H	-7.77040400	0.16062000	-0.39405800
H	-7.01924500	1.71614300	-0.75269000
C	-3.67092000	-1.34479000	2.21760500
H	-2.89878400	-0.73982500	2.70233600
H	-4.55486200	-1.34323900	2.85685300
H	-3.28496900	-2.36755900	2.16298800
C	-2.43860900	-0.73135800	-2.65424500
H	-1.42514000	-0.44183700	-2.37583000
H	-2.39070400	-1.78731900	-2.94046800
H	-2.75719200	-0.15913200	-3.52757300
H	-0.97918300	0.76490400	1.08695900
B	1.36401600	-1.17728100	-2.39863900
F	0.46456600	-0.46890200	-1.55555900
F	0.73795200	-1.39033900	-3.62651700
F	1.65833800	-2.40091600	-1.78588800
F	2.51943700	-0.41630200	-2.56128900

N	-1.01713500	2.00815700	1.44136300
C	-0.19041800	1.91230700	2.67567000
C	0.05420900	3.22019100	3.41661500
H	0.76849500	1.47916900	2.36983600
H	-0.68739800	1.18487500	3.32808100
H	0.70921200	3.02177300	4.26752400
H	0.55175000	3.95412800	2.77857400
H	-0.86632300	3.66009200	3.80428700
C	-0.41097300	2.93728800	0.44273900
C	-0.61683000	2.51373800	-1.00769000
H	0.66516500	2.96890200	0.64333100
H	-0.79502300	3.94821800	0.62292400
H	-0.01489800	3.16780800	-1.64395400
H	-0.27912800	1.48905300	-1.18345600
H	-1.65599200	2.59174100	-1.32757100
C	-2.42853800	2.32321700	1.79436400
C	-3.35242800	2.58985100	0.61742800
H	-2.43789700	3.18920000	2.46424200
H	-2.79555200	1.46262900	2.36490100
H	-4.36979500	2.69475500	1.00251400
H	-3.09444500	3.51789900	0.10221500
H	-3.35083700	1.76752600	-0.10099900

NHC-Et₃NH⁺·BF₄⁻

C	-3.67466200	-1.08632600	-1.45343100
C	-2.41686900	-0.57028200	-1.14701000
C	-2.25526000	0.54014900	-0.34232400
C	-3.40258700	1.14793800	0.14843800
C	-4.67441000	0.67479600	-0.15437000
C	-4.81225100	-0.45743600	-0.96288100
C	-3.52874200	-2.33291000	-2.29949800
C	-2.06732300	-2.74108200	-2.05844600
C	-1.34806100	-1.39107700	-1.82198700
H	-1.27294600	0.87302500	-0.03634500
H	-5.54783100	1.16905500	0.25509800
H	-5.80267300	-0.84545600	-1.17910300
H	-4.20350200	-3.14117100	-2.00946500
H	-1.62074100	-3.30922000	-2.88558100
H	-1.07110500	-0.94490000	-2.78496000
H	-3.69081300	-2.11478200	-3.36095900
Br	-3.17917000	2.63587000	1.29939500
O	-2.05243900	-3.50252000	-0.86669400
C	-0.76462900	-3.90666900	-0.45491400
H	-0.86616100	-4.33537000	0.54100700

H	-0.35701300	-4.66230700	-1.14214300
N	-0.12784900	-1.57512900	-1.05744800
C	0.88191800	-0.67715100	-0.89446900
C	0.16891400	-2.73584400	-0.39875700
N	1.34437500	-2.66310200	0.15030300
N	1.75470900	-1.39115500	-0.16965600
C	3.08124700	-0.95464800	0.14906700
C	3.42951700	-0.68886200	1.47706200
C	3.98853200	-0.81258300	-0.91080800
C	4.71574600	-0.19704500	1.71552900
C	5.25780000	-0.31726700	-0.61905000
C	5.63208300	0.01252300	0.68566300
H	5.00389500	0.02853400	2.73941200
H	5.97463500	-0.19547500	-1.42768100
C	6.99153500	0.59778400	0.96707800
H	7.29796600	0.41041900	1.99826500
H	7.74782900	0.18009700	0.29838000
H	6.98065200	1.68244700	0.81566300
C	3.62374400	-1.22393400	-2.31552100
H	2.85016800	-0.58135000	-2.74587500
H	4.50199000	-1.18817600	-2.96201500
H	3.22595000	-2.24350200	-2.32571300
C	2.47472300	-0.94516200	2.61014600
H	1.46079400	-0.62212300	2.37346400
H	2.41646700	-2.01837300	2.81853900
H	2.81882500	-0.44251800	3.51625600
H	1.00812800	1.08682200	-1.04651500
B	-1.33856600	-1.18434900	2.37721000
F	-0.42046000	-0.47391200	1.55825300
F	-0.69856800	-1.50925200	3.57429300
F	-1.71660200	-2.34861100	1.70052500
F	-2.44491700	-0.37081400	2.61781000
N	1.02283600	2.13429400	-1.36139100
C	0.20021800	2.06586300	-2.61422500
C	-0.03940200	3.40328100	-3.29379100
H	-0.74957500	1.60924000	-2.31944000
H	0.71437200	1.36460300	-3.27799800
H	-0.68493100	3.23531200	-4.15796800
H	-0.54828900	4.10759900	-2.63228500
H	0.88279400	3.86094400	-3.65562500
C	0.38893800	3.01400700	-0.32055500
C	0.59341800	2.52391300	1.10688200
H	-0.68376600	3.03294900	-0.53599400
H	0.77029500	4.02867800	-0.46774100

H	-0.05897500	3.11089400	1.75777000
H	0.30585700	1.47513800	1.22131800
H	1.61882400	2.64429700	1.45438200
C	2.44808300	2.46772200	-1.68048900
C	3.35302800	2.62274200	-0.47122700
H	2.44738300	3.38501300	-2.27333900
H	2.80308800	1.65058700	-2.31535800
H	4.37928200	2.72231900	-0.83256000
H	3.11299700	3.51940400	0.10374700
H	3.31433500	1.74809800	0.18277600
R2C			
C	4.52701800	0.36627900	-1.46959100
C	3.14921100	0.39709900	-1.25445200
C	2.50072600	-0.59265300	-0.52244400
C	3.28339700	-1.64429100	-0.05419000
C	4.66088400	-1.69793100	-0.25554600
C	5.29169600	-0.67604500	-0.95933800
C	4.97503800	1.53551700	-2.31335100
C	3.76993000	2.48137000	-2.30116600
C	2.56462400	1.54009900	-2.05389800
H	1.44005100	-0.56945900	-0.27894800
H	5.22945900	-2.53190300	0.13905400
H	6.36597300	-0.70355000	-1.11062000
H	5.85660800	2.04572200	-1.91886000
H	3.65131000	3.04820200	-3.23342000
H	2.17431800	1.16524700	-3.00437400
H	5.19629100	1.21658500	-3.33722300
Br	2.44092700	-3.07919900	0.85069200
O	3.92618400	3.37086500	-1.21211800
C	2.87653800	4.30876700	-1.13399900
H	3.04441300	4.93003200	-0.25836500
H	2.83371300	4.92811900	-2.04107800
N	1.47864700	2.28210700	-1.41499100
C	0.23908500	1.87948700	-1.12808600
C	1.58478400	3.57097500	-0.96930800
N	0.45488300	3.98630400	-0.47258300
N	-0.37276200	2.91182500	-0.57509300
C	-1.75329900	2.99894900	-0.18891600
C	-2.04584500	3.38057400	1.12575000
C	-2.73174600	2.74704200	-1.15749300
C	-3.39331900	3.50586100	1.45816400
C	-4.06184300	2.89065900	-0.76380100
C	-4.41056900	3.26591200	0.53221200

H	-3.65200600	3.79288500	2.47481200
H	-4.84368100	2.70546900	-1.49420700
C	-5.85455000	3.41063200	0.93456200
H	-6.03418100	4.38336100	1.40051900
H	-6.51634100	3.31025400	0.07188100
H	-6.13088400	2.64146700	1.66272300
C	-2.39473300	2.36655300	-2.57792400
H	-1.60276000	3.00197800	-2.98633200
H	-2.06052200	1.32572700	-2.66079600
H	-3.27903600	2.47649100	-3.20779800
C	-0.96524600	3.62717200	2.14358500
H	-0.14741100	2.90795600	2.05977600
H	-0.52593100	4.62037900	2.01102200
H	-1.38157200	3.56914700	3.15139700
H	-0.20071700	0.91523600	-1.34635400
B	2.56191100	2.51695500	2.15474700
F	1.70627500	1.85461600	1.23654800
F	1.83627300	2.79024000	3.32052000
F	2.98742100	3.72228100	1.57835600
F	3.65415000	1.70440900	2.43488600
N	-0.25393900	-1.36784400	1.93865400
C	-1.03855400	-2.54684900	1.59758100
C	-2.09559200	-3.05394400	2.58927900
H	-0.32326200	-3.36236500	1.42188700
H	-1.51687100	-2.35253400	0.63207300
H	-2.46607100	-4.02564000	2.24710000
H	-1.67590500	-3.19083600	3.59020300
H	-2.95593800	-2.38457900	2.67133000
C	0.47159600	-1.51232500	3.19430400
C	1.60327900	-0.50559500	3.33024400
H	0.88833500	-2.52689800	3.20362300
H	-0.19379500	-1.44423400	4.07348800
H	2.19453800	-0.72486700	4.22445200
H	2.25985600	-0.54743500	2.45760500
H	1.24357600	0.52254800	3.41319400
C	-0.92603600	-0.08128000	1.77352800
C	-1.86232700	0.36133900	2.90648300
H	-1.48358900	-0.13005300	0.82758000
H	-0.15353400	0.68598400	1.63838900
H	-2.42201300	1.25033600	2.60391600
H	-2.58525200	-0.41397600	3.17276800
H	-1.29508400	0.61299300	3.80820900
C	0.24969200	-3.41649700	-1.83208300
C	-0.23330600	-2.19488100	-2.18029600

H	1.28716800	-3.60165300	-2.11191800
C	0.67119700	-1.31459800	-2.94396300
H	1.64473200	-1.76081200	-3.21715100
O	0.39162400	-0.17223900	-3.26177900
C	-0.39602500	-4.51921800	-1.13227000
C	0.43038800	-5.53005800	-0.61346500
C	-1.78551200	-4.61750800	-0.95105300
C	-0.10996100	-6.58498500	0.11024200
H	1.50496100	-5.45989800	-0.75509500
C	-2.32316000	-5.68430300	-0.24234800
H	-2.44145500	-3.86199000	-1.36668000
C	-1.48884700	-6.66215400	0.30003600
H	0.54085000	-7.34960300	0.52035300
H	-3.39776100	-5.75237800	-0.10925400
H	-1.91407600	-7.48679300	0.86260400
C	-1.51576300	-1.65092300	-1.86402000
C	-2.58348900	-1.14014000	-1.59467800
C	-3.87151800	-0.62144000	-1.23362200
C	-4.24425300	-0.55507400	0.11741700
C	-4.77625000	-0.21714300	-2.22594200
C	-5.50552100	-0.08850100	0.46647400
H	-3.54288200	-0.87577900	0.88133100
C	-6.04107000	0.23567200	-1.86704200
H	-4.48288500	-0.27428500	-3.26912000
C	-6.40679500	0.30248700	-0.52298500
H	-5.78734000	-0.03826200	1.51341600
H	-6.74238100	0.53811800	-2.63774700
H	-7.39406500	0.65840800	-0.24637400

R2C'

C	2.31327200	-3.53966700	-1.11632700
C	1.72901200	-2.31008700	-0.79586900
C	0.78896900	-2.19530900	0.21848600
C	0.47992100	-3.35761900	0.91970300
C	1.07618900	-4.58327300	0.64624200
C	2.00079900	-4.67939300	-0.39106100
C	3.25045200	-3.39859300	-2.29073600
C	3.56949400	-1.90596500	-2.26802900
C	2.24493700	-1.27030500	-1.77607700
H	0.30543400	-1.25947700	0.48341400
H	0.80700800	-5.45498700	1.23165100
H	2.46716200	-5.63197400	-0.62173300
H	4.16297600	-3.99205800	-2.20752800
H	3.90134200	-1.48974200	-3.22767400

H	1.54637200	-1.14290600	-2.61063000
H	2.74289900	-3.66357200	-3.22616800
Br	-0.86558200	-3.29633100	2.25182700
O	4.56613200	-1.73959300	-1.27391800
C	4.97732200	-0.40862000	-1.08017100
H	5.60552800	-0.38045600	-0.19215400
H	5.53756000	-0.03669900	-1.94983300
N	2.53916300	0.06627100	-1.24916700
C	1.72198100	1.10645300	-1.05547300
C	3.78872100	0.47506200	-0.86991200
N	3.77368700	1.71541800	-0.47195000
N	2.47274500	2.09178400	-0.59037800
C	2.08241700	3.45844900	-0.34986000
C	1.96837900	3.91036700	0.96597100
C	1.89484200	4.27904900	-1.46786400
C	1.58147200	5.24054600	1.14266600
C	1.51187800	5.59611500	-1.23272300
C	1.33686100	6.08838000	0.06339700
H	1.47186400	5.61821800	2.15612200
H	1.35504100	6.25630000	-2.08187900
C	0.88220600	7.50704000	0.28672900
H	1.21370300	7.88032300	1.25781100
H	1.26543200	8.17110800	-0.49127400
H	-0.21067900	7.56695800	0.26298600
C	2.11211500	3.76431900	-2.86548200
H	3.05565100	3.21541900	-2.94305200
H	1.29902900	3.09556000	-3.16061000
H	2.14162900	4.59460900	-3.57253300
C	2.27528400	3.02959100	2.14440600
H	2.03054500	1.98283200	1.96370100
H	3.34617300	3.06078200	2.37139300
H	1.73605500	3.37910200	3.02791400
H	0.66349200	1.17033000	-1.28494200
B	3.08570200	-0.58838300	2.32147300
F	2.15418200	-0.02112300	1.41026100
F	3.25035600	0.28880100	3.39265800
F	4.30236100	-0.75831600	1.64275600
F	2.60038000	-1.81759500	2.75734100
N	-1.67912600	0.04714900	1.87123400
C	-3.09069100	0.10002400	1.50558600
C	-3.91295600	-1.07723900	2.01778300
H	-3.13382100	0.09916500	0.41215700
H	-3.57545100	1.03858100	1.84025900
H	-4.88979900	-1.07609500	1.52421500

H	-3.40360600	-2.01949400	1.79676700
H	-4.08488400	-1.02716400	3.09611200
C	-1.48277800	0.01204900	3.31780200
C	-0.01692600	-0.02660400	3.72717200
H	-1.96268900	-0.90036100	3.68775900
H	-1.99490100	0.85966500	3.81499100
H	0.05485400	-0.18700200	4.80690800
H	0.50734100	-0.84092000	3.22073100
H	0.51252000	0.90179800	3.49588600
C	-0.91530200	1.09802200	1.19977400
C	-1.22721900	2.54428300	1.60016400
H	-1.10081900	0.97632400	0.12566100
H	0.14865500	0.89557600	1.36023000
H	-0.61891100	3.23266900	1.00450000
H	-2.27996300	2.79611300	1.43354900
H	-0.99726400	2.72598000	2.65548500
C	-4.10807000	2.25800000	-1.11139900
C	-2.89622700	1.92728100	-1.62618900
H	-4.22203300	3.30326300	-0.82285900
C	-1.87094500	2.99099500	-1.66437000
H	-2.23321900	4.00788600	-1.42563200
O	-0.69887600	2.78489300	-1.90745300
C	-5.26169500	1.41702400	-0.81525400
C	-6.24376600	1.95012100	0.03643700
C	-5.42691300	0.10903200	-1.30393700
C	-7.34617100	1.19414100	0.41355200
H	-6.12610800	2.96279600	0.41185800
C	-6.53904500	-0.63809500	-0.93634200
H	-4.69205700	-0.31631400	-1.97616900
C	-7.49553100	-0.10349100	-0.07262100
H	-8.08910100	1.61646900	1.08141200
H	-6.65953300	-1.64428500	-1.32354300
H	-8.35746600	-0.69593600	0.21610000
C	-2.45681000	0.62186600	-1.99575600
C	-2.00292000	-0.47638900	-2.23890200
C	-1.54113400	-1.81835600	-2.42690500
C	-0.78908700	-2.17918200	-3.55474000
C	-1.83510300	-2.77763000	-1.44671100
C	-0.33090700	-3.48491200	-3.68948700
H	-0.57319700	-1.43393500	-4.31381000
C	-1.38244300	-4.08241800	-1.59650700
H	-2.38576300	-2.48000300	-0.55793300
C	-0.62537700	-4.43617200	-2.71155200
H	0.25115700	-3.76390000	-4.56199700

H	-1.59286400	-4.81105300	-0.82011300
H	-0.25830700	-5.45198200	-2.81682400
TS1			
C	4.55725900	0.37670700	0.14214100
C	3.20891200	0.14857800	0.40257700
C	2.24923700	1.12722100	0.22210000
C	2.67700100	2.36808800	-0.22998400
C	4.01885200	2.63680100	-0.48648300
C	4.96916900	1.62974200	-0.29879000
C	5.35064300	-0.88521900	0.40211900
C	4.27734600	-1.98461000	0.37493000
C	2.99868700	-1.26695800	0.87664200
H	1.20143400	0.92829900	0.40197900
H	4.31794400	3.61685300	-0.83985200
H	6.01388500	1.83112400	-0.51355300
H	6.12075400	-1.08671000	-0.34573400
H	4.52834500	-2.86176000	0.98407700
H	2.89871200	-1.29807700	1.96481600
H	5.82982200	-0.85147700	1.38633500
Br	1.35998200	3.70982800	-0.50591900
O	4.12597500	-2.36932200	-0.98557800
C	3.12631600	-3.34977200	-1.16978300
H	3.08079500	-3.59026900	-2.23208400
H	3.36452900	-4.26383000	-0.60767200
N	1.79491300	-1.86950400	0.30460500
C	0.51270500	-1.50019800	0.53735000
C	1.81553200	-2.79413000	-0.70782100
N	0.61249800	-3.05033400	-1.12861200
N	-0.17030000	-2.24044200	-0.33809000
C	-1.58659800	-2.15042000	-0.54195300
C	-2.41352000	-3.08949700	0.07370400
C	-2.07504700	-1.07685000	-1.29363900
C	-3.79241700	-2.91889700	-0.06353300
C	-3.45686900	-0.95149900	-1.40583700
C	-4.32780500	-1.85510400	-0.79140100
H	-4.46079700	-3.62930900	0.41630900
H	-3.86546500	-0.10905500	-1.95956900
C	-5.81709500	-1.67078200	-0.92185600
H	-6.09105800	-0.62734200	-0.73895900
H	-6.15386400	-1.92579000	-1.93142000
H	-6.35974000	-2.30182800	-0.21514700
C	-1.14430800	-0.05864500	-1.89393500
H	-0.76424900	0.61269400	-1.11329600

H	-0.28199900	-0.53217200	-2.37173300
H	-1.66673200	0.54916900	-2.63448800
C	-1.82689300	-4.22267400	0.87279700
H	-1.16555800	-4.83585800	0.25401200
H	-1.22923200	-3.84457600	1.70896400
H	-2.61579100	-4.85918700	1.27585300
C	-2.18870200	0.39120600	1.47645200
C	-0.87860400	0.52159700	1.70256900
H	-2.65649800	-0.57708800	1.67010100
H	-0.37250200	1.47916800	1.57942700
C	-0.01449300	-0.60963200	2.19537200
H	-0.64539600	-1.48998300	2.46743400
O	1.03135700	-0.35530300	2.84362600
C	-3.08843800	1.42456100	0.93994600
C	-4.47363500	1.22635100	1.01617800
C	-2.61260100	2.58238200	0.30775300
C	-5.36151100	2.16139300	0.49420700
H	-4.85049300	0.32078800	1.48596900
C	-3.50007500	3.51716300	-0.21488600
H	-1.54309400	2.74739900	0.20484200
C	-4.87640800	3.31245300	-0.12396200
H	-6.43116300	1.99029500	0.56686500
H	-3.11540500	4.40580400	-0.70534900
H	-5.56484200	4.04158000	-0.53849900
MI			
C	-4.46021500	-1.67798600	-0.36084200
C	-3.26361700	-0.96521300	-0.43405800
C	-3.24136000	0.40744700	-0.62842500
C	-4.46958800	1.05578200	-0.70166800
C	-5.68032500	0.37264500	-0.61754600
C	-5.67611000	-1.01252500	-0.45685600
C	-4.18163500	-3.15403300	-0.19660000
C	-2.75310100	-3.15941000	0.35223000
C	-2.09856700	-1.92542100	-0.31893000
H	-2.30266700	0.92957700	-0.77223800
H	-6.61431600	0.91897300	-0.68139100
H	-6.61506700	-1.55381000	-0.39805500
H	-4.85878500	-3.66222300	0.49311800
H	-2.19751200	-4.08614900	0.16225300
H	-1.68078100	-2.13541900	-1.30401900
H	-4.22101200	-3.66940700	-1.16217600
Br	-4.49332900	2.94110200	-0.93781200
O	-2.88476100	-2.94542100	1.75338200

C	-1.65011200	-2.89640900	2.42344000
H	-1.84043500	-2.67425000	3.47391800
H	-1.12199700	-3.85854000	2.35564500
N	-0.98340200	-1.43916000	0.51585000
C	-0.01813500	-0.54482600	0.22174000
C	-0.79484200	-1.82812900	1.81865600
N	0.21662800	-1.21384400	2.35635400
N	0.68375800	-0.41743000	1.34903800
C	1.80729300	0.45123100	1.55742500
C	1.56935500	1.81822500	1.70110600
C	3.08675800	-0.11438300	1.56906200
C	2.68577700	2.64902000	1.82114500
C	4.16397900	0.75551200	1.69901800
C	3.98309200	2.13752000	1.81354500
H	2.53320700	3.72003800	1.92545200
H	5.17189300	0.34802400	1.68514500
C	5.17761100	3.04600800	1.94476000
H	5.59663900	2.99031600	2.95427000
H	5.96727400	2.75282200	1.24727100
H	4.90958600	4.08574300	1.74810100
C	3.28210500	-1.59493700	1.39593900
H	2.82820300	-2.15325600	2.21957200
H	2.81387600	-1.93187500	0.46435100
H	4.34512100	-1.83692900	1.35059300
C	0.16969500	2.37573300	1.72575400
H	-0.27211700	2.39656600	0.72355400
H	-0.48451900	1.77306200	2.36206100
H	0.17559600	3.39758200	2.10752000
C	2.76069800	0.21100500	-1.52018000
C	1.62994700	-0.49802300	-1.57393000
H	2.69732400	1.24517700	-1.17401500
H	1.60816300	-1.53627500	-1.90593500
C	0.25620300	0.06531200	-1.19838400
H	0.43161600	1.15162000	-0.97085600
O	-0.71475100	-0.22913500	-2.04228700
C	4.12569900	-0.26061900	-1.80721000
C	5.20252200	0.59643900	-1.54339900
C	4.40382600	-1.54407100	-2.29992000
C	6.51580800	0.18829100	-1.75719600
H	4.99796900	1.59203300	-1.15682000
C	5.71443200	-1.95268300	-2.51609500
H	3.58845300	-2.22700100	-2.51863300
C	6.77698200	-1.09010400	-2.24380900
H	7.33423400	0.86879700	-1.54384700

H	5.90968700	-2.94931000	-2.89928100
H	7.79903600	-1.41335000	-2.41225200
TS2			
C	2.74070600	4.37952500	0.81176900
C	1.79089200	3.36716300	0.69274200
C	0.43632300	3.61712100	0.83651400
C	0.04934200	4.93142300	1.06113700
C	0.97094500	5.96747300	1.18231700
C	2.33447700	5.68522700	1.06554500
C	4.12818000	3.80263600	0.63234300
C	3.85894200	2.48646800	-0.11085700
C	2.46689700	2.04668100	0.41302300
H	-0.29783200	2.82857300	0.76125300
H	0.63021000	6.98108500	1.35964400
H	3.05935200	6.48802600	1.15792100
H	4.80395800	4.43654500	0.05400300
H	4.62035900	1.71061600	0.05597700
H	2.54836800	1.47168500	1.33725400
H	4.59403000	3.60095800	1.60325000
Br	-1.81605300	5.28249000	1.19093500
O	3.80731800	2.81930000	-1.49085700
C	3.48907300	1.70217700	-2.29455400
H	3.47193400	2.02103100	-3.33710500
H	4.24393000	0.91325800	-2.17391500
N	1.76288200	1.22789800	-0.57462600
C	0.46678700	0.75656400	-0.49653700
C	2.14029300	1.19769700	-1.89811500
N	1.20704500	0.73933400	-2.66286600
N	0.16649000	0.45786500	-1.80197400
C	-1.10041100	0.08579000	-2.33781800
C	-1.33963000	-1.26223400	-2.61079100
C	-2.07178800	1.07605800	-2.52655800
C	-2.61405800	-1.62240500	-3.05203200
C	-3.32635800	0.67190600	-2.97550300
C	-3.61858500	-0.67078200	-3.22926000
H	-2.82766500	-2.67069500	-3.24744800
H	-4.10715600	1.41916600	-3.10016700
C	-5.00151500	-1.07150900	-3.67261500
H	-5.11616600	-2.15783600	-3.68042900
H	-5.75463200	-0.64853400	-3.00014000
H	-5.21487100	-0.69988100	-4.67949100
C	-1.79705300	2.51348500	-2.17753600
H	-1.96345600	2.68088300	-1.10505600

H	-0.76378500	2.79329100	-2.40029400
H	-2.46669600	3.17779300	-2.72725900
C	-0.27694300	-2.29715700	-2.36228300
H	0.68051500	-2.01679300	-2.81246600
H	-0.11306200	-2.41310900	-1.28282700
H	-0.58041200	-3.26750800	-2.76071800
C	-2.72144500	0.14457600	0.28400900
C	-1.66210300	0.76032200	0.83057200
H	-2.58148000	-0.75656800	-0.31277500
C	-0.19991600	0.45373400	0.74362000
H	-0.05395300	-0.96135000	0.71814200
O	0.47467600	0.72677600	1.87545700
C	-4.11104000	0.61872700	0.37507100
C	-5.13791100	-0.18815800	-0.14001800
C	-4.46489700	1.86957600	0.90658800
C	-6.46889200	0.21256400	-0.09160000
H	-4.87018600	-1.14177500	-0.58894200
C	-5.79671300	2.26880200	0.96091300
H	-3.69309300	2.55180500	1.25271800
C	-6.80727900	1.44335300	0.46919100
H	-7.24131600	-0.43550000	-0.49686300
H	-6.04633900	3.23990000	1.37758200
H	-7.84350900	1.76304100	0.50811700
C	4.79018900	-1.37311300	1.18761000
C	3.45088900	-1.48041600	0.81003800
C	3.07297400	-1.58758000	-0.51994000
C	4.08728700	-1.59050200	-1.47328700
C	5.43180700	-1.48139900	-1.12492900
C	5.78769500	-1.36843100	0.21995500
C	4.90062300	-1.28410600	2.69311500
C	3.54706800	-1.82384400	3.16889000
C	2.57245800	-1.43057800	2.03715500
H	2.02968700	-1.66328500	-0.81643000
H	6.19024300	-1.48748900	-1.89935600
H	6.83458100	-1.29382200	0.49660400
H	5.72079300	-1.87145200	3.11144200
H	3.23304000	-1.43850100	4.14646000
H	2.10561300	-0.43717400	2.16759700
H	5.02389000	-0.24421000	3.01547800
Br	3.61669200	-1.69176200	-3.30590000
O	3.66875500	-3.24263800	3.21997400
C	2.48954800	-3.88752400	3.65055000
H	2.66138800	-4.96334800	3.60082100
H	2.24700700	-3.61626000	4.68765800

N	1.44702100	-2.35468200	2.00744000
C	0.28807800	-2.16573200	1.34386400
C	1.35055600	-3.49431900	2.75803200
N	0.18270100	-4.05007500	2.60553700
N	-0.44913300	-3.20937000	1.72210100
C	-1.83294500	-3.37266400	1.38816000
C	-2.19063600	-4.24421800	0.35738300
C	-2.75399400	-2.59461200	2.09491000
C	-3.53958200	-4.29639100	0.00760100
C	-4.09214900	-2.69657100	1.71850400
C	-4.49799600	-3.52877600	0.67386300
H	-3.84828200	-4.95180200	-0.80363800
H	-4.83128700	-2.08808700	2.23309000
C	-5.94643600	-3.59325700	0.26170800
H	-6.52885000	-2.81212200	0.75535700
H	-6.04945800	-3.46480600	-0.82057400
H	-6.38483000	-4.56223800	0.51902000
C	-2.30995400	-1.69064800	3.21552100
H	-1.87802800	-2.27815400	4.03280500
H	-1.55245200	-0.97144700	2.88375200
H	-3.16097400	-1.12935300	3.60541700
C	-1.16716600	-5.11983300	-0.31582600
H	-0.22235700	-4.59418000	-0.47449400
H	-0.95002800	-5.99542900	0.30421400
H	-1.53604500	-5.47136800	-1.28133200
H	-1.83587200	1.59290500	1.52109000

TS2^N

C	-4.43141400	-1.76298100	-1.47936700
C	-3.34081500	-1.01427900	-1.02874100
C	-3.50778500	0.30075800	-0.62694700
C	-4.79716000	0.81370300	-0.59401800
C	-5.90558000	0.07586800	-0.99509500
C	-5.71264200	-1.22486300	-1.46408200
C	-3.97174900	-3.11421300	-1.97069900
C	-2.64031600	-3.27105900	-1.24192900
C	-2.06192400	-1.83141400	-1.16937700
H	-2.61914600	0.88609300	-0.43367600
H	-6.89748700	0.51160200	-0.95750100
H	-6.56258100	-1.80723100	-1.80625200
H	-4.64820400	-3.93560300	-1.72547200
H	-1.94539900	-3.98443500	-1.70433900
H	-1.55595100	-1.55804100	-2.09795900
H	-3.81724000	-3.10273100	-3.05520500

Br	-5.02255300	2.60937100	0.00172400
O	-2.99080500	-3.69256900	0.07034300
C	-1.87819600	-3.95755300	0.88549300
H	-2.23132000	-3.99553700	1.91860000
H	-1.42209600	-4.92597200	0.63840200
N	-1.03745400	-1.79777100	-0.09932600
C	0.15748400	-1.07736000	-0.09650600
C	-0.84043200	-2.89001800	0.72165100
N	0.34345200	-2.93305200	1.22893100
N	0.97965300	-1.82120200	0.71209100
C	2.39325100	-1.73058000	0.84809800
C	2.92751200	-1.34592700	2.08038000
C	3.20199200	-2.03032400	-0.25633400
C	4.31048400	-1.17345600	2.16800300
C	4.57546400	-1.84660000	-0.12233800
C	5.14471100	-1.39912900	1.07253300
H	4.74189100	-0.85010500	3.11226200
H	5.21873900	-2.04329500	-0.97721400
C	6.63028400	-1.16492500	1.15872100
H	6.93402800	-0.39237700	0.44445200
H	6.92564400	-0.84318500	2.15936600
H	7.18609300	-2.07406300	0.91188500
C	2.60243000	-2.50337200	-1.55181500
H	1.80313400	-3.22930900	-1.37443700
H	2.17179900	-1.66111300	-2.10468700
H	3.36525500	-2.97009300	-2.17756400
C	2.03289200	-1.12686500	3.27028600
H	1.15142200	-0.54371600	2.98940000
H	1.66971200	-2.08103500	3.66355300
H	2.56292200	-0.59933600	4.06607300
C	2.77809200	0.90685300	-0.74390400
C	1.55217100	0.71783500	-1.25672500
H	2.96822900	0.68005000	0.29988000
H	1.35984100	1.01347600	-2.29056900
C	0.26383600	0.26278100	-0.63019600
H	0.19697800	0.96708500	0.62633100
O	-0.81938000	0.71460500	-1.26780500
C	3.96443400	1.37124700	-1.47626400
C	5.13372500	1.64250500	-0.74848200
C	4.00399200	1.54044300	-2.86905800
C	6.29401100	2.07917500	-1.37975500
H	5.11986300	1.50198400	0.33073200
C	5.16151600	1.98111700	-3.50075700
H	3.12528000	1.31360100	-3.46501200

C	6.31326800	2.25334000	-2.76224800
H	7.18355800	2.28385100	-0.79125900
H	5.16836700	2.10461000	-4.57945800
H	7.21604000	2.59131100	-3.26043900
N	-0.36071600	1.77766600	1.56623400
C	0.53869500	2.30429900	2.63255700
C	2.01457200	2.29546400	2.25998700
H	0.39087800	1.69782300	3.53130200
H	0.21728400	3.32201500	2.88407100
H	2.58468600	2.81730600	3.03320600
H	2.39385600	1.27339500	2.19419700
H	2.19744900	2.78360700	1.30091000
C	-1.00562300	2.89225300	0.81802500
C	-0.01615600	3.69659900	-0.00654500
H	-1.51833900	3.54226700	1.53989400
H	-1.74637000	2.45228000	0.15367600
H	-0.56814900	4.42683700	-0.60322500
H	0.69194300	4.24742200	0.61812200
H	0.53071000	3.03847500	-0.68530000
C	-1.37097500	0.83206800	2.11081600
C	-2.48346100	1.46851500	2.93391800
H	-0.82330400	0.09612100	2.70827100
H	-1.78733600	0.29800600	1.25593200
H	-3.06392500	0.67942500	3.41753000
H	-2.08828600	2.12342800	3.71656800
H	-3.16769100	2.04193100	2.30308100

TS2^{NH}

C	-5.51853500	-0.43248200	-0.33136400
C	-4.12578200	-0.37549200	-0.32147100
C	-3.44666700	0.82525500	-0.43425300
C	-4.19704400	1.98452400	-0.59528100
C	-5.58654400	1.95514900	-0.64448800
C	-6.25350000	0.73391900	-0.50522100
C	-5.97306900	-1.85470100	-0.08536200
C	-4.73849100	-2.50127600	0.56217000
C	-3.55912000	-1.76281300	-0.11969200
H	-2.36867800	0.89788300	-0.35127500
H	-6.14515300	2.87579700	-0.76664200
H	-7.33853300	0.71288200	-0.51073300
H	-6.83607900	-1.93153000	0.57907000
H	-4.68030200	-3.58760300	0.42106000
H	-3.31515800	-2.23953500	-1.06967200
H	-6.21554800	-2.36326400	-1.02454800

Br	-3.25288100	3.62413000	-0.71709100
O	-4.79350200	-2.19015400	1.94436300
C	-3.65477800	-2.64643700	2.64300000
H	-3.76676800	-2.37705800	3.69283700
H	-3.55400300	-3.73753700	2.55943000
N	-2.35644600	-1.74729200	0.72431300
C	-1.16304000	-1.11836600	0.49450600
C	-2.44017700	-1.98051000	2.07856300
N	-1.39475500	-1.54700200	2.70339700
N	-0.60911400	-1.00779300	1.71622100
C	0.60483900	-0.33009500	2.06159200
C	1.76969000	-1.08869900	2.20961800
C	0.57062700	1.05832400	2.20517500
C	2.95957500	-0.40119200	2.43066700
C	1.78467600	1.69922800	2.44789300
C	2.98548300	0.99339500	2.53078300
H	3.89665500	-0.94678500	2.47848400
H	1.79528700	2.78341200	2.53459800
C	4.29352500	1.72063700	2.68063000
H	4.78622200	1.80306500	1.70616900
H	4.14072100	2.72534900	3.08176900
H	4.97675000	1.17209800	3.33175100
C	-0.69708500	1.85073800	2.02967800
H	-0.81020300	2.16862700	0.98473700
H	-1.58622600	1.27795700	2.30776500
H	-0.66781500	2.75476000	2.64122300
C	1.72804700	-2.59299800	2.14149400
H	1.39996000	-3.01358900	3.09746000
H	1.02297900	-2.94331500	1.38033900
H	2.71723000	-2.99573000	1.91251700
C	1.27873600	0.91502100	-0.72486600
C	0.04516600	0.50901600	-1.05070600
H	1.98433800	0.22275300	-0.26728300
H	-0.61749400	1.21609400	-1.56469000
C	-0.56061200	-0.83865900	-0.81412600
H	0.41414900	-1.79407200	-1.14910900
O	-1.47090400	-1.18602900	-1.85131800
C	1.79287000	2.28530400	-0.88149100
C	3.17442400	2.48516500	-0.74767800
C	0.96583000	3.39460300	-1.11045000
C	3.71847600	3.75975100	-0.86430100
H	3.81938700	1.63446200	-0.54560400
C	1.51523600	4.66725000	-1.22901000
H	-0.11319400	3.27517500	-1.17496100

C	2.89222300	4.85524600	-1.10878700
H	4.79108900	3.89023400	-0.75755300
H	0.86466200	5.51874500	-1.40275900
H	3.31412200	5.85159600	-1.19399200
N	1.23071700	-2.57710000	-1.82755900
C	0.89573500	-3.97835800	-1.48953900
C	-0.59961500	-4.26491200	-1.52466900
H	1.27588600	-4.15630500	-0.47937300
H	1.43777300	-4.65943000	-2.15566900
H	-0.76679000	-5.30431800	-1.23394400
H	-1.14157200	-3.62370200	-0.82363900
H	-1.02921500	-4.12178100	-2.51794700
C	2.58162300	-2.17246000	-1.34771600
C	3.70568700	-3.19461300	-1.47282900
H	2.47810200	-1.89372400	-0.29475600
H	2.84526600	-1.25382000	-1.87626600
H	4.62898600	-2.68936000	-1.17953100
H	3.55643100	-4.04813100	-0.80623100
H	3.82486900	-3.57276700	-2.48998300
C	0.98142400	-2.21260200	-3.24595600
C	1.97225200	-2.77202700	-4.25863400
H	0.98542200	-1.11789900	-3.27704600
H	-0.03589700	-2.52457200	-3.48373000
H	1.63000200	-2.51131200	-5.26296300
H	2.96956900	-2.34725100	-4.12698500
H	2.04502900	-3.86183400	-4.20607600
H	-1.93857600	-0.39306100	-2.15665500
B	5.69434200	-0.28148200	0.17197400
F	6.03729400	1.05413800	-0.08639600
F	5.95111900	-0.58818700	1.51426000
F	6.41773400	-1.13736100	-0.66212800
F	4.31778100	-0.44947400	-0.09101400

TS2^{NHCH}

C	-0.37550300	5.37551300	-0.67846200
C	0.14941500	4.09322500	-0.52536500
C	1.49501600	3.82889300	-0.71115600
C	2.31390300	4.88844900	-1.08119700
C	1.81621200	6.17523700	-1.26530000
C	0.45676400	6.42169400	-1.05846200
C	-1.85188400	5.37070800	-0.34563800
C	-2.00322600	4.09648700	0.49660900
C	-0.95425200	3.14224900	-0.12291600
H	1.91259700	2.84116900	-0.56661600

H	2.48453800	6.97887200	-1.55202800
H	0.06844800	7.42808200	-1.17803300
H	-2.17941700	6.24487500	0.22066700
H	-3.01225900	3.66099500	0.48484600
H	-1.38047400	2.63629500	-0.99022200
H	-2.46327400	5.29882200	-1.25175900
Br	4.16220900	4.53139700	-1.33024500
O	-1.62814800	4.44274600	1.81984000
C	-1.67000800	3.33705700	2.69348100
H	-1.34260300	3.66652800	3.67986700
H	-2.68711000	2.93146200	2.77346200
N	-0.52283900	2.12593300	0.84176700
C	0.33276100	1.07579100	0.67912500
C	-0.75127400	2.26585000	2.19192800
N	-0.10033700	1.38285600	2.87731400
N	0.56303300	0.63982600	1.93468100
C	1.42958900	-0.42468300	2.35504100
C	0.92466300	-1.72280100	2.39234200
C	2.75507800	-0.10734500	2.67307400
C	1.81615100	-2.74677400	2.72428900
C	3.60047600	-1.15927600	3.00788800
C	3.15153300	-2.48471400	3.02414900
H	1.45198600	-3.77132200	2.73663900
H	4.64381600	-0.94681500	3.22914600
C	4.10853500	-3.60054100	3.35136900
H	5.01694500	-3.51611700	2.74597600
H	4.41144000	-3.56096700	4.40201600
H	3.65609000	-4.57706400	3.16498100
C	3.25749800	1.30546900	2.56248300
H	4.24841100	1.39883000	3.00899000
H	3.33402500	1.59559800	1.50606300
H	2.58310700	2.01272400	3.05271700
C	-0.49491300	-2.02165600	2.01197300
H	-1.20073500	-1.29518700	2.42459400
H	-0.61797300	-2.01557000	0.92382700
H	-0.79193700	-3.01442200	2.35489900
C	2.93841100	-0.84937900	-0.29249200
C	2.26521800	0.23472200	-0.69658300
H	2.39482500	-1.68358100	0.15246600
H	2.79825900	1.03838700	-1.21236400
C	0.79829000	0.48425200	-0.56194700
H	0.00131100	-0.66015500	-0.90599900
O	0.34150600	1.27329900	-1.65869900
C	4.40054900	-1.01115900	-0.34753000

C	4.94687500	-2.24530900	0.03094800
C	5.27712800	0.01870400	-0.71981700
C	6.32028000	-2.46245600	0.01058000
H	4.27104600	-3.03399800	0.35110100
C	6.65089300	-0.19873500	-0.74382900
H	4.89358200	1.00340900	-0.97324700
C	7.17909700	-1.43833200	-0.38417000
H	6.71806700	-3.42859900	0.30745000
H	7.31531500	0.60876900	-1.03430600
H	8.25203400	-1.59904200	-0.39971400
C	-4.56493100	1.25433800	-1.32394200
C	-3.39259000	0.57080300	-0.99730900
C	-3.01865700	0.33486100	0.31289600
C	-3.87590800	0.79165700	1.30816600
C	-5.03436200	1.50602200	1.01861700
C	-5.38011300	1.74839700	-0.31362700
C	-4.75939300	1.26262000	-2.82479100
C	-3.86223300	0.10474300	-3.28515500
C	-2.69900800	0.13601200	-2.26639300
H	-2.14987600	-0.26414400	0.56071700
H	-5.67798200	1.83770000	1.82532800
H	-6.30005100	2.27559100	-0.54506600
H	-5.79353200	1.09227100	-3.13072400
H	-3.51027400	0.19400300	-4.32112100
H	-1.94593100	0.86984200	-2.57262900
H	-4.41883700	2.20392900	-3.27021700
Br	-3.47920400	0.34226900	3.09981500
O	-4.61188800	-1.08238800	-3.10964000
C	-3.91188600	-2.26940200	-3.41313800
H	-4.53422800	-3.10146500	-3.08941000
H	-3.71822700	-2.34361400	-4.49278600
N	-2.04733500	-1.16366800	-2.19524800
C	-0.84606000	-1.46028200	-1.65492600
C	-2.60500300	-2.31442900	-2.68113900
N	-1.80241700	-3.32436300	-2.50460100
N	-0.72833700	-2.77018400	-1.86210300
C	0.45332900	-3.53290200	-1.56988800
C	0.41120100	-4.52583400	-0.58300800
C	1.61442200	-3.22717200	-2.28984600
C	1.61184900	-5.16714100	-0.27625900
C	2.78209200	-3.91114000	-1.95283700
C	2.80293100	-4.87050900	-0.94102000
H	1.60963500	-5.92827100	0.50107500
H	3.69947900	-3.67818300	-2.48780600

C	4.07934000	-5.58675300	-0.58069600
H	4.25635600	-5.55163200	0.49917300
H	4.02920500	-6.64130400	-0.86780000
H	4.93837900	-5.13637300	-1.08329200
C	1.63003200	-2.19917300	-3.39173500
H	0.70591400	-2.21586200	-3.97552800
H	1.76097100	-1.19228100	-2.98016200
H	2.46756700	-2.38736200	-4.06577300
C	-0.87086800	-4.93703700	0.08768300
H	-1.57243400	-4.11177100	0.20376200
H	-1.37133300	-5.70332400	-0.51407900
H	-0.65952600	-5.37167200	1.06792000
H	0.27529800	0.67149500	-2.41589000
B	-4.07278700	-2.87611200	0.43122700
F	-4.02287400	-4.20930200	0.84012800
F	-4.76724000	-2.76722800	-0.78010800
F	-2.74440100	-2.42056800	0.22120600
F	-4.67001600	-2.08648700	1.41218500
M2			
C	-5.78078600	-1.14901500	-0.44438500
C	-4.50318100	-0.60709700	-0.57463600
C	-4.20686900	0.33515600	-1.54755800
C	-5.25894300	0.78041200	-2.33841900
C	-6.55067400	0.27456400	-2.22052700
C	-6.81023700	-0.71817100	-1.27365600
C	-5.78525100	-2.18987300	0.65131000
C	-4.56644600	-1.79811500	1.49429000
C	-3.57028000	-1.18915300	0.46752800
H	-3.18655400	0.66596800	-1.69508800
H	-7.34129800	0.65010800	-2.86003600
H	-7.81147600	-1.12795800	-1.18203800
H	-6.68960700	-2.19414800	1.26394300
H	-4.12007200	-2.63571500	2.04508300
H	-2.93521400	-1.96283300	0.02934700
H	-5.64980500	-3.19359600	0.23251000
Br	-4.89913600	2.14311000	-3.61766900
O	-5.03587900	-0.81984300	2.41311800
C	-3.99722300	-0.27745800	3.19792600
H	-4.42979200	0.44949500	3.88573000
H	-3.48817200	-1.06455900	3.77845900
N	-2.70512400	-0.19948000	1.10201800
C	-1.63416200	0.51971600	0.54570800
C	-2.99425300	0.37442800	2.30821900

N	-2.27577800	1.40654000	2.58173000
N	-1.43048300	1.54825200	1.47821800
C	-0.88755500	2.84235200	1.26832100
C	0.05531500	3.30275900	2.20769100
C	-1.25260700	3.62840900	0.16683600
C	0.63916700	4.54986500	2.01340100
C	-0.61992100	4.86481300	0.00493200
C	0.32874800	5.34125600	0.90480000
H	1.37497000	4.90323400	2.73312100
H	-0.89480600	5.47773000	-0.85090900
C	1.02524400	6.65898400	0.68218200
H	2.03451300	6.50006200	0.28778900
H	0.48171800	7.27820600	-0.03489400
H	1.12356900	7.21873200	1.61612700
C	-2.29695000	3.19795700	-0.82688100
H	-1.86636500	2.53248300	-1.58381200
H	-3.10851600	2.64765800	-0.34191700
H	-2.72009000	4.06875000	-1.33302700
C	0.46221700	2.43571900	3.36791700
H	-0.35445100	2.32204500	4.08686000
H	0.69985700	1.42147600	3.02716600
H	1.33119500	2.85795700	3.87733700
C	1.25755200	1.35842200	-0.19629600
C	0.30594700	0.74777400	-0.97231800
H	1.07610600	1.47942200	0.86586500
C	-0.96530700	0.15526200	-0.62655200
H	2.33906200	-0.49044600	-0.63120900
O	-1.49017600	-0.74714400	-1.43219700
C	2.54508100	1.86228300	-0.65277400
C	3.38086600	2.52903200	0.26799800
C	3.04746600	1.67493400	-1.95965100
C	4.64631400	2.97339300	-0.08917200
H	3.00884600	2.69510200	1.27735500
C	4.31815000	2.11692700	-2.31029400
H	2.43539000	1.18274900	-2.71058700
C	5.12989800	2.76713800	-1.38148700
H	5.26590700	3.47707800	0.64783500
H	4.67944000	1.95015600	-3.32164100
H	6.12447800	3.10190600	-1.65830300
C	-0.94085900	-3.86422900	0.05847900
C	0.00009700	-2.83504900	0.06186200
C	0.19754000	-2.02697500	1.17243700
C	-0.56877800	-2.30918300	2.30116100
C	-1.47922700	-3.35987500	2.34188600

C	-1.67758200	-4.14280000	1.20235400
C	-1.03320700	-4.48320000	-1.31555500
C	0.29677000	-4.08901900	-1.95943100
C	0.62191600	-2.72121800	-1.31132800
H	0.89328200	-1.19207300	1.17589100
H	-2.03592000	-3.55562000	3.25204800
H	-2.40319500	-4.95034000	1.21803200
H	-1.15853400	-5.56799400	-1.31764800
H	0.26788500	-4.03578200	-3.05412900
H	0.13275700	-1.88416900	-1.83352900
H	-1.86096900	-4.03155500	-1.87329600
Br	-0.39560800	-1.18349300	3.81437400
O	1.24515900	-5.06922500	-1.54602800
C	2.53871500	-4.83932800	-2.05017400
H	3.19780000	-5.62039700	-1.67060200
H	2.55203300	-4.86347100	-3.14879500
N	2.08098200	-2.53085700	-1.29035000
C	2.76668700	-1.44262700	-0.93242600
C	3.00600800	-3.49789500	-1.57785300
N	4.21935300	-3.05526000	-1.39803100
N	4.04925500	-1.76497500	-0.99260100
C	5.16784300	-0.94602300	-0.61209000
C	5.21982700	-0.45430500	0.69583500
C	6.15638100	-0.69794400	-1.56923500
C	6.34095600	0.29939600	1.04097500
C	7.25450500	0.05617400	-1.16648900
C	7.36170700	0.56356100	0.12944300
H	6.40966600	0.69740500	2.05020400
H	8.03534600	0.27101700	-1.89157800
C	8.52514500	1.43646400	0.51746700
H	9.41668900	1.19448100	-0.06477500
H	8.28197900	2.48856400	0.33170900
H	8.76202800	1.33485700	1.57875300
C	6.01830800	-1.18457400	-2.98676600
H	6.15029400	-2.26717600	-3.05547300
H	5.02352200	-0.94792800	-3.37910800
H	6.76148700	-0.70237100	-3.62336600
C	4.12204700	-0.69532600	1.70028200
H	3.27244300	-0.02410800	1.51665600
H	3.75377400	-1.72542800	1.67202200
H	4.48587300	-0.49297600	2.70856800
H	0.54196800	0.56535400	-2.02509100

M2^H

C	-4.62819100	0.34005800	-0.74930800
C	-3.23473500	0.27062900	-0.73828500
C	-2.46901500	1.17417800	-0.01849200
C	-3.14392300	2.13791300	0.72305700
C	-4.53189800	2.23570700	0.72480200
C	-5.28271300	1.33045700	-0.02780600
C	-5.19344800	-0.78220900	-1.59005000
C	-4.04510700	-1.79750000	-1.60140300
C	-2.77332800	-0.90995500	-1.56892300
H	-1.38708400	1.13152000	-0.01810900
H	-5.02031700	3.00156100	1.31615700
H	-6.36636400	1.39306200	-0.02219600
H	-6.09962700	-1.23154900	-1.17838200
H	-4.05276800	-2.47483100	-2.46504700
H	-2.51767900	-0.59433600	-2.58256300
H	-5.40925000	-0.44198200	-2.60882500
Br	-2.11454300	3.33149700	1.78221900
O	-4.16859800	-2.54150400	-0.39871800
C	-3.12022700	-3.47069200	-0.22909700
H	-3.27713300	-3.99414000	0.71403600
H	-3.11751100	-4.20402800	-1.04891000
N	-1.64083900	-1.63855700	-1.00283600
C	-0.32542500	-1.20866000	-0.82935400
C	-1.81313900	-2.74618400	-0.20114100
N	-0.75756600	-3.05969500	0.46343800
N	0.18404600	-2.10725200	0.09346800
C	1.36414800	-1.96135200	0.87778300
C	2.40631300	-2.87333200	0.67504400
C	1.46797700	-0.90301900	1.79167000
C	3.58585300	-2.69599600	1.39703900
C	2.67102900	-0.75914500	2.48196700
C	3.74041800	-1.63688100	2.29359900
H	4.40678200	-3.39245900	1.24524500
H	2.77432100	0.06181300	3.18802800
C	5.04005400	-1.42169800	3.02544800
H	5.59431900	-0.58635300	2.58495800
H	4.86476500	-1.17787400	4.07634400
H	5.67470300	-2.30876100	2.97708800
C	0.35114100	0.08594800	1.99382300
H	0.43999400	0.91233900	1.27842400
H	-0.63038700	-0.37507600	1.85034500
H	0.39251300	0.51031100	2.99898500
C	2.25170100	-3.98648500	-0.32574200
H	1.42264000	-4.64561000	-0.05364800

H	2.02584200	-3.58113400	-1.31749200
H	3.16579900	-4.57867900	-0.39112600
C	2.28009600	1.28069800	-1.80118900
C	1.69053200	0.16562400	-1.31214400
H	1.67422500	2.01330200	-2.33014500
C	0.30460900	-0.16297500	-1.45816100
H	-0.13490200	0.66493400	-3.13630900
O	-0.49602500	0.67065700	-2.23858700
C	3.70277800	1.59675900	-1.66319400
C	4.24098600	2.67654600	-2.38217500
C	4.57193800	0.87511200	-0.82311200
C	5.58707100	3.01364400	-2.28474300
H	3.58574000	3.25393900	-3.02941500
C	5.91700400	1.20934400	-0.73041200
H	4.19018300	0.05410700	-0.22074800
C	6.43660600	2.27909200	-1.46086700
H	5.97329100	3.85279100	-2.85539500
H	6.56559600	0.63497700	-0.07542000
H	7.48714600	2.53881500	-1.38221700
H	2.30703400	-0.56749200	-0.80320200

M2^{NH}

C	-5.00080200	0.83559700	-0.66075600
C	-3.67102800	0.46656400	-0.46296800
C	-3.32550400	-0.61458000	0.32630100
C	-4.35461100	-1.33445200	0.92108100
C	-5.69088600	-0.98418900	0.75110500
C	-6.01726200	0.11426000	-0.04672000
C	-5.07578400	2.02930300	-1.58519700
C	-3.72052300	1.98298200	-2.30000000
C	-2.76672500	1.41099300	-1.22065000
H	-2.29441200	-0.89559800	0.48209800
H	-6.46847400	-1.56861400	1.22908500
H	-7.05833300	0.38341100	-0.19303300
H	-5.89054900	1.97848300	-2.31018400
H	-3.38154300	2.95175400	-2.68691800
H	-2.38199700	2.19772900	-0.57163700
H	-5.17471600	2.96203800	-1.01994100
Br	-3.89260000	-2.83381100	1.98761800
O	-3.86446500	1.05151100	-3.36166600
C	-2.68055500	0.88678800	-4.10224900
H	-2.85492700	0.12313900	-4.86057800
H	-2.38828700	1.82175100	-4.60037800
N	-1.60564300	0.75433700	-1.85205200

C	-0.45198300	0.29362000	-1.32172600
C	-1.57328600	0.45316000	-3.19172600
N	-0.47536400	-0.16453600	-3.51168000
N	0.20892100	-0.25504700	-2.33938700
C	1.51186900	-0.86549500	-2.28143600
C	2.62447100	-0.02929500	-2.31677200
C	1.58001100	-2.25374800	-2.12558400
C	3.87022800	-0.62814300	-2.11217100
C	2.84436700	-2.80371800	-1.95626800
C	3.99311300	-2.00337700	-1.92304100
H	4.74442400	0.01318200	-2.06002800
H	2.93526200	-3.87648200	-1.80304800
C	5.33910900	-2.63636500	-1.68583100
H	5.27975300	-3.37808000	-0.88365100
H	5.68976700	-3.15293600	-2.58487900
H	6.08492700	-1.88733900	-1.41315400
C	0.33198500	-3.09013200	-2.06975500
H	-0.26394500	-2.82780000	-1.18669200
H	-0.29650400	-2.93256200	-2.95088900
H	0.58287800	-4.14967700	-2.00469800
C	2.49029000	1.44587200	-2.57784200
H	2.00933200	1.62000100	-3.54572100
H	1.90418900	1.94769000	-1.80333700
H	3.47259500	1.91676500	-2.56947700
C	1.57935400	-1.40924800	0.85828300
C	0.33680100	-0.94054100	0.71165000
H	2.40814000	-0.76709600	0.55389700
H	-0.53006200	-1.51384600	1.03348900
C	0.05805500	0.41982200	0.11134100
H	1.02385600	0.94659400	0.03107000
O	-0.89055900	1.13777200	0.83521200
C	1.95497200	-2.74042500	1.35830100
C	3.31805700	-3.04487500	1.46755700
C	1.01696200	-3.72930100	1.68733100
C	3.73855000	-4.29993100	1.89583900
H	4.04875200	-2.28384100	1.20428900
C	1.43679600	-4.98309600	2.11653800
H	-0.04733400	-3.52585700	1.60571300
C	2.79719100	-5.27400100	2.22114400
H	4.79916000	-4.51681400	1.97425900
H	0.69990600	-5.73939200	2.36693700
H	3.11965100	-6.25563400	2.55256600
N	0.11198800	3.13398300	2.16579100
C	0.77917900	2.71967500	3.40900400

C	1.84370500	1.66142300	3.15549700
H	0.00180900	2.31158000	4.06413200
H	1.21758400	3.58222400	3.93052500
H	2.27763400	1.34379900	4.10742100
H	1.40034000	0.78323900	2.67557800
H	2.65109500	2.02285600	2.51456000
C	-1.15031000	3.85257900	2.40146500
C	-1.05788200	5.24265800	3.02766900
H	-1.76406000	3.20296500	3.03555800
H	-1.66314600	3.92264100	1.43450000
H	-2.06264200	5.60335900	3.26327200
H	-0.48057400	5.22835000	3.95634900
H	-0.59804700	5.96025400	2.34440500
C	1.01126000	3.78973000	1.18801700
C	2.01188100	4.80743100	1.73488800
H	0.36401100	4.25762600	0.43708400
H	1.58478300	3.01234000	0.67692900
H	2.52332800	5.26935400	0.88872200
H	1.54215500	5.58748900	2.33757500
H	2.78310600	4.31255400	2.33008800
H	-0.42904500	1.87272100	1.39944500
B	4.10812700	2.37652400	0.08830800
F	3.52532300	3.47923600	-0.54784300
F	3.12093100	1.36735400	0.24751400
F	4.57797300	2.74248000	1.35059100
F	5.14855400	1.87268000	-0.69809000

M2^{NHCH}

C	3.03631100	3.66101200	0.35726100
C	1.85080300	2.93346500	0.49989800
C	1.71208500	1.97948800	1.49890800
C	2.80138900	1.77202600	2.34088200
C	4.00100200	2.45981400	2.19673800
C	4.11772200	3.41840500	1.19303300
C	2.94744800	4.63772800	-0.78795600
C	1.44908400	4.69088000	-1.07595600
C	0.93110000	3.29251600	-0.65231300
H	0.81103400	1.38839000	1.60185600
H	4.82901400	2.24745600	2.86305400
H	5.04535800	3.96907000	1.07316300
H	3.31826400	5.63521800	-0.54183200
H	1.19914000	4.92754100	-2.11755900
H	1.06776600	2.56438900	-1.45566500
H	3.49657000	4.26389600	-1.65588300

Br	2.66189100	0.49218800	3.73682600
O	0.90848500	5.67562500	-0.20538900
C	-0.45878300	5.89431900	-0.43013400
H	-0.82790700	6.57358000	0.33960300
H	-0.63795400	6.34585500	-1.41590800
N	-0.53123300	3.38690200	-0.40167200
C	-1.48758900	2.43533400	-0.39344600
C	-1.19649900	4.59269000	-0.35662700
N	-2.48622900	4.42878000	-0.32371400
N	-2.64917000	3.07889600	-0.35182200
C	-3.95668800	2.47806200	-0.41324100
C	-4.40859500	2.00311300	-1.64436700
C	-4.68418900	2.36108200	0.77730400
C	-5.64924800	1.35741900	-1.65706000
C	-5.91314400	1.71731600	0.70704200
C	-6.40803800	1.20494200	-0.49871900
H	-6.03211900	0.98128500	-2.60232200
H	-6.49681000	1.59844900	1.61643900
C	-7.74661600	0.51482100	-0.52653700
H	-7.74392800	-0.36724400	0.12304200
H	-8.53197800	1.18135500	-0.15956600
H	-8.01109600	0.19728800	-1.53700700
C	-4.12322700	2.86094900	2.07905200
H	-4.85192400	2.74005100	2.88128200
H	-3.22416200	2.29297500	2.34554000
H	-3.84370300	3.91591700	2.01542700
C	-3.61187900	2.15883800	-2.91401800
H	-3.01541200	3.07420800	-2.91276100
H	-2.93230800	1.31187500	-3.06608100
H	-4.28260500	2.19132000	-3.77411400
C	-3.08760700	-0.39015800	0.77089700
C	-1.96075400	0.32372800	0.81980900
H	-3.59176900	-0.49454900	-0.19327100
H	-1.41125300	0.48495900	1.74605000
C	-1.34996000	0.93188100	-0.42387400
H	-1.94652800	0.58783300	-1.28795500
O	-0.00131100	0.64432000	-0.56195500
C	-3.75306700	-1.05546800	1.89970800
C	-5.07412400	-1.49020100	1.73421000
C	-3.11220000	-1.29721900	3.12202300
C	-5.74628800	-2.14023800	2.76414800
H	-5.56545800	-1.31335100	0.78016500
C	-3.78211300	-1.94811400	4.15171500
H	-2.07708600	-0.99747900	3.25908300

C	-5.10019900	-2.37079400	3.97711200
H	-6.77008500	-2.47009500	2.61927000
H	-3.27234500	-2.13593600	5.09103400
H	-5.61769800	-2.88334200	4.78130800
C	4.53041800	-1.36654800	1.21666700
C	3.28581500	-1.19100200	0.61655900
C	3.08883300	-0.30633600	-0.42857300
C	4.18862300	0.42897900	-0.84188700
C	5.43996600	0.30841400	-0.24698600
C	5.61490200	-0.60629000	0.79349100
C	4.45020500	-2.43925600	2.28165200
C	3.12559400	-3.15453400	1.97027400
C	2.26673200	-2.05493800	1.31132500
H	2.13940800	-0.21632500	-0.94067700
H	6.27087500	0.90482800	-0.60651900
H	6.59467100	-0.72878700	1.24472600
H	5.28464600	-3.14396200	2.26103600
H	2.63967000	-3.58018400	2.85907800
H	1.75423500	-1.47178800	2.08374400
H	4.40006900	-1.98681900	3.27856000
Br	3.94990300	1.60045300	-2.31790000
O	3.39036000	-4.17652400	1.02472500
C	2.23914400	-4.89907700	0.63365200
H	2.53831000	-5.56848100	-0.17043300
H	1.84295700	-5.48129300	1.47851700
N	1.25076800	-2.63603800	0.46102800
C	0.20737800	-1.96836400	-0.07983100
C	1.18295400	-3.95920500	0.13326100
N	0.10771600	-4.20138600	-0.55808900
N	-0.46940900	-2.95672900	-0.67738000
C	-1.78341600	-2.79953700	-1.22650400
C	-1.96558200	-2.02578300	-2.37618500
C	-2.85728700	-3.36233700	-0.52159300
C	-3.27986200	-1.81590900	-2.81077100
C	-4.14189700	-3.15309900	-1.01565800
C	-4.37439900	-2.37302200	-2.15138300
H	-3.44394100	-1.21840500	-3.70503400
H	-4.98558400	-3.58008400	-0.47787200
C	-5.78306300	-2.13860100	-2.63164100
H	-6.38511100	-1.66664000	-1.84738900
H	-5.80134200	-1.49095100	-3.51099200
H	-6.27118700	-3.08208900	-2.89236800
C	-2.63742300	-4.11175500	0.76535100
H	-2.20065900	-5.09759000	0.58548100

H	-1.94770300	-3.56009700	1.41335200
H	-3.58312700	-4.23078200	1.29908900
C	-0.80314700	-1.42898000	-3.12486400
H	-0.40194200	-0.55208100	-2.60411600
H	0.02666200	-2.13301100	-3.20161900
H	-1.12037600	-1.12172000	-4.12375500
H	0.09227200	-0.37521300	-0.32153300
B	3.12601900	-3.02230800	-2.67473200
F	2.98111600	-3.33598600	-4.03030100
F	3.21602700	-4.20712700	-1.92546800
F	1.98978100	-2.30172300	-2.24934900
F	4.26976300	-2.24776700	-2.48321300
TS3			
C	-5.69422500	-0.87113500	0.29206600
C	-4.53780500	-0.20938600	-0.12629900
C	-4.49861400	0.50698500	-1.31267300
C	-5.67160400	0.55812600	-2.05923800
C	-6.83879200	-0.09132600	-1.66740400
C	-6.84794300	-0.82199000	-0.47925000
C	-5.45250200	-1.56251000	1.61489800
C	-4.25395900	-0.78768400	2.15977900
C	-3.43550200	-0.45145700	0.88949500
H	-3.57010500	0.95046300	-1.65309500
H	-7.72862800	-0.02405000	-2.28277300
H	-7.75372600	-1.32947100	-0.16234500
H	-6.29743300	-1.51225700	2.30470600
H	-3.66080500	-1.31907000	2.91245700
H	-2.80554400	-1.28569500	0.57082800
H	-5.18359000	-2.61534200	1.46901500
Br	-5.67481000	1.54373400	-3.68624400
O	-4.78427000	0.40838800	2.71957300
C	-3.78724100	1.23862500	3.26215500
H	-4.25760900	2.16313600	3.59868300
H	-3.29231900	0.75336300	4.11668900
N	-2.55556900	0.68574500	1.16785000
C	-1.42518000	1.09014900	0.51663900
C	-2.74161100	1.52678200	2.23106200
N	-1.85301100	2.46888500	2.26079300
N	-1.05147900	2.21174200	1.17764100
C	-0.06887900	3.18350800	0.80917200
C	0.97434500	3.43742300	1.70800900
C	-0.18011300	3.83871600	-0.42061100
C	1.95328800	4.34713400	1.32114800

C	0.83672900	4.73059600	-0.76438800
C	1.91960700	4.97734400	0.07703100
H	2.78794700	4.53560900	1.99238700
H	0.77997300	5.23864100	-1.72430100
C	3.06247200	5.85297500	-0.36306900
H	2.76056400	6.53436400	-1.16157700
H	3.45700300	6.44256300	0.46838100
H	3.87748600	5.22557000	-0.74251100
C	-1.33005400	3.60874600	-1.36535100
H	-1.11878600	2.76642800	-2.03142900
H	-2.25681500	3.38044600	-0.83085300
H	-1.49746500	4.49910700	-1.97489400
C	1.06034800	2.74081200	3.04027400
H	0.43142600	3.24004600	3.78383500
H	0.71473300	1.70485600	2.98071700
H	2.09079800	2.74706400	3.40224700
C	1.57662000	0.83450400	-0.06978100
C	0.46447800	0.57806100	-0.95340100
H	1.36949200	0.93211300	0.99601100
C	-0.88309800	0.42925100	-0.68232700
H	2.10256400	-0.53685800	-0.37376600
O	-1.73451000	-0.26374500	-1.37663300
C	2.78354200	1.50479200	-0.53074400
C	3.83408300	1.78928900	0.37161500
C	3.02337800	1.79043400	-1.89102000
C	5.03593800	2.32996200	-0.05350300
H	3.68127900	1.57441000	1.42895000
C	4.24039900	2.32256200	-2.31787200
H	2.22885200	1.63624600	-2.61496600
C	5.25697100	2.60048100	-1.40935300
H	5.81732200	2.53430800	0.67464200
H	4.38553700	2.53347500	-3.37460000
H	6.20362700	3.01449800	-1.74289700
C	-1.42580900	-3.70496200	0.23513000
C	-0.39875200	-2.76371800	0.15949300
C	-0.10505400	-1.91921200	1.22165100
C	-0.86716400	-2.06822400	2.37615700
C	-1.82996100	-3.06480900	2.51445000
C	-2.12483800	-3.88433700	1.42359900
C	-1.62821600	-4.36525000	-1.10711200
C	-0.29885700	-4.11213600	-1.82169300
C	0.19979100	-2.76588800	-1.22965700
H	0.66092700	-1.15258400	1.15752900
H	-2.36427200	-3.17855700	3.45132800

H	-2.89751200	-4.64206700	1.50866400
H	-1.84108600	-5.43505300	-1.05717600
H	-0.38105400	-4.07551100	-2.91472100
H	-0.20228500	-1.90507300	-1.78198300
H	-2.44458500	-3.87193800	-1.64552000
Br	-0.65361300	-0.78421700	3.75926300
O	0.56113300	-5.17790400	-1.43687400
C	1.84619800	-5.07858000	-2.00771500
H	2.43846600	-5.92594100	-1.66145600
H	1.79465500	-5.10489500	-3.10536200
N	1.66652300	-2.72502300	-1.24708600
C	2.46346100	-1.69099700	-0.89583800
C	2.46697900	-3.79437900	-1.55963000
N	3.72440400	-3.49549200	-1.41476400
N	3.69248700	-2.18787400	-0.99941900
C	4.90348400	-1.50984800	-0.63046700
C	5.18331100	-1.35473000	0.72767300
C	5.73958200	-1.03588100	-1.64313600
C	6.38011000	-0.72351000	1.06589300
C	6.92252700	-0.41391900	-1.25488000
C	7.25751500	-0.25102500	0.09085000
H	6.62420600	-0.58852900	2.11678000
H	7.58936200	-0.02794800	-2.02230300
C	8.51830300	0.47926900	0.47261300
H	8.77713600	0.30835300	1.51950800
H	9.36132000	0.16736000	-0.14908700
H	8.38804700	1.55772300	0.32981700
C	5.34170700	-1.16589400	-3.08772100
H	5.20038000	-2.21280500	-3.37103400
H	4.39575900	-0.64107700	-3.25945500
H	6.10112300	-0.72684900	-3.73660900
C	4.20570000	-1.80259100	1.78219900
H	3.34318700	-1.12451100	1.81164000
H	3.82658200	-2.80965800	1.58457300
H	4.67387900	-1.79573500	2.76772900
H	0.73195000	0.19153800	-1.94522100
TS3 ^H			
C	4.37362600	-0.05281500	-1.44896400
C	3.08205700	-0.14487900	-0.92828600
C	2.81511300	-0.84894700	0.23641500
C	3.89401400	-1.45158100	0.87645700
C	5.19111900	-1.37936900	0.37651600
C	5.43349600	-0.67548700	-0.80273800

C	4.37383800	0.77869800	-2.71086800
C	3.07655500	1.57984100	-2.57749600
C	2.12753100	0.60701600	-1.83523500
H	1.80852500	-0.94699400	0.62500500
H	6.00202600	-1.86403600	0.90774500
H	6.44325500	-0.60769000	-1.19484300
H	5.23172600	1.44835900	-2.79998300
H	2.65796800	1.92584100	-3.53061400
H	1.63409600	-0.07439700	-2.52955300
H	4.33725600	0.14356600	-3.60245100
Br	3.57976600	-2.40560100	2.48769200
O	3.38416300	2.68927000	-1.74363100
C	2.27298600	3.51760700	-1.49996700
H	2.58005500	4.30705500	-0.81355200
H	1.91128300	3.97801900	-2.43056300
N	1.08414400	1.36412700	-1.13294900
C	-0.06667700	0.92259500	-0.55136600
C	1.16618600	2.71222400	-0.89338900
N	0.16952800	3.13682000	-0.18183500
N	-0.59038700	2.01644700	0.03657400
C	-1.77795300	2.09738900	0.83219400
C	-2.94799200	2.56210000	0.22745800
C	-1.71464500	1.68252900	2.16401100
C	-4.09800300	2.60812900	1.01212200
C	-2.89226500	1.74401800	2.90712400
C	-4.08701300	2.20448200	2.35003400
H	-5.02578700	2.95744200	0.56646000
H	-2.87585500	1.42091400	3.94478100
C	-5.33882200	2.28689000	3.18388700
H	-5.34360800	1.52329000	3.96449400
H	-5.40909700	3.26321300	3.67408600
H	-6.23186900	2.16052300	2.56817500
C	-0.43335000	1.14968700	2.74535000
H	0.41029400	1.80869100	2.52071400
H	-0.51485100	1.04443100	3.82784200
H	-0.20731700	0.16396200	2.32249500
C	-2.95493200	2.94625700	-1.22762500
H	-2.24450100	3.75374400	-1.42635000
H	-2.66388900	2.09277400	-1.85041000
H	-3.94909400	3.27226400	-1.53570600
C	-2.05871600	-2.19790300	-0.65354600
C	-1.85709300	-0.80721500	-0.28573200
H	-1.54427400	-2.91470300	-0.00287100
C	-0.57094800	-0.41466000	-0.58711500

H	-0.81941900	-2.07063000	-1.37722800
O	0.18942800	-1.36098600	-1.14865800
C	-3.39413800	-2.64249700	-1.07400500
C	-3.81002000	-3.97336600	-0.88984000
C	-4.29849900	-1.76864800	-1.70489500
C	-5.06377700	-4.40678000	-1.30510900
H	-3.13143800	-4.67165100	-0.40573400
C	-5.55799400	-2.19830100	-2.11051500
H	-3.99832500	-0.73943200	-1.88671500
C	-5.95192400	-3.52111800	-1.91573000
H	-5.35330400	-5.44156700	-1.14556900
H	-6.23395600	-1.49652900	-2.59101700
H	-6.93209700	-3.85758100	-2.23750000
H	-2.65192000	-0.12623700	0.00055200

TS3^{NHCH}

C	-6.59568000	-1.35059700	-0.55407000
C	-5.39685000	-0.64409600	-0.44674600
C	-5.14718700	0.48756900	-1.20853900
C	-6.14844900	0.90149800	-2.08240700
C	-7.35011700	0.21109500	-2.21348700
C	-7.57546700	-0.92985600	-1.44365600
C	-6.60044000	-2.52638300	0.39534900
C	-5.51820900	-2.14610200	1.40937500
C	-4.50639100	-1.33469800	0.56329700
H	-4.21551700	1.03825500	-1.14075400
H	-8.10384800	0.56772000	-2.90579700
H	-8.51403800	-1.46712900	-1.53420200
H	-7.55659400	-2.68749000	0.89735400
H	-5.04975700	-3.00645400	1.90580300
H	-3.80725300	-2.00764300	0.06544800
H	-6.32328500	-3.45220900	-0.12123500
Br	-5.86022300	2.46121900	-3.12199500
O	-6.13650100	-1.30910800	2.37329300
C	-5.23095600	-0.87330700	3.35856000
H	-5.76077700	-0.21380600	4.04583800
H	-4.82236100	-1.72351900	3.92347300
N	-3.72787600	-0.42867700	1.42132200
C	-2.65077600	0.35564500	1.12611200
C	-4.10535100	-0.13028900	2.70872600
N	-3.35477400	0.78640000	3.22981100
N	-2.45044300	1.08739100	2.24467200
C	-1.48747700	2.12672600	2.46566400
C	-0.27131500	1.79403800	3.06450600

C	-1.79229900	3.41449500	2.01349600
C	0.67596700	2.80959600	3.19673000
C	-0.81034400	4.39213000	2.15883800
C	0.42826100	4.10681400	2.74147400
H	1.63206500	2.58284400	3.66298900
H	-1.01250700	5.39759200	1.79925100
C	1.47270100	5.18283600	2.87654700
H	1.50632300	5.80680800	1.98025200
H	1.24567700	5.83571100	3.72491400
H	2.46364300	4.75350600	3.03891000
C	-3.10431700	3.69799800	1.33357900
H	-3.13482000	3.22398200	0.34511700
H	-3.94481500	3.30830400	1.91432700
H	-3.24209200	4.77068800	1.19520400
C	0.01179400	0.37963000	3.48853700
H	-0.77560200	-0.00752500	4.14144900
H	0.06525100	-0.27056000	2.60720000
H	0.96376200	0.31361500	4.01966800
C	0.09652300	0.94047100	-1.40863400
C	-0.83763900	1.15813600	-0.36188500
H	-0.26419800	0.36895500	-2.26482900
C	-1.89741200	0.33194200	-0.09324600
H	-1.62583400	-1.29012800	-1.11980600
O	-2.31602700	-0.61521800	-1.00868300
C	1.18024500	1.90987400	-1.70044200
C	1.85035500	1.84210500	-2.93042600
C	1.65432900	2.82231800	-0.74511300
C	2.95042700	2.65052200	-3.19764300
H	1.50265600	1.13776100	-3.68240800
C	2.76178000	3.62372500	-1.00854300
H	1.16347000	2.91690800	0.22138400
C	3.41950900	3.54044900	-2.23350400
H	3.45789100	2.56579000	-4.15284900
H	3.11409600	4.31331700	-0.24656300
H	4.28840400	4.15872400	-2.43356300
H	-0.58673800	1.90624500	0.37954100
C	5.37649100	1.28370000	1.08213700
C	4.27090600	0.71402100	0.45307900
C	4.26476500	0.41061300	-0.89633700
C	5.41394000	0.71641500	-1.61225700
C	6.52304500	1.31599000	-1.02401300
C	6.50759900	1.60106000	0.34152800
C	5.11799400	1.43307500	2.56511700
C	3.93992600	0.48081100	2.80421700

C	3.16859200	0.52146600	1.46557000
H	3.42206700	-0.07787100	-1.37123900
H	7.39944100	1.53334000	-1.62373600
H	7.38045500	2.04172600	0.81287700
H	5.96874900	1.15430500	3.19058400
H	3.31163300	0.76495800	3.66078100
H	2.47610500	1.37335200	1.45039100
H	4.82677200	2.45916600	2.81972000
Br	5.48096700	0.25396100	-3.44992200
O	4.47407400	-0.81408900	3.00538200
C	3.48836400	-1.80134600	3.21967700
H	3.99433700	-2.76304800	3.26163700
H	2.94946100	-1.61519400	4.16114700
N	2.37945100	-0.68774500	1.29733600
C	1.43282700	-0.91176600	0.36482200
C	2.51376200	-1.80188500	2.08177700
N	1.66810000	-2.72151900	1.72211900
N	1.01338100	-2.14528100	0.66162600
C	-0.04619100	-2.82188300	-0.02241800
C	0.04345000	-2.98180800	-1.41482000
C	-1.15751300	-3.26422800	0.71296100
C	-1.04751800	-3.56820300	-2.06772300
C	-2.18929300	-3.88737200	0.01343800
C	-2.16920900	-4.02331300	-1.37664500
H	-1.00269100	-3.68380100	-3.14727300
H	-3.04587500	-4.26039600	0.57128100
C	-3.35097200	-4.60951600	-2.10270900
H	-3.06532400	-4.98871300	-3.08551100
H	-3.79976600	-5.42509100	-1.53088100
H	-4.12118700	-3.84449900	-2.25237200
C	-1.27384500	-3.05176600	2.19940000
H	-0.53490300	-3.63819700	2.74880600
H	-1.10434100	-2.00132300	2.45676100
H	-2.27241500	-3.33015400	2.54385300
C	1.25329000	-2.55437200	-2.20612800
H	1.22842700	-1.48050400	-2.42388400
H	2.17879600	-2.75083400	-1.66255300
H	1.27180300	-3.08418300	-3.15996200
H	0.77780200	0.02871500	-0.64488100
B	5.04343800	-2.95784500	-0.02943300
F	6.05664000	-2.03855200	-0.28364300
F	5.24466500	-4.12032300	-0.77639200
F	3.79498000	-2.39590700	-0.38870800
F	5.00962500	-3.27684200	1.33826900

M3

C	2.90101400	2.73140800	-0.26317300
C	1.86958700	1.79137700	-0.28879700
C	2.00370800	0.54040100	0.29474200
C	3.21469900	0.25801900	0.92138400
C	4.26347900	1.17246200	0.95369700
C	4.10658100	2.42240600	0.35277200
C	2.47080900	4.00352600	-0.95759100
C	0.94311200	3.89050100	-0.95482400
C	0.69051200	2.36656300	-1.04328800
H	1.20941600	-0.20017600	0.26980000
H	5.19000300	0.91209200	1.45242700
H	4.91706900	3.14357700	0.38545900
H	2.78878300	4.91542800	-0.44771700
H	0.44924400	4.44499100	-1.76187600
H	0.65812100	1.99670600	-2.07265100
H	2.84387800	4.03683200	-1.98677500
Br	3.42275400	-1.42725100	1.76002500
O	0.50721500	4.37473400	0.31067600
C	-0.89101200	4.32506800	0.47608800
H	-1.12461100	4.66963300	1.48374000
H	-1.40075600	4.97524100	-0.24863900
N	-0.61323300	2.04848200	-0.45697800
C	-1.27836100	0.87835500	-0.51269200
C	-1.36301300	2.91562800	0.28763800
N	-2.46268000	2.35312500	0.69699800
N	-2.39415100	1.08427900	0.18636200
C	-3.48940100	0.17055900	0.35689900
C	-4.31070500	-0.08384200	-0.74431100
C	-3.67195900	-0.41490900	1.60948200
C	-5.36111500	-0.97906300	-0.55436700
C	-4.74009900	-1.30017100	1.74754200
C	-5.59123400	-1.59154200	0.68014600
H	-6.01664000	-1.20332700	-1.39189800
H	-4.90458700	-1.77837300	2.70961700
C	-6.75460500	-2.53175300	0.86027300
H	-6.95184100	-3.09433200	-0.05492000
H	-6.56839900	-3.23981300	1.67040900
H	-7.66375200	-1.97446900	1.10790100
C	-2.73844300	-0.10727200	2.74986900
H	-1.69554300	-0.27837600	2.46192200
H	-2.82233800	0.94016200	3.05347300
H	-2.96437700	-0.73744700	3.61084100

C	-4.06372400	0.58241500	-2.07265300
H	-4.04173000	1.67157600	-1.96202500
H	-3.10510900	0.27814500	-2.50696700
H	-4.85600400	0.32705700	-2.77755700
C	-0.46017800	-2.75683400	-1.46492700
C	-0.91543900	-1.51597300	-0.74393200
H	-0.67428500	-2.62439700	-2.53264800
C	-0.84537900	-0.29714900	-1.34908600
O	-0.44597500	0.04400700	-2.51604200
C	1.02420300	-3.03603200	-1.30961400
C	1.49673800	-4.21293500	-0.72946500
C	1.95383800	-2.09047300	-1.76517300
C	2.86727700	-4.45300200	-0.61382400
H	0.78593100	-4.95240400	-0.36841000
C	3.31888500	-2.32752000	-1.64987300
H	1.57807800	-1.17083100	-2.21000500
C	3.78162500	-3.51375000	-1.07826900
H	3.21671600	-5.37603700	-0.16067900
H	4.02720100	-1.58224000	-2.00118800
H	4.84779200	-3.69624600	-0.98556000
H	-1.27779800	-1.59079400	0.27703400
H	-1.02871400	-3.62833300	-1.12377300

M3^{NHCH}

C	-6.90656500	-1.05399000	-0.66799300
C	-5.61788800	-0.52914900	-0.56532900
C	-5.33678300	0.78039800	-0.92058500
C	-6.39830400	1.56986500	-1.34977900
C	-7.69264500	1.07252700	-1.46537200
C	-7.94778500	-0.25863700	-1.12939000
C	-6.91607500	-2.49227800	-0.20125500
C	-5.66047700	-2.56454000	0.67471900
C	-4.68017200	-1.58382600	-0.01760000
H	-4.33480100	1.18621200	-0.86036000
H	-8.49325600	1.71997100	-1.80381100
H	-8.95673700	-0.65087600	-1.20885900
H	-7.80271900	-2.76791900	0.37324400
H	-5.23626300	-3.57373100	0.77020100
H	-4.15919700	-2.09503300	-0.82984700
H	-6.82533000	-3.18147000	-1.04837700
Br	-6.04678500	3.38947600	-1.76066100
O	-6.04170600	-2.07896100	1.95234200
C	-4.95546700	-2.00982400	2.84866100
H	-5.31953000	-1.62095600	3.79950400

H	-4.52485100	-3.00935100	3.01313800
N	-3.68645500	-1.08054200	0.93124200
C	-2.63503800	-0.19694900	0.70195500
C	-3.90920600	-1.09951800	2.29096600
N	-3.11895600	-0.32233600	2.94389100
N	-2.31350600	0.25765800	1.97082700
C	-1.51753600	1.38772900	2.31882600
C	-0.37876100	1.18447900	3.10999100
C	-1.87815000	2.66372400	1.85714300
C	0.43799400	2.28224900	3.38314400
C	-1.01702000	3.72478700	2.13801500
C	0.15153700	3.55346900	2.88215100
H	1.31750700	2.14457300	4.00923700
H	-1.27366900	4.71599000	1.77155600
C	1.07963100	4.71350800	3.13012300
H	1.64581400	4.95193300	2.22372800
H	0.52279800	5.61071800	3.41112100
H	1.79440700	4.48685900	3.92379000
C	-3.12590500	2.89826400	1.04844900
H	-2.92594900	2.75847600	-0.02056000
H	-3.92651300	2.20884500	1.33143000
H	-3.48227900	3.92025100	1.18994700
C	-0.04266600	-0.18239700	3.64529000
H	-0.91517700	-0.65585400	4.10119100
H	0.29596400	-0.84766100	2.84209600
H	0.74702800	-0.11935300	4.39724100
C	-0.26799600	1.16634100	-1.85663700
C	-0.89188200	0.90101300	-0.68146900
H	-0.67786800	0.77200600	-2.78393300
C	-2.04845100	0.08507000	-0.51177500
H	-2.01849400	-1.13618200	-1.99987100
O	-2.63461600	-0.47723700	-1.64013600
C	1.00065800	1.89597400	-1.94688500
C	1.78049400	1.78885500	-3.11183800
C	1.50972200	2.67666000	-0.88875900
C	3.02034200	2.41201000	-3.21222600
H	1.40316500	1.19989100	-3.94423800
C	2.74912200	3.29901900	-0.99290600
H	0.91481700	2.82882100	0.01039700
C	3.51494200	3.16726000	-2.15137500
H	3.61258700	2.29221600	-4.11361500
H	3.12144600	3.89083100	-0.16143700
H	4.49357700	3.63130000	-2.22126500
H	-0.43737800	1.27710200	0.23024000

C	5.38415900	1.24266400	1.71031400
C	4.42036200	0.74557600	0.83231400
C	4.64554800	0.62733100	-0.52639500
C	5.89235500	1.02956900	-0.99212500
C	6.87084600	1.54265300	-0.14750400
C	6.61685700	1.65107500	1.22121400
C	4.85969400	1.23175400	3.12949200
C	3.68990400	0.24442700	3.05057300
C	3.16429200	0.44633800	1.60937600
H	3.91083800	0.20739300	-1.20575200
H	7.83005900	1.84027100	-0.55514000
H	7.38422200	2.03395000	1.88622300
H	5.59125600	0.90047800	3.86915200
H	2.91025800	0.41242100	3.80459900
H	2.45859800	1.28726000	1.57158400
H	4.49265800	2.22139100	3.42581300
Br	6.25765400	0.85871500	-2.83915600
O	4.24027000	-1.05151700	3.18176200
C	3.31921900	-2.10880900	3.06079100
H	3.89230400	-3.03205200	2.99403900
H	2.64574100	-2.15101800	3.92910300
N	2.43350700	-0.74538200	1.18641700
C	1.55589600	-0.87241500	0.19229500
C	2.48948400	-1.95223700	1.82233900
N	1.65850900	-2.79944000	1.27978400
N	1.07457900	-2.10274300	0.26383800
C	0.01743500	-2.66619700	-0.53729400
C	0.11569100	-2.61722500	-1.93603000
C	-1.09024400	-3.21418300	0.12614200
C	-0.95135500	-3.14577900	-2.66980400
C	-2.11119200	-3.74267000	-0.66182000
C	-2.07042400	-3.71053800	-2.05542900
H	-0.89346000	-3.12128800	-3.75476100
H	-2.97109500	-4.18410200	-0.16393500
C	-3.22402500	-4.22303900	-2.87541100
H	-2.87282200	-4.78193600	-3.74567100
H	-3.87293100	-4.87127100	-2.28280000
H	-3.82758500	-3.38653100	-3.24454600
C	-1.24039000	-3.20826400	1.62417400
H	-0.49767600	-3.84168900	2.11170500
H	-1.12520500	-2.19401600	2.02131300
H	-2.23736500	-3.56423400	1.89274500
C	1.30188100	-2.03841900	-2.66101100
H	1.26356500	-0.94300200	-2.67391100

H	2.24234100	-2.33211600	-2.19491400
H	1.29554200	-2.37426800	-3.69889900
H	1.26935200	-0.11186400	-0.52051600
B	4.99356800	-2.67364500	-0.41398700
F	5.99622600	-1.98183800	-1.08672200
F	5.06152700	-4.03438200	-0.69938100
F	3.72861300	-2.17685200	-0.83180400
F	5.09193900	-2.46702300	0.96965300

TS4-RS

C	1.84048500	-0.17806600	4.19342200
C	1.17657000	-0.31855300	2.97097300
C	1.86454200	-0.35815400	1.76951000
C	3.24874500	-0.18670000	1.82106200
C	3.92451000	0.01017600	3.01997600
C	3.21486700	0.00231900	4.22193900
C	0.86586700	-0.33035000	5.34041800
C	-0.29808800	-1.06211300	4.66726500
C	-0.30824100	-0.44505400	3.25120500
H	1.36891200	-0.53894300	0.81815900
H	5.00061100	0.13907600	3.01588900
H	3.74317400	0.11071800	5.16363400
H	1.26356400	-0.91318100	6.17336000
H	-1.26261000	-0.96954100	5.18017000
H	-0.79647200	0.53499300	3.25366800
H	0.53075200	0.63990600	5.72282900
Br	4.22554900	-0.25099000	0.19929700
O	0.09580000	-2.42388000	4.56253100
C	-0.83027300	-3.24852200	3.89742100
H	-0.35312400	-4.21403800	3.72577600
H	-1.73254800	-3.40404500	4.50493000
N	-1.05718300	-1.30926600	2.34033600
C	-1.73227900	-0.99888200	1.20853100
C	-1.25917500	-2.63785500	2.59405800
N	-1.98509300	-3.17892100	1.66029400
N	-2.27455500	-2.15113200	0.81278000
C	-3.00995300	-2.44583700	-0.39127000
C	-4.40168500	-2.35224000	-0.37572700
C	-2.27582200	-2.91866500	-1.47969200
C	-5.06321700	-2.67158000	-1.56035000
C	-2.98658700	-3.23434500	-2.63464000
C	-4.37399800	-3.09392200	-2.69848300
H	-6.14723400	-2.59820200	-1.58879900
H	-2.44252700	-3.59379100	-3.50457700

C	-5.11488400	-3.38769800	-3.97639800
H	-4.59789000	-4.14581100	-4.56867700
H	-6.13055800	-3.73487700	-3.77451900
H	-5.18933200	-2.48279800	-4.58784700
C	-0.78189000	-3.08641200	-1.39557300
H	-0.28664600	-2.15398600	-1.10298700
H	-0.51636600	-3.84997100	-0.65724500
H	-0.37525300	-3.38517000	-2.36343400
C	-5.14952900	-1.98272400	0.87607500
H	-4.96097800	-2.72078300	1.66299000
H	-4.82530800	-1.00542300	1.23954000
H	-6.22303200	-1.95734500	0.68319200
C	-1.45117500	2.81164400	1.18691100
C	-1.12564000	1.41313600	0.67201300
H	-0.50331500	3.32819900	1.36925600
C	-2.13860000	0.44458700	0.85277900
O	-3.35859200	0.62356700	0.97531800
C	-2.32664700	3.73792100	0.35879500
C	-3.30343700	3.28452300	-0.53315700
C	-2.16348700	5.11890400	0.51938300
C	-4.07711500	4.19257700	-1.25612200
H	-3.44524900	2.21785600	-0.67692300
C	-2.94185800	6.02630200	-0.19251900
H	-1.39872300	5.48489700	1.20093100
C	-3.90274700	5.56395000	-1.09019100
H	-4.82049300	3.82077700	-1.95469500
H	-2.79093600	7.09268000	-0.05485900
H	-4.50634000	6.26617500	-1.65641400
H	-0.12374700	1.07133600	0.91239400
H	-1.93994400	2.71045100	2.16887600
C	-0.50246300	1.72020400	-1.38496700
C	-0.30033600	0.52119200	-2.09664300
H	-1.46543100	2.17337700	-1.58741800
C	-1.48616400	-0.14562900	-2.57172700
H	-1.31023100	-1.01176500	-3.24155300
O	-2.63338500	0.17952100	-2.26982800
C	0.59383900	2.67846700	-1.11670500
C	1.83884200	2.26178800	-0.63067800
C	0.39177000	4.04259800	-1.35859300
C	2.85453300	3.17695900	-0.38384700
H	2.01721600	1.20860500	-0.45833600
C	1.40960800	4.96238600	-1.11619800
H	-0.56957500	4.38001400	-1.73546600
C	2.64141000	4.53446800	-0.62415700

H	3.80853500	2.81591800	-0.00983800
H	1.23720200	6.01638700	-1.31021500
H	3.43094100	5.25398200	-0.43196300
C	0.95824100	-0.06697100	-2.37373400
C	2.02121300	-0.59714300	-2.64675300
C	3.29861000	-1.13741600	-2.98733300
C	4.42657600	-0.29703800	-3.02618700
C	3.45980600	-2.50327400	-3.26662900
C	5.68109400	-0.81830300	-3.31763100
H	4.30026900	0.76059700	-2.81378900
C	4.71709800	-3.01434300	-3.56953200
H	2.59249700	-3.15498500	-3.23738300
C	5.83189700	-2.17795400	-3.59132800
H	6.54416900	-0.16044600	-3.33718100
H	4.82797800	-4.07265700	-3.78318700
H	6.81206700	-2.58210400	-3.82156800

TS4-RR

C	4.76476400	0.63458800	1.21976400
C	3.64450200	0.31074600	0.44661800
C	3.40508600	0.90863300	-0.77904300
C	4.31749500	1.87461300	-1.19986100
C	5.42448000	2.23675800	-0.44129800
C	5.65336500	1.60566300	0.78310200
C	4.81747000	-0.22896100	2.46002900
C	3.92016100	-1.40057600	2.05872500
C	2.82336500	-0.71227900	1.21359700
H	2.54035600	0.65673200	-1.38521400
H	6.10816700	2.99328200	-0.80855000
H	6.52872500	1.86389800	1.37031600
H	5.82202100	-0.57403100	2.71181100
H	3.51197100	-1.98134200	2.89480100
H	2.11662500	-0.20406200	1.87257800
H	4.39731200	0.28749700	3.33066800
Br	4.02530800	2.71851300	-2.87335400
O	4.70549700	-2.21630500	1.20241700
C	4.01969800	-3.31580900	0.65767600
H	4.64097100	-3.73771000	-0.13324700
H	3.84557400	-4.09028900	1.41793800
N	2.08832000	-1.72432000	0.44492100
C	0.81249000	-1.76871700	-0.02755200
C	2.68022000	-2.91722000	0.10932200
N	1.86858800	-3.67462600	-0.56402400
N	0.71842100	-2.94869100	-0.64496300

C	-0.46658000	-3.58156300	-1.17114400
C	-1.27258300	-4.27645600	-0.27166500
C	-0.74110100	-3.46235900	-2.53191600
C	-2.41509000	-4.88720000	-0.78890800
C	-1.88949900	-4.09551900	-2.99968800
C	-2.73418400	-4.80996300	-2.14495000
H	-3.07058400	-5.42914900	-0.11168600
H	-2.13841500	-4.01846800	-4.05517100
C	-3.95936100	-5.49986100	-2.68697600
H	-4.69369500	-5.67766000	-1.89847500
H	-4.43110300	-4.90413300	-3.47195300
H	-3.69620000	-6.46905600	-3.12277000
C	0.15536700	-2.64720100	-3.42045300
H	0.20237500	-1.61180800	-3.06329300
H	1.17610000	-3.04329000	-3.41810200
H	-0.21249700	-2.65296800	-4.44769500
C	-0.93676200	-4.32714800	1.19437000
H	0.09535300	-4.65540300	1.35346700
H	-1.05854900	-3.33785000	1.65423500
H	-1.60506400	-5.01275500	1.71699000
C	-1.87453100	0.17150400	1.88758300
C	-0.48754100	-0.16019600	1.38499800
H	-2.44141400	0.65246800	1.08386700
C	-0.42171500	-0.93402500	0.21658200
O	-1.32884500	-0.99832900	-0.63309400
C	-2.59282000	-1.08585300	2.33348600
C	-2.37498900	-1.61474400	3.61012000
C	-3.44001600	-1.77319900	1.45802300
C	-2.98774800	-2.80143000	4.00558200
H	-1.71985600	-1.08665300	4.29951400
C	-4.05597700	-2.95927700	1.85235100
H	-3.59342900	-1.37803300	0.45920000
C	-3.83238300	-3.47765000	3.12634000
H	-2.81133600	-3.19500000	5.00202700
H	-4.71115700	-3.47950700	1.15980600
H	-4.31370800	-4.40090600	3.43367300
H	0.27717800	-0.27535700	2.14677200
H	-1.80133200	0.87515200	2.72180500
C	0.07371800	1.74801400	0.32354200
C	-0.78497500	1.79591900	-0.77957000
H	1.05732100	1.36850200	0.06650100
C	-0.38402100	1.05667800	-1.95952700
H	-1.11968900	1.05650900	-2.78397000
O	0.69403900	0.47112600	-2.09426900

C	0.09057300	2.62903700	1.50735800
C	1.31696300	2.79683800	2.17044800
C	-1.03364100	3.30363900	2.00536500
C	1.42218400	3.61068600	3.29194200
H	2.20188000	2.29616000	1.78053500
C	-0.92695900	4.11644500	3.13030100
H	-1.99134800	3.18558600	1.51288900
C	0.29656900	4.27380700	3.77804200
H	2.38246800	3.73142600	3.78301200
H	-1.80762600	4.63042300	3.50246200
H	0.37307100	4.91035900	4.65345800
C	-2.05616300	2.42784100	-0.82501400
C	-3.14553800	2.95782800	-0.93924400
C	-4.42434500	3.58845900	-1.03916100
C	-4.85425600	4.48508400	-0.04669300
C	-5.26971200	3.32048800	-2.12832400
C	-6.09967600	5.09360100	-0.14364700
H	-4.20112500	4.69874600	0.79355600
C	-6.51250800	3.93583700	-2.21824500
H	-4.94027000	2.62735400	-2.89512400
C	-6.93311200	4.82273700	-1.22815600
H	-6.42071200	5.78400300	0.62969200
H	-7.15664200	3.72092700	-3.06484500
H	-7.90443300	5.30052900	-1.30144300

TS4-SS

C	4.64251900	-1.45874500	-1.71343200
C	3.70324900	-0.80214800	-0.91583000
C	3.68197600	-0.96061400	0.46270000
C	4.60788900	-1.83791200	1.02109400
C	5.53424100	-2.52673100	0.24413700
C	5.55749600	-2.32930000	-1.13690200
C	4.49292900	-1.03641000	-3.15740000
C	3.71768600	0.27837900	-3.03717000
C	2.80996700	0.03947800	-1.80794400
H	2.97879500	-0.42841400	1.09573200
H	6.23981400	-3.19987800	0.71708100
H	6.29580600	-2.84321000	-1.74376400
H	5.44477300	-0.87781700	-3.66811900
H	3.14295000	0.55183500	-3.93018100
H	1.91252100	-0.50105800	-2.12174800
H	3.91094400	-1.76671000	-3.72974500
Br	4.59165600	-2.09877300	2.89792300
O	4.66766200	1.28487400	-2.72472700

C	4.08542400	2.55665700	-2.56553200
H	4.86153000	3.24260700	-2.22466800
H	3.67725600	2.92764100	-3.51604900
N	2.37375200	1.31150500	-1.23846700
C	1.31174600	1.59895000	-0.44613300
C	2.97204400	2.49924400	-1.56300400
N	2.38712400	3.49646500	-0.97457800
N	1.36603500	2.92348500	-0.27195600
C	0.53854700	3.78998700	0.52748400
C	-0.31977800	4.66270700	-0.13760000
C	0.68500700	3.76081900	1.91606800
C	-1.07483900	5.53335300	0.65006900
C	-0.08837200	4.65076100	2.65510500
C	-0.97572300	5.53897500	2.04047700
H	-1.75883400	6.22141500	0.15958400
H	0.00243500	4.65039300	3.73854400
C	-1.82406900	6.46509500	2.87297300
H	-2.68680500	5.93093800	3.28347900
H	-1.25685300	6.86786700	3.71569900
H	-2.20045700	7.29965400	2.27794700
C	1.61860000	2.78761300	2.58383700
H	1.20138300	1.77500300	2.54883400
H	2.59700400	2.76518100	2.09396800
H	1.76602400	3.05514300	3.63110600
C	-0.41944600	4.67536800	-1.64022300
H	0.39634400	5.26318800	-2.07342600
H	-0.35084400	3.66519400	-2.05510800
H	-1.36353000	5.12584300	-1.95234500
C	-0.00944200	-1.44461400	1.46586200
C	0.39023300	-0.67654100	0.20458000
H	0.22808700	-0.79517900	2.32130200
C	0.25496500	0.72902700	0.19750100
O	-0.71665700	1.34886100	0.66195800
C	-1.41917100	-1.95520900	1.67988100
C	-2.52165400	-1.10155600	1.61157700
C	-1.62354100	-3.29390600	2.02288900
C	-3.80299800	-1.58597700	1.86071500
H	-2.36262500	-0.06225800	1.34112900
C	-2.90336600	-3.77964100	2.27567400
H	-0.77210300	-3.96905700	2.06596100
C	-4.00103200	-2.92554200	2.19111200
H	-4.65227400	-0.91259300	1.78684600
H	-3.04358000	-4.82740900	2.52496200
H	-5.00311800	-3.29897500	2.38196900

H	1.28998500	-1.07573500	-0.24133400
H	0.67051400	-2.29986400	1.54241200
C	-0.96529500	-1.15469200	-1.51762600
C	-1.91936200	-0.12815200	-1.65216200
H	-0.09106100	-0.95993400	-2.12930800
C	-1.41914600	1.12310300	-2.15323500
H	-2.15571300	1.94228800	-2.23726600
O	-0.23335400	1.32044500	-2.45788700
C	-1.21162300	-2.59914900	-1.30702900
C	-2.48892200	-3.15832800	-1.18439800
C	-0.10365700	-3.46074700	-1.27987400
C	-2.64738600	-4.53257300	-1.03283200
H	-3.36051600	-2.51638400	-1.19778400
C	-0.26055400	-4.83046600	-1.11404700
H	0.89647200	-3.04373200	-1.38153500
C	-1.53930100	-5.37358200	-0.98906100
H	-3.64709000	-4.94463100	-0.93445100
H	0.61233100	-5.47510400	-1.08857400
H	-1.66782700	-6.44371400	-0.86126100
C	-3.29930200	-0.16342300	-1.32110300
C	-4.49594700	-0.12200600	-1.10613100
C	-5.89715600	-0.15218600	-0.82808900
C	-6.49422000	-1.33177200	-0.34886900
C	-6.69831900	0.98326000	-1.02985000
C	-7.85673800	-1.36788000	-0.07874900
H	-5.87292300	-2.20727200	-0.18388900
C	-8.06076900	0.93684600	-0.75824900
H	-6.24025200	1.89490900	-1.39883800
C	-8.64540700	-0.23589900	-0.28248900
H	-8.30562600	-2.28376900	0.29224800
H	-8.66928000	1.82116500	-0.91806200
H	-9.70908800	-0.26764800	-0.07102300

TS4-SR

C	4.31124700	-1.21595800	-1.52357800
C	3.27111200	-0.53915100	-0.88673600
C	3.19244000	-0.44570500	0.49282900
C	4.17712900	-1.09130800	1.23462700
C	5.20147600	-1.81140900	0.62783200
C	5.27407100	-1.86940300	-0.76572300
C	4.20260100	-1.03867400	-3.02230600
C	3.31572500	0.20692200	-3.14499600
C	2.36309300	0.07167900	-1.93332000
H	2.40540400	0.11539000	0.98642300

H	5.94996100	-2.30161700	1.23945200
H	6.09267900	-2.40003100	-1.24086600
H	5.16331200	-0.87750300	-3.51516200
H	2.77355400	0.28548700	-4.09484800
H	1.53075300	-0.58687400	-2.19366900
H	3.71165500	-1.89678800	-3.49426300
Br	4.12127500	-0.94650200	3.12256400
O	4.16105500	1.33070200	-2.95783700
C	3.46299400	2.55538000	-2.97924200
H	4.17431900	3.35398200	-2.76880400
H	3.00770500	2.73335600	-3.96337300
N	1.81380800	1.36610600	-1.54470300
C	0.79634900	1.66983000	-0.70437100
C	2.38080500	2.54666200	-1.94262700
N	1.81284500	3.55792700	-1.36053000
N	0.84078100	3.00088400	-0.58174600
C	0.09225300	3.86283100	0.29431300
C	-0.74904900	4.81539600	-0.28080900
C	0.29757800	3.74913700	1.67241400
C	-1.42332500	5.67333200	0.58822600
C	-0.39935000	4.63170600	2.49377500
C	-1.26613600	5.59409000	1.97158700
H	-2.09087400	6.42154200	0.16813300
H	-0.25934200	4.56654100	3.56982300
C	-2.03387700	6.51056000	2.88846500
H	-2.96931200	6.03918100	3.20647200
H	-1.45881100	6.74103800	3.78820900
H	-2.28802000	7.44790900	2.38899600
C	1.21633100	2.70939600	2.25895900
H	0.73558800	1.72364200	2.25373300
H	2.15475500	2.63294700	1.69970400
H	1.45888400	2.95607700	3.29365500
C	-0.91978300	4.92142000	-1.77301400
H	-1.83387900	5.47005700	-2.00766800
H	-0.07691700	5.45908400	-2.21869400
H	-0.96422900	3.93237300	-2.23908500
C	-0.99833000	-1.32924700	0.97943800
C	-0.16490100	-0.59704000	-0.06205800
H	-1.97763800	-1.61985500	0.58064800
C	-0.25080100	0.80988600	-0.04477000
O	-1.24911900	1.42221900	0.37871900
C	-0.28257600	-2.54872500	1.51351400
C	-0.76420600	-3.83584000	1.27298900
C	0.90748000	-2.40718000	2.23626500

C	-0.07315100	-4.95531600	1.73396800
H	-1.67922700	-3.96110400	0.70019600
C	1.60663300	-3.52063800	2.69186500
H	1.29026100	-1.41067800	2.44837900
C	1.11614100	-4.80204700	2.44122300
H	-0.46248100	-5.94822300	1.52902900
H	2.53685800	-3.38125400	3.23409800
H	1.65949800	-5.67293200	2.79410500
H	0.76932700	-1.07655300	-0.33071300
H	-1.20754200	-0.62361100	1.79288000
C	-1.34096900	-0.92811900	-1.89337300
C	-2.39995300	-0.01267700	-1.79528400
H	-0.54480000	-0.55140600	-2.53066400
C	-2.09607200	1.33814200	-2.20593600
H	-2.90498300	2.07892600	-2.07394800
O	-1.00301200	1.68094200	-2.67254100
C	-1.43207000	-2.40795800	-1.87154700
C	-0.25666200	-3.15660700	-2.04001600
C	-2.64327600	-3.10311900	-1.75421100
C	-0.28067500	-4.54381400	-2.07271800
H	0.69623800	-2.64117100	-2.13812000
C	-2.67027200	-4.49663600	-1.79467600
H	-3.57104200	-2.55383100	-1.65326000
C	-1.49270000	-5.22261300	-1.94608700
H	0.64505100	-5.09658000	-2.19484400
H	-3.62107800	-5.01338300	-1.70940500
H	-1.51679000	-6.30722500	-1.97211100
C	-3.64788400	-0.23780200	-1.15890000
C	-4.72996100	-0.38826900	-0.62292000
C	-5.97712400	-0.63272200	0.02933100
C	-6.22937900	-1.88699500	0.61118500
C	-6.96407600	0.36356200	0.10176300
C	-7.44009900	-2.13435600	1.24609100
H	-5.46430500	-2.65572000	0.56049900
C	-8.17180300	0.10708200	0.74001300
H	-6.77098800	1.33334300	-0.34457300
C	-8.41570300	-1.14016300	1.31329000
H	-7.62285600	-3.10666500	1.69229200
H	-8.92661900	0.88525300	0.79064800
H	-9.35986800	-1.33600800	1.81060400
TS4C-RS			
C	-3.73599400	-1.38864400	3.47183500
C	-3.43670200	-0.83604900	2.22361500

C	-3.74747500	-1.48567100	1.04078200
C	-4.38438700	-2.71839700	1.15061400
C	-4.68735000	-3.29834300	2.37673200
C	-4.35738300	-2.62622300	3.55468000
C	-3.29191800	-0.46401500	4.58386600
C	-3.13342000	0.87678600	3.86165900
C	-2.69688000	0.46274300	2.43872300
H	-3.54066900	-1.06400400	0.06150500
H	-5.18327800	-4.26159700	2.40948300
H	-4.60013600	-3.06620400	4.51680500
H	-4.01347800	-0.37794200	5.39908500
H	-2.41666400	1.56737200	4.32602000
H	-1.60933900	0.32868700	2.38598600
H	-2.33256800	-0.78229100	5.00792400
Br	-4.83571900	-3.64458000	-0.43821500
O	-4.42718900	1.45484600	3.81110600
C	-4.49627300	2.69301600	3.14581100
H	-5.55016300	2.92020700	2.99058200
H	-4.02793900	3.49004400	3.74030900
N	-3.00268800	1.55709000	1.52128200
C	-2.44223800	1.82212500	0.34434500
C	-3.80415400	2.62137500	1.81982800
N	-3.74629500	3.53078600	0.88537600
N	-2.88937500	3.00554100	-0.03614300
C	-2.34454600	3.77388200	-1.12777000
C	-2.84882000	3.61297700	-2.41785200
C	-1.27581700	4.63248600	-0.82226200
C	-2.16795600	4.26766300	-3.44978200
C	-0.63444700	5.25510800	-1.88820600
C	-1.05117700	5.06292600	-3.21018900
H	-2.52818100	4.14144000	-4.46784500
H	0.21158500	5.90683600	-1.68551500
C	-0.30004600	5.70729300	-4.34521700
H	-0.02993300	6.73844000	-4.10240100
H	0.63287100	5.16783000	-4.54036500
H	-0.89234900	5.70819200	-5.26236200
C	-0.89098300	4.94756700	0.60107600
H	-1.57909300	5.69586600	1.00770600
H	-0.92650000	4.07657300	1.26035200
H	0.11840900	5.36421300	0.63468100
C	-4.10145500	2.83481500	-2.71437400
H	-4.35274100	2.11509300	-1.93546500
H	-4.94303700	3.53017300	-2.80336100
H	-4.00520500	2.31298800	-3.66954800

H	-1.72918200	1.20784100	-0.18861100
B	-6.09469000	0.63866100	0.14913000
F	-4.80580200	0.80494400	-0.43089500
F	-7.00266200	1.43051900	-0.54752300
F	-6.01935100	1.04915100	1.48832000
F	-6.45197500	-0.70655600	0.07410700
N	-2.71611100	-1.76807100	-2.54740300
C	-1.61862900	-2.61563800	-3.00311700
C	-1.97597200	-4.09925300	-3.03154400
H	-0.78334900	-2.45242700	-2.31114000
H	-1.25260200	-2.32010600	-4.00470700
H	-1.06564600	-4.70356000	-3.09453600
H	-2.52297300	-4.37792900	-2.12650700
H	-2.59531400	-4.35350300	-3.89564800
C	-3.90849500	-1.93203600	-3.37661100
C	-5.06102800	-1.02543600	-2.96976300
H	-4.23723900	-2.97091100	-3.26844400
H	-3.67330700	-1.78809500	-4.44930200
H	-5.95591400	-1.30421900	-3.53382000
H	-5.27631900	-1.12269000	-1.90323400
H	-4.85357100	0.02869400	-3.17569400
C	-2.28224300	-0.37722900	-2.40386400
C	-1.89719900	0.35775900	-3.69065900
H	-1.40962100	-0.39280400	-1.73663500
H	-3.08243700	0.16870100	-1.88917700
H	-1.59742900	1.38423800	-3.45404400
H	-1.04973300	-0.12017300	-4.18983800
H	-2.73514000	0.40291000	-4.39507800
C	1.56834100	1.37246500	-1.25745200
C	0.80121300	1.02825000	-0.13322200
H	1.73934100	2.44505700	-1.33343300
C	0.57521300	2.05482200	0.85014800
H	1.00151300	3.03780000	0.57769900
O	-0.09130300	1.93107500	1.88300900
C	1.53275800	0.69657600	-2.57538400
C	1.52287600	1.50068600	-3.72418400
C	1.51650100	-0.69442400	-2.73558600
C	1.53126700	0.93137900	-4.99426600
H	1.50370400	2.58123800	-3.61345200
C	1.53722600	-1.26483200	-4.00405600
H	1.48054500	-1.33696500	-1.86601200
C	1.55344000	-0.45474100	-5.13897800
H	1.52230000	1.57270100	-5.87003800
H	1.53569200	-2.34765000	-4.08940400

H	1.57268900	-0.90069200	-6.12819300
C	0.39264100	-0.30158700	0.16216000
C	0.06929300	-1.44051100	0.44823200
C	-0.19082300	-2.80945700	0.78625500
C	0.73283700	-3.52044900	1.56738200
C	-1.31906300	-3.46451100	0.27711200
C	0.53256700	-4.87135200	1.82414700
H	1.61334800	-3.01088700	1.94820000
C	-1.52068200	-4.81254000	0.55470700
H	-2.02022000	-2.91838700	-0.34979800
C	-0.59403800	-5.51952500	1.31889100
H	1.25607100	-5.42017500	2.41821200
H	-2.41683200	-5.29898300	0.17996900
H	-0.75113000	-6.57330000	1.52525400
C	5.88931000	-3.25145700	-1.12054700
C	4.91521900	-2.39845900	-0.59308200
C	3.56122500	-2.63380900	-0.77019400
C	3.20617000	-3.73734700	-1.54995100
C	4.15874600	-4.56955800	-2.12803800
C	5.51552900	-4.33180200	-1.90401200
C	7.26277100	-2.84109900	-0.63848200
C	6.92212900	-2.01398800	0.60355600
C	5.61810800	-1.30071400	0.18047600
H	2.80071200	-2.00477100	-0.31130200
H	3.83974900	-5.41500700	-2.72641600
H	6.25929500	-5.00418200	-2.31906700
H	7.90367900	-3.68619900	-0.38045200
H	7.70540700	-1.31633400	0.92349000
H	5.84455200	-0.43974100	-0.45602800
H	7.78475600	-2.21942200	-1.37398200
Br	1.37210300	-4.13186000	-1.81472500
O	6.61759800	-2.94614100	1.63025300
C	6.20853600	-2.35617900	2.83889400
H	5.81834100	-3.14694900	3.48093600
H	7.05033000	-1.87094400	3.35184300
N	4.91347000	-0.79889800	1.36208900
C	4.06434500	0.25111300	1.51102500
C	5.15525800	-1.31175600	2.60563000
N	4.48899800	-0.66022700	3.51312000
N	3.82367400	0.30739800	2.82848700
C	3.02965600	1.22474500	3.62059700
C	3.62931900	2.40573700	4.06857300
C	1.76488300	0.80506800	4.02166900
C	2.86660500	3.22483900	4.89458400

C	1.04500400	1.66039600	4.85591800
C	1.56887000	2.87650700	5.28461100
H	3.29968600	4.15580100	5.25174700
H	0.04973000	1.35963800	5.17379200
C	0.75352600	3.80812300	6.14259500
H	0.27180500	4.57244200	5.52432200
H	-0.03201000	3.26891000	6.67636300
H	1.38034600	4.32377500	6.87395700
C	1.21937100	-0.52721000	3.59650200
H	1.25975000	-0.63724300	2.51100100
H	1.79230300	-1.34408200	4.04881700
H	0.17594000	-0.63211500	3.90053700
C	5.03917900	2.76247600	3.68666700
H	5.72314700	1.93112700	3.88620500
H	5.08989900	2.99723800	2.62060900
H	5.38141200	3.62810200	4.25567500
C	4.35389900	2.00728200	-1.91574200
C	3.72355100	1.08904100	-0.86504900
H	4.32249600	1.44460000	-2.85437800
C	3.72336900	1.35964000	0.51910600
O	3.41574100	2.42322400	1.08149600
C	3.84982700	3.41030600	-2.23110300
C	3.86108800	3.81713300	-3.57162900
C	3.45220200	4.34118800	-1.26538100
C	3.47548200	5.10209000	-3.94332900
H	4.16219400	3.10684800	-4.33818800
C	3.05864500	5.62689700	-1.63578600
H	3.43715200	4.04676600	-0.22237900
C	3.06588500	6.01482800	-2.97296900
H	3.48814500	5.38730800	-4.99096000
H	2.74773700	6.33018000	-0.86817900
H	2.75649000	7.01585500	-3.25740100
H	3.85556100	0.04217700	-1.12803300
H	5.42244600	2.10358900	-1.67231200

TS4C-SS

C	-6.10900300	-1.97407600	2.39436500
C	-5.24010800	-1.26411700	1.56086800
C	-4.91077400	-1.72101200	0.29142700
C	-5.50735800	-2.91125600	-0.11693500
C	-6.39414200	-3.62321600	0.68398800
C	-6.69707600	-3.15215600	1.95875500
C	-6.26419000	-1.28246400	3.72707000
C	-5.82565800	0.14371200	3.40356400

C	-4.72819500	-0.05985200	2.33027100
H	-4.23506600	-1.19528000	-0.37788200
H	-6.83773900	-4.53935800	0.31120700
H	-7.38487500	-3.70025400	2.59514900
H	-7.28333600	-1.29516800	4.11885500
H	-5.46403900	0.72128200	4.26407300
H	-3.76633600	-0.28612400	2.80405300
H	-5.59384600	-1.72566700	4.47286400
Br	-5.06906400	-3.63122000	-1.81422400
O	-6.95042600	0.77371700	2.81249800
C	-6.72614000	2.10397600	2.41319000
H	-7.58520100	2.42460700	1.82742100
H	-6.59784700	2.76186500	3.28475000
N	-4.56255900	1.19058900	1.58855900
C	-3.53076400	1.60649900	0.84679500
C	-5.49404500	2.19183800	1.56898600
N	-5.07450700	3.20442800	0.86606100
N	-3.84848700	2.81747000	0.41802400
C	-3.01714100	3.76051800	-0.28529100
C	-3.30508900	4.06062000	-1.61673400
C	-2.00523400	4.39219100	0.44684700
C	-2.50527500	5.02664200	-2.23365200
C	-1.25279300	5.35908200	-0.21157400
C	-1.48544100	5.68692500	-1.55068500
H	-2.70536700	5.27876100	-3.27230800
H	-0.47915300	5.88125600	0.34500600
C	-0.64921500	6.73594900	-2.23833500
H	-0.29174400	7.48325200	-1.52517700
H	0.22840700	6.28702400	-2.71636900
H	-1.21962900	7.24772900	-3.01645400
C	-1.73785500	4.04676000	1.88620100
H	-2.66274100	4.01267500	2.47044000
H	-1.24989200	3.06953100	1.94641600
H	-1.07494200	4.78775300	2.33611500
C	-4.44124000	3.41711200	-2.36425700
H	-4.77423500	2.48276700	-1.91257500
H	-5.30507500	4.08985100	-2.38639800
H	-4.14607400	3.22634200	-3.39974000
H	-2.57724000	1.10980000	0.67452700
B	-6.89654900	0.75129600	-1.22444400
F	-5.51428200	0.80108200	-0.90730600
F	-7.11514200	1.50672800	-2.37705300
F	-7.61096800	1.29876500	-0.14716400
F	-7.27159600	-0.57506900	-1.42169400

N	-2.77569200	-1.20966600	-2.65443700
C	-1.52285800	-1.93924200	-2.83238000
C	-1.65474000	-3.44079400	-2.60938300
H	-0.80423600	-1.55200600	-2.10522200
H	-1.08590600	-1.74979600	-3.83217000
H	-0.68628300	-3.92671500	-2.76569900
H	-1.97981800	-3.63485600	-1.58406200
H	-2.38365900	-3.89783100	-3.28526800
C	-3.58212200	-1.24385600	-3.86941300
C	-4.93597000	-0.56375200	-3.72615200
H	-3.74447700	-2.29983800	-4.11871900
H	-3.03153400	-0.80786600	-4.72657200
H	-5.52876500	-0.73584200	-4.62977800
H	-5.48538400	-0.95925700	-2.86900600
H	-4.84919700	0.51771200	-3.58974100
C	-2.56118900	0.13194600	-2.11542200
C	-1.74197600	1.09300800	-2.98131400
H	-2.04930000	-0.00038100	-1.15663700
H	-3.53957300	0.56831200	-1.89106900
H	-1.60725200	2.04329700	-2.45434000
H	-0.74678200	0.68250000	-3.19110500
H	-2.23554500	1.29676100	-3.93770000
C	1.50850700	-1.04432600	-0.81347600
C	0.42678000	-0.44043600	-0.15229600
H	1.94315800	-0.40854300	-1.58562100
C	0.22436700	0.97844800	-0.31751400
H	0.95368500	1.47559700	-0.98532600
O	-0.70324300	1.62940700	0.16509800
C	1.59788700	-2.48214200	-1.17133500
C	2.01969300	-2.80984200	-2.46849900
C	1.27174100	-3.52367000	-0.29184700
C	2.13337600	-4.13615800	-2.87519200
H	2.23558200	-2.00931200	-3.17381200
C	1.38385800	-4.84929600	-0.70044900
H	0.93160100	-3.29501700	0.71117000
C	1.81935600	-5.16245000	-1.98722600
H	2.45685200	-4.36463500	-3.88571400
H	1.13021300	-5.64366700	-0.00607200
H	1.90625500	-6.19851800	-2.29704400
C	-0.49798100	-1.16106400	0.65669300
C	-1.28932900	-1.79399900	1.33072500
C	-2.11911400	-2.58769200	2.19020700
C	-2.21244500	-2.27915000	3.55667900
C	-2.83376000	-3.68563500	1.68488200

C	-3.01276900	-3.04743000	4.39662200
H	-1.64793500	-1.43794400	3.94756600
C	-3.62068500	-4.45518200	2.53255700
H	-2.80133000	-3.90222100	0.62104400
C	-3.71633300	-4.13747500	3.88713500
H	-3.07965600	-2.79971700	5.45140200
H	-4.17864500	-5.29418500	2.12989500
H	-4.34070300	-4.73609900	4.54274000
C	6.80191700	-2.48237700	-2.18509700
C	6.17395200	-1.57188300	-1.33227500
C	6.59486900	-1.38772100	-0.02304800
C	7.65837100	-2.17197200	0.41936000
C	8.28617900	-3.10134900	-0.40392100
C	7.85704600	-3.25547100	-1.72203600
C	6.17945400	-2.43440200	-3.56141500
C	5.48158400	-1.07282300	-3.55886900
C	5.03157700	-0.92013100	-2.08738200
H	6.12655900	-0.67365600	0.64742600
H	9.11126600	-3.68997200	-0.02032600
H	8.35670900	-3.96367500	-2.37478700
H	6.90400000	-2.49654600	-4.37555500
H	4.64433100	-0.99216500	-4.26351400
H	4.09675000	-1.46787800	-1.93726100
H	5.44076100	-3.23342300	-3.69086300
Br	8.26992300	-1.96333200	2.20164900
O	6.47366200	-0.10166900	-3.84796400
C	5.97411100	1.21359700	-3.85063200
H	6.81555000	1.89537800	-3.97687800
H	5.26517600	1.36932800	-4.67592600
N	4.78414200	0.49123000	-1.77576800
C	4.09866300	1.06767400	-0.75703900
C	5.26989700	1.50447400	-2.55907100
N	4.94704500	2.66656700	-2.07344900
N	4.22258600	2.38208900	-0.95750100
C	3.74835000	3.48480800	-0.15830700
C	2.77413700	4.31178600	-0.70812300
C	4.32875000	3.69935300	1.09827600
C	2.39465800	5.42841200	0.04043200
C	3.89893700	4.81482900	1.80741400
C	2.93716000	5.69268000	1.29381400
H	1.65271000	6.10315500	-0.37929100
H	4.32615900	5.00688200	2.78849100
C	2.48033900	6.87936200	2.10129200
H	1.83273200	6.55691400	2.92285000

H	3.32971700	7.40703900	2.54240700
H	1.91704300	7.58396900	1.48569900
C	5.33637100	2.74425000	1.68012700
H	4.83267600	1.84158600	2.04883900
H	6.08683000	2.44275400	0.94212900
H	5.85499300	3.20481600	2.52247300
C	2.11552500	4.03925400	-2.03559200
H	2.29051500	3.02075800	-2.38732600
H	1.03434100	4.18209400	-1.94074400
H	2.48537400	4.72397800	-2.80506500
C	2.71371900	-1.37462500	1.88705400
C	3.22235000	-0.91341700	0.53765400
H	2.79582600	-2.46384500	1.95073300
C	3.27677200	0.47955200	0.36119400
O	2.55443800	1.28422300	0.97501600
C	3.50658800	-0.72206300	3.00496900
C	4.84089500	-1.07270100	3.23408300
C	2.94349800	0.29870300	3.77394200
C	5.59597400	-0.41694500	4.20318700
H	5.29769400	-1.86735300	2.64595700
C	3.69241300	0.95198500	4.75093900
H	1.91700100	0.59522300	3.58129800
C	5.02222700	0.59832600	4.96703300
H	6.63244300	-0.69986000	4.35710800
H	3.23824800	1.74590300	5.33588900
H	5.60881000	1.11064300	5.72301200
H	3.95693100	-1.55154700	0.06279700
H	1.65784200	-1.10609400	1.99843600

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C	-1.09717300	-4.17117700	1.08131200
C	-1.49958200	-2.85453000	0.85210000
C	-1.29949400	-2.23612000	-0.37794400
C	-0.66868900	-2.98607400	-1.36647500
C	-0.27630500	-4.30881100	-1.16651300
C	-0.49012400	-4.90753800	0.07116400
C	-1.38798700	-4.60011800	2.49771000
C	-2.30975500	-3.50029800	3.03650000
C	-2.00072200	-2.26267300	2.15093400
H	-1.62331600	-1.22339700	-0.60966300
H	0.19004900	-4.86081600	-1.97588900
H	-0.19077200	-5.93749800	0.23693000
H	-1.89542800	-5.56583500	2.56123400
H	-2.14738000	-3.27878700	4.09975200

H	-1.21448700	-1.64128300	2.59211100
H	-0.46943400	-4.67147200	3.09007000
Br	-0.29302300	-2.17079700	-3.02761200
O	-3.64070900	-3.93796700	2.84061700
C	-4.58602000	-3.01657600	3.33313000
H	-5.57752800	-3.40268000	3.11065400
H	-4.46442900	-2.86761800	4.41571700
N	-3.18768200	-1.40896700	2.06429200
C	-3.33082700	-0.21992300	1.47188100
C	-4.40055900	-1.71754400	2.61744200
N	-5.25761600	-0.75601900	2.43482700
N	-4.57148200	0.16841500	1.70970100
C	-5.17302700	1.42294200	1.35700000
C	-6.36580000	1.39205100	0.62472000
C	-4.56722700	2.60287100	1.80241100
C	-6.96002000	2.61915700	0.33920000
C	-5.21032600	3.79964500	1.48436800
C	-6.39983300	3.82771500	0.75933800
H	-7.88296200	2.62837400	-0.23617400
H	-4.76472200	4.73325900	1.81446800
C	-7.07617100	5.13200200	0.42814600
H	-8.12206500	5.12137900	0.74751700
H	-6.57236300	5.97143900	0.91162800
H	-7.06348100	5.30916700	-0.65197100
C	-3.29529000	2.60937400	2.61355200
H	-3.33733100	1.87823200	3.42772000
H	-2.41130700	2.37475200	2.00904800
H	-3.14398700	3.59794600	3.05070100
C	-6.96527300	0.09968200	0.14024900
H	-6.20575700	-0.58833000	-0.23810200
H	-7.48151300	-0.42317900	0.95050000
H	-7.68512300	0.29711300	-0.65665600
H	-2.56211800	0.35001200	0.96491700
B	-5.54499800	-3.22440800	-0.28072500
F	-4.57298500	-2.21094900	-0.09734200
F	-6.57491600	-2.71450500	-1.08302700
F	-6.06689600	-3.58052700	0.97252100
F	-4.95710600	-4.32701800	-0.89009300
N	-2.93634500	-0.11311700	-2.92124100
C	-2.03655600	0.86578900	-3.51692300
C	-2.54335800	1.72452600	-4.68556900
H	-1.14954800	0.31870200	-3.86333400
H	-1.68574100	1.51765300	-2.71004100
H	-1.69716800	2.25975300	-5.12742700

H	-2.99329500	1.10949900	-5.47080900
H	-3.27929900	2.47231300	-4.37859500
C	-3.45268900	-1.07859500	-3.88203100
C	-4.01455900	-2.32277000	-3.20913700
H	-2.61178800	-1.36467400	-4.52531000
H	-4.21852500	-0.64147100	-4.54811900
H	-4.27724300	-3.07073300	-3.96351600
H	-3.27252000	-2.75388400	-2.53189600
H	-4.91054000	-2.11192600	-2.62108400
C	-3.93909600	0.42389900	-2.00553300
C	-5.19784900	1.03067700	-2.64319900
H	-3.43370600	1.17718300	-1.38419900
H	-4.24572800	-0.38437500	-1.32998500
H	-5.77759300	1.57226200	-1.89114200
H	-4.95591400	1.73170700	-3.44591900
H	-5.83936400	0.24944500	-3.06388200
C	1.40800100	0.64969300	-1.12421100
C	0.36600500	0.99362700	-0.23267400
H	1.79519800	-0.35568600	-0.95250500
C	0.24651700	0.22935000	0.97892400
H	1.00667900	-0.56923200	1.08866200
O	-0.63088500	0.35400500	1.84051200
C	1.48197900	1.01873600	-2.56198000
C	2.13085600	0.13275500	-3.43436900
C	0.94308700	2.19805800	-3.09500600
C	2.22425400	0.40202600	-4.79507000
H	2.53592300	-0.79615300	-3.04311500
C	1.04974600	2.47452200	-4.45541200
H	0.43454600	2.90150000	-2.44657700
C	1.68223500	1.57706500	-5.31257700
H	2.71752700	-0.30833600	-5.45075700
H	0.62972600	3.39623100	-4.84597100
H	1.75466400	1.79259500	-6.37365700
C	-0.54699500	2.07537200	-0.37349400
C	-1.37226000	2.96925800	-0.42286500
C	-2.29731400	4.06153900	-0.52748800
C	-3.29850000	4.05773400	-1.51129900
C	-2.19186100	5.16209000	0.33726200
C	-4.17181400	5.13273400	-1.62645600
H	-3.37972900	3.20850600	-2.18220500
C	-3.06256300	6.23910600	0.20935500
H	-1.41547600	5.16398700	1.09568900
C	-4.05374800	6.22762200	-0.77131800
H	-4.94353800	5.11674600	-2.39016700

H	-2.96736000	7.08971400	0.87683700
H	-4.73263300	7.06892800	-0.86877000
C	6.89670800	-1.06725000	-1.70741200
C	5.79125600	-0.66802000	-0.96030700
C	4.58841100	-1.34360200	-1.01089200
C	4.49185200	-2.43423500	-1.86537000
C	5.56006100	-2.83038700	-2.66364200
C	6.77605700	-2.14253000	-2.57977100
C	8.09753500	-0.23284800	-1.31326400
C	7.70499200	0.26458600	0.08808000
C	6.17222800	0.46419000	-0.03583500
H	3.74304800	-1.06504200	-0.39187100
H	5.45741900	-3.68397100	-3.32360700
H	7.62185800	-2.47723700	-3.17137800
H	9.03041800	-0.79783100	-1.26909300
H	8.22151000	1.17679100	0.40851500
H	5.94153900	1.45738300	-0.43529900
H	8.23791200	0.61659800	-1.99013700
Br	2.83650600	-3.35205600	-1.86585700
O	7.98435200	-0.80748700	0.97533600
C	7.56173500	-0.57105800	2.29898400
H	7.79359200	-1.45522900	2.89226000
H	8.07608200	0.29750000	2.73298300
N	5.49424100	0.31253800	1.25370900
C	4.17868000	0.45476900	1.54801500
C	6.08494600	-0.32162500	2.31169700
N	5.21410400	-0.58991600	3.24076400
N	4.03933900	-0.10532800	2.75310500
C	2.81872600	-0.37512100	3.46981900
C	2.40235400	0.54198300	4.43591700
C	2.15434100	-1.57143600	3.19293000
C	1.22201300	0.25477900	5.11419200
C	0.99382700	-1.82062000	3.92553700
C	0.49978300	-0.91283600	4.86184500
H	0.85866300	0.95870600	5.85783700
H	0.46878700	-2.75830800	3.76236100
C	-0.80147300	-1.17867200	5.57081200
H	-0.88599900	-0.58681400	6.48409500
H	-1.64681700	-0.90827700	4.92513800
H	-0.90275600	-2.23503700	5.83411700
C	2.63790500	-2.55657300	2.15564100
H	2.23495800	-2.33532400	1.15810600
H	3.72866400	-2.57366500	2.08030100
H	2.30203800	-3.56369800	2.41193400

C	3.19914500	1.78679200	4.70824500
H	4.22783300	1.54034600	4.98881000
H	3.23002000	2.40788800	3.80816900
H	2.74912600	2.36082100	5.51923000
C	2.85548800	3.11603600	-0.79885500
C	3.18005200	1.66509400	-0.48321000
H	1.85620000	3.35474100	-0.41907100
C	3.14814300	1.35710300	0.89659500
O	2.30539400	1.82262300	1.68139600
C	3.88506900	4.02031200	-0.15645500
C	5.12611200	4.22746100	-0.76857900
C	3.64643200	4.60438400	1.09135600
C	6.11021200	4.99197200	-0.14645200
H	5.31701300	3.78796500	-1.74593200
C	4.62906300	5.37086200	1.71524800
H	2.68696500	4.44169500	1.57329100
C	5.86430400	5.56481600	1.10071700
H	7.06564600	5.14757800	-0.63805300
H	4.42773000	5.81954500	2.68323500
H	6.62816000	6.16351400	1.58628200
H	3.94015200	1.20737100	-1.10920500
H	2.85560300	3.26399000	-1.88062900

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C	1.62459000	-4.35071700	0.50766700
C	1.99730200	-3.02615400	0.27009100
C	2.25108100	-2.13352600	1.30476300
C	2.12587400	-2.62769000	2.60081700
C	1.72857200	-3.93539700	2.86535700
C	1.47155200	-4.80775000	1.80911500
C	1.46534400	-5.10467700	-0.79307900
C	2.24053000	-4.23932400	-1.79255400
C	2.05928500	-2.81204100	-1.22705800
H	2.60728000	-1.11721700	1.15214900
H	1.64886600	-4.27383800	3.89193800
H	1.18521300	-5.83504800	2.01005200
H	1.87151800	-6.11796400	-0.76674700
H	1.87623900	-4.31470000	-2.82615700
H	1.13756400	-2.38314600	-1.62507000
H	0.41025800	-5.16413900	-1.08693000
Br	2.57489100	-1.51109000	4.06379800
O	3.59969400	-4.62247400	-1.72716800
C	4.43576000	-3.87608000	-2.58122000
H	5.46318600	-4.16800400	-2.37434100

H	4.19352700	-4.06758700	-3.63622800
N	3.14674500	-1.95502200	-1.68673100
C	3.26754900	-0.63043000	-1.59166200
C	4.27883500	-2.41257800	-2.29956100
N	5.06029800	-1.42295300	-2.62743800
N	4.41371600	-0.31524400	-2.17006700
C	4.95186200	1.00062600	-2.37445500
C	6.26904900	1.25244900	-1.96322500
C	4.14350800	1.96221600	-2.99232500
C	6.77453200	2.52629000	-2.21149700
C	4.70347200	3.22645600	-3.19680600
C	6.01110500	3.52541300	-2.81879500
H	7.79031800	2.75035300	-1.89537900
H	4.09644000	3.99123300	-3.67578700
C	6.58547000	4.90199100	-3.02707300
H	7.56995800	4.84896700	-3.49882600
H	5.93382900	5.51368600	-3.65439100
H	6.71097500	5.41255700	-2.06685700
C	2.72670300	1.68712200	-3.43548700
H	2.63333100	0.71030900	-3.91915800
H	2.01435900	1.69918500	-2.60082100
H	2.41069200	2.45158100	-4.14750900
C	7.10333800	0.22356200	-1.24911000
H	6.51496900	-0.34539400	-0.52630100
H	7.52814100	-0.49529700	-1.95559800
H	7.92588800	0.71697700	-0.72740200
H	2.55595200	0.05310700	-1.15061700
B	5.69458100	-2.54957900	0.83482400
F	4.91057000	-1.46383500	0.36344100
F	7.00361400	-2.10203900	1.02467500
F	5.67385700	-3.55684600	-0.14081000
F	5.15401000	-3.02121400	2.02844100
N	3.65015100	1.22169700	2.34725700
C	2.46181600	1.87296200	2.88198600
C	2.53586400	3.38046500	3.15093800
H	2.20114300	1.35309300	3.81256800
H	1.63955200	1.67854500	2.18736200
H	1.61348600	3.71041400	3.64050700
H	3.37643700	3.63266100	3.80625300
H	2.63808700	3.95042000	2.22290600
C	4.75740700	1.16831600	3.29093400
C	5.78835500	0.11249400	2.91778000
H	4.32915000	0.91281800	4.26870400
H	5.25065400	2.14940800	3.41690000

H	6.60502000	0.11025000	3.64642800
H	5.32501700	-0.87551800	2.89765200
H	6.22208100	0.28736700	1.92911000
C	4.02510200	1.62414800	0.99305800
C	4.94759300	2.84222400	0.84658500
H	3.08745000	1.81778100	0.45173700
H	4.50989900	0.76566100	0.50914100
H	5.02335500	3.12030500	-0.20943100
H	4.57882800	3.71029400	1.39833900
H	5.95926100	2.61648700	1.20115100
C	-0.93640900	-0.02981700	1.39591000
C	-0.27433000	0.43230700	0.24390200
H	-1.04502100	-1.11484100	1.45595000
C	-0.13860300	-0.49468200	-0.84082700
H	-0.53232200	-1.50984500	-0.61418000
O	0.35251200	-0.26370200	-1.95364500
C	-0.89388900	0.66118000	2.69534500
C	-0.55954700	-0.09535100	3.82311800
C	-1.14881100	2.03225400	2.84239200
C	-0.43000700	0.51281500	5.06885200
H	-0.35207700	-1.15583200	3.71215200
C	-1.04646000	2.63123900	4.09079600
H	-1.43657900	2.62489100	1.97910000
C	-0.67579100	1.87545000	5.20583300
H	-0.13767200	-0.08225600	5.92800300
H	-1.25198000	3.69169900	4.19747600
H	-0.58461900	2.35104100	6.17686300
C	0.22263700	1.75394500	0.07742700
C	0.63713700	2.89113400	-0.04387900
C	1.19713400	4.20531100	-0.12509200
C	2.37533100	4.41658200	-0.85529800
C	0.61040700	5.28064200	0.56090500
C	2.95656900	5.67782600	-0.89834700
H	2.84127000	3.57999400	-1.36468800
C	1.19661100	6.54007900	0.51059600
H	-0.28820200	5.11294900	1.14746000
C	2.36896900	6.74314300	-0.21759500
H	3.87628800	5.82269500	-1.45813200
H	0.74142100	7.36540400	1.04790700
H	2.82511700	7.72690900	-0.24815200
C	-3.98740800	4.05224200	-1.08055000
C	-4.11263700	2.67468100	-0.88618700
C	-5.30261100	2.09827100	-0.46581600
C	-6.37048700	2.95718200	-0.21461100

C	-6.26681900	4.33476200	-0.38082000
C	-5.06475800	4.88852200	-0.82301200
C	-2.60350400	4.39057800	-1.58867900
C	-2.10641100	3.04762300	-2.12676600
C	-2.77277800	2.02968000	-1.17192100
H	-5.41348900	1.02652500	-0.32439900
H	-7.12291400	4.96737200	-0.17728500
H	-4.98640200	5.96035300	-0.97324100
H	-2.59594900	5.14957200	-2.37348700
H	-1.01589200	2.93731800	-2.14344000
H	-2.17420400	1.94277600	-0.26315400
H	-1.94841400	4.72864300	-0.77692400
Br	-8.01483900	2.21995300	0.37335600
O	-2.64667700	2.89697000	-3.43096700
C	-2.26974500	1.67909800	-4.02541200
H	-2.76384000	1.60127100	-4.99400000
H	-1.18109400	1.62579200	-4.17048800
N	-2.83259000	0.70598700	-1.79796400
C	-3.07650300	-0.51615600	-1.26807000
C	-2.67958300	0.53653100	-3.14759600
N	-2.86120200	-0.70595800	-3.48661000
N	-3.10435900	-1.34722500	-2.31539800
C	-3.42944700	-2.74968800	-2.34429100
C	-2.47154300	-3.62936000	-2.84606700
C	-4.69392000	-3.15414600	-1.89978500
C	-2.80339100	-4.98531000	-2.86782100
C	-4.97191100	-4.51643000	-1.95039900
C	-4.03965100	-5.44595500	-2.42019600
H	-2.07141100	-5.69554100	-3.24436100
H	-5.94496300	-4.86236900	-1.61039000
C	-4.36940200	-6.91566400	-2.42543600
H	-3.64963900	-7.48140600	-3.01995300
H	-4.35507300	-7.31608500	-1.40704800
H	-5.36877100	-7.09168300	-2.83155200
C	-5.71523100	-2.18317300	-1.36800200
H	-5.50731000	-1.93243600	-0.32035900
H	-5.73792100	-1.25596900	-1.94958300
H	-6.71085600	-2.62852700	-1.40467100
C	-1.13787700	-3.16091900	-3.36759800
H	-1.21487200	-2.88221900	-4.42296700
H	-0.76050800	-2.28057100	-2.83898400
H	-0.40577300	-3.96801500	-3.28976600
C	-3.65384800	-0.62316100	2.54515200
C	-3.22882600	-0.06970400	1.20502500

H	-3.66183200	0.18107900	3.28739600
C	-3.12157200	-0.99993500	0.16441500
O	-2.92176400	-2.22130900	0.30746100
C	-5.02547900	-1.25577200	2.40964100
C	-5.17054200	-2.64457000	2.39866300
C	-6.15589800	-0.46067300	2.18450900
C	-6.41705600	-3.22936400	2.17725300
H	-4.29292700	-3.26681000	2.54380900
C	-7.40039600	-1.04172900	1.95863900
H	-6.05953400	0.62424500	2.17279100
C	-7.53532400	-2.43018400	1.95614800
H	-6.51023000	-4.31107800	2.16904900
H	-8.26322400	-0.40845000	1.77882600
H	-8.50543400	-2.88339800	1.77866800
H	-3.49140600	0.95945500	0.99673300
H	-2.93933100	-1.38021800	2.88882900

M4C

C	2.24051500	-4.38464100	0.82162300
C	2.36792900	-3.03403000	0.49357700
C	2.61359400	-2.06285900	1.45840900
C	2.74664100	-2.50701600	2.77140200
C	2.61201000	-3.84696200	3.12597700
C	2.35207900	-4.79774800	2.14238900
C	1.98368100	-5.21772000	-0.41262300
C	2.44147900	-4.30273000	-1.55199800
C	2.16740500	-2.88335100	-1.00014100
H	2.75266300	-1.00811500	1.23150000
H	2.72733700	-4.14127400	4.16269400
H	2.26081900	-5.84587000	2.40901000
H	2.53767300	-6.15864000	-0.43257400
H	1.91685600	-4.47439400	-2.50183700
H	1.14937700	-2.57829700	-1.25219000
H	0.91635500	-5.44614900	-0.51660200
Br	3.15109300	-1.25839800	4.14129300
O	3.82989300	-4.50914400	-1.72364600
C	4.38997100	-3.70616400	-2.73617900
H	5.46585900	-3.86560500	-2.72965100
H	3.97482900	-3.96774300	-3.72020400
N	3.04927700	-1.92211600	-1.65490600
C	3.02065400	-0.58954600	-1.60034200
C	4.10637000	-2.26410700	-2.45007300
N	4.69610500	-1.20368700	-2.92108900
N	4.00885200	-0.16341500	-2.37079300

C	4.36161600	1.19318900	-2.68339200
C	5.69406300	1.59160300	-2.49942400
C	3.36999200	2.04379100	-3.18389400
C	6.01832600	2.89701300	-2.85993200
C	3.75369100	3.34889900	-3.50570200
C	5.06680500	3.79041800	-3.35688000
H	7.04244100	3.23386700	-2.71899600
H	2.99961300	4.03134700	-3.89072600
C	5.45634100	5.20505200	-3.69734200
H	6.28932200	5.22178700	-4.40538300
H	4.61988500	5.75226400	-4.13665300
H	5.78113700	5.74010300	-2.79964300
C	1.93989800	1.60540900	-3.37957800
H	1.87829200	0.62385200	-3.85964300
H	1.39095900	1.51995200	-2.43325300
H	1.41775400	2.33010000	-4.00831100
C	6.73117700	0.68250300	-1.89758500
H	6.32536000	0.10071300	-1.06729600
H	7.10335100	-0.03249100	-2.63676500
H	7.57491900	1.27498000	-1.53803500
H	2.30400100	0.01513900	-1.06149700
B	6.05878700	-2.16973700	0.38382100
F	5.05792100	-1.22093600	0.05415100
F	7.29575800	-1.52001000	0.42173200
F	6.07641100	-3.15503500	-0.61553200
F	5.76054100	-2.74113200	1.61813400
N	3.77081000	1.45489900	2.18925800
C	2.65316500	2.08127200	2.88455100
C	2.71789100	3.59424000	3.12733300
H	2.56292700	1.57115100	3.85042400
H	1.73377200	1.84613400	2.33418000
H	1.86697700	3.89741800	3.74751900
H	3.63771700	3.88070500	3.64851500
H	2.65717600	4.15869200	2.19259600
C	5.00841700	1.47888700	2.95599000
C	6.02789000	0.46507100	2.45718800
H	4.74460500	1.23438300	3.99295000
H	5.46603900	2.48486400	2.98366400
H	6.93463300	0.51499200	3.06844000
H	5.62216100	-0.54794900	2.50875900
H	6.31674200	0.64229800	1.41795300
C	3.92272100	1.81940200	0.78269200
C	4.74035200	3.07967200	0.46661800
H	2.90748900	1.93372500	0.37704900

H	4.38763200	0.96950300	0.26417700
H	4.63066800	3.33457900	-0.59186000
H	4.41502100	3.94110400	1.05454800
H	5.80676900	2.91685200	0.65889100
C	-1.30691700	-0.25802300	1.68926800
C	-0.48448100	0.12558800	0.46220600
H	-1.08726100	-1.31171600	1.91066300
C	-0.27613900	-0.80995100	-0.54713200
H	-0.57948700	-1.84743400	-0.27223300
O	0.18345100	-0.61664000	-1.71023200
C	-0.94742300	0.54639000	2.91901300
C	-0.12179400	-0.01751800	3.89016500
C	-1.38244600	1.86602500	3.08578900
C	0.25978600	0.71463200	5.01256300
H	0.25113100	-1.02950100	3.75499300
C	-1.00342400	2.59976600	4.20534500
H	-2.01726700	2.32860000	2.33245700
C	-0.18213800	2.02368600	5.17534600
H	0.92063600	0.26013700	5.74462400
H	-1.34843800	3.62260800	4.32228400
H	0.11487300	2.59735900	6.04751000
C	-0.02496500	1.44752600	0.29192900
C	0.31628200	2.61562400	0.18958400
C	0.77673600	3.96499000	0.14009600
C	1.81423400	4.33169400	-0.73076200
C	0.21063200	4.94393500	0.97608200
C	2.28548300	5.63858700	-0.75439200
H	2.26261200	3.57643000	-1.36713400
C	0.68618300	6.24943900	0.94423700
H	-0.58534000	4.65932300	1.65796900
C	1.72545700	6.60300800	0.08255200
H	3.09979300	5.89778700	-1.42566500
H	0.24802300	6.99503700	1.60000300
H	2.09644800	7.62231300	0.06635200
C	-3.73820400	3.84814000	-1.28879000
C	-3.98680500	2.50255200	-1.00374600
C	-5.20434400	2.07213600	-0.50048400
C	-6.17302100	3.04730400	-0.26461200
C	-5.94622400	4.39468100	-0.52475300
C	-4.71753600	4.79998200	-1.04625600
C	-2.34633700	4.02512000	-1.85071700
C	-1.98302200	2.60930700	-2.30086500
C	-2.71993400	1.72367500	-1.27250100
H	-5.41838400	1.02547500	-0.29907400

H	-6.72874300	5.11875000	-0.33031100
H	-4.54186800	5.84801600	-1.26597400
H	-2.29759800	4.72179000	-2.69015000
H	-0.90794200	2.39387000	-2.31805900
H	-2.10536200	1.65598200	-0.37752300
H	-1.64617800	4.36252400	-1.07800200
Br	-7.85627900	2.52790000	0.43365800
O	-2.56279700	2.42430100	-3.58482100
C	-2.32146400	1.14174600	-4.10289800
H	-2.86574600	1.04018900	-5.04210400
H	-1.24954800	0.97777100	-4.28740700
N	-2.89159900	0.36496200	-1.79986700
C	-3.12918300	-0.81280600	-1.18028800
C	-2.77090200	0.09410400	-3.13090500
N	-2.98396800	-1.16978000	-3.37499800
N	-3.20758000	-1.71684300	-2.16115900
C	-3.53095900	-3.11923100	-2.08563700
C	-2.54080400	-4.03320300	-2.43607400
C	-4.82428600	-3.47783300	-1.68909200
C	-2.88051300	-5.38620600	-2.35728700
C	-5.10693900	-4.83727400	-1.63405800
C	-4.14728400	-5.80385600	-1.95661700
H	-2.12945000	-6.12793900	-2.61663000
H	-6.10182900	-5.15315900	-1.33057900
C	-4.48565900	-7.26780000	-1.85413100
H	-3.72407900	-7.88558700	-2.33319300
H	-4.55787100	-7.57188500	-0.80538200
H	-5.44996100	-7.47985200	-2.32280400
C	-5.85569900	-2.44688100	-1.31296600
H	-5.67363400	-2.05572100	-0.30430000
H	-5.86303900	-1.60497900	-2.01267000
H	-6.85122800	-2.89322900	-1.30782100
C	-1.17234400	-3.60670800	-2.90058400
H	-1.15953400	-3.50028200	-3.99005400
H	-0.85233100	-2.64626700	-2.48325100
H	-0.44033400	-4.37314800	-2.63554500
C	-3.63593500	-0.70302400	2.67043200
C	-2.85807500	-0.23612400	1.41610300
H	-3.64531600	0.13710900	3.37088500
C	-3.07906100	-1.22154500	0.29140900
O	-3.11420700	-2.40897300	0.50494900
C	-5.04300700	-1.18947100	2.40707800
C	-5.33351400	-2.55612900	2.47941000
C	-6.07218000	-0.30563100	2.06657900

C	-6.61544500	-3.03226100	2.21979600
H	-4.53818900	-3.25088500	2.73237000
C	-7.35569800	-0.78124800	1.79629200
H	-5.87961500	0.76558100	2.02674500
C	-7.63138100	-2.14394000	1.87408200
H	-6.81800500	-4.09675000	2.28317100
H	-8.13946600	-0.08187200	1.52878100
H	-8.63183800	-2.50990000	1.66733800
H	-3.19146700	0.76562000	1.12437800
H	-3.06230000	-1.50562000	3.14486400
M4			
C	0.50108200	-1.24360200	2.27986900
C	1.07224500	-2.17347600	1.21101900
H	-0.25627100	-1.80256900	2.84766100
C	0.21605300	-3.05124500	0.51990100
H	-0.77795700	-3.19029200	1.00897600
O	0.42150100	-3.62814900	-0.57322400
C	1.53456000	-0.73857600	3.26537000
C	1.56063000	-1.23232800	4.56999300
C	2.48195400	0.22353500	2.89496800
C	2.51198700	-0.78528900	5.48580600
H	0.82854500	-1.97734000	4.87039000
C	3.42878100	0.67762100	3.80771900
H	2.48539500	0.61980700	1.88170500
C	3.44838100	0.17194800	5.10732900
H	2.51582900	-1.18270000	6.49574300
H	4.15237200	1.42815800	3.50441900
H	4.18707600	0.52588400	5.81903800
C	2.41601800	-2.07349300	0.81154300
C	3.57923600	-1.95247800	0.45506800
C	4.92507600	-1.77378100	0.02473400
C	5.43073300	-2.47915400	-1.08356400
C	5.76391500	-0.84910900	0.67549300
C	6.73076600	-2.26069600	-1.52359500
H	4.79092600	-3.19606700	-1.58876800
C	7.06194400	-0.63868400	0.22681500
H	5.37822100	-0.30611200	1.53326000
C	7.55300400	-1.34035500	-0.87426300
H	7.10474800	-2.81299600	-2.38008800
H	7.69544900	0.07805200	0.74019300
H	8.56681800	-1.17236800	-1.22194600
C	2.47395800	1.54594200	-2.14354900
C	1.22264200	1.28839000	-1.57598400

C	0.33612900	2.30667300	-1.26254100
C	0.75614400	3.61277500	-1.51179500
C	2.00203000	3.89792500	-2.05994700
C	2.86885800	2.85376100	-2.38395000
C	3.21449400	0.25459900	-2.40591000
C	2.09465600	-0.78747700	-2.37425200
C	1.10945000	-0.19968000	-1.34177200
H	-0.65045000	2.11544800	-0.84822500
H	2.28681300	4.92774800	-2.24086300
H	3.83535200	3.07084400	-2.82705600
H	3.73475400	0.23423200	-3.36589600
H	2.40640500	-1.79987200	-2.09207500
H	1.45699400	-0.47159000	-0.34695300
H	3.94085200	0.04664800	-1.61245000
Br	-0.40266500	5.05259500	-1.08995600
O	1.48893400	-0.77585100	-3.66071600
C	0.41971800	-1.68144600	-3.75670800
H	-0.05477000	-1.55279400	-4.73000100
H	0.76291300	-2.72089900	-3.65588000
N	-0.22403500	-0.78454800	-1.51699600
C	-1.27068600	-0.89518400	-0.66926600
C	-0.57338100	-1.43486200	-2.66264400
N	-1.79899500	-1.87751000	-2.59783700
N	-2.21763200	-1.53486300	-1.36126800
C	-3.57531800	-1.84005500	-0.98718300
C	-3.92464400	-3.18024200	-0.84789500
C	-4.46681300	-0.77398200	-0.81731900
C	-5.25235900	-3.44645000	-0.49954900
C	-5.77333500	-1.09926400	-0.47555300
C	-6.18188300	-2.42809100	-0.30794500
H	-5.55897100	-4.48161700	-0.37426600
H	-6.49348600	-0.29693900	-0.33529800
C	-7.60542600	-2.73577400	0.07653600
H	-7.78108500	-3.81211100	0.11796100
H	-7.84058100	-2.31312600	1.05772700
H	-8.30521900	-2.30011400	-0.64210800
C	-4.02940500	0.65909600	-0.97047900
H	-3.45574300	0.99373100	-0.09745600
H	-3.41097000	0.80180700	-1.86232300
H	-4.89918400	1.31281200	-1.05114900
C	-2.94485800	-4.30285700	-1.07333500
H	-2.99741400	-4.63995100	-2.11377700
H	-1.90560400	-4.01862700	-0.88081300
H	-3.20116700	-5.15196900	-0.43664400

C	-0.92566300	0.83665500	2.78550300
C	-0.30048000	-0.02954000	1.66540700
H	-0.11641900	1.43264200	3.21749500
C	-1.40281500	-0.64007000	0.83105500
O	-2.41577700	-1.04984700	1.34474200
C	-2.06234800	1.73093800	2.34496700
C	-3.37764200	1.41919300	2.70587800
C	-1.83825800	2.86477200	1.55706700
C	-4.44293200	2.21460700	2.29364500
H	-3.56296600	0.53444300	3.30766400
C	-2.90511000	3.65720600	1.13240300
H	-0.82225500	3.14500200	1.28286400
C	-4.20906900	3.33640400	1.50127800
H	-5.45505700	1.95371300	2.58664400
H	-2.71191900	4.52771700	0.51561700
H	-5.03646600	3.95697100	1.17270300
H	0.35569400	0.58840700	1.04303300
H	-1.28267600	0.16558500	3.57348600
TS5			
C	0.53636400	0.34312400	2.73950500
C	1.12031000	-1.04459200	2.53223200
H	0.11937000	0.37507500	3.75614100
C	0.24387300	-2.06428400	2.43223800
H	0.55839500	-3.10121700	2.32175100
O	-1.08283100	-1.87592800	2.43172400
C	1.53206800	1.47639800	2.59464200
C	1.75994400	2.37186200	3.63907600
C	2.17980600	1.69711500	1.37339800
C	2.60276300	3.47047900	3.46552200
H	1.26278500	2.21702700	4.59313100
C	3.00398400	2.80191000	1.18741600
H	2.04282600	0.99219300	0.55974100
C	3.21850400	3.69477400	2.23789200
H	2.76586900	4.15765200	4.28956400
H	3.46349000	2.96868700	0.21669000
H	3.85966400	4.55898200	2.09840400
C	2.49503200	-1.26683900	2.23958000
C	3.61970500	-1.41840600	1.80636100
C	4.91630300	-1.53953000	1.21138400
C	5.66655000	-2.71923900	1.32907200
C	5.41998200	-0.47257400	0.44939300
C	6.89896500	-2.82554400	0.69417400
H	5.27414000	-3.54273000	1.91640600

C	6.65349100	-0.58859000	-0.18030700
H	4.82905000	0.43403900	0.35703000
C	7.39485400	-1.76364800	-0.06102600
H	7.47427800	-3.74057500	0.78867100
H	7.03601400	0.23960600	-0.76824000
H	8.35649000	-1.85167900	-0.55560000
C	2.69765600	-1.08323000	-1.92864100
C	1.43324700	-0.68057100	-1.48506700
C	0.98829700	0.62312800	-1.64553900
C	1.89069800	1.53959900	-2.18787800
C	3.16861400	1.17233700	-2.59578200
C	3.57137800	-0.15903000	-2.48160300
C	2.89137200	-2.56619100	-1.70958000
C	1.46247500	-3.05507300	-1.46241600
C	0.80872100	-1.85369100	-0.75522700
H	-0.00676700	0.94004200	-1.34411600
H	3.83705000	1.91928200	-3.00807000
H	4.55877900	-0.45878700	-2.81848500
H	3.33824200	-3.07641400	-2.56561800
H	1.39672100	-3.97705400	-0.87066900
H	1.14179000	-1.82872600	0.28070800
H	3.51411500	-2.75686400	-0.82716500
Br	1.39958100	3.36669800	-2.31070400
O	0.84737700	-3.23078500	-2.73070900
C	-0.49744300	-3.64193000	-2.63629300
H	-0.92943600	-3.60496900	-3.63696700
H	-0.56585400	-4.67340200	-2.26228600
N	-0.64481000	-1.97661200	-0.76570800
C	-1.59251300	-1.40918800	0.03781500
C	-1.27274000	-2.75431500	-1.70481700
N	-2.56052600	-2.69021100	-1.56802300
N	-2.73547500	-1.85312100	-0.49452800
C	-4.09232600	-1.45370700	-0.21120500
C	-4.84192000	-2.17810800	0.71616600
C	-4.60515600	-0.40116500	-0.96284400
C	-6.16182400	-1.78419700	0.90806200
C	-5.93592400	-0.04224900	-0.73456200
C	-6.72170900	-0.71572000	0.19812800
H	-6.77122000	-2.32165100	1.63091400
H	-6.36306900	0.77855600	-1.30551300
C	-8.15185200	-0.30977500	0.44685700
H	-8.27236000	0.08554100	1.46004700
H	-8.47321000	0.46047100	-0.25711500
H	-8.82522600	-1.16602800	0.34991200

C	-3.75004700	0.30435600	-1.98087800
H	-2.90369300	0.80555800	-1.49606300
H	-3.35197600	-0.40419600	-2.71416400
H	-4.32715300	1.06540900	-2.50733500
C	-4.21773900	-3.30777800	1.48533300
H	-3.77993800	-4.04922600	0.80930800
H	-3.41778100	-2.91292000	2.11916200
H	-4.95959600	-3.80664200	2.11132400
C	-1.41817500	1.82303200	2.06680800
C	-0.64146600	0.53576600	1.74780400
H	-0.70184500	2.57809300	2.40661900
C	-1.64116500	-0.65996600	1.73877000
O	-2.81852800	-0.48098400	2.05194200
C	-2.17235000	2.39723400	0.89300000
C	-3.56693900	2.39992700	0.83521600
C	-1.45594600	2.99648900	-0.14915300
C	-4.22976300	3.02785900	-0.21833900
H	-4.12655400	1.89830200	1.61868000
C	-2.11359500	3.59753200	-1.21933700
H	-0.36740400	3.00876400	-0.10639200
C	-3.50740800	3.63086400	-1.24574200
H	-5.31563800	3.03288900	-0.24143300
H	-1.53509600	4.04465200	-2.02211800
H	-4.02646200	4.11198700	-2.06893900
H	-0.19306600	0.62429200	0.75378500
H	-2.10526300	1.61481900	2.88947000
P			
C	-0.34286000	-0.68744000	0.85526800
C	0.50639700	-1.71701300	0.11970300
H	-0.33458900	-0.93036100	1.92710700
C	-0.05974800	-2.83752100	-0.34497600
H	0.46961000	-3.61440900	-0.88111400
O	-1.37494300	-3.16901200	-0.14370000
C	0.19861400	0.71908500	0.68776900
C	0.57955600	1.46916100	1.79882300
C	0.33990200	1.27628100	-0.58747400
C	1.09090500	2.75783700	1.64453300
H	0.47828100	1.04144500	2.79260300
C	0.84827400	2.56104600	-0.74494900
H	0.07096900	0.69249100	-1.46496700
C	1.22563500	3.30654200	0.37277800
H	1.38276200	3.32952700	2.51948200
H	0.95701800	2.97938100	-1.74028600

H	1.62308800	4.30867000	0.24975300
C	1.89523300	-1.46110800	-0.06096900
C	3.05123100	-1.11321100	-0.17017500
C	4.38788800	-0.61627800	-0.28566100
C	5.44702800	-1.44603700	-0.67931000
C	4.63380500	0.73623700	0.00114900
C	6.73260600	-0.92717100	-0.78323400
H	5.25237500	-2.49018700	-0.89980900
C	5.92257200	1.24440300	-0.10434800
H	3.80445500	1.36997300	0.30265300
C	6.97349900	0.41552200	-0.49623100
H	7.54936000	-1.57284500	-1.08848900
H	6.10837500	2.28992800	0.11845500
H	7.97869200	0.81564900	-0.57805300
C	-2.78997700	0.10123800	1.06293300
C	-1.78893000	-0.79991900	0.32707800
H	-2.26753100	1.02043100	1.34646800
C	-2.25465300	-2.24161200	0.34355800
O	-3.32947200	-2.62688700	0.71269500
C	-3.98728800	0.45953500	0.21282400
C	-5.23290700	-0.13880000	0.40678100
C	-3.84569300	1.40685400	-0.80656100
C	-6.31673200	0.20448200	-0.39916600
H	-5.34487200	-0.88590100	1.18642300
C	-4.92457300	1.74907400	-1.61605500
H	-2.87747300	1.88058300	-0.96025300
C	-6.16576400	1.14770100	-1.41265800
H	-7.28019700	-0.26805100	-0.23573000
H	-4.79893700	2.48781100	-2.40134700
H	-7.00999400	1.41405200	-2.04042500
H	-1.76091400	-0.51878800	-0.73664700
H	-3.10926500	-0.39554100	1.98363600
TS1'			
C	-4.50501800	-1.67997900	-0.79178900
C	-3.17207000	-1.26161400	-0.78532500
C	-2.83522000	0.08486900	-0.81777700
C	-3.88363300	1.00297500	-0.82104800
C	-5.21897900	0.60973300	-0.80463700
C	-5.53415600	-0.74803000	-0.79863300
C	-4.58905600	-3.18772700	-0.81358500
C	-3.21070400	-3.59598900	-0.29720800
C	-2.26954300	-2.48365000	-0.82427400
H	-1.80109100	0.40540800	-0.88360700

H	-6.00144700	1.35981600	-0.80450400
H	-6.57249800	-1.06447700	-0.79489700
H	-5.37710200	-3.59927300	-0.17937000
H	-2.88787800	-4.59955700	-0.60198100
H	-1.95515700	-2.67760100	-1.85377100
H	-4.73832900	-3.55696100	-1.83412700
Br	-3.48859900	2.85941000	-0.87766200
O	-3.29310600	-3.51304900	1.12056900
C	-2.09662000	-3.86832900	1.77091900
H	-2.22343600	-3.67203900	2.83648800
H	-1.87680300	-4.93712500	1.63519900
N	-1.05399900	-2.44860200	-0.00337800
C	0.15471300	-1.91354300	-0.32102300
C	-0.95844000	-3.06679200	1.22087600
N	0.23495400	-2.93959600	1.71604000
N	0.89772400	-2.22549700	0.74593600
C	2.26818400	-1.85032300	0.93667900
C	3.25154500	-2.50248300	0.19060900
C	2.55565300	-0.81164700	1.82610200
C	4.56437800	-2.05191100	0.32167900
C	3.88367300	-0.40061200	1.92594400
C	4.89405900	-0.99268900	1.16775700
H	5.34613300	-2.53399000	-0.26064600
H	4.12995200	0.42113900	2.59439300
C	6.30032300	-0.45958200	1.21731100
H	6.42206300	0.32456700	0.46149800
H	6.52612800	-0.02132100	2.19225400
H	7.03183300	-1.24392000	1.00908400
C	1.47240100	-0.17031200	2.64967300
H	0.56739500	-0.02364600	2.05612800
H	1.21024100	-0.80035800	3.50536100
H	1.79816900	0.80274400	3.02334400
C	2.90709500	-3.63405900	-0.74109200
H	2.19902600	-4.32788200	-0.27992200
H	2.44616000	-3.26121200	-1.66187300
H	3.80662900	-4.18698500	-1.01704500
C	2.75228700	0.09250300	-1.88055200
C	1.45090800	0.11809800	-1.53213300
H	3.03820800	-0.71346500	-2.55808000
C	0.52117800	-0.94064500	-2.11571000
H	1.10390700	-1.79559700	-2.51769300
O	-0.57543600	-0.63697500	-2.60572900
C	3.85232700	0.99282200	-1.51824900
C	5.04623400	0.89028600	-2.24929500

C	3.78346400	1.94323000	-0.48696100
C	6.12352000	1.73133700	-1.99125400
H	5.11820000	0.14780400	-3.03973000
C	4.86528600	2.77569700	-0.22197500
H	2.88637400	2.01854400	0.11595300
C	6.03416500	2.68359100	-0.97774800
H	7.03163500	1.64167100	-2.57863700
H	4.79505500	3.50321900	0.58058600
H	6.87174800	3.34183700	-0.77062900
C	0.81416100	1.05424400	-0.66752300
C	0.16159800	1.74292100	0.09074300
C	-0.64508800	2.51422600	0.98664200
C	-1.57184300	1.86375400	1.81588600
C	-0.56488200	3.91324200	1.00137600
C	-2.41443000	2.60588400	2.63358900
H	-1.64312600	0.78032900	1.78821800
C	-1.41393200	4.64767500	1.82077800
H	0.14999500	4.41118100	0.35487600
C	-2.34122400	3.99767600	2.63424000
H	-3.13631800	2.09771900	3.26438500
H	-1.35510500	5.73115100	1.82223500
H	-3.00587900	4.57589000	3.26768800

TS1'C

C	-1.70081900	-3.23529800	2.48012800
C	-0.79586000	-2.47090400	1.74350400
C	-0.05582400	-1.44708600	2.32580900
C	-0.28471000	-1.19659400	3.67535600
C	-1.17733700	-1.94960500	4.43577900
C	-1.88711800	-2.98541500	3.83473700
C	-2.40629300	-4.23937300	1.59904000
C	-1.57563800	-4.24985300	0.31293200
C	-0.91927300	-2.84900800	0.28684200
H	0.68319100	-0.85254800	1.79082600
H	-1.31154200	-1.72270800	5.48703200
H	-2.57947200	-3.58110200	4.42104600
H	-2.45856700	-5.24258400	2.02823000
H	-2.17558000	-4.42718700	-0.58748600
H	-1.56388200	-2.12911800	-0.22239500
H	-3.42820400	-3.91105000	1.37324900
Br	0.61392200	0.25274000	4.49878300
O	-0.58071900	-5.25041400	0.42939200
C	0.20547500	-5.35107800	-0.73793200
H	0.96513300	-6.11027700	-0.56863900

H	-0.41615900	-5.61013200	-1.60762200
N	0.32115500	-2.89395100	-0.47679200
C	1.09976700	-1.88321800	-0.86175700
C	0.86986300	-4.03395900	-0.99170800
N	1.92263700	-3.76186000	-1.70934100
N	2.05168000	-2.40985800	-1.60936500
C	3.05771000	-1.69044600	-2.33493200
C	4.39955500	-2.01409900	-2.10419800
C	2.64152900	-0.71555200	-3.24868800
C	5.35184300	-1.31859300	-2.84596700
C	3.64221200	-0.05334400	-3.96075200
C	4.99368200	-0.33516100	-3.77093400
H	6.40357700	-1.54010300	-2.68019900
H	3.35236700	0.70235900	-4.68376500
C	6.05365100	0.41798400	-4.53091800
H	6.57568600	1.11546700	-3.86768900
H	6.80020000	-0.26408200	-4.94617100
H	5.61729500	0.99766800	-5.34720500
C	1.18967500	-0.36954400	-3.47168400
H	0.54675800	-1.25526300	-3.49638300
H	0.80135300	0.28058500	-2.67741300
H	1.07863300	0.16075100	-4.41969200
C	4.79990300	-3.03051500	-1.07005000
H	4.20422900	-2.93863400	-0.15855200
H	4.65159300	-4.04951100	-1.43967100
H	5.85453100	-2.90783900	-0.81536000
H	0.94551200	-0.83352100	-0.65244200
B	2.86289600	-4.28918200	1.80550700
F	2.40178000	-3.08155900	1.22365400
F	4.26124100	-4.30486500	1.74928200
F	2.34926700	-5.36379300	1.06289900
F	2.42598000	-4.36494600	3.12362600
N	3.12838300	0.53684100	2.22954200
C	2.90584600	1.97383600	2.32569400
C	4.11410900	2.90264800	2.51074600
H	2.22792900	2.13546000	3.17467800
H	2.34626500	2.27857400	1.43544500
H	3.75335500	3.92348200	2.67413700
H	4.71033800	2.61668100	3.38217300
H	4.77751300	2.92080800	1.64189900
C	3.87578800	0.00485900	3.36217100
C	3.71944900	-1.50009300	3.51688500
H	3.48061500	0.49803200	4.25896600
H	4.94828600	0.26570200	3.31518900

H	4.21428600	-1.83355800	4.43421900
H	2.66181100	-1.76887600	3.57249700
H	4.15027100	-2.05884900	2.68271100
C	3.56300000	0.04316800	0.92430700
C	5.05564600	0.16530700	0.59136900
H	2.97420800	0.57990900	0.16639100
H	3.27891700	-1.01532000	0.85465300
H	5.22634300	-0.12400200	-0.44935000
H	5.42721900	1.18526400	0.72027200
H	5.65635700	-0.49410300	1.22605800
C	-0.77101700	2.27167700	1.92441500
C	-0.57360700	1.80808800	0.67094500
H	-1.51020700	1.72275500	2.51155300
C	-1.36975500	0.61650400	0.20285200
H	-1.94281600	0.13097000	1.01261500
O	-0.97981200	-0.03484000	-0.78221500
C	-0.18008800	3.42070000	2.60970100
C	-0.43052400	3.56362400	3.98380900
C	0.59096100	4.39946900	1.96159100
C	0.09533000	4.63356900	4.69773900
H	-1.02265700	2.80850000	4.49288200
C	1.10499100	5.47567600	2.67656700
H	0.77948000	4.32131300	0.89734800
C	0.86606400	5.59455000	4.04544800
H	-0.10028800	4.72173500	5.76131900
H	1.69629600	6.22584700	2.16040600
H	1.27491300	6.43327000	4.59939900
C	0.41168600	2.24579900	-0.26327000
C	1.27163200	2.48270700	-1.08743900
C	2.34371300	2.79161000	-1.98673200
C	3.65515700	2.88716800	-1.49550800
C	2.10242200	3.00031700	-3.35229000
C	4.70138700	3.19666900	-2.35646000
H	3.83839200	2.71628000	-0.43892500
C	3.15043400	3.33781300	-4.20179300
H	1.09253300	2.89018300	-3.73187900
C	4.45051400	3.43504600	-3.70735300
H	5.71340600	3.26110300	-1.96945900
H	2.95418000	3.51038400	-5.25526700
H	5.26776000	3.68981900	-4.37443800
C	-5.71146500	-2.19990000	-0.66348700
C	-4.66067800	-1.28476600	-0.72292100
C	-3.54126700	-1.50135500	-1.50999400
C	-3.47435600	-2.71106300	-2.19429600

C	-4.49952500	-3.65156600	-2.15110400
C	-5.63728800	-3.38611800	-1.38510900
C	-6.79686200	-1.69508700	0.26046400
C	-6.46159000	-0.20658200	0.42141500
C	-4.92455700	-0.14788800	0.23896600
H	-2.71860000	-0.79328400	-1.55763500
H	-4.40973700	-4.57995600	-2.70356900
H	-6.44688700	-4.10827500	-1.35634500
H	-7.80629000	-1.81786500	-0.13812100
H	-6.78057400	0.21599200	1.38244300
H	-4.42922400	-0.34542800	1.19680200
H	-6.75063800	-2.19948200	1.23154800
Br	-1.87113000	-3.11228500	-3.14134900
O	-7.09049500	0.48451500	-0.64657300
C	-6.85923100	1.87730700	-0.60012800
H	-7.34203400	2.32594300	-1.46866700
H	-7.29103100	2.31539200	0.31072900
N	-4.50384300	1.16973900	-0.21868000
C	-3.22886100	1.63860300	-0.31842200
C	-5.38375600	2.13639700	-0.63444200
N	-4.74824100	3.20958100	-0.99416300
N	-3.42791400	2.87483700	-0.78665500
C	-2.41014200	3.82727900	-1.12558200
C	-1.76655800	3.69695300	-2.35934200
C	-2.11503100	4.84367100	-0.21675900
C	-0.81471500	4.65740300	-2.68781000
C	-1.11987300	5.75605400	-0.57330300
C	-0.46274300	5.67752700	-1.80015600
H	-0.31759200	4.60228800	-3.65268700
H	-0.85059000	6.53883900	0.13173700
C	0.63083700	6.64690500	-2.16614100
H	0.39329200	7.17667100	-3.09316800
H	0.78724600	7.38670800	-1.37859200
H	1.57306800	6.11276900	-2.32777400
C	-2.84414900	4.94504700	1.09507800
H	-2.89207600	3.97034400	1.59117000
H	-2.33654300	5.64362100	1.76334500
H	-3.87266200	5.28710900	0.94236000
C	-2.04720300	2.51742800	-3.25133200
H	-1.64407500	1.60547000	-2.79167100
H	-3.12073400	2.36746700	-3.39978100
H	-1.57779900	2.65037800	-4.22841500

TS1'C'

C	-5.50560600	-0.79970000	-2.45807100
C	-4.38959600	-0.81235700	-1.61601500
C	-4.38736800	-0.14304100	-0.39976200
C	-5.56512500	0.50746900	-0.04308100
C	-6.69495800	0.51946100	-0.85398800
C	-6.66462100	-0.13730000	-2.08164000
C	-5.23097700	-1.56134600	-3.73274200
C	-4.04073300	-2.43533100	-3.34355600
C	-3.27347900	-1.55860500	-2.32310200
H	-3.53879100	-0.13910700	0.27785400
H	-7.58792200	1.03790500	-0.52395600
H	-7.53959800	-0.13619000	-2.72403200
H	-6.06721200	-2.17687700	-4.07052200
H	-3.40641700	-2.74604700	-4.18375200
H	-2.61073900	-0.85592200	-2.84178900
H	-4.95096100	-0.88127500	-4.54570900
Br	-5.63590700	1.43360800	1.60582900
O	-4.57878700	-3.56448500	-2.67699000
C	-3.61508600	-4.48978400	-2.23479500
H	-4.11927800	-5.21453200	-1.59858100
H	-3.13930900	-5.00176500	-3.08325600
N	-2.41528200	-2.43291200	-1.51923000
C	-1.33518300	-2.11785800	-0.80105900
C	-2.55567100	-3.79176100	-1.44186000
N	-1.60076500	-4.32068800	-0.72964500
N	-0.84655100	-3.25662800	-0.33785700
C	0.39766400	-3.42384500	0.37170700
C	0.38754400	-3.48071200	1.76788900
C	1.56377100	-3.54916600	-0.39338900
C	1.62894700	-3.51197100	2.40626300
C	2.77413500	-3.59349100	0.29787900
C	2.82724500	-3.53383400	1.69283700
H	1.65313700	-3.52519800	3.49345000
H	3.70141200	-3.69254200	-0.26332700
C	4.14630200	-3.51591600	2.41755700
H	4.19321900	-4.31121500	3.16666100
H	4.98059500	-3.63980200	1.72236500
H	4.28556400	-2.56347400	2.93985800
C	1.51164600	-3.66131800	-1.89414200
H	0.74053900	-4.37177300	-2.20593800
H	1.29055400	-2.68593300	-2.33403100
H	2.47185100	-4.01498300	-2.27713300
C	-0.88744600	-3.59710700	2.55652500
H	-1.73239900	-3.09066400	2.09011200

H	-1.16099800	-4.65490100	2.63971900
H	-0.74720400	-3.21025900	3.56798800
H	-0.88841100	-1.13698300	-0.68726900
B	-4.49039100	-3.13248700	1.34286500
F	-3.33425000	-2.37618200	1.00900500
F	-4.25895500	-3.78112600	2.55471200
F	-4.70039900	-4.07320800	0.32185000
F	-5.58423200	-2.27766300	1.43767600
N	-2.39635600	0.95039600	2.77440900
C	-1.80740900	2.27617000	2.93050200
C	-2.82701300	3.37414000	3.21495200
H	-1.29011800	2.50107500	1.99137400
H	-1.03040300	2.30738800	3.72007700
H	-2.35911700	4.35286400	3.07023900
H	-3.68165600	3.28357000	2.53821600
H	-3.20145500	3.33701400	4.24125700
C	-3.16015300	0.53708900	3.94741800
C	-3.77460500	-0.84790400	3.80030000
H	-3.97512400	1.25764500	4.07815900
H	-2.54666400	0.58823000	4.86903000
H	-4.43024700	-1.05061200	4.65247300
H	-4.36725200	-0.90953900	2.88471200
H	-3.02546500	-1.64384800	3.76268800
C	-1.38669200	-0.02722000	2.36480500
C	-0.31619100	-0.36952200	3.40715100
H	-0.89695100	0.38416100	1.47634700
H	-1.90728300	-0.93616300	2.04726200
H	0.43499200	-1.03281900	2.96637500
H	0.20257600	0.52663500	3.75967000
H	-0.74815000	-0.87702200	4.27648900
C	1.93346600	1.42337100	1.33098600
C	1.31270400	1.10022000	0.17521500
H	2.71933700	0.74532000	1.66777200
C	1.75576400	-0.12620600	-0.59127100
H	2.50362200	-0.72952400	-0.04270600
O	1.00994900	-0.65564900	-1.42885400
C	1.69025300	2.55938700	2.22104700
C	2.16379700	2.48173500	3.54010900
C	1.03034400	3.72783900	1.80926300
C	1.93844600	3.51761000	4.43942400
H	2.71051100	1.59521100	3.85250900
C	0.81739400	4.76754900	2.70715600
H	0.68545400	3.81724300	0.78471600
C	1.25753800	4.66199200	4.02658300

H	2.29818300	3.43536400	5.45974600
H	0.30575500	5.66576200	2.37492300
H	1.08254000	5.47316400	4.72578900
C	0.14333000	1.71749300	-0.35349600
C	-0.92740700	2.05259000	-0.81725300
C	-2.21158500	2.40843100	-1.33329900
C	-2.57735400	2.01315300	-2.62998600
C	-3.13126000	3.10361700	-0.53485300
C	-3.85083400	2.29358800	-3.10928000
H	-1.85086100	1.48802700	-3.24412700
C	-4.39865700	3.39250100	-1.02797200
H	-2.84534900	3.40015800	0.46927200
C	-4.76358200	2.98045900	-2.30814400
H	-4.13445900	1.97589100	-4.10789000
H	-5.11453800	3.90704900	-0.39529400
H	-5.76131300	3.18802800	-2.68068300
C	6.58980200	-2.13102100	-0.60210800
C	5.50242200	-1.26010500	-0.56675400
C	5.17970700	-0.53438600	0.56714100
C	5.95776400	-0.73696100	1.69966100
C	7.05076800	-1.59910900	1.69976500
C	7.37590800	-2.29650300	0.53392100
C	6.70754800	-2.76354000	-1.97116000
C	5.83734100	-1.86228800	-2.85986100
C	4.77663100	-1.28279600	-1.88869700
H	4.36139900	0.17598800	0.56786100
H	7.63839300	-1.72789300	2.60147200
H	8.23578500	-2.95865600	0.52558500
H	7.73024900	-2.80040500	-2.35278000
H	5.37690800	-2.39262600	-3.70279400
H	3.90145000	-1.94351700	-1.83559400
H	6.30988400	-3.78451800	-1.96680600
Br	5.44172500	0.14314200	3.29804100
O	6.66489800	-0.81495200	-3.34158500
C	5.96981800	0.08453800	-4.18284600
H	6.67146000	0.85744500	-4.49714500
H	5.58646500	-0.43073300	-5.07451800
N	4.31424900	0.02026900	-2.33872900
C	3.31576100	0.75254700	-1.78040300
C	4.83565000	0.69090700	-3.41401400
N	4.21305000	1.81627800	-3.59505000
N	3.28133400	1.82482400	-2.57762600
C	2.32774100	2.89385900	-2.49534100
C	2.52902400	3.91308200	-1.56551000

C	1.20977900	2.83655500	-3.33285500
C	1.55544300	4.91249700	-1.48888500
C	0.27831300	3.86444100	-3.23477200
C	0.42556400	4.89833700	-2.30567200
H	1.68104700	5.71136900	-0.76152600
H	-0.60718500	3.83822500	-3.86585400
C	-0.65270800	5.94072100	-2.16710000
H	-0.89085400	6.39472900	-3.13288400
H	-1.57176300	5.48050600	-1.78676400
H	-0.35654000	6.73262100	-1.47628600
C	0.98674500	1.64387300	-4.22244900
H	1.85501500	1.44176400	-4.85565700
H	0.81408400	0.75946100	-3.59556800
H	0.11694000	1.79787900	-4.86433800
C	3.73172700	3.90911300	-0.66143500
H	3.69194200	3.05723500	0.02737000
H	4.65800000	3.82214800	-1.23706900
H	3.77109400	4.82399000	-0.06787900
MI'			
C	-4.48622600	-1.59346800	-0.86411100
C	-3.14497900	-1.20338800	-0.86926300
C	-2.77855100	0.13479000	-0.91789700
C	-3.80717200	1.07402500	-0.89905100
C	-5.15088000	0.71079200	-0.86223700
C	-5.49546300	-0.63972900	-0.85881600
C	-4.60233900	-3.09832400	-0.90296000
C	-3.23315900	-3.54017500	-0.39110700
C	-2.27070400	-2.44378700	-0.91405700
H	-1.73576000	0.41536900	-1.02072100
H	-5.91664800	1.47785200	-0.84839400
H	-6.54024000	-0.93406600	-0.84832400
H	-5.39732000	-3.50310100	-0.27312000
H	-2.93319800	-4.54880800	-0.70199100
H	-1.93401300	-2.62277900	-1.93600500
H	-4.75871400	-3.45167400	-1.92788900
Br	-3.37145900	2.92141000	-0.95336800
O	-3.31993100	-3.46767700	1.02792600
C	-2.13818400	-3.86749300	1.67071600
H	-2.25217900	-3.68217400	2.73970200
H	-1.94377000	-4.93888900	1.51851800
N	-1.05190500	-2.43884300	-0.07427000
C	0.17800600	-1.94285100	-0.33064400
C	-0.97813000	-3.08883400	1.13417900

N	0.21359600	-3.01040400	1.64713700
N	0.91832300	-2.29943300	0.72119400
C	2.29083300	-1.94126300	0.94468600
C	3.28516900	-2.58661100	0.21215000
C	2.55021600	-0.88297800	1.82600000
C	4.58184900	-2.07714300	0.31141300
C	3.85753800	-0.41348200	1.88453100
C	4.87604000	-0.97263700	1.10686300
H	5.37292900	-2.54467100	-0.27020000
H	4.08357500	0.43063700	2.53168500
C	6.24564500	-0.35116200	1.09377100
H	6.24732500	0.50777000	0.41179800
H	6.52894200	0.01073900	2.08510000
H	7.00287500	-1.05856500	0.74921100
C	1.46990400	-0.28683100	2.68832000
H	0.50962500	-0.25068600	2.17038800
H	1.33753500	-0.88267600	3.59705900
H	1.73396600	0.73170100	2.98024100
C	3.00112500	-3.76102500	-0.68768400
H	2.05490600	-4.24822700	-0.44368200
H	2.96209100	-3.45002200	-1.73677900
H	3.79936600	-4.50094400	-0.59581800
C	2.77076700	0.06254000	-1.71208200
C	1.50721800	-0.02337300	-1.25356400
H	3.09652600	-0.76267000	-2.34647700
C	0.60063500	-1.22499600	-1.65791200
H	1.31391600	-1.97262500	-2.09990800
O	-0.45190700	-0.91607600	-2.38092600
C	3.80170300	1.08105000	-1.47710900
C	4.95491800	1.04324100	-2.27645300
C	3.72420000	2.05892100	-0.47174400
C	5.98230300	1.96524300	-2.10542000
H	5.03670700	0.28032000	-3.04625800
C	4.75504500	2.97571800	-0.29639800
H	2.86167600	2.08754100	0.18373900
C	5.88440100	2.94015700	-1.11463700
H	6.85980800	1.92003200	-2.74250100
H	4.67793400	3.72234000	0.48791300
H	6.68398500	3.66032400	-0.97453700
C	0.83919600	0.93395400	-0.43856600
C	0.14663900	1.62383000	0.28359800
C	-0.70012900	2.40771100	1.12740900
C	-1.70746300	1.77691400	1.87374200
C	-0.57410500	3.80314300	1.17400800

C	-2.58575200	2.53550900	2.63711000
H	-1.80955600	0.69683000	1.82142700
C	-1.45732100	4.55385800	1.94007100
H	0.20424400	4.28530600	0.59186800
C	-2.46611900	3.92387700	2.66814100
H	-3.37045900	2.04344600	3.20237700
H	-1.36240200	5.63448700	1.96595800
H	-3.15803700	4.51496800	3.25911200

MI'C

C	-3.09066700	0.04363700	3.21837400
C	-2.13405700	-0.31847700	2.26973400
C	-0.79827900	-0.50398600	2.61008300
C	-0.45857200	-0.30815500	3.94499300
C	-1.40055800	0.02211100	4.91804800
C	-2.73155800	0.19702000	4.55242300
C	-4.43292400	0.29271700	2.57363600
C	-4.28416000	-0.29666600	1.16837400
C	-2.76057400	-0.25193800	0.89690000
H	-0.03142200	-0.78695200	1.89161000
H	-1.08672300	0.14840700	5.94770000
H	-3.47117500	0.46181200	5.30149400
H	-5.26845200	-0.18070700	3.09442900
H	-4.84388600	0.25730800	0.40294300
H	-2.45643300	0.68349800	0.42261100
H	-4.63967700	1.36783600	2.51267000
Br	1.35743400	-0.44547600	4.45927600
O	-4.74021300	-1.63749500	1.22362300
C	-4.66398100	-2.28587700	-0.02569900
H	-5.00060500	-3.31132600	0.10493100
H	-5.27880200	-1.76822100	-0.77860400
N	-2.39834900	-1.30035200	-0.05257700
C	-1.22257000	-1.50938100	-0.64964000
C	-3.24416200	-2.27979200	-0.49035700
N	-2.65627100	-3.05524500	-1.35419700
N	-1.38828400	-2.56002100	-1.43380700
C	-0.42427100	-3.12408500	-2.33496700
C	-0.12313600	-4.48597000	-2.21163700
C	0.14766700	-2.29368600	-3.30562400
C	0.78872300	-5.01709200	-3.12175400
C	1.05214400	-2.88454000	-4.18873900
C	1.38846000	-4.23418900	-4.11006300
H	1.05029500	-6.06965900	-3.04043200
H	1.50522100	-2.26697900	-4.95776000

C	2.39444400	-4.83708700	-5.05509000
H	3.32898400	-5.05732500	-4.52871000
H	2.02523800	-5.77514100	-5.47815100
H	2.62668500	-4.15228200	-5.87364200
C	-0.18789200	-0.82837200	-3.42263400
H	-1.26893800	-0.66057900	-3.39422200
H	0.24745300	-0.23749200	-2.60683400
H	0.19740800	-0.43620200	-4.36640900
C	-0.71286900	-5.33389000	-1.11781700
H	-0.73440500	-4.80556800	-0.16191700
H	-1.74665600	-5.61119700	-1.34371400
H	-0.12857500	-6.24888800	-1.00044000
H	-0.35620200	-0.86139100	-0.55702200
B	-2.23202800	-4.34899000	2.05796500
F	-1.45417500	-3.35348800	1.41843500
F	-1.62002400	-5.59274000	1.85762200
F	-3.51058200	-4.35719200	1.47943500
F	-2.31884900	-4.06516300	3.41739000
N	2.27046400	-2.50814500	1.95215800
C	3.47906300	-1.69838700	1.88100200
C	4.84199300	-2.40143600	1.80541300
H	3.48718500	-1.05391700	2.77082600
H	3.36844700	-1.02057600	1.02770800
H	5.63312700	-1.64710400	1.86952700
H	4.97860700	-3.09926900	2.63686500
H	4.98855300	-2.95651700	0.87492600
C	2.28044100	-3.46105900	3.05340800
C	0.88739000	-3.96540300	3.40233000
H	2.69881300	-2.93658900	3.92140700
H	2.94908000	-4.31950700	2.85990000
H	0.93055200	-4.59357900	4.29742900
H	0.21605100	-3.12533900	3.59579600
H	0.43809400	-4.55642600	2.60064500
C	1.78260800	-3.04663700	0.68491400
C	2.45138100	-4.32990400	0.17385500
H	1.88765900	-2.25009200	-0.06474400
H	0.70633000	-3.23281300	0.79049700
H	2.10164400	-4.55398800	-0.83754200
H	3.54089300	-4.24443600	0.13950900
H	2.20284100	-5.18376000	0.81258500
C	2.02032500	1.87102900	1.77040900
C	1.47454000	1.55012400	0.57737400
H	1.33530500	2.31460700	2.49631300
C	0.00179600	1.90622800	0.27588000

H	-0.48971100	1.93171800	1.28221100
O	-0.59276000	1.11319000	-0.62275700
C	3.40780100	1.76402700	2.23295100
C	3.66205400	1.95429700	3.60062500
C	4.49645500	1.52488600	1.37865400
C	4.95162500	1.85878200	4.10973900
H	2.82801500	2.14829000	4.26872200
C	5.78754700	1.43851900	1.88934200
H	4.33129800	1.41159700	0.31380600
C	6.02070800	1.59489000	3.25492000
H	5.12412300	1.99546500	5.17235400
H	6.61691500	1.24957700	1.21446600
H	7.02913300	1.52049300	3.64879600
C	2.12413700	0.81146600	-0.45616300
C	2.61325000	0.14202800	-1.34439400
C	3.25730400	-0.64678800	-2.35302000
C	3.94664900	-1.81685200	-1.99907500
C	3.21941500	-0.25370700	-3.69862000
C	4.58183400	-2.57582400	-2.97483700
H	3.97643700	-2.11991900	-0.95768600
C	3.87975900	-1.00317400	-4.66578800
H	2.66436100	0.63710200	-3.97087500
C	4.55848700	-2.16719600	-4.30783600
H	5.10402000	-3.48426400	-2.69114500
H	3.85248000	-0.68570000	-5.70338400
H	5.06481600	-2.75628600	-5.06574900
C	-4.86405300	3.28963100	-0.28592300
C	-3.55559400	2.89021200	-0.57136700
C	-3.28595700	1.87878100	-1.48522800
C	-4.38033900	1.24584000	-2.06626000
C	-5.69461300	1.62972700	-1.81060100
C	-5.93796700	2.67044400	-0.91466000
C	-4.87670900	4.39726300	0.74170800
C	-3.43930800	4.91265700	0.68546700
C	-2.61193500	3.64538700	0.35587900
H	-2.26271100	1.55167700	-1.65739800
H	-6.51528700	1.11129600	-2.29312700
H	-6.95700700	2.98105000	-0.70809600
H	-5.58275100	5.19868300	0.51543200
H	-3.09612600	5.41445100	1.59834500
H	-2.42706200	3.06344700	1.26700200
H	-5.10440900	4.01065100	1.74123200
Br	-4.07026500	-0.27543600	-3.16002300
O	-3.37989200	5.79425300	-0.42652800

C	-2.11122200	6.36834900	-0.62676100
H	-2.13577400	6.91743100	-1.56858900
H	-1.85862500	7.06691600	0.18303900
N	-1.30346900	4.05184100	-0.16675700
C	-0.13438200	3.36962300	-0.18958400
C	-1.05918300	5.30147900	-0.67393700
N	0.17907600	5.42005200	-1.04712500
N	0.73844800	4.20814800	-0.74217400
C	2.09080500	3.95088200	-1.16654500
C	2.26196100	3.34387600	-2.40999500
C	3.14607800	4.35740200	-0.34751700
C	3.57319200	3.12913800	-2.83316200
C	4.43471400	4.09196300	-0.80296600
C	4.66463700	3.47796800	-2.03761600
H	3.74765700	2.66319700	-3.79902200
H	5.27899500	4.36357300	-0.17416200
C	6.07271200	3.20301600	-2.49656800
H	6.55639100	4.12132900	-2.84370100
H	6.67591400	2.80442100	-1.67638000
H	6.08621200	2.48209100	-3.31645100
C	2.89207900	5.04650900	0.96360600
H	2.21141000	4.46010000	1.58880400
H	3.82531500	5.18337800	1.51191800
H	2.43262200	6.02694500	0.80366200
C	1.06668700	2.90089100	-3.21054300
H	0.52437500	2.11407300	-2.66808100
H	0.37258300	3.73142400	-3.37714900
H	1.37117200	2.51719900	-4.18625600

MI'C'

C	-5.35500100	0.42862200	1.81745300
C	-4.15101900	0.65503200	1.14419200
C	-3.91286000	0.13481200	-0.11989600
C	-4.94500100	-0.60005900	-0.69840800
C	-6.15826600	-0.82337500	-0.05597000
C	-6.36732600	-0.30585600	1.22022000
C	-5.33314300	1.06739900	3.18595700
C	-4.23640600	2.11858600	3.03116400
C	-3.23495300	1.44376000	2.06136000
H	-2.98828800	0.29452100	-0.66513200
H	-6.93018000	-1.39865300	-0.55426500
H	-7.31024500	-0.47523400	1.73082300
H	-6.27768800	1.53211000	3.47575800
H	-3.76203900	2.43363900	3.96974300

H	-2.55677800	0.77640700	2.60690900
H	-5.05317600	0.33875600	3.95639700
Br	-4.70790300	-1.31694200	-2.43331400
O	-4.84671500	3.22009200	2.38010500
C	-3.97980300	4.29592300	2.11141400
H	-4.50659100	4.98721200	1.45631500
H	-3.68482800	4.80613400	3.03947400
N	-2.40785600	2.48246700	1.44983600
C	-1.21287000	2.36621800	0.86001900
C	-2.74475200	3.80861000	1.42184900
N	-1.80539700	4.51589500	0.86284700
N	-0.86228100	3.59571300	0.51553600
C	0.40695800	4.00776300	-0.01989500
C	0.48455700	4.41105400	-1.35332100
C	1.50314700	4.01689200	0.85140000
C	1.74565800	4.77206800	-1.83628300
C	2.72757900	4.41682300	0.32361700
C	2.87493000	4.76991100	-1.02113300
H	1.83834600	5.06459200	-2.87893700
H	3.58772400	4.47118400	0.98812100
C	4.23376100	5.12557800	-1.56577300
H	4.15786200	5.60718300	-2.54226500
H	4.76481800	5.80084100	-0.88875400
H	4.84659000	4.22433000	-1.68400400
C	1.37716400	3.59170000	2.28947900
H	0.48198900	4.01365800	2.75641900
H	1.31107900	2.49702000	2.33103900
H	2.24620500	3.92546400	2.86151300
C	-0.73239700	4.48218400	-2.23190300
H	-1.47929000	3.72831700	-1.97916600
H	-1.22230600	5.45515400	-2.11656300
H	-0.44896500	4.37385400	-3.28140800
H	-0.56401400	1.47429800	0.76187400
B	-4.26366900	3.29520700	-1.64346100
F	-3.08812300	2.67049700	-1.15466800
F	-3.92182700	4.10295200	-2.72904600
F	-4.79973300	4.07986600	-0.60936800
F	-5.17470800	2.31418800	-2.02677400
N	-1.43023900	-0.38210300	-2.85123200
C	-0.71349200	-1.64494800	-2.95511800
C	-1.47185700	-2.75155600	-3.67969600
H	-0.52783400	-1.97934200	-1.93254900
H	0.27963600	-1.52937900	-3.43448100
H	-0.95449200	-3.70293000	-3.51317400

H	-2.48914400	-2.82715800	-3.28576300
H	-1.53078700	-2.58833200	-4.75923000
C	-1.81100900	0.16370900	-4.14612800
C	-2.61515400	1.45182500	-4.03801600
H	-2.43988600	-0.58705100	-4.63828200
H	-0.93098900	0.31533000	-4.80429300
H	-3.01611200	1.71953200	-5.02018600
H	-3.44815000	1.32229400	-3.34181300
H	-2.01629000	2.29521000	-3.68561800
C	-0.73971300	0.55571400	-1.96872100
C	0.64530000	1.05293400	-2.39905500
H	-0.63459600	0.05670100	-0.99869300
H	-1.39909200	1.41475600	-1.80787400
H	1.07029400	1.65689600	-1.58850800
H	1.33360200	0.22197500	-2.58997200
H	0.59810400	1.67527900	-3.30012300
C	1.83698900	-2.29985400	-0.79332800
C	1.16813500	-1.54984300	0.11177600
H	2.77357400	-1.88730800	-1.16929000
C	1.78347700	-0.23281900	0.62197900
H	2.43439300	0.11518300	-0.21009000
O	0.93625200	0.69781400	1.08066500
C	1.47605000	-3.58075800	-1.40992700
C	2.11561400	-3.92350700	-2.61247200
C	0.53812300	-4.47702900	-0.87063900
C	1.80315800	-5.10280800	-3.27830500
H	2.86859600	-3.25138600	-3.01820300
C	0.23348400	-5.66031600	-1.53672500
H	0.06145600	-4.25488200	0.07693900
C	0.85431600	-5.97415000	-2.74487800
H	2.30188300	-5.34414600	-4.21133000
H	-0.49308400	-6.34214700	-1.10548100
H	0.60817600	-6.89584000	-3.26202000
C	-0.15074200	-1.86413000	0.54410700
C	-1.30284700	-2.16672700	0.78015000
C	-2.61569600	-2.71793300	0.90870000
C	-3.41276700	-2.50390000	2.04334400
C	-3.10074900	-3.51288300	-0.14125100
C	-4.66402000	-3.09833300	2.13203300
H	-3.04121500	-1.86967600	2.84280700
C	-4.35917800	-4.09715400	-0.04688100
H	-2.48015400	-3.65691500	-1.02150900
C	-5.13811200	-3.89765900	1.09027800
H	-5.28034900	-2.92718000	3.00900800

H	-4.73393800	-4.70040000	-0.86733800
H	-6.12073100	-4.35268800	1.16215000
C	6.22088900	1.93628100	-0.05609900
C	5.19511200	1.00432300	0.09607000
C	5.07724700	-0.08926600	-0.74276200
C	5.97881900	-0.19968800	-1.79519900
C	6.98661300	0.73838700	-1.99741300
C	7.11680300	1.81009200	-1.11115800
C	6.17004400	2.96171400	1.05424900
C	5.25705700	2.29962200	2.09589600
C	4.30940000	1.41446500	1.25027200
H	4.32573800	-0.85139300	-0.58433300
H	7.67368200	0.62402400	-2.82762000
H	7.92241100	2.52466600	-1.24560200
H	7.14713600	3.17706100	1.49221500
H	4.71176700	3.00957200	2.73194600
H	3.43638600	1.98041600	0.90011700
H	5.74045200	3.90690800	0.70589600
Br	5.79736900	-1.67615200	-2.97082000
O	6.08577600	1.46204400	2.88978400
C	5.38881000	0.77414500	3.90517700
H	6.09782000	0.11946500	4.41219400
H	4.96355400	1.47322400	4.63832800
N	3.80111000	0.31310900	2.06134900
C	2.76337300	-0.49810100	1.78042600
C	4.27839700	-0.02934100	3.29638400
N	3.60148000	-1.02169300	3.79529600
N	2.66418300	-1.30343400	2.83490000
C	1.67367100	-2.32330300	3.06123700
C	1.93097900	-3.61824700	2.60400200
C	0.49416300	-1.95145900	3.70700700
C	0.91672600	-4.55965000	2.76755800
C	-0.47171700	-2.94055400	3.87925800
C	-0.29459700	-4.23302600	3.38370000
H	1.07379900	-5.56931000	2.39589400
H	-1.40149800	-2.68558200	4.38086200
C	-1.41108100	-5.24017300	3.45909600
H	-2.08022100	-5.03072500	4.29670100
H	-2.00980300	-5.19670200	2.54129600
H	-1.02643900	-6.25736300	3.56158000
C	0.25636000	-0.52169200	4.10787400
H	1.04788500	-0.15362900	4.76844300
H	0.25187500	0.10183500	3.20299600
H	-0.69942200	-0.42279000	4.62642700

C	3.24073600	-3.96633600	1.95201400
H	3.38728200	-3.38569400	1.03468500
H	4.08016000	-3.74915900	2.61939700
H	3.26896700	-5.02482600	1.68994300
TS2'			
C	-5.01663400	-0.81961700	-0.30649200
C	-3.72379900	-0.29276200	-0.26702900
C	-3.42810600	0.94137500	-0.83505600
C	-4.48945900	1.65188500	-1.39075800
C	-5.79767900	1.17315000	-1.38813900
C	-6.06262900	-0.08428800	-0.85049200
C	-5.03269500	-2.23843400	0.20712300
C	-3.73448700	-2.32819800	1.00477300
C	-2.77395300	-1.34078300	0.29080700
H	-2.39743400	1.27525800	-0.91315600
H	-6.59065300	1.76729900	-1.82783900
H	-7.07162900	-0.48451200	-0.87478600
H	-5.88984900	-2.48056400	0.83958900
H	-3.30974800	-3.33958200	1.05608500
H	-2.28309800	-1.83533400	-0.54545500
H	-5.01361500	-2.94791800	-0.62866500
Br	-4.14636700	3.30639000	-2.26350500
O	-4.04605300	-1.86862100	2.31264600
C	-2.92629100	-1.93266100	3.16220300
H	-3.20848000	-1.53282400	4.13701800
H	-2.58661100	-2.97174800	3.29010400
N	-1.72398100	-0.91589600	1.22216200
C	-0.54695400	-0.22684400	0.98443600
C	-1.81054900	-1.12695500	2.58156700
N	-0.81733600	-0.61630600	3.22491700
N	-0.02084100	-0.06752000	2.24373800
C	1.11170500	0.70428900	2.63970900
C	2.38566600	0.14078200	2.55162100
C	0.89902200	2.00208000	3.11907200
C	3.47512300	0.92881700	2.92081300
C	2.01647000	2.75407700	3.47609400
C	3.31011400	2.23909200	3.37077700
H	4.47712500	0.51111200	2.84256500
H	1.87441900	3.77118400	3.83379200
C	4.50267000	3.10077800	3.69159200
H	4.68714900	3.80375300	2.87120800
H	4.33742000	3.68950800	4.59741100
H	5.40384000	2.49855500	3.82814600

C	-0.49524900	2.55202300	3.25261600
H	-1.10305200	2.28355300	2.38472100
H	-0.98627600	2.14520100	4.14251900
H	-0.47570800	3.64076100	3.33334100
C	2.58065200	-1.25609900	2.03426900
H	1.87322300	-1.95695500	2.48740900
H	2.42019900	-1.28147700	0.94850900
H	3.59709300	-1.60478700	2.23039800
C	2.05120100	1.61325200	-0.37055300
C	0.71397400	1.44775400	-0.32315200
H	2.67290300	0.72921900	-0.23277500
C	0.00094400	0.09318000	-0.29489000
H	1.05383000	-0.88347000	-0.71793200
O	-0.76623300	-0.12043700	-1.38200800
C	2.78325100	2.88003500	-0.54059900
C	4.01869700	3.05438400	0.10048400
C	2.31827200	3.90629200	-1.37455000
C	4.75200300	4.22506700	-0.05917700
H	4.39748100	2.25040300	0.72609200
C	3.05390900	5.07696900	-1.53949000
H	1.38222200	3.77452600	-1.90718200
C	4.26973500	5.24461700	-0.87999000
H	5.70504200	4.33912400	0.44990600
H	2.67920100	5.85758100	-2.19428500
H	4.84182700	6.15743400	-1.01125300
C	-0.19168200	2.55908700	-0.29376800
C	-1.02822400	3.42129200	-0.11011100
C	-2.04466900	4.39563600	0.14175000
C	-3.15748400	4.04962900	0.92406700
C	-1.97150000	5.67619700	-0.42331100
C	-4.18288400	4.96545100	1.12235200
H	-3.22000900	3.04928000	1.34188700
C	-3.00302900	6.58607800	-0.22267600
H	-1.10888000	5.93973900	-1.02683500
C	-4.11119800	6.23300500	0.54646200
H	-5.04490100	4.68709400	1.72001000
H	-2.94431100	7.57333600	-0.66953100
H	-4.91641400	6.94474000	0.69700500
C	-1.65038700	-4.78352500	-1.07132100
C	-0.72167200	-3.76948300	-0.83008400
C	-0.19822500	-3.54279200	0.43357900
C	-0.62932400	-4.37707300	1.46202600
C	-1.53767800	-5.41048400	1.24649500
C	-2.05806300	-5.61342300	-0.03395500

C	-2.05794300	-4.77458100	-2.52740100
C	-0.91758300	-3.99847600	-3.19607600
C	-0.46157500	-3.00082100	-2.10679100
H	0.51315300	-2.74338100	0.62572900
H	-1.83874400	-6.04424500	2.07271400
H	-2.76675100	-6.41704200	-0.20715900
H	-2.15899100	-5.76924400	-2.96640700
H	-1.20389500	-3.49955600	-4.12956000
H	-0.99819000	-2.03772500	-2.11243700
H	-3.00509300	-4.24005500	-2.66228800
Br	0.02658900	-4.07081900	3.21313100
O	0.11536200	-4.94733200	-3.44350000
C	1.26405100	-4.38021200	-4.03378200
H	2.00911300	-5.16880800	-4.14321300
H	1.03613600	-3.96832300	-5.02692700
N	0.93853500	-2.64763100	-2.29217300
C	1.61140800	-1.66098500	-1.66108600
C	1.78662700	-3.28701100	-3.15297500
N	2.97781600	-2.76793400	-3.09743100
N	2.84395500	-1.77144200	-2.16340100
C	3.98070200	-0.97866600	-1.79763500
C	4.84970100	-1.48075600	-0.82530300
C	4.15084000	0.26133100	-2.41599400
C	5.90564700	-0.66014200	-0.43017800
C	5.23378300	1.03466300	-2.00212800
C	6.10416800	0.59975100	-1.00139900
H	6.58969200	-1.01449900	0.33733000
H	5.37773900	2.01706300	-2.44496600
C	7.20936200	1.49420200	-0.50480000
H	7.41434400	2.30131700	-1.21101000
H	6.92538600	1.95200200	0.45002400
H	8.13138900	0.93209500	-0.33696900
C	3.17033100	0.75001000	-3.44779500
H	3.08220600	0.03817700	-4.27429900
H	2.17473400	0.86919000	-3.00515900
H	3.48567600	1.71504800	-3.84744200
C	4.66734500	-2.86630100	-0.26387400
H	3.62634600	-3.06001400	0.01245300
H	4.94789000	-3.61802300	-1.00824400
H	5.29152800	-3.00937100	0.61983200
TS2 ^N			
C	3.52692500	-3.29148800	-0.56013000
C	2.49630600	-2.42559000	-0.19748700

C	2.71093900	-1.06756000	-0.01484700
C	3.97671500	-0.58157600	-0.32590400
C	5.01663400	-1.41562300	-0.72917900
C	4.79713700	-2.79085600	-0.82122500
C	3.02939900	-4.71794800	-0.55940700
C	1.51316200	-4.55280800	-0.71140900
C	1.20371000	-3.19216700	-0.02137400
H	1.93241700	-0.43505500	0.40212100
H	5.98897400	-0.99535500	-0.95967500
H	5.60985700	-3.45051300	-1.10892200
H	3.42578400	-5.33475300	-1.36899200
H	0.92969600	-5.37296100	-0.27163300
H	0.98542900	-3.32595000	1.03925500
H	3.26708700	-5.20666700	0.39162600
Br	4.26652900	1.29337600	-0.20276000
O	1.27830200	-4.50039900	-2.11179900
C	-0.07627300	-4.26548900	-2.42456100
H	-0.18501300	-4.27035300	-3.50908200
H	-0.71730100	-5.05000300	-1.99483500
N	0.04245700	-2.54578300	-0.65076500
C	-0.49493800	-1.29714900	-0.37213900
C	-0.45482800	-2.93124700	-1.87541900
N	-1.21222600	-2.03886000	-2.41517800
N	-1.21943000	-0.98861100	-1.50394600
C	-1.59655000	0.30729900	-1.98049100
C	-2.94672900	0.57965500	-2.22913700
C	-0.59939300	1.26962400	-2.20238400
C	-3.29241600	1.85767100	-2.66826800
C	-0.99959500	2.54015700	-2.61458400
C	-2.33936300	2.85835300	-2.84136900
H	-4.34109100	2.07919200	-2.85571800
H	-0.23649000	3.29732300	-2.78288400
C	-2.74753000	4.25179700	-3.24017000
H	-3.01385700	4.83303500	-2.35052500
H	-1.93523000	4.77379000	-3.75119100
H	-3.61960300	4.23686100	-3.89836900
C	0.86355900	0.96874700	-2.00910400
H	1.16545900	1.12853500	-0.96920800
H	1.10229600	-0.06712300	-2.26853100
H	1.47053700	1.62941700	-2.63272300
C	-4.03116000	-0.43903100	-1.99416800
H	-4.80009800	-0.35996600	-2.76636500
H	-3.64626300	-1.45936700	-1.99179300
H	-4.52250000	-0.24934800	-1.03190900

C	-2.34408400	0.95511800	0.88563900
C	-1.03432300	0.67482900	1.05426000
H	-2.98668800	0.08878300	0.72438000
C	-0.51363500	-0.75116300	0.95976100
H	-1.59421300	-1.57105500	1.24880300
O	0.39947500	-1.13217900	1.83722800
C	-3.05191100	2.23415000	0.79631900
C	-4.45498200	2.20804600	0.84841700
C	-2.41725100	3.47021600	0.59526900
C	-5.20357900	3.37129900	0.71590300
H	-4.95823200	1.25427000	0.99386300
C	-3.16761800	4.63459800	0.46894800
H	-1.33771900	3.51263500	0.51669000
C	-4.56037100	4.59321700	0.52607600
H	-6.28709500	3.32530400	0.75866500
H	-2.66031100	5.58205600	0.31323000
H	-5.13906000	5.50518000	0.42045700
C	-0.01352600	1.64324300	1.30819100
C	0.94155300	2.37691300	1.46379000
C	2.08449700	3.23572900	1.53454900
C	2.34226900	4.12519300	0.48068400
C	2.99353400	3.13852100	2.59639700
C	3.50601200	4.88471300	0.47953600
H	1.63751700	4.18647900	-0.34319600
C	4.15131600	3.90770400	2.59164400
H	2.79347100	2.44247300	3.40383400
C	4.41503900	4.77425800	1.53179900
H	3.70768500	5.56047400	-0.34523000
H	4.85670500	3.82226800	3.41169500
H	5.32546400	5.36456200	1.52651400
N	-2.44483700	-2.49991700	1.81878300
C	-3.09215900	-1.85368800	2.98134300
C	-2.07392100	-1.32260600	3.98402500
H	-3.79067200	-2.55083800	3.46175400
H	-3.68482700	-1.02481100	2.58218700
H	-2.57380700	-0.64229600	4.67704300
H	-1.62692100	-2.12827100	4.57195100
H	-1.26125700	-0.79937400	3.47243200
C	-3.37982100	-2.80244500	0.71621000
C	-4.32308500	-3.98437400	0.90765900
H	-2.76975000	-2.95922900	-0.18392900
H	-3.96328100	-1.89129400	0.54839300
H	-5.03822100	-4.00040100	0.08143100
H	-3.78519600	-4.93464400	0.89805100

H	-4.88865800	-3.90799000	1.84004500
C	-1.53252400	-3.61639300	2.17919500
C	-2.05251600	-4.62662200	3.19991000
H	-0.61681600	-3.13760700	2.53951700
H	-1.28504400	-4.12319600	1.23859600
H	-1.28544200	-5.39134000	3.34610200
H	-2.24035500	-4.16409600	4.17126500
H	-2.96757900	-5.12550200	2.87910500
M2'			
C	-5.87041200	-0.26447000	-0.70424500
C	-4.52816500	-0.03030300	-0.41010800
C	-4.01933300	1.25643600	-0.31551400
C	-4.91765100	2.30619600	-0.44945900
C	-6.26877500	2.10769400	-0.71948300
C	-6.74671100	0.80356500	-0.86725300
C	-6.11654400	-1.75100400	-0.82738300
C	-4.94110200	-2.35820300	-0.05200300
C	-3.78300100	-1.34042300	-0.24880300
H	-2.95599300	1.41880500	-0.19861200
H	-6.93592600	2.95646600	-0.81800300
H	-7.79531500	0.63653300	-1.09401800
H	-7.06687800	-2.08626200	-0.40564200
H	-4.65687900	-3.36333100	-0.39121100
H	-3.21344300	-1.56958600	-1.15361400
H	-6.07955000	-2.06169000	-1.87769600
Br	-4.23855700	4.07438700	-0.24225700
O	-5.36724400	-2.41593300	1.30328200
C	-4.34525900	-2.85332100	2.17341800
H	-4.75137000	-2.89951200	3.18406500
H	-3.98201100	-3.85205500	1.88016600
N	-2.86499300	-1.37351500	0.88489700
C	-1.68324000	-0.63615700	1.06846300
C	-3.20396200	-1.89781900	2.10419000
N	-2.41359700	-1.55100200	3.06023800
N	-1.47702300	-0.71971800	2.45271600
C	-0.71039000	0.15233900	3.26243300
C	0.26768900	-0.41144000	4.09887200
C	-0.87904200	1.54539300	3.18474300
C	1.08948500	0.43793800	4.83683300
C	-0.01679000	2.35272500	3.92612600
C	0.98220500	1.82395900	4.74403400
H	1.85989600	0.00276800	5.47019000
H	-0.13719700	3.43274600	3.86552900

C	1.94477500	2.72281600	5.47491700
H	2.86816900	2.83434100	4.89511800
H	1.52251500	3.71904800	5.62715700
H	2.21495600	2.30870400	6.44974600
C	-1.94194100	2.18931100	2.33418000
H	-1.57210100	2.38114300	1.31976000
H	-2.82583200	1.55221100	2.24269200
H	-2.24390300	3.14537400	2.76939300
C	0.44791600	-1.90283000	4.17802400
H	-0.28218700	-2.35250300	4.85908900
H	0.28659900	-2.37142400	3.20342100
H	1.45064800	-2.14760900	4.53649700
C	1.26963000	-0.06989500	1.16046600
C	0.34334700	0.54750400	0.34482200
H	1.00059400	-1.06691200	1.50717500
C	-0.98012900	-0.00506200	0.04328400
H	2.19878200	-0.50520500	-0.72036800
O	-1.51610200	0.16059700	-1.14012600
C	2.52845800	0.43588900	1.68496700
C	3.47418300	-0.49099100	2.17414800
C	2.84824400	1.80455200	1.78331200
C	4.66898700	-0.07583500	2.74402800
H	3.24213300	-1.55279900	2.11365200
C	4.05577100	2.21567700	2.33931800
H	2.12766200	2.54364900	1.45172600
C	4.96858300	1.28497600	2.83386300
H	5.37420400	-0.81465000	3.11477300
H	4.27396000	3.27785700	2.40991400
H	5.90181500	1.61502100	3.28026200
C	0.61461800	1.76028100	-0.37099900
C	0.70528200	2.80233000	-0.99137100
C	0.71346100	4.04622000	-1.69804400
C	-0.50430900	4.70276400	-1.94577900
C	1.90986300	4.62496800	-2.14704200
C	-0.51638400	5.91055300	-2.63245500
H	-1.42807800	4.26421600	-1.58009900
C	1.88722300	5.83308000	-2.83451900
H	2.85034400	4.12041400	-1.95034100
C	0.67618900	6.47793500	-3.08087400
H	-1.46077700	6.41243600	-2.81716800
H	2.81755800	6.27326400	-3.17854300
H	0.66186100	7.42105800	-3.61720200
C	-1.37168600	-2.78473500	-2.96932300
C	-0.34023300	-2.30348400	-2.16454700

C	-0.15210100	-2.75581700	-0.86697400
C	-1.04540200	-3.71404300	-0.39679500
C	-2.06117100	-4.24031300	-1.18849900
C	-2.22914300	-3.76900000	-2.49236300
C	-1.41181100	-2.03463800	-4.27985400
C	-0.02689300	-1.38824100	-4.35751900
C	0.35774600	-1.16799800	-2.87641600
H	0.63391000	-2.37206300	-0.22437400
H	-2.72065300	-5.00046600	-0.78405400
H	-3.02916000	-4.16211100	-3.11212300
H	-1.59314100	-2.66329500	-5.15444700
H	-0.00022000	-0.45939600	-4.93951800
H	-0.04726900	-0.23011100	-2.46371500
H	-2.18175800	-1.25629500	-4.24482800
Br	-0.91039600	-4.25928500	1.41167700
O	0.84320100	-2.35322200	-4.94396400
C	2.16171900	-1.88576300	-5.09782100
H	2.76307200	-2.69316500	-5.51678200
H	2.20527300	-1.02124000	-5.77458900
N	1.82294900	-1.15957700	-2.75556900
C	2.56431800	-0.81520100	-1.69989900
C	2.69744400	-1.48908700	-3.75588100
N	3.93489400	-1.36128400	-3.35949900
N	3.82742300	-0.94137500	-2.06898500
C	4.97562600	-0.67299600	-1.24482400
C	5.71420400	-1.76109500	-0.77709600
C	5.26941300	0.65804400	-0.93767600
C	6.80540300	-1.47716900	0.04124200
C	6.37322300	0.88370400	-0.11942100
C	7.14175600	-0.16648700	0.38396300
H	7.39936800	-2.30127400	0.42773200
H	6.62596700	1.90655800	0.14696500
C	8.27986900	0.11146800	1.32847500
H	8.77243300	1.05670700	1.08993800
H	7.90206400	0.18597600	2.35448900
H	9.02393500	-0.68733100	1.30465400
C	4.43405900	1.79568400	-1.46289500
H	4.25954900	1.70234900	-2.53965100
H	3.45833900	1.83619600	-0.96438600
H	4.93966000	2.74512000	-1.27626400
C	5.33346400	-3.17332300	-1.13339300
H	4.28876600	-3.37606100	-0.87510900
H	5.44555500	-3.35455300	-2.20592200
H	5.96156400	-3.88400500	-0.59515100

M2^H

C	-4.99213900	0.16009600	-0.71518500
C	-3.61248200	-0.06285200	-0.73927600
C	-2.71044100	0.98557300	-0.60885300
C	-3.23802000	2.26491400	-0.45133400
C	-4.60619100	2.51276000	-0.43137300
C	-5.49451100	1.44526000	-0.56538800
C	-5.73890800	-1.14737300	-0.84852000
C	-4.68241400	-2.17626100	-0.43813400
C	-3.35759900	-1.54847700	-0.93628800
H	-1.63698500	0.83051800	-0.61895200
H	-4.97157600	3.52514000	-0.30380700
H	-6.56459800	1.62513200	-0.53603900
H	-6.61983200	-1.21892300	-0.20700100
H	-4.84401000	-3.17879200	-0.85506900
H	-3.22696600	-1.76090900	-2.00018700
H	-6.05187400	-1.31933100	-1.88428600
Br	-2.03493700	3.72279500	-0.26450500
O	-4.70849600	-2.22876100	0.98071100
C	-3.70865900	-3.07458000	1.51116400
H	-3.77829100	-3.04400700	2.59833500
H	-3.85980200	-4.10943700	1.17042000
N	-2.22128700	-2.10109300	-0.21000200
C	-0.88393500	-1.73473900	-0.35985600
C	-2.36415200	-2.59639400	1.06908600
N	-1.25924600	-2.61851100	1.72589300
N	-0.31623700	-2.10086400	0.84651600
C	1.06396900	-2.20220100	1.17530900
C	1.91481100	-2.98849100	0.39040500
C	1.52859700	-1.49612000	2.29601100
C	3.27559000	-2.99370700	0.71210000
C	2.88584000	-1.55842700	2.59191000
C	3.78047100	-2.28053400	1.79613200
H	3.95180000	-3.58999300	0.10368600
H	3.26023400	-1.00341500	3.44959800
C	5.25611400	-2.26830500	2.10241600
H	5.71283800	-1.33093500	1.76657500
H	5.43789400	-2.35282200	3.17687600
H	5.77297400	-3.08791300	1.59874900
C	0.58887400	-0.66838900	3.12937500
H	-0.06973100	-0.07670100	2.48528600
H	-0.04995400	-1.30195500	3.75117800
H	1.14906700	0.01453500	3.77233900

C	1.41169000	-3.82519500	-0.75675400
H	0.39415800	-4.18062300	-0.57324500
H	1.40385600	-3.24984700	-1.68870900
H	2.06088100	-4.69180900	-0.89860200
C	1.69609500	-0.55947400	-2.73077200
C	0.96597500	-0.53269800	-1.58218400
H	1.25543700	-1.10787400	-3.56049200
C	-0.32177200	-1.21143900	-1.49661300
H	-0.94257300	-2.26653800	-2.99461000
O	-1.04292600	-1.35606300	-2.68443700
C	2.97022800	0.10148100	-3.01668300
C	3.28101900	0.41671700	-4.35026500
C	3.93070700	0.38657900	-2.03077900
C	4.48326800	1.02899500	-4.68434700
H	2.55821200	0.18330800	-5.12758800
C	5.13372400	0.99727900	-2.36691800
H	3.73928900	0.10259600	-1.00200600
C	5.41452400	1.32919800	-3.69152800
H	4.69490100	1.27103000	-5.72116400
H	5.86223700	1.20560400	-1.58923700
H	6.35479500	1.80587000	-3.94893900
C	1.32179800	0.30491900	-0.47145900
C	1.56014300	1.06540600	0.44313900
C	1.90576700	1.88871900	1.56364600
C	0.97085300	2.77644600	2.11551500
C	3.17813100	1.77616100	2.14437400
C	1.30284600	3.52689900	3.23752600
H	-0.00455100	2.87535900	1.65006600
C	3.50130900	2.52967500	3.26717800
H	3.89607700	1.08450600	1.71459600
C	2.56398700	3.40214000	3.81891900
H	0.57405000	4.21013300	3.66117600
H	4.48559700	2.43440100	3.71405000
H	2.81735500	3.98637600	4.69747200
TS3'			
C	-5.84147100	0.30906600	-0.84445600
C	-4.66489200	0.15017500	-0.10820900
C	-4.54798500	0.63543700	1.18516500
C	-5.66012500	1.27370800	1.72608300
C	-6.84253700	1.45035000	1.01369500
C	-6.93204700	0.96651200	-0.29155500
C	-5.69832900	-0.33002400	-2.20701500
C	-4.56111800	-1.32097800	-1.96877500

C	-3.64369500	-0.57749000	-0.96668400
H	-3.60933400	0.55732500	1.72011500
H	-7.68300400	1.95533800	1.47587500
H	-7.85194600	1.09164200	-0.85410500
H	-6.59788600	-0.84175300	-2.55507100
H	-4.02807400	-1.64149800	-2.87039500
H	-2.98806300	0.14020200	-1.46687400
H	-5.40037200	0.40645900	-2.96272200
Br	-5.55319800	1.93773500	3.50438300
O	-5.14974800	-2.44742600	-1.32942300
C	-4.21280900	-3.45471000	-1.03815000
H	-4.71907100	-4.24041500	-0.47642200
H	-3.79470600	-3.88301200	-1.96107400
N	-2.79256100	-1.55109500	-0.27791700
C	-1.60950400	-1.36992000	0.37967700
C	-3.07947000	-2.88875900	-0.24067900
N	-2.20194700	-3.54901600	0.44759200
N	-1.30444200	-2.59770200	0.85456000
C	-0.31440300	-2.96865700	1.81987200
C	0.64709200	-3.91327200	1.44667600
C	-0.37538800	-2.41653700	3.10417600
C	1.58649200	-4.28969800	2.40280700
C	0.59074500	-2.82854700	4.02187900
C	1.58179000	-3.75121500	3.68884200
H	2.35965600	-5.00198900	2.12464500
H	0.56347400	-2.41402400	5.02683500
C	2.64652300	-4.14169500	4.67938300
H	3.60150800	-3.69071600	4.39007400
H	2.39794500	-3.80120400	5.68690600
H	2.78542500	-5.22601900	4.70448700
C	-1.43176900	-1.42415900	3.51517200
H	-1.13508900	-0.40538500	3.24492200
H	-2.39194000	-1.62692600	3.03085800
H	-1.58168500	-1.46316500	4.59586900
C	0.68527200	-4.51132000	0.06535600
H	0.08092300	-5.42305100	0.02091600
H	0.28982600	-3.82926000	-0.69197000
H	1.71390100	-4.76826900	-0.19735500
C	1.38040100	-0.97751400	0.27915900
C	0.41164300	-0.02301700	0.81445900
H	0.95191900	-1.74774100	-0.36490700
C	-0.97459700	-0.05461900	0.59078800
H	1.94641400	0.09402200	-0.69575300
O	-1.76835600	0.95294200	0.53992600

C	2.59141400	-1.40686700	0.96430800
C	3.46365700	-2.31027200	0.31203400
C	2.99148100	-0.95121600	2.23700200
C	4.63064000	-2.76233200	0.90650600
H	3.19214300	-2.66276000	-0.68245800
C	4.17996800	-1.38534300	2.81954600
H	2.34474400	-0.27082400	2.78243600
C	5.00610600	-2.30308200	2.17297900
H	5.26532000	-3.46663600	0.37327600
H	4.45083600	-1.01758900	3.80687500
H	5.92482200	-2.64787500	2.63850000
C	0.88508300	1.22800700	1.31656900
C	1.28007300	2.30192200	1.73816900
C	1.74569400	3.57474100	2.19346800
C	1.07487200	4.75088100	1.81650000
C	2.88427900	3.67597100	3.01118000
C	1.53739900	5.99137200	2.23956700
H	0.18949800	4.67395500	1.19316100
C	3.34352100	4.92061700	3.42581900
H	3.39623200	2.76852600	3.31611200
C	2.67435000	6.08211900	3.04173400
H	1.00925900	6.89149800	1.94140800
H	4.22511500	4.98441100	4.05563700
H	3.03470700	7.05193200	3.36858000
C	-1.62870100	1.82293300	-3.32440400
C	-0.61538400	1.23643200	-2.56842300
C	-0.42213600	-0.13806900	-2.54670600
C	-1.27507800	-0.91113500	-3.32476700
C	-2.23854100	-0.34808100	-4.15942300
C	-2.42667600	1.03474600	-4.14879400
C	-1.70196400	3.30507300	-3.04730800
C	-0.34474900	3.62367000	-2.40866000
C	0.10175200	2.28571900	-1.75324400
H	0.33955000	-0.60647300	-1.93236300
H	-2.85313700	-0.98346500	-4.78766600
H	-3.19453400	1.47949000	-4.77407100
H	-1.85686800	3.92058800	-3.93612300
H	-0.38746600	4.43740800	-1.67452100
H	-0.22867100	2.22341900	-0.70719100
H	-2.51072300	3.51438400	-2.33955200
Br	-1.18122300	-2.79847000	-3.13447300
O	0.52850300	3.98647900	-3.46922400
C	1.82535000	4.30406500	-3.01190900
H	2.42631900	4.60360800	-3.87055800

H	1.79768600	5.13015500	-2.28750900
N	1.56233400	2.16422300	-1.79950900
C	2.31355900	1.14636300	-1.33285000
C	2.40338300	3.08044600	-2.37632200
N	3.64390100	2.69521900	-2.29307600
N	3.55696900	1.49249700	-1.64097300
C	4.72391700	0.70665600	-1.34844300
C	5.14812600	-0.22321400	-2.29572500
C	5.34105500	0.87925400	-0.10695100
C	6.25290900	-1.00955100	-1.96728600
C	6.44133600	0.07585100	0.17128000
C	6.90190600	-0.87690300	-0.74034200
H	6.60317700	-1.74975700	-2.68227500
H	6.93320900	0.17334900	1.13591400
C	8.05054600	-1.77518700	-0.36592800
H	8.90382400	-1.19691100	-0.00124300
H	7.74496200	-2.45118700	0.44030200
H	8.37924100	-2.38080400	-1.21280900
C	4.79842800	1.86786400	0.88646600
H	4.69541700	2.86596600	0.44846900
H	3.80544200	1.55020100	1.22363700
H	5.45211200	1.93512300	1.75837800
C	4.41158000	-0.38763800	-3.59861300
H	3.40052600	-0.77360700	-3.42616700
H	4.31011300	0.56780200	-4.12135000
H	4.93521300	-1.08718100	-4.25167700

TS3^H

C	4.96548500	-0.32005600	0.69816100
C	3.57452300	-0.42612300	0.66328700
C	2.75133900	0.68226700	0.79553800
C	3.37124100	1.91656100	0.96916100
C	4.75520800	2.05013000	1.02484400
C	5.56171400	0.91946200	0.88851600
C	5.60211400	-1.67263200	0.47105400
C	4.47600600	-2.46075500	-0.20595400
C	3.19606200	-1.87833800	0.44349200
H	1.66824200	0.61918400	0.75930700
H	5.19775200	3.03023400	1.15944300
H	6.64196000	1.02018700	0.91157500
H	6.48637400	-1.64094100	-0.16853700
H	4.54819900	-3.54823200	-0.08888600
H	2.94502800	-2.38706300	1.37916400
H	5.87773900	-2.14664600	1.41900400

Br	2.27706500	3.45727900	1.12432200
O	4.51769200	-2.10460900	-1.58250100
C	3.49939700	-2.69482400	-2.35862000
H	3.59880500	-2.33033400	-3.38089100
H	3.58196600	-3.79044000	-2.35980900
N	2.05959100	-2.04277600	-0.46286100
C	0.76565300	-1.77049400	-0.20418700
C	2.16663900	-2.30586300	-1.79689100
N	1.00705500	-2.21228700	-2.38307400
N	0.14263300	-1.88180500	-1.38172200
C	-1.25633400	-1.70178700	-1.66474200
C	-2.19680200	-2.52885000	-1.04927100
C	-1.59857800	-0.66466300	-2.54391600
C	-3.54114000	-2.28731400	-1.35086300
C	-2.94903400	-0.47808600	-2.81261500
C	-3.93447600	-1.27421800	-2.22078600
H	-4.29636700	-2.90999100	-0.87745900
H	-3.24167500	0.33107900	-3.47727400
C	-5.38888100	-1.02956100	-2.52604200
H	-5.63253300	-1.35612600	-3.54170900
H	-6.03604900	-1.56927100	-1.83214300
H	-5.62468900	0.03643400	-2.46085200
C	-0.55702500	0.24471800	-3.13877800
H	0.14591200	0.58164600	-2.36873200
H	0.01799300	-0.26196500	-3.91833800
H	-1.03460300	1.12803500	-3.56747700
C	-1.83862500	-3.60974900	-0.06398200
H	-1.88797300	-3.22286600	0.96102400
H	-2.54618200	-4.43693300	-0.14671000
H	-0.83045800	-4.00222600	-0.21676400
C	-1.21260300	-0.87186900	2.87014800
C	-0.70344500	-0.62524200	1.50029700
H	-0.55090800	-0.48823300	3.65293900
C	0.20663800	-1.57040300	1.12419000
H	-0.32290600	-2.23725100	2.70938600
O	0.49929400	-2.52525600	2.02120200
C	-2.62892400	-0.65250000	3.12611700
C	-3.10715000	-0.35143900	4.41962100
C	-3.60362100	-0.78273100	2.11050300
C	-4.46275200	-0.19428600	4.68088900
H	-2.38787300	-0.23943100	5.22788700
C	-4.95758200	-0.61277300	2.37221000
H	-3.28373200	-1.02455500	1.09936900
C	-5.40655000	-0.31880600	3.66011800

H	-4.78692300	0.03704800	5.69226300
H	-5.67172800	-0.71824100	1.55866600
H	-6.46453500	-0.19093400	3.86423300
C	-1.07361600	0.44961900	0.64176300
C	-1.36405800	1.39975200	-0.05842400
C	-1.74164400	2.45580400	-0.94936400
C	-0.79222700	3.38504700	-1.40020000
C	-3.06330200	2.53807600	-1.41390500
C	-1.15912500	4.36672300	-2.31381700
H	0.22220700	3.33191800	-1.01713300
C	-3.42153600	3.52345900	-2.32698000
H	-3.79161900	1.81650300	-1.05680900
C	-2.47026700	4.43516800	-2.78357100
H	-0.41959400	5.08118700	-2.66043500
H	-4.44474100	3.57902500	-2.68452300
H	-2.75153900	5.20089700	-3.49906200
M3'			
C	4.92412800	-0.62227200	0.65480800
C	3.52920900	-0.60542200	0.66742400
C	2.80976300	0.57413700	0.77956400
C	3.54010500	1.75451000	0.87922000
C	4.93165600	1.76897900	0.88346500
C	5.63216700	0.56693100	0.77155800
C	5.42977400	-2.03610400	0.47656000
C	4.21348500	-2.75432200	-0.11737600
C	3.01127200	-2.02183800	0.52794800
H	1.72482400	0.60362800	0.77805900
H	5.46148000	2.71132200	0.96089700
H	6.71732800	0.57361200	0.75700600
H	6.28782100	-2.11699500	-0.19386400
H	4.19297700	-3.83530700	0.06423600
H	2.72782600	-2.45763600	1.49132900
H	5.69993100	-2.48484700	1.43831900
Br	2.58637200	3.38912100	1.00055200
O	4.23761600	-2.48806800	-1.51472500
C	3.15668600	-3.05660300	-2.21801600
H	3.24193100	-2.76125600	-3.26388800
H	3.17280100	-4.15355600	-2.15509600
N	1.84035500	-2.13082900	-0.34002800
C	0.57285400	-1.78655800	-0.04889900
C	1.87038400	-2.55204600	-1.63864000
N	0.68610500	-2.49050400	-2.17419700
N	-0.11065800	-2.01170500	-1.17100600

C	-1.50873900	-1.77526900	-1.41327300
C	-2.45206500	-2.58746300	-0.78411800
C	-1.84404900	-0.73719600	-2.29178200
C	-3.79800700	-2.30099100	-1.02944000
C	-3.19859800	-0.48971400	-2.49175100
C	-4.18685900	-1.25173600	-1.86019600
H	-4.55661800	-2.91044700	-0.54488500
H	-3.48840700	0.32359100	-3.15304100
C	-5.64255900	-0.93306200	-2.08291900
H	-5.87546100	0.07306700	-1.72007100
H	-5.89128800	-0.96040200	-3.14750600
H	-6.28873200	-1.64187800	-1.56109700
C	-0.78751700	0.05484100	-3.01376800
H	0.02769100	0.33349900	-2.33916800
H	-0.35956100	-0.53403200	-3.83054800
H	-1.21570300	0.97094200	-3.42539600
C	-2.05387400	-3.71555400	0.12995700
H	-1.22058700	-4.28891700	-0.28699100
H	-1.73332900	-3.34585700	1.10905200
H	-2.89720100	-4.39192800	0.27723300
C	-1.24405900	-0.20774600	3.00179800
C	-0.61215600	-0.38782500	1.64505100
H	-0.83934000	0.68232000	3.50068400
C	0.08092000	-1.54945200	1.37188700
O	0.36936300	-2.52260600	2.12158300
C	-2.76098000	-0.09641500	2.98528000
C	-3.43881000	0.27773400	4.15045500
C	-3.51241500	-0.37610700	1.84235700
C	-4.82775200	0.36103500	4.17656700
H	-2.86693100	0.50528900	5.04722700
C	-4.90411600	-0.29536200	1.86405800
H	-3.00499200	-0.65476700	0.92473400
C	-5.56862600	0.07298500	3.03034600
H	-5.33367200	0.65279500	5.09192000
H	-5.46486100	-0.52328900	0.96092200
H	-6.65188000	0.13879000	3.04855300
C	-0.75001000	0.64372200	0.68524400
C	-0.88181100	1.58643300	-0.07653800
C	-1.20061600	2.58419800	-1.05420700
C	-0.19591100	3.33212000	-1.68583600
C	-2.53953100	2.77644200	-1.43312900
C	-0.52461200	4.23672500	-2.68967900
H	0.83478500	3.19894600	-1.37289600
C	-2.86110500	3.68710600	-2.43323200

H	-3.31117100	2.19091600	-0.94221400
C	-1.85457600	4.41396000	-3.06909700
H	0.25961600	4.80676700	-3.17744200
H	-3.89821200	3.82652000	-2.72159100
H	-2.10665500	5.11956400	-3.85401700
H	-0.95215200	-1.06982100	3.61206800

TS4'-RS

C	-5.02040600	-0.23526100	0.22904900
C	-3.64402200	-0.37544900	0.04404000
C	-2.79909700	0.72483500	0.01158800
C	-3.37009700	1.97588100	0.22676700
C	-4.74155300	2.14521700	0.38656600
C	-5.57829700	1.02799100	0.37302600
C	-5.67681300	-1.59534000	0.29795700
C	-4.51114300	-2.50566300	0.70156800
C	-3.29749800	-1.85251500	-0.00614700
H	-1.72830300	0.64821500	-0.15299900
H	-5.14840500	3.13683500	0.54731400
H	-6.64653000	1.15182700	0.51898400
H	-6.48416400	-1.65917500	1.03017200
H	-4.63825700	-3.55539100	0.41121600
H	-3.19770900	-2.22623100	-1.02309500
H	-6.07045300	-1.89751500	-0.67836900
Br	-2.22507400	3.47801500	0.39034000
O	-4.39367200	-2.39946700	2.11260200
C	-3.29340000	-3.11857200	2.62152000
H	-3.26330200	-2.98002000	3.70196200
H	-3.38060400	-4.19073200	2.39764800
N	-2.04641100	-2.13642200	0.71730000
C	-0.78436200	-1.73980000	0.41898400
C	-2.04038500	-2.58171700	2.00573600
N	-0.86528500	-2.45072200	2.54174700
N	-0.09229200	-1.89923500	1.55779300
C	1.18366900	-1.38209700	2.00308500
C	2.30343200	-2.21293500	2.05855000
C	1.16801000	-0.08311500	2.53248900
C	3.48222800	-1.65086800	2.55802700
C	2.36218000	0.41450600	3.04276600
C	3.53553300	-0.34308400	3.03559000
H	4.37732800	-2.26845400	2.58639100
H	2.38460000	1.43107800	3.42914400
C	4.83390600	0.24097200	3.52583400
H	5.35028200	-0.45041100	4.19684900

H	5.50308300	0.44221200	2.68219600
H	4.67014600	1.18445300	4.05053000
C	-0.07329400	0.76882900	2.51838900
H	-0.25976300	1.16142900	1.51234000
H	-0.95902400	0.20878600	2.83429300
H	0.04782800	1.62400000	3.18592700
C	2.26667800	-3.66886100	1.67869200
H	2.15577700	-4.27582500	2.58369400
H	1.44535000	-3.90163600	0.99834900
H	3.20923800	-3.95539000	1.20380600
C	0.52993600	-0.15999700	-2.92629300
C	0.70519700	-0.65737600	-1.47936000
H	0.28265200	-1.02574100	-3.54711900
C	-0.46993000	-1.36720000	-1.02565700
O	-1.25633900	-1.84055200	-1.84441000
C	-0.54139300	0.90133300	-3.04261300
C	-0.24748200	2.23688100	-2.74146400
C	-1.84594000	0.57544700	-3.42877200
C	-1.23541100	3.21457200	-2.80371300
H	0.76484900	2.50531600	-2.45210600
C	-2.83724800	1.55304600	-3.48413300
H	-2.07938800	-0.45584800	-3.67029800
C	-2.53769400	2.87472800	-3.16479800
H	-0.99155700	4.24310000	-2.55607000
H	-3.84709400	1.27929000	-3.77527300
H	-3.31108400	3.63600900	-3.19805100
C	1.33022500	0.32988400	-0.64796900
C	1.92073700	1.25931100	-0.13751500
C	2.54759300	2.33796400	0.56452200
C	1.77183300	3.39806900	1.05502700
C	3.92679900	2.31452100	0.81708700
C	2.36694800	4.40336500	1.81037300
H	0.70712300	3.41483000	0.84178700
C	4.51455400	3.32408800	1.56917000
H	4.51706400	1.48969300	0.42908800
C	3.73535300	4.36575400	2.07408400
H	1.76152000	5.21779500	2.19463900
H	5.58102800	3.29579300	1.76899700
H	4.19543900	5.14926000	2.66717400
H	1.49166600	0.24414500	-3.25299900
C	1.92606300	-2.20742200	-1.64098700
C	1.29303400	-3.23647300	-2.39248700
H	1.95765800	-2.40651500	-0.57159300
H	1.46632500	-3.35009700	-3.45633700

C	0.37592800	-4.08872600	-1.75866100
H	-0.09000300	-4.86277700	-2.40010300
O	0.04977000	-4.03890400	-0.54665900
C	3.18852200	-1.58053600	-2.12529200
C	4.11873800	-1.10871500	-1.19062800
C	3.49255900	-1.46015100	-3.48719200
C	5.32305000	-0.54448000	-1.60283300
H	3.88785100	-1.18861700	-0.13079000
C	4.69105400	-0.88653400	-3.90065300
H	2.78457200	-1.81326900	-4.23086200
C	5.61267700	-0.42887200	-2.96030100
H	6.03817100	-0.19902200	-0.86183100
H	4.90786200	-0.80064200	-4.96064500
H	6.54983800	0.01213200	-3.28408900

TS4'-RR

C	-2.52905400	-3.53701600	-1.00002800
C	-1.66360900	-2.52452100	-0.57480600
C	-2.07900600	-1.53872800	0.30398800
C	-3.40364200	-1.58110900	0.73402300
C	-4.28955000	-2.56477500	0.30837100
C	-3.84657400	-3.55673500	-0.56728400
C	-1.79105400	-4.53010500	-1.86982600
C	-0.34291000	-4.27777900	-1.44964800
C	-0.31527700	-2.74565700	-1.24277000
H	-1.41277000	-0.75516600	0.64052300
H	-5.31255100	-2.56066800	0.66702400
H	-4.52408600	-4.34370000	-0.88360000
H	-2.07734500	-5.56825100	-1.69094100
H	0.41990200	-4.62818100	-2.15475700
H	-0.24681000	-2.22655100	-2.20434000
H	-1.91798200	-4.31080800	-2.93602400
Br	-4.01715300	-0.24457000	1.92957900
O	-0.20404000	-4.90869100	-0.18172000
C	1.02879700	-4.70853600	0.46191400
H	0.91075200	-5.00832500	1.50427900
H	1.81991700	-5.32207800	0.00902400
N	0.88666100	-2.39206300	-0.47870800
C	1.67968700	-1.28848600	-0.54612500
C	1.47912000	-3.27894000	0.37197600
N	2.55814700	-2.77362900	0.88588600
N	2.67150900	-1.53484200	0.31286300
C	3.87655800	-0.82232000	0.67892100
C	5.03112300	-1.10837700	-0.05479900

C	3.86234300	-0.02010900	1.81429300
C	6.21067700	-0.50525100	0.36562000
C	5.07749600	0.54974000	2.20573900
C	6.25216400	0.32625900	1.49216900
H	7.12470000	-0.69416200	-0.19201900
H	5.09713900	1.18253900	3.08905100
C	7.54919100	0.96936800	1.90919200
H	7.46342900	1.43312800	2.89367100
H	8.35824900	0.23488300	1.94182400
H	7.84113900	1.74466300	1.19415000
C	2.59276500	0.23587600	2.57567600
H	1.92745700	0.88259800	1.99421900
H	2.06090700	-0.69964700	2.77511700
H	2.80399400	0.72211800	3.52933000
C	4.96999300	-2.02009300	-1.24776900
H	4.23019200	-1.64169900	-1.95903100
H	5.94126200	-2.07144500	-1.74210000
H	4.68258700	-3.03382800	-0.94897800
C	-0.50475800	0.95480100	-2.65249600
C	0.54618100	0.85442000	-1.51358400
H	-0.23631500	0.19733600	-3.39282500
C	1.40833400	-0.31783300	-1.72956000
O	1.59946400	-0.87462000	-2.80832300
C	-1.94997000	0.77567800	-2.25470000
C	-2.59105400	1.70622900	-1.42752100
C	-2.69061200	-0.30127800	-2.74661300
C	-3.92412300	1.53631200	-1.06946500
H	-2.03207500	2.56524700	-1.06260600
C	-4.03218500	-0.46444100	-2.40536100
H	-2.21049400	-1.02204800	-3.40595100
C	-4.64873300	0.44827000	-1.55543200
H	-4.39911100	2.25265600	-0.40575500
H	-4.58747200	-1.31514100	-2.78863300
H	-5.68602400	0.31117100	-1.26487200
C	0.09816000	1.03025200	-0.16980300
C	-0.32341500	1.27380200	0.94412600
C	-0.98541000	1.51588700	2.18948700
C	-0.83418800	0.64192500	3.27579100
C	-1.86956500	2.60103000	2.29450300
C	-1.55946800	0.84898700	4.44321000
H	-0.16685600	-0.20886500	3.18517200
C	-2.59922100	2.79330400	3.46095300
H	-1.98525100	3.26994600	1.44659000
C	-2.44733400	1.91887100	4.53752100

H	-1.44220200	0.16442600	5.27694700
H	-3.28987500	3.62747500	3.53168500
H	-3.01959000	2.07189100	5.44660300
H	-0.41258000	1.91765500	-3.15866600
C	1.60333700	2.58038700	-1.79180400
C	2.70131700	2.66644000	-0.89877800
H	1.83953500	2.22321900	-2.79601300
H	2.75550000	3.43832100	-0.14022100
C	3.64963600	1.65339400	-0.95937700
H	4.52622300	1.69743400	-0.28923200
O	3.50375500	0.65013900	-1.71155100
C	0.59168900	3.66875600	-1.73100500
C	0.05140300	4.21715300	-2.90146400
C	0.16971900	4.19157400	-0.49861300
C	-0.89860000	5.23436900	-2.84832500
H	0.39095000	3.84837400	-3.86595900
C	-0.77992300	5.20715600	-0.44333300
H	0.58070700	3.78428000	0.41926000
C	-1.32356200	5.72760300	-1.61778600
H	-1.30297400	5.64203100	-3.76911000
H	-1.09474900	5.59600900	0.52055600
H	-2.06606500	6.51768500	-1.57255900

TS4'-SS

C	5.08063300	-0.22522200	-0.37113700
C	3.70817400	0.00925500	-0.41190200
C	2.79210400	-0.91321700	0.06290600
C	3.29656900	-2.09926600	0.58535100
C	4.66253800	-2.36631900	0.63407300
C	5.56496500	-1.41893200	0.15021600
C	5.82660300	0.95895000	-0.94388700
C	4.78910400	2.08266300	-0.84739900
C	3.45230800	1.34232100	-1.07402200
H	1.72231200	-0.73185600	0.04882000
H	5.01482200	-3.30271000	1.05081800
H	6.63120300	-1.61670600	0.19444200
H	6.73135900	1.22353900	-0.39260300
H	4.94495300	2.90396100	-1.55722100
H	3.23033300	1.18282700	-2.13347900
H	6.09651500	0.78532500	-1.99093200
Br	2.07068300	-3.38620200	1.24883700
O	4.85621800	2.56690600	0.48934700
C	3.91821600	3.57877400	0.75228200
H	3.98316400	3.84045200	1.80883400

H	4.11915800	4.47711500	0.15158400
N	2.33711800	2.09390700	-0.48170100
C	1.00402500	1.93096100	-0.61088500
C	2.53681600	3.09167100	0.43498200
N	1.40686300	3.55452300	0.87983100
N	0.46478400	2.82707500	0.22322900
C	-0.92444200	3.06959700	0.52135800
C	-1.72950200	3.72302500	-0.41635400
C	-1.36619400	2.72396000	1.80616800
C	-3.06426200	3.93426500	-0.06268000
C	-2.70019800	2.98238400	2.11186800
C	-3.56817100	3.56196400	1.18250400
H	-3.71826200	4.42708500	-0.77772700
H	-3.07169700	2.71287600	3.09732000
C	-5.02550400	3.75489700	1.50393800
H	-5.60612100	2.91724800	1.10222100
H	-5.19358900	3.79417500	2.58206900
H	-5.41273700	4.67202100	1.05445200
C	-0.43635800	2.14372200	2.83731500
H	0.29882900	1.47288200	2.38719500
H	0.10909900	2.94328200	3.34800900
H	-0.99968800	1.57692100	3.58109500
C	-1.20721800	4.25199700	-1.72853800
H	-0.12108500	4.36015400	-1.72476800
H	-1.46381900	3.59426400	-2.56277600
H	-1.64958400	5.23121100	-1.92243700
C	-2.15138300	0.46420900	-2.04651700
C	-0.76894100	0.15149900	-1.39612800
H	-2.13843400	0.06560400	-3.06659100
C	0.16677800	1.24109100	-1.70859700
O	0.22427000	1.79147500	-2.79457200
C	-3.39909300	0.00772800	-1.32311300
C	-3.65329200	0.41413800	-0.00891500
C	-4.38510700	-0.72464900	-1.98715500
C	-4.83868800	0.06895000	0.63413100
H	-2.91381200	1.00661900	0.51567400
C	-5.57474100	-1.07341900	-1.34946500
H	-4.22069000	-1.02753200	-3.01609100
C	-5.80443400	-0.68406600	-0.03307200
H	-5.00542400	0.39467400	1.65791300
H	-6.32196400	-1.64994500	-1.88599400
H	-6.72861800	-0.95733700	0.46613600
C	-0.75767800	-0.23823800	-0.01060100
C	-0.72870800	-0.66569000	1.12571500

C	-0.82379900	-1.15873800	2.46587000
C	0.30703400	-1.25139400	3.29065100
C	-2.08012900	-1.53243100	2.96714300
C	0.17799800	-1.70618300	4.59724500
H	1.27872400	-0.97141100	2.89536100
C	-2.19823100	-1.98895000	4.27520300
H	-2.94827500	-1.45723900	2.31898900
C	-1.07244100	-2.07457400	5.09313400
H	1.05619200	-1.77505300	5.23080500
H	-3.17192900	-2.27740600	4.65756600
H	-1.16815900	-2.42942000	6.11401100
H	-2.21940600	1.55272300	-2.15488500
C	-0.12673100	-1.35126500	-2.35899900
C	0.22661900	-0.97707900	-3.69541200
H	0.75629700	-1.54458200	-1.74856800
H	-0.47228200	-1.03495200	-4.52084400
C	1.50127000	-0.45883800	-3.91305500
H	1.74852700	-0.17263000	-4.95525000
O	2.37682200	-0.31352800	-3.02009500
C	-1.16982900	-2.41074900	-2.15704200
C	-1.16793300	-3.17206300	-0.98024500
C	-2.12302300	-2.71560700	-3.13503800
C	-2.11469600	-4.16926000	-0.76853700
H	-0.39629400	-2.99294500	-0.23926200
C	-3.06603700	-3.71913500	-2.93047200
H	-2.13218700	-2.16891000	-4.07274100
C	-3.07474000	-4.44211600	-1.74077200
H	-2.09346200	-4.74226200	0.15338000
H	-3.79740500	-3.93369900	-3.70392700
H	-3.81179900	-5.22237800	-1.57954900

TS4'-SR

C	-4.40098100	-2.87492300	-0.45771300
C	-3.37559100	-1.95096900	-0.25546600
C	-3.46912400	-0.64905900	-0.71783100
C	-4.60192500	-0.31350700	-1.45096900
C	-5.62455700	-1.22464400	-1.70068400
C	-5.52747600	-2.51845900	-1.18794700
C	-4.07828100	-4.17129500	0.25414700
C	-3.05789100	-3.69991000	1.29470500
C	-2.25983900	-2.63024400	0.51745000
H	-2.67523100	0.06764400	-0.54051100
H	-6.48981200	-0.92250300	-2.27915500
H	-6.33265800	-3.22727600	-1.35292300

H	-4.94216600	-4.63276300	0.73664600
H	-2.42591700	-4.48876000	1.71938300
H	-1.52431200	-3.06973600	-0.15834700
H	-3.62210800	-4.90318800	-0.42105500
Br	-4.73002800	1.44195700	-2.17285700
O	-3.83175600	-3.06419300	2.30794300
C	-3.08441700	-2.42084000	3.30638100
H	-3.76832700	-1.80904000	3.89606200
H	-2.60149100	-3.14835100	3.97463200
N	-1.53374500	-1.76600500	1.45332200
C	-0.40730400	-1.02376900	1.30628800
C	-1.99484600	-1.56847300	2.72438800
N	-1.25232600	-0.71784400	3.36831400
N	-0.27419400	-0.39218700	2.47819500
C	0.74322400	0.52654300	2.91476500
C	1.96896000	0.02057000	3.34429000
C	0.39548000	1.87987100	2.98326000
C	2.91502900	0.94943900	3.78603300
C	1.37765000	2.76310900	3.41952500
C	2.64509500	2.31718400	3.80907200
H	3.88429800	0.58859000	4.12028700
H	1.14402200	3.82386300	3.46892500
C	3.69748600	3.30333000	4.24333000
H	4.47788300	2.81656300	4.83141800
H	4.17304300	3.76253400	3.37086300
H	3.26129700	4.10745400	4.84063400
C	-1.00035100	2.33966100	2.66115000
H	-1.39129300	1.83946900	1.77092700
H	-1.67180900	2.11132600	3.49513800
H	-1.02046300	3.41595000	2.48152300
C	2.27000300	-1.45571100	3.33122200
H	1.39789700	-2.04358000	3.63091400
H	2.57098400	-1.79908900	2.33485100
H	3.08718100	-1.67690100	4.01950700
C	3.05614700	-0.06060400	0.14552900
C	1.56688200	-0.23310200	-0.23373600
H	3.10693300	0.13811400	1.22264600
C	0.76671100	-1.31779900	0.33863800
O	1.01406700	-2.51998300	0.31530600
C	4.14566500	-1.06377100	-0.18929000
C	5.41510900	-0.53677500	-0.45987600
C	3.99551700	-2.45296600	-0.19069700
C	6.49699900	-1.36218900	-0.74121700
H	5.54690900	0.54246600	-0.47833800

C	5.07919900	-3.28300400	-0.47993800
H	3.02264800	-2.88573000	0.00654300
C	6.33201200	-2.74605200	-0.75880000
H	7.46576700	-0.92413000	-0.96227100
H	4.93670600	-4.35971600	-0.48887500
H	7.17082000	-3.39623100	-0.98693200
C	0.88319500	1.02072500	-0.20964600
C	0.28864200	2.07170700	-0.35065900
C	-0.45202900	3.29304000	-0.43237900
C	-1.76344500	3.26977800	-0.92891300
C	0.08922200	4.50560000	0.02019100
C	-2.52584800	4.42998200	-0.95644200
H	-2.17542500	2.33363000	-1.29030900
C	-0.67645900	5.66635500	-0.02019500
H	1.10170000	4.52136900	0.41121200
C	-1.98491600	5.63268800	-0.50258700
H	-3.54430300	4.38808200	-1.33118400
H	-0.25261600	6.60129400	0.33199900
H	-2.57899000	6.54030800	-0.52481600
H	3.35175900	0.88264600	-0.32203100
C	1.59912900	-0.71622000	-2.27836000
C	0.46568500	-0.09874300	-2.85295000
H	1.49256100	-1.76530900	-1.99426100
H	0.56365000	0.72717000	-3.54827600
C	-0.76877600	-0.44098500	-2.31151100
H	-1.68344400	0.07698400	-2.66573300
O	-0.87025300	-1.28932400	-1.38521700
C	2.92137000	-0.33903800	-2.83796200
C	3.80196600	-1.32131800	-3.30427500
C	3.28886300	1.00646900	-2.95482300
C	5.02030400	-0.96970100	-3.87390200
H	3.52897900	-2.36802600	-3.20316100
C	4.51801200	1.35980000	-3.50514400
H	2.60643400	1.77085900	-2.58949000
C	5.38589500	0.37246300	-3.96856700
H	5.69282900	-1.74406500	-4.22963600
H	4.79710300	2.40662100	-3.57663100
H	6.34295700	0.64774300	-4.40056000

TS4^H-RS

C	-2.72618700	-3.02576200	-1.73675900
C	-1.82579200	-2.27156300	-0.97893500
C	-2.14157300	-1.81875100	0.29031600
C	-3.42127100	-2.10387200	0.76653700

C	-4.34917300	-2.81990500	0.01880600
C	-3.99430600	-3.29559200	-1.24473500
C	-2.07790900	-3.47485500	-3.02652600
C	-0.59057700	-3.33945800	-2.69384200
C	-0.55478000	-2.08967300	-1.78417000
H	-1.43673000	-1.25746400	0.89894700
H	-5.33271900	-3.01884700	0.42817500
H	-4.70239600	-3.88254500	-1.82059600
H	-2.32219700	-4.50194500	-3.30412300
H	0.07048400	-3.25041300	-3.56429300
H	-0.59728400	-1.17696200	-2.38731000
H	-2.34043100	-2.81637600	-3.86145300
Br	-3.91473100	-1.47579500	2.48579300
O	-0.25488500	-4.47732900	-1.91424500
C	1.08390300	-4.49507600	-1.48550800
H	1.18528000	-5.28762000	-0.74264900
H	1.76638900	-4.70653100	-2.32020400
N	0.70354700	-2.05348700	-1.03301700
C	1.41964500	-0.99760400	-0.55808000
C	1.47959600	-3.17356600	-0.89335200
N	2.61994900	-2.88141700	-0.34613500
N	2.57527400	-1.53529100	-0.14914900
C	3.76622200	-0.91929800	0.38881600
C	4.72048900	-0.45086000	-0.52394900
C	3.98650500	-0.97185600	1.76284000
C	5.88875300	0.09136300	0.00019600
C	5.17674600	-0.41239500	2.23588300
C	6.12269100	0.14106500	1.37819600
H	6.64358300	0.47014900	-0.68425700
H	5.36704600	-0.42616400	3.30646200
C	7.37945200	0.77416100	1.91595900
H	7.60962600	0.40843400	2.91884300
H	8.23380500	0.56917600	1.26619700
H	7.26546200	1.86126900	1.97528600
C	3.05242000	-1.65661800	2.72262400
H	2.11500500	-1.95011500	2.25084300
H	3.53337800	-2.55204000	3.12881000
H	2.81199200	-0.98783300	3.55148500
C	4.51814400	-0.59018600	-2.00807000
H	4.32835900	-1.63604600	-2.27282300
H	3.66256200	0.00758300	-2.32862200
H	5.40897200	-0.26056500	-2.54529400
C	-0.43222600	2.06541700	-1.89383900
C	-0.18342500	0.98038600	-0.84609700

H	-1.50012400	2.05317400	-2.13456600
C	1.14903400	0.48775000	-0.80512700
O	2.16635000	1.11659900	-1.14362700
C	-0.05599800	3.51074300	-1.60768800
C	1.03003200	3.88733000	-0.81143000
C	-0.82999700	4.52147800	-2.18855300
C	1.30346600	5.23447100	-0.57437200
H	1.66085700	3.11824000	-0.37966200
C	-0.55348200	5.86625900	-1.96425800
H	-1.68449000	4.24599000	-2.80258200
C	0.51294100	6.22972300	-1.14380600
H	2.14278800	5.50459300	0.05944300
H	-1.17890100	6.62945200	-2.41759800
H	0.72704300	7.27677100	-0.95382300
H	-0.97998800	0.24953000	-0.76728400
H	0.09677900	1.77557400	-2.81506900
C	-0.81445100	1.82849800	1.05644700
C	-0.81308100	0.83758500	2.04529100
H	0.06668400	2.45964100	1.00826300
C	0.42384400	0.26788500	2.40676400
H	0.41528300	-0.52150500	3.18738300
O	1.50131800	0.56411700	1.85449000
C	-2.09969800	2.47150500	0.69036100
C	-3.25073700	1.70146900	0.47554100
C	-2.19899800	3.86438900	0.60419900
C	-4.46737000	2.30594800	0.18040600
H	-3.18774400	0.61930500	0.54158100
C	-3.41917500	4.47177700	0.31918800
H	-1.31029100	4.47262500	0.75302200
C	-4.55544300	3.69600400	0.10261800
H	-5.34739500	1.69227800	0.01432400
H	-3.47714200	5.55399400	0.25627700
H	-5.50444500	4.17014800	-0.12674600
H	-1.73660400	0.44225500	2.45465300

TS4^H-RR

C	3.69104100	-0.61531100	2.22671500
C	2.70810800	-0.74280300	1.23873600
C	3.02824000	-1.05491200	-0.07252100
C	4.38060300	-1.20766100	-0.37177800
C	5.38081300	-1.06192700	0.58225400
C	5.03055000	-0.76560500	1.90074200
C	3.05727900	-0.36258300	3.57591000
C	1.63199600	-0.86506300	3.34554300

C	1.35902100	-0.45480500	1.87944400
H	2.26510500	-1.16626600	-0.83976200
H	6.41975400	-1.19189700	0.30227900
H	5.80143700	-0.67487200	2.65928000
H	3.53559600	-0.90580800	4.39309500
H	0.88208200	-0.47200500	4.04303800
H	1.14572800	0.61467700	1.83869400
H	3.04635800	0.70424600	3.82617400
Br	4.86222800	-1.63293000	-2.15724100
O	1.70361300	-2.28069000	3.41413600
C	0.48707900	-2.93432500	3.15314600
H	0.70258100	-3.99367600	3.00765900
H	-0.20705600	-2.83099900	3.99898600
N	0.17676300	-1.17237600	1.38464200
C	-0.76649800	-0.85914600	0.45282200
C	-0.19594700	-2.37235300	1.94033400
N	-1.28276900	-2.82871400	1.39801000
N	-1.62389100	-1.88293400	0.47852900
C	-2.90827300	-1.98735100	-0.16944500
C	-3.98679500	-1.35235100	0.44296300
C	-3.00309700	-2.71721600	-1.35213400
C	-5.22694900	-1.46668900	-0.18506000
C	-4.26427700	-2.80798200	-1.93577800
C	-5.38248900	-2.19006900	-1.36813500
H	-6.08725000	-0.97421700	0.26166400
H	-4.37445400	-3.36385700	-2.86366200
C	-6.73677300	-2.32331700	-2.01579400
H	-7.40670200	-1.52105300	-1.69931500
H	-6.65602000	-2.29752300	-3.10510100
H	-7.20408200	-3.27513600	-1.74338900
C	-1.77783800	-3.33688200	-1.96280700
H	-1.00249900	-2.57673900	-2.11594600
H	-1.35922000	-4.10384400	-1.30256600
H	-2.01911200	-3.80376500	-2.91920300
C	-3.80363400	-0.55607400	1.70662200
H	-3.27026800	-1.13723100	2.46610900
H	-3.23239100	0.36037700	1.50988000
H	-4.76995500	-0.25524500	2.11375900
C	-1.39651500	2.83705800	-0.35665500
C	-0.58434300	1.63631600	0.08325900
H	-1.47739600	2.81940700	-1.44933200
C	-1.09684400	0.38771900	-0.32875800
O	-1.81376500	0.24557000	-1.33164100
C	-2.77975100	2.81708700	0.25842100

C	-2.97930400	3.26371400	1.56927000
C	-3.87235100	2.30246800	-0.44680400
C	-4.23718800	3.19744800	2.16333500
H	-2.13728700	3.66875900	2.12642100
C	-5.13271700	2.23730700	0.14408600
H	-3.71740300	1.93366300	-1.45530600
C	-5.31987500	2.68385600	1.45050000
H	-4.37420500	3.55248600	3.18023200
H	-5.96931000	1.83372800	-0.41873600
H	-6.30181300	2.63390300	1.91066700
H	-0.11835500	1.72231600	1.06029600
H	-0.87238800	3.75345400	-0.06980600
C	1.07572300	1.66742400	-1.27168800
C	0.58674400	1.28272100	-2.52242600
H	1.59122800	0.88311500	-0.72637300
C	0.39596400	-0.09676200	-2.78475000
H	-0.05584600	-0.35198600	-3.76106100
O	0.69896400	-1.02453800	-2.00305500
C	1.58918700	3.02151900	-0.95895300
C	2.43291800	3.18372400	0.14762600
C	1.26611400	4.14997800	-1.72232500
C	2.93840500	4.43380000	0.48741100
H	2.70392200	2.30874200	0.73686800
C	1.76897300	5.40244400	-1.38301100
H	0.61426500	4.04948200	-2.58460800
C	2.60494700	5.55022700	-0.27756600
H	3.59559500	4.53673000	1.34499800
H	1.50821200	6.26670000	-1.98551600
H	2.99688500	6.52783100	-0.01671100
H	0.25158100	2.00274100	-3.26057400

TS4^H-SS

C	-2.00953700	-3.65959200	-1.24264000
C	-1.20476700	-2.71493400	-0.60262700
C	-1.26546800	-2.51730100	0.76944500
C	-2.19134300	-3.27240800	1.48480700
C	-3.02397100	-4.19973100	0.86604800
C	-2.92782200	-4.40066600	-0.51144200
C	-1.67393800	-3.72326900	-2.71551300
C	-0.27795400	-3.09579000	-2.76147200
C	-0.33464500	-2.03143200	-1.64086600
H	-0.62251700	-1.80729000	1.28013000
H	-3.73009800	-4.76970800	1.45859500
H	-3.55649400	-5.14168900	-0.99443500

H	-1.65477400	-4.73843500	-3.11696400
H	-0.00390800	-2.66324000	-3.73114600
H	-0.80078300	-1.12173000	-2.02825000
H	-2.37486800	-3.12896600	-3.31160700
Br	-2.31453200	-3.01922400	3.35924500
O	0.63728500	-4.11481300	-2.39063000
C	1.97294600	-3.66962800	-2.36342700
H	2.59013100	-4.47956500	-1.97342900
H	2.32411300	-3.41082400	-3.37209400
N	1.01081500	-1.68293100	-1.19621400
C	1.46279600	-0.58281400	-0.54462400
C	2.10129000	-2.45717500	-1.49114500
N	3.18858500	-1.94276600	-1.00712800
N	2.77757500	-0.78747100	-0.40398500
C	3.76861800	-0.00297200	0.28457800
C	4.72623400	0.65753600	-0.48264800
C	3.76402600	0.00251200	1.68131300
C	5.71348200	1.36544400	0.20492400
C	4.77124000	0.72138700	2.31860200
C	5.75006400	1.41099100	1.59782300
H	6.47062300	1.89548800	-0.36760800
H	4.79266300	0.74389100	3.40544300
C	6.80807100	2.20576200	2.31882400
H	6.40774600	3.16964500	2.64884000
H	7.16096000	1.67645000	3.20738600
H	7.66443800	2.40426300	1.67111700
C	2.69714600	-0.71484700	2.46354800
H	1.75486600	-0.15708400	2.42067900
H	2.51125900	-1.71811800	2.06757600
H	2.98658600	-0.80774600	3.51134700
C	4.69943300	0.60112200	-1.98696700
H	5.13127800	-0.34004700	-2.34275100
H	3.67442200	0.65740200	-2.36753600
H	5.28504300	1.42168200	-2.40598700
C	-1.25910700	1.43648400	1.25331000
C	-0.65094400	0.70255200	0.05181700
H	-0.57690400	1.27542300	2.10033100
C	0.75984000	0.63535200	-0.00736600
O	1.50851100	1.57653400	0.31130800
C	-1.56284600	2.92133300	1.20905600
C	-0.57417600	3.86479300	0.91028200
C	-2.84161500	3.37318000	1.53984100
C	-0.87577100	5.22427100	0.90578900
H	0.42176100	3.50981700	0.66590000

C	-3.14238800	4.73311800	1.54731100
H	-3.61948200	2.64865600	1.76864100
C	-2.16101300	5.66479700	1.22119200
H	-0.10105300	5.94533900	0.66063500
H	-4.14783300	5.06175100	1.79349400
H	-2.39261900	6.72552100	1.21715300
H	-1.19311700	-0.20082000	-0.19355600
H	-2.18819600	0.91580000	1.50804900
C	-1.03622300	1.78253100	-1.79140500
C	0.04451600	2.63019800	-2.04108800
H	-0.96329400	0.83318800	-2.31376200
C	1.24725400	2.02978000	-2.47957600
H	2.12106800	2.68958900	-2.63027500
O	1.37422900	0.79910700	-2.67320500
C	-2.43329000	2.25288700	-1.60371900
C	-2.78649300	3.59536400	-1.77556000
C	-3.44488300	1.33231300	-1.30046800
C	-4.10647200	4.00762400	-1.62562600
H	-2.02196500	4.32371600	-2.02427000
C	-4.76386500	1.74205500	-1.14363200
H	-3.18989300	0.28191400	-1.17456300
C	-5.09935500	3.08609900	-1.30240300
H	-4.35810000	5.05578000	-1.75453200
H	-5.53070300	1.01314600	-0.90061500
H	-6.12806300	3.41012100	-1.18080800
H	0.03286200	3.68353800	-1.78898000

TS4^H-SR

C	-2.63924500	1.53515900	-2.09477700
C	-1.63282800	0.71475900	-1.57853400
C	-1.75681200	-0.66702000	-1.57669000
C	-2.95404900	-1.20451200	-2.04478800
C	-3.98901600	-0.40566900	-2.51901500
C	-3.82430900	0.97922700	-2.55665200
C	-2.20252400	2.98100200	-2.08292300
C	-0.68540700	2.86905500	-1.91740800
C	-0.50770100	1.59201100	-1.06556000
H	-0.95812500	-1.31415400	-1.22727700
H	-4.90487600	-0.86458500	-2.87260400
H	-4.61361300	1.60643100	-2.95850400
H	-2.44987400	3.51636700	-3.00216100
H	-0.21046900	3.74341700	-1.45455600
H	-0.63546800	1.82927900	-0.00452900
H	-2.63400400	3.51934400	-1.23389500

Br	-3.18042000	-3.08694500	-2.03083700
O	-0.15871100	2.63662700	-3.21738900
C	1.24065300	2.49622400	-3.23283700
H	1.53756700	2.19502000	-4.23824600
H	1.73743800	3.44544000	-2.98761500
N	0.84564600	1.06752100	-1.22186300
C	1.57901900	0.30059200	-0.37960200
C	1.67790600	1.46869400	-2.23228200
N	2.85808800	0.94437300	-2.10775300
N	2.77929200	0.20619100	-0.96148900
C	3.94357100	-0.53846800	-0.56087700
C	5.05057500	0.18010800	-0.11225200
C	3.93025900	-1.92733900	-0.69664800
C	6.19141300	-0.55162600	0.21771500
C	5.09470200	-2.61105400	-0.35560400
C	6.23089200	-1.94148700	0.10491000
H	7.06912700	-0.01897100	0.57543200
H	5.11462600	-3.69378400	-0.45224500
C	7.46481900	-2.71162400	0.49896400
H	7.38950100	-3.05452600	1.53589100
H	7.59671800	-3.59472000	-0.13055900
H	8.36044500	-2.09186000	0.41887700
C	2.69924700	-2.65493400	-1.16561600
H	1.93674600	-2.66274500	-0.37843400
H	2.26203000	-2.17896700	-2.04876300
H	2.93709400	-3.68994400	-1.41540500
C	5.01048700	1.68052400	0.00888600
H	5.80217800	2.02711800	0.67578200
H	5.15947300	2.15008400	-0.96880200
H	4.04299300	2.02214000	0.39180800
C	-0.28935800	-1.70553400	2.32934300
C	-0.05776400	-0.53794600	1.37875000
H	0.23282500	-1.53631600	3.27675100
C	1.26212500	-0.36855000	0.93088100
O	2.25512900	-0.69381000	1.61193900
C	-1.76344600	-1.94184000	2.55070700
C	-2.38767200	-1.70012500	3.77542900
C	-2.55248100	-2.35564600	1.47171000
C	-3.76990600	-1.84083500	3.90970900
H	-1.79003500	-1.39485100	4.63105200
C	-3.93001800	-2.49104600	1.59552900
H	-2.07655600	-2.57623200	0.51972500
C	-4.54549000	-2.22641200	2.81974400
H	-4.23958300	-1.64355400	4.86820400

H	-4.51241800	-2.80175900	0.73271200
H	-5.62098800	-2.32690100	2.92400500
H	-0.88507600	-0.28676100	0.72631300
H	0.16344400	-2.60861400	1.89609700
C	-0.15056400	1.08266600	2.92352400
C	1.17525500	1.32523700	3.27496800
H	-0.68799800	0.41992900	3.60047800
C	2.10300600	1.94134000	2.38927300
H	3.14805100	2.00748900	2.74647300
O	1.83010500	2.33412300	1.23880100
C	-1.08940400	2.04839300	2.28422100
C	-0.77658500	3.40480400	2.13112200
C	-2.37850100	1.61875800	1.92985800
C	-1.71180600	4.29642800	1.61259000
H	0.20551200	3.75617700	2.42279900
C	-3.31384500	2.50804100	1.41191600
H	-2.64418500	0.57119200	2.05776700
C	-2.98451300	3.85444300	1.25420200
H	-1.45007300	5.34428200	1.50325700
H	-4.30161000	2.15073000	1.13772400
H	-3.71549900	4.55366000	0.85947700
H	1.59189500	0.80734200	4.13184000

TS4^H-RS

C	-2.94995800	-4.39720400	0.21415500
C	-2.19873100	-3.22254300	0.27641300
C	-2.38812400	-2.18921300	-0.62997500
C	-3.39939500	-2.34426100	-1.57362600
C	-4.14258900	-3.51581000	-1.67511700
C	-3.90499100	-4.56046500	-0.78040500
C	-2.58911900	-5.30669700	1.36655700
C	-1.99953800	-4.32718100	2.38785800
C	-1.29464400	-3.27601000	1.49430600
H	-1.80350700	-1.27410500	-0.61975200
H	-4.91850200	-3.59991400	-2.42717500
H	-4.49726700	-5.46784400	-0.84034800
H	-3.44189300	-5.83833700	1.79318800
H	-1.30878200	-4.78565500	3.10532000
H	-0.28088100	-3.58992500	1.25375200
H	-1.83404300	-6.04313200	1.07178100
Br	-3.83038700	-0.87431100	-2.69024600
O	-3.10390100	-3.75228000	3.07075300
C	-2.71711000	-2.75472200	3.98790300
H	-3.61469600	-2.35562000	4.45962000

H	-2.05307100	-3.16171500	4.76282200
N	-1.22655300	-1.96765300	2.16972500
C	-0.70197700	-0.80535000	1.70964800
C	-2.00853100	-1.66656500	3.24475500
N	-2.03031600	-0.38658300	3.46359200
N	-1.23409800	0.14833600	2.48980300
C	-1.34416700	1.58396500	2.33590600
C	-0.56280300	2.44099000	3.11066600
C	-2.39798700	2.03381400	1.52498400
C	-0.78589100	3.81312500	2.95627600
C	-2.58819100	3.40746000	1.42691000
C	-1.77390600	4.31291800	2.11196500
H	-0.17208100	4.50354400	3.53086500
H	-3.37727200	3.78246500	0.77887600
C	-1.95365000	5.79720000	1.93611500
H	-1.90424700	6.31825600	2.89555200
H	-1.15995200	6.20234300	1.29904000
H	-2.90861500	6.02650000	1.45885100
C	-3.27586100	1.08315400	0.75566600
H	-2.75379100	0.70824700	-0.13158000
H	-3.57978400	0.22342700	1.36137100
H	-4.17714600	1.59478400	0.41300100
C	0.43690600	1.95807600	4.12685900
H	0.01403900	2.06513300	5.13105500
H	0.71870800	0.91662700	3.97347500
H	1.34159400	2.57200100	4.08532400
C	1.62659200	-0.30737400	-1.41171000
C	0.80761300	0.19004700	-0.20962900
H	2.45487900	-0.91616100	-1.03946000
C	0.37492000	-0.88893700	0.63073600
O	0.96405500	-1.97276800	0.60853500
C	0.77118800	-1.10795300	-2.36964000
C	-0.03208200	-0.45671600	-3.31292800
C	0.73979300	-2.50557300	-2.31393500
C	-0.85625600	-1.18290200	-4.16718400
H	-0.00943100	0.62820300	-3.37163800
C	-0.09226500	-3.23213900	-3.16305700
H	1.36322100	-3.01550200	-1.58729100
C	-0.89807800	-2.57341000	-4.08814000
H	-1.47863500	-0.66116600	-4.88739100
H	-0.11166700	-4.31609700	-3.09940300
H	-1.55258000	-3.13783400	-4.74529900
C	-0.05346900	1.28006100	-0.54598300
C	-0.65512400	2.22392500	-1.01650300

C	-1.48082200	3.28301600	-1.51215200
C	-2.68576600	2.98001400	-2.16271400
C	-1.12476900	4.62252200	-1.30113400
C	-3.53236900	4.00588000	-2.56987100
H	-2.94576000	1.93948300	-2.33372800
C	-1.97408100	5.64158900	-1.71447800
H	-0.18728900	4.84253200	-0.79924000
C	-3.18236600	5.33595000	-2.34170900
H	-4.46742900	3.76716100	-3.06598700
H	-1.69759900	6.67679500	-1.54125300
H	-3.84683400	6.13360100	-2.65718400
H	2.03494800	0.56957800	-1.92035100
C	2.25908100	0.90587700	1.08761100
C	3.07741600	-0.19150700	1.48321400
H	1.53874000	1.16933000	1.85909100
C	2.61267200	-1.01340700	2.56418000
H	3.28279200	-1.85231300	2.83250800
O	1.55630500	-0.84630800	3.18929300
C	2.73980900	2.09860100	0.34721400
C	2.14240700	3.33275700	0.64168400
C	3.74632600	2.06429900	-0.62906300
C	2.55681900	4.50075700	0.00956400
H	1.34133600	3.36973400	1.37538800
C	4.15096100	3.23161900	-1.27030500
H	4.21176100	1.12143100	-0.88796300
C	3.56473400	4.45454400	-0.95096200
H	2.09139100	5.44727600	0.26914200
H	4.93122100	3.18345500	-2.02348100
H	3.88867800	5.36284900	-1.44859500
C	4.29751100	-0.57234300	0.86992600
C	5.35633300	-0.93664900	0.39045400
C	6.59756700	-1.31992100	-0.20337300
C	7.22388400	-0.47846600	-1.13925900
C	7.21283700	-2.53739700	0.13307600
C	8.42859600	-0.85029300	-1.72283400
H	6.75672800	0.46706900	-1.39672500
C	8.41992300	-2.89930600	-0.45312100
H	6.73303000	-3.19030800	0.85465600
C	9.03235600	-2.06055600	-1.38327300
H	8.90025900	-0.19104500	-2.44458700
H	8.88443400	-3.84246500	-0.18350600
H	9.97387200	-2.34740900	-1.83972900

TS4^H-RR

C	-5.04410500	0.85506700	-1.20684500
C	-3.69309600	0.73238100	-0.87290500
C	-3.01085800	-0.45816700	-1.01408800
C	-3.73572500	-1.55734300	-1.46486200
C	-5.08048400	-1.47104700	-1.80201400
C	-5.74223000	-0.24543500	-1.68038800
C	-5.49731800	2.28173700	-0.99482600
C	-4.16967600	3.04299600	-1.05091400
C	-3.18839900	2.06393200	-0.36213000
H	-1.96246600	-0.56080000	-0.76023500
H	-5.60828300	-2.35093900	-2.15193900
H	-6.78872000	-0.16591100	-1.95698600
H	-6.18914500	2.64817800	-1.75547800
H	-4.18213100	4.03549100	-0.58532000
H	-3.26320600	2.13555800	0.72753600
H	-5.96009600	2.40608300	-0.00887700
Br	-2.85463200	-3.23541000	-1.49883600
O	-3.84073300	3.13142600	-2.43122000
C	-2.59789200	3.72947900	-2.69499900
H	-2.37722000	3.59353400	-3.75431300
H	-2.61528300	4.80604500	-2.47429000
N	-1.80781600	2.39529600	-0.73352300
C	-0.63857800	2.14533700	-0.09443100
C	-1.51609500	3.11429900	-1.85704500
N	-0.23663500	3.30228300	-1.96435800
N	0.29962600	2.69744900	-0.86213900
C	1.71640600	2.93256200	-0.68330800
C	2.07723700	4.14793600	-0.09407600
C	2.61665000	2.07380900	-1.31124300
C	3.42773800	4.48289600	-0.12084600
C	3.95895900	2.44847100	-1.29421300
C	4.37873900	3.64378000	-0.70932100
H	3.74584900	5.41498700	0.33876400
H	4.68761800	1.78598600	-1.75534700
C	5.84122100	4.00141700	-0.67122800
H	6.37959900	3.55574900	-1.51058400
H	5.98649100	5.08367300	-0.69687200
H	6.29752100	3.62803000	0.25184000
C	2.15266700	0.81217200	-1.98047900
H	1.71318900	0.13670600	-1.24116700
H	1.39788700	1.02920500	-2.74480200
H	2.99134500	0.29453900	-2.45026300
C	1.04329800	5.02953300	0.54891100
H	0.53214800	4.48485400	1.34924100

H	1.51412500	5.91153600	0.98456200
H	0.29741100	5.36171800	-0.18129900
C	-1.26577500	-0.23921900	2.87321600
C	-0.34086900	0.27659300	1.75078300
H	-1.18333800	0.45176300	3.71824500
C	-0.66652000	1.64374200	1.37220900
O	-1.12983000	2.49037700	2.12452600
C	-2.71359700	-0.41054900	2.48580400
C	-3.14283100	-1.60744300	1.90448100
C	-3.65588800	0.59336800	2.73533400
C	-4.48094000	-1.79629600	1.57013500
H	-2.41656000	-2.39055800	1.69599600
C	-4.99349100	0.41186100	2.38859300
H	-3.33096800	1.51700500	3.20786600
C	-5.40874600	-0.78435700	1.80404500
H	-4.78923600	-2.72704000	1.10237900
H	-5.71515900	1.19811900	2.59086800
H	-6.45048600	-0.92642700	1.53407700
C	-0.08817000	-0.65410900	0.69403900
C	0.17602400	-1.52901300	-0.10682900
C	0.56856500	-2.57762700	-0.99519900
C	0.71994100	-2.34535900	-2.37014800
C	0.83013700	-3.85548700	-0.47566600
C	1.16130300	-3.36656400	-3.20247100
H	0.49426800	-1.36325800	-2.77268200
C	1.26469100	-4.87289200	-1.31799200
H	0.69825700	-4.03030500	0.58787300
C	1.43962400	-4.62967100	-2.68010900
H	1.28701800	-3.17777400	-4.26351500
H	1.47130500	-5.85676400	-0.90973800
H	1.78517400	-5.42383200	-3.33378900
H	-0.88014900	-1.20632400	3.19581400
C	1.41517500	0.33538700	2.74716000
C	2.52568900	0.81896400	1.99178600
H	1.05924200	1.10356200	3.43580500
C	2.83434100	2.21088400	2.12019400
H	3.78988800	2.51161400	1.64816800
O	2.14102100	3.05228900	2.70298300
C	1.49252700	-1.01529900	3.37314800
C	1.19840200	-1.12737000	4.73922700
C	1.88556600	-2.16982700	2.67991200
C	1.28890800	-2.34982100	5.39770300
H	0.89479800	-0.24005300	5.28853500
C	1.96602100	-3.39408500	3.33759000

H	2.13085600	-2.10640100	1.62713600
C	1.66806200	-3.49140100	4.69567500
H	1.05947200	-2.40970700	6.45670700
H	2.27256100	-4.27692000	2.78420200
H	1.73551700	-4.44833600	5.20303100
C	3.34084300	0.03845200	1.14246800
C	4.05327600	-0.56077400	0.35342700
C	4.78331200	-1.23729200	-0.66832100
C	6.01778800	-0.73894900	-1.12330700
C	4.26134300	-2.39838300	-1.26956300
C	6.70232100	-1.38047700	-2.14960200
H	6.42809800	0.15366000	-0.66052900
C	4.95654000	-3.03508400	-2.29019400
H	3.30314200	-2.78657600	-0.93601200
C	6.17808900	-2.53120500	-2.73720800
H	7.65260900	-0.98111200	-2.49007200
H	4.53269300	-3.92667400	-2.74288600
H	6.71590200	-3.02952100	-3.53698600

TS4^H-SS

C	3.96583100	-1.09233600	-3.09098500
C	3.06680300	-0.59367200	-2.14414300
C	3.11421200	-0.99203500	-0.81971500
C	4.07515800	-1.94011800	-0.46574700
C	4.96124200	-2.47241900	-1.39533400
C	4.90962300	-2.03922900	-2.72207100
C	3.74346500	-0.41869600	-4.42657300
C	3.00144100	0.85346600	-4.01315300
C	2.12394700	0.36709600	-2.84077600
H	2.43242800	-0.58846800	-0.07990100
H	5.69414800	-3.20722100	-1.08308100
H	5.61583200	-2.43226200	-3.44640200
H	4.66645300	-0.18002000	-4.95847500
H	2.42354700	1.33301600	-4.81199200
H	1.23274800	-0.16576600	-3.19766400
H	3.10720100	-1.02600700	-5.07939300
Br	4.16668800	-2.51047100	1.34156300
O	3.99479100	1.73773600	-3.50253800
C	3.49313000	2.95469300	-3.01262000
H	4.29812800	3.45586200	-2.47324700
H	3.15828900	3.60832000	-3.83012200
N	1.66715800	1.52719900	-2.06774900
C	0.54591300	1.70511200	-1.34143000
C	2.31595600	2.73389300	-2.10589400

N	1.67218200	3.63327600	-1.42080000
N	0.57578700	2.97736100	-0.94936600
C	-0.44691400	3.73360300	-0.26432300
C	-1.44894300	4.30851100	-1.06304800
C	-0.32816700	3.96893300	1.10367900
C	-2.40215600	5.08886800	-0.41895100
C	-1.29418300	4.79102100	1.69032800
C	-2.34260500	5.33670400	0.95768900
H	-3.19654300	5.53858300	-1.00884600
H	-1.22392200	4.98885300	2.75691700
C	-3.40530600	6.16913300	1.62496600
H	-4.33891200	5.60220500	1.70394600
H	-3.10360900	6.46511100	2.63169700
H	-3.62060900	7.07107900	1.04653500
C	0.75842800	3.37524900	1.95572900
H	1.57189800	2.95710400	1.36130000
H	1.16980700	4.13615400	2.62278200
H	0.34484300	2.56875500	2.56985600
C	-1.45284000	4.14206500	-2.55948700
H	-0.52195200	4.52758300	-2.98856100
H	-1.54673400	3.09137500	-2.84479200
H	-2.28347700	4.69679800	-2.99741200
C	-2.31527700	-0.06496700	0.51357600
C	-0.87350000	-0.02245700	-0.03682900
H	-2.64038500	-1.10022700	0.61887400
C	-0.71531900	0.83788100	-1.19224000
O	-1.53535100	0.96417300	-2.09082400
C	-2.46676400	0.61270700	1.85241800
C	-2.90876600	1.93037500	1.95709600
C	-2.15210800	-0.09098500	3.02165700
C	-3.04982800	2.53228600	3.20780900
H	-3.14119700	2.49192700	1.05354600
C	-2.27900100	0.51052600	4.26872400
H	-1.80179100	-1.11866500	2.93958900
C	-2.73412900	1.82636300	4.36491900
H	-3.40585600	3.55639600	3.27494300
H	-2.02944500	-0.04625300	5.16663600
H	-2.84359400	2.29592100	5.33729300
C	0.18068900	0.08404000	0.92798100
C	1.08554600	0.08302200	1.73736100
C	2.19412800	0.01170000	2.63596000
C	3.36558800	0.73893400	2.37687400
C	2.14107900	-0.84935300	3.74201900
C	4.47058300	0.59536200	3.20709000

H	3.40844600	1.39198600	1.51003000
C	3.25306400	-0.98951800	4.56300000
H	1.23345100	-1.41506000	3.92744900
C	4.41923200	-0.27094300	4.29732400
H	5.37716100	1.15326000	2.99716500
H	3.21237000	-1.66343700	5.41259900
H	5.28617000	-0.38762500	4.93918500
H	-2.96469400	0.39248900	-0.23744100
C	-0.69097200	-1.83401700	-0.89869000
C	-1.66336100	-1.93190400	-1.94789600
H	0.30606500	-1.71247200	-1.32492700
C	-1.23006400	-1.70003000	-3.28960700
H	-2.03492200	-1.76605800	-4.04771300
O	-0.06654400	-1.47807600	-3.65924200
C	-0.65373200	-2.72684600	0.29477800
C	0.59015700	-2.96721500	0.89562400
C	-1.78067700	-3.35489100	0.84723800
C	0.70972600	-3.76304800	2.02836500
H	1.48107300	-2.52936900	0.46175900
C	-1.66365700	-4.15301700	1.98330100
H	-2.75051800	-3.23795300	0.37791900
C	-0.42348700	-4.35103400	2.58691400
H	1.69333500	-3.91731000	2.46202600
H	-2.54960400	-4.62750900	2.39333700
H	-0.33956200	-4.97209200	3.47302900
C	-3.04854000	-2.15735300	-1.76054000
C	-4.24958900	-2.33116200	-1.64510800
C	-5.64854900	-2.52108400	-1.43755800
C	-6.17155600	-2.53851900	-0.13197900
C	-6.52721300	-2.68960400	-2.52128300
C	-7.53260300	-2.72232900	0.07802900
H	-5.49763900	-2.40243500	0.70857800
C	-7.88752700	-2.87007400	-2.30126200
H	-6.12946300	-2.67704600	-3.53067600
C	-8.39712200	-2.88861600	-1.00350500
H	-7.92137600	-2.73357900	1.09141300
H	-8.55406900	-2.99852900	-3.14826700
H	-9.45960100	-3.03088800	-0.83615800

TS4^H-SR

C	-4.93496000	-1.16730300	-2.23311400
C	-3.79668600	-0.99304600	-1.44593800
C	-3.49770300	0.22189200	-0.85517100
C	-4.33796500	1.29292900	-1.14170100

C	-5.45867600	1.15978900	-1.95658300
C	-5.76915500	-0.08890100	-2.49703400
C	-5.06930000	-2.62164700	-2.63202800
C	-4.21047900	-3.31184600	-1.56680900
C	-3.05007600	-2.31080900	-1.37835600
H	-2.62762500	0.34437000	-0.21800600
H	-6.08742300	2.01980900	-2.15572800
H	-6.65935100	-0.20769000	-3.10637000
H	-6.09652800	-2.99031000	-2.60272300
H	-3.87290200	-4.32283700	-1.82337500
H	-2.30470100	-2.38464500	-2.17200200
H	-4.65892400	-2.80909400	-3.63008500
Br	-3.90318100	3.00173200	-0.43273900
O	-5.01417000	-3.32431200	-0.39102300
C	-4.36287500	-3.78432400	0.76437200
H	-5.00621700	-3.57306000	1.61934300
H	-4.18589900	-4.86857100	0.71817300
N	-2.36658300	-2.55677500	-0.10665300
C	-1.11075900	-2.25734200	0.30658600
C	-3.02607100	-3.12594100	0.94535900
N	-2.27154800	-3.16900100	2.00331900
N	-1.09124300	-2.62959000	1.59318500
C	-0.02613500	-2.54177400	2.55785200
C	0.95899600	-3.52848500	2.56187100
C	-0.10092100	-1.51464100	3.50197900
C	1.97181900	-3.40315400	3.51406100
C	0.93331100	-1.43554300	4.43071400
C	1.98523800	-2.35572700	4.43676600
H	2.76298300	-4.14800000	3.53746200
H	0.91337700	-0.63859600	5.17000400
C	3.11708400	-2.21568400	5.42048800
H	3.57078600	-3.18381700	5.64240700
H	3.89934900	-1.56848400	5.01104100
H	2.77423500	-1.76824000	6.35592900
C	-1.27589900	-0.57592900	3.54107600
H	-1.55132900	-0.23663200	2.53845700
H	-2.14573500	-1.07843300	3.97617600
H	-1.04415100	0.30424300	4.14315300
C	0.90488000	-4.69784900	1.61172500
H	-0.02266600	-5.26158500	1.75438000
H	0.93888900	-4.38816000	0.56260500
H	1.74519000	-5.36975000	1.79180700
C	2.63107200	-1.93482500	0.04478100
C	1.26081600	-1.28280800	-0.25516900

H	2.47633600	-2.70568100	0.80933400
C	0.15054800	-2.16565400	-0.59839800
O	0.13869300	-3.06073900	-1.43681800
C	3.52792000	-2.52939400	-1.02743600
C	4.90848900	-2.39924700	-0.83551600
C	3.08063500	-3.23580000	-2.14721300
C	5.81813600	-2.93859000	-1.73781700
H	5.27380900	-1.83989200	0.02240000
C	3.99174900	-3.76986500	-3.05786100
H	2.01709100	-3.35303400	-2.31353600
C	5.36187100	-3.62388900	-2.86175000
H	6.88339000	-2.80886200	-1.57138200
H	3.62280500	-4.30397900	-3.92869900
H	6.06669500	-4.03879100	-3.57552500
C	0.90642800	-0.25516100	0.66850100
C	0.62574100	0.74820200	1.29462300
C	0.26813900	1.92580800	2.02008900
C	-0.79138500	2.71885400	1.55382300
C	0.94777300	2.30125000	3.18883000
C	-1.17229900	3.85870700	2.24894700
H	-1.29732900	2.43456100	0.63720800
C	0.56991100	3.45429200	3.87154000
H	1.76427900	1.68353800	3.54988800
C	-0.49027500	4.23296200	3.40704500
H	-1.99903400	4.45780200	1.87911900
H	1.10200400	3.74361400	4.77212000
H	-0.78177800	5.12904500	3.94509400
H	3.21256200	-1.15705000	0.54713000
C	1.61556600	-0.06065500	-1.98065000
C	0.70437800	1.02176800	-1.89336900
H	1.27907600	-0.88860300	-2.60458000
C	-0.66436800	0.67147600	-1.94423000
H	-1.40767800	1.48872600	-1.85149300
O	-1.04411800	-0.51187100	-2.02693300
C	3.06885400	0.23186300	-2.02888100
C	3.81779300	-0.19162300	-3.13261600
C	3.70507900	0.96347300	-1.01946600
C	5.17178800	0.10733400	-3.22858300
H	3.33152300	-0.77245400	-3.91125000
C	5.06618600	1.24281500	-1.10406400
H	3.12498000	1.29921900	-0.16439700
C	5.80201700	0.81954400	-2.20938600
H	5.73886200	-0.23067900	-4.09022000
H	5.55179600	1.79966500	-0.30860900

H	6.86226100	1.04303900	-2.27565200
C	1.03611700	2.35939900	-1.53114300
C	1.22851200	3.51513700	-1.20554000
C	1.45948100	4.84982600	-0.73126200
C	1.67442700	5.07873100	0.63774100
C	1.46220700	5.94177800	-1.61241300
C	1.88553000	6.36939700	1.10893200
H	1.66353700	4.23549900	1.32184200
C	1.67307300	7.23067100	-1.13421700
H	1.29637400	5.76664400	-2.67032300
C	1.88534500	7.44863700	0.22631100
H	2.04478900	6.53183100	2.17058600
H	1.67196300	8.06758800	-1.82521000
H	2.04849200	8.45558900	0.59680100

R2CF

C	-3.97461600	1.06986100	0.00432200
C	-2.85154700	1.83048000	0.00048300
H	-4.90973600	1.62854500	-0.03798100
C	-3.04297700	3.30412100	-0.03199700
H	-4.10363600	3.62289100	-0.04911400
O	-2.14124900	4.11009200	-0.03871500
C	-4.14416000	-0.37822900	0.03875000
C	-5.43459000	-0.88249200	-0.19583200
C	-3.10377400	-1.28531500	0.30326000
C	-5.67849700	-2.24962800	-0.19088900
H	-6.24716600	-0.18775600	-0.38897100
C	-3.35325100	-2.65163700	0.31568900
H	-2.10719900	-0.91829300	0.51329900
C	-4.63584900	-3.13850300	0.06384400
H	-6.67970500	-2.62149000	-0.38035400
H	-2.54308300	-3.34179800	0.52663500
H	-4.82251000	-4.20733400	0.07290300
C	-1.50338900	1.36970800	0.00013700
C	-0.33347100	1.05254500	-0.01497300
C	1.03620800	0.63942200	-0.03014900
C	1.36201100	-0.70767600	-0.25189500
C	2.05826000	1.57814200	0.17404700
C	2.68997900	-1.10835100	-0.26407900
H	0.56941900	-1.42865000	-0.41986500
C	3.38588900	1.17369500	0.16149000
H	1.80090200	2.61822200	0.33876100
C	3.69621900	-0.16672000	-0.05641800
H	2.94666900	-2.14696100	-0.44173900

H	4.17939000	1.89680900	0.31365900
C	5.12732300	-0.61724100	-0.01340700
F	5.34863600	-1.65313200	-0.83678800
F	5.48362600	-1.02022200	1.21844200
F	5.97307400	0.36357300	-0.36074500

TS4CCF-RS

C	3.91919600	0.81315600	3.23555400
C	3.50084700	0.16933200	2.06771400
C	3.90318700	0.59442600	0.81262500
C	4.75158400	1.69697000	0.76615800
C	5.17466500	2.36615400	1.90838200
C	4.75284200	1.91947300	3.16148300
C	3.34093500	0.13152100	4.45582700
C	2.92799000	-1.23868200	3.91112400
C	2.54221200	-0.93443200	2.44652700
H	3.60783300	0.09370100	-0.10482900
H	5.83364400	3.22208200	1.81876500
H	5.08809300	2.42767000	4.06004600
H	4.05311900	0.02021100	5.27617700
H	2.10892000	-1.72192200	4.46020700
H	1.49677000	-0.60953700	2.37660900
H	2.46385800	0.66939500	4.83354400
Br	5.32958100	2.32312800	-0.92469100
O	4.09373800	-2.04578400	3.93459000
C	3.91997000	-3.34955400	3.43319900
H	4.91080900	-3.78463100	3.30881300
H	3.32808200	-3.96557300	4.12465100
N	2.62238600	-2.17202600	1.67583400
C	2.00145800	-2.47299700	0.53870300
C	3.22258600	-3.31972900	2.10800300
N	2.98122500	-4.31165200	1.29445100
N	2.21722000	-3.75609600	0.31106000
C	1.51878600	-4.53790500	-0.67889500
C	2.01341800	-4.62718700	-1.97943600
C	0.31803500	-5.14223000	-0.27049200
C	1.19861700	-5.26130600	-2.92389000
C	-0.45211000	-5.75655600	-1.25242100
C	-0.03932100	-5.80132700	-2.58900600
H	1.55265900	-5.32653400	-3.94995900
H	-1.39765000	-6.21304800	-0.97119700
C	-0.92274700	-6.42265300	-3.63827900
H	-1.41211200	-7.32298400	-3.25792700
H	-1.71496500	-5.72554500	-3.93143000

H	-0.35228200	-6.68501500	-4.53149500
C	-0.08340300	-5.21161200	1.18126300
H	0.47113500	-6.01617700	1.67508600
H	0.12044600	-4.28863400	1.72991600
H	-1.14939400	-5.43497600	1.26694100
C	3.38000200	-4.13879800	-2.37645200
H	3.82558900	-3.46054700	-1.64889100
H	4.04833400	-4.99976500	-2.48288400
H	3.33488500	-3.64064400	-3.34827600
H	1.40616300	-1.80771700	-0.07153900
B	5.79265400	-2.01317600	0.19150100
F	4.47979400	-2.00694600	-0.35891400
F	6.51756200	-3.04127000	-0.40366800
F	5.68014400	-2.23256200	1.57208300
F	6.38992400	-0.77844400	-0.05685100
N	2.84784400	0.61973200	-2.78143500
C	1.91214400	1.59357400	-3.33688600
C	2.52917100	2.97485300	-3.54061400
H	1.07294100	1.66514800	-2.63392800
H	1.48037400	1.25459900	-4.29726900
H	1.74089000	3.72290500	-3.66942500
H	3.14303800	3.25260400	-2.67913500
H	3.16122000	3.01185000	-4.43153600
C	4.03475100	0.47183100	-3.62306400
C	5.01474600	-0.57622000	-3.11615600
H	4.54563700	1.44010300	-3.63430700
H	3.75529000	0.25290200	-4.67196400
H	5.93162500	-0.52931900	-3.71073700
H	5.26876100	-0.40124700	-2.06827600
H	4.61662600	-1.59164200	-3.19977800
C	2.17338200	-0.64656500	-2.48543000
C	1.63523100	-1.43272700	-3.68412300
H	1.33135900	-0.40158600	-1.82350000
H	2.87235800	-1.27043000	-1.91457200
H	1.16270900	-2.35767700	-3.33674000
H	0.87609500	-0.86635900	-4.23059600
H	2.43602000	-1.70177600	-4.38181000
C	-1.89310700	-1.50678300	-1.13855800
C	-1.06775900	-1.17518500	-0.05623000
H	-2.26161700	-2.53020500	-1.08780700
C	-1.01214700	-2.10001300	1.04840900
H	-1.61059800	-3.01661000	0.89750700
O	-0.31553900	-1.96792300	2.05904600
C	-1.76796000	-0.99711300	-2.52225900

C	-1.93634200	-1.90809800	-3.57515500
C	-1.50258600	0.34166800	-2.83517700
C	-1.87325900	-1.48654300	-4.90008500
H	-2.11413900	-2.95500200	-3.34594500
C	-1.45142400	0.76661400	-4.15842100
H	-1.33035800	1.05745800	-2.04256800
C	-1.64447400	-0.14395100	-5.19675000
H	-2.00509100	-2.20846700	-5.69987300
H	-1.25456500	1.81508500	-4.36297100
H	-1.60739600	0.18895700	-6.22895800
C	-0.40945000	0.07738400	0.08273300
C	0.13715600	1.15308600	0.24479200
C	0.66541600	2.47208100	0.42858300
C	-0.07450200	3.41966100	1.15290500
C	1.87275600	2.84207300	-0.17609400
C	0.38336800	4.72444200	1.25994300
H	-1.01797200	3.12936600	1.60463600
C	2.33901200	4.14476200	-0.04941300
H	2.43124500	2.11312400	-0.75913600
C	1.58865800	5.08112200	0.65649900
H	-0.19347000	5.46683600	1.80102000
H	3.28950300	4.42191500	-0.49509800
C	-5.31054100	3.81092000	-1.57677600
C	-4.50920400	2.85769400	-0.94134900
C	-3.13547400	2.82007500	-1.11848400
C	-2.58596000	3.74663800	-2.00781500
C	-3.36963000	4.67014800	-2.69095000
C	-4.74636400	4.71112400	-2.46676800
C	-6.73466700	3.71625400	-1.07712500
C	-6.54925800	2.98428300	0.25422100
C	-5.39952200	2.00146500	-0.06347600
H	-2.50324800	2.11735300	-0.57880500
H	-2.90169800	5.37114900	-3.37228200
H	-5.35485600	5.45819100	-2.96576600
H	-7.20746600	4.68824400	-0.92497600
H	-7.44651900	2.48112600	0.63374300
H	-5.78289100	1.13010600	-0.60346000
H	-7.36459400	3.12303500	-1.74876100
Br	-0.71113100	3.76582200	-2.28430500
O	-6.07728200	3.95257800	1.17883300
C	-5.78829100	3.43288200	2.45262900
H	-5.26345700	4.20450500	3.01738300
H	-6.70705000	3.16557900	2.99296100
N	-4.79487000	1.51559100	1.17868100

C	-4.14760400	0.35361300	1.45733400
C	-4.94201800	2.19648700	2.35492200
N	-4.40519700	1.54002000	3.34096200
N	-3.92276700	0.40072300	2.77779700
C	-3.33341800	-0.56282400	3.68478300
C	-4.16786700	-1.53641800	4.24209700
C	-2.00811500	-0.37705900	4.06371600
C	-3.59786500	-2.39650000	5.17435200
C	-1.48577100	-1.26580400	5.00433200
C	-2.25630400	-2.28524000	5.55604700
H	-4.21775300	-3.17013300	5.62045400
H	-0.44889400	-1.14943900	5.30886500
C	-1.65900300	-3.26094300	6.53602400
H	-1.37115100	-4.18609300	6.02647500
H	-0.76489400	-2.84972300	7.00928000
H	-2.37557400	-3.52561400	7.31723900
C	-1.19025900	0.75020100	3.50167700
H	-1.15839900	0.70331100	2.41066100
H	-1.60862200	1.71890400	3.79603900
H	-0.16237700	0.69690200	3.86584400
C	-5.61557500	-1.64089400	3.84982500
H	-6.11796300	-0.67146400	3.93111600
H	-5.69644300	-1.98091000	2.81394000
H	-6.13673700	-2.34976600	4.49481600
C	-4.76206400	-1.71778400	-1.74633800
C	-3.98690500	-0.80137700	-0.79788700
H	-4.61770600	-1.29583800	-2.74634300
C	-4.00471300	-0.90507000	0.60586500
O	-3.86349000	-1.93041800	1.29462600
C	-4.52824300	-3.21876800	-1.86857400
C	-4.63044900	-3.78589400	-3.14599900
C	-4.30019600	-4.07544100	-0.78649500
C	-4.49783400	-5.15725300	-3.34419300
H	-4.80343100	-3.13674600	-4.00133700
C	-4.15947800	-5.44914200	-0.98349300
H	-4.21834000	-3.65818500	0.21026200
C	-4.25570700	-5.99801100	-2.25917700
H	-4.57636000	-5.56755900	-4.34643400
H	-3.97682400	-6.09317000	-0.12771600
H	-4.14462300	-7.06761900	-2.40820000
H	-3.94150500	0.21407300	-1.18419100
H	-5.83234900	-1.58331300	-1.52970900
C	2.10979400	6.47659500	0.83045800
F	2.94088100	6.83159400	-0.15984800

F	2.79421800	6.61379500	1.98016000
F	1.11634600	7.37959500	0.86651600
TS4CCF-SS			
C	6.14451700	-1.74834300	-1.37619200
C	5.17035600	-0.91459000	-0.81856900
C	4.79331000	-1.02148700	0.51392100
C	5.45350500	-1.98427400	1.27251900
C	6.44804900	-2.80444500	0.74985300
C	6.79501300	-2.69210400	-0.59425900
C	6.33288700	-1.45035900	-2.84371900
C	5.77400800	-0.03485500	-2.95946400
C	4.62439400	-0.02447200	-1.92104500
H	4.03053900	-0.39942100	0.97497300
H	6.93665100	-3.53072400	1.38938600
H	7.55837300	-3.33553200	-1.01927800
H	7.37313400	-1.48736900	-3.17370600
H	5.42989000	0.24353300	-3.96396100
H	3.71368200	-0.45424400	-2.35377300
H	5.74913000	-2.14375500	-3.45925100
Br	4.94337100	-2.24395400	3.07815100
O	6.80778500	0.83203800	-2.52356100
C	6.46177600	2.19549900	-2.53289700
H	7.25815400	2.74456200	-2.03523300
H	6.33568300	2.56436000	-3.56093800
N	4.32297300	1.36394900	-1.57109500
C	3.22170600	1.87770600	-1.01412500
C	5.17883700	2.40773100	-1.79337400
N	4.64705500	3.53422800	-1.41460500
N	3.42706600	3.18171800	-0.92435500
C	2.48652800	4.20273900	-0.54089500
C	2.66778700	4.87958000	0.66547700
C	1.47523300	4.51538200	-1.45683700
C	1.75365300	5.89390700	0.96355400
C	0.60539000	5.54617100	-1.11699000
C	0.72529000	6.24226000	0.08975200
H	1.86792400	6.43547700	1.89958200
H	-0.17096000	5.82281400	-1.82522800
C	-0.23711800	7.34956900	0.43654900
H	-0.62729500	7.82972900	-0.46473100
H	-1.09112900	6.96309000	1.00418900
H	0.24487300	8.11269900	1.05144200
C	1.33254100	3.77640900	-2.75952500
H	2.29579500	3.66954100	-3.26806200

H	0.92050900	2.77956500	-2.57687100
H	0.65168000	4.31100400	-3.42404500
C	3.80581500	4.57856400	1.60254900
H	4.26306300	3.60563600	1.42267100
H	4.59183700	5.33269900	1.49019900
H	3.45691200	4.62025200	2.63823000
H	2.29618300	1.36749300	-0.75279800
B	6.51750200	1.92245500	1.33190200
F	5.15436000	1.76270000	0.96773400
F	6.61056000	2.97472600	2.24309500
F	7.24665100	2.22167700	0.17061100
F	6.98243800	0.73662600	1.89435200
N	2.42279800	0.12700800	3.08958100
C	1.21788100	-0.62497800	3.43474800
C	1.45699800	-2.12383400	3.56439700
H	0.48196600	-0.46913100	2.64132800
H	0.75814100	-0.23732600	4.36372000
H	0.53000400	-2.62853700	3.85541500
H	1.78032600	-2.52476200	2.59972400
H	2.22651400	-2.35625500	4.30591600
C	3.16645900	0.50588800	4.28555300
C	4.48137600	1.21388800	3.99384600
H	3.37810300	-0.41922900	4.83681600
H	2.54720900	1.12924900	4.96076200
H	5.03316600	1.35782000	4.92788900
H	5.10143900	0.62993400	3.31023400
H	4.33594100	2.19889500	3.54194500
C	2.14471800	1.23167700	2.17519000
C	1.20157200	2.32258900	2.69007000
H	1.70604300	0.78333400	1.27755400
H	3.10073100	1.67151700	1.87218400
H	1.02017400	3.05920200	1.90061800
H	0.23302600	1.89893100	2.98242100
H	1.62107000	2.84400300	3.55721200
C	-1.74096600	-0.64757600	1.13611800
C	-0.66719400	-0.18728000	0.35924700
H	-2.26876900	0.15405100	1.65345800
C	-0.57437500	1.22595500	0.07549700
H	-1.38054900	1.84085500	0.51799500
O	0.33754200	1.77154400	-0.54653200
C	-1.75638400	-1.91066700	1.91416100
C	-2.22411800	-1.86069900	3.23593900
C	-1.32207300	-3.14177300	1.40446300
C	-2.27608500	-3.00682600	4.02410800

H	-2.52729800	-0.90305200	3.65552900
C	-1.37421800	-4.28677600	2.19351200
H	-0.94515900	-3.20160500	0.39036300
C	-1.85492500	-4.22732200	3.50082000
H	-2.63600700	-2.94331000	5.04603000
H	-1.03789400	-5.23303700	1.78247000
H	-1.89446800	-5.12485800	4.10889700
C	0.35988600	-1.03912800	-0.13767300
C	1.24350600	-1.76966400	-0.54471100
C	2.20912300	-2.67922100	-1.08531800
C	2.37559200	-2.77339400	-2.47752500
C	2.99373100	-3.48155400	-0.24242800
C	3.32237800	-3.63534900	-3.01373100
H	1.75439400	-2.16579000	-3.12738200
C	3.92759300	-4.35553700	-0.78149400
H	2.91282100	-3.37436000	0.83505900
C	4.09656100	-4.42179200	-2.16207900
H	3.45294200	-3.70630900	-4.08893200
H	4.54255600	-4.96570600	-0.12969600
C	-7.01718200	-2.18975300	2.57559300
C	-6.39259900	-1.47680300	1.55011700
C	-6.74132000	-1.64984500	0.21838500
C	-7.73238600	-2.58970500	-0.05910700
C	-8.35400600	-3.32940800	0.94228100
C	-7.99639700	-3.12547400	2.27478900
C	-6.48250400	-1.75693700	3.92139800
C	-5.86914700	-0.39053300	3.60808000
C	-5.34303600	-0.57455900	2.16635800
H	-6.27221600	-1.08910700	-0.58580500
H	-9.12135500	-4.04884800	0.68139100
H	-8.49385800	-3.68415900	3.06071500
H	-7.24915500	-1.66998700	4.69364700
H	-5.07942000	-0.07874500	4.30346300
H	-4.36729300	-1.06668300	2.20372100
H	-5.70471800	-2.44165100	4.27772100
Br	-8.25792900	-2.86470200	-1.85858500
O	-6.93085800	0.54901600	3.60416200
C	-6.50603000	1.85542600	3.30062800
H	-7.38956300	2.48883000	3.21785200
H	-5.85558100	2.25669200	4.09022200
N	-5.16886800	0.72748800	1.51551400
C	-4.47154200	1.07848500	0.40577800
C	-5.74831200	1.86680200	2.00629100
N	-5.46777200	2.89257800	1.25846100

N	-4.67649400	2.39112700	0.27186400
C	-4.21824900	3.30162900	-0.74774200
C	-3.31940600	4.29436600	-0.36919800
C	-4.75119700	3.18803400	-2.03759300
C	-2.96543500	5.23097900	-1.34252400
C	-4.34996800	4.13795100	-2.97011900
C	-3.46126300	5.16760600	-2.64071400
H	-2.28254500	6.02952200	-1.06514700
H	-4.74280500	4.07574600	-3.98183600
C	-3.02822100	6.16661200	-3.68157600
H	-2.28846200	5.72168500	-4.35499000
H	-3.87328600	6.49231200	-4.29304600
H	-2.57514800	7.04692200	-3.21997400
C	-5.68185600	2.06689700	-2.41624000
H	-5.11304700	1.14248900	-2.57489800
H	-6.43176300	1.87778700	-1.64149800
H	-6.20518300	2.30464600	-3.34359500
C	-2.71852500	4.38445500	1.01013400
H	-2.85203400	3.46701000	1.58730400
H	-1.64396900	4.57743600	0.92712400
H	-3.16950500	5.20213200	1.58072800
C	-2.73848500	-1.86396700	-1.39829900
C	-3.38233000	-1.09186500	-0.26970400
H	-2.69664100	-2.92439400	-1.13211700
C	-3.56400100	0.28163500	-0.49997300
O	-2.89003800	0.94679200	-1.30612100
C	-3.51161700	-1.68406200	-2.69157700
C	-4.76549200	-2.27830300	-2.86734600
C	-3.00715000	-0.87113100	-3.70948800
C	-5.49286000	-2.07028300	-4.03708400
H	-5.17997600	-2.90861600	-2.08170200
C	-3.73163800	-0.66211000	-4.88099000
H	-2.04679200	-0.38573100	-3.56531300
C	-4.97722000	-1.26223900	-5.04877700
H	-6.46400400	-2.53922800	-4.15558100
H	-3.32423700	-0.02518900	-5.66015200
H	-5.54428100	-1.10086700	-5.96001800
H	-4.08372400	-1.64217000	0.34326700
H	-1.71302000	-1.50966800	-1.54888400
C	5.17236800	-5.28545000	-2.74756500
F	4.78505400	-5.85716100	-3.89837800
F	6.28138200	-4.57190300	-3.03542300
F	5.54963900	-6.26435300	-1.91506300

TS4CCF-RR

C	0.14574300	-4.65887500	0.78667000
C	-0.53451500	-3.44758200	0.65920900
C	-0.53077900	-2.73230900	-0.53306300
C	0.18972500	-3.27385900	-1.59308300
C	0.84997300	-4.49831500	-1.49906400
C	0.83068700	-5.19739700	-0.29588500
C	0.03720900	-5.20501400	2.18864800
C	-1.07481500	-4.36591400	2.82829500
C	-1.08774000	-3.04755500	2.00837300
H	-1.06335800	-1.79546200	-0.67822200
H	1.37650100	-4.89389700	-2.36134800
H	1.34464800	-6.14951400	-0.21125300
H	-0.23456200	-6.26264900	2.22448800
H	-0.91163900	-4.16851100	3.89655300
H	-0.43943100	-2.29014000	2.46058200
H	0.98069100	-5.08671700	2.73259900
Br	0.32159000	-2.28898900	-3.19868600
O	-2.28534300	-5.07644100	2.65565100
C	-3.38631600	-4.41059600	3.23057800
H	-4.27708000	-5.00127700	3.03285200
H	-3.24470100	-4.27913800	4.31308100
N	-2.43675500	-2.47729700	2.00759500
C	-2.86254400	-1.32513800	1.48315200
C	-3.52967600	-3.07585800	2.57279500
N	-4.58544300	-2.32295800	2.46313400
N	-4.14844900	-1.23493700	1.77270400
C	-5.02108600	-0.12638600	1.50826800
C	-6.19908200	-0.37350100	0.79353900
C	-4.67260700	1.12982300	2.01696700
C	-7.05107700	0.71001700	0.59219400
C	-5.56491100	2.17587700	1.77858500
C	-6.75128400	1.98663300	1.07243300
H	-7.96980800	0.55182100	0.03205700
H	-5.32613500	3.16275300	2.16477500
C	-7.69473500	3.13244200	0.82157500
H	-8.70943100	2.87954600	1.14157100
H	-7.37770300	4.03132900	1.35376200
H	-7.73840600	3.37258900	-0.24510800
C	-3.41392600	1.36264300	2.81539600
H	-3.28212900	0.59329300	3.58350600
H	-2.51242400	1.35600100	2.19163600
H	-3.46764400	2.33329500	3.31163200
C	-6.52092100	-1.73354500	0.23616500

H	-5.64382100	-2.21183900	-0.20584400
H	-6.88159100	-2.40532700	1.02066800
H	-7.29644900	-1.64851500	-0.52767600
H	-2.26124800	-0.58014300	0.97920200
B	-4.34012900	-4.57795500	-0.40673100
F	-3.67078900	-3.34257300	-0.22391500
F	-5.49246500	-4.35405500	-1.17008100
F	-4.70749900	-5.07801100	0.85220400
F	-3.49086900	-5.46927700	-1.05190100
N	-2.67047900	-0.77651600	-2.91700600
C	-2.00269900	0.39640000	-3.46508700
C	-2.70535500	1.19965900	-4.56955000
H	-1.03335400	0.06030200	-3.85851200
H	-1.76761200	1.05885000	-2.62524700
H	-2.00172900	1.92821000	-4.98404200
H	-3.03392600	0.55316900	-5.38872300
H	-3.57564500	1.75320300	-4.20707100
C	-3.01892500	-1.76273700	-3.93086200
C	-3.30117900	-3.13503400	-3.33730800
H	-2.16021600	-1.83440100	-4.60967400
H	-3.87748500	-1.44427300	-4.54937400
H	-3.45281200	-3.86435300	-4.13895100
H	-2.45988600	-3.46212800	-2.72101200
H	-4.19023100	-3.14541500	-2.70292400
C	-3.72486800	-0.50993600	-1.94261500
C	-5.10287300	-0.13031600	-2.50321100
H	-3.35647900	0.28939800	-1.28364300
H	-3.83657800	-1.40337800	-1.31562900
H	-5.75698900	0.20661500	-1.69490100
H	-5.04162600	0.67403300	-3.24085600
H	-5.58036300	-0.98952600	-2.98514100
C	1.48713000	0.69539600	-1.09653600
C	0.42681700	0.77257100	-0.16685200
H	2.07988300	-0.21335200	-0.98724300
C	0.50517600	-0.05971400	1.00493200
H	1.42259400	-0.68004800	1.06031400
O	-0.35604800	-0.17145700	1.88265300
C	1.44690200	1.15294400	-2.50811100
C	2.23680500	0.46762100	-3.44274800
C	0.66878200	2.22843200	-2.95915800
C	2.23567100	0.82667600	-4.78570900
H	2.83084400	-0.38090500	-3.11516100
C	0.68013300	2.59808000	-4.30126600
H	0.05038300	2.77938600	-2.26048000

C	1.45491600	1.89581600	-5.22149900
H	2.84267400	0.26891200	-5.49152700
H	0.07483800	3.43792000	-4.62793500
H	1.45327400	2.18130200	-6.26842200
C	-0.69134400	1.64824700	-0.22605200
C	-1.68566900	2.35044400	-0.20065300
C	-2.80860000	3.24099200	-0.20066600
C	-3.80239100	3.14060500	-1.18571100
C	-2.90779400	4.24618200	0.77644000
C	-4.86687900	4.03330700	-1.20416100
H	-3.72930800	2.36286300	-1.93870500
C	-3.96724000	5.14101000	0.75342900
H	-2.13959500	4.32057400	1.53856100
C	-4.94276200	5.03326000	-0.23851600
H	-5.63219500	3.95477800	-1.96888900
H	-4.03972500	5.92267800	1.50304100
C	7.21089800	0.12529500	-1.74712300
C	6.05516300	0.27692300	-0.98521100
C	4.99903500	-0.60790100	-1.07160500
C	5.10050600	-1.65523200	-1.97766900
C	6.21995300	-1.80963700	-2.78912300
C	7.28779000	-0.91309400	-2.66814100
C	8.23558900	1.15385000	-1.31709400
C	7.76294400	1.51790900	0.10039800
C	6.21911400	1.42321100	-0.01534900
H	4.12003500	-0.52038000	-0.44362700
H	6.27357600	-2.63510000	-3.48949700
H	8.17786700	-1.05648000	-3.27199200
H	9.25774900	0.77176500	-1.29040000
H	8.09655700	2.50144200	0.45121500
H	5.79910500	2.36849000	-0.37587700
H	8.21317100	2.03865800	-1.96180900
Br	3.63868600	-2.85672500	-2.02926200
O	8.24949600	0.49198100	0.95162000
C	7.80177900	0.60741100	2.28307400
H	8.20685400	-0.22923100	2.85173000
H	8.14094400	1.54834700	2.73771300
N	5.59291700	1.09587400	1.26847000
C	4.27737500	0.96496100	1.56839300
C	6.30511900	0.56244000	2.30695200
N	5.51143900	0.09980800	3.22867700
N	4.26009000	0.35436200	2.75737500
C	3.12493300	-0.18768000	3.46236400
C	2.50802000	0.59630000	4.43795200

C	2.75100500	-1.50073200	3.16704500
C	1.41551000	0.04034700	5.09741100
C	1.67336300	-2.01816400	3.88510600
C	0.97730400	-1.25617300	4.82355700
H	0.89719800	0.63327200	5.84599900
H	1.37747400	-3.04995100	3.70751200
C	-0.23827000	-1.81795900	5.51126500
H	-0.47044300	-1.26737400	6.42475500
H	-1.11218000	-1.74331900	4.85179700
H	-0.10017700	-2.87147400	5.76911100
C	3.45757900	-2.33584700	2.12691000
H	3.05910600	-2.16549800	1.11779300
H	4.53219900	-2.13670600	2.10066400
H	3.31782700	-3.39711700	2.34256400
C	3.01074800	1.97836800	4.74836900
H	4.06690600	1.95422900	5.03421500
H	2.90985200	2.61532400	3.86488300
H	2.44244300	2.41724600	5.56949000
C	2.44643500	3.39588900	-0.68446200
C	3.04838100	2.02626700	-0.42061300
H	1.43159100	3.43321600	-0.27374400
C	3.08534200	1.66804200	0.94590500
O	2.17242600	1.93203400	1.74624900
C	3.31085200	4.45824100	-0.04045200
C	4.46398700	4.91592800	-0.68727800
C	3.01970400	4.94477200	1.23759400
C	5.31305600	5.83145000	-0.07009500
H	4.69194500	4.55155200	-1.68718400
C	3.86688600	5.86218300	1.85651300
H	2.12856000	4.58778600	1.74546600
C	5.01692000	6.30605400	1.20693700
H	6.20083900	6.18054500	-0.58844600
H	3.62628200	6.23294300	2.84820200
H	5.67474500	7.02195200	1.68903100
H	3.87570700	1.74749300	-1.06587200
H	2.38806400	3.57052600	-1.76047700
C	-6.03640100	6.05828200	-0.28243200
F	-7.05762600	5.68468200	-1.06697100
F	-5.59374500	7.23769000	-0.74966100
F	-6.53851000	6.30212300	0.94243100
TS4CCF-SR			
C	0.66981500	-4.99424200	0.48054000
C	1.21759400	-3.73373500	0.23711200

C	1.57363000	-2.87346700	1.26863800
C	1.36891100	-3.33235700	2.56667700
C	0.81197600	-4.57925300	2.83684000
C	0.45687700	-5.42041400	1.78437100
C	0.39430200	-5.72059700	-0.81594800
C	1.25803600	-4.96530300	-1.83202700
C	1.29877600	-3.52819100	-1.25993300
H	2.04795000	-1.90868700	1.11060300
H	0.67795300	-4.89527200	3.86488000
H	0.03838200	-6.40051100	1.98937900
H	0.66783900	-6.77763100	-0.79516400
H	0.85934500	-4.98152000	-2.85556100
H	0.44810700	-2.96238700	-1.64609800
H	-0.66490000	-5.64565600	-1.08969800
Br	1.90659200	-2.24827900	4.02447000
O	2.54753700	-5.54328700	-1.80327700
C	3.46133000	-4.91892400	-2.67481800
H	4.43708700	-5.37075500	-2.51084000
H	3.15668200	-5.04735600	-3.72331200
N	2.50019900	-2.84063200	-1.72544600
C	2.83163900	-1.55448100	-1.60225500
C	3.54110700	-3.45627700	-2.36173900
N	4.46787900	-2.59590400	-2.67587100
N	4.00816900	-1.41155600	-2.18703200
C	4.73632300	-0.18812600	-2.37868000
C	6.06203300	-0.12059800	-1.93352300
C	4.08834500	0.86923200	-3.03089900
C	6.74179300	1.07717300	-2.15529900
C	4.82119000	2.04026100	-3.22045800
C	6.13922300	2.16850100	-2.78074200
H	7.76688300	1.16275800	-1.80426800
H	4.35100800	2.87154800	-3.74136200
C	6.87018300	3.47593800	-2.93161400
H	7.95071500	3.32547300	-2.97483300
H	6.55497100	4.00415600	-3.83490700
H	6.65866800	4.12744200	-2.07639600
C	2.66750000	0.77019800	-3.53103100
H	2.48198100	-0.18096900	-4.03901000
H	1.93179200	0.84913400	-2.72076300
H	2.46957400	1.57610700	-4.24120200
C	6.73391000	-1.26404400	-1.22271600
H	6.05489100	-1.77334000	-0.53557700
H	7.08725300	-2.01121700	-1.93967900
H	7.59562300	-0.89448600	-0.66323300

H	2.24406500	-0.77417200	-1.13883000
B	4.91762800	-3.90126000	0.75475300
F	4.31716000	-2.69193100	0.31477600
F	6.26459200	-3.65570300	1.02941900
F	4.81036400	-4.84403800	-0.27872000
F	4.25468900	-4.35580900	1.89122500
N	3.53813600	0.25772400	2.41858800
C	2.58759400	1.18625900	3.02024300
C	3.14408000	2.39984100	3.77820200
H	1.96494300	0.61084200	3.72134600
H	1.91452100	1.52618700	2.22687300
H	2.30805900	2.99361300	4.16452700
H	3.74931400	2.09218000	4.63583900
H	3.75797400	3.04773900	3.14685600
C	4.60555800	-0.12401700	3.33207000
C	5.34171900	-1.38468100	2.90739700
H	4.13077900	-0.30809800	4.30577600
H	5.32860900	0.69623400	3.49593200
H	6.09819700	-1.63988200	3.65608700
H	4.64496300	-2.21984600	2.81027800
H	5.85227700	-1.27099600	1.94812000
C	3.95412100	0.56178300	1.05483500
C	4.90279700	1.74723400	0.84322200
H	3.03741700	0.74848500	0.47972000
H	4.40503500	-0.34767900	0.63652800
H	5.08569000	1.88555600	-0.22699200
H	4.47351100	2.67806900	1.22367800
H	5.86924100	1.58371800	1.33250200
C	-1.14840300	-0.18514700	1.42437000
C	-0.42168500	0.07983900	0.25123900
H	-1.50127300	-1.21370000	1.52407200
C	-0.50679700	-0.87716100	-0.81562600
H	-1.09062900	-1.78884300	-0.56415000
O	-0.00589500	-0.75859300	-1.94084700
C	-0.95826100	0.53828000	2.69110700
C	-0.84853500	-0.21772100	3.86305900
C	-0.87591900	1.93717100	2.77225700
C	-0.59983800	0.40254700	5.08501000
H	-0.90420400	-1.30070500	3.80555800
C	-0.65183200	2.55507700	3.99522300
H	-0.99765000	2.54154000	1.87838400
C	-0.50107700	1.78842200	5.15385500
H	-0.48685700	-0.20089100	5.97978300
H	-0.59716800	3.63795100	4.04948600

H	-0.31435300	2.27520000	6.10549500
C	0.35499500	1.24762800	0.04481900
C	1.01226800	2.25862300	-0.11591100
C	1.88990900	3.38382800	-0.14676600
C	2.61541400	3.69439500	-1.30553900
C	2.07659100	4.14990500	1.01607600
C	3.54555800	4.72287700	-1.29090000
H	2.45470800	3.10919400	-2.20355400
C	3.00189900	5.18425100	1.02517100
H	1.51404900	3.90325900	1.91170700
C	3.74315000	5.45814000	-0.12364300
H	4.12695400	4.94776200	-2.17986600
H	3.16546400	5.76257700	1.92814200
C	-3.28730800	4.41095600	-1.13444300
C	-3.69599100	3.09321200	-0.91763200
C	-4.98066300	2.78275700	-0.49568300
C	-5.84843100	3.84827700	-0.26617800
C	-5.46109600	5.17132900	-0.45499200
C	-4.16908700	5.45652200	-0.89837600
C	-1.86085100	4.44556500	-1.63781100
C	-1.65236400	3.01896600	-2.15047200
C	-2.51870600	2.17888400	-1.18285400
H	-5.31082000	1.75981900	-0.33579300
H	-6.16793400	5.97107800	-0.26737000
H	-3.87022900	6.48620500	-1.06538700
H	-1.69292000	5.17294300	-2.43448100
H	-0.60850900	2.68307600	-2.15863200
H	-1.95594000	1.98471900	-0.26762000
H	-1.15496700	4.65411400	-0.82504800
Br	-7.61097300	3.47673200	0.32388700
O	-2.20678800	2.95915600	-3.45553100
C	-2.08954300	1.67808100	-4.02551800
H	-2.58402000	1.68730900	-4.99691600
H	-1.03515500	1.39631100	-4.16018300
N	-2.85245300	0.88653900	-1.78658600
C	-3.35385000	-0.24498600	-1.23718800
C	-2.73349200	0.66305200	-3.13160100
N	-3.17417000	-0.51858300	-3.45021700
N	-3.55385900	-1.07086400	-2.26979900
C	-4.18186900	-2.36684700	-2.27683700
C	-3.44435000	-3.44705800	-2.75975600
C	-5.50661000	-2.47037700	-1.83507300
C	-4.07365400	-4.69305700	-2.76721900
C	-6.08387900	-3.73592300	-1.86939300

C	-5.38348500	-4.85755600	-2.32175100
H	-3.51942500	-5.55478700	-3.13090600
H	-7.11099500	-3.84921600	-1.53141700
C	-6.03291500	-6.21653800	-2.30771000
H	-5.50201400	-6.91653100	-2.95573400
H	-6.03323600	-6.63070800	-1.29456400
H	-7.07293200	-6.15812700	-2.63785800
C	-6.28720300	-1.28695600	-1.32513100
H	-6.02688800	-1.06458500	-0.28254500
H	-6.10889100	-0.38985000	-1.92709000
H	-7.35644100	-1.50341200	-1.35348500
C	-2.03633600	-3.30087600	-3.27651800
H	-2.04335000	-3.05288700	-4.34237500
H	-1.47976000	-2.50489300	-2.77385300
H	-1.49808400	-4.24446900	-3.15815600
C	-3.94863100	-0.15806900	2.57485500
C	-3.42183000	0.26864200	1.22542200
H	-3.78894400	0.64445800	3.30165400
C	-3.50058700	-0.68273600	0.20327400
O	-3.55312400	-1.91716700	0.36772400
C	-5.42209500	-0.49466900	2.44644800
C	-5.85072500	-1.82366000	2.45190500
C	-6.36377500	0.51414900	2.20975100
C	-7.19110900	-2.14093200	2.23428900
H	-5.12017800	-2.61186700	2.60557600
C	-7.70162500	0.19996000	1.98857900
H	-6.04539200	1.55543900	2.18451500
C	-8.12024100	-1.13064000	2.00173900
H	-7.50560400	-3.18010000	2.23838700
H	-8.41512400	0.99568500	1.79979900
H	-9.16310200	-1.37578500	1.82759700
H	-3.45793100	1.32620000	0.99847700
H	-3.40764300	-1.04073700	2.93557700
C	4.72870000	6.58851300	-0.12737100
F	5.21741600	6.83406200	1.09581700
F	5.77174200	6.33578300	-0.93688600
F	4.17513000	7.73331600	-0.56327300
R2Cl			
C	-3.24643000	1.17519500	-0.00536300
C	-2.07112900	1.85263900	-0.00936400
H	-4.13789200	1.80174900	-0.03675500
C	-2.15884200	3.33637600	-0.03754900
H	-3.19456200	3.72871300	-0.05166000

O	-1.20323800	4.07786900	-0.04438000
C	-3.52549700	-0.25584900	0.02396100
C	-4.86578100	-0.65364700	-0.11921800
C	-2.54376200	-1.24724200	0.19410800
C	-5.21755500	-1.99701200	-0.10862000
H	-5.63277100	0.10579200	-0.24314000
C	-2.89993700	-2.58965500	0.20918800
H	-1.50704700	-0.96405700	0.32397600
C	-4.23304800	-2.96970600	0.05472000
H	-6.25682000	-2.28532300	-0.22447100
H	-2.13322200	-3.34534300	0.34455400
H	-4.50316500	-4.02054400	0.06606100
C	-0.75722100	1.30267400	-0.00445400
C	0.39167000	0.91519100	-0.00991600
C	1.73621100	0.42792800	-0.01428100
C	1.99322500	-0.93887100	-0.19735900
C	2.80937000	1.31289300	0.16584100
C	3.29709400	-1.41540800	-0.19892100
H	1.16576100	-1.62532500	-0.34189300
C	4.11577000	0.84288100	0.16534700
H	2.61153500	2.36968400	0.30621500
C	4.34478600	-0.51765400	-0.01675200
H	3.50208100	-2.47021400	-0.34008100
H	4.94914000	1.52162600	0.30459800
Cl	5.98525500	-1.11318300	-0.01768100

TS4CCI-RS

C	-3.74617700	-1.31616300	3.35553000
C	-3.43155000	-0.68139200	2.15046800
C	-3.79396600	-1.21661000	0.92570600
C	-4.49556500	-2.41876700	0.94882600
C	-4.81556500	-3.07798500	2.12950800
C	-4.43567300	-2.51978300	3.35093100
C	-3.23926800	-0.50967200	4.53020800
C	-3.02146700	0.87475400	3.91480900
C	-2.62001700	0.55620500	2.45726400
H	-3.57673700	-0.73026500	-0.02056700
H	-5.36259900	-4.01305600	2.09400500
H	-4.69111500	-3.02062600	4.27936400
H	-3.94354900	-0.45397700	5.36294000
H	-2.26827700	1.49065300	4.42376900
H	-1.54197200	0.36887200	2.37839700
H	-2.29194900	-0.91065800	4.90892900
Br	-5.00893600	-3.19424100	-0.70103000

O	-4.28624800	1.51700700	3.92495300
C	-4.29458100	2.81006900	3.36831600
H	-5.33592400	3.10367000	3.24264000
H	-3.78208800	3.52789400	4.02387500
N	-2.87518300	1.73797000	1.63734400
C	-2.31623500	2.06982100	0.47633400
C	-3.61573100	2.81447000	2.03407500
N	-3.52005200	3.79355000	1.17678600
N	-2.70359000	3.30209500	0.20145100
C	-2.13828600	4.12894200	-0.83554800
C	-2.66040700	4.08961400	-2.12777200
C	-1.03302000	4.91931800	-0.47710400
C	-1.96259100	4.79708600	-3.11357400
C	-0.37931800	5.60064200	-1.49795000
C	-0.81494400	5.52907400	-2.82621400
H	-2.33824900	4.76655700	-4.13356900
H	0.49201100	6.20352600	-1.25478800
C	-0.05074600	6.23544400	-3.91454600
H	0.24763900	7.23818000	-3.59706200
H	0.86637700	5.68691200	-4.15401900
H	-0.64604700	6.32090100	-4.82567700
C	-0.61908200	5.10278600	0.96107200
H	-1.27686400	5.83525500	1.44018000
H	-0.67331400	4.18127900	1.54614300
H	0.40361600	5.48354900	1.01214900
C	-3.94585400	3.39015800	-2.47904700
H	-4.29420800	2.70744200	-1.70450700
H	-4.72618400	4.14118600	-2.64012200
H	-3.82986500	2.83727000	-3.41494700
H	-1.64848100	1.46290700	-0.11947700
B	-6.00720500	1.13333700	0.16889800
F	-4.68701400	1.22425000	-0.35422600
F	-6.82391900	2.00825300	-0.54105200
F	-5.96022800	1.49892600	1.52238200
F	-6.45199300	-0.18050900	0.03408700
N	-2.78876400	-1.27575500	-2.67876400
C	-1.74187200	-2.14764500	-3.20426600
C	-2.17971300	-3.60385900	-3.33709300
H	-0.89448600	-2.08033900	-2.51069000
H	-1.36510700	-1.80098700	-4.18487900
H	-1.30384100	-4.25073400	-3.44612600
H	-2.74353300	-3.91768900	-2.45401100
H	-2.81147600	-3.76160300	-4.21492700
C	-3.99407100	-1.32009800	-3.50565400

C	-5.09702400	-0.38856900	-3.02487200
H	-4.37391400	-2.34625600	-3.46838900
H	-3.75805900	-1.11191000	-4.56733400
H	-6.00603600	-0.57772600	-3.60320600
H	-5.31568300	-0.55404300	-1.96742700
H	-4.83557200	0.66585500	-3.15252200
C	-2.27880700	0.07874100	-2.45129100
C	-1.85785500	0.87104900	-3.69216900
H	-1.40573000	-0.02630400	-1.79296000
H	-3.04560100	0.63453900	-1.89784500
H	-1.50636000	1.86446200	-3.39308300
H	-1.03648800	0.38294900	-4.22405600
H	-2.69297800	1.00205500	-4.38919900
C	1.65245000	1.52023100	-1.22301800
C	0.87930100	1.15293600	-0.11363600
H	1.88820400	2.58300800	-1.23655000
C	0.71747800	2.12715200	0.93631100
H	1.18938300	3.10307800	0.72019600
O	0.05541500	1.96810900	1.96631500
C	1.58603100	0.91980800	-2.57470600
C	1.63084600	1.78384700	-3.67858000
C	1.48828700	-0.45706900	-2.81049400
C	1.61171000	1.28443800	-4.97758300
H	1.67460300	2.85598700	-3.51036900
C	1.48160400	-0.95817200	-4.10798800
H	1.41085300	-1.14354600	-1.97799900
C	1.55131100	-0.09059400	-5.19724700
H	1.64520900	1.97145800	-5.81727700
H	1.41636800	-2.03263300	-4.25258100
H	1.54872900	-0.48301400	-6.20903700
C	0.39220400	-0.16482100	0.10491900
C	-0.00307300	-1.29548800	0.32377200
C	-0.34447400	-2.66363400	0.57445500
C	0.52322800	-3.46887500	1.32631000
C	-1.49472000	-3.22647300	0.00805700
C	0.25507700	-4.81991900	1.50117900
H	1.42137600	-3.03394400	1.75451500
C	-1.77928100	-4.57382600	0.19504800
H	-2.15792500	-2.61093300	-0.59603600
C	-0.89553800	-5.35604000	0.93065900
H	0.92708900	-5.45213200	2.07001600
H	-2.68873900	-5.00082200	-0.21549300
C	5.71062800	-3.34564500	-1.40335000
C	4.79019600	-2.47153200	-0.81739300

C	3.42409700	-2.61934300	-0.99356200
C	3.00179300	-3.65345400	-1.83241600
C	3.90109400	-4.50151400	-2.46951100
C	5.27080500	-4.35406200	-2.24612500
C	7.10699500	-3.04648300	-0.90548400
C	6.81767800	-2.28179800	0.38881000
C	5.55729400	-1.46757600	0.01889900
H	2.70585100	-1.97605600	-0.48876400
H	3.53024300	-5.29105500	-3.11267800
H	5.97201700	-5.04198200	-2.70714400
H	7.69846800	-3.94179000	-0.70534600
H	7.64109500	-1.65325500	0.74828600
H	5.83322600	-0.58176000	-0.56164800
H	7.66221600	-2.41047500	-1.60332300
Br	1.14642000	-3.93183800	-2.09783500
O	6.46003900	-3.25829700	1.35544700
C	6.08827200	-2.72389500	2.60143000
H	5.65294500	-3.52983800	3.19363600
H	6.95790700	-2.32309700	3.14026500
N	4.88421400	-1.00232300	1.23315600
C	4.10085100	0.08590700	1.45327800
C	5.09884700	-1.60584700	2.44067600
N	4.47781400	-0.97263100	3.39201500
N	3.86989800	0.07471800	2.77376200
C	3.17822500	1.01255100	3.63527300
C	3.90110700	2.10239700	4.13119300
C	1.88771500	0.69564300	4.04644500
C	3.24472500	2.94043700	5.02566800
C	1.27598600	1.56767400	4.94855800
C	1.92846300	2.69738100	5.43315800
H	3.77651400	3.80150400	5.42255200
H	0.26338800	1.34906600	5.27773300
C	1.23354900	3.64898500	6.37152100
H	0.85473600	4.51756600	5.82349700
H	0.38506400	3.17007300	6.86454800
H	1.91834900	4.01820300	7.13879400
C	1.19924300	-0.54772600	3.56177900
H	1.16946700	-0.57780800	2.47035500
H	1.71620700	-1.44451100	3.92049200
H	0.16914700	-0.57959900	3.92326200
C	5.32736600	2.34654500	3.72245800
H	5.93292700	1.44254800	3.84470500
H	5.36920700	2.64573400	2.67206600
H	5.76936800	3.13658400	4.33126900

C	4.47405500	2.06287100	-1.84807300
C	3.81344500	1.10067400	-0.85785600
H	4.40673400	1.57229200	-2.82451800
C	3.81896500	1.27478700	0.53921600
O	3.56170100	2.31113800	1.17586100
C	4.03483100	3.50757600	-2.05479900
C	4.04880500	4.00886500	-3.36299500
C	3.69388700	4.38448600	-1.01929200
C	3.71759500	5.33316900	-3.63637000
H	4.30815700	3.34300400	-4.18284900
C	3.35452700	5.70947600	-1.29115900
H	3.67861100	4.01740200	0.00025000
C	3.36175900	6.19129700	-2.59749500
H	3.73061300	5.69206200	-4.66109400
H	3.08630500	6.36901900	-0.47050300
H	3.09459100	7.22284200	-2.80547600
H	3.89257500	0.06999200	-1.19555500
H	5.54838500	2.09040000	-1.61265500
Cl	-1.24159400	-7.05473000	1.15225600

TS4CCl-SS

C	-6.27739300	-1.87556500	1.81675600
C	-5.31185500	-1.12012900	1.14491700
C	-4.92385800	-1.42217600	-0.15378200
C	-5.55901700	-2.50324800	-0.75925200
C	-6.54000000	-3.25502800	-0.12088000
C	-6.90252500	-2.94187300	1.18702600
C	-6.48434600	-1.36157800	3.22063500
C	-5.94602100	0.06432600	3.12420800
C	-4.79045900	-0.06047900	2.09944500
H	-4.17423000	-0.85725500	-0.70159800
H	-7.00872800	-4.08128400	-0.64311400
H	-7.66236100	-3.52353700	1.69944900
H	-7.52734200	-1.35976000	3.54341300
H	-5.61318100	0.49664200	4.07656000
H	-3.87516200	-0.40128500	2.59548800
H	-5.89742200	-1.94469100	3.94096300
Br	-5.03212100	-3.02097200	-2.50461000
O	-6.99319400	0.83646600	2.56081300
C	-6.67000400	2.19154900	2.36678500
H	-7.47275200	2.64588400	1.78989800
H	-6.55602300	2.71176700	3.32861100
N	-4.51151000	1.26477800	1.54244800
C	-3.41913200	1.71080400	0.91158400

C	-5.38734900	2.31338100	1.60659500
N	-4.87757300	3.38003300	1.06184600
N	-3.65019100	2.98253600	0.62736200
C	-2.73980600	3.96460900	0.09506200
C	-2.94215600	4.45197200	-1.19610900
C	-1.75204500	4.45314400	0.95844800
C	-2.07887600	5.46106200	-1.63226400
C	-0.93504800	5.47192400	0.47951500
C	-1.08243900	5.98714600	-0.81223600
H	-2.21313600	5.85940500	-2.63513600
H	-0.18175500	5.88701400	1.14369400
C	-0.18618400	7.09508400	-1.30455100
H	0.15797600	7.72031200	-0.47644300
H	0.69992900	6.69135300	-1.80709300
H	-0.70651700	7.73216800	-2.02297000
C	-1.58386400	3.90837200	2.35033300
H	-2.54249900	3.84620000	2.87499300
H	-1.14464500	2.90758400	2.30439700
H	-0.91678300	4.54880300	2.92971300
C	-4.05437100	3.96453600	-2.08456800
H	-4.47194000	3.01088500	-1.76324600
H	-4.87331400	4.69127500	-2.09271600
H	-3.69361500	3.86500200	-3.11230000
H	-2.48546200	1.18389100	0.72263600
B	-6.68283600	1.33053800	-1.41703500
F	-5.31981600	1.24759800	-1.02913500
F	-6.78494100	2.21974500	-2.48731100
F	-7.41792300	1.80921400	-0.32119800
F	-7.13142700	0.06332600	-1.77907200
N	-2.57382000	-0.62034300	-2.90437000
C	-1.34873500	-1.37813900	-3.14601500
C	-1.55141600	-2.88784200	-3.12323300
H	-0.63491000	-1.12223300	-2.35928100
H	-0.87558500	-1.08155400	-4.10213200
H	-0.60623600	-3.39375900	-3.34527300
H	-1.88582800	-3.20030100	-2.13034300
H	-2.29936800	-3.21621200	-3.85086300
C	-3.33029200	-0.44142300	-4.13889700
C	-4.65582300	0.28016400	-3.94771500
H	-3.52894800	-1.44248200	-4.54184500
H	-2.72504900	0.08260200	-4.90511100
H	-5.21710000	0.26947100	-4.88709900
H	-5.25920900	-0.20360100	-3.17675100
H	-4.52546900	1.32488400	-3.65332300

C	-2.32068300	0.61783400	-2.17009000
C	-1.41367400	1.64423200	-2.85466800
H	-1.86340300	0.32365900	-1.21953400
H	-3.28675400	1.07146800	-1.92723200
H	-1.25607400	2.50069200	-2.19066300
H	-0.43184000	1.21145300	-3.08233700
H	-1.85030700	2.01029700	-3.79016100
C	1.65116900	-0.85838800	-0.98051800
C	0.57227000	-0.35193000	-0.24166100
H	2.12479400	-0.10950500	-1.61636600
C	0.40326500	1.08047100	-0.14995300
H	1.16549200	1.67152300	-0.69161700
O	-0.52823300	1.65335300	0.41545300
C	1.71452800	-2.21466200	-1.57905700
C	2.14644200	-2.32738900	-2.90913300
C	1.35539100	-3.38179300	-0.89131300
C	2.23889600	-3.56878600	-3.53209300
H	2.38984800	-1.42464800	-3.46703900
C	1.44886600	-4.62227100	-1.51506800
H	1.00568500	-3.31635400	0.13229300
C	1.89549600	-4.72322300	-2.83189200
H	2.57046000	-3.63144700	-4.56361900
H	1.17196700	-5.51682300	-0.96680000
H	1.96783400	-5.69399800	-3.31073100
C	-0.40221900	-1.17217200	0.39392500
C	-1.25966500	-1.85433600	0.92216700
C	-2.20778200	-2.67362200	1.61505800
C	-2.39437000	-2.50920200	2.99655200
C	-2.97076400	-3.63462600	0.93357800
C	-3.34723300	-3.25721000	3.67811500
H	-1.79207400	-1.78129600	3.53069600
C	-3.90860500	-4.40159400	1.61095800
H	-2.86995600	-3.74153100	-0.14223300
C	-4.09901600	-4.19132800	2.97273100
H	-3.50326400	-3.12175600	4.74277100
H	-4.51448300	-5.12814100	1.08203800
C	6.95955900	-2.31648500	-2.37446600
C	6.32465500	-1.50617500	-1.43098400
C	6.71268500	-1.48834600	-0.09897000
C	7.75543600	-2.33705700	0.26780200
C	8.38961700	-3.17073400	-0.64835100
C	7.99118100	-3.15859300	-1.98484400
C	6.37078700	-2.08868000	-3.74783500
C	5.69599800	-0.72370400	-3.59498600

C	5.21590900	-0.74211200	-2.12566600
H	6.23329200	-0.85106600	0.63937300
H	9.19757000	-3.81403300	-0.32002600
H	8.49705900	-3.79153800	-2.70647200
H	7.11243400	-2.06703500	-4.54853300
H	4.87348400	-0.54454900	-4.29941000
H	4.26553000	-1.28018800	-2.06791500
H	5.62054300	-2.85043200	-3.98812600
Br	8.33543600	-2.35266400	2.07202000
O	6.70818600	0.25748100	-3.74701000
C	6.22750800	1.57145200	-3.59782400
H	7.08016300	2.25003100	-3.62952100
H	5.53365300	1.83631500	-4.40795500
N	4.99384200	0.62383000	-1.64304800
C	4.31163400	1.08195400	-0.56393000
C	5.50909500	1.71553800	-2.28938300
N	5.20284300	2.81459300	-1.66595700
N	4.46080700	2.40847700	-0.60033000
C	3.98158300	3.41844900	0.31016900
C	3.02845900	4.31418800	-0.16531400
C	4.54121500	3.48831300	1.59174600
C	2.64742000	5.34672100	0.69388200
C	4.11067400	4.52620600	2.41040500
C	3.16809500	5.46604000	1.97837600
H	1.92231900	6.07324600	0.33751000
H	4.52259600	4.60621100	3.41326400
C	2.70501800	6.56395600	2.89979200
H	2.01225500	6.16785400	3.64929500
H	3.54571600	7.01173200	3.43546600
H	2.18742900	7.35154400	2.34740700
C	5.53156300	2.46656800	2.08332500
H	5.01257900	1.54173900	2.36430400
H	6.27876700	2.22202800	1.32166400
H	6.05587300	2.83937700	2.96459100
C	2.40021600	4.20383300	-1.53101100
H	2.52580800	3.21241100	-1.97187000
H	1.32662900	4.40297100	-1.45495100
H	2.83619100	4.93036900	-2.22371800
C	2.77298500	-1.66911500	1.66503900
C	3.34622200	-1.02798300	0.42156400
H	2.79193600	-2.75721200	1.55185000
C	3.46165900	0.37081600	0.46005500
O	2.77107900	1.10612200	1.18733700
C	3.56058400	-1.25973100	2.89593900

C	4.85732500	-1.73804400	3.11033400
C	3.02598200	-0.34331100	3.80448400
C	5.59982100	-1.31151200	4.20909000
H	5.29407300	-2.44850500	2.40977400
C	3.76424500	0.08207500	4.90672000
H	2.03069900	0.05219000	3.62557900
C	5.05457900	-0.40052900	5.11214700
H	6.60578600	-1.69048600	4.35634700
H	3.33311100	0.79721700	5.60056500
H	5.63324500	-0.06846700	5.96823200
H	4.06048100	-1.62132800	-0.13379600
H	1.73066500	-1.35812100	1.79505800
Cl	-5.33797600	-5.09351300	3.80980600

TS4CCI-RR

C	-0.57651600	-4.49183100	0.86480100
C	-1.10043700	-3.20661400	0.72416100
C	-0.96589400	-2.49001700	-0.45910700
C	-0.27253200	-3.10530700	-1.49661100
C	0.24492900	-4.39515800	-1.38615700
C	0.09400000	-5.09539000	-0.19251800
C	-0.82845800	-5.03930300	2.24814900
C	-1.85222000	-4.06960100	2.85101000
C	-1.65597200	-2.75218300	2.05372500
H	-1.38403900	-1.49905300	-0.61630100
H	0.75790400	-4.84430600	-2.23025700
H	0.48998600	-6.10146100	-0.09827700
H	-1.24019400	-6.05151600	2.24479600
H	-1.71512700	-3.90717900	3.92847400
H	-0.93132400	-2.09163100	2.54073900
H	0.09117900	-5.05906600	2.84286800
Br	0.00724600	-2.14200700	-3.09585200
O	-3.13779500	-4.61040700	2.61207900
C	-4.16357900	-3.81470900	3.16155400
H	-5.11598200	-4.27215300	2.90550900
H	-4.05650600	-3.73151700	4.25257700
N	-2.91674500	-2.00880800	2.00947500
C	-3.16622500	-0.80470300	1.48839200
C	-4.09653300	-2.45772100	2.53721400
N	-5.03585900	-1.56609900	2.41063300
N	-4.43557400	-0.54190600	1.74564500
C	-5.14184300	0.67567200	1.46451000
C	-6.33384300	0.58768600	0.73545700
C	-4.62946800	1.87636800	1.96882800

C	-7.02616500	1.77616900	0.51562800
C	-5.36743800	3.03268100	1.71305800
C	-6.56086900	3.00271400	0.99432300
H	-7.95260900	1.74019100	-0.05288800
H	-4.99871400	3.98063700	2.09498700
C	-7.33553000	4.26558400	0.72777900
H	-8.39659700	4.12935200	0.95336700
H	-6.95571300	5.09709200	1.32529500
H	-7.25800100	4.55206500	-0.32645300
C	-3.36115100	1.94371400	2.78299300
H	-3.34405900	1.17112600	3.55880500
H	-2.46110700	1.81146200	2.17157900
H	-3.29012800	2.91742500	3.27105200
C	-6.83433300	-0.72101300	0.18831400
H	-6.02848600	-1.31828000	-0.24378500
H	-7.28529200	-1.33030200	0.97667600
H	-7.58670200	-0.54128100	-0.58221300
H	-2.45171200	-0.14393200	1.01438400
B	-5.13838900	-3.85545200	-0.45507800
F	-4.24283100	-2.78621800	-0.20869200
F	-6.19837200	-3.37615100	-1.23761700
F	-5.63886000	-4.31528900	0.77284000
F	-4.47341500	-4.87892300	-1.11964000
N	-2.84127200	-0.36994500	-2.92058800
C	-2.05702200	0.72908000	-3.46576400
C	-2.67226100	1.60094800	-4.57023200
H	-1.12542400	0.29645500	-3.85587000
H	-1.75877500	1.36431000	-2.62457200
H	-1.89716000	2.25278000	-4.98537400
H	-3.06855000	0.99263500	-5.38893200
H	-3.47911100	2.24208700	-4.20491800
C	-3.25079600	-1.33815700	-3.92878400
C	-3.66917600	-2.66878200	-3.32046000
H	-2.38536600	-1.49693100	-4.58359700
H	-4.06277300	-0.95640000	-4.57387700
H	-3.85692800	-3.40042600	-4.11223200
H	-2.87917200	-3.05259700	-2.66927300
H	-4.57708600	-2.58582300	-2.71929900
C	-3.89089700	0.00735100	-1.97794400
C	-5.22287000	0.47636700	-2.58180400
H	-3.47329700	0.79453500	-1.33342600
H	-4.08843100	-0.85540600	-1.32904900
H	-5.85672700	0.91052100	-1.80427900
H	-5.08031900	1.23213100	-3.35817800

H	-5.76723500	-0.36300000	-3.02682900
C	1.44346500	0.66563900	-1.08648600
C	0.38964500	0.85524300	-0.16463200
H	1.92898000	-0.30500400	-0.97902400
C	0.36131200	0.01025700	0.99947500
H	1.19911500	-0.71289900	1.05616500
O	-0.51480000	-0.00613000	1.87048500
C	1.46516800	1.12988400	-2.49717900
C	2.19409700	0.37307700	-3.42650000
C	0.80172500	2.27771600	-2.95257400
C	2.24350500	0.73462700	-4.76779800
H	2.69809400	-0.53098800	-3.09610500
C	0.86283500	2.64758000	-4.29353900
H	0.23235500	2.88432300	-2.25863000
C	1.57542100	1.87596900	-5.20813300
H	2.80114200	0.12226900	-5.46909700
H	0.34514100	3.54301300	-4.62319200
H	1.61277000	2.16266300	-6.25406500
C	-0.61910000	1.85573000	-0.22642700
C	-1.52119900	2.67329700	-0.21340500
C	-2.51190700	3.70927400	-0.23170200
C	-3.51540000	3.73000500	-1.21211800
C	-2.46219700	4.74570200	0.71346400
C	-4.43663900	4.76878900	-1.26193500
H	-3.56289200	2.93022400	-1.94459500
C	-3.37684600	5.79056800	0.66910500
H	-1.68791000	4.73328900	1.47326300
C	-4.35113400	5.79399200	-0.32484700
H	-5.20472200	4.79069700	-2.02732700
H	-3.33046900	6.59994300	1.38903600
C	7.07999000	-0.48529500	-1.76794900
C	5.94612100	-0.23137700	-1.00013600
C	4.80957500	-1.00966000	-1.09040600
C	4.80955600	-2.05498500	-2.00466900
C	5.90616200	-2.30706800	-2.82276600
C	7.05444000	-1.51669500	-2.69941700
C	8.20121400	0.43183800	-1.32646900
C	7.77068100	0.81291100	0.09987700
C	6.22539100	0.87738500	-0.01313800
H	3.94450500	-0.84404000	-0.45822900
H	5.87904400	-3.12824000	-3.52963900
H	7.92466900	-1.73872300	-3.30839600
H	9.18178300	-0.04749800	-1.31258200
H	8.20350700	1.74973000	0.46937200

H	5.90268900	1.86600800	-0.35675800
H	8.26164100	1.32689400	-1.95448100
Br	3.24369000	-3.11635200	-2.05893900
O	8.15160900	-0.27523700	0.92747600
C	7.71736400	-0.14704000	2.26223200
H	8.03374800	-1.03494500	2.80906700
H	8.15181700	0.74220400	2.73959100
N	5.57038700	0.59213500	1.26611000
C	4.24856100	0.59215900	1.56725400
C	6.22396800	-0.03767900	2.28909400
N	5.38731600	-0.43665200	3.20239700
N	4.16905300	-0.04195900	2.74100600
C	2.98404300	-0.46565900	3.44370200
C	2.48181300	0.35750400	4.45246400
C	2.44405600	-1.70980300	3.11159400
C	1.33811700	-0.07902400	5.11388300
C	1.31293800	-2.10712200	3.82467900
C	0.73321100	-1.29792800	4.80174700
H	0.90955100	0.54743800	5.89133700
H	0.88174000	-3.08293600	3.61272900
C	-0.53385600	-1.72417100	5.49418200
H	-0.65853000	-1.21007000	6.44910100
H	-1.40572700	-1.47932100	4.87421900
H	-0.54305000	-2.80164500	5.67935200
C	3.03583800	-2.59665800	2.04270000
H	2.66342800	-2.34683400	1.04026700
H	4.12730300	-2.53520500	2.01816200
H	2.76045300	-3.63735100	2.22650400
C	3.15514400	1.65827100	4.78837200
H	4.20315800	1.49758200	5.05952600
H	3.12495600	2.32272500	3.91999200
H	2.65376900	2.14579900	5.62544400
C	2.67238600	3.23695200	-0.63990200
C	3.13151900	1.80924500	-0.39743200
H	1.66556000	3.36981500	-0.22970600
C	3.13486200	1.42732800	0.96341400
O	2.25638000	1.77043500	1.77206600
C	3.63639600	4.19824200	0.02063100
C	4.83638300	4.53996600	-0.61257900
C	3.38494300	4.70231500	1.30021400
C	5.76902100	5.35890300	0.01927900
H	5.03461200	4.16156100	-1.61372100
C	4.31590700	5.52341500	1.93391700
H	2.45717900	4.43530100	1.79780000

C	5.51125100	5.85186400	1.29779900
H	6.69260900	5.61923000	-0.48864400
H	4.10546600	5.90948200	2.92662600
H	6.23433900	6.49321500	1.79120800
H	3.92553400	1.45647800	-1.04850900
H	2.63386400	3.43244300	-1.71332600
Cl	-5.47443200	7.12983800	-0.41160200

TS4CCl-SR

C	1.30778500	-4.74019500	0.52068900
C	1.71161100	-3.42914000	0.26436200
C	1.99239000	-2.53061800	1.28666200
C	1.85750800	-3.00216600	2.58932600
C	1.43235900	-4.29746800	2.87280500
C	1.15264600	-5.17737200	1.82914500
C	1.10579700	-5.50200800	-0.76912000
C	1.87391300	-4.66298900	-1.79687100
C	1.75779500	-3.22648000	-1.23445400
H	2.36454900	-1.52367200	1.11692500
H	1.34581200	-4.61953600	3.90407000
H	0.84193900	-6.19461200	2.04454500
H	1.49508500	-6.52197100	-0.74286800
H	1.47175100	-4.72990000	-2.81698500
H	0.84622300	-2.76415500	-1.61930200
H	0.04340400	-5.54724500	-1.03607100
Br	2.31820800	-1.86534400	4.03288200
O	3.22005200	-5.09335800	-1.77404200
C	4.05480200	-4.37651800	-2.65354400
H	5.07573000	-4.71447200	-2.48969400
H	3.76412500	-4.54695200	-3.69995400
N	2.87125400	-2.41168900	-1.71288800
C	3.05559300	-1.09486800	-1.60395600
C	3.97075000	-2.91162000	-2.35211300
N	4.79167900	-1.95491700	-2.68153100
N	4.20414600	-0.82542700	-2.19935400
C	4.78911200	0.46941600	-2.41034700
C	6.10611200	0.68534200	-1.98510300
C	4.02124800	1.44244900	-3.06271800
C	6.65023900	1.94476700	-2.23380000
C	4.62188100	2.68298300	-3.27913400
C	5.92580400	2.95573800	-2.86596800
H	7.66557900	2.14450900	-1.90111800
H	4.05721500	3.45134100	-3.80267300
C	6.51874800	4.32708800	-3.05145500

H	7.59694600	4.27522800	-3.21688200
H	6.06032600	4.84732900	-3.89559200
H	6.35078700	4.93361200	-2.15436300
C	2.61104900	1.18696000	-3.53672800
H	2.51598200	0.21160500	-4.02333300
H	1.88291300	1.20595100	-2.71583800
H	2.32065100	1.95335600	-4.25859500
C	6.90523600	-0.36831100	-1.26730600
H	6.29506300	-0.93207800	-0.55924700
H	7.32285900	-1.08888300	-1.97686000
H	7.73255100	0.09965300	-0.72993400
H	2.38687000	-0.38126300	-1.14306900
B	5.43323900	-3.14364000	0.74726700
F	4.68035300	-2.01976700	0.31569300
F	6.75555800	-2.74200300	0.94898700
F	5.38494800	-4.11741300	-0.26123200
F	4.87988000	-3.64081400	1.92381700
N	3.61960900	0.81914800	2.39201700
C	2.56283300	1.62585200	2.99273200
C	2.96727100	2.90893600	3.73237600
H	2.02496200	0.98357700	3.70569300
H	1.84560300	1.86752700	2.20213600
H	2.06636400	3.39667900	4.12108600
H	3.61426900	2.69020400	4.58687400
H	3.48835400	3.62185200	3.08792400
C	4.73429900	0.58840100	3.29930900
C	5.62303600	-0.57206600	2.88076400
H	4.29494600	0.35589700	4.27930000
H	5.34725100	1.49642900	3.44835000
H	6.41283900	-0.71913700	3.62420300
H	5.03828700	-1.49019700	2.79966800
H	6.10609700	-0.40425500	1.91495500
C	3.98195900	1.16077800	1.02176000
C	4.76917400	2.45589600	0.79053500
H	3.04380200	1.22383400	0.45455600
H	4.54101700	0.31241200	0.60669100
H	4.93292700	2.59961500	-0.28219800
H	4.22277000	3.32952600	1.15680800
H	5.74851700	2.42642900	1.28065400
C	-1.01987100	-0.17341800	1.41000700
C	-0.32874600	0.16583400	0.23376900
H	-1.26247500	-1.23332100	1.51033500
C	-0.32565500	-0.79358200	-0.83235300
H	-0.81501300	-1.75800200	-0.57551700

O	0.15208300	-0.62853500	-1.96237300
C	-0.88777200	0.56044800	2.67912700
C	-0.67193800	-0.18289900	3.84405700
C	-0.96423100	1.95904600	2.76708800
C	-0.47666900	0.45681300	5.06586000
H	-0.60443100	-1.26514400	3.78145800
C	-0.79202700	2.59361100	3.98997200
H	-1.17108000	2.54803000	1.87843500
C	-0.53631100	1.84441900	5.14162900
H	-0.27987300	-0.13364000	5.95479000
H	-0.85985000	3.67548800	4.04969100
H	-0.39132600	2.34549500	6.09314000
C	0.31780700	1.41102900	0.02411100
C	0.85708800	2.48934800	-0.13704100
C	1.58059400	3.71981800	-0.16985400
C	2.26298700	4.12620400	-1.32415100
C	1.65511800	4.51135600	0.98796800
C	3.03812500	5.27801800	-1.31704700
H	2.19284400	3.52439000	-2.22309400
C	2.42268300	5.66840200	0.99998300
H	1.12663400	4.19740100	1.88357300
C	3.11570700	6.03398900	-0.15139300
H	3.57978400	5.58781200	-2.20437300
H	2.49525500	6.27480300	1.89572600
C	-3.60711100	4.19018000	-1.14457600
C	-3.88946900	2.84037500	-0.92270700
C	-5.13666200	2.41236800	-0.49138500
C	-6.09825800	3.39317800	-0.25772400
C	-5.83775900	4.74612700	-0.45226200
C	-4.58095700	5.14948600	-0.90518000
C	-2.19285400	4.35673900	-1.65561000
C	-1.85580000	2.95523700	-2.16840500
C	-2.63245700	2.04086200	-1.19261300
H	-5.36956600	1.36341200	-0.32845000
H	-6.61506100	5.47681800	-0.26138900
H	-4.38038100	6.20204500	-1.07663300
H	-2.09675900	5.09639100	-2.45285700
H	-0.78527400	2.71827600	-2.18345300
H	-2.04798200	1.90780600	-0.28055800
H	-1.50525200	4.62938400	-0.84588100
Br	-7.81342500	2.86161700	0.34955200
O	-2.41194400	2.83968800	-3.46903200
C	-2.17718200	1.57372700	-4.03640200
H	-2.67997700	1.53129100	-5.00270100

H	-1.10180400	1.39478100	-4.18138400
N	-2.84259700	0.71930900	-1.78842500
C	-3.22293200	-0.45520400	-1.23185400
C	-2.71084500	0.50378800	-3.13353600
N	-3.03244500	-0.71750100	-3.44508300
N	-3.34590000	-1.30104700	-2.26043200
C	-3.84066000	-2.65377600	-2.26241700
C	-3.00310800	-3.65396200	-2.75421200
C	-5.14540300	-2.89041200	-1.81122600
C	-3.50648700	-4.95623500	-2.76415900
C	-5.59493100	-4.20637600	-1.84893200
C	-4.79088000	-5.25127800	-2.31310200
H	-2.87196600	-5.75729900	-3.13502500
H	-6.60324400	-4.42212100	-1.50423100
C	-5.30589000	-6.66675700	-2.30594100
H	-4.68062600	-7.31941500	-2.91812000
H	-5.31478400	-7.06687800	-1.28730700
H	-6.33017100	-6.71325700	-2.68426100
C	-6.03492300	-1.79448500	-1.28482500
H	-5.79309000	-1.56334600	-0.23985600
H	-5.94470500	-0.87576200	-1.87329600
H	-7.07858300	-2.11196100	-1.31510700
C	-1.61860800	-3.36912700	-3.27681300
H	-1.65438000	-3.12553800	-4.34312100
H	-1.14195100	-2.52058900	-2.77809700
H	-0.98896500	-4.25442000	-3.15902300
C	-3.79146900	-0.40816400	2.58525200
C	-3.31631500	0.05919800	1.22987800
H	-3.69875800	0.40898200	3.30747000
C	-3.31826300	-0.89969200	0.21082500
O	-3.25647000	-2.13273900	0.37923000
C	-5.22921700	-0.87839500	2.47369800
C	-5.53701000	-2.24000100	2.50729900
C	-6.25975400	0.03724500	2.22793600
C	-6.84506900	-2.68034800	2.30783000
H	-4.73802600	-2.95674100	2.67023500
C	-7.56549500	-0.39977800	2.02475900
H	-6.03696300	1.10247200	2.18221100
C	-7.86285700	-1.76209400	2.06544400
H	-7.06501400	-3.74323500	2.33385300
H	-8.34906500	0.32498700	1.82860900
H	-8.88074300	-2.10308400	1.90544900
H	-3.45629800	1.10729900	0.99847000
H	-3.16882100	-1.23591600	2.94439500

Cl	4.10457800	7.47207000	-0.13370500
R2F			
C	-2.77090000	1.28580800	-0.00296800
C	-1.55073500	1.87850000	-0.00564800
H	-3.61639300	1.97315800	-0.03269200
C	-1.53600400	3.36488500	-0.03066900
H	-2.54230000	3.82780000	-0.04332900
O	-0.53183100	4.03924200	-0.03643900
C	-3.14941300	-0.12239200	0.02304300
C	-4.51454200	-0.42576500	-0.11623600
C	-2.23854900	-1.18026800	0.18625200
C	-4.95891200	-1.74140000	-0.10830000
H	-5.22728900	0.38555400	-0.23489100
C	-2.68726800	-2.49476400	0.19880400
H	-1.18411200	-0.97013400	0.31208300
C	-4.04401600	-2.78086200	0.04844000
H	-6.01619100	-1.95608600	-0.22110100
H	-1.97431600	-3.30229300	0.32878000
H	-4.38667100	-3.81035600	0.05758700
C	-0.27769000	1.23946200	-0.00192100
C	0.84290600	0.77597100	-0.00905800
C	2.15304500	0.20216200	-0.01513800
C	2.31963800	-1.18202100	-0.17909400
C	3.28254200	1.02014100	0.14407900
C	3.58967900	-1.74220100	-0.18242200
H	1.44717400	-1.81378200	-0.30700100
C	4.55620800	0.46807400	0.14189300
H	3.15149700	2.08916900	0.26930700
C	4.68406800	-0.90416700	-0.02108600
H	3.74340500	-2.80755800	-0.30756800
H	5.44299700	1.07888800	0.26336800
F	5.91294700	-1.44169700	-0.02365000
TS4CF-RS			
C	-3.68614900	-1.38995500	3.40051100
C	-3.40429600	-0.78703800	2.17163500
C	-3.75496000	-1.37651200	0.96882700
C	-4.41432600	-2.60042600	1.03852500
C	-4.70258700	-3.22873400	2.24397400
C	-4.33249400	-2.61671000	3.44265400
C	-3.19522600	-0.52724700	4.54209400
C	-3.02529300	0.84182400	3.87762300
C	-2.63191300	0.48482200	2.42716200

H	-3.56123200	-0.91509500	0.00492600
H	-5.21705700	-4.18278000	2.24526900
H	-4.56272700	-3.09468400	4.38959100
H	-3.89480800	-0.46362700	5.37827900
H	-2.28291800	1.49629800	4.35387800
H	-1.54923100	0.32989400	2.34300000
H	-2.23359000	-0.88591000	4.92724100
Br	-4.91438900	-3.44827300	-0.57929900
O	-4.30784800	1.44590900	3.88656200
C	-4.37307400	2.71169500	3.27503500
H	-5.42688700	2.95815100	3.15143500
H	-3.88312600	3.47714400	3.89298300
N	-2.93414100	1.62616100	1.56826000
C	-2.39096800	1.93742000	0.39452900
C	-3.70826200	2.68958000	1.93354700
N	-3.64980000	3.64215400	1.04307300
N	-2.82071800	3.14630100	0.08065900
C	-2.27954200	3.95847200	-0.98059700
C	-2.78816300	3.85198200	-2.27431600
C	-1.20726900	4.80178700	-0.64344800
C	-2.11103700	4.55065300	-3.28025300
C	-0.57342200	5.47265900	-1.68373100
C	-0.99577200	5.33784200	-3.01132800
H	-2.47602200	4.46812000	-4.30120400
H	0.27254300	6.11651700	-1.45666000
C	-0.25101900	6.03390100	-4.11957200
H	0.01227100	7.05587500	-3.83415400
H	0.68477700	5.50867600	-4.33825000
H	-0.84500200	6.06970600	-5.03487700
C	-0.80624900	5.04528700	0.78943600
H	-1.49436900	5.76430800	1.24570800
H	-0.82466600	4.13984200	1.40141900
H	0.20026800	5.46800900	0.83093700
C	-4.04038500	3.08695100	-2.60716000
H	-4.35144400	2.40293100	-1.81776900
H	-4.85732800	3.79657100	-2.77481400
H	-3.90351800	2.52437000	-3.53415900
H	-1.70141500	1.33578100	-0.18165400
B	-6.05315600	0.81334200	0.22102100
F	-4.77762300	1.00121800	-0.38284300
F	-6.96639800	1.66424800	-0.39407900
F	-5.93589500	1.12745200	1.58271200
F	-6.43307300	-0.51830100	0.06038300
N	-2.74880400	-1.54491700	-2.62613800

C	-1.67299600	-2.39991000	-3.11925600
C	-2.06452600	-3.87315600	-3.19953500
H	-0.82951100	-2.28069700	-2.42800800
H	-1.30624200	-2.07657300	-4.11161300
H	-1.16860800	-4.49612300	-3.28247700
H	-2.62116600	-4.17092600	-2.30637500
H	-2.68810600	-4.08266700	-4.07244200
C	-3.94896500	-1.65518600	-3.45391300
C	-5.07892400	-0.73680700	-3.01218500
H	-4.29979300	-2.68953800	-3.37779700
H	-3.71536800	-1.48134100	-4.52237900
H	-5.98376400	-0.98115000	-3.57620200
H	-5.28867500	-0.85827000	-1.94683200
H	-4.85067500	0.31777900	-3.19190700
C	-2.28414400	-0.16892300	-2.43822100
C	-1.87676100	0.59621300	-3.70047300
H	-1.41476100	-0.22472700	-1.76898700
H	-3.07387300	0.37929700	-1.90924900
H	-1.56271600	1.61072100	-3.43185600
H	-1.03301200	0.11913800	-4.20680300
H	-2.70791000	0.67455500	-4.41007100
C	1.60087600	1.44831600	-1.26583500
C	0.83123200	1.10066900	-0.14723800
H	1.80302000	2.51659500	-1.31971400
C	0.63521300	2.10970000	0.86293600
H	1.07464900	3.09194000	0.60909500
O	-0.02268100	1.97046500	1.89872300
C	1.55828200	0.79668700	-2.59501600
C	1.57824200	1.62186200	-3.72891400
C	1.50517400	-0.59017000	-2.78180900
C	1.57771900	1.07650300	-5.00941500
H	1.58770500	2.70015300	-3.59880300
C	1.51744200	-1.13688300	-4.06078300
H	1.44733400	-1.24831400	-1.92526400
C	1.56158800	-0.30668900	-5.18017900
H	1.59134500	1.73405100	-5.87293800
H	1.48698600	-2.21737400	-4.16708000
H	1.57358600	-0.73457000	-6.17743400
C	0.38751000	-0.22387500	0.11955300
C	0.03144500	-1.35975100	0.37650800
C	-0.26421300	-2.72934200	0.67459700
C	0.63113800	-3.47982200	1.45177200
C	-1.39482300	-3.34952400	0.12592000
C	0.40941600	-4.83286200	1.67083200

H	1.51278700	-2.99909000	1.86501500
C	-1.63390600	-4.69896300	0.35508200
H	-2.07718100	-2.77527600	-0.49689700
C	-0.72071500	-5.41544100	1.11423200
H	1.09087000	-5.43735600	2.25794100
H	-2.52203700	-5.18463700	-0.03596000
C	5.80534100	-3.29477200	-1.23758400
C	4.85238800	-2.42984600	-0.69125500
C	3.49320200	-2.62720600	-0.87350500
C	3.11159400	-3.70424500	-1.67730000
C	4.04322300	-4.54624100	-2.27476800
C	5.40544700	-4.34706300	-2.04585300
C	7.18747100	-2.93180400	-0.74232500
C	6.86355000	-2.12958200	0.52052600
C	5.58067000	-1.37091300	0.11178800
H	2.74978200	-1.98883100	-0.39976100
H	3.70353200	-5.37009000	-2.89159000
H	6.13231900	-5.02837500	-2.47591700
H	7.80639800	-3.79914600	-0.50545900
H	7.66364700	-1.46204200	0.86209300
H	5.83229700	-0.49970900	-0.50085000
H	7.72663000	-2.30392700	-1.45997500
Br	1.26840100	-4.05031900	-1.94901600
O	6.52953600	-3.08083900	1.52021200
C	6.12939200	-2.51388800	2.74281500
H	5.71298700	-3.31131200	3.35970500
H	6.98096200	-2.06763700	3.27464500
N	4.88441800	-0.88162000	1.30334200
C	4.06640900	0.18935100	1.47765400
C	5.10773600	-1.43343400	2.53370700
N	4.45985500	-0.78540000	3.45668200
N	3.82492900	0.21917900	2.79607400
C	3.08675500	1.15785900	3.61716100
C	3.75474100	2.29575800	4.07949200
C	1.80775500	0.79706000	4.03019500
C	3.05084700	3.13550300	4.93650200
C	1.14902100	1.67037500	4.89586500
C	1.74382800	2.84719600	5.34242500
H	3.53880400	4.03402400	5.30554900
H	0.14569300	1.41512600	5.22761600
C	0.99284700	3.79917300	6.23607200
H	0.49942600	4.57322000	5.63948200
H	0.22122500	3.27951200	6.80821600
H	1.66591800	4.30093200	6.93508200

C	1.18092100	-0.49157600	3.58231700
H	1.15180400	-0.55258400	2.49216600
H	1.74132800	-1.35179600	3.96429100
H	0.15367300	-0.56439500	3.94593500
C	5.17363700	2.58949000	3.67764800
H	5.81784600	1.71914700	3.84006800
H	5.21496000	2.85164500	2.61744600
H	5.57166700	3.42029100	4.26210000
C	4.40954900	2.05062500	-1.89166000
C	3.76491600	1.10636700	-0.87326000
H	4.37642300	1.51909500	-2.84820200
C	3.75719900	1.33339600	0.51659700
O	3.46636600	2.38637600	1.10969700
C	3.92302100	3.46906600	-2.16390100
C	3.93341900	3.91588600	-3.49152100
C	3.53991500	4.37519500	-1.16901600
C	3.55737600	5.21473500	-3.82323100
H	4.22504700	3.22632500	-4.28034000
C	3.15496900	5.67409000	-1.49929300
H	3.52709600	4.05016900	-0.13519600
C	3.15908000	6.10136500	-2.82450600
H	3.56857900	5.53096800	-4.86191000
H	2.85421600	6.35685500	-0.70950600
H	2.85665000	7.11286900	-3.07777300
H	3.87569600	0.06655700	-1.17169500
H	5.47788400	2.12636900	-1.64013100
F	-0.93971800	-6.72352300	1.32659700

TS4CF-SS

C	-6.20517100	-1.95232200	2.10272500
C	-5.28588200	-1.21424400	1.35121700
C	-4.92911400	-1.58852500	0.06217100
C	-5.55118300	-2.72343700	-0.45220000
C	-6.48202600	-3.46442900	0.26872000
C	-6.81033800	-3.07937700	1.56638500
C	-6.40202600	-1.34098100	3.46884400
C	-5.91817900	0.09090800	3.25074700
C	-4.77848200	-0.07299300	2.21453700
H	-4.21897400	-1.03716000	-0.54870700
H	-6.94289400	-4.33479800	-0.18430200
H	-7.53409300	-3.64977500	2.14013000
H	-7.43865400	-1.34985500	3.81159700
H	-5.58559300	0.60932700	4.15925700
H	-3.84174200	-0.34884800	2.71130200

H	-5.78171000	-1.84534900	4.21897700
Br	-5.10077900	-3.31368600	-2.19519300
O	-7.00296300	0.77655400	2.64668000
C	-6.73832100	2.12371500	2.33891800
H	-7.56296900	2.49395800	1.73341500
H	-6.64079000	2.72646200	3.25307800
N	-4.55540700	1.21625300	1.55824800
C	-3.48515900	1.65328800	0.88583800
C	-5.46699600	2.23614600	1.55825500
N	-4.99981300	3.27822800	0.93328400
N	-3.76369800	2.89226400	0.51355500
C	-2.88730300	3.86143600	-0.09306300
C	-3.10299500	4.24499400	-1.41654700
C	-1.91294800	4.43964200	0.72891900
C	-2.26746100	5.24209200	-1.92879200
C	-1.12590400	5.44303200	0.17437100
C	-1.28613600	5.85519600	-1.15228200
H	-2.41163200	5.55974400	-2.95877000
H	-0.38537100	5.92776600	0.80467300
C	-0.41584000	6.94324900	-1.72796200
H	-0.07462100	7.62858400	-0.94768700
H	0.47228700	6.52088400	-2.21125500
H	-0.95434000	7.52101600	-2.48230900
C	-1.72572700	4.00358500	2.15610800
H	-2.68116100	3.94691100	2.68710400
H	-1.25208000	3.01778200	2.18186500
H	-1.08036200	4.70672900	2.68517200
C	-4.19787600	3.65870400	-2.26641200
H	-4.61899300	2.74324400	-1.85189100
H	-5.01695500	4.37747400	-2.37108900
H	-3.81657500	3.44865200	-3.27006400
H	-2.53330400	1.14868800	0.72809600
B	-6.79322700	1.02838600	-1.37538900
F	-5.42940200	1.01789200	-0.98166800
F	-6.91958400	1.82524000	-2.51370700
F	-7.54707500	1.57081900	-0.32288100
F	-7.20159600	-0.27754200	-1.63412700
N	-2.66845000	-0.92998100	-2.74434500
C	-1.43889100	-1.69640700	-2.92359000
C	-1.64364800	-3.20505700	-2.87113300
H	-0.75632200	-1.42032200	-2.11635000
H	-0.92805400	-1.42586600	-3.86862500
H	-0.68423400	-3.71339400	-3.00988200
H	-2.05388700	-3.48965700	-1.89911800

H	-2.33560800	-3.55824000	-3.64159700
C	-3.42127000	-0.83990200	-3.99068800
C	-4.74927800	-0.11141500	-3.84922500
H	-3.61781100	-1.86624700	-4.32370300
H	-2.81541800	-0.36882500	-4.78998700
H	-5.31297600	-0.19060800	-4.78381600
H	-5.34757100	-0.54310900	-3.04396200
H	-4.62327000	0.95192100	-3.62912900
C	-2.42075300	0.35933000	-2.10125000
C	-1.52281600	1.34026300	-2.86072300
H	-1.95747100	0.13648700	-1.13406700
H	-3.38914400	0.82301000	-1.88773500
H	-1.38327100	2.24991400	-2.26718500
H	-0.53287100	0.90525900	-3.04470700
H	-1.95665700	1.62245300	-3.82608300
C	1.57487700	-0.95849700	-0.86124000
C	0.50872700	-0.39917800	-0.13697800
H	2.01578800	-0.26246200	-1.57541500
C	0.32559300	1.03226800	-0.16774400
H	1.07238700	1.58112200	-0.77259200
O	-0.60159700	1.64656400	0.36193500
C	1.63556200	-2.36033000	-1.34746700
C	2.05154100	-2.58199800	-2.66898600
C	1.28908600	-3.46886500	-0.56246900
C	2.14529400	-3.87014800	-3.18797500
H	2.27893400	-1.72816600	-3.30480600
C	1.38304400	-4.75627800	-1.08266100
H	0.94778000	-3.32224400	0.45532000
C	1.81727000	-4.96449400	-2.39090200
H	2.46527900	-4.01590400	-4.21475800
H	1.11584900	-5.60331000	-0.45921400
H	1.89013700	-5.97132600	-2.78826600
C	-0.43799300	-1.17238600	0.59295100
C	-1.26424800	-1.83089900	1.19593200
C	-2.17308500	-2.64071400	1.95094900
C	-2.35509200	-2.40477900	3.32278200
C	-2.89760300	-3.67373600	1.33265200
C	-3.26339200	-3.15856800	4.05797400
H	-1.78164800	-1.62050200	3.80644200
C	-3.79030400	-4.44539000	2.06222900
H	-2.79054400	-3.84073800	0.26550100
C	-3.96913300	-4.16025400	3.40818700
H	-3.42572600	-2.98526100	5.11595000
H	-4.37437200	-5.23131700	1.59801300

C	6.88238400	-2.33987900	-2.34474200
C	6.25161400	-1.49424400	-1.42972700
C	6.67638700	-1.39068300	-0.11292600
C	7.75203100	-2.19007200	0.26971700
C	8.38231100	-3.05847100	-0.61636900
C	7.94657600	-3.13228100	-1.93912900
C	6.25212800	-2.20304900	-3.71167000
C	5.54707200	-0.84847100	-3.61474900
C	5.10398800	-0.79938400	-2.13431500
H	6.20215700	-0.72404900	0.60252100
H	9.21629500	-3.66123000	-0.27645400
H	8.44919500	-3.79177800	-2.63894500
H	6.97199400	-2.20774500	-4.53227400
H	4.70439900	-0.72710600	-4.30731300
H	4.17160200	-1.36010600	-2.02189000
H	5.51541600	-2.99454700	-3.88957900
Br	8.38466700	-2.08669700	2.05276800
O	6.52980600	0.14730300	-3.84429700
C	6.01751400	1.45464800	-3.75397100
H	6.85020800	2.15255200	-3.84407000
H	5.29694800	1.65663600	-4.55890900
N	4.85455000	0.58467400	-1.72075000
C	4.18788200	1.08468100	-0.64999600
C	5.32743700	1.65149200	-2.43716500
N	5.01023100	2.77513000	-1.86542200
N	4.30459000	2.41056700	-0.76073300
C	3.82363600	3.45984500	0.10366700
C	2.84237200	4.30864500	-0.40037600
C	4.41101800	3.61599600	1.36502100
C	2.45997000	5.38270300	0.40564700
C	3.97819400	4.69240900	2.13133000
C	3.00747800	5.58746600	1.66805700
H	1.71354500	6.07378800	0.02345100
H	4.41216400	4.83985000	3.11710600
C	2.54481900	6.72938000	2.53455900
H	1.86151000	6.36864900	3.31015900
H	3.38710300	7.21006000	3.03816200
H	2.01657200	7.48335100	1.94660700
C	5.43369500	2.64548100	1.89284500
H	4.94032800	1.73093300	2.24445800
H	6.16653200	2.36751300	1.12874500
H	5.97235600	3.08262700	2.73501500
C	2.18579200	4.10773000	-1.74207600
H	2.35158700	3.10621300	-2.14410000

H	1.10562000	4.25722000	-1.64508200
H	2.56675700	4.82481700	-2.47586000
C	2.79048100	-1.58136900	1.77081600
C	3.30436800	-0.99270200	0.47578500
H	2.83772000	-2.67281100	1.71251400
C	3.38780400	0.40986200	0.43726500
O	2.69993500	1.16514800	1.14531100
C	3.60437000	-1.08822200	2.95228700
C	4.91701900	-1.52726900	3.15316400
C	3.07516300	-0.13607300	3.82666800
C	5.67996400	-1.02848900	4.20661100
H	5.34961200	-2.26460200	2.47821200
C	3.83438500	0.36218000	4.88325400
H	2.06653400	0.22808300	3.65703000
C	5.14008500	-0.08264200	5.07630000
H	6.69741900	-1.37895500	4.34480500
H	3.40707200	1.10382800	5.55112500
H	5.73474500	0.30540300	5.89717800
H	4.02081000	-1.59570800	-0.06678300
H	1.74370700	-1.29362700	1.91771500
F	-4.87259500	-4.86920500	4.10506800

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C	-0.85838500	-4.34042200	0.96846200
C	-1.31145200	-3.03387700	0.78107400
C	-1.14622800	-2.37262100	-0.43067400
C	-0.49963100	-3.06915300	-1.44750400
C	-0.05708000	-4.38177700	-1.29004200
C	-0.23520400	-5.02400000	-0.06836200
C	-1.12144800	-4.81819500	2.37485200
C	-2.08728900	-3.77398800	2.94564100
C	-1.82743100	-2.49969100	2.09792000
H	-1.50711200	-1.36492500	-0.62375500
H	0.42094200	-4.89201700	-2.11977500
H	0.10421000	-6.04632000	0.06391700
H	-1.58376000	-5.80736500	2.41708600
H	-1.93458300	-3.57920600	4.01552400
H	-1.06311000	-1.86321500	2.55576400
H	-0.19682100	-4.86045300	2.96049400
Br	-0.17295200	-2.19148100	-3.08638300
O	-3.40066600	-4.25539700	2.73259400
C	-4.38015200	-3.38829600	3.25778500
H	-5.35686900	-3.80125000	3.01803300
H	-4.26501000	-3.27593900	4.34540100

N	-3.04596300	-1.68970000	2.03998600
C	-3.23402200	-0.48816700	1.48747900
C	-4.24316300	-2.05708600	2.59129900
N	-5.13269100	-1.11835300	2.44886300
N	-4.48376400	-0.14788300	1.74964400
C	-5.12299000	1.10384200	1.45795100
C	-6.32132000	1.07429000	0.73472400
C	-4.54752500	2.27795300	1.95531500
C	-6.94893700	2.29669000	0.50605900
C	-5.22934100	3.46893200	1.70315400
C	-6.42119400	3.49944200	0.98231400
H	-7.87488500	2.30717100	-0.06436100
H	-4.81305900	4.39621400	2.08532400
C	-7.13357500	4.79984300	0.71776800
H	-8.16075500	4.76380900	1.09175700
H	-6.62003500	5.63781700	1.19344500
H	-7.18176800	5.00548700	-0.35602700
C	-3.26542400	2.28393600	2.74955900
H	-3.27129800	1.51108800	3.52539500
H	-2.38448700	2.10751300	2.12123600
H	-3.13850300	3.25292700	3.23560600
C	-6.89317300	-0.21321800	0.20666400
H	-6.12081100	-0.86649800	-0.20554300
H	-7.38620800	-0.77810100	1.00320300
H	-7.62742500	-0.00503300	-0.57412400
H	-2.48986600	0.12032500	0.98981800
B	-5.39668200	-3.48486500	-0.34362300
F	-4.42950500	-2.47187900	-0.13335600
F	-6.42821900	-2.95885500	-1.13411600
F	-5.91813600	-3.87439100	0.89964500
F	-4.80456800	-4.56901700	-0.98074400
N	-2.89955300	-0.24648600	-2.92491000
C	-2.04888500	0.78399600	-3.50531000
C	-2.60570600	1.65124600	-4.64440300
H	-1.14456500	0.28285400	-3.87705600
H	-1.71302600	1.42823700	-2.68547300
H	-1.78811200	2.23216600	-5.08236700
H	-3.04017900	1.03837800	-5.43989000
H	-3.36806400	2.35974400	-4.30963800
C	-3.38863100	-1.20762000	-3.90373000
C	-3.89337400	-2.48898500	-3.25582100
H	-2.54419500	-1.44383800	-4.56273800
H	-4.17938400	-0.78527700	-4.55016800
H	-4.12829400	-3.23077700	-4.02520400

H	-3.12959400	-2.90254700	-2.59176600
H	-4.79404700	-2.32879800	-2.65944100
C	-3.90702300	0.21886100	-1.97671700
C	-5.19745700	0.80277500	-2.57196500
H	-3.41907600	0.96531300	-1.33366700
H	-4.17379100	-0.62420100	-1.32758000
H	-5.77886600	1.30402000	-1.79332600
H	-4.99551800	1.53360500	-3.35926800
H	-5.82257700	0.01321100	-3.00179800
C	1.43364500	0.64736200	-1.10181100
C	0.38863800	0.92666100	-0.19221900
H	1.86704100	-0.34283000	-0.95462300
C	0.31082600	0.12432400	0.99869300
H	1.10151100	-0.64863300	1.07888600
O	-0.56162400	0.19045300	1.87146600
C	1.47596700	1.04909600	-2.53156400
C	2.15233800	0.20982200	-3.42893000
C	0.88029600	2.21416800	-3.03496200
C	2.21520800	0.50819400	-4.78528500
H	2.60244100	-0.70784400	-3.06098800
C	0.95701100	2.52096600	-4.39082700
H	0.35140000	2.88316800	-2.36681100
C	1.61541100	1.66776500	-5.27319200
H	2.72979200	-0.16768200	-5.46072600
H	0.49310400	3.43118500	-4.75794200
H	1.66393700	1.90591200	-6.33080600
C	-0.57017900	1.97218700	-0.30231800
C	-1.43434600	2.82926400	-0.33409400
C	-2.41748600	3.87016100	-0.42139200
C	-3.42746700	3.81570800	-1.39579200
C	-2.36919400	4.96945800	0.45027100
C	-4.37306300	4.82735900	-1.49628100
H	-3.46482600	2.97309300	-2.07750800
C	-3.30575600	5.99205300	0.35316200
H	-1.58681000	5.01639700	1.20038300
C	-4.29194800	5.89807000	-0.61801300
H	-5.16125900	4.79763000	-2.24060200
H	-3.28389300	6.85102200	1.01426700
C	6.98543900	-0.84428300	-1.72592900
C	5.86983200	-0.49151700	-0.97071000
C	4.68943200	-1.20491700	-1.02946700
C	4.62595700	-2.28636500	-1.89837400
C	5.70469700	-2.63746500	-2.70348300
C	6.89776400	-1.91145900	-2.61228700

C	8.15848900	0.02604200	-1.32650000
C	7.75440900	0.49625900	0.08088700
C	6.21465500	0.64250100	-0.03404700
H	3.83670900	-0.96191900	-0.40592200
H	5.62839900	-3.48472600	-3.37509700
H	7.75253900	-2.21001600	-3.21030400
H	9.11023100	-0.50721000	-1.29091100
H	8.23965100	1.42344100	0.40716400
H	5.94685700	1.63139200	-0.42118700
H	8.26756600	0.88616900	-1.99539400
Br	2.99858400	-3.25330700	-1.90902100
O	8.07631600	-0.57255000	0.95732100
C	7.65408500	-0.36001200	2.28513100
H	7.92236500	-1.23861800	2.87133100
H	8.13884600	0.52432000	2.72127300
N	5.54894000	0.45264800	1.25744600
C	4.22993500	0.53879000	1.55838400
C	6.16916500	-0.16655600	2.30752700
N	5.31391200	-0.47827800	3.23741000
N	4.11836600	-0.03726500	2.75915700
C	2.91090600	-0.38078800	3.46736300
C	2.43792800	0.49587600	4.44413000
C	2.31710600	-1.60869500	3.16824900
C	1.26931500	0.13208300	5.10669300
C	1.16320700	-1.93276100	3.88145800
C	0.61231000	-1.06736500	4.82670000
H	0.86209300	0.80180400	5.85917600
H	0.68978600	-2.89405000	3.69450800
C	-0.68001300	-1.41222900	5.51762800
H	-0.79732800	-0.85114700	6.44665000
H	-1.53227100	-1.16105800	4.87335700
H	-0.73550100	-2.47911400	5.75039600
C	2.87557600	-2.55097700	2.12956400
H	2.52900400	-2.30590900	1.11667300
H	3.96916700	-2.54675700	2.11766100
H	2.54335100	-3.57101300	2.33348600
C	3.16533000	1.77597400	4.74511600
H	4.20116700	1.57795300	5.03761700
H	3.17746500	2.41010500	3.85393500
H	2.67517900	2.31480100	5.55698500
C	2.79102700	3.16799000	-0.75825900
C	3.17484200	1.72888200	-0.45707300
H	1.78963800	3.36731900	-0.36156800
C	3.16066300	1.40525400	0.91914700

O	2.30264900	1.82690900	1.71208400
C	3.79756300	4.10569200	-0.12756500
C	5.01627300	4.36637200	-0.76355800
C	3.56273800	4.66894900	1.13045700
C	5.98301700	5.16309400	-0.15485300
H	5.20274100	3.94267900	-1.74869900
C	4.52782600	5.46792000	1.74077300
H	2.62041300	4.46502100	1.63040600
C	5.74135800	5.71513600	1.10250500
H	6.92109900	5.36007200	-0.66469000
H	4.32987600	5.90033200	2.71681000
H	6.49138700	6.33918800	1.57755900
H	3.94962100	1.30875200	-1.09124300
H	2.76879000	3.32250200	-1.83879800
F	-5.20743700	6.87874300	-0.70683600

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C	1.55732000	-4.57397200	0.56878500
C	1.90080600	-3.24884400	0.29690400
C	2.14845000	-2.32948300	1.30929600
C	2.04635100	-2.79560200	2.61693500
C	1.68342400	-4.10632800	2.91532700
C	1.43355300	-5.00666500	1.88192000
C	1.37888900	-5.35707000	-0.71146100
C	2.10340000	-4.49706000	-1.75267800
C	1.92850400	-3.06075400	-1.20447600
H	2.47150800	-1.30796000	1.12730500
H	1.62136700	-4.42284200	3.95007400
H	1.17075900	-6.03498500	2.10828200
H	1.81090400	-6.35949800	-0.67754100
H	1.69803900	-4.59236700	-2.76917500
H	0.99529300	-2.64374800	-1.58854600
H	0.31764000	-5.44961300	-0.97071800
Br	2.46840100	-1.62891300	4.04837200
O	3.46719300	-4.86813000	-1.73614500
C	4.25857000	-4.12543000	-2.63465700
H	5.29530600	-4.41704800	-2.48206900
H	3.96074200	-4.31927500	-3.67501500
N	3.00189200	-2.20356500	-1.69975000
C	3.13290000	-0.87955900	-1.60053900
C	4.11519000	-2.66241900	-2.34590600
N	4.89282200	-1.67511800	-2.68917500
N	4.26426900	-0.56734100	-2.20812600
C	4.79902100	0.74765400	-2.42768700

C	6.11276500	1.01114600	-2.01850400
C	3.98938900	1.69186500	-3.07170500
C	6.60968400	2.28756800	-2.27810500
C	4.54336300	2.95254400	-3.29759400
C	5.84289500	3.27066300	-2.90435300
H	7.62206100	2.52319200	-1.96014800
H	3.94479200	3.70063000	-3.81256800
C	6.38826400	4.65942400	-3.10519600
H	7.46289300	4.64005200	-3.29879900
H	5.89248100	5.16446600	-3.93725200
H	6.22550300	5.26110000	-2.20431000
C	2.58387000	1.38557200	-3.52880200
H	2.51832100	0.40694600	-4.01364600
H	1.86517600	1.37865100	-2.69961800
H	2.25758100	2.14059100	-4.24745700
C	6.95787600	-0.01048700	-1.30673700
H	6.37718300	-0.58905500	-0.58570800
H	7.38887000	-0.72168800	-2.01765100
H	7.77667500	0.48890000	-0.78487500
H	2.43986800	-0.19117400	-1.13693100
B	5.59932600	-2.81425000	0.74623400
F	4.80393300	-1.72119900	0.31166600
F	6.89911200	-2.35620000	0.97309000
F	5.61160700	-3.77877000	-0.27219100
F	5.04962400	-3.34640400	1.90906400
N	3.64280600	1.09046300	2.37074100
C	2.55848600	1.85770700	2.97381100
C	2.91493000	3.16370200	3.69772500
H	2.05466200	1.20051700	3.69776200
H	1.82471900	2.06165800	2.18751800
H	1.99790200	3.61489200	4.09305500
H	3.58077900	2.98120400	4.54629600
H	3.39604400	3.89302300	3.04076200
C	4.77278600	0.90865200	3.27039000
C	5.70286400	-0.21982900	2.85290100
H	4.35051600	0.66716500	4.25564900
H	5.35221100	1.84027500	3.40797700
H	6.50321900	-0.33069400	3.59137900
H	5.15549800	-1.16187600	2.78152500
H	6.17232100	-0.03944700	1.88292500
C	3.97966500	1.43570600	0.99513400
C	4.70171700	2.76501900	0.74607400
H	3.03601200	1.44890000	0.43368600
H	4.57612000	0.61108600	0.58430100

H	4.86061100	2.90029600	-0.32851200
H	4.11048400	3.61546100	1.09745100
H	5.67999000	2.79234600	1.23850500
C	-0.96459700	-0.12211900	1.39850600
C	-0.29002400	0.24301200	0.21896000
H	-1.15172000	-1.19245400	1.50686500
C	-0.24819800	-0.71795500	-0.84309000
H	-0.69512600	-1.70162500	-0.58135000
O	0.21920000	-0.53783900	-1.97586300
C	-0.85643400	0.62435200	2.66360000
C	-0.59391000	-0.10015000	3.83056600
C	-0.99965100	2.01812900	2.74434900
C	-0.42051100	0.55571000	5.04722800
H	-0.47404600	-1.17821900	3.77366200
C	-0.84884300	2.66786000	3.96216900
H	-1.24046700	2.59131400	1.85380500
C	-0.54784200	1.93907800	5.11597600
H	-0.18654600	-0.01918800	5.93739100
H	-0.96932600	3.74550100	4.01621000
H	-0.42010800	2.45233800	6.06347900
C	0.30363700	1.51485300	0.00532200
C	0.79724000	2.61476500	-0.15566000
C	1.45618000	3.88213800	-0.18963800
C	2.12199300	4.32173000	-1.34244300
C	1.48107800	4.67900400	0.96759200
C	2.82888600	5.51693200	-1.33733400
H	2.09024300	3.71245700	-2.23844000
C	2.17827600	5.87973900	0.97930000
H	0.96730800	4.33543600	1.86087800
C	2.84711600	6.27161200	-0.17296000
H	3.36209800	5.86826900	-2.21405900
H	2.22012900	6.50495700	1.86379200
C	-3.75547000	4.10848800	-1.13730800
C	-3.97007200	2.74627600	-0.91552300
C	-5.19351800	2.25711800	-0.48108700
C	-6.20202300	3.18876600	-0.24451000
C	-6.00923900	4.55306500	-0.43859900
C	-4.77502800	5.01830400	-0.89436300
C	-2.35279100	4.34450300	-1.65277000
C	-1.94838100	2.96178400	-2.16800000
C	-2.67670300	2.00916700	-1.19141000
H	-5.37435100	1.19796300	-0.31808000
H	-6.82133200	5.24422700	-0.24546100
H	-4.62741000	6.07960000	-1.06562000

H	-2.29532800	5.08899000	-2.44925300
H	-0.86751500	2.77904200	-2.18432400
H	-2.08160000	1.90158800	-0.28261600
H	-1.67641800	4.64899300	-0.84481100
Br	-7.88730100	2.57142700	0.36446200
O	-2.49920500	2.81909200	-3.46832600
C	-2.20143500	1.56623400	-4.03571500
H	-2.69823400	1.50010100	-5.00374000
H	-1.11812000	1.43914500	-4.17664400
N	-2.82687500	0.68034000	-1.78952600
C	-3.15434100	-0.50999100	-1.23383200
C	-2.68622200	0.47181000	-3.13469200
N	-2.95360900	-0.76251200	-3.44706400
N	-3.24055700	-1.35974100	-2.26272400
C	-3.67898500	-2.73150800	-2.26249100
C	-2.80049700	-3.69897900	-2.74783600
C	-4.97335600	-3.01891600	-1.81107400
C	-3.25026900	-5.02070300	-2.75094700
C	-5.36885800	-4.35230600	-1.84197900
C	-4.52196200	-5.36581900	-2.29939400
H	-2.58284400	-5.79710200	-3.11638600
H	-6.36801700	-4.60706700	-1.49722700
C	-4.97745700	-6.80149900	-2.28400700
H	-4.33099300	-7.42920000	-2.90025300
H	-4.96005600	-7.19873300	-1.26433000
H	-6.00231000	-6.89202100	-2.65261300
C	-5.90723100	-1.95744500	-1.29085900
H	-5.67661000	-1.71182500	-0.24655200
H	-5.85393500	-1.03871500	-1.88396700
H	-6.93696800	-2.31759200	-1.32018400
C	-1.42750800	-3.36113300	-3.26900400
H	-1.46909300	-3.13397300	-4.33876100
H	-0.98982900	-2.48636900	-2.77994100
H	-0.76098000	-4.21687600	-3.13668700
C	-3.70585300	-0.49657800	2.58593600
C	-3.25607100	-0.00313200	1.23057800
H	-3.65252900	0.32277300	3.30956000
C	-3.22373400	-0.95975600	0.20855600
O	-3.10527000	-2.18828400	0.37541200
C	-5.11893700	-1.03694100	2.47543000
C	-5.35852800	-2.41260400	2.49716800
C	-6.19489000	-0.17171300	2.24188700
C	-6.64380400	-2.91568500	2.29831200
H	-4.52457700	-3.09039000	2.65080200

C	-7.47834500	-0.67142600	2.03997000
H	-6.02551000	0.90362500	2.20470600
C	-7.70728900	-2.04712800	2.06889500
H	-6.81020400	-3.98845000	2.31505400
H	-8.29796900	0.01521900	1.85414800
H	-8.70765900	-2.43688500	1.90968800
H	-3.45053300	1.03696900	1.00228400
H	-3.04207600	-1.29307000	2.94224100
F	3.53101700	7.42591400	-0.16188000

R2Me

C	-2.81332700	1.26049600	-0.00118100
C	-1.60289600	1.87317000	-0.00548600
H	-3.67044700	1.93342200	-0.02799000
C	-1.61349000	3.35958200	-0.02932000
H	-2.62755000	3.80552800	-0.03946000
O	-0.62106200	4.05122900	-0.03683400
C	-3.16762700	-0.15416300	0.02387300
C	-4.52830600	-0.48114300	-0.10595300
C	-2.23734700	-1.19662600	0.17685500
C	-4.94963700	-1.80435100	-0.09798200
H	-5.25600000	0.31790500	-0.21715400
C	-2.66299300	-2.51879600	0.18901100
H	-1.18574400	-0.96846000	0.29440800
C	-4.01564800	-2.82825400	0.04867300
H	-6.00389800	-2.03710200	-0.20318500
H	-1.93487000	-3.31402700	0.31063900
H	-4.34022800	-3.86360100	0.05749100
C	-0.31992100	1.25479800	-0.00361500
C	0.80746200	0.80703000	-0.01158500
C	2.12351200	0.24653100	-0.01778600
C	2.30751600	-1.13400000	-0.18657500
C	3.24741000	1.07013200	0.14173700
C	3.58746000	-1.67099200	-0.19132100
H	1.44206900	-1.77527200	-0.32019400
C	4.52150900	0.51861400	0.13491600
H	3.10933600	2.13887800	0.26676200
C	4.71358600	-0.85731700	-0.02773000
H	3.71830900	-2.74096500	-0.32661400
H	5.38507000	1.16646300	0.25620900
C	6.09680000	-1.45248000	-0.00209300
H	6.37241100	-1.74297800	1.01707600
H	6.84220400	-0.73581700	-0.35377000
H	6.15346700	-2.34719400	-0.62617300

TS4CMe-RS

C	-3.68056000	-1.39363400	3.39901900
C	-3.40022500	-0.79114200	2.16959200
C	-3.74567200	-1.38451800	0.96718100
C	-4.39801000	-2.61208100	1.03779700
C	-4.68458200	-3.23988600	2.24390100
C	-4.31996100	-2.62393200	3.44220600
C	-3.19499000	-0.52733800	4.54015100
C	-3.02940600	0.84144300	3.87408000
C	-2.63399300	0.48466700	2.42405700
H	-3.55185800	-0.92472200	0.00254600
H	-5.19342500	-4.19696500	2.24584900
H	-4.54864400	-3.10176000	4.38961600
H	-3.89637600	-0.46492900	5.37495500
H	-2.28970300	1.49925600	4.34994800
H	-1.55050100	0.33482900	2.34003200
H	-2.23288500	-0.88179900	4.92786600
Br	-4.89111800	-3.46507500	-0.57915100
O	-4.31430300	1.44071300	3.88223600
C	-4.38402200	2.70578100	3.26987900
H	-5.43868900	2.94827700	3.14568800
H	-3.89717000	3.47351500	3.88748100
N	-2.94128900	1.62393200	1.56401300
C	-2.39852600	1.93656600	0.39050500
C	-3.71863600	2.68511700	1.92874400
N	-3.66298700	3.63763500	1.03808900
N	-2.83189800	3.14410000	0.07612800
C	-2.29253600	3.95765500	-0.98494100
C	-2.79667900	3.84537300	-2.27993000
C	-1.22611100	4.80793100	-0.64665400
C	-2.11987400	4.54456400	-3.28572800
C	-0.59232000	5.47904600	-1.68684200
C	-1.00935000	5.33798900	-3.01546000
H	-2.48117600	4.45732100	-4.30760400
H	0.24954500	6.12795900	-1.45884900
C	-0.26411900	6.03420300	-4.12330400
H	-0.00524700	7.05778100	-3.83958600
H	0.67416200	5.51186300	-4.33826100
H	-0.85572700	6.06572400	-5.04031500
C	-0.83131600	5.05789200	0.78682400
H	-1.52661500	5.77227100	1.23948900
H	-0.84398000	4.15348400	1.40047100
H	0.17160100	5.48891500	0.83012700

C	-4.04476400	3.07412100	-2.61397400
H	-4.35386400	2.38956100	-1.82426000
H	-4.86473600	3.77984400	-2.78342400
H	-3.90401100	2.51117400	-3.54012200
H	-1.70640400	1.33708400	-0.18495100
B	-6.05655700	0.79708500	0.21737800
F	-4.78224000	0.98957100	-0.38691400
F	-6.97393900	1.64285000	-0.39912600
F	-5.94083300	1.11458000	1.57852200
F	-6.43109300	-0.53638400	0.05962100
N	-2.74337400	-1.55144800	-2.62543800
C	-1.66414800	-2.40488700	-3.11312500
C	-2.05005000	-3.87965000	-3.18844000
H	-0.82290800	-2.28149700	-2.42008300
H	-1.29651200	-2.08391500	-4.10618200
H	-1.15170500	-4.49806900	-3.27937900
H	-2.59535200	-4.17847100	-2.28885300
H	-2.68040900	-4.09317600	-4.05560100
C	-3.94135900	-1.66601300	-3.45485000
C	-5.07524700	-0.75187600	-3.01419800
H	-4.28890200	-2.70151400	-3.37882100
H	-3.70750600	-1.49165300	-4.52335300
H	-5.97859500	-0.99878300	-3.57956000
H	-5.28552700	-0.87516400	-1.94910000
H	-4.85039900	0.30368100	-3.19255800
C	-2.28248000	-0.17459400	-2.43736200
C	-1.87449100	0.59088300	-3.69934300
H	-1.41431300	-0.22809600	-1.76628100
H	-3.07442300	0.37227500	-1.91025600
H	-1.56266000	1.60615100	-3.43090800
H	-1.02917500	0.11498400	-4.20415900
H	-2.70476900	0.66725300	-4.41024900
C	1.59530400	1.46618300	-1.26786400
C	0.82333000	1.12113500	-0.14988100
H	1.79355000	2.53499300	-1.32583900
C	0.62211600	2.13224600	0.85635200
H	1.05528900	3.11641500	0.59865100
O	-0.03488200	1.99308400	1.89315700
C	1.55549800	0.81059100	-2.59577100
C	1.57517100	1.63382800	-3.73111500
C	1.50574500	-0.57679900	-2.78062700
C	1.57779300	1.08681600	-5.01089600
H	1.58193400	2.71235500	-3.60257800
C	1.52141900	-1.12507800	-4.05901700

H	1.44747300	-1.23423700	-1.92347400
C	1.56536100	-0.29662000	-5.17965800
H	1.59112300	1.74325400	-5.87529600
H	1.49364000	-2.20578100	-4.16363800
H	1.57995600	-0.72601900	-6.17624800
C	0.39248500	-0.20653000	0.12249300
C	0.05178100	-1.34730800	0.37948500
C	-0.22455500	-2.72206300	0.67264200
C	0.68404800	-3.46957700	1.43503600
C	-1.35352500	-3.35461900	0.13745700
C	0.47178900	-4.82689200	1.63878700
H	1.56365300	-2.98198300	1.84657600
C	-1.56302500	-4.70847100	0.36651100
H	-2.05201900	-2.78550300	-0.47170700
C	-0.65000900	-5.46845800	1.10438500
H	1.18734800	-5.40059300	2.22152200
H	-2.46388700	-5.17449300	-0.02701300
C	5.81253100	-3.26895300	-1.22922700
C	4.85178800	-2.41063600	-0.68603600
C	3.49478000	-2.61544800	-0.87525000
C	3.12285200	-3.69268800	-1.68351800
C	4.06264900	-4.52735300	-2.27863700
C	5.42265000	-4.32124000	-2.04231800
C	7.18976200	-2.90030600	-0.72440300
C	6.85370100	-2.10327900	0.53860300
C	5.56994000	-1.34976000	0.12339200
H	2.74514700	-1.98380900	-0.40238200
H	3.73082200	-5.35153500	-2.89932300
H	6.15556600	-4.99745700	-2.47024100
H	7.81162500	-3.76516500	-0.48606300
H	7.64827900	-1.43285700	0.88746000
H	5.82134900	-0.47635300	-0.48625100
H	7.73042600	-2.26749800	-1.43659900
Br	1.28310300	-4.04887000	-1.96076300
O	6.51739700	-3.05898600	1.53332400
C	6.10531500	-2.49814200	2.75481200
H	5.68506200	-3.29924700	3.36431700
H	6.95130800	-2.05279200	3.29619100
N	4.86499600	-0.86514200	1.31171500
C	4.04572900	0.20528300	1.48409500
C	5.08352000	-1.41844700	2.54221200
N	4.43202800	-0.77167100	3.46348700
N	3.79914900	0.23355400	2.80173300
C	3.06099000	1.17299400	3.62212300

C	3.72910800	2.31200300	4.08215600
C	1.78309700	0.81175500	4.03823700
C	3.02576400	3.15325400	4.93796200
C	1.12505200	1.68679500	4.90301500
C	1.71922200	2.86517300	5.34583100
H	3.51382900	4.05259200	5.30494900
H	0.12266300	1.43123000	5.23734300
C	0.96955900	3.81893600	6.23868800
H	0.49883800	4.60820400	5.64373700
H	0.18065000	3.30552600	6.79252000
H	1.63958700	4.30143000	6.95413200
C	1.15618900	-0.47834200	3.59494300
H	1.11181500	-0.53599500	2.50514900
H	1.72546700	-1.33756000	3.96553200
H	0.13477300	-0.55739100	3.97333700
C	5.14822900	2.60501300	3.68037700
H	5.79187200	1.73415600	3.84242100
H	5.19000700	2.86790000	2.62041800
H	5.54675100	3.43510700	4.26552800
C	4.40232400	2.06793500	-1.88238600
C	3.75163400	1.12316200	-0.86789900
H	4.37617800	1.53606200	-2.83893900
C	3.74024200	1.34930200	0.52241700
O	3.44574600	2.40213900	1.11383300
C	3.91480500	3.48532700	-2.15806200
C	3.92693000	3.93053700	-3.48611900
C	3.52796200	4.39187800	-1.16495700
C	3.54864000	5.22820400	-3.82014600
H	4.22140600	3.24058900	-4.27353300
C	3.14057100	5.68939600	-1.49752600
H	3.51327100	4.06771300	-0.13086700
C	3.14626500	6.11506000	-2.82331500
H	3.56113300	5.54319100	-4.85919400
H	2.83656500	6.37238900	-0.70918400
H	2.84181800	7.12550100	-3.07842000
H	3.86379700	0.08341200	-1.16632600
H	5.46880200	2.14545000	-1.62371500
C	-0.85978600	-6.94740400	1.29663900
H	-0.44610400	-7.50712100	0.45113500
H	-0.36637100	-7.30485400	2.20322100
H	-1.92321100	-7.18955400	1.36119600
TS4CMe-SS			
C	-6.28879900	-1.90793700	2.05946000

C	-5.33801600	-1.19353700	1.32467900
C	-4.93666000	-1.60458100	0.05985400
C	-5.54303500	-2.75201700	-0.44566900
C	-6.51911800	-3.45767700	0.25070000
C	-6.89745900	-3.03264200	1.52133100
C	-6.49844900	-1.28883000	3.41925500
C	-5.98749900	0.13354000	3.20617200
C	-4.83341000	-0.05061800	2.18868700
H	-4.19117000	-1.08033700	-0.53269200
H	-6.96974300	-4.33574900	-0.19761500
H	-7.65958400	-3.57328400	2.07453300
H	-7.53880100	-1.28130400	3.75080700
H	-5.66030700	0.64713100	4.11939300
H	-3.90967800	-0.33799000	2.70256900
H	-5.89054600	-1.80074000	4.17571400
Br	-4.98056600	-3.43943500	-2.12003800
O	-7.05195200	0.83664900	2.58684400
C	-6.75781000	2.18016400	2.29180100
H	-7.56692700	2.57166700	1.67892500
H	-6.65881100	2.77446500	3.21141000
N	-4.58152700	1.23510500	1.53267900
C	-3.49727300	1.65683700	0.87141300
C	-5.47570700	2.27048200	1.52685900
N	-4.98558100	3.30644200	0.91015500
N	-3.75164000	2.90258200	0.50249700
C	-2.86646900	3.86171800	-0.10705900
C	-3.10982700	4.26183300	-1.42162300
C	-1.86750200	4.41858500	0.69757000
C	-2.27403400	5.25100300	-1.94555000
C	-1.07940800	5.41632900	0.13189600
C	-1.26511700	5.84269600	-1.18609000
H	-2.43771000	5.58065200	-2.96862900
H	-0.31702100	5.88455600	0.74835900
C	-0.39363500	6.92437100	-1.77208200
H	-0.03173100	7.60240600	-0.99467200
H	0.48155900	6.49555800	-2.27284700
H	-0.93924400	7.51158800	-2.51391900
C	-1.65340400	3.97002700	2.11697600
H	-2.59830000	3.91308100	2.66638900
H	-1.18416100	2.98194400	2.12474000
H	-0.99444000	4.66616600	2.63856700
C	-4.24259100	3.69540500	-2.23275100
H	-4.52666400	2.69078000	-1.91873300
H	-5.13538800	4.32025100	-2.12347400

H	-3.97604100	3.67859800	-3.29240900
H	-2.55407800	1.13588900	0.71413800
B	-6.80238600	1.11577800	-1.42587400
F	-5.45289500	1.01168700	-1.00003800
F	-6.84782500	1.91301200	-2.57158700
F	-7.54143100	1.71800500	-0.39513100
F	-7.29900500	-0.15761000	-1.68738500
N	-2.67098300	-0.99128700	-2.75974100
C	-1.42007900	-1.71395700	-2.97257600
C	-1.56672900	-3.22793800	-2.88118100
H	-0.71541300	-1.39549500	-2.20016100
H	-0.95966500	-1.44474900	-3.94328000
H	-0.59922400	-3.70662800	-3.06252000
H	-1.91182400	-3.50718500	-1.88254600
H	-2.28600500	-3.61916000	-3.60714800
C	-3.45810300	-0.92991800	-3.98619300
C	-4.81073300	-0.25527100	-3.81440200
H	-3.62039700	-1.96315900	-4.31684900
H	-2.89199400	-0.43319900	-4.79908500
H	-5.38920600	-0.35560100	-4.73798100
H	-5.37923500	-0.71009200	-2.99985500
H	-4.72592400	0.81185900	-3.59385100
C	-2.45802100	0.30484300	-2.11902600
C	-1.62262100	1.32428900	-2.89844400
H	-1.96186100	0.09918800	-1.16464000
H	-3.43862600	0.72852400	-1.88000100
H	-1.48306700	2.22709000	-2.29487700
H	-0.62959300	0.92218100	-3.13315000
H	-2.10686300	1.61077900	-3.83822900
C	1.58674200	-0.97746400	-0.88061900
C	0.51205700	-0.41831900	-0.17242600
H	2.03378700	-0.28609900	-1.59531600
C	0.31846000	1.01197600	-0.22087700
H	1.06215300	1.56063900	-0.82980000
O	-0.61593500	1.62316400	0.29919200
C	1.66329800	-2.38401500	-1.34884300
C	2.10105100	-2.61924000	-2.66098000
C	1.31098900	-3.48483300	-0.55563900
C	2.20956500	-3.91300900	-3.16285300
H	2.33369800	-1.77190600	-3.30360200
C	1.41832700	-4.77771300	-1.05925900
H	0.95333600	-3.32736000	0.45492700
C	1.87348600	-4.99929800	-2.35815700
H	2.54630800	-4.06941900	-4.18272600

H	1.14521700	-5.61860600	-0.43008800
H	1.95690900	-6.01040300	-2.74241500
C	-0.43507900	-1.18562300	0.56371900
C	-1.26745400	-1.82763600	1.17608300
C	-2.19191100	-2.60716100	1.94425000
C	-2.38732500	-2.33139000	3.30556800
C	-2.92323600	-3.65050900	1.35393500
C	-3.31699700	-3.05654800	4.04346700
H	-1.80833500	-1.54106900	3.77395800
C	-3.83160100	-4.37992100	2.10642100
H	-2.81234000	-3.85046800	0.29187600
C	-4.05881900	-4.08446900	3.45519000
H	-3.46666300	-2.82366800	5.09477200
H	-4.40318200	-5.17259700	1.63124700
C	6.90985800	-2.36709800	-2.29492300
C	6.27132800	-1.51247100	-1.39374500
C	6.68149600	-1.40017500	-0.07301700
C	7.75000700	-2.20003200	0.32812100
C	8.38775500	-3.07702700	-0.54401300
C	7.96697400	-3.15949400	-1.87111600
C	6.29532800	-2.23939400	-3.66986800
C	5.59289400	-0.88227400	-3.59131000
C	5.13308400	-0.82029400	-2.11649100
H	6.20070200	-0.72716300	0.63192300
H	9.21569200	-3.67996000	-0.18991700
H	8.47538000	-3.82597400	-2.56006600
H	7.02433600	-2.25212000	-4.48227300
H	4.75882700	-0.76374500	-4.29464600
H	4.19849400	-1.37812000	-2.00865100
H	5.55882800	-3.03057100	-3.84991200
Br	8.36129900	-2.08617700	2.11809400
O	6.58179400	0.10842700	-3.81719700
C	6.07469500	1.41874200	-3.74071800
H	6.91156700	2.11210300	-3.82706400
H	5.36332900	1.61862900	-4.55434700
N	4.88284500	0.56740200	-1.71695600
C	4.20503000	1.07710500	-0.65790600
C	5.37188100	1.62755400	-2.43257800
N	5.05525100	2.75611200	-1.87045300
N	4.33303000	2.40149200	-0.77301000
C	3.85544300	3.45649200	0.08583600
C	2.88822600	4.31574800	-0.42674900
C	4.43336700	3.60630600	1.35241300
C	2.51258500	5.39595800	0.37447400

C	4.00636500	4.68795600	2.11440300
C	3.05123000	5.59491600	1.64158900
H	1.77836100	6.09607500	-0.01522500
H	4.43273800	4.83050700	3.10421400
C	2.59628900	6.74347700	2.50343000
H	1.91472300	6.38989800	3.28379600
H	3.44256000	7.22344600	3.00112600
H	2.06903100	7.49639800	1.91335500
C	5.44111200	2.62472100	1.88875700
H	4.93723100	1.71112800	2.22833900
H	6.18292100	2.34690900	1.13316600
H	5.97072800	3.05260000	2.74140700
C	2.23727300	4.11675100	-1.77134000
H	2.39841000	3.11318500	-2.17005100
H	1.15768400	4.27248000	-1.67920700
H	2.62553000	4.83020300	-2.50482000
C	2.77831900	-1.55564700	1.77782700
C	3.30645500	-0.98582500	0.48005100
H	2.82957500	-2.64778700	1.73858700
C	3.38458600	0.41527400	0.42100700
O	2.68198600	1.17959900	1.10586700
C	3.57993800	-1.03837400	2.95749600
C	4.89017500	-1.47435300	3.17992400
C	3.04506900	-0.06430100	3.80415100
C	5.64566300	-0.95118500	4.22681700
H	5.32692100	-2.22821300	2.52624500
C	3.79670700	0.45798900	4.85459000
H	2.03885000	0.29772600	3.61687700
C	5.10019300	0.01633200	5.06887900
H	6.66154400	-1.29947300	4.38146100
H	3.36539900	1.21645700	5.50067700
H	5.68886200	0.42355500	5.88479000
H	4.03024700	-1.59501900	-0.04572300
H	1.72926800	-1.26892700	1.90887200
C	-5.11702400	-4.82066400	4.23123300
H	-6.10774100	-4.41201300	3.99695900
H	-5.13532000	-5.88211100	3.97208200
H	-4.96220300	-4.72724300	5.30839600

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C	-0.81316900	-4.36134400	0.91715800
C	-1.28192400	-3.05884300	0.74323900
C	-1.16264600	-2.39830200	-0.47491500
C	-0.54249900	-3.09065300	-1.51037900

C	-0.09006600	-4.40177600	-1.36754900
C	-0.22373800	-5.04375800	-0.14013400
C	-1.01726800	-4.83595300	2.33419600
C	-1.96848400	-3.79797500	2.94099900
C	-1.75846000	-2.52529100	2.07607000
H	-1.53717800	-1.39368200	-0.65885100
H	0.36460500	-4.90921100	-2.21196200
H	0.12617400	-6.06383200	-0.01814000
H	-1.46899400	-5.82881700	2.39830800
H	-1.76909300	-3.59413900	4.00165900
H	-0.98975500	-1.87447800	2.50561700
H	-0.06906800	-4.86815100	2.88182900
Br	-0.25503100	-2.20533000	-3.15377400
O	-3.28361200	-4.29756900	2.79333700
C	-4.25135000	-3.43239100	3.34099400
H	-5.23118800	-3.86800400	3.16332200
H	-4.08513600	-3.28831500	4.41851500
N	-2.98968200	-1.73290700	2.05395000
C	-3.21520300	-0.54341200	1.48968400
C	-4.16663000	-2.11725000	2.63597800
N	-5.07942500	-1.19998600	2.49893100
N	-4.46586500	-0.22584500	1.77338300
C	-5.13810200	1.00335800	1.46226600
C	-6.34703000	0.93095200	0.76029500
C	-4.57062200	2.20265200	1.90709000
C	-7.00015300	2.13525000	0.50803300
C	-5.26580300	3.37575200	1.61190100
C	-6.47386000	3.36182100	0.91814400
H	-7.93802700	2.11235000	-0.04232500
H	-4.84620600	4.32456300	1.93368500
C	-7.19833200	4.64256600	0.59931300
H	-8.25222300	4.57970800	0.88401400
H	-6.74695600	5.49149400	1.11764300
H	-7.15957800	4.84646900	-0.47594900
C	-3.28509500	2.25241100	2.69463800
H	-3.28376300	1.51212400	3.50173700
H	-2.40346700	2.05830400	2.07320100
H	-3.16609300	3.24224300	3.13896500
C	-6.90254100	-0.37707200	0.26522500
H	-6.12344800	-1.02149800	-0.14892300
H	-7.37337000	-0.93775700	1.07797100
H	-7.65269700	-0.19456000	-0.50700800
H	-2.49910600	0.07106200	0.96051700
B	-5.20005500	-3.56884700	-0.30348000

F	-4.34631400	-2.44959700	-0.14690800
F	-6.31989600	-3.17373400	-1.04661300
F	-5.61365400	-3.99819600	0.96667200
F	-4.51232000	-4.58454800	-0.95669600
N	-2.94708700	-0.17775200	-2.89771800
C	-2.08756600	0.84826900	-3.47392500
C	-2.64218100	1.72596600	-4.60563300
H	-1.18884400	0.34009200	-3.85028900
H	-1.74591800	1.48570800	-2.65172600
H	-1.82529400	2.31468700	-5.03436900
H	-3.07248000	1.12119400	-5.40958000
H	-3.40790900	2.42736300	-4.26377700
C	-3.45017600	-1.12239100	-3.88599000
C	-3.96267200	-2.40879400	-3.25551700
H	-2.61237600	-1.35807900	-4.55333400
H	-4.23957500	-0.68383000	-4.52291200
H	-4.22671200	-3.12843000	-4.03667400
H	-3.19556300	-2.85220800	-2.61574600
H	-4.84736600	-2.24959400	-2.63467500
C	-3.95174300	0.29652100	-1.94897700
C	-5.24639500	0.86705300	-2.54516700
H	-3.46667500	1.05517300	-1.31798100
H	-4.21164600	-0.54004100	-1.28830900
H	-5.84499000	1.33522300	-1.75985000
H	-5.05093400	1.62223200	-3.31086800
H	-5.84999700	0.07596900	-3.00191900
C	1.41492800	0.65770600	-1.10251200
C	0.37311700	0.93246600	-0.18676500
H	1.84668600	-0.33413100	-0.96204000
C	0.30276100	0.12708400	1.00187800
H	1.09340000	-0.64764800	1.07480500
O	-0.56323000	0.19194200	1.88156100
C	1.44264500	1.05993600	-2.53308900
C	2.09307000	0.21157200	-3.44060400
C	0.85638700	2.23399000	-3.02703700
C	2.14218400	0.51122300	-4.79748700
H	2.53317800	-0.71378900	-3.08040600
C	0.92091000	2.54249800	-4.38297300
H	0.34351900	2.90775800	-2.35118000
C	1.55506200	1.68114500	-5.27540400
H	2.63659300	-0.17183700	-5.48079500
H	0.46591500	3.46023400	-4.74249800
H	1.59387200	1.92083500	-6.33309700
C	-0.58061400	1.98393800	-0.28457900

C	-1.43686400	2.84951400	-0.30344300
C	-2.38783200	3.92247300	-0.35383300
C	-3.38974300	3.95698000	-1.33453300
C	-2.31112900	4.97767000	0.56896600
C	-4.28080300	5.02212500	-1.39127700
H	-3.46166800	3.14389600	-2.05038900
C	-3.20369800	6.03925800	0.49796200
H	-1.53897000	4.95626300	1.33158200
C	-4.19882600	6.08366600	-0.48534200
H	-5.05044100	5.03299000	-2.15917600
H	-3.12672800	6.85270000	1.21493600
C	6.93215400	-0.85865400	-1.77417700
C	5.82905300	-0.49553400	-1.00578400
C	4.64248800	-1.19975800	-1.04799100
C	4.55856100	-2.28163500	-1.91444500
C	5.62422500	-2.64288400	-2.73246800
C	6.82446800	-1.92684700	-2.65722300
C	8.11650500	0.00455100	-1.39283700
C	7.73370600	0.48503500	0.01717600
C	6.19340400	0.63940500	-0.07787400
H	3.79970600	-0.94878600	-0.41444900
H	5.53236700	-3.49021900	-3.40205300
H	7.66908300	-2.23341000	-3.26554400
H	9.06465500	-0.53561100	-1.36638000
H	8.22822700	1.41156500	0.33124900
H	5.92627300	1.62838300	-0.46512200
H	8.22384300	0.86058000	-2.06726300
Br	2.92221700	-3.23397600	-1.90261100
O	8.06164800	-0.57965500	0.89631000
C	7.65875700	-0.35499400	2.22826900
H	7.93188100	-1.22993500	2.81769300
H	8.15276700	0.53092300	2.65044800
N	5.54353400	0.45839900	1.22287000
C	4.22815600	0.54785900	1.53852000
C	6.17495600	-0.15627900	2.26898400
N	5.33011000	-0.46167500	3.21045300
N	4.12968800	-0.02145800	2.74377100
C	2.92880500	-0.36574700	3.46283800
C	2.45785200	0.51519500	4.43690400
C	2.33738800	-1.59723400	3.17412900
C	1.29309100	0.15228300	5.10634600
C	1.18908200	-1.92156800	3.89650100
C	0.63859300	-1.05106600	4.83710400
H	0.88637000	0.82603000	5.85549300

H	0.71896000	-2.88639500	3.71892300
C	-0.65203600	-1.39271100	5.53260000
H	-0.77308900	-0.81814100	6.45284200
H	-1.50409000	-1.15514100	4.88311600
H	-0.70304300	-2.45613900	5.78124000
C	2.88937100	-2.54301400	2.13501100
H	2.49906000	-2.32922900	1.13092900
H	3.98102000	-2.50695700	2.08346200
H	2.59800900	-3.56861400	2.37119000
C	3.18221100	1.79964600	4.72662000
H	4.22205700	1.60759000	5.00866300
H	3.18181200	2.43143200	3.83360800
H	2.69794500	2.33828200	5.54215900
C	2.76512100	3.17830100	-0.75788100
C	3.15096400	1.73651400	-0.46864200
H	1.76220900	3.37218400	-0.36261200
C	3.15098300	1.40985700	0.90786200
O	2.29734700	1.82767800	1.70706200
C	3.76631800	4.11402700	-0.11593200
C	4.98941400	4.37906500	-0.74158600
C	3.52102700	4.67239500	1.14229500
C	5.95026200	5.17499700	-0.12266400
H	5.18371000	3.96011500	-1.72723300
C	4.48037200	5.47028000	1.76307900
H	2.57501700	4.46559800	1.63407000
C	5.69835500	5.72168400	1.13503400
H	6.89176500	5.37559500	-0.62473700
H	4.27429500	5.89862800	2.73923900
H	6.44384100	6.34497100	1.61819500
H	3.92249300	1.32161900	-1.11024500
H	2.74574900	3.34185300	-1.83711000
C	-5.12724400	7.26624300	-0.58373500
H	-5.42483200	7.62036500	0.40697700
H	-6.02980300	7.01738000	-1.14653800
H	-4.63573600	8.10074700	-1.09460600

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C	1.56564400	-4.59141600	0.56344000
C	1.90426200	-3.26454700	0.29384500
C	2.14972000	-2.34642300	1.30793200
C	2.05076700	-2.81572300	2.61467700
C	1.69355000	-4.12855600	2.91074600
C	1.44570800	-5.02760000	1.87577800
C	1.38658100	-5.37218600	-0.71807300

C	2.10525600	-4.50735700	-1.75924100
C	1.92772600	-3.07281600	-1.20718100
H	2.46781800	-1.32303300	1.12766100
H	1.63389500	-4.44740500	3.94492000
H	1.18694000	-6.05737600	2.10020300
H	1.82217700	-6.37319000	-0.68764600
H	1.69703100	-4.60152200	-2.77470300
H	0.99222300	-2.65750000	-1.58758400
H	0.32501000	-5.46791600	-0.97466500
Br	2.46760700	-1.64991200	4.04833100
O	3.47015500	-4.87474600	-1.74767400
C	4.25651300	-4.12758000	-2.64684500
H	5.29455700	-4.41672600	-2.49852800
H	3.95566800	-4.31951300	-3.68672400
N	2.99733100	-2.21136500	-1.70351500
C	3.12519100	-0.88711400	-1.60170900
C	4.10999600	-2.66580300	-2.35387700
N	4.88422100	-1.67585100	-2.69707900
N	4.25410800	-0.57081200	-2.21182800
C	4.78380500	0.74635600	-2.43076200
C	6.09608900	1.01537200	-2.02133000
C	3.96949600	1.68750900	-3.07360000
C	6.58574200	2.29580300	-2.27614300
C	4.51619600	2.95169000	-3.29525200
C	5.81276100	3.27672100	-2.89783900
H	7.59620300	2.53646200	-1.95587400
H	3.91315700	3.69848400	-3.80662900
C	6.34424800	4.67255000	-3.08606400
H	7.42563500	4.67020300	-3.23810500
H	5.87192800	5.16590100	-3.93868400
H	6.13580500	5.27513700	-2.19482000
C	2.56584900	1.37442200	-3.53149000
H	2.50573200	0.39619900	-4.01792600
H	1.84759500	1.36307500	-2.70204100
H	2.23562400	2.12919600	-4.24857900
C	6.94666700	-0.00414800	-1.31296500
H	6.36917000	-0.58787900	-0.59342700
H	7.38109100	-0.71102500	-2.02615000
H	7.76312100	0.49773400	-0.78977300
H	2.43155500	-0.20118000	-1.13504900
B	5.60131800	-2.82286800	0.73461600
F	4.80246500	-1.73091100	0.30459500
F	6.89964400	-2.36164400	0.96383200
F	5.61708000	-3.78316800	-0.28789400

F	5.05331700	-3.36216400	1.89500900
N	3.63903300	1.07321300	2.37583900
C	2.55568600	1.83981400	2.98187100
C	2.91340400	3.14383300	3.70860900
H	2.05197200	1.18096900	3.70452700
H	1.82188800	2.04719800	2.19667100
H	1.99701500	3.59197200	4.10881300
H	3.58321500	2.95988200	4.55384800
H	3.38907000	3.87615300	3.05112300
C	4.76975600	0.88877300	3.27370600
C	5.69887300	-0.23916000	2.85250800
H	4.34861000	0.64525300	4.25898200
H	5.35006900	1.81966900	3.41295100
H	6.50014600	-0.35234200	3.58970800
H	5.15093500	-1.18080800	2.77955500
H	6.16709100	-0.05695900	1.88231200
C	3.97495800	1.42339900	1.00095000
C	4.69522600	2.75433600	0.75679500
H	3.03090800	1.43842700	0.44036900
H	4.57139100	0.60029800	0.58698600
H	4.85558400	2.89232200	-0.31705100
H	4.10068100	3.60253400	1.10741300
H	5.67268800	2.78177300	1.25114300
C	-0.97287300	-0.14029900	1.40471700
C	-0.29367100	0.22369200	0.22660600
H	-1.16224700	-1.21039800	1.51188100
C	-0.25469300	-0.73572200	-0.83602500
H	-0.70290400	-1.71918700	-0.57517800
O	0.21119500	-0.55572900	-1.97000000
C	-0.85932500	0.60218000	2.67228700
C	-0.59851800	-0.12698300	3.83671900
C	-0.99648000	1.99621900	2.75766400
C	-0.42238000	0.52406300	5.05554800
H	-0.48256900	-1.20531500	3.77620000
C	-0.84271700	2.64130500	3.97760200
H	-1.23324200	2.57356400	1.86882200
C	-0.54467000	1.90766100	5.12899500
H	-0.19013700	-0.05469100	5.94368700
H	-0.95773400	3.71937600	4.03473800
H	-0.41470300	2.41728200	6.07818500
C	0.30054900	1.49557700	0.01393800
C	0.79047700	2.59748900	-0.14655400
C	1.44583600	3.86672700	-0.18700100
C	2.10160400	4.30927400	-1.34330800

C	1.48698400	4.66504200	0.96731000
C	2.81150000	5.50239700	-1.33148500
H	2.06299400	3.70051100	-2.24002000
C	2.19414200	5.86018800	0.96216200
H	0.98458900	4.32236800	1.86802000
C	2.87432000	6.29546800	-0.18103200
H	3.33245100	5.82378000	-2.23047400
H	2.23255600	6.46095800	1.86692200
C	-3.72591800	4.11374900	-1.13140000
C	-3.95199400	2.75295200	-0.91168200
C	-5.17911300	2.27345000	-0.47694200
C	-6.17948000	3.21333800	-0.23815500
C	-5.97535900	4.57623300	-0.43029000
C	-4.73756500	5.03171600	-0.88623000
C	-2.32152000	4.33880300	-1.64711300
C	-1.92874600	2.95353900	-2.16406200
C	-2.66458000	2.00597300	-1.18824800
H	-5.36857700	1.21558000	-0.31528100
H	-6.78142300	5.27391900	-0.23532600
H	-4.58096600	6.09202300	-1.05571200
H	-2.25824700	5.08378600	-2.44271000
H	-0.84948400	2.76224700	-2.18051100
H	-2.07014900	1.89440700	-0.27971100
H	-1.64165300	4.63635500	-0.83942900
Br	-7.86958100	2.60995700	0.37185900
O	-2.48092700	2.81592600	-3.46451600
C	-2.19039600	1.56166600	-4.03227300
H	-2.68744800	1.49848600	-5.00039200
H	-1.10779500	1.42831300	-4.17300100
N	-2.82372700	0.67827800	-1.78685000
C	-3.15769300	-0.51086200	-1.23230100
C	-2.68146800	0.46959000	-3.13173800
N	-2.95407800	-0.76335600	-3.44517600
N	-3.24587700	-1.35981800	-2.26180000
C	-3.69018600	-2.72980800	-2.26461700
C	-2.81473200	-3.70019000	-2.74962000
C	-4.98747900	-3.01229200	-1.81836200
C	-3.27110800	-5.01971500	-2.75820700
C	-5.38947700	-4.34354000	-1.85462800
C	-4.54605700	-5.35987700	-2.31234300
H	-2.60620200	-5.79831300	-3.12357900
H	-6.39101200	-4.59442000	-1.51393900
C	-5.00892300	-6.79326000	-2.30314500
H	-4.36241700	-7.42263500	-2.91763800

H	-4.99900200	-7.19327800	-1.28445700
H	-6.03225700	-6.87755800	-2.67742900
C	-5.91746600	-1.94774800	-1.29754900
H	-5.68765600	-1.70612300	-0.25216800
H	-5.85819800	-1.02764400	-1.88789900
H	-6.94890400	-2.30268800	-1.33027000
C	-1.43811300	-3.36810000	-3.26503500
H	-1.47407100	-3.14369600	-4.33560000
H	-0.99965200	-2.49366300	-2.77619000
H	-0.77512500	-4.22584700	-3.12754900
C	-3.71212100	-0.49581400	2.58733100
C	-3.25397100	-0.00515400	1.23344200
H	-3.65345900	0.32284000	3.31133400
C	-3.23288500	-0.96114100	0.20974900
O	-3.12793700	-2.19066900	0.37578800
C	-5.12931500	-1.02453900	2.47418700
C	-5.38035500	-2.39810300	2.49809700
C	-6.19776700	-0.15100000	2.23724800
C	-6.66927800	-2.89108900	2.29770900
H	-4.55231300	-3.08242300	2.65473600
C	-7.48486400	-0.64059200	2.03361200
H	-6.01968300	0.92289500	2.19906100
C	-7.72514400	-2.01430400	2.06449000
H	-6.84446500	-3.96242600	2.31614100
H	-8.29848400	0.05238800	1.84498800
H	-8.72835400	-2.39615600	1.90398900
H	-3.43976900	1.03677700	1.00582800
H	-3.05574300	-1.29775000	2.94512000
C	3.63280700	7.59666000	-0.18184500
H	2.99267100	8.41954600	-0.51674700
H	3.99264900	7.84429300	0.81915300
H	4.49100700	7.55168300	-0.85664000

R2NH

C	-2.79781600	1.27274100	-0.00630600
C	-1.58108000	1.87382200	-0.00698800
H	-3.64912300	1.95276000	-0.03483400
C	-1.58289100	3.36044600	-0.03082200
H	-2.59451600	3.81218400	-0.04253400
O	-0.58717100	4.04760400	-0.03683600
C	-3.16323400	-0.13912300	0.01785200
C	-4.52703200	-0.45679600	-0.10320600
C	-2.23973300	-1.18885500	0.16205400
C	-4.95788800	-1.77689100	-0.09345600

H	-5.24980200	0.34755600	-0.20861500
C	-2.67489400	-2.50813300	0.17568600
H	-1.18562600	-0.96785900	0.27096400
C	-4.03056000	-2.80806500	0.04534300
H	-6.01462400	-2.00174200	-0.19142600
H	-1.95136200	-3.30864700	0.29052100
H	-4.36263900	-3.84103500	0.05536700
C	-0.30276800	1.24841100	-0.00078900
C	0.82315000	0.79372400	-0.00517200
C	2.13347200	0.22894200	-0.00860400
C	2.31942700	-1.15582900	-0.15377400
C	3.26770600	1.04537500	0.13211500
C	3.58925000	-1.70520000	-0.15687500
H	1.45310900	-1.79959000	-0.27050400
C	4.53925600	0.49979600	0.13028100
H	3.13811000	2.11708700	0.24178200
C	4.72360400	-0.88665900	-0.01425400
H	3.71758000	-2.77755700	-0.26970000
H	5.40674600	1.14329300	0.24233300
N	5.98818900	-1.43905000	0.03924400
H	6.09116800	-2.35220700	-0.37976900
H	6.75321500	-0.81795900	-0.18210300

TS4CNH-RS

C	-3.78918700	-1.21517100	3.49278100
C	-3.45192600	-0.66720700	2.25170000
C	-3.78521400	-1.29343300	1.06125600
C	-4.48382800	-2.49395100	1.15776600
C	-4.82709600	-3.06600100	2.37684000
C	-4.47381000	-2.41965500	3.56189500
C	-3.30692200	-0.32691300	4.61772000
C	-3.07457900	1.01104900	3.91198200
C	-2.65011200	0.59270200	2.48673900
H	-3.54990000	-0.87680800	0.08626500
H	-5.37292700	-4.00220300	2.39821500
H	-4.74653000	-2.85271300	4.51912900
H	-4.02868400	-0.21350900	5.42944600
H	-2.32702000	1.65826900	4.38936500
H	-1.57051300	0.40552800	2.43735100
H	-2.36785500	-0.69916900	5.04298700
Br	-4.97656300	-3.38720100	-0.43839100
O	-4.33697500	1.65684200	3.85851400
C	-4.32809300	2.91036100	3.21836300
H	-5.36508800	3.20696000	3.06718200

H	-3.81047400	3.66391600	3.82845800
N	-2.89531200	1.71517500	1.58386300
C	-2.32741100	1.95850600	0.40606500
C	-3.64058000	2.81720800	1.89159000
N	-3.53946500	3.72905300	0.96265300
N	-2.71434000	3.16612700	0.03511800
C	-2.14812800	3.89594000	-1.07196000
C	-2.70191700	3.77122900	-2.34639200
C	-1.00768000	4.66940900	-0.80462200
C	-1.99332700	4.35081800	-3.40350500
C	-0.33442200	5.21200200	-1.89593500
C	-0.79748600	5.03610500	-3.20425200
H	-2.39217200	4.24891700	-4.41010200
H	0.57017000	5.78956600	-1.72234400
C	-0.01822800	5.57970900	-4.37310100
H	0.54290900	6.47426200	-4.09299300
H	0.70888700	4.83944600	-4.72604000
H	-0.67812800	5.82299700	-5.20873600
C	-0.58402500	5.00253300	0.60350400
H	-1.18269200	5.84357600	0.96872600
H	-0.71914800	4.17581400	1.30468600
H	0.46578000	5.30506900	0.62099400
C	-4.03053700	3.11248600	-2.59955100
H	-4.34971700	2.45880000	-1.78792900
H	-4.79395400	3.88807000	-2.72243600
H	-3.99648800	2.53836900	-3.52874300
H	-1.65176600	1.30949300	-0.13419000
B	-6.04206100	0.99423100	0.18021600
F	-4.71842200	1.05670800	-0.33574400
F	-6.86504800	1.77982300	-0.62246500
F	-6.01867600	1.49288300	1.49108200
F	-6.46563100	-0.33337000	0.17320400
N	-2.85366500	-1.52844900	-2.55855400
C	-1.80392100	-2.41210100	-3.05734400
C	-2.22165200	-3.87895300	-3.11065400
H	-0.94846300	-2.29730700	-2.38082300
H	-1.44732900	-2.11115100	-4.06068500
H	-1.33753200	-4.51699800	-3.20555600
H	-2.75998900	-4.15714400	-2.20071300
H	-2.86760800	-4.08838300	-3.96733900
C	-4.07664900	-1.63319800	-3.35197000
C	-5.18561800	-0.70129900	-2.88486800
H	-4.43596500	-2.66318700	-3.25779300
H	-3.87185900	-1.47069700	-4.42823700

H	-6.10433000	-0.93029900	-3.43294300
H	-5.37573100	-0.82706800	-1.81662700
H	-4.94750100	0.35172200	-3.06011300
C	-2.35682000	-0.15729300	-2.41998800
C	-1.99027400	0.56719000	-3.71772700
H	-1.46057800	-0.21523000	-1.78649400
H	-3.11264300	0.41843700	-1.87209900
H	-1.61705800	1.57009400	-3.48891700
H	-1.19832000	0.04547400	-4.26073300
H	-2.85634000	0.66867100	-4.38121200
C	1.58405900	1.46740200	-1.18401600
C	0.83505500	1.10099000	-0.05565000
H	1.79858100	2.53498500	-1.21645700
C	0.68579900	2.08869400	0.98125100
H	1.17718200	3.05083600	0.75263400
O	0.02235300	1.95863000	2.01527100
C	1.47543700	0.85527500	-2.52966800
C	1.45267900	1.71264100	-3.63874600
C	1.40996400	-0.52585900	-2.75386900
C	1.40995200	1.20467300	-4.93420200
H	1.46770500	2.78668600	-3.47444700
C	1.37945400	-1.03529500	-4.04790500
H	1.37651700	-1.20787400	-1.91450000
C	1.39130500	-0.17307000	-5.14407000
H	1.39405500	1.88739200	-5.77834200
H	1.34148100	-2.11242400	-4.18337100
H	1.37236600	-0.57204900	-6.15319300
C	0.36550100	-0.22034700	0.17938100
C	-0.00241700	-1.35846400	0.41362800
C	-0.29282600	-2.72972500	0.69778300
C	0.62441500	-3.50375700	1.42558100
C	-1.44078600	-3.35093900	0.18741900
C	0.40973100	-4.85683800	1.62726100
H	1.52281400	-3.03434200	1.81770500
C	-1.66704000	-4.70078400	0.40201600
H	-2.15025400	-2.77132800	-0.39892600
C	-0.74109200	-5.47915100	1.11518300
H	1.13316100	-5.44732300	2.18205300
H	-2.58099000	-5.15477200	0.02690100
C	5.71994700	-3.32918400	-1.42632400
C	4.79428300	-2.47010100	-0.82650400
C	3.42784500	-2.65059200	-0.96568400
C	3.00803000	-3.70288400	-1.78334800
C	3.91113200	-4.53694700	-2.43384900

C	5.28236600	-4.35656900	-2.24695700
C	7.12115600	-2.99287300	-0.96676900
C	6.84619200	-2.22104900	0.32642100
C	5.55894900	-1.43985900	-0.02082200
H	2.70678400	-2.01939800	-0.44926200
H	3.54241800	-5.34163300	-3.05928000
H	5.98734700	-5.03364300	-2.71825800
H	7.73781900	-3.87224100	-0.77192600
H	7.66374800	-1.57065800	0.65957400
H	5.79933400	-0.55462600	-0.61773000
H	7.64458900	-2.35201100	-1.68444300
Br	1.15430600	-4.02428400	-1.99686900
O	6.53457200	-3.19606800	1.31063300
C	6.17536100	-2.66085500	2.56002600
H	5.76845200	-3.47195500	3.16534200
H	7.04650500	-2.23854600	3.07966500
N	4.90598100	-0.97691600	1.20474000
C	4.10710700	0.09775200	1.43288900
C	5.15969700	-1.56490000	2.41211100
N	4.54764000	-0.93528300	3.37173500
N	3.90528700	0.09409200	2.75821000
C	3.21363300	1.02659200	3.62563900
C	3.92760900	2.13163600	4.09971200
C	1.93495200	0.69315100	4.06113600
C	3.27336600	2.96775600	4.99784800
C	1.32499000	1.56424000	4.96520100
C	1.96792500	2.70840200	5.42879500
H	3.79825100	3.84045100	5.37814200
H	0.32070600	1.33413800	5.31181800
C	1.27167400	3.65814500	6.36813300
H	0.82744800	4.48913300	5.81091900
H	0.46922400	3.15767100	6.91418600
H	1.97148800	4.08398600	7.09109600
C	1.25826800	-0.56440200	3.59753500
H	1.18625500	-0.59116100	2.50796900
H	1.81141900	-1.44935600	3.93062300
H	0.24418000	-0.62448200	3.99802100
C	5.34283700	2.39396700	3.66453400
H	5.96594200	1.50254200	3.79093400
H	5.36297000	2.67731800	2.60907400
H	5.78049800	3.20098400	4.25393600
C	4.34602800	2.04970100	-1.89886100
C	3.72994300	1.08601200	-0.88070100
H	4.23428700	1.56016800	-2.87175700

C	3.78440600	1.27290200	0.51543300
O	3.53325000	2.31154000	1.14921500
C	3.89959100	3.49585200	-2.08330200
C	3.81744200	3.98856800	-3.39226400
C	3.65892400	4.38715200	-1.03113200
C	3.49757400	5.31929300	-3.64929800
H	3.99714000	3.31241900	-4.22492700
C	3.33491100	5.71936000	-1.28585200
H	3.71338600	4.02753000	-0.01066400
C	3.25264300	6.19372100	-2.59288300
H	3.43621900	5.67069300	-4.67488600
H	3.14822100	6.39057900	-0.45229900
H	3.00073300	7.23195300	-2.78674700
H	3.82175300	0.05369000	-1.21120400
H	5.42983300	2.07808200	-1.71256200
N	-0.93120900	-6.84374600	1.26391900
H	-1.88821700	-7.15757400	1.18191600
H	-0.45668600	-7.26592400	2.04968400

TS4CNH-SS

C	-6.19542700	-1.86419400	2.15975900
C	-5.29006700	-1.14801000	1.37074200
C	-5.01165700	-1.51427000	0.06095200
C	-5.70753500	-2.61187100	-0.44028800
C	-6.60487500	-3.34789600	0.32665300
C	-6.84871500	-2.97497200	1.64703100
C	-6.34609300	-1.22774300	3.52063900
C	-5.85768300	0.19594300	3.25787300
C	-4.74054100	-0.00460700	2.20453600
H	-4.33019900	-0.96727600	-0.58464400
H	-7.12547600	-4.18915600	-0.11670600
H	-7.56461700	-3.52751900	2.24834100
H	-7.37285500	-1.22066300	3.89235700
H	-5.50436700	0.73591900	4.14579800
H	-3.79879200	-0.28887200	2.68595000
H	-5.70412700	-1.71804100	4.26126200
Br	-5.48537300	-3.09659400	-2.25695700
O	-6.95125200	0.87070200	2.65645500
C	-6.69028600	2.20195900	2.28397700
H	-7.51989400	2.54118900	1.66678400
H	-6.59088500	2.84763300	3.16825300
N	-4.51059500	1.26936600	1.52095100
C	-3.42853600	1.69909400	0.86243300
C	-5.42046000	2.29012500	1.49647100

N	-4.94401600	3.32364500	0.86342100
N	-3.70164800	2.93169000	0.46589400
C	-2.80787500	3.89704700	-0.12386100
C	-2.95890000	4.25086200	-1.46395200
C	-1.87722400	4.50064400	0.73115200
C	-2.10888500	5.24754100	-1.95400600
C	-1.07431400	5.50235700	0.19717800
C	-1.17463800	5.88800200	-1.14346200
H	-2.20613200	5.54338400	-2.99604800
H	-0.36696200	6.00452600	0.85199900
C	-0.28815200	6.97227400	-1.70045700
H	0.03152700	7.66299000	-0.91594100
H	0.61240800	6.54468500	-2.15528200
H	-0.80437400	7.54465300	-2.47433500
C	-1.74441000	4.08197700	2.16962800
H	-2.71887900	4.02544900	2.66476700
H	-1.26771900	3.09844600	2.22266100
H	-1.12285600	4.79324400	2.71588900
C	-3.99465900	3.63652900	-2.36668600
H	-4.52682100	2.80357700	-1.90865300
H	-4.73399600	4.39062600	-2.65376400
H	-3.51685000	3.28273300	-3.28605100
H	-2.46922800	1.19944000	0.73955000
B	-6.72817400	1.04367400	-1.42822100
F	-5.35493600	1.08599400	-1.07148000
F	-6.94657700	1.95206100	-2.46320300
F	-7.48209300	1.40346200	-0.30118100
F	-7.05196400	-0.25099200	-1.83157400
N	-2.66223600	-1.02065000	-2.56796700
C	-1.50642000	-1.90627900	-2.49079200
C	-1.83278800	-3.37385200	-2.74142600
H	-1.10463400	-1.81732900	-1.47740400
H	-0.69644600	-1.59396900	-3.18033400
H	-0.97424800	-3.98882500	-2.45434400
H	-2.70303800	-3.66507900	-2.14718400
H	-2.05882400	-3.58239800	-3.79140800
C	-3.24630900	-0.98286300	-3.90273100
C	-4.46944800	-0.07955100	-3.98896500
H	-3.55518600	-2.00331800	-4.15258700
H	-2.49692500	-0.68784700	-4.66432400
H	-4.95362700	-0.20596200	-4.96173400
H	-5.18384400	-0.33334300	-3.20227300
H	-4.21195800	0.97835300	-3.88077500
C	-2.35988100	0.30015700	-2.01691000

C	-1.37597200	1.17096500	-2.80585500
H	-1.94707600	0.12639700	-1.01706600
H	-3.30493600	0.83703000	-1.88498400
H	-1.23199300	2.12255600	-2.28229700
H	-0.39647100	0.68731500	-2.89603900
H	-1.74564400	1.38627000	-3.81427900
C	1.55441000	-0.98774700	-0.69483900
C	0.53271100	-0.34309100	0.03213300
H	1.96960600	-0.35859000	-1.48355800
C	0.37793800	1.08090600	-0.10925900
H	1.12738400	1.56447100	-0.76596900
O	-0.52881500	1.75850100	0.38100500
C	1.54696300	-2.42016000	-1.09494200
C	1.91444700	-2.73893900	-2.41085600
C	1.18871600	-3.46684200	-0.23398700
C	1.95053200	-4.05868900	-2.85140800
H	2.14765900	-1.93401100	-3.10573000
C	1.22647800	-4.78705800	-0.67452200
H	0.88027100	-3.24694500	0.78091300
C	1.61443200	-5.09085100	-1.97855100
H	2.23283800	-4.27731600	-3.87635600
H	0.95055400	-5.58358000	0.00895500
H	1.64327600	-6.12212500	-2.31420000
C	-0.40431200	-1.04017200	0.84406900
C	-1.21791300	-1.67321500	1.49125700
C	-2.16318500	-2.52623200	2.14089600
C	-2.49863900	-2.37968500	3.49407900
C	-2.78988600	-3.54668200	1.40368000
C	-3.45880100	-3.19241100	4.07976400
H	-2.00470400	-1.61383500	4.08492100
C	-3.74020900	-4.36451100	1.98584800
H	-2.52547900	-3.67049200	0.35694100
C	-4.11271300	-4.18116500	3.32817700
H	-3.71362800	-3.06345500	5.12835900
H	-4.23255300	-5.13177100	1.39555000
C	6.72416000	-2.49201500	-2.42334500
C	6.15945000	-1.60855100	-1.50087700
C	6.65344500	-1.48032200	-0.21069400
C	7.73094800	-2.29276400	0.13785100
C	8.29693300	-3.19734200	-0.75539700
C	7.79158500	-3.29646900	-2.05144800
C	6.02599900	-2.37873900	-3.75903800
C	5.35396200	-1.00739100	-3.66370500
C	4.99087000	-0.90825900	-2.16428100

H	6.23022200	-0.78562400	0.51007300
H	9.13514400	-3.80879700	-0.44240200
H	8.24347900	-3.98502400	-2.75786600
H	6.70174500	-2.42081600	-4.61534500
H	4.47888400	-0.88637000	-4.31479600
H	4.05550100	-1.44586900	-1.98581300
H	5.26576300	-3.15933000	-3.87645600
Br	8.45768600	-2.15673100	1.88257300
O	6.34303800	-0.03910200	-3.97106900
C	5.86179100	1.28093600	-3.89444100
H	6.70376700	1.95762000	-4.04272700
H	5.10931500	1.47655600	-4.67106600
N	4.79033500	0.49172700	-1.77930000
C	4.18304300	1.03497900	-0.69445300
C	5.23840900	1.52886600	-2.55316000
N	4.96446600	2.67466900	-2.00285400
N	4.31030900	2.35474100	-0.85381000
C	3.89095300	3.43030900	0.00970800
C	2.87719500	4.26877900	-0.44386600
C	4.55764800	3.60705300	1.22867600
C	2.54431900	5.35432300	0.36954000
C	4.17433700	4.69543900	2.00347600
C	3.17261700	5.58089300	1.58959200
H	1.76863700	6.03485700	0.02921800
H	4.67007500	4.85886700	2.95709500
C	2.76339700	6.73516000	2.46665800
H	2.13991900	6.38365500	3.29501500
H	3.63550500	7.23065800	2.90039100
H	2.18859800	7.47482300	1.90472100
C	5.60893800	2.64109000	1.70696800
H	5.13695800	1.73477000	2.10703400
H	6.29006300	2.34587200	0.90255600
H	6.20200500	3.09027900	2.50514600
C	2.13020000	4.04509200	-1.73377500
H	2.32326500	3.06253400	-2.16847600
H	1.05342500	4.12869700	-1.54989800
H	2.40927200	4.79527700	-2.48014900
C	2.86917600	-1.52806200	1.87932700
C	3.31390300	-0.99196300	0.53460600
H	2.90171800	-2.62132200	1.85698500
C	3.42719500	0.40935900	0.45063900
O	2.78382800	1.19630300	1.16370700
C	3.75576900	-1.00330600	2.99259800
C	5.06930200	-1.46013200	3.14195000

C	3.29325200	-0.00260800	3.85070500
C	5.89874600	-0.92998500	4.12788000
H	5.45015300	-2.23672300	2.47997300
C	4.11912100	0.52733300	4.83954400
H	2.28323100	0.37343900	3.72074600
C	5.42556900	0.06544000	4.98084300
H	6.91568600	-1.29504600	4.22672700
H	3.74287900	1.30676800	5.49503600
H	6.07200300	0.47799100	5.74893300
H	4.00156400	-1.62189700	-0.01559400
H	1.83543300	-1.22324300	2.07454600
N	-5.07490800	-4.99476900	3.90758200
H	-5.74154700	-5.39015300	3.25820000
H	-5.52694800	-4.61233500	4.72698700

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C	-0.84778400	-4.36414600	0.89540200
C	-1.31274500	-3.05891300	0.73309300
C	-1.18303300	-2.38433000	-0.47646800
C	-0.55623200	-3.06581900	-1.51506000
C	-0.10830500	-4.37983500	-1.38437100
C	-0.25243700	-5.03578100	-0.16560900
C	-1.05871000	-4.85307100	2.30669700
C	-2.00840700	-3.81840800	2.92194200
C	-1.79567700	-2.53835800	2.06859000
H	-1.55396300	-1.37669600	-0.65153000
H	0.35164000	-4.87849400	-2.23119600
H	0.09463300	-6.05789000	-0.05280600
H	-1.51430300	-5.84489700	2.35877900
H	-1.80955500	-3.62415900	3.98448200
H	-1.02952000	-1.88914800	2.50494000
H	-0.11245300	-4.89481400	2.85705600
Br	-0.25176000	-2.16080600	-3.14486300
O	-3.32392500	-4.31550700	2.76918300
C	-4.29356000	-3.45332300	3.31842500
H	-5.27257200	-3.88986600	3.13827200
H	-4.12902500	-3.31285900	4.39668500
N	-3.02800700	-1.74824500	2.04587500
C	-3.25086700	-0.55866700	1.48219800
C	-4.20872100	-2.13615400	2.61744600
N	-5.12241100	-1.22057600	2.47407600
N	-4.50457900	-0.24395900	1.75537800
C	-5.17421700	0.98374700	1.43469500
C	-6.38238800	0.91098600	0.73098900

C	-4.59808700	2.18514800	1.86220600
C	-7.02778600	2.11640200	0.46440100
C	-5.28091000	3.35966800	1.54482100
C	-6.48945600	3.34496900	0.85246600
H	-7.96444500	2.09299500	-0.08803700
H	-4.84776400	4.30981000	1.84487600
C	-7.20057400	4.62727700	0.50909700
H	-8.23392400	4.61229100	0.86699100
H	-6.69264100	5.48952500	0.94650500
H	-7.23308400	4.76798000	-0.57674400
C	-3.31401100	2.23852800	2.65244700
H	-3.31485800	1.50264200	3.46352400
H	-2.43038300	2.04274900	2.03427100
H	-3.19664700	3.23088300	3.09161200
C	-6.94063000	-0.39697800	0.23833200
H	-6.16092100	-1.04058000	-0.17707500
H	-7.41070500	-0.95759900	1.05139200
H	-7.69149300	-0.21292800	-0.53279600
H	-2.52840500	0.05487300	0.96125700
B	-5.18463600	-3.57124100	-0.34098100
F	-4.36877700	-2.42444900	-0.18063200
F	-6.29265100	-3.22234200	-1.12306200
F	-5.62388000	-3.98922400	0.92473700
F	-4.44789700	-4.57799400	-0.95363800
N	-2.92899200	-0.11048900	-2.89714600
C	-2.05986900	0.91276300	-3.46388600
C	-2.60649700	1.80209300	-4.59024000
H	-1.16436900	0.39996200	-3.84151300
H	-1.71620800	1.54171400	-2.63632900
H	-1.78533900	2.38863200	-5.01376500
H	-3.04024400	1.20622300	-5.39905200
H	-3.36779900	2.50595800	-4.24348800
C	-3.43187000	-1.04746900	-3.89259000
C	-3.94701600	-2.33801600	-3.27293000
H	-2.59291400	-1.28018800	-4.55954900
H	-4.21884300	-0.60338300	-4.52869400
H	-4.21538800	-3.04913800	-4.06046600
H	-3.17821600	-2.78941300	-2.64071500
H	-4.82904700	-2.18341200	-2.64723400
C	-3.93473200	0.36816500	-1.95194100
C	-5.22662100	0.93977100	-2.55310600
H	-3.44845600	1.12883700	-1.32383900
H	-4.19991400	-0.46601000	-1.28935900
H	-5.82954600	1.40419000	-1.76899400

H	-5.02715000	1.69749100	-3.31523700
H	-5.82752600	0.15017600	-3.01592900
C	1.42267700	0.66980900	-1.10751800
C	0.37360300	0.94273600	-0.19858500
H	1.84397000	-0.32761600	-0.97369200
C	0.28468800	0.11904600	0.97580400
H	1.07153500	-0.65987000	1.04739700
O	-0.59136700	0.17316400	1.84686100
C	1.46382500	1.08229900	-2.53547800
C	2.11550600	0.23636500	-3.44437900
C	0.88905900	2.26376400	-3.02507200
C	2.17760700	0.54601900	-4.79857300
H	2.54670600	-0.69463200	-3.08766900
C	0.96660900	2.58209700	-4.37812900
H	0.37400100	2.93430200	-2.34748100
C	1.60229700	1.72352500	-5.27216900
H	2.67290100	-0.13516700	-5.48315000
H	0.52031000	3.50543200	-4.73429300
H	1.65110400	1.97096900	-6.32767700
C	-0.56415600	2.00975600	-0.28672300
C	-1.40423600	2.89190000	-0.28626400
C	-2.34276400	3.97443400	-0.30697500
C	-3.34829400	4.05113700	-1.28377500
C	-2.26068200	5.00803600	0.64005400
C	-4.23329700	5.11679000	-1.31723900
H	-3.42957200	3.25978800	-2.02343100
C	-3.14059500	6.07882800	0.60898800
H	-1.48799100	4.96420600	1.40140900
C	-4.14198000	6.15291300	-0.37351500
H	-5.00145400	5.15896500	-2.08470700
H	-3.05503300	6.87413800	1.34419100
C	6.93262800	-0.87154600	-1.76310200
C	5.82683000	-0.51103400	-0.99733200
C	4.63837000	-1.21129000	-1.05054600
C	4.55584800	-2.28655700	-1.92535700
C	5.62444500	-2.64485500	-2.74083200
C	6.82629800	-1.93279000	-2.65461700
C	8.11750000	-0.01456300	-1.36963000
C	7.72924600	0.45643000	0.04207000
C	6.18985400	0.61568000	-0.05905600
H	3.79304100	-0.96232500	-0.41951100
H	5.53339800	-3.48702000	-3.41702200
H	7.67296700	-2.23723900	-3.26115500
H	9.06402200	-0.55756700	-1.34264400

H	8.22470600	1.37931900	0.36525100
H	5.92741900	1.60829300	-0.44016700
H	8.23049300	0.84616900	-2.03711100
Br	2.91715500	-3.23451200	-1.92836000
O	8.05039300	-0.61560100	0.91482000
C	7.64144100	-0.39974400	2.24638100
H	7.90957100	-1.27962300	2.83072400
H	8.13558400	0.48189900	2.67739000
N	5.53318300	0.42677500	1.23705900
C	4.21645000	0.51817200	1.54753500
C	6.15797200	-0.19746500	2.28146500
N	5.30819800	-0.50708000	3.21702100
N	4.11109900	-0.05973600	2.74822200
C	2.90631300	-0.40384300	3.46054600
C	2.43754600	0.47122400	4.44092300
C	2.30879400	-1.62937200	3.15958300
C	1.27020100	0.10812000	5.10577300
C	1.15786600	-1.95447300	3.87751100
C	0.61079300	-1.09014500	4.82583600
H	0.86567300	0.77734600	5.86013700
H	0.68344500	-2.91541500	3.69067000
C	-0.68101400	-1.43256900	5.51898100
H	-0.79936200	-0.86480600	6.44380700
H	-1.53297500	-1.18714300	4.87229500
H	-0.73546900	-2.49767600	5.75957300
C	2.85860400	-2.56874500	2.11359100
H	2.47733300	-2.33985600	1.10941900
H	3.95096900	-2.54216400	2.07018500
H	2.55565000	-3.59405900	2.33602800
C	3.16746500	1.74991600	4.74192400
H	4.20475600	1.55041800	5.02821900
H	3.17529200	2.38675300	3.85253700
H	2.68196400	2.28669800	5.55795300
C	2.78348800	3.17625600	-0.73126600
C	3.15432700	1.72788400	-0.45397400
H	1.78191200	3.37660100	-0.33612700
C	3.14522700	1.38849300	0.91983900
O	2.28741000	1.80056800	1.71769800
C	3.79441400	4.09473300	-0.07989600
C	5.01899700	4.35595200	-0.70426300
C	3.55679100	4.63946800	1.18583200
C	5.98877800	5.13428900	-0.07683300
H	5.20767800	3.94782000	-1.69552000
C	4.52494300	5.41983100	1.81506900

H	2.60944800	4.43582700	1.67634900
C	5.74442900	5.66718200	1.18821600
H	6.93136400	5.33201000	-0.57803800
H	4.32464400	5.83777800	2.79693400
H	6.49686200	6.27680000	1.67801200
H	3.92892700	1.31525000	-1.09351500
H	2.76773500	3.34965800	-1.80898300
N	-4.98030200	7.25575800	-0.44833900
H	-5.10157600	7.77091200	0.41264300
H	-5.85617100	7.10358900	-0.92923900

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C	1.61049600	-4.59473400	0.57007700
C	1.93205000	-3.26340300	0.30129000
C	2.17563600	-2.34531600	1.31599900
C	2.09465900	-2.81990500	2.62209500
C	1.75600000	-4.13785600	2.91741300
C	1.50848300	-5.03644900	1.88207900
C	1.42650600	-5.37347100	-0.71193900
C	2.12595100	-4.49842300	-1.75750800
C	1.93968900	-3.06720800	-1.19942300
H	2.47800700	-1.31707900	1.13594700
H	1.70997700	-4.46048700	3.95111000
H	1.26347900	-6.06979100	2.10563400
H	1.87240800	-6.37014000	-0.68901600
H	1.70820800	-4.59355800	-2.76902200
H	0.99668500	-2.66046000	-1.57010400
H	0.36351800	-5.47906200	-0.95832800
Br	2.50915200	-1.65366400	4.05619500
O	3.49422700	-4.85323300	-1.76071900
C	4.26498200	-4.09516000	-2.66406300
H	5.30709500	-4.37490700	-2.52654000
H	3.95641100	-4.28593400	-3.70194400
N	2.99596000	-2.19367900	-1.70353100
C	3.11169700	-0.86828600	-1.60010500
C	4.10715000	-2.63597400	-2.36468400
N	4.86898800	-1.63812800	-2.71234400
N	4.23254100	-0.54009600	-2.21925000
C	4.74813400	0.78211400	-2.44205500
C	6.06056400	1.06415900	-2.04248800
C	3.92048800	1.71474400	-3.08058200
C	6.53572500	2.34960400	-2.30080300
C	4.45316600	2.98384000	-3.30676200
C	5.74876200	3.32241000	-2.91726900

H	7.54596700	2.60017400	-1.98751100
H	3.83946400	3.72412100	-3.81485600
C	6.26314200	4.72422800	-3.10952400
H	7.34714600	4.73696400	-3.24056800
H	5.80023800	5.20148100	-3.97645200
H	6.02763400	5.33330400	-2.22924900
C	2.51731300	1.38696800	-3.52889100
H	2.46495000	0.40931500	-4.01741200
H	1.80577500	1.36458900	-2.69397300
H	2.17309100	2.13986400	-4.24142400
C	6.92694600	0.05311000	-1.34116900
H	6.36041400	-0.53993100	-0.62044000
H	7.36632300	-0.64639800	-2.05862200
H	7.74000900	0.56332400	-0.82070000
H	2.41522900	-0.18970900	-1.12629600
B	5.62639800	-2.78934700	0.71008100
F	4.81392300	-1.70427500	0.28921700
F	6.92366300	-2.31737900	0.92398100
F	5.63795800	-3.75007800	-0.31189400
F	5.09733800	-3.33236400	1.87747900
N	3.64191900	1.08211300	2.37384500
C	2.55506500	1.83716300	2.98805300
C	2.90555000	3.14222000	3.71656800
H	2.06142800	1.17215500	3.71189200
H	1.81508100	2.03998100	2.20744500
H	1.98775500	3.58004600	4.12496800
H	3.58321200	2.96198800	4.55637700
H	3.36894700	3.88139700	3.05798000
C	4.78013200	0.90608400	3.26355800
C	5.71658100	-0.21251300	2.83357400
H	4.36817100	0.65666500	4.25123500
H	5.35312100	1.84191500	3.40090100
H	6.52385100	-0.32005600	3.56510800
H	5.17674200	-1.15898200	2.76202700
H	6.17650300	-0.02410900	1.86054800
C	3.96532100	1.43812500	0.99742400
C	4.67296400	2.77550800	0.75204900
H	3.01716800	1.44764200	0.44404000
H	4.56556400	0.62091000	0.57745300
H	4.82247800	2.91872800	-0.32267400
H	4.07397100	3.61718500	1.11057400
H	5.65464100	2.80903300	1.23783900
C	-0.98282200	-0.17076700	1.40076300
C	-0.29967100	0.19879200	0.22501900

H	-1.16723800	-1.24210000	1.50438100
C	-0.26435600	-0.75304100	-0.84165600
H	-0.71366500	-1.73742900	-0.58494700
O	0.19859600	-0.56956400	-1.97764000
C	-0.85599300	0.56276600	2.67380000
C	-0.57726400	-0.17310800	3.82952700
C	-0.99919600	1.95528700	2.77107100
C	-0.39329700	0.46964400	5.05170500
H	-0.45531400	-1.25032700	3.75978500
C	-0.83723700	2.59214700	3.99439000
H	-1.24631600	2.53781800	1.88837600
C	-0.52404400	1.85172600	5.13735700
H	-0.14732800	-0.11455100	5.93261700
H	-0.95748500	3.66917400	4.06057600
H	-0.38814100	2.35485200	6.08921100
C	0.29225600	1.47422700	0.01916700
C	0.77436500	2.58092500	-0.13481000
C	1.41530400	3.85576700	-0.17730000
C	2.05272700	4.31663600	-1.33793600
C	1.47078800	4.65359500	0.97813400
C	2.75404200	5.51057900	-1.33912000
H	2.00500400	3.71706000	-2.24065600
C	2.16536200	5.85174600	0.97923300
H	0.98226500	4.30683100	1.88507200
C	2.83323800	6.29483800	-0.17605900
H	3.25156400	5.84728500	-2.24499100
H	2.20888900	6.45146100	1.88387900
C	-3.70291700	4.10431000	-1.12396100
C	-3.93978100	2.74500000	-0.90557100
C	-5.16862700	2.27534000	-0.46509900
C	-6.15963600	3.22354900	-0.21998100
C	-5.94489800	4.58490300	-0.41127600
C	-4.70545700	5.03048300	-0.87247300
C	-2.29861100	4.31854900	-1.64443500
C	-1.91837200	2.93082400	-2.16356300
C	-2.65941000	1.98834300	-1.18702500
H	-5.36596800	1.21887100	-0.30361800
H	-6.74398000	5.28913900	-0.21115900
H	-4.54037600	6.08972000	-1.04066700
H	-2.23221800	5.06373900	-2.43962000
H	-0.84081700	2.73086500	-2.18117200
H	-2.06225800	1.87355900	-0.28098000
H	-1.61267300	4.60953200	-0.83941600
Br	-7.85188800	2.63480000	0.39881100

O	-2.47335600	2.79781900	-3.46342700
C	-2.18928900	1.54229000	-4.03123600
H	-2.68744800	1.48093400	-4.99893200
H	-1.10741500	1.40367300	-4.17256200
N	-2.82839400	0.66171900	-1.78568300
C	-3.16615400	-0.52673000	-1.23171200
C	-2.68421800	0.45244300	-3.13011900
N	-2.95940900	-0.77988800	-3.44401700
N	-3.25432700	-1.37565900	-2.26143000
C	-3.69863300	-2.74574300	-2.26696200
C	-2.82169800	-3.71536400	-2.75077600
C	-4.99787200	-3.02874400	-1.82645300
C	-3.27942900	-5.03453500	-2.76538800
C	-5.40097700	-4.35934800	-1.86877100
C	-4.55658700	-5.37497100	-2.32656200
H	-2.61349700	-5.81258400	-3.13007600
H	-6.40402900	-4.61050100	-1.53277000
C	-5.02114800	-6.80784400	-2.32456700
H	-4.37041400	-7.43647900	-2.93533700
H	-5.02011500	-7.21038500	-1.30683000
H	-6.04149200	-6.88999600	-2.70744500
C	-5.92803600	-1.96506800	-1.30428300
H	-5.69953600	-1.72731100	-0.25774900
H	-5.86629900	-1.04299900	-1.89119300
H	-6.95980100	-2.31870500	-1.34056600
C	-1.44188000	-3.38449000	-3.25883000
H	-1.47088100	-3.16931300	-4.33153700
H	-1.00760400	-2.50560500	-2.77438900
H	-0.77860500	-4.24017500	-3.10973400
C	-3.70567500	-0.51077600	2.59024200
C	-3.24231600	-0.02222200	1.23661300
H	-3.63908700	0.30688200	3.31469400
C	-3.24304800	-0.97724400	0.21002200
O	-3.15441800	-2.20749400	0.37518800
C	-5.12731400	-1.02754800	2.47935400
C	-5.39016500	-2.39876900	2.50888000
C	-6.18879600	-0.14593900	2.24116500
C	-6.68341800	-2.88169600	2.31227900
H	-4.56771300	-3.08946900	2.66707300
C	-7.48026800	-0.62543000	2.04101100
H	-6.00198900	0.92636400	2.19983300
C	-7.73213800	-1.99690100	2.07709500
H	-6.86761000	-3.95143800	2.33501400
H	-8.28829000	0.07370500	1.85118600

H	-8.73876900	-2.37082100	1.91935100
H	-3.42233500	1.02134000	1.01093900
H	-3.05560400	-1.31819400	2.94723300
N	3.50016600	7.50866900	-0.18660600
H	4.22255700	7.59926300	-0.88761300
H	3.80315600	7.84437800	0.71711300

R2NO

C	3.52529700	1.16513300	-0.00548500
C	2.34489900	1.83410200	-0.01084100
H	4.41058700	1.80101900	-0.02446700
C	2.41849100	3.31940900	-0.03030500
H	3.45028300	3.72160100	-0.03861800
O	1.45528800	4.05058500	-0.03654000
C	3.82068400	-0.26183100	0.01591200
C	5.17186300	-0.63935900	-0.06846500
C	2.84503700	-1.26818900	0.12036100
C	5.54119800	-1.97793100	-0.05868400
H	5.93312100	0.13196200	-0.14450300
C	3.21818600	-2.60561100	0.13277600
H	1.79896700	-1.00106200	0.19768700
C	4.56296700	-2.96530000	0.04149200
H	6.58868300	-2.25100700	-0.12697500
H	2.45640300	-3.37358600	0.21587800
H	4.84654900	-4.01257300	0.05113100
C	1.03350500	1.27888600	-0.00806900
C	-0.12041400	0.90698800	-0.01136000
C	-1.47873200	0.46320300	-0.01209200
C	-1.77922200	-0.90499600	-0.11348200
C	-2.51735600	1.40348800	0.08988900
C	-3.09811100	-1.33119700	-0.11205500
H	-0.97451100	-1.62662900	-0.19494100
C	-3.83885800	0.98545500	0.09234400
H	-2.27572900	2.45711900	0.16663600
C	-4.10181800	-0.37552100	-0.00846300
H	-3.35581700	-2.37956600	-0.18908100
H	-4.65660200	1.69026900	0.17022200
N	-5.49890100	-0.82342000	-0.00566800
O	-6.36869800	0.02476600	0.09022500
O	-5.71350600	-2.01959900	-0.09920100

TS4CNO-RS

C	3.82805900	1.23834100	3.31557700
C	3.46354500	0.59574500	2.12888000

C	3.79020200	1.11260700	0.88621700
C	4.51002800	2.30413700	0.87111200
C	4.87613300	2.97330700	2.03287700
C	4.53011600	2.43416500	3.27311000
C	3.35947400	0.44467700	4.51522700
C	3.11124700	-0.94409300	3.92058200
C	2.65728500	-0.63387800	2.47668100
H	3.54017800	0.61487700	-0.04608500
H	5.43603900	3.89915700	1.96818300
H	4.82426600	2.94184000	4.18625600
H	4.09309700	0.39293300	5.32245000
H	2.37346100	-1.55010800	4.46306900
H	1.57793700	-0.44291900	2.43692200
H	2.42729800	0.85217300	4.92374000
Br	4.99768200	3.04019900	-0.80449100
O	4.37010700	-1.59650500	3.88840700
C	4.34579700	-2.89413800	3.34267900
H	5.37909500	-3.20144600	3.18738900
H	3.84489000	-3.60019700	4.01965200
N	2.87822200	-1.82064000	1.65451400
C	2.28763000	-2.14840900	0.50836200
C	3.62668900	-2.89967300	2.02933100
N	3.50248900	-3.87813400	1.17447800
N	2.66150700	-3.38239300	0.22284600
C	2.05820400	-4.20051900	-0.79944500
C	2.56906700	-4.19267300	-2.09698000
C	0.92668700	-4.94255800	-0.42313600
C	1.83291600	-4.87827900	-3.06948400
C	0.23059500	-5.59940700	-1.43280900
C	0.65492000	-5.55466000	-2.76546800
H	2.19868400	-4.87143000	-4.09353500
H	-0.66399300	-6.16127100	-1.17639100
C	-0.15263300	-6.22518700	-3.84543800
H	-0.59670200	-7.15646100	-3.48508500
H	-0.97665800	-5.57742400	-4.16354500
H	0.46214700	-6.44477000	-4.72070500
C	0.53012000	-5.10944600	1.02207900
H	1.15985900	-5.87565700	1.48591500
H	0.64141000	-4.19470400	1.60967600
H	-0.50894200	-5.43971500	1.09218900
C	3.87792900	-3.54622200	-2.46218200
H	4.23201300	-2.83326900	-1.71763200
H	4.64148200	-4.32382900	-2.56942500
H	3.79095100	-3.04067700	-3.42741700

H	1.60996700	-1.53730800	-0.07169600
B	5.98429400	-1.24424200	0.09901300
F	4.64815400	-1.33504900	-0.38325600
F	6.77697800	-2.12075100	-0.63567900
F	5.97758000	-1.60785400	1.45375700
F	6.42684400	0.06908800	-0.05003400
N	2.73947800	1.11149900	-2.73943200
C	1.69447100	1.97948000	-3.27526200
C	2.14619500	3.42687700	-3.45325800
H	0.85496300	1.93788300	-2.57008600
H	1.30166300	1.61137000	-4.24151000
H	1.27655200	4.08323600	-3.55553600
H	2.73732100	3.75467700	-2.59333100
H	2.75726100	3.55537100	-4.35017400
C	3.93983700	1.13316800	-3.57518500
C	5.03972100	0.20388100	-3.08405000
H	4.32644000	2.15734200	-3.55952700
H	3.69487900	0.90708800	-4.63099700
H	5.94526500	0.37411900	-3.67354100
H	5.26750300	0.39097400	-2.03246800
H	4.76978900	-0.85114600	-3.18646700
C	2.22335800	-0.23647500	-2.48617300
C	1.79841800	-1.04884200	-3.71246100
H	1.35090200	-0.11627500	-1.82968700
H	2.98800500	-0.78502700	-1.92271900
H	1.43853000	-2.03324200	-3.39555900
H	0.98178400	-0.56450100	-4.25481900
H	2.63354800	-1.19956900	-4.40539700
C	-1.69242400	-1.60967200	-1.14485400
C	-0.90861400	-1.19837100	-0.06009400
H	-1.93648800	-2.67035900	-1.10749400
C	-0.74466400	-2.12682200	1.03201400
H	-1.23074700	-3.10401800	0.86335600
O	-0.06814900	-1.93031100	2.04462300
C	-1.63793600	-1.06861700	-2.52087200
C	-1.69235400	-1.98013500	-3.58517500
C	-1.54159600	0.29654000	-2.81671600
C	-1.68418800	-1.53778700	-4.90470500
H	-1.73561500	-3.04356800	-3.36813400
C	-1.54577900	0.74094800	-4.13455100
H	-1.45814000	1.01826500	-2.01516500
C	-1.62556500	-0.17356700	-5.18424100
H	-1.72506200	-2.26055200	-5.71353200
H	-1.48162000	1.80801300	-4.32657100

H	-1.63179900	0.17443000	-6.21207900
C	-0.40932900	0.12274800	0.09603900
C	-0.00249800	1.25761400	0.26592800
C	0.35292700	2.63008900	0.46291500
C	-0.51304900	3.47455000	1.17797700
C	1.52075600	3.14721000	-0.11457800
C	-0.22633800	4.82422700	1.30314500
H	-1.42217200	3.06963000	1.61008100
C	1.82719700	4.49355300	0.02550000
H	2.17525600	2.49506100	-0.68848100
C	0.94045300	5.30592300	0.72051400
H	-0.88493600	5.49931100	1.83401200
H	2.74264100	4.90287200	-0.38579500
C	-5.75061100	3.25184200	-1.47421800
C	-4.83108600	2.39474000	-0.86247200
C	-3.46537700	2.52692900	-1.05632200
C	-3.04421900	3.52693800	-1.93584600
C	-3.94307600	4.35740800	-2.59610500
C	-5.31159600	4.22610800	-2.35682700
C	-7.14551900	2.97869800	-0.95822000
C	-6.85403600	2.25992700	0.36142100
C	-5.59779700	1.42763200	0.01755000
H	-2.74623000	1.89746200	-0.53551300
H	-3.57292500	5.12068300	-3.27057300
H	-6.01260700	4.90054700	-2.83757000
H	-7.73083100	3.88409300	-0.78757200
H	-7.67803300	1.64727300	0.74617800
H	-5.88008600	0.52024700	-0.52538000
H	-7.70783700	2.32154700	-1.63008700
Br	-1.18889800	3.78299200	-2.23151900
O	-6.49122700	3.26947400	1.29133300
C	-6.12145000	2.77610700	2.55463400
H	-5.69435000	3.60198800	3.12479300
H	-6.99098500	2.38477200	3.10067400
N	-4.91759700	1.01067800	1.24531000
C	-4.11798900	-0.05797900	1.49928200
C	-5.12298000	1.66199600	2.42955600
N	-4.48039600	1.07718900	3.39724300
N	-3.86816600	0.01225000	2.81487100
C	-3.10764000	-0.85035400	3.69666000
C	-3.75321800	-1.94992300	4.27121300
C	-1.82227600	-0.44751200	4.04438100
C	-3.01934300	-2.70811300	5.17696500
C	-1.13249100	-1.23816700	4.96387900

C	-1.70426700	-2.37685100	5.52283900
H	-3.48841300	-3.57659700	5.63265500
H	-0.12200400	-0.94915700	5.24212300
C	-0.92439100	-3.24663400	6.47369100
H	-0.54343500	-4.13231700	5.95533900
H	-0.06917300	-2.71035300	6.89028700
H	-1.55206700	-3.59382600	7.29806700
C	-1.22160400	0.80440100	3.47358700
H	-1.30917400	0.81470600	2.38536600
H	-1.72608700	1.69261000	3.86976500
H	-0.16023200	0.87402700	3.72185200
C	-5.17970800	-2.28400600	3.93345100
H	-5.82736800	-1.40931000	4.05267800
H	-5.24904900	-2.62004100	2.89593100
H	-5.55206900	-3.07441600	4.58671900
C	-4.51646900	-2.18281500	-1.71061000
C	-3.85786000	-1.17216800	-0.76942600
H	-4.43840900	-1.74672900	-2.71186100
C	-3.83474800	-1.28233000	0.63335700
O	-3.54830100	-2.28463000	1.31140900
C	-4.09025100	-3.64093300	-1.83470400
C	-4.08410700	-4.20707900	-3.11639500
C	-3.79142300	-4.47176000	-0.74906400
C	-3.77702400	-5.55040300	-3.31585600
H	-4.31206100	-3.57847100	-3.97410300
C	-3.47817600	-5.81633500	-0.94676800
H	-3.78939800	-4.05524200	0.25118100
C	-3.46730500	-6.36324600	-2.22741000
H	-3.77510200	-5.95971300	-4.32160300
H	-3.24367000	-6.43986600	-0.08852500
H	-3.22260800	-7.41042600	-2.37654900
H	-3.95254200	-0.15894200	-1.15275600
H	-5.59284200	-2.18870200	-1.48297800
N	1.25067700	6.73278100	0.85321000
O	0.45637400	7.43617100	1.45490900
O	2.28483600	7.14106800	0.35419100

TS4CNO-SS

C	-6.63424800	-1.35999300	1.89365400
C	-5.55849000	-0.76150700	1.22636800
C	-5.10419000	-1.24510000	0.00689200
C	-5.78993700	-2.33354500	-0.52858100
C	-6.88608600	-2.91838700	0.09573100
C	-7.31557900	-2.42596200	1.32619600

C	-6.86743100	-0.70730800	3.23242300
C	-6.20791600	0.65516100	3.04086300
C	-5.00536100	0.34407900	2.11172500
H	-4.26028100	-0.82185600	-0.53116200
H	-7.38329100	-3.76330700	-0.36670800
H	-8.15427800	-2.88750900	1.83841100
H	-7.92069000	-0.59402700	3.49584400
H	-5.90015700	1.15607400	3.96741300
H	-4.15321300	-0.01916000	2.69699800
H	-6.36910400	-1.27351200	4.02860200
Br	-5.15335200	-3.12938500	-2.12487300
O	-7.15514600	1.43741900	2.33415800
C	-6.71932100	2.74069800	2.03742300
H	-7.44079900	3.18627400	1.35568600
H	-6.63638700	3.34793600	2.95019100
N	-4.58175700	1.59060200	1.46321300
C	-3.41678800	1.90875400	0.88240200
C	-5.38035400	2.69844100	1.37316600
N	-4.75791800	3.67620500	0.78267200
N	-3.53449500	3.16407100	0.47914600
C	-2.54039600	4.04343100	-0.08490800
C	-2.67224700	4.42541500	-1.42198300
C	-1.57338900	4.56843900	0.77679500
C	-1.76041900	5.36610400	-1.90219600
C	-0.70101900	5.51826200	0.24905900
C	-0.78333400	5.93292900	-1.08253300
H	-1.84103300	5.68623500	-2.93809100
H	0.03882200	5.96406500	0.90880800
C	0.14773400	6.98719700	-1.62671400
H	0.56538000	7.59933200	-0.82309400
H	0.98328400	6.53589000	-2.17334000
H	-0.37551500	7.64725700	-2.32235200
C	-1.48845400	4.14751000	2.21828900
H	-2.47080800	4.17411100	2.70030500
H	-1.09407200	3.12960300	2.28466000
H	-0.81941500	4.81163000	2.76786800
C	-3.77227200	3.89132200	-2.29617500
H	-4.04085000	2.86312900	-2.05177200
H	-4.68517300	4.48170500	-2.16687500
H	-3.48115300	3.94807700	-3.34746200
H	-2.51361200	1.30776300	0.80162800
B	-6.54724000	1.57597500	-1.65698500
F	-5.24703300	1.37435700	-1.12488100
F	-6.44156400	2.34609700	-2.81633200

F	-7.30866400	2.25745500	-0.69464600
F	-7.12136500	0.33955500	-1.93628500
N	-2.52685800	-0.94558700	-2.61992900
C	-1.31609900	-1.75325000	-2.70849600
C	-1.56262100	-3.19410400	-3.14237300
H	-0.86722500	-1.76472600	-1.71155300
H	-0.56415900	-1.30282600	-3.38713500
H	-0.66233900	-3.78799300	-2.95809000
H	-2.39390500	-3.61819200	-2.57255400
H	-1.80563200	-3.27597200	-4.20545800
C	-3.19170100	-0.81514900	-3.91237800
C	-4.45060600	0.03928700	-3.86689500
H	-3.47552600	-1.82336600	-4.23410200
H	-2.49756400	-0.42503300	-4.68379900
H	-4.95914700	-0.01215100	-4.83426700
H	-5.14011500	-0.31627900	-3.09680300
H	-4.24375100	1.09251800	-3.65950300
C	-2.26945100	0.32987700	-1.95212800
C	-1.34564800	1.31708800	-2.67348800
H	-1.83284200	0.08739000	-0.97637800
H	-3.23504500	0.80822500	-1.75996700
H	-1.22448100	2.21767900	-2.06240700
H	-0.34935300	0.89092200	-2.83731300
H	-1.75616600	1.61713100	-3.64377100
C	1.74056500	-0.87191200	-0.79016000
C	0.69152600	-0.34924200	-0.01819100
H	2.18142300	-0.13929900	-1.46641500
C	0.47300100	1.07957800	0.02261300
H	1.20378400	1.68150200	-0.54820200
O	-0.47388900	1.63033800	0.58487100
C	1.78672500	-2.24797500	-1.34451600
C	2.15829900	-2.40852800	-2.68757000
C	1.47385200	-3.39155100	-0.59667900
C	2.24227300	-3.67308800	-3.26413300
H	2.36518200	-1.52595700	-3.29079100
C	1.55840300	-4.65513500	-1.17383200
H	1.17129400	-3.29069900	0.43923100
C	1.95036800	-4.80326400	-2.50397500
H	2.52820600	-3.77235200	-4.30641200
H	1.32086100	-5.53037900	-0.57804200
H	2.01791300	-5.79155700	-2.94618700
C	-0.26247100	-1.15636000	0.65325800
C	-1.15104700	-1.80654400	1.16874600
C	-2.25421100	-2.58203800	1.62976700

C	-2.80166500	-2.36688000	2.90719800
C	-2.83420100	-3.53123500	0.77125500
C	-3.94452500	-3.04411900	3.29824000
H	-2.32844100	-1.65681500	3.57664300
C	-3.96834900	-4.22598300	1.16153800
H	-2.40515100	-3.68752300	-0.21351200
C	-4.51551000	-3.94946400	2.40889700
H	-4.39720800	-2.88291200	4.26890500
H	-4.46100400	-4.92031300	0.49140800
C	6.99297100	-2.61791400	-2.22848000
C	6.40866100	-1.72257100	-1.32992600
C	6.82757700	-1.62791600	-0.01067900
C	7.84832300	-2.48735000	0.39198800
C	8.43024700	-3.40532500	-0.47705300
C	8.00178200	-3.46990400	-1.80273000
C	6.38530400	-2.45848900	-3.60340300
C	5.76794400	-1.06018500	-3.52893200
C	5.31439800	-0.96534300	-2.05404000
H	6.38934200	-0.92311100	0.69118000
H	9.22233500	-4.05402100	-0.12180800
H	8.46834200	-4.16875100	-2.48921500
H	7.11129200	-2.51858800	-4.41638200
H	4.94142700	-0.89046500	-4.23108600
H	4.34587200	-1.46180200	-1.94526300
H	5.60182000	-3.20403000	-3.77978800
Br	8.47385800	-2.39862300	2.17847100
O	6.81639600	-0.13362900	-3.75807900
C	6.39098500	1.20556900	-3.68964000
H	7.26984400	1.84536100	-3.77354700
H	5.69821700	1.44600200	-4.50825200
N	5.15065100	0.43746500	-1.66036500
C	4.49908300	0.99347700	-0.60871700
C	5.69473800	1.46306400	-2.38651200
N	5.43349900	2.61299700	-1.83829200
N	4.69431300	2.30724500	-0.73900000
C	4.23486900	3.39308200	0.09014200
C	3.25908700	4.23150400	-0.43970400
C	4.81643600	3.57373900	1.34921300
C	2.87593600	5.32386800	0.33951200
C	4.38834800	4.67226000	2.08702200
C	3.42192900	5.55799200	1.59822400
H	2.12728800	6.00323000	-0.05651700
H	4.81716700	4.84030700	3.07174800
C	2.95501300	6.72033600	2.43503300

H	2.27234500	6.37736600	3.21930400
H	3.79508100	7.21718800	2.92649200
H	2.42439000	7.45730800	1.82737800
C	5.81681500	2.59581600	1.90486000
H	5.30269400	1.69277400	2.25745400
H	6.55688300	2.29835500	1.15542800
H	6.34757300	3.03312300	2.75191500
C	2.61636800	3.99087700	-1.78158700
H	2.66626900	2.94100100	-2.08282900
H	1.56100700	4.27557900	-1.74027300
H	3.10237800	4.58171200	-2.56426100
C	2.94441900	-1.53701100	1.85909400
C	3.48629000	-1.00461200	0.55246300
H	2.93721500	-2.63066400	1.82744500
C	3.64509300	0.38986600	0.48266200
O	3.00439300	1.19962900	1.17341200
C	3.78195800	-1.05729200	3.03014900
C	5.06272100	-1.57218800	3.25448400
C	3.31039000	-0.04426700	3.86858400
C	5.85157500	-1.08730700	4.29538600
H	5.44981400	-2.35837900	2.60774800
C	4.09539000	0.44027400	4.91253800
H	2.32797000	0.37737500	3.68017000
C	5.36936000	-0.07980100	5.12888700
H	6.84403200	-1.49681400	4.45199200
H	3.71338000	1.22983800	5.55235500
H	5.98399800	0.29756800	5.93996200
H	4.16050700	-1.65786600	0.01455800
H	1.91345200	-1.19336800	1.99973400
N	-5.77100700	-4.59464900	2.78524700
O	-6.33140400	-4.20385100	3.79765700
O	-6.20742500	-5.47032700	2.05849700

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C	-0.28243800	-4.54642400	0.82768800
C	-0.87104600	-3.28828700	0.69735300
C	-0.79437500	-2.56881700	-0.49018000
C	-0.09460400	-3.15336500	-1.54109900
C	0.47929500	-4.42009800	-1.44218900
C	0.38772500	-5.12307000	-0.24464500
C	-0.46860700	-5.10048000	2.21817100
C	-1.52804600	-4.18538100	2.84303100
C	-1.42465400	-2.86079900	2.03789200
H	-1.25831900	-1.59686600	-0.63879800

H	0.99260600	-4.84738200	-2.29733900
H	0.83117900	-6.10976700	-0.15759200
H	-0.82571800	-6.13307500	2.22861400
H	-1.37503600	-4.01123000	3.91665700
H	-0.73205700	-2.15738800	2.51122000
H	0.46609500	-5.06891600	2.78834100
Br	0.12316400	-2.17775000	-3.14269600
O	-2.78484800	-4.80087800	2.63610200
C	-3.84310700	-4.06107200	3.20041800
H	-4.77185800	-4.58086100	2.98044300
H	-3.71155700	-3.95196000	4.28654700
N	-2.72813700	-2.19284600	2.01588800
C	-3.05697900	-1.00768400	1.49555400
C	-3.87318300	-2.71332900	2.55508500
N	-4.86807000	-1.88375400	2.43220400
N	-4.33853500	-0.82550700	1.76058300
C	-5.12143700	0.34976600	1.50398200
C	-6.30333400	0.20655700	0.76721000
C	-4.69466100	1.56321700	2.05427100
C	-7.07189300	1.35386700	0.58115900
C	-5.51407800	2.67291300	1.84503700
C	-6.69642600	2.59007400	1.11225400
H	-7.98908800	1.27693900	0.00190600
H	-5.22063400	3.62453800	2.27845200
C	-7.55766300	3.80612200	0.89336600
H	-8.58374800	3.62382100	1.22426500
H	-7.17145300	4.66881100	1.44276300
H	-7.60161900	4.06670300	-0.16938200
C	-3.42673200	1.68960000	2.86133800
H	-3.34320400	0.88902900	3.60343300
H	-2.52736600	1.64693000	2.23517100
H	-3.41973300	2.64453700	3.38976200
C	-6.72062700	-1.11649200	0.18352700
H	-5.87447300	-1.66630700	-0.23566900
H	-7.16223400	-1.75912700	0.95113500
H	-7.46267700	-0.96005800	-0.60188300
H	-2.38956400	-0.30442800	1.01473700
B	-4.73100200	-4.14617400	-0.44144200
F	-3.99024200	-2.95647800	-0.23051400
F	-5.84174700	-3.84145000	-1.23786200
F	-5.16904700	-4.62582100	0.80217300
F	-3.92197100	-5.08753800	-1.06621400
N	-2.76270600	-0.49710200	-2.94901900
C	-2.01451300	0.62782700	-3.49156500

C	-2.64886300	1.46946400	-4.60903400
H	-1.06364900	0.22964800	-3.87222500
H	-1.74551100	1.27634600	-2.65057300
H	-1.89659100	2.15492900	-5.01140600
H	-2.99894800	0.84072200	-5.43307600
H	-3.49327300	2.07297800	-4.26535800
C	-3.15948700	-1.46370000	-3.96359100
C	-3.52088600	-2.81764900	-3.37089100
H	-2.30111300	-1.58416800	-4.63615700
H	-3.99425700	-1.09877200	-4.58893700
H	-3.70906100	-3.53793300	-4.17295600
H	-2.70090400	-3.19050800	-2.75196100
H	-4.41288600	-2.77763400	-2.74186800
C	-3.80310400	-0.16462500	-1.98066100
C	-5.14728200	0.31616300	-2.54577200
H	-3.38406100	0.60083400	-1.31175800
H	-3.98265100	-1.05158700	-1.36100800
H	-5.78390800	0.68524900	-1.73722500
H	-5.02689800	1.12524500	-3.27087200
H	-5.67798600	-0.50164400	-3.04383300
C	1.46190900	0.70267400	-1.08987100
C	0.40986600	0.85922600	-0.16243100
H	1.98834100	-0.24593200	-0.98022700
C	0.41640900	0.01983900	1.00871700
H	1.28300400	-0.66866200	1.06780500
O	-0.45988200	-0.02757500	1.87688700
C	1.46595900	1.17040400	-2.49777400
C	2.21369100	0.43667600	-3.43070500
C	0.76779900	2.29961800	-2.94821900
C	2.24741000	0.80210700	-4.77138000
H	2.74535700	-0.45248800	-3.10365300
C	0.81399000	2.67415300	-4.28825100
H	0.18454600	2.88959400	-2.25131500
C	1.54526000	1.92471100	-5.20672900
H	2.82000300	0.20770700	-5.47599800
H	0.27038600	3.55531700	-4.61444500
H	1.57082900	2.21464900	-6.25208600
C	-0.64444700	1.80872800	-0.22981600
C	-1.59181000	2.57380100	-0.21559300
C	-2.67913000	3.50259600	-0.24875900
C	-3.63567200	3.43623800	-1.27735500
C	-2.79086400	4.49865500	0.73693500
C	-4.68591000	4.33913100	-1.32240300
H	-3.54586700	2.67038000	-2.03955700

C	-3.83379600	5.41150700	0.69716000
H	-2.04729600	4.55146300	1.52428800
C	-4.76435800	5.31139600	-0.33142800
H	-5.43327300	4.29942100	-2.10534600
H	-3.93591200	6.18920200	1.44373000
C	7.14006100	-0.23464400	-1.76974400
C	6.00098400	-0.01585200	-0.99897600
C	4.89041700	-0.83142600	-1.08327500
C	4.92162600	-1.87857700	-1.99469900
C	6.02339100	-2.09717800	-2.81554700
C	7.14552000	-1.26932800	-2.69802200
C	8.23131900	0.72132000	-1.33578600
C	7.79279100	1.09522700	0.09009400
C	6.24569400	1.10536500	-0.01704900
H	4.02259100	-0.69283300	-0.44820000
H	6.02092100	-2.92090800	-3.51998200
H	8.02070000	-1.46436900	-3.30915000
H	9.22744900	0.27519400	-1.32265300
H	8.19437200	2.04856100	0.45244500
H	5.88664600	2.08077900	-0.36226300
H	8.25977900	1.61474000	-1.96834100
Br	3.39122000	-2.99070000	-2.04041300
O	8.21389700	0.02599700	0.92283600
C	7.78174500	0.14939100	2.25879200
H	8.13206000	-0.72223300	2.81105400
H	8.18643600	1.05733200	2.72691400
N	5.60562800	0.80158500	1.26556700
C	4.28563100	0.75141400	1.56949800
C	6.28548400	0.20494000	2.29121200
N	5.46679600	-0.21990500	3.20931500
N	4.23325900	0.12401400	2.74808900
C	3.06657400	-0.34441300	3.45310700
C	2.52694400	0.46252100	4.45525900
C	2.58151800	-1.61277900	3.12771400
C	1.40139900	-0.01919000	5.11672300
C	1.46943600	-2.05617700	3.84329500
C	0.85183400	-1.26590800	4.81287000
H	0.94354300	0.59364700	5.88825700
H	1.08413900	-3.05276000	3.63947300
C	-0.39780300	-1.74197300	5.50431700
H	-0.55623000	-1.21642900	6.44788200
H	-1.27520700	-1.55316300	4.87276800
H	-0.35493500	-2.81469400	5.71041900
C	3.21071400	-2.47505600	2.06042700

H	2.83945100	-2.23154600	1.05595400
H	4.29979400	-2.37860200	2.04579500
H	2.96756300	-3.52487800	2.23612900
C	3.14183100	1.79324200	4.78561100
H	4.19512200	1.68004900	5.06017500
H	3.08472700	2.45132400	3.91378700
H	2.61741600	2.26234500	5.61910000
C	2.60662000	3.32756700	-0.64195700
C	3.12352800	1.92112300	-0.39678200
H	1.59812800	3.42306700	-0.22496100
C	3.13821800	1.53860300	0.96274600
O	2.24761100	1.84917800	1.77192900
C	3.53797400	4.32758200	0.00870300
C	4.71338300	4.72115700	-0.64022800
C	3.28387300	4.81668200	1.29361700
C	5.61957300	5.57705500	-0.01877800
H	4.91341600	4.35401200	-1.64509200
C	4.18836300	5.67457900	1.91681700
H	2.37573800	4.50896400	1.80362200
C	5.35948300	6.05522000	1.26478500
H	6.52412000	5.87724800	-0.53878700
H	3.97608200	6.04857200	2.91373500
H	6.06183300	6.72516300	1.75009000
H	3.92646000	1.59553600	-1.05061100
H	2.55428900	3.51795600	-1.71565600
N	-5.87216100	6.26689300	-0.37123200
O	-5.98837600	7.04643400	0.56012300
O	-6.62825200	6.22768800	-1.32762400

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C	0.81360200	-4.75416000	0.48397900
C	1.37280200	-3.49795100	0.24134100
C	1.72100700	-2.63309500	1.27160000
C	1.49675500	-3.08430700	2.56975800
C	0.91090100	-4.31838500	2.83879600
C	0.56284400	-5.16340200	1.78625600
C	0.59230200	-5.50233900	-0.81110200
C	1.49802100	-4.76092300	-1.80113200
C	1.49712000	-3.31475700	-1.25513300
H	2.21494500	-1.67738400	1.11511000
H	0.75826600	-4.62648800	3.86667600
H	0.13049000	-6.13733100	1.99170500
H	0.86570600	-6.55834500	-0.75947300
H	1.14806400	-4.80188700	-2.84158600

H	0.65006000	-2.77120200	-1.67917400
H	-0.45374700	-5.43390200	-1.13354200
Br	2.07152700	-2.01768200	4.02541800
O	2.79312100	-5.31917800	-1.70088800
C	3.73674900	-4.70016900	-2.54567700
H	4.71147000	-5.12739900	-2.32044900
H	3.48653300	-4.86591300	-3.60325700
N	2.70033200	-2.61597000	-1.69373700
C	2.99443900	-1.31856200	-1.60446300
C	3.77495100	-3.22574800	-2.27670800
N	4.68920600	-2.35148800	-2.59196900
N	4.18392600	-1.16373600	-2.15855900
C	4.87469600	0.07764000	-2.37248400
C	6.18330800	0.21227600	-1.89305400
C	4.20432000	1.08903500	-3.07358500
C	6.81846400	1.43205500	-2.12697900
C	4.89265600	2.28532600	-3.27295100
C	6.18969700	2.48169100	-2.79691300
H	7.82861100	1.56944300	-1.75005500
H	4.40365700	3.08114000	-3.83119800
C	6.87074900	3.81452200	-2.95998800
H	7.95677300	3.70549300	-2.98826700
H	6.54653400	4.31646200	-3.87496200
H	6.62496800	4.47263500	-2.11811200
C	2.80642600	0.91762200	-3.61786600
H	2.67562700	-0.05668100	-4.09809100
H	2.03766700	0.99609100	-2.83870400
H	2.60479700	1.69004200	-4.36297300
C	6.88200800	-0.88491000	-1.13703100
H	6.20780800	-1.40362500	-0.45235400
H	7.28147400	-1.63516500	-1.82605000
H	7.71505900	-0.46762300	-0.56777400
H	2.37236900	-0.54038000	-1.18447600
B	5.08161400	-3.50200800	0.88504800
F	4.46275400	-2.31926300	0.39889200
F	6.43181000	-3.23511600	1.11719400
F	4.95547300	-4.49496300	-0.09719000
F	4.44742500	-3.90223000	2.05843500
N	3.58327500	0.57953800	2.40681700
C	2.56931800	1.46149700	2.97586800
C	3.04232300	2.71762200	3.72126700
H	1.96863300	0.86250800	3.67644400
H	1.89216200	1.74996800	2.16594200
H	2.16741200	3.27495600	4.07360300

H	3.64029600	2.45971200	4.60001300
H	3.63884500	3.38318500	3.09152800
C	4.65886500	0.28995600	3.34436800
C	5.49182900	-0.91935600	2.95248600
H	4.18078300	0.08565400	4.31260800
H	5.31664600	1.16335200	3.50765600
H	6.25684000	-1.10279700	3.71341700
H	4.85833300	-1.80320100	2.86651300
H	6.00292300	-0.78485200	1.99566500
C	4.00133300	0.88224600	1.04343200
C	4.90198000	2.10352200	0.82632600
H	3.08347200	1.02014800	0.45572600
H	4.49580600	-0.01179300	0.64303600
H	5.09556000	2.23319100	-0.24321800
H	4.43003600	3.02100900	1.18907000
H	5.86699500	1.98723200	1.33155900
C	-1.06011800	-0.09518700	1.38744700
C	-0.36193200	0.22677200	0.21022400
H	-1.34199500	-1.14621000	1.47917900
C	-0.38555300	-0.73253100	-0.85975100
H	-0.91923000	-1.67540800	-0.61276200
O	0.11854000	-0.58558500	-1.97916200
C	-0.91414100	0.62677600	2.65916500
C	-0.77202600	-0.13190500	3.82614000
C	-0.90686700	2.02745400	2.75092700
C	-0.56613000	0.49091400	5.05452300
H	-0.77094400	-1.21593100	3.76013100
C	-0.72626800	2.64640700	3.98030900
H	-1.05300400	2.63081000	1.86010300
C	-0.54315200	1.87947800	5.13424100
H	-0.42605700	-0.11280200	5.94519300
H	-0.72987300	3.73008100	4.04405500
H	-0.39016600	2.36817400	6.09087700
C	0.35314600	1.43065300	0.00528600
C	0.97633100	2.46175000	-0.16924300
C	1.84176700	3.59200300	-0.21363500
C	2.61876300	3.84849000	-1.35475000
C	1.97189900	4.41616200	0.91951300
C	3.54815700	4.87500000	-1.35279600
H	2.50002600	3.22085700	-2.22982200
C	2.89040200	5.45386400	0.92495000
H	1.36926200	4.21209500	1.79897300
C	3.67322800	5.65380700	-0.20816700
H	4.17391000	5.07532900	-2.21424000

H	3.02232700	6.08886200	1.79203200
C	-3.55164100	4.35859900	-1.10435900
C	-3.86444400	3.01261100	-0.90183500
C	-5.12256600	2.60652500	-0.48092300
C	-6.06284900	3.60505100	-0.23621400
C	-5.77132500	4.95449200	-0.41039000
C	-4.50453900	5.33603000	-0.85413900
C	-2.13330000	4.50076100	-1.61141100
C	-1.82724800	3.09915400	-2.14350800
C	-2.62492400	2.18875600	-1.18126200
H	-5.37989100	1.56083000	-0.33460800
H	-6.53265600	5.69967000	-0.21139100
H	-4.28018300	6.38610900	-1.01055800
H	-2.02015400	5.24851000	-2.39873600
H	-0.76244300	2.83793500	-2.16301600
H	-2.04613900	2.02680800	-0.26982700
H	-1.44130600	4.74771200	-0.79751800
Br	-7.79183800	3.10306000	0.35640900
O	-2.38679100	3.01632800	-3.44499400
C	-2.18695400	1.75401700	-4.03356400
H	-2.69329700	1.74098100	-4.99883700
H	-1.11718700	1.54964300	-4.18524500
N	-2.86584400	0.88172300	-1.79716100
C	-3.27721300	-0.29001400	-1.25745000
C	-2.74633700	0.68403200	-3.14641500
N	-3.10277700	-0.52287900	-3.47526100
N	-3.42767100	-1.11610600	-2.29808800
C	-3.95627800	-2.45588200	-2.31618300
C	-3.14634800	-3.46927400	-2.82684100
C	-5.26286000	-2.66734200	-1.85800400
C	-3.67934700	-4.75949200	-2.84761300
C	-5.74275300	-3.97223800	-1.90703500
C	-4.96651100	-5.03008700	-2.38889200
H	-3.06668200	-5.57027000	-3.23386300
H	-6.75325000	-4.16871800	-1.55727700
C	-5.51477100	-6.43296500	-2.39456400
H	-4.90132700	-7.09611800	-3.00737600
H	-5.54001300	-6.83943300	-1.37877300
H	-6.53738300	-6.45234600	-2.77982000
C	-6.12368600	-1.55674300	-1.31491900
H	-5.87266700	-1.34290500	-0.26846100
H	-6.01428800	-0.63398500	-1.89380300
H	-7.17472600	-1.84904100	-1.34387700
C	-1.76111300	-3.20935700	-3.35980800

H	-1.80196500	-2.94365400	-4.42059100
H	-1.25688200	-2.38384100	-2.84968800
H	-1.15299900	-4.11245300	-3.26662400
C	-3.85386600	-0.27966600	2.55786000
C	-3.37125700	0.19559400	1.20872500
H	-3.74463000	0.52510900	3.29149500
C	-3.38122700	-0.75117300	0.17918300
O	-3.33936600	-1.98730300	0.33251100
C	-5.30093900	-0.71897100	2.43889200
C	-5.63564600	-2.07457300	2.45021500
C	-6.31242900	0.22114500	2.20704100
C	-6.95217500	-2.48516900	2.24291500
H	-4.85110300	-2.80973200	2.60096400
C	-7.62645100	-0.18623900	1.99601800
H	-6.06817400	1.28222200	2.17812100
C	-7.95108900	-1.54280600	2.01489200
H	-7.19348200	-3.54368800	2.25156100
H	-8.39508200	0.55716400	1.81074000
H	-8.97545200	-1.86068400	1.84884200
H	-3.48798500	1.24909900	0.99055000
H	-3.24890500	-1.12548100	2.90463900
N	4.67581000	6.71943900	-0.19402000
O	4.71964100	7.44975700	0.78071100
O	5.41693700	6.81860200	-1.15891000

R2OMe

C	3.23775400	1.23560900	-0.00139900
C	2.03573800	1.86490300	0.00572700
H	4.10437500	1.89628600	0.02247300
C	2.06807500	3.35101500	0.02938000
H	3.08856500	3.78216600	0.03611000
O	1.08595400	4.05735400	0.04023300
C	3.57120700	-0.18412900	-0.02696400
C	4.92798000	-0.53159700	0.09046900
C	2.62404800	-1.21288200	-0.16878800
C	5.32925600	-1.86101700	0.08006700
H	5.66865500	0.25654500	0.19373900
C	3.02952700	-2.54140700	-0.18302000
H	1.57484400	-0.96892000	-0.27566800
C	4.37867500	-2.87110300	-0.05589400
H	6.38090400	-2.10946600	0.17531900
H	2.28826500	-3.32575800	-0.29578300
H	4.68753400	-3.91123600	-0.06632000
C	0.74373300	1.26663600	0.00684100

C	-0.39138300	0.83789900	0.01763200
C	-1.71509100	0.30022900	0.02864500
C	-1.92548500	-1.08092300	0.19685300
C	-2.82556100	1.13724600	-0.12865400
C	-3.20582200	-1.59943500	0.20469400
H	-1.07223500	-1.73922600	0.32464500
C	-4.11781000	0.62333400	-0.12240500
H	-2.67172700	2.20327100	-0.25775100
C	-4.31121300	-0.75131900	0.04468700
H	-3.38346600	-2.66131200	0.33398600
H	-4.95698000	1.29595800	-0.24727100
O	-5.52218900	-1.35460400	0.06651000
C	-6.66934000	-0.53586200	-0.08779300
H	-6.66056800	-0.02227700	-1.05491100
H	-7.52659300	-1.20518900	-0.03965300
H	-6.73742000	0.20399600	0.71668100

TS4COMe-RS

C	-3.74762600	-1.14092300	3.36737400
C	-3.42347000	-0.53292300	2.15113800
C	-3.81526400	-1.07111600	0.93704300
C	-4.55537100	-2.24917500	0.98250900
C	-4.88591700	-2.88189100	2.17461400
C	-4.47660300	-2.32085500	3.38524600
C	-3.20352600	-0.33612100	4.52656600
C	-2.94434400	1.03189100	3.89028300
C	-2.56783400	0.68004300	2.43405700
H	-3.59035500	-0.60470600	-0.01750000
H	-5.46415900	-3.79868500	2.15621200
H	-4.73974500	-2.80061700	4.32264100
H	-3.89822300	-0.24532600	5.36431600
H	-2.16513000	1.62837000	4.38341300
H	-1.49739100	0.45498900	2.34857100
H	-2.26737900	-0.76451100	4.90270900
Br	-5.11096600	-3.02944600	-0.65108600
O	-4.18680600	1.71655000	3.90382900
C	-4.16007100	3.00017200	3.32664200
H	-5.19312100	3.32336400	3.20468200
H	-3.62096600	3.71241200	3.96684500
N	-2.79032900	1.85838500	1.60009400
C	-2.22379500	2.15774700	0.43418200
C	-3.49097000	2.96434500	1.98774400
N	-3.36524500	3.92989700	1.11891200
N	-2.56946700	3.39974000	0.14654500

C	-1.97499000	4.19618300	-0.89807300
C	-2.48824100	4.15078200	-2.19365900
C	-0.85040500	4.96073900	-0.54384000
C	-1.76324200	4.82113400	-3.18558500
C	-0.16985300	5.60589100	-1.57078800
C	-0.59688000	5.52421600	-2.90116800
H	-2.13203100	4.78446000	-4.20786800
H	0.71679100	6.18727800	-1.33060000
C	0.19656300	6.18784600	-3.99546500
H	0.53851200	7.17924300	-3.68661600
H	1.08869400	5.59770100	-4.23042900
H	-0.39481800	6.29099200	-4.90736900
C	-0.44046700	5.15441400	0.89407200
H	-1.08575500	5.90584200	1.36057800
H	-0.51595800	4.24122400	1.48975100
H	0.58953500	5.51485500	0.94545800
C	-3.79116400	3.48308800	-2.54191500
H	-4.16163300	2.82287500	-1.75808500
H	-4.54935000	4.25349700	-2.71694000
H	-3.68751600	2.91317600	-3.46882300
H	-1.57608400	1.52203700	-0.15412900
B	-5.95499300	1.32081600	0.17842400
F	-4.64536400	1.39523500	-0.37265600
F	-6.77797500	2.20410900	-0.51368500
F	-5.87584900	1.68658800	1.53024100
F	-6.41845800	0.01189400	0.05412400
N	-2.82285700	-1.22293400	-2.65969600
C	-1.80745000	-2.13989800	-3.16941200
C	-2.29582300	-3.58205000	-3.27416800
H	-0.95784700	-2.09032100	-2.47727400
H	-1.42023000	-1.82435900	-4.15666800
H	-1.44306600	-4.25991100	-3.37860200
H	-2.86077300	-3.85985100	-2.37997000
H	-2.94016600	-3.73315800	-4.14412500
C	-4.02751200	-1.23443500	-3.48772100
C	-5.09467200	-0.25408900	-3.02316300
H	-4.44630400	-2.24470900	-3.43435500
H	-3.78334800	-1.05242400	-4.55254100
H	-6.01220600	-0.42150500	-3.59470300
H	-5.31462000	-0.39033400	-1.96180400
H	-4.79589800	0.78755400	-3.17238600
C	-2.26341400	0.11367400	-2.44649400
C	-1.80565800	0.87307200	-3.69505500
H	-1.39892900	-0.01624500	-1.78115600

H	-3.01170900	0.70555500	-1.90498700
H	-1.42285800	1.85840600	-3.40765600
H	-0.99735000	0.34947600	-4.21304600
H	-2.63043000	1.02200100	-4.40089600
C	1.72296600	1.45186900	-1.24794600
C	0.93154000	1.13771100	-0.13463100
H	1.99310500	2.50580500	-1.28662100
C	0.80117100	2.13957900	0.89221600
H	1.30094300	3.09664100	0.65363700
O	0.13624800	2.02422200	1.92707400
C	1.63658300	0.82461000	-2.58729000
C	1.71735100	1.66321300	-3.70860600
C	1.48542500	-0.55211400	-2.79587500
C	1.68075300	1.13920700	-4.99749000
H	1.80280400	2.73607500	-3.56193800
C	1.46154700	-1.07828000	-4.08336200
H	1.37787200	-1.21788500	-1.95005600
C	1.56691600	-0.23653600	-5.18982600
H	1.74260000	1.80742600	-5.85067100
H	1.35437800	-2.15218100	-4.20608000
H	1.55066700	-0.64881800	-6.19359800
C	0.40826300	-0.16120200	0.11281300
C	-0.01544900	-1.27798300	0.35198900
C	-0.40761400	-2.62716300	0.62431600
C	0.42695600	-3.46434700	1.38588800
C	-1.57588200	-3.15735100	0.07141800
C	0.10050600	-4.79376700	1.57885500
H	1.34382700	-3.06293500	1.80819000
C	-1.92125500	-4.48932200	0.27704100
H	-2.21641600	-2.52749200	-0.54216800
C	-1.07837100	-5.31340700	1.02616000
H	0.73777900	-5.45428900	2.15663600
H	-2.85744500	-4.85312400	-0.13072800
C	5.59362600	-3.55715700	-1.34460500
C	4.70115600	-2.64704900	-0.77022000
C	3.33082200	-2.75491700	-0.94299600
C	2.87571900	-3.78601000	-1.76863200
C	3.74826600	-4.66925900	-2.39532300
C	5.12207800	-4.56205100	-2.17422900
C	6.99867300	-3.29630800	-0.84951600
C	6.73328100	-2.50648500	0.43484200
C	5.50007700	-1.65708100	0.05301800
H	2.63247400	-2.08463400	-0.44516100
H	3.35263700	-5.45500000	-3.02832000

H	5.80128600	-5.27755000	-2.62617400
H	7.56117800	-4.20749800	-0.63771200
H	7.57623300	-1.90003500	0.78693500
H	5.80499700	-0.78830100	-0.53886400
H	7.57432400	-2.68714100	-1.55471000
Br	1.01273600	-4.01101400	-2.02735000
O	6.34387700	-3.45841800	1.41353100
C	5.98686300	-2.89683000	2.65188900
H	5.52309300	-3.68066800	3.25216600
H	6.86809700	-2.51916200	3.18859000
N	4.84179200	-1.15398900	1.26005000
C	4.09513200	-0.03714100	1.46482900
C	5.03593800	-1.74805000	2.47555200
N	4.43642200	-1.08184100	3.41803200
N	3.86343300	-0.02329600	2.78540900
C	3.20357800	0.94881100	3.63348100
C	3.96255300	2.02104500	4.11330000
C	1.90200000	0.68344300	4.04709700
C	3.33384600	2.89640500	4.99212500
C	1.31911700	1.59142600	4.93257500
C	2.00902900	2.70637400	5.39950200
H	3.89445700	3.74495800	5.37605400
H	0.29914400	1.41272500	5.26362200
C	1.34400700	3.69755000	6.31837700
H	0.97216500	4.55571800	5.74947500
H	0.49414900	3.24859100	6.83672900
H	2.04560700	4.07735500	7.06491400
C	1.17176200	-0.54311200	3.58189400
H	1.11406100	-0.57283000	2.49157800
H	1.67474600	-1.45237500	3.92846700
H	0.15089800	-0.54982300	3.97006500
C	5.39730900	2.20876100	3.70435500
H	5.97141000	1.28707200	3.84511800
H	5.45189600	2.48668200	2.64868600
H	5.86465600	2.99455700	4.29960400
C	4.55965300	1.87893000	-1.85741300
C	3.85162000	0.95669700	-0.86122500
H	4.48392000	1.37764000	-2.82774800
C	3.85846400	1.14840700	0.53429400
O	3.63333300	2.20216600	1.15402100
C	4.17621900	3.33574800	-2.08797300
C	4.20876700	3.81618800	-3.40350500
C	3.86761500	4.24026500	-1.06604800
C	3.92588600	5.14746700	-3.69726400

H	4.44395700	3.12895100	-4.21296400
C	3.57620100	5.57222200	-1.35825800
H	3.83759900	3.88924900	-0.04120600
C	3.60088800	6.03346600	-2.67188000
H	3.95221300	5.48997900	-4.72733000
H	3.33144400	6.25342500	-0.54803000
H	3.37084000	7.07065200	-2.89564000
H	3.89405700	-0.08071200	-1.18462300
H	5.63159300	1.86893500	-1.61031400
O	-1.32122800	-6.62344700	1.27597300
C	-2.51767800	-7.17390300	0.75263900
H	-2.53184300	-8.21787900	1.06149700
H	-3.39790500	-6.66051900	1.15514000
H	-2.53472800	-7.11492900	-0.34094600

TS4COMe-SS

C	-6.11817300	-1.80406600	1.92980300
C	-5.22081400	-1.03570400	1.18114200
C	-4.98169800	-1.28853500	-0.16209800
C	-5.71339200	-2.32343100	-0.73938700
C	-6.60688500	-3.10741200	-0.01746400
C	-6.80645900	-2.85277800	1.33837200
C	-6.21487300	-1.28701400	3.34640200
C	-5.70329200	0.14463900	3.19727900
C	-4.62056200	0.01355000	2.09858800
H	-4.30040400	-0.70155900	-0.77101300
H	-7.15145300	-3.90035500	-0.51726100
H	-7.50896500	-3.45273000	1.90892700
H	-7.22899200	-1.29659000	3.75156600
H	-5.31207000	0.59436400	4.11901900
H	-3.67345300	-0.33448500	2.52656200
H	-5.55897300	-1.84966200	4.02068700
Br	-5.52316300	-2.66228200	-2.59283800
O	-6.79600800	0.89405000	2.69188900
C	-6.51522400	2.24557200	2.42149000
H	-7.35328600	2.64972700	1.85705300
H	-6.38047300	2.81489100	3.35236900
N	-4.37607300	1.33774900	1.52714700
C	-3.29510800	1.80230400	0.89208600
C	-5.26269400	2.37543900	1.61213500
N	-4.77278000	3.45161400	1.06592300
N	-3.54584500	3.07035800	0.61232100
C	-2.63349500	4.06612800	0.10790500
C	-2.76380400	4.52936300	-1.20046800

C	-1.70140300	4.58136100	1.01771600
C	-1.89484300	5.55054600	-1.59805700
C	-0.87870800	5.61150600	0.57623800
C	-0.96012100	6.10813900	-0.72875000
H	-1.97711900	5.93299200	-2.61287300
H	-0.17032300	6.04705000	1.27625800
C	-0.05214700	7.22005500	-1.18843900
H	0.29494800	7.82218000	-0.34469300
H	0.83110200	6.81715200	-1.69712100
H	-0.56247000	7.87869000	-1.89474500
C	-1.58532000	4.03546300	2.41430300
H	-2.56372600	3.95138800	2.89766200
H	-1.12571100	3.04263000	2.38035600
H	-0.95534100	4.68414000	3.02500100
C	-3.78414800	3.99503300	-2.16942800
H	-4.44497200	3.24677300	-1.73411000
H	-4.39488900	4.81522600	-2.55693300
H	-3.27122000	3.54039600	-3.02433100
H	-2.34727800	1.29746200	0.71616600
B	-6.60951000	1.42285200	-1.38046400
F	-5.22126000	1.41679300	-1.08493900
F	-6.87339900	2.48678000	-2.24264100
F	-7.31159500	1.58945800	-0.17734100
F	-6.95045000	0.20894400	-1.97485800
N	-2.58561200	-0.70132000	-2.71212200
C	-1.45990200	-1.62734400	-2.67419900
C	-1.82265700	-3.05100600	-3.08240500
H	-1.09830000	-1.64574900	-1.64148200
H	-0.61193200	-1.27913600	-3.29750100
H	-1.02457900	-3.73349400	-2.77397200
H	-2.75908700	-3.34458300	-2.59969800
H	-1.95506600	-3.15737300	-4.16303800
C	-3.14225900	-0.55705800	-4.05143700
C	-4.32427600	0.40201600	-4.10142800
H	-3.48863300	-1.54634500	-4.36833300
H	-2.36780700	-0.24761500	-4.78166500
H	-4.80255400	0.34700700	-5.08361600
H	-5.05893800	0.14164000	-3.33515500
H	-4.01989800	1.44065300	-3.93883900
C	-2.25223700	0.56887100	-2.06823100
C	-1.22717400	1.45935100	-2.77930600
H	-1.86225000	0.31322200	-1.07685200
H	-3.18172700	1.12764900	-1.91380700
H	-1.06956800	2.37090300	-2.19231200

H	-0.25865900	0.95649600	-2.88063600
H	-1.56770800	1.74904500	-3.77937400
C	1.59692800	-0.93970800	-0.74658700
C	0.58069700	-0.29831600	-0.00265700
H	2.03999400	-0.28771900	-1.50081900
C	0.47807400	1.13386900	-0.06388500
H	1.25550300	1.62684000	-0.67974400
O	-0.41162400	1.81764300	0.45012500
C	1.54110400	-2.34999000	-1.21883400
C	1.90775100	-2.61643800	-2.54656200
C	1.13560400	-3.42478000	-0.41442000
C	1.89438500	-3.91236900	-3.05413900
H	2.17915600	-1.78830800	-3.19880600
C	1.12111300	-4.72078100	-0.92308800
H	0.83183400	-3.24700300	0.60981200
C	1.50673400	-4.97285100	-2.23875800
H	2.17721100	-4.08966400	-4.08683600
H	0.80684800	-5.53919400	-0.28340900
H	1.49492300	-5.98567900	-2.62741900
C	-0.40194400	-1.01945200	0.73025400
C	-1.24256500	-1.70272600	1.28544600
C	-2.21356600	-2.64034700	1.76250500
C	-2.59701200	-2.71623500	3.10432400
C	-2.80258400	-3.52951200	0.84104900
C	-3.56413300	-3.62846200	3.52474900
H	-2.13341300	-2.05444700	3.82974400
C	-3.75526200	-4.44006500	1.24933500
H	-2.51070900	-3.47212200	-0.20406200
C	-4.15845100	-4.48082400	2.59112600
H	-3.84339800	-3.66189700	4.57113400
H	-4.23610500	-5.10721000	0.54211000
C	6.72917100	-2.45208800	-2.53217500
C	6.17688900	-1.60775800	-1.56666900
C	6.67094800	-1.55230700	-0.27150300
C	7.73645800	-2.39657200	0.03614500
C	8.28989200	-3.26332600	-0.90135000
C	7.78409800	-3.29008800	-2.20080400
C	6.03308800	-2.26285500	-3.86021100
C	5.37936400	-0.88908000	-3.69695600
C	5.01908200	-0.85822500	-2.19382000
H	6.25702500	-0.88898000	0.48326000
H	9.11890600	-3.90189200	-0.61945100
H	8.22598800	-3.94938500	-2.94066700
H	6.70844100	-2.27134400	-4.71779300

H	4.50489400	-0.72539400	-4.33931800
H	4.07578500	-1.38996600	-2.04185200
H	5.26253000	-3.02637200	-4.01604100
Br	8.46325900	-2.35661800	1.78498800
O	6.37953800	0.08063900	-3.95945500
C	5.91187300	1.40037400	-3.82079100
H	6.75987600	2.07519800	-3.94026800
H	5.15880600	1.63892600	-4.58471400
N	4.83969300	0.52429300	-1.74001600
C	4.24850200	1.02274400	-0.62524700
C	5.29595400	1.59142300	-2.46681300
N	5.03955500	2.71298800	-1.86054100
N	4.38983900	2.34724200	-0.72319600
C	3.99763300	3.38636000	0.19651000
C	3.00102600	4.27047100	-0.20837400
C	4.67698100	3.48858200	1.41631700
C	2.69660200	5.31852900	0.66197400
C	4.32307200	4.54514700	2.24808500
C	3.33719700	5.46969800	1.88798600
H	1.93344700	6.03126300	0.36249400
H	4.83062800	4.65078400	3.20351300
C	2.95158300	6.58466500	2.82439100
H	2.22489000	6.22912800	3.56229200
H	3.81895400	6.96081100	3.37167400
H	2.49565600	7.41621800	2.28200300
C	5.71320500	2.48102600	1.83804300
H	5.22661700	1.57023300	2.20869200
H	6.37492100	2.20302200	1.01167800
H	6.32879400	2.88447600	2.64351100
C	2.25069300	4.13948200	-1.50930800
H	2.37610600	3.15891900	-1.97287500
H	1.18125800	4.29451900	-1.33069600
H	2.58956500	4.88937600	-2.23092200
C	2.86433700	-1.64877500	1.80271800
C	3.33356100	-1.05257900	0.49233800
H	2.85655600	-2.73925700	1.71606100
C	3.48727000	0.34963900	0.49086600
O	2.86843600	1.10862400	1.25182800
C	3.76149600	-1.22464100	2.94995500
C	5.06309500	-1.72303500	3.06789500
C	3.31996700	-0.27932800	3.87884600
C	5.89984100	-1.28922400	4.09391100
H	5.42853000	-2.45667100	2.35045400
C	4.15344100	0.15486600	4.90712700

H	2.31967400	0.12964500	3.77525500
C	5.44708400	-0.34920700	5.01777200
H	6.90677500	-1.68602700	4.16866400
H	3.79316800	0.89231200	5.61780300
H	6.09958800	-0.01182200	5.81677500
H	4.01146300	-1.66823700	-0.08563600
H	1.84122900	-1.31647800	2.01064700
O	-5.13681000	-5.37265100	2.88258900
C	-5.67344600	-5.34879900	4.19231400
H	-6.47816800	-6.08221700	4.20525900
H	-4.92008400	-5.62247900	4.93871100
H	-6.07798900	-4.35807000	4.43181000

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C	-0.55096300	-4.47196800	0.92409600
C	-1.08060700	-3.19145100	0.76251500
C	-0.94441600	-2.49150700	-0.43057400
C	-0.24339000	-3.11898600	-1.45567700
C	0.28043500	-4.40425100	-1.32393200
C	0.12800000	-5.08746000	-0.12082900
C	-0.80926000	-5.00262700	2.31261900
C	-1.84002500	-4.02897900	2.89704700
C	-1.64745700	-2.72161300	2.08182700
H	-1.36710400	-1.50505500	-0.60411000
H	0.79907900	-4.86319700	-2.15924100
H	0.52830000	-6.09013100	-0.00996500
H	-1.21857500	-6.01583400	2.31892500
H	-1.70823600	-3.85042600	3.97260500
H	-0.93054200	-2.04876400	2.56347300
H	0.10662300	-5.01353300	2.91319600
Br	0.03582000	-2.18034500	-3.06917800
O	-3.12153400	-4.58069200	2.66108900
C	-4.15387100	-3.78246400	3.19405600
H	-5.10258300	-4.24911500	2.94112800
H	-4.05176300	-3.68220800	4.28410200
N	-2.91269800	-1.98732600	2.01906400
C	-3.16721900	-0.79269900	1.47832100
C	-4.09176300	-2.43506900	2.54913400
N	-5.03592900	-1.55137900	2.40518800
N	-4.43926700	-0.53390400	1.72659400
C	-5.15044600	0.67786000	1.43308000
C	-6.34209700	0.57883300	0.70512500
C	-4.64392800	1.88447500	1.92854200
C	-7.03902000	1.76275100	0.47395800

C	-5.38860200	3.03442400	1.66584300
C	-6.57935800	2.99512100	0.94329600
H	-7.96418300	1.71804700	-0.09606600
H	-5.02362900	3.98669600	2.03936800
C	-7.35441000	4.25519100	0.66292800
H	-8.41974100	4.11352900	0.86365900
H	-6.99181700	5.08399600	1.27614700
H	-7.24774300	4.55264900	-0.38485700
C	-3.37195400	1.96672400	2.73490000
H	-3.34014800	1.19660000	3.51282800
H	-2.47595600	1.84304900	2.11576500
H	-3.30787700	2.94268900	3.21939900
C	-6.83836400	-0.73776300	0.17214200
H	-6.03022000	-1.34122400	-0.24735700
H	-7.29429000	-1.33633100	0.96592000
H	-7.58614500	-0.56886400	-0.60533700
H	-2.45465500	-0.13371200	0.99851300
B	-5.11907000	-3.89301900	-0.41931500
F	-4.22032100	-2.82421700	-0.18632400
F	-6.17641600	-3.42141800	-1.21026800
F	-5.62361100	-4.33389400	0.81417000
F	-4.45703400	-4.92875600	-1.06805400
N	-2.82831300	-0.43128100	-2.91042700
C	-2.04494200	0.66499600	-3.46362000
C	-2.64732400	1.50919400	-4.59672500
H	-1.10394100	0.23350000	-3.83153700
H	-1.76384200	1.31785300	-2.63008300
H	-1.86971200	2.16009300	-5.00864000
H	-3.01984100	0.88049200	-5.41116800
H	-3.46797000	2.14975500	-4.26288300
C	-3.22606800	-1.41188600	-3.91144800
C	-3.64095800	-2.73910000	-3.29324400
H	-2.35582100	-1.57210600	-4.55948900
H	-4.03610600	-1.04100600	-4.56534200
H	-3.81368600	-3.48077000	-4.07914800
H	-2.85572000	-3.10934400	-2.62844600
H	-4.55646600	-2.65663400	-2.70369600
C	-3.88816300	-0.05159300	-1.97938100
C	-5.21071800	0.42350100	-2.59912500
H	-3.48013200	0.73313700	-1.32606600
H	-4.09542600	-0.91561000	-1.33550900
H	-5.85128500	0.86219900	-1.82976600
H	-5.05491100	1.17927300	-3.37298600
H	-5.75383900	-0.41279600	-3.05142200

C	1.44875600	0.67449600	-1.07376600
C	0.38782500	0.87648300	-0.16090400
H	1.93170700	-0.29602000	-0.95054900
C	0.35360400	0.04350400	1.01059600
H	1.19222400	-0.67777100	1.07910100
O	-0.52677900	0.03335500	1.87844700
C	1.47287500	1.11412200	-2.49348900
C	2.20842700	0.34506800	-3.40721700
C	0.80635300	2.25108900	-2.97149800
C	2.26211800	0.68361600	-4.75442800
H	2.71488600	-0.55108100	-3.06000800
C	0.87159300	2.59797600	-4.31848900
H	0.23088900	2.86603400	-2.29019300
C	1.59117700	1.81425700	-5.21714000
H	2.82532700	0.06144100	-5.44259500
H	0.35106200	3.48525900	-4.66540100
H	1.63154800	2.08328000	-6.26768600
C	-0.62381400	1.87354100	-0.24979000
C	-1.52629200	2.69096400	-0.26961900
C	-2.55276100	3.68826700	-0.35220400
C	-3.53167000	3.62906900	-1.36173600
C	-2.58802200	4.75852200	0.54825000
C	-4.50854900	4.60197700	-1.45718500
H	-3.51610200	2.80688100	-2.06988600
C	-3.56380000	5.74851900	0.45619800
H	-1.83449300	4.81813100	1.32720200
C	-4.53072100	5.66964800	-0.54955600
H	-5.26790000	4.56166700	-2.23145600
H	-3.55889500	6.56638700	1.16636600
C	7.08857500	-0.46094700	-1.75979900
C	5.95286800	-0.21160800	-0.99299500
C	4.82279300	-1.00009800	-1.07737100
C	4.83160200	-2.05117500	-1.98529400
C	5.92977000	-2.29869500	-2.80266100
C	7.07138900	-1.49797600	-2.68502100
C	8.20287900	0.46716800	-1.32369000
C	7.76968600	0.85174700	0.10081500
C	6.22434300	0.90563000	-0.01328700
H	3.95629000	-0.83785300	-0.44586400
H	5.90903300	-3.12435700	-3.50450900
H	7.94314300	-1.71630600	-3.29316500
H	9.18715900	-0.00444200	-1.30813600
H	8.19649100	1.79279300	0.46659700
H	5.89529000	1.88972700	-0.36385400

H	8.25582300	1.35972300	-1.95594900
Br	3.27597200	-3.12749600	-2.03359700
O	8.15676200	-0.23074000	0.93316900
C	7.72099400	-0.10039100	2.26721100
H	8.04093000	-0.98531900	2.81681500
H	8.15165800	0.79202700	2.74211200
N	5.57116800	0.62536800	1.26753500
C	4.24954600	0.62466900	1.56978300
C	6.22710000	0.00341700	2.29380100
N	5.39222900	-0.39172000	3.21037800
N	4.17259300	-0.00241400	2.74754900
C	2.98872500	-0.42257200	3.45380700
C	2.48969900	0.40509000	4.46056200
C	2.44504300	-1.66618500	3.12632200
C	1.34720800	-0.02725100	5.12659600
C	1.31511900	-2.05916800	3.84378700
C	0.73987000	-1.24648700	4.82048400
H	0.92157700	0.60260700	5.90291200
H	0.88090100	-3.03419700	3.63491500
C	-0.52491900	-1.66895400	5.51939100
H	-0.64532700	-1.15078500	6.47266600
H	-1.39908400	-1.42604400	4.90198900
H	-0.53400700	-2.74562200	5.70931000
C	3.02952200	-2.55638700	2.05620300
H	2.64012300	-2.31629600	1.05771800
H	4.12001400	-2.48680100	2.01561900
H	2.76518400	-3.59790000	2.25145500
C	3.16553400	1.70643500	4.78911500
H	4.21342100	1.54542400	5.06058800
H	3.13601100	2.36593600	3.91693600
H	2.66537800	2.19959300	5.62360700
C	2.66623200	3.24670100	-0.65935000
C	3.12525700	1.82102700	-0.40283200
H	1.66021500	3.38338400	-0.24869000
C	3.13468300	1.45443000	0.96264800
O	2.25843100	1.80439900	1.77080000
C	3.63193600	4.21517700	-0.01219000
C	4.82827000	4.55381300	-0.65396800
C	3.38558700	4.73022000	1.26412200
C	5.76243500	5.37987600	-0.03358400
H	5.02254700	4.16733200	-1.65280400
C	4.31799900	5.55841500	1.88629300
H	2.46061400	4.46586900	1.76823800
C	5.50983200	5.88343700	1.24182200

H	6.68312700	5.63747100	-0.54814700
H	4.11147100	5.95273100	2.87659600
H	6.23409900	6.53028900	1.72627800
H	3.91963900	1.46298100	-1.05086400
H	2.62502400	3.43021400	-1.73479900
O	-5.52468600	6.57549600	-0.72908900
C	-5.60918500	7.64603500	0.19388300
H	-4.71245300	8.27380800	0.15623100
H	-6.47723400	8.23357600	-0.10070200
H	-5.74794100	7.27649600	1.21654600

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C	1.32860600	-4.75554600	0.46787600
C	1.72357000	-3.43751300	0.23425600
C	2.00366600	-2.55630200	1.27177300
C	1.87684400	-3.05308500	2.56589900
C	1.45941100	-4.35559100	2.82706700
C	1.18063000	-5.21777200	1.76848700
C	1.12937600	-5.49563300	-0.83499800
C	1.89109000	-4.63378900	-1.84847800
C	1.76551400	-3.20841100	-1.26084400
H	2.37100600	-1.54471200	1.11914700
H	1.37894200	-4.69706500	3.85257000
H	0.87690100	-6.24072200	1.96614400
H	1.52479300	-6.51355700	-0.82714700
H	1.48836000	-4.68554500	-2.86930400
H	0.85045800	-2.74658500	-1.63721500
H	0.06711300	-5.54246000	-1.10196000
Br	2.33923000	-1.94223800	4.02891400
O	3.24026300	-5.05527200	-1.83440700
C	4.06845500	-4.31693400	-2.70224800
H	5.09213200	-4.64987300	-2.54554000
H	3.77772800	-4.47150800	-3.75110700
N	2.87206800	-2.37704700	-1.72604100
C	3.04721100	-1.06097000	-1.59357200
C	3.97390200	-2.85814900	-2.37536900
N	4.78774700	-1.89035300	-2.68877300
N	4.19354500	-0.77352000	-2.18553800
C	4.77409400	0.52683900	-2.37336800
C	6.09421100	0.73608400	-1.95088100
C	4.00172600	1.51108700	-3.00105600
C	6.63547600	1.99921900	-2.17980100
C	4.59991500	2.75743600	-3.19672700
C	5.90626400	3.02137800	-2.79001700

H	7.65261300	2.19432500	-1.84936000
H	4.02931400	3.53647200	-3.69713400
C	6.50979800	4.39011300	-2.95986300
H	7.52828700	4.32876900	-3.35115500
H	5.91496800	5.00785400	-3.63653000
H	6.56186800	4.89940200	-1.99157500
C	2.58930600	1.26346800	-3.47189000
H	2.49441600	0.30008400	-3.98196800
H	1.86693300	1.25946100	-2.64601500
H	2.29189900	2.04707900	-4.17217000
C	6.89868600	-0.32926700	-1.25635600
H	6.29332500	-0.90584100	-0.55444100
H	7.31306900	-1.03688400	-1.98061300
H	7.72840700	0.13062700	-0.71572100
H	2.37385400	-0.36048100	-1.11862000
B	5.44314400	-3.14127500	0.71984400
F	4.68585200	-2.01456300	0.30508400
F	6.76124000	-2.73523000	0.93949700
F	5.40982100	-4.09552700	-0.30807300
F	4.88467100	-3.66593300	1.88209400
N	3.61158300	0.77822600	2.42357500
C	2.54414800	1.56053400	3.03858300
C	2.93303000	2.83407700	3.80254200
H	2.01413400	0.89804800	3.73855000
H	1.82513600	1.80934400	2.25200100
H	2.02641100	3.30012300	4.20433500
H	3.58692100	2.60790400	4.64999300
H	3.43898900	3.56793600	3.16986500
C	4.72830700	0.54374600	3.32720000
C	5.62866300	-0.60114500	2.89043900
H	4.29126400	0.29098300	4.30317800
H	5.33256200	1.45502000	3.49172600
H	6.42057100	-0.75170000	3.63102600
H	5.05320600	-1.52381800	2.79548700
H	6.10915600	-0.41395300	1.92696000
C	3.97102600	1.15292000	1.06107900
C	4.73129500	2.46845200	0.85655800
H	3.03362100	1.20874400	0.49224100
H	4.54801700	0.32363500	0.63221000
H	4.90557100	2.62839200	-0.21229800
H	4.15834200	3.32482700	1.22335800
H	5.70435000	2.45566800	1.36000000
C	-1.04056300	-0.24027200	1.39611300
C	-0.33553900	0.12347000	0.23272800

H	-1.27833900	-1.30324100	1.47363900
C	-0.33561500	-0.80559700	-0.85576600
H	-0.83105900	-1.77384300	-0.62411900
O	0.14440800	-0.61711100	-1.98299500
C	-0.89942500	0.46065900	2.68488400
C	-0.67198600	-0.31129200	3.82828500
C	-0.98415500	1.85575900	2.81028900
C	-0.47717100	0.29678800	5.06633100
H	-0.59761800	-1.39114400	3.73668500
C	-0.81267000	2.45879400	4.04921900
H	-1.19620900	2.46655200	1.93754900
C	-0.54796500	1.68119500	5.17985800
H	-0.27087400	-0.31603900	5.93788200
H	-0.88779200	3.53830200	4.13776200
H	-0.40367500	2.15778600	6.14401200
C	0.31296100	1.37495800	0.05730200
C	0.84504100	2.46119300	-0.07285200
C	1.53678300	3.71072500	-0.07274300
C	2.22453000	4.16547000	-1.20104200
C	1.57496600	4.48603300	1.10228100
C	2.96101700	5.34555800	-1.16832900
H	2.19148300	3.57898800	-2.11263700
C	2.29692600	5.66386400	1.14106500
H	1.04734700	4.13741300	1.98594300
C	3.00118200	6.09892700	0.00826400
H	3.49529400	5.66310700	-2.05602100
H	2.34267600	6.26599200	2.04211100
C	-3.53484700	4.19848700	-1.06794900
C	-3.84684800	2.85051500	-0.87567000
C	-5.10015000	2.44082300	-0.44477500
C	-6.03738000	3.43745400	-0.18077000
C	-5.74736100	4.78827900	-0.34575700
C	-4.48489200	5.17359900	-0.79876200
C	-2.11986400	4.34467700	-1.58353200
C	-1.81628000	2.94755900	-2.12775800
C	-2.60893900	2.03043200	-1.16837300
H	-5.35455000	1.39357200	-0.30504900
H	-6.50619500	5.53175600	-0.13140400
H	-4.26153400	6.22517900	-0.94648000
H	-2.01164600	5.09919800	-2.36519900
H	-0.75140100	2.68780400	-2.15108600
H	-2.02278600	1.86840800	-0.26272500
H	-1.42093100	4.58336000	-0.77254700
Br	-7.76015300	2.93199900	0.42808300

O	-2.37986000	2.86989600	-3.42844100
C	-2.16872700	1.61193900	-4.02192100
H	-2.67715600	1.59648100	-4.98615400
H	-1.09713600	1.41857200	-4.17600700
N	-2.84530600	0.72477600	-1.78922900
C	-3.23446500	-0.45658300	-1.25387900
C	-2.71354200	0.53195500	-3.13748600
N	-3.04391500	-0.68143800	-3.47078100
N	-3.36233400	-1.28354500	-2.29719500
C	-3.85685300	-2.63637100	-2.32471500
C	-3.01494000	-3.62727000	-2.82752800
C	-5.16435600	-2.88166700	-1.88619000
C	-3.51797500	-4.92939100	-2.86467400
C	-5.61327100	-4.19661100	-1.95130600
C	-4.80553700	-5.23274900	-2.42893500
H	-2.88027200	-5.72356800	-3.24475800
H	-6.62375800	-4.41895400	-1.61734700
C	-5.32069000	-6.64803100	-2.45198600
H	-4.68621000	-7.29113900	-3.06477600
H	-5.34549900	-7.06419200	-1.44008000
H	-6.33904200	-6.68814300	-2.84680700
C	-6.05594000	-1.79562700	-1.34337300
H	-5.81342800	-1.57962600	-0.29541900
H	-5.96767900	-0.86823600	-1.91810200
H	-7.09897700	-2.11470700	-1.37786100
C	-1.62629100	-3.33365600	-3.33443100
H	-1.65373700	-3.07685100	-4.39792000
H	-1.15410800	-2.49118000	-2.82141100
H	-0.99654800	-4.21972300	-3.22283200
C	-3.79342200	-0.47210100	2.56463200
C	-3.30404700	0.01418600	1.21993600
H	-3.68883000	0.32956600	3.30240900
C	-3.33380300	-0.92526200	0.18071300
O	-3.29562100	-2.16091100	0.32737000
C	-5.23839700	-0.91616700	2.44231800
C	-5.57009900	-2.27245900	2.45770100
C	-6.25267100	0.02031300	2.20789300
C	-6.88530700	-2.68734800	2.25077500
H	-4.78419500	-3.00531300	2.61264500
C	-7.56535600	-0.39114500	1.99626800
H	-6.01174500	1.08216400	2.17886700
C	-7.88647500	-1.74848600	2.01844000
H	-7.12376900	-3.74649000	2.26279500
H	-8.33574700	0.34978900	1.80852200

H	-8.90982900	-2.06957300	1.85225600
H	-3.43398300	1.06796600	1.00827500
H	-3.18497600	-1.31628100	2.90951800
O	3.68387300	7.25985200	0.14987400
C	4.40928200	7.73613600	-0.96995100
H	4.88140200	8.66440600	-0.65285700
H	5.18027300	7.02032000	-1.27491700
H	3.74368500	7.93479700	-1.81692900