

Supplementary Information for
Combined Molecular Dynamics and Coordinate Driving Method for Automatically
Searching Complicated Reaction Pathways

Guoao Li, Zhenxing Li, Liuzhou Gao, Shengda Chen, Guoqiang Wang*, Shuhua Li*

*School of Chemistry and Chemical Engineering, Key Laboratory of Mesoscopic
Chemistry of Ministry of Education, Institute of Theoretical and Computational
Chemistry, Nanjing University, Nanjing, 210023, P. R. China.*

E-mail: shuhua@nju.edu.cn; wangguoqiang710@nju.edu.cn

Tel: +86-25-89686465

Table of Contents

1. Evaluation of activation barriers for single electron transfer processes	3
The Marcus Theory	3
The solvation reorganization energy	4
The Wolynes Theory	4
Calculation procedure of the activation barriers of SET processes	5
2. Details of the improved CD procedure	7
3. Reaction pathways for the Organocatalytic trans phosphinoboration reaction	9
4. Reaction pathways for the phosphine-catalyzed hydroboration reaction	15
5. Reaction pathways for the Fe(II) complex mediated C-H borylation reaction	17
6. Reaction pathways for the SET-triggered deaminative cross-coupling reaction	19
7. Optimized structures of local minima and transition states along main reaction pathways	20
8. References	24
9. DFT-optimized cartesian coordinates of all species involved in the organocatalytic trans phosphinoboration reaction	25
10. DFT-optimized cartesian coordinates of all species involved in the phosphine-catalyzed hydroboration reaction	211
11. DFT-optimized cartesian coordinates of all species involved in the Fe(II) complex mediated C-H borylation reaction	247
12. DFT-optimized cartesian coordinates of all species involved in the SET-triggered deaminative cross-coupling reaction	268

1. Evaluation of free energy barriers and reaction rate constants for single electron transfer processes.

The Marcus theory

Single electron transfer (SET) processes can be described as $[D] + [A] \rightarrow [D^+] + [A^-]$, where $[D]$, $[A]$ are the electron donor and acceptor respectively, and $[D^+]$, $[A^-]$ are electron-transferred species. To evaluate the free energy barrier ΔG^\ddagger for a SET process, the Marcus theory^{1,2} makes the following assumptions:

(a) The entropy exchange of the SET process is ignored. As a result, the free energies can be replaced by potential energies.

(b) The free energy surfaces V_R of $[D A]$ and V_P of $[D^+ A^-]$ are parabolas of the same shape.

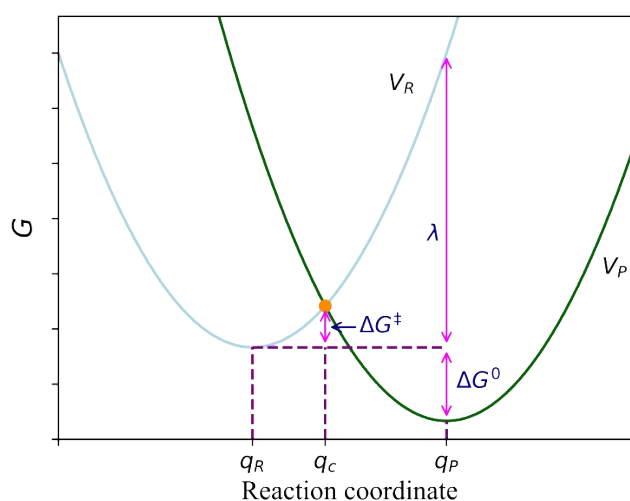


Fig. S1 Schematic diagram of the Marcus theory.

The schematic diagram of the Marcus theory is shown in **Figure S1**. Along the reaction coordinate of a certain SET process, the positions of local minima of V_R and V_P can be denoted as q_R and q_P . Then the Gibbs free energy change can be expressed as Eq. (S1).

$$\Delta G^0 = V_P(q_P) - V_R(q_R) \quad (\text{S1})$$

Supposing that $V_R(q_R)$ is zero. Then the expressions of parabola V_R and V_P can be written as:

$$V_R(q) = \frac{1}{2}f(q - q_R)^2 \quad (\text{S2})$$

$$V_P(q) = \frac{1}{2}f(q - q_P)^2 + \Delta G^0 \quad (\text{S3})$$

At the crossing point q_c , we have $V_R(q_c) = V_P(q_c)$, leading to Eq. (S4).

$$\frac{1}{2}f(q_c - q_R)^2 = \frac{1}{2}f(q_c - q_P)^2 + \Delta G^0 \quad (\text{S4})$$

Solving this equation, we obtain

$$q_c = \frac{\Delta G^0}{q_P - q_R} + \frac{q_P + q_R}{2} \quad (\text{S5})$$

As in Eq. (S6), the reorganization energy (λ) is defined as the change in Gibbs free energy if the reactant state $[D A]$ distorts to the equilibrium conformation of the product state $[D^+ A^-]$ without transfer of an electron.

$$\lambda = V_R(q_P) - V_R(q_R) = \frac{1}{2}f(q_P - q_R)^2 \quad (\text{S6})$$

Thus, the free energy barrier ΔG^\ddagger can be expressed as Eq. (S7), which is exactly Eq. (1) in the main text of the manuscript.

$$\Delta G^\ddagger = \frac{1}{2}f(q_c - q_R)^2 = \frac{(\lambda + \Delta G^0)^2}{4\lambda} = \frac{\lambda}{4}\left(1 + \frac{\Delta G^0}{\lambda}\right)^2 \quad (\text{S7})$$

The solvation reorganization energy

In more realistic situations, the reorganization energy λ should be divided into the vibrational (inner-sphere) part λ_i and the solvation (outer-sphere) part λ_o . λ_i represents the distortion of $[D A]$, which can be estimated with Eq. (S6), while λ_o represents the distortion of the solvents. According to the Marcus equation, λ_o can be calculated with Eq. (S8),

$$\lambda_o = \frac{e^2}{4\pi\epsilon_0} \left(\frac{1}{2r_D} + \frac{1}{2r_A} - \frac{1}{R} \right) \left(\frac{1}{\epsilon_{op,r}} - \frac{1}{\epsilon_{s,r}} \right) \quad (\text{S8})$$

where e is the elementary charge, ϵ_0 is the permittivity of vacuum, $\epsilon_{op,r}$ and $\epsilon_{s,r}$ are relative optical and static dielectric constants of the solvent, r_D , r_A and R are the radii of the donor $[D]$, the acceptor $[A]$ and the donor-acceptor complex $[D A]$. For the solvent acetonitrile, we refer to $\epsilon_{s,r} = 35.688$ and $\epsilon_{op,r} = 1.806874$. For the solvent DMSO, we refer to $\epsilon_{s,r} = 46.826$ and $\epsilon_{op,r} = 2.007889$. These data are obtained from the output results of the Gaussian 16 software package.³ The total reorganization energy λ used in Eq. (S7) in this work is the summation of λ_i and λ_o .

$$\lambda = \lambda_i + \lambda_o \quad (\text{S9})$$

The Wolynes theory

Traditional Marcus theory gives the electron transfer rate constants as Eq. (S10),

$$k_{MT} = \frac{\Delta^2}{\hbar} \sqrt{\frac{\pi}{k_B T \lambda}} \exp\left(-\frac{\Delta G^\ddagger}{k_B T}\right) \quad (\text{S10})$$

where Δ is the electronic coupling, \hbar is the reduced Planck's constant, k_B is the Boltzmann constant and T is the temperature. However, in the Marcus inverted regime ($\lambda < -\Delta G^0$), the SET rate could be significantly enhanced by nuclear quantum effects, introducing a correction factor r to the Marcus rate k_{MT} . The correction factor r can be evaluated by the analytic continuation version of the Wolynes theory.⁴

First, based on the harmonic oscillator approximation, the total reorganization energy λ can be

decomposed into the contribution of each vibrational modes of the donor-acceptor complex $[D A]$.

$$\lambda = \sum_{j=1}^f \lambda_j, \quad \lambda_j = \mu_j \omega_j^2 d_j^2 \quad (\text{S11})$$

In Eq. (S11), f is the total number of vibrational modes, and μ_j , ω_j , d_j are the reduced mass, harmonic vibrational frequencies, geometry displacements between $[D A]$ and $[D^+ A^-]$ for the vibrational mode j . Since Gaussian 16 can provide Huang-Rhys factors S_j using the local minimum structures of $[D A]$ and $[D^+ A^-]$, λ_j can be directly derived with Eq. (S12) instead of computing d_j ,

$$\lambda_j = 2\pi\hbar\omega_j S_j \quad (\text{S12})$$

Then, the rate constant predicted by the Wolynes theory can be written as Eq. (S13),

$$k_W = \frac{\Delta^2}{\hbar} \sqrt{\frac{2\pi k_B T}{F''(x)|_{x=x_{sp}}}} \exp\left(-\frac{F(x)|_{x=x_{sp}}}{k_B T}\right) \quad (\text{S13})$$

where $F(x)$ is in the free energy form with x as the hypothesized reaction coordinate, and x_{sp} is the saddle point of $F(x)$. Using Eq. (S12), the formula of $F(x)$ is given as follows:

$$F(x) = \left(\frac{1}{2} + k_B T x\right) \Delta G^0 + \sum_{j=1}^f 2\pi S_j k_B T \frac{\cosh\left(\frac{\hbar\omega_j}{2k_B T}\right) - \cosh(x\hbar\omega_j)}{\sinh\left(\frac{\hbar\omega_j}{2k_B T}\right)} \quad (\text{S14})$$

At the saddle point $x = x_{sp}$, we have

$$F'(x)|_{x=x_{sp}} = k_B T \Delta G^0 - \sum_{j=1}^f 2\pi S_j k_B T \cdot \hbar\omega_j \frac{\sinh(x_{sp}\hbar\omega_j)}{\sinh\left(\frac{\hbar\omega_j}{2k_B T}\right)} = 0 \quad (\text{S15})$$

and

$$F''(x)|_{x=x_{sp}} = - \sum_{j=1}^f 2\pi S_j k_B T \cdot \hbar^2 \omega_j^2 \frac{\cosh(x_{sp}\hbar\omega_j)}{\sinh\left(\frac{\hbar\omega_j}{2k_B T}\right)} \quad (\text{S16})$$

Since $F'(x)$ is monotonous, Eq. (S15) can be solved easily using the bisection method. Finally, the correction ratio r to the Marcus rate k_{MT} can be evaluated as Eq. (S17) with the quantities obtained above:

$$r = \frac{k_W}{k_{MT}} = k_B T \sqrt{\frac{2\lambda}{F''(x)|_{x=x_{sp}}}} \exp\left(\frac{\Delta G^\ddagger - F(x)|_{x=x_{sp}}}{k_B T}\right) \quad (\text{S17})$$

Calculation procedure of the activation barriers of SET processes

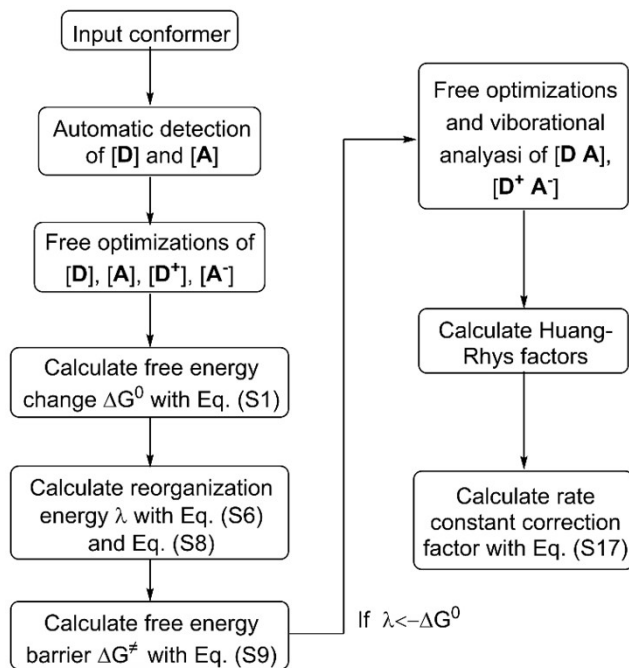
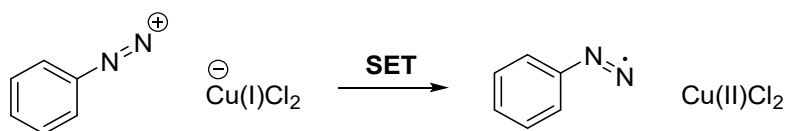


Fig. S2 Flowchart of the calculation procedure of SET processes.

The calculation flowchart of the barriers of SET processes is shown in **Figure S2**. For a given conformer, the electron donor $[D]$ and acceptor $[A]$ are detected with the following steps. First, the conformer is divided into single molecules based on the bonding relationships. If the relative distance λ_{ij} between atom i and j is less than 1.25, atom i and j are considered to be connected with a chemical bond. Regarding the conformer as an undirected graph with atoms as its vertices and bonds as its edges, the single molecules are exactly the connected components of the graph.



Scheme S1. The SET process in the **CuCl** catalyzed Sandmeyer reaction of **PhN₂Cl**.

For example, consider the outer-sphere SET process in the traditional Sandmeyer reaction⁴ of **PhN₂Cl** (**Scheme S1**). An electron is about to transfer from the **Cu(I)Cl₂** anion to the phenyl diazo cation. We divide the encounter complex into two single molecules **SM(a)** (**PhN₂⁺**) and **SM(b)** (**Cu(I)Cl₂⁻**) via bonding connections as shown in **Figure S3**. Since the donor will have a higher HOMO energy, while the acceptor will have a lower LUMO energy, **SM(b)** is automatically detected as the electron donor $[D]$ and **SM(a)** as the electron acceptor $[A]$.

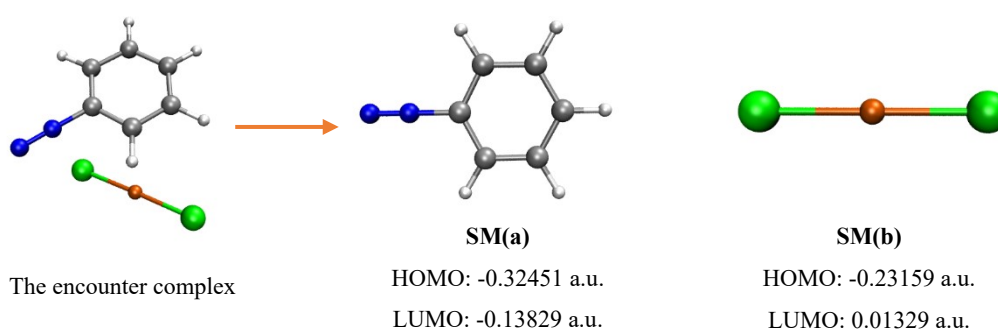


Fig. S3. Schematic diagram of dividing an encounter complex into two separate reactants. Frontier orbital energies are calculated at the PBE0-D3/def-TZVP level with the PCM model (MeCN as the solvent).

Then free optimizations of $[D]$, $[A]$ and their electron transferred species $[D^+]$ and $[A^-]$ are performed to obtain the structures at q_R and q_P described in **Figure S1**. To find the ground state spin multiplicities of $[D^+]$ and $[A^-]$, odd or even numbers from 1 to the user-defined largest possible spin multiplicities are assigned to the real spin multiplicities of $[D^+]$ and $[A^-]$ to perform single point calculations at the initial structures. If $[D^+]$ or $[A^-]$ has an even number of electrons, its spin multiplicity should be an odd number, vice versa. The spin multiplicity with the lowest electronic energy is taken as the ground state spin multiplicity and will be used in the optimizations and following calculations. Finally, by applying Eq. (S1), Eq. (S6), Eq. (S7) and Eq. (S8), the free energy changes and barriers of the SET process from **SM(b)** to **SM(a)** can be evaluated. For the reactant complex **SM(a)** and **SM(b)**, the computed results at the uESE(MeCN)/RI- ω B97M-V/ma-def2-TZVPP//PCM(MeCN)/PBE0-D3/def-TZVP level are $\lambda = 51.53$ kcal/mol, $\Delta G^0 = 31.09$ kcal/mol and $\Delta G^\ddagger = 33.12$ kcal/mol.

2. Details of the improved CD procedure

In the improved CD procedure, a reaction coordinate (RC) consists of one or several primary reaction coordinates (PRC). A PRC (i,j,k) is a tuple with three numbers. The first two numbers i,j are atom labels between which a bond change may occur. The third number k is 1 or 2, where 1 means to form a bond along this PRC and 2 means to break the bond. For a given structure, all the PRCs are generated according to the relative distance λ_{ij} and bond order L_{ij} between all the active atoms. The bond order L_{ij} of atom i and j is defined according to their relative distance λ_{ij} :

$$L_{ij} = \begin{cases} 0, & \lambda_{ij} > 1.25 \\ 1, & 0.93 < \lambda_{ij} < 1.25 \\ 2, & 0.81 < \lambda_{ij} < 0.93 \\ 3, & \lambda_{ij} < 0.81 \end{cases} \quad (\text{S10})$$

If $L_{ij} = 0$ and $\lambda_{ij} < 5.0$, it is possible to form a bond between atom i and j , then the PRC $(i,j,1)$ is generated. If $L_{ij} > 0$ and $\lambda_{ij} > 0.90$, the bond between atom i and j is possible to break, then the PRC $(i,j,2)$ is generated. We choose 12 fixed relative distance values for each PRC. The fixed values along PRC $(i,j,1)$ are

$$F_1(1,2,\dots,12) = [4.5, 4.0, 3.5, 3.0, 2.5, 2.0, 1.5, 1.4, 1.3, 1.2, 1.1, 1.0].$$

For PRC $(i,j,2)$, the fixed values are

$$F_2(1,2,\dots,12) = [1.0, 1.1, 1.2, 1.3, 1.4, 1.5, 1.6, 1.7, 1.8, 1.9, 2.0, 2.15].$$

It should be mentioned that for judging the criterion $\lambda_{ij} < 5.0$, the radius of H atoms is doubled to avoid missing the reaction possibilities of H atoms because their radius is too small (0.30 Å).

In the first CD stage, 12 points along every RC from the starting conformer are explored to obtain the local potential energy surface. For each PRC (i,j,k) constituting the current RC, on the m th point, the relative distance λ_{ij} is fixed at $F_k(m)$. If $k = 1$, meaning to form a bond, but $F_k(m)$ is greater than the initial relative distance λ_{ij}^0 in the starting conformer, λ_{ij} is fixed at λ_{ij}^0 . Similarly, if $k = 2$ but $F_k(m) < \lambda_{ij}^0$, λ_{ij} is also fixed at λ_{ij}^0 .

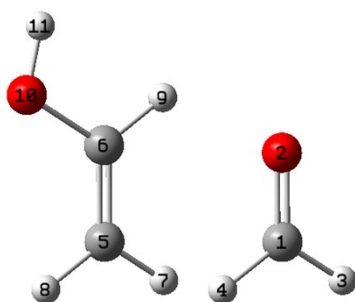


Fig S4. A conformer for the complex of the formaldehyde and the vinyl alcohol.

For example, as shown in **Figure S4**, we suppose to apply the traditional CD technique on the RC containing PRCs $(1,5,1)$ and $(2,11,1)$, which is a typical RC for the intermolecular Aldol reaction. In the starting conformer, $\lambda_{1,5}^0 = 2.45$, and $\lambda_{2,11}^0 = 4.20$. Thus, on the 12 points along the current RC, $\lambda_{1,5}$ and $\lambda_{2,11}$ are fixed at $[2.45, 2.45, 2.45, 2.45, 2.45, 2.0, 1.5, 1.4, 1.3, 1.2, 1.1, 1.0]$ and

[4.2, 4.0, 3.5, 3.0, 2.5, 2.0, 1.5, 1.4, 1.3, 1.2, 1.1, 1.0], respectively.

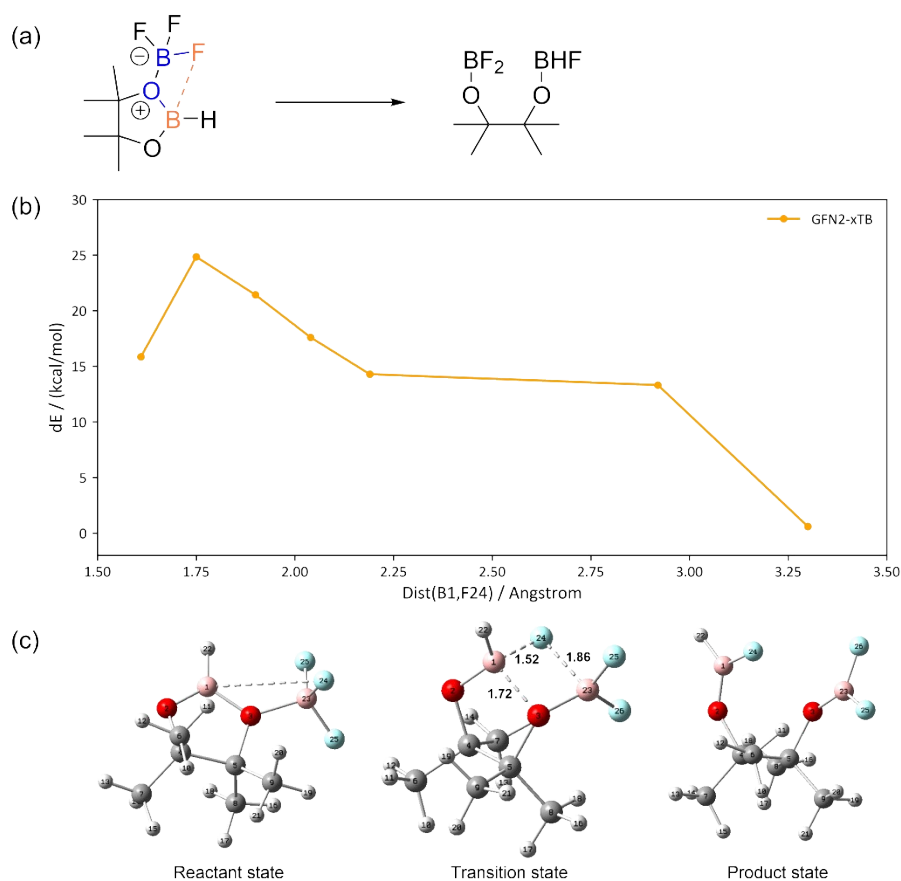
In the second CD stage, if we need to perform CD calculations directly with *ab initio* methods, 20 points along one RC are chosen to obtain the local potential energy surface with

$$F_{1,r} = [4.5, 4.0, 3.5, 3.0, 2.5, 2.0, 1.8, 1.6, 1.55, 1.5, 1.45, 1.4, 1.35, 1.3, 1.25, 1.2, 1.15, 1.1, 1.05, 1.0]$$

and

$$F_{2,r} = [1.0, 1.05, 1.1, 1.15, 1.2, 1.25, 1.3, 1.35, 1.4, 1.45, 1.5, 1.55, 1.6, 1.65, 1.7, 1.8, 1.9, 2.0, 2.15, 2.3]$$

The following example shows that the RC used in the constrained optimizations does not need to contain all bond-forming and bond-breaking atom pairs along the elementary reaction step. For the ring-opening 1,4-fluorine migration step shown in Scheme S2(a), concerted bond formation and breakage happens among three atom pairs. However, with the RC that contains only one B-F distance (in dotted line), the reasonable local potential energy surface can be obtained (Scheme S2(b)), and further free optimizations will lead to the desired product and transition state (Scheme S2(c)).



Scheme S2. (a) The ring-opening 1,4-fluorine migration. Atom pairs involved in bond changes are colored with orange (included in RC) and blue (not included in RC). (b) The local potential energy surface along the B-F distance (in dotted line). (c) Optimized structure of the reactant, transition state and product of this reaction step. Bond distances are in Å.

3. Reaction pathways for the organocatalytic *trans* phosphinoboration reaction.

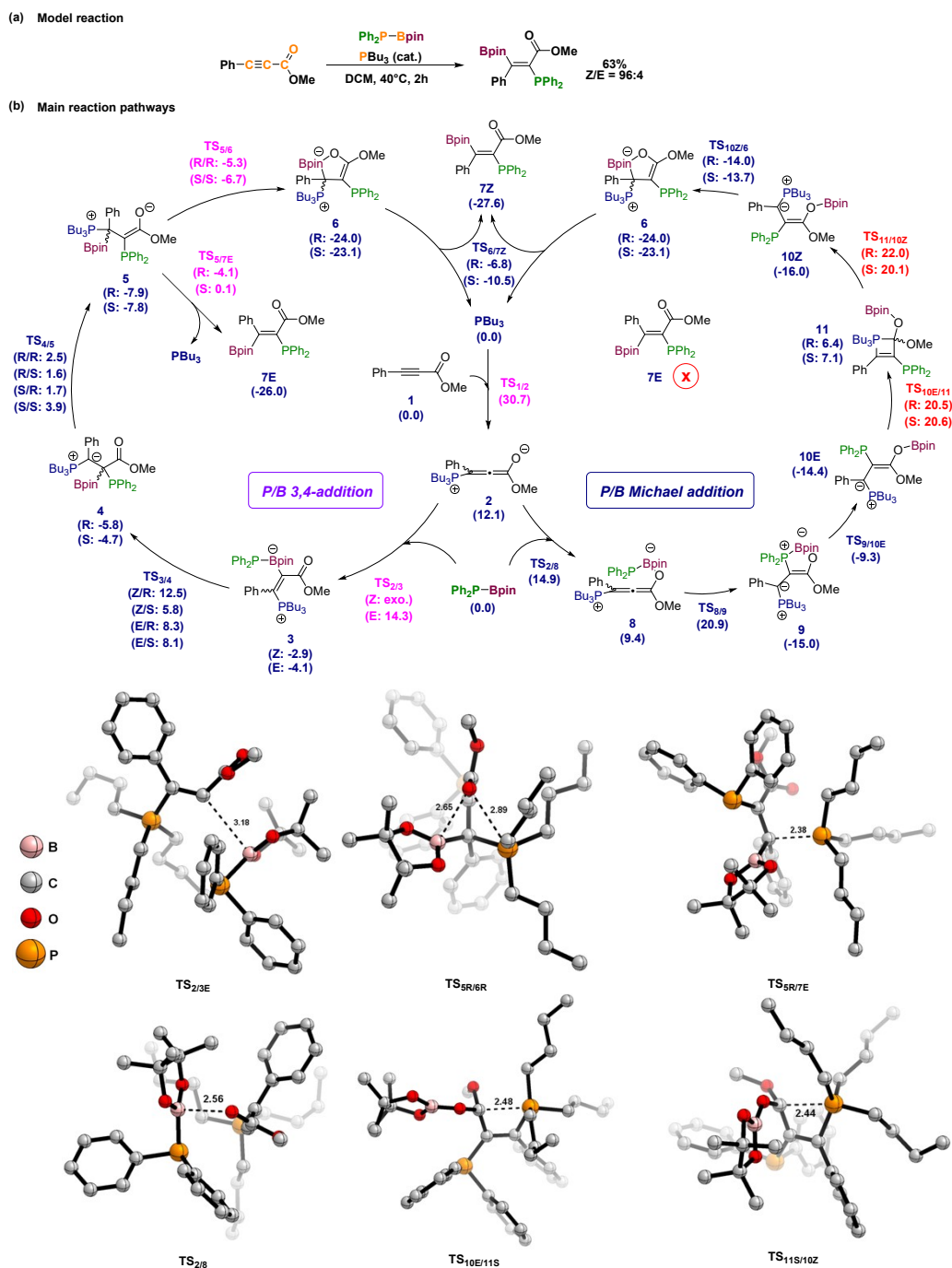


Fig S5. P/B 3,4-addition and 1,4-addition pathways for the organocatalytic *trans* phosphinoboration reaction.

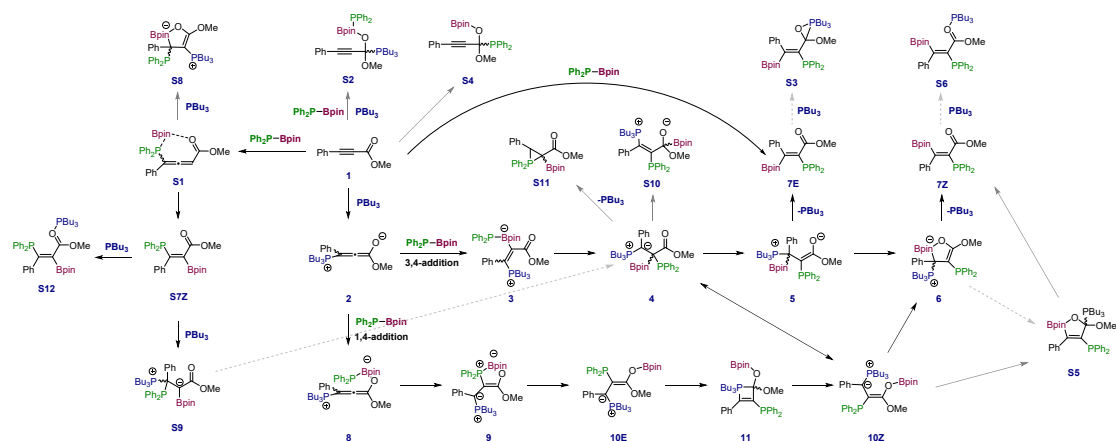


Fig. S6. Overall reaction pathways for the organocatalytic *trans* phosphinoboration reaction. (Black arrows: MD/CD method found all the TS structures among different stereoisomers; Brown arrows: MD/CD method found part of TS structures among different stereoisomers; Dashed arrows: Intermediates were connected during MD/CD explorations, but TS locations failed.)

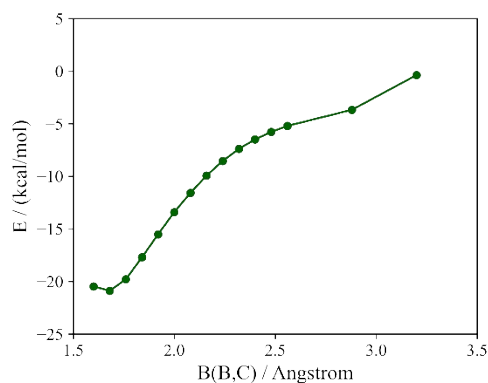


Fig. S7. Local potential energy surface of the coordination from **2** to **3Z** obtained in the second CD stage at the B3LYP-D3/6-31G(d) level.

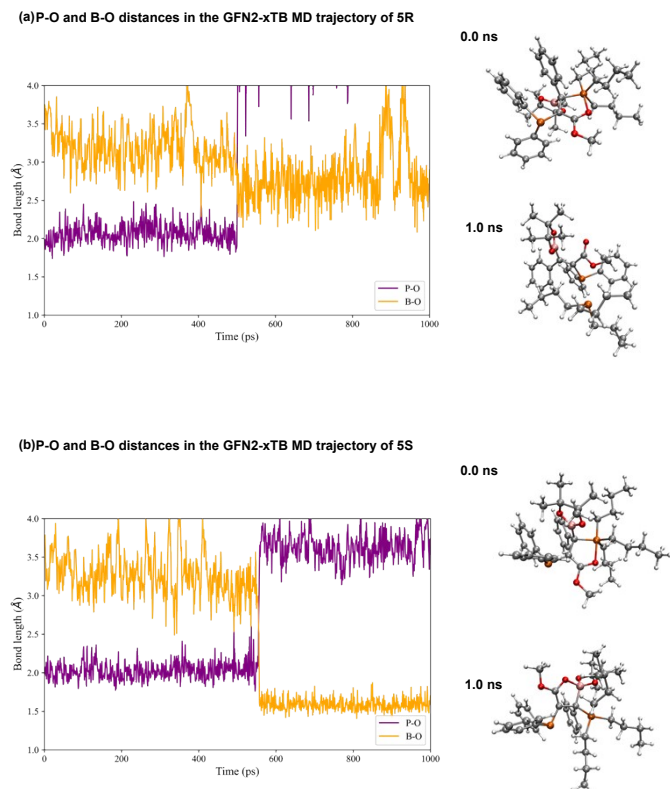


Fig. S8. P-O and B-O distances among the P atom from **PBu₃**, the B atom from **PPh₂-Bpin** and the carbonyl O atom from **1** as functions of time in the MD trajectories of (a) **5R** and (b) **5S**.

Table S1. B3LYP-D3/6-31G(d) computed imaginary frequency (ImF); Grimme's QRRHO approximated gas-phase Gibbs free energy corrections (Gc); the solvation free energies (Gsol) computed with the SMD model at the M05-2X/6-31G(d) level in CH₂Cl₂ solution; the RI- ω B97M-V/def2-TZVPP single point energies (Esp); the total Gibbs free energies (G); relative electronic energies (ΔE) and relative Gibbs free energies (ΔG).

Species	ImF cm ⁻¹	Gc/Eh	Gsol/Eh	Esp/Eh	G/Eh	ΔE (kcal/mol)	ΔG (kcal/mol)
PBu₃	0	0.319962	-0.014557	-814.792781	-814.484364	0.00	0.00
PPh₂- Bpin	0	0.312950	-0.026361	-1215.904501	-1215.614901	0.00	0.00
1	0	0.114093	-0.016473	-536.286267	-536.185636	0.00	0.00
2	0	0.463120	-0.041108	-1351.075713	-1350.650689	2.09	12.12
3Z	0	0.808029	-0.057088	-2567.043525	-2566.289571	-37.63	-2.93
3E	0	0.809072	-0.051622	-2567.051968	-2566.291506	-42.93	-4.14
4R	0	0.811617	-0.043209	-2567.065570	-2566.294150	-51.47	-5.80
4S	0	0.812015	-0.045396	-2567.061991	-2566.292360	-49.22	-4.68
5R	0	0.812810	-0.045332	-2567.067970	-2566.297480	-52.97	-7.89
5S	0	0.812820	-0.045117	-2567.068106	-2566.297391	-53.06	-7.84
6R	0	0.812801	-0.046703	-2567.092225	-2566.323114	-68.19	-23.98
7Z	0	0.456138	-0.035865	-1752.267848	-1751.844563	-48.37	-27.63
7E	0	0.455801	-0.036316	-1752.264484	-1751.841987	-46.26	-26.01

8	0	0.806270	-0.051276	-2567.027996	-2566.269991	-27.89	9.36
9	0	0.808726	-0.048325	-2567.072155	-2566.308742	-55.60	-14.96
10Z	0	0.809776	-0.046857	-2567.076389	-2566.310458	-58.26	-16.04
10E	0	0.808695	-0.045232	-2567.074241	-2566.307766	-56.91	-14.35
11R	0	0.807026	-0.043341	-2567.041470	-2566.274774	-36.35	6.35
12R	0	0.808392	-0.047633	-2567.078090	-2566.314319	-59.32	-18.46
12S	0	0.809915	-0.047309	-2567.080854	-2566.315236	-61.06	-19.04
S1	0	0.458655	-0.035583	-1752.212235	-1751.786151	-13.47	9.03
S2R	0	0.805833	-0.052156	-2567.004806	-2566.248117	-13.34	23.08
S2S	0	0.806978	-0.052587	-2567.008586	-2566.251183	-15.71	21.16
S3	0	0.809270	-0.045149	-2567.017093	-2566.249960	-21.05	21.93
S4R	0	0.454056	-0.037375	-1752.225788	-1751.806095	-21.98	-3.49
S4S	0	0.455326	-0.034377	-1752.231348	-1751.807387	-25.46	-4.30
S5R	0	0.808392	-0.047633	-2567.078090	-2566.314319	-59.32	-18.46
S5S	0	0.809915	-0.047309	-2567.080854	-2566.315236	-61.06	-19.04
S6	0	0.805466	-0.058495	-2567.026827	-2566.276844	-27.16	5.06
S7Z	0	0.457661	-0.036530	-1752.269031	-1751.844889	-49.11	-27.83
S8S	0	0.814619	-0.045678	-2567.091649	-2566.319696	-67.83	-21.83
S9R	0	0.812443	-0.044548	-2567.064977	-2566.294070	-51.10	-5.75
S9S	0	0.814270	-0.046364	-2567.057888	-2566.286970	-46.65	-1.30
S10R	0	0.811770	-0.039177	-2567.047303	-2566.271698	-40.01	8.28
S11	0	0.455938	-0.038957	-1752.197445	-1751.777452	-4.19	14.49
S12	0	0.809077	-0.055063	-2567.012271	-2566.255245	-18.02	18.61
TS_{1/2}	138i	0.462205	-0.029077	-1351.057160	-1350.621020	13.74	30.73
TS_{2/3E}	20i	0.807987	-0.049718	-2567.023459	-2566.262179	-25.04	14.26
TS_{3Z/4R}	21i	0.809309	-0.049348	-2567.027962	-2566.264989	-27.87	12.49
TS_{3Z/4S}	123i	0.809933	-0.052016	-2567.036586	-2566.275657	-33.28	5.80
TS_{3E/4R}	106i	0.812126	-0.049674	-2567.037213	-2566.271749	-33.67	8.25
TS_{3E/4S}	105i	0.811950	-0.049710	-2567.037173	-2566.271922	-33.65	8.14
TS_{4R/5R}	246i	0.809849	-0.043378	-2567.050374	-2566.280891	-41.93	2.52
TS_{4R/5S}	151i	0.812180	-0.044018	-2567.053438	-2566.282265	-43.86	1.65
TS_{4S/5R}	185i	0.812107	-0.042871	-2567.054464	-2566.282216	-44.50	1.68
TS_{4S/5S}	250i	0.810401	-0.042815	-2567.049268	-2566.278670	-41.24	3.91
TS_{4R/10Z}	282i	0.810619	-0.047848	-2567.019064	-2566.253282	-22.29	19.84
TS_{4S/10Z}	242i	0.811739	-0.046567	-2567.014711	-2566.246527	-19.55	24.08
TS_{5R/7E}	122i	0.808461	-0.044797	-2567.058172	-2566.291496	-46.83	-4.14
TS_{5S/7E}	142i	0.809669	-0.044865	-2567.052584	-2566.284768	-43.32	0.08
TS_{5R/6R}	25i	0.807875	-0.048348	-2567.055924	-2566.293385	-45.42	-5.32
TS_{5S/6S}	32i	0.807740	-0.049778	-2567.056504	-2566.295531	-45.78	-6.67
TS_{6R/7Z}	156i	0.808880	-0.041816	-2567.065880	-2566.295804	-51.66	-6.84
TS_{6S/7Z}	125i	0.808171	-0.042363	-2567.070440	-2566.301620	-54.52	-10.49
TS_{2/8}	19i	0.805248	-0.049871	-2567.019554	-2566.261165	-22.59	14.89
TS_{8/9}	130i	0.808418	-0.049019	-2567.014076	-2566.251664	-19.16	20.86

TS_{9/10E}	103i	0.810402	-0.045773	-2567.067418	-2566.299777	-52.63	-9.33
TS_{10E/11R}	194i	0.809494	-0.042829	-2567.021977	-2566.252300	-24.11	20.46
TS_{10E/11S}	247i	0.806761	-0.043585	-2567.018241	-2566.252053	-21.77	20.61
TS_{11R/10Z}	187i	0.809494	-0.042829	-2567.019591	-2566.249915	-22.62	21.95
TS_{11S/10Z}	261i	0.808831	-0.041812	-2567.022894	-2566.252863	-24.69	20.10
TS_{10Z/6R}	141i	0.810384	-0.045579	-2567.075080	-2566.307263	-57.44	-14.03
TS_{10Z/6S}	89i	0.810429	-0.045713	-2567.074395	-2566.306666	-57.01	-13.66
TS_{11R/12R}	201i	0.807726	-0.046441	-2567.003028	-2566.238731	-12.22	28.97
TS_{1/7E}	196i	0.453791	-0.040192	-1752.160040	-1751.743429	19.28	35.84
TS_{1/S1}	211i	0.453805	-0.038671	-1752.159837	-1751.741691	19.41	36.93
TS_{1/S2S}	171i	0.802504	-0.048722	-2566.958713	-2566.201919	15.59	52.07
TS_{1/S4S}	137i	0.454396	-0.033897	-1752.158121	-1751.734610	20.49	41.37
TS_{7Z/55S}	142i	0.809470	-0.043203	-2567.057719	-2566.288440	-46.54	-2.22
TS_{10Z/55S}	183i	0.808378	-0.045256	-2567.007633	-2566.241499	-15.11	27.23
TS_{S1/S7Z}	360i	0.456768	-0.033678	-1752.212386	-1751.786284	-13.56	8.94
TS_{S1/S8S}	127i	0.809775	-0.040906	-2567.035263	-2566.263382	-32.45	13.50
TS_{S7Z/S9R}	159i	0.809517	-0.043545	-2567.046569	-2566.277585	-39.54	4.59
TS_{S7Z/S9S}	135i	0.812259	-0.044335	-2567.050204	-2566.279268	-41.83	3.53
TS_{4R/S10R}	468i	0.807061	-0.043392	-2566.996958	-2566.230278	-8.41	34.28
TS_{4R/S11}	248i	0.806703	-0.041525	-2566.988203	-2566.220013	-2.92	40.72
TS_{S7Z/S12}	435i	0.806487	-0.051010	-2566.985634	-2566.227145	-1.31	36.24
5'R	0	0.794250	-0.041931	-2452.696933	-2451.941602	0.00	0.00
5'S	0	0.793623	-0.041394	-2452.697618	-2451.942378	-0.43	-0.49
TS_{5'R/7'E}	120i	0.790429	-0.040837	-2452.695690	-2451.943086	0.78	-0.93
TS_{5'S/7'E}	137i	0.789205	-0.043412	-2452.694872	-2451.946067	1.29	-2.80
TS_{5'R/6'R}	41i	0.793687	-0.044181	-2452.706565	-2451.954047	-6.04	-7.81
TS_{5'S/6'S}	32i	0.793126	-0.043814	-2452.704990	-2451.952666	-5.06	-6.94

Investigation on the sampling efficiency of the present MD procedure

For the intermediate **5R**, at the GFN2-xTB level, 10 conformers are obtained from the MD procedure for subsequent CD calculations. Here we also adopted the iMTD-GC algorithm to explore its possible lowest energy conformers for comparison. Our calculations for this intermediate lead to 298 conformers. The lowest-energy conformers found in the two methods differ by 0.06 kcal/mol at the same theory level. Taking 10 conformers from the MD procedure as reference structures, the 298 conformers are classified into the corresponding 10 groups according to the minimum RMSD values of seven active atoms. The results are illustrated in **Table S2**. The maximum RMSD value of active atoms compared with the reference structures among the 10 groups is only 0.171 Å. These results indicate that the lowest energy conformers from the iMTD-GC algorithm are energetically and spatially close to those conformers from our MD simulations.

Table S2. Number of conformers in each group and maximum RMSD values of active atoms compared with the reference structure in each group.

Group	1	2	3	4	5	6	7	8	9	10
Number	77	13	0	22	0	0	0	69	9	108
Max. RMSD / Å	0.090	0.107	-	0.134	-	-	-	0.171	0.137	0.054

4. Reaction pathways for the phosphine-catalyzed hydroboration reaction.

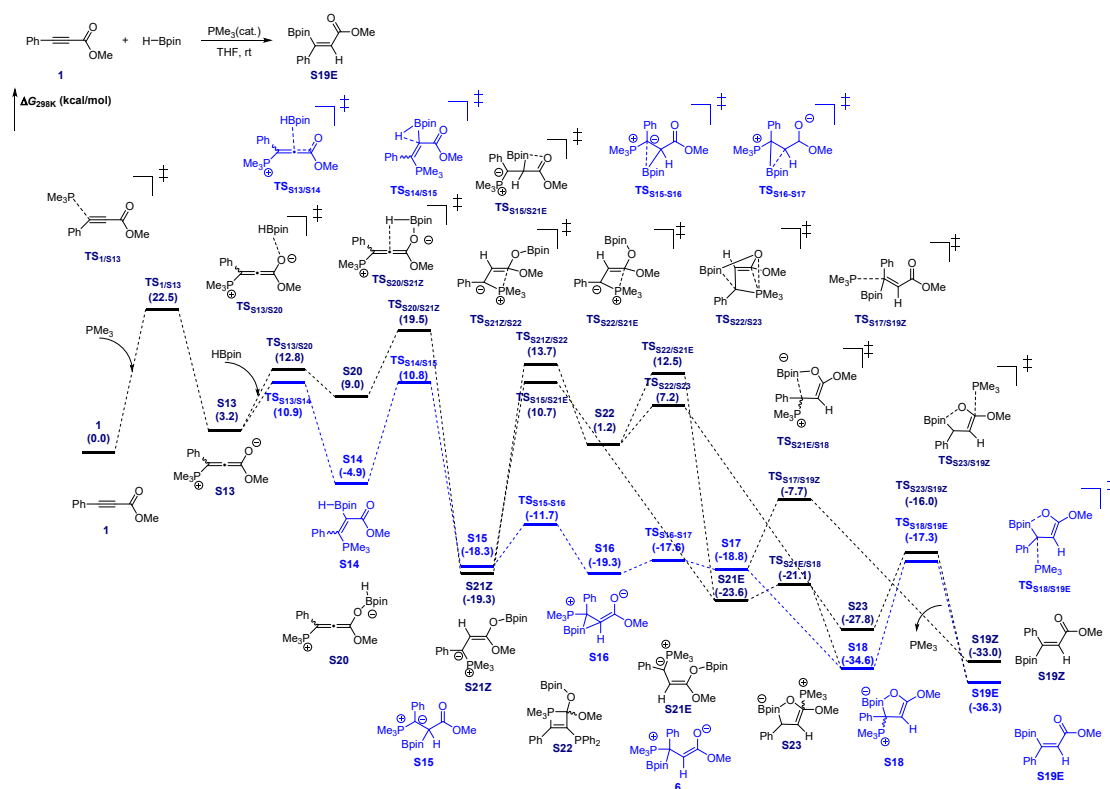


Fig. S9. Free energy profiles of the reaction networks for phosphine catalyzed hydroboration reaction. The 3,4-addition pathway (blue curve) is the most favored.

Table S3. RI-r²SCAN-3c(CPCM(THF)) computed imaginary frequency (ImF); Grimme's QRRHO approximated gas-phase Gibbs free energy corrections (Gc); the solvation free energies (Gsol) computed with the SMD model at the M06-2X/6-31G(d) level in THF solution; the RI- ω B97M-V/def2-TZVPPD single point energies (Esp); the total Gibbs free energies (G); relative electronic energies (ΔE) and relative Gibbs free energies (ΔG).

Species	ImF cm ⁻¹	Gc/Eh	Gsol/Eh	Esp/Eh	G/Eh	ΔE (kcal/mol)	ΔG (kcal/mol)
PMe ₃	0	0.082471	-0.003574	-461.052599	-460.970690	0.00	0.00
1	0	0.114849	-0.015097	-536.287677	-536.184913	0.00	0.00
HBpin	0	0.156806	-0.007796	-411.853774	-411.701753	0.00	0.00
S13	0	0.221261	-0.034333	-997.340479	-997.150539	-0.13	3.18
S14	0	0.403465	-0.036089	-1409.235549	-1408.865162	-26.04	-4.90
S15	0	0.406045	-0.031534	-1409.264093	-1408.886569	-43.95	-18.33
S16	0	0.405946	-0.033061	-1409.263948	-1408.888051	-43.86	-19.26
S17	0	0.405037	-0.039675	-1409.255619	-1408.887245	-38.63	-18.76
S18	0	0.407361	-0.026315	-1409.296583	-1408.912525	-64.34	-34.62
S19Z	0	0.298581	-0.021839	-948.218955	-947.939201	-48.63	-32.97
S19E	0	0.299607	-0.019456	-948.227669	-947.944506	-54.10	-36.30
S20	0	0.402448	-0.035982	-1409.212553	-1408.843075	-11.61	8.96
S21Z	0	0.405088	-0.031721	-1409.264478	-1408.888100	-44.19	-19.29

S21E	0	0.406308	-0.024851	-1409.279454	-1408.894986	-53.59	-23.61
S22	0	0.404367	-0.019697	-1409.243135	-1408.855453	-30.80	1.19
S23	0	0.405743	-0.031597	-1409.278840	-1408.901683	-53.21	-27.82
TS_{S1/S13}	151i	0.218498	-0.016326	-997.324949	-997.119766	9.62	22.49
TS_{S13/S14}	36i	0.401525	-0.032231	-1409.212275	-1408.839969	-11.44	10.91
TS_{S14/S15}	706i	0.401913	-0.028643	-1409.216409	-1408.840126	-14.03	10.81
TS_{S15/S16}	15i	0.406834	-0.030582	-1409.255194	-1408.875930	-38.37	-11.65
TS_{S15/S21E}	242i	0.404752	-0.028064	-1409.220023	-1408.840322	-16.30	10.69
TS_{S16/S17}	214i	0.405385	-0.036984	-1409.256896	-1408.885483	-39.44	-17.65
TS_{S17/S19Z}	139i	0.404356	-0.025554	-1409.251510	-1408.869696	-36.06	-7.74
TS_{S21E/S18}	132i	0.406840	-0.023608	-1409.277191	-1408.890948	-52.17	-21.08
TS_{S18/S19E}	97i	0.404453	-0.019689	-1409.272695	-1408.884919	-49.35	-17.30
TS_{S13/S20}	126i	0.401377	-0.037076	-1409.204192	-1408.836879	-6.36	12.85
TS_{S20/S21Z}	411i	0.401115	-0.032096	-1409.198270	-1408.826240	-2.65	19.53
TS_{S21Z/S22}	305i	0.404425	-0.022144	-1409.220769	-1408.835476	-16.77	13.73
TS_{S22/S21E}	260i	0.404424	-0.022312	-1409.222504	-1408.837380	-17.85	12.54
TS_{S22/S23}	89i	0.402304	-0.036327	-1409.214925	-1408.845937	-13.10	7.17
TS_{S23/S19Z}	159i	0.404921	-0.024280	-1409.266544	-1408.882892	-45.49	-16.02

5. Reaction pathways for the Fe(II) boryl complex mediated C-H borylation reaction.

Table S4. PBE0-D3(PCM(C₆H₆))/def2-SVP computed imaginary frequency (ImF); Grimme's QRRHO approximated gas-phase Gibbs free energy corrections (Gc); the solvation free energies (Gsol) computed with the SMD model at the M05-2X/6-31G(d) level in C₆H₆ solution; the RI- ω B97M-V/ma-def2-TZVPP single point energies (Esp); the total Gibbs free energies (G); relative electronic energies (ΔE) and relative Gibbs free energies (ΔG).

Species	ImF cm ⁻¹	Gc/Eh	Gsol/Eh	Esp/Eh	G/Eh	ΔE (kcal/mol)	ΔG (kcal/mol)
PEt ₃	0	0.164741	-0.006690	-578.960384	-578.799321	0.00	0.00
C ₆ H ₆	0	0.076138	-0.008533	-232.229151	-232.158535	0.00	0.00
Ph-Bpin	0	0.235303	-0.013189	-642.920608	-642.695483	-	-
HBpin	0	0.158563	-0.006582	-411.852466	-411.697472	-	-
12	0	0.612487	-0.017985	-3026.442937	-3025.845423	0.00	0.00
13	0	0.416659	-0.018202	-2447.415574	-2447.014105	42.03	20.08
14	0	0.516313	-0.020818	-2679.690683	-2679.192176	13.19	7.82
15	0	0.513708	-0.022402	-2679.675942	-2679.181624	22.44	14.44
16	0	0.516077	-0.020539	-2679.679945	-2679.181395	-22.10	14.58
17	0	0.445134	-0.016994	-2615.749956	-2615.318805	0.96	-6.48
S24	0	0.515764	-0.022533	-2679.652224	-2679.155981	37.32	30.53
S25	0	0.515127	-0.021624	-2679.657803	-2679.161288	33.82	27.20
S26	0	0.329390	-0.020454	-2267.781515	-2267.469567	48.77	23.59
TS _{13/14}	703i	0.512490	-0.020703	-2679.653703	-2679.158904	36.40	28.70
TS _{14/15}	18i	0.516170	-0.022325	-2679.663364	-2679.166508	30.33	23.93
TS _{S24/S25a}	97i	0.516322	-0.021616	-2679.640242	-2679.142524	44.84	38.98
TS _{S24/S25b}	171i	0.515386	-0.021182	-2679.626493	-2679.129277	53.47	47.29

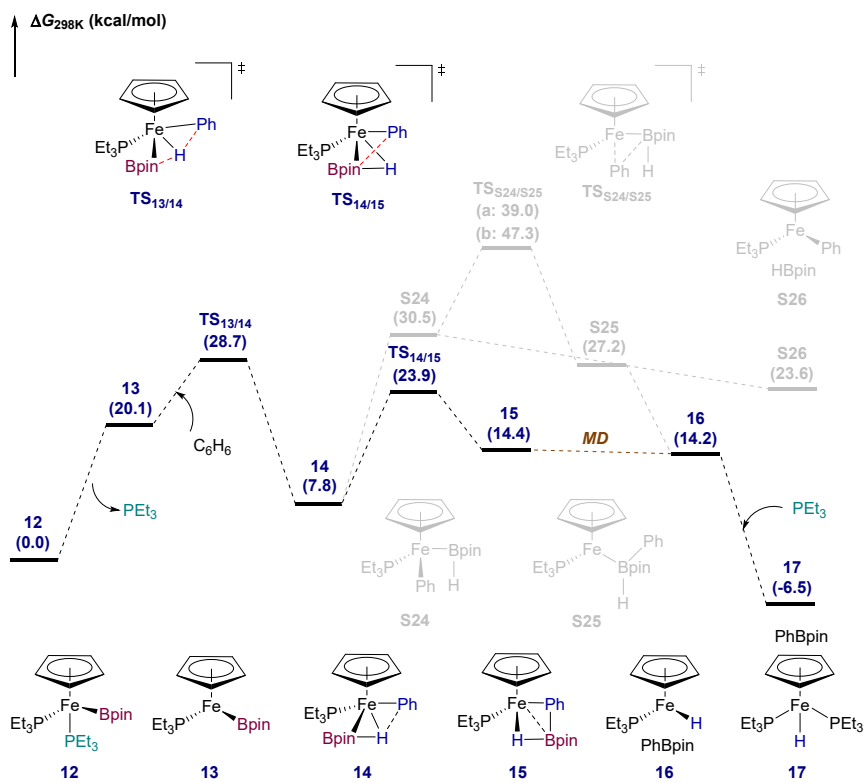


Fig. S10. Free energy profiles of the reaction networks for Fe(II) complex mediated C-H borylation explored by the improved MD/CD method.

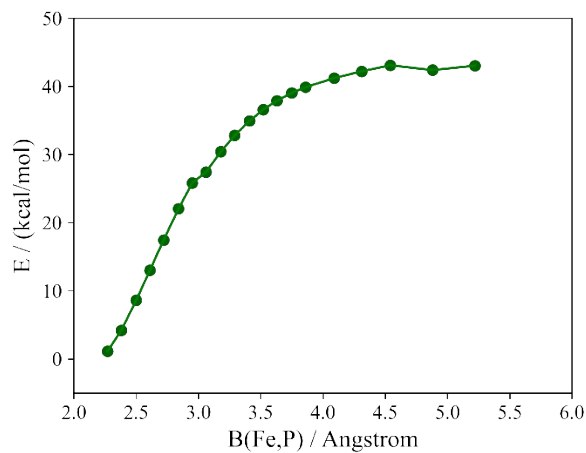


Fig. S11. Local potential energy surface of the PEt_3 disassociation of **12** obtained in the second CD stage at the PCM(C_6H_6)/PBE0-D3/def2-SVP level.

6. Reaction pathways for the SET-triggered deaminative cross-coupling reaction.

Table S4. PCM(DMSO)-(U)B3LYP-D3/6-31G(d) computed imaginary frequency (ImF); Grimme's QRRHO approximated gas-phase Gibbs free energy corrections (Gc); the solvation free energies (Gsol) computed with the uESE model at the (U)B3LYP/def2-TZVP level in DMSO solution; the RI-(U)ωB97M-V/ma-def2-TZVPP single point energies (Esp); the total Gibbs free energies (G); relative electronic energies (ΔE) and relative Gibbs free energies (ΔG).

Species	ImF cm ⁻¹	Gc/Eh	Gsol/Eh	Esp/Eh	G/Eh	ΔE (kcal/mol)	ΔG (kcal/mol)
18	0	0.468041	-0.109909	-1576.281404	-1575.920260	0.00	0.00
19	0	0.387754	-0.105850	-1248.325945	-1248.041029	0.00	0.00
20	-	0.376371	-0.034380	-1231.230206	-1230.885204	-	-
21	0	0.282988	-0.032604	-941.445279	-941.191882	-	-
22R	0	0.168072	-0.020028	-652.099703	-651.948647	-	-
22S	0	0.168016	-0.020245	-652.099703	-651.948920	-	-
23	0	0.383414	-0.044599	-1248.509112	-1248.167285	-	-
24	0	0.468915	-0.048995	-1576.246548	-1575.823616	-	-
25	0	0.071549	-0.007770	-307.048426	-306.981635	-	-
26R	0	0.573829	-0.069161	-1883.336212	-1882.828532	-	-
26S	0	0.572401	-0.068660	-1883.334333	-1882.827581	-	-
TSI	608i	0.380378	-0.045803	-1248.499013	-1248.161426	-	-
TSIIR	30i	0.565854	-0.053550	-1883.315920	-1882.800604	-	-
TSIIS	32i	0.566055	-0.053389	-1883.315849	-1882.800171	-	-
TSIIR	186i	0.572651	-0.063508	-1883.329564	-1882.817409	-	-
TSIIS	211i	0.571570	-0.063443	-1883.325360	-1882.814221	-	-
18@24	-	-	-0.108881	-1576.274664	-1576.380533	-	-
19@23	-	-	-0.104276	-1248.320285	-1248.421549	-	-
24@18	-	-	-0.051253	-1576.229342	-1576.277583	-	-
23@19	-	-	-0.045647	-1248.496725	-1248.539360	-	-
18@24+19@23	-	-	-	-	-	7.78	9.41
24@18+23@19	-	-	-	-	-	18.57	16.50
23+24	-	-	-	-	-	-93.07	-18.58
24+TSI	-	-	-	-	-	-86.73	-14.91
21+24+25	-	-	-	-	-	-83.40	-22.49
21+ TSIIR	-	-	-	-	-	-96.54	-19.58
21+ TSIIS	-	-	-	-	-	-96.50	-19.30
21+26R	-	-	-	-	-	-109.28	-37.10
21+26S	-	-	-	-	-	-108.10	-36.50
21+ TSIIR	-	-	-	-	-	-105.10	-30.12
21+ TSIIS	-	-	-	-	-	-102.47	-28.12
20+21+22R	-	-	-	-	-	-105.32	-40.44
20+21+22S	-	-	-	-	-	-105.32	-40.61

7. Optimized structures of local minima and transition states along main reaction pathways.

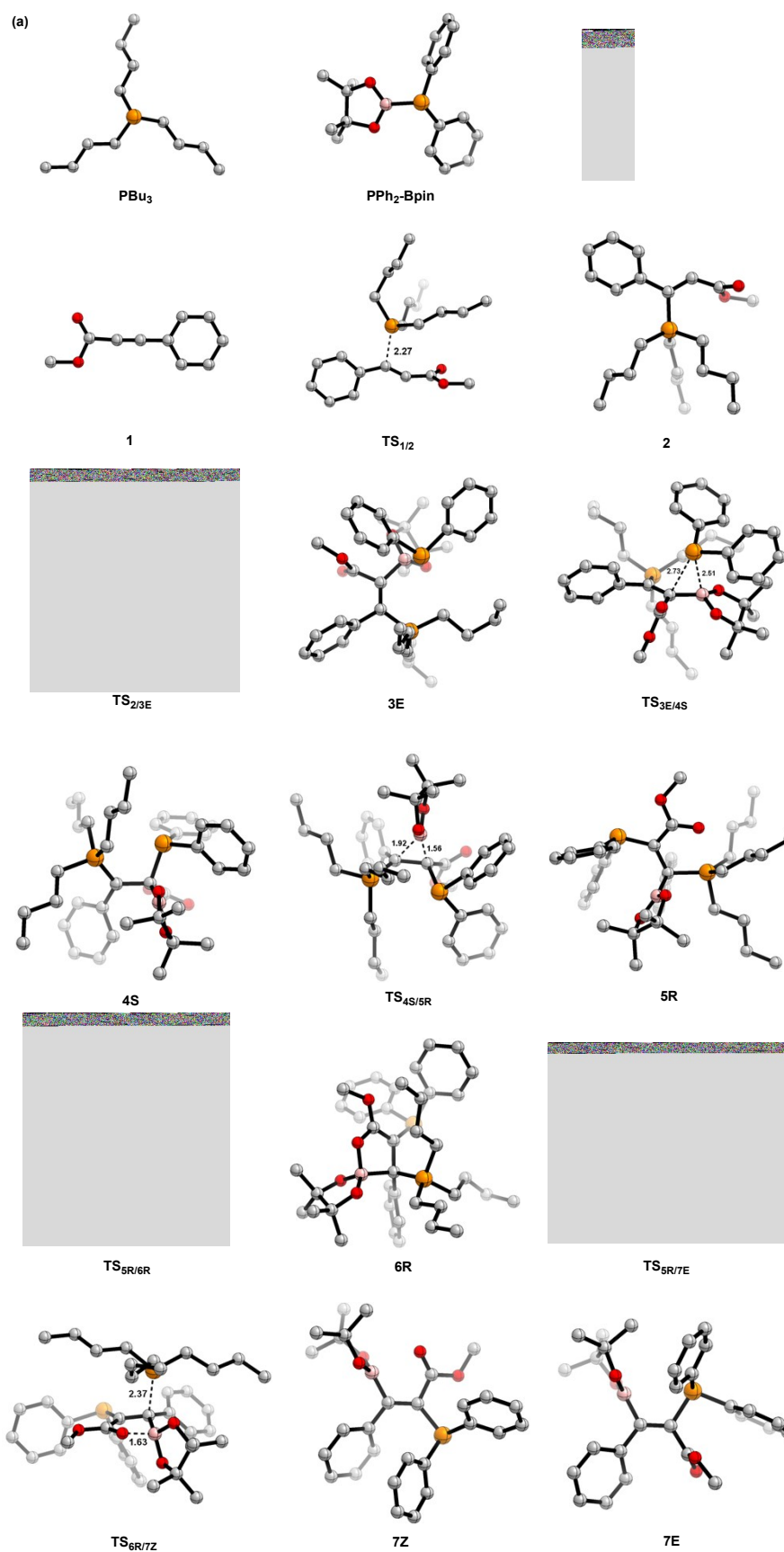


Fig. S12. Optimized structures of the P/B 3,4-addition pathway in the organocatalytic trans

phosphinoboration reaction.

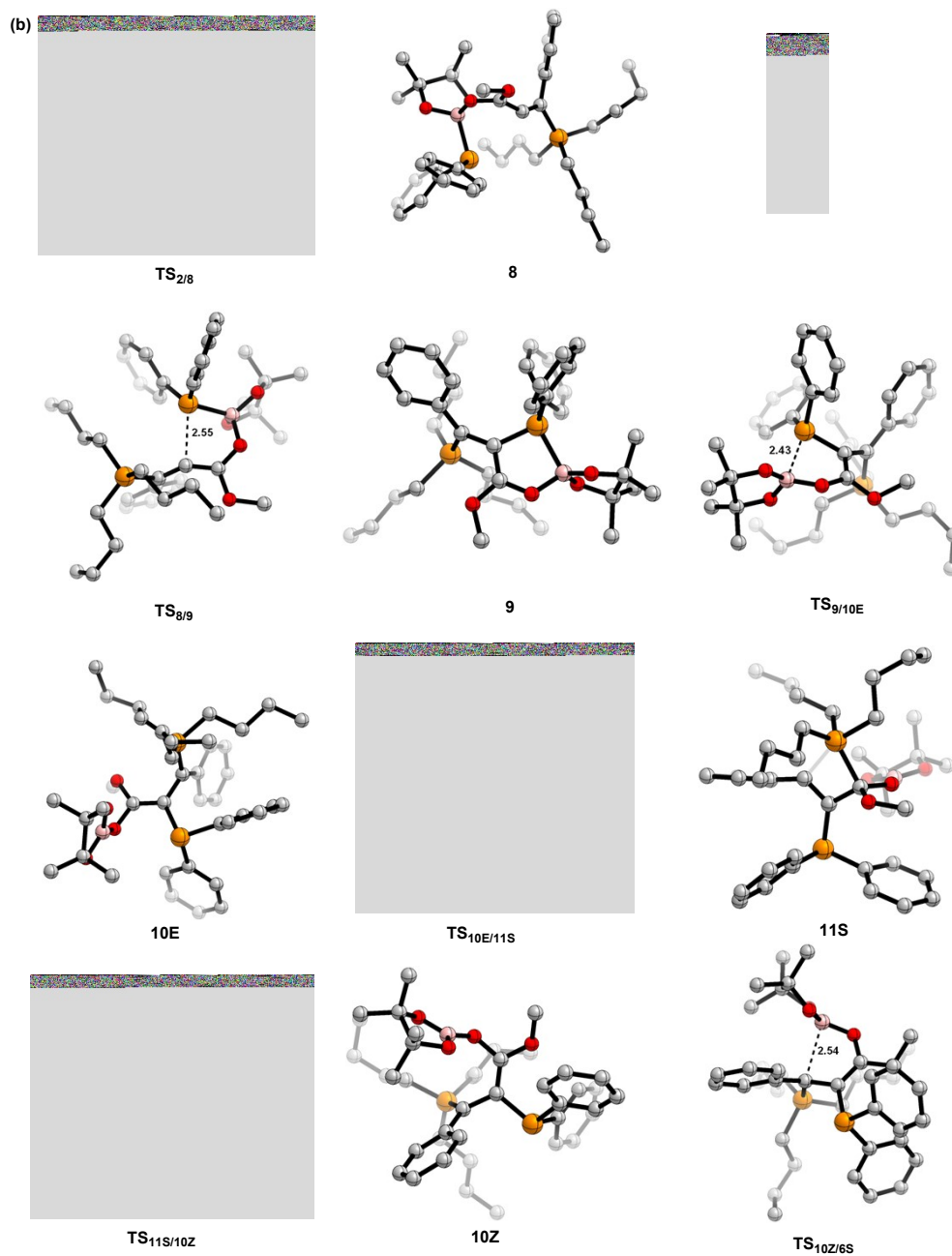


Fig. S13. Optimized structures of the P/B Michael addition pathway in the organocatalytic trans phosphinoboration reaction.

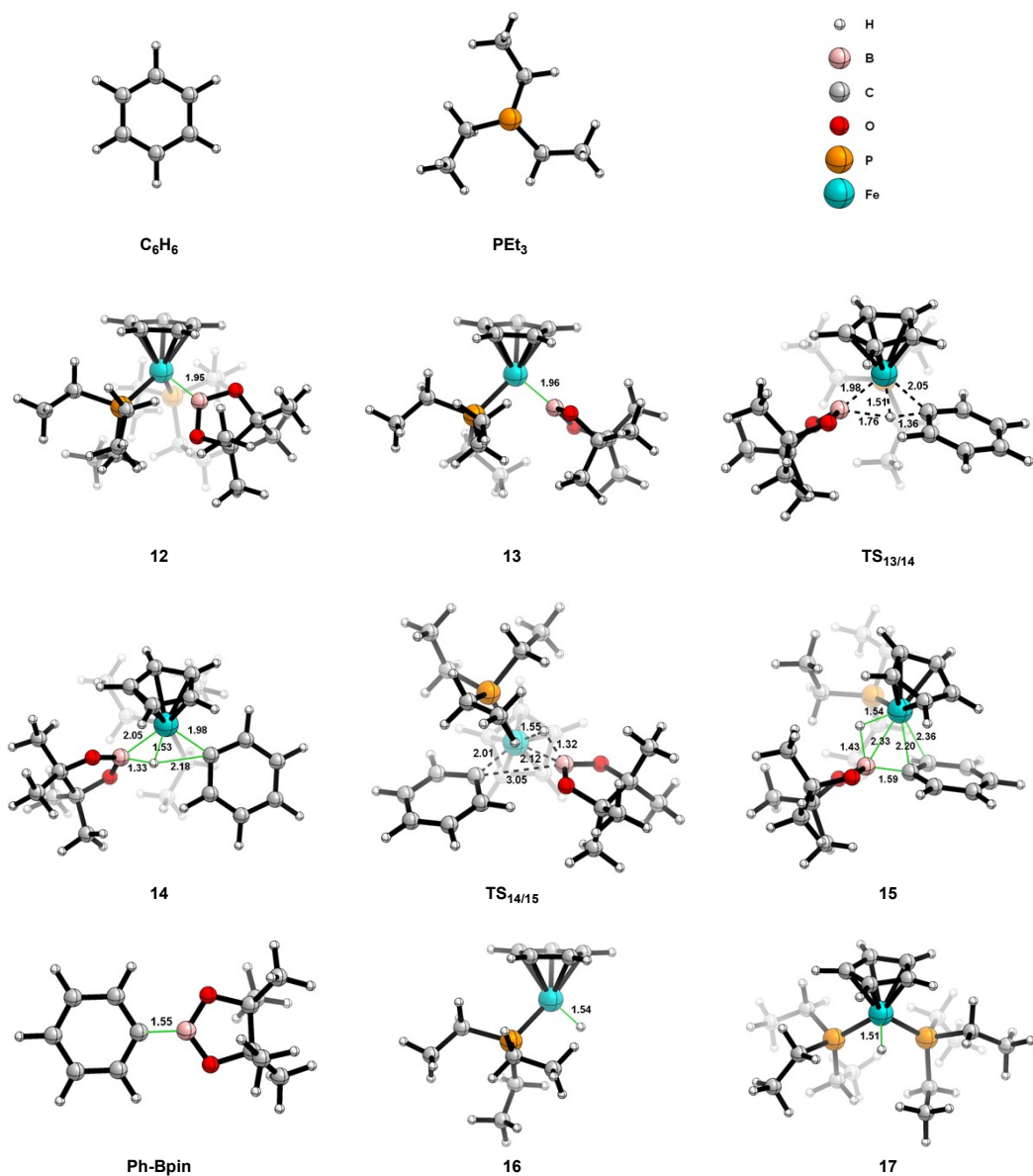


Fig. S14. Optimized structures along the main pathway of the Fe(II) complex mediated C-H borylation reaction.

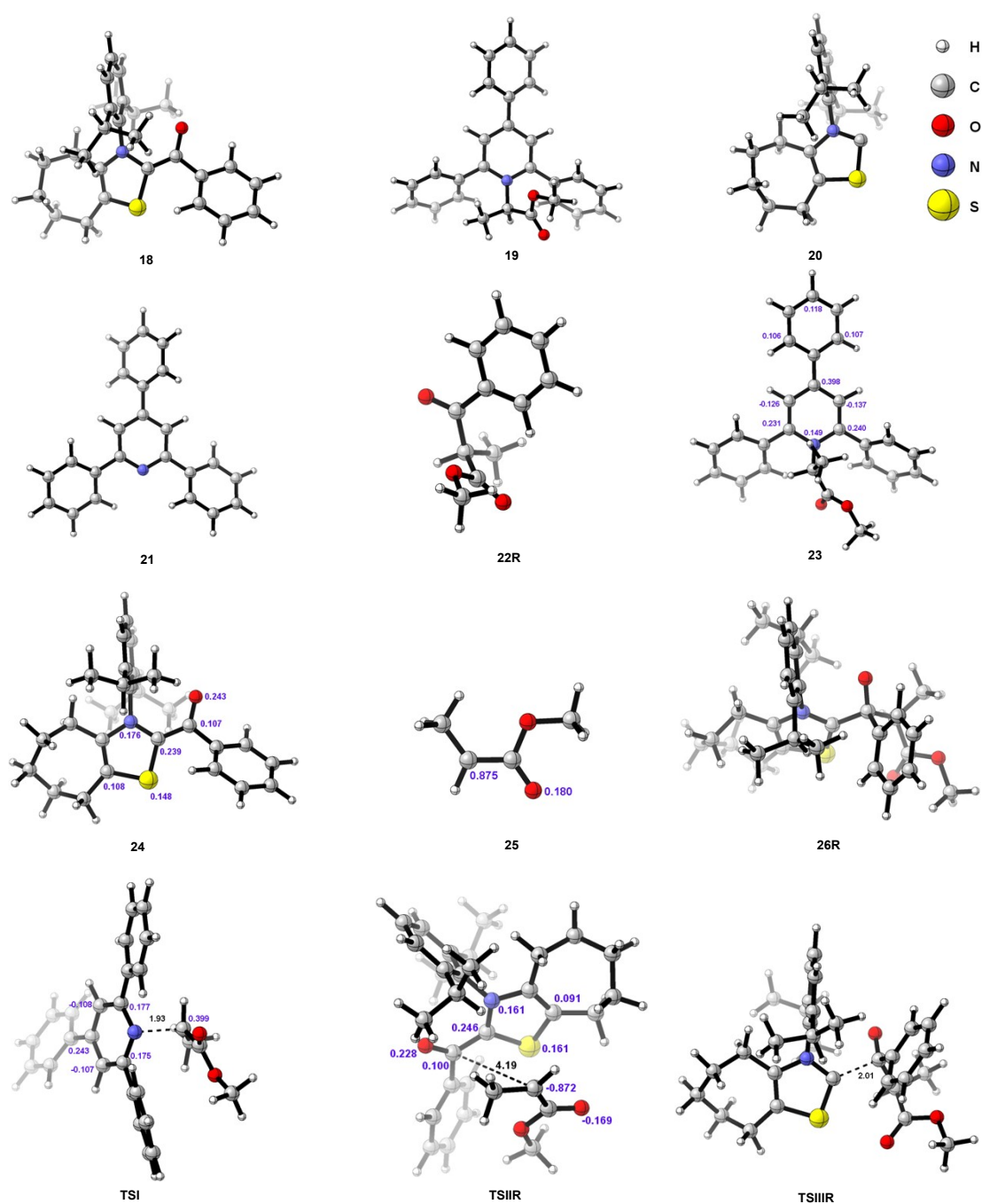


Fig. S15. Optimized structures along the main pathway of the SET-triggered deaminative cross-coupling reaction.

Reference

- (1) Marcus, R. A. On the Theory of Oxidation-Reduction Reactions Involving Electron Transfer. *J. Chem. Phys.* **1956**, 966-978.
- (2) Marcus, R. A. Chemical and Electrochemical Electron-Transfer Theory. *Annu. Rev. Phys. Chem.* **1964** 155-196.
- (3) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; et al. *Gaussian 16*, revision A.03; Gaussian, Inc., Wallingford CT, **2016**.
- (4) Lawrence, J. E.; Manolopoulos, D. E. Analytic continuation of Wolynes theory into the Marcus inverted regime. *J. Chem. Phys.* **2018**, 148, 102313.
- (5) Sandmeyer, T. Ueber die Ersetzung der Amidgruppe durch Chlor in den aromatischen Substanzen. *Ber. Dtsch. Chem. Ges.* **1884**, 17, 1633-1635.

9. DFT-optimized cartesian coordinates of all species involved in the organocatalytic *trans* phosphinoboration reaction.

PBu₃

P	0.718356000	0.010562000	-0.010459000
C	-0.175378000	1.655649000	0.041995000
C	0.241032000	2.606610000	-1.085985000
H	0.059024000	2.118458000	1.009408000
H	-1.263183000	1.493858000	0.022992000
C	-0.429152000	3.981672000	-0.986878000
H	1.332491000	2.731517000	-1.073616000
H	-0.003652000	2.160689000	-2.059943000
C	-0.012985000	4.928712000	-2.114903000
H	-1.520606000	3.853564000	-0.995467000
H	-0.182430000	4.432716000	-0.015608000
H	-0.504260000	5.903837000	-2.023309000
H	1.070631000	5.097695000	-2.107339000
H	-0.275273000	4.512822000	-3.095396000
C	-0.180790000	-0.770899000	-1.455754000
C	0.247609000	-2.216845000	-1.730211000
H	0.035181000	-0.157174000	-2.339802000
H	-1.267286000	-0.720112000	-1.292717000
C	-0.443554000	-2.819073000	-2.958844000
H	1.336840000	-2.254764000	-1.868167000
H	0.028982000	-2.845028000	-0.855626000
C	-0.020924000	-4.264468000	-3.232057000
H	-1.532719000	-2.773010000	-2.819453000
H	-0.221902000	-2.196703000	-3.837067000
H	-0.526590000	-4.670929000	-4.115079000
H	1.060058000	-4.333125000	-3.403928000
H	-0.261647000	-4.913080000	-2.380898000
C	-0.167299000	-0.856474000	1.393412000
C	0.273155000	-0.373148000	2.779806000
H	0.049706000	-1.928342000	1.298895000
H	-1.255140000	-0.742498000	1.277877000
C	-0.410187000	-1.132804000	3.922504000
H	1.362886000	-0.476800000	2.873144000
H	0.058695000	0.699069000	2.887708000
C	0.032471000	-0.650594000	5.305993000
H	-1.499842000	-1.027615000	3.825611000
H	-0.196810000	-2.205906000	3.819492000
H	-0.469759000	-1.206866000	6.105332000
H	1.113842000	-0.776039000	5.439173000
H	-0.195967000	0.413255000	5.444267000

PPh₂-Bpin

P	0.781132000	1.352854000	-0.033682000
B	-0.961033000	0.549756000	0.138372000
O	-1.566112000	0.291906000	1.339983000
O	-1.751034000	0.275729000	-0.944516000
C	-2.968828000	-0.001425000	1.057045000
C	-2.914189000	-0.450656000	-0.445919000
C	-3.443579000	-1.068588000	2.034585000
C	-3.736664000	1.304922000	1.271376000
C	-4.124753000	-0.059659000	-1.283185000
C	-2.598487000	-1.938775000	-0.622005000
H	-3.423677000	-0.668944000	3.052990000
H	-4.472184000	-1.369854000	1.807058000
H	-2.804381000	-1.953147000	2.005463000
H	-4.814752000	1.161880000	1.147966000
H	-3.548639000	1.663449000	2.287495000
H	-3.403674000	2.076679000	0.571073000
H	-3.976734000	-0.387607000	-2.316414000
H	-5.031222000	-0.540701000	-0.898939000
H	-4.277111000	1.021409000	-1.289768000
H	-3.449952000	-2.567562000	-0.343323000
H	-2.356439000	-2.125356000	-1.672182000
H	-1.735325000	-2.232896000	-0.016854000
C	1.742979000	0.429194000	1.248977000
C	2.985072000	-0.150035000	0.952655000
C	1.278861000	0.388148000	2.573764000
C	3.737723000	-0.766033000	1.953232000
H	3.363174000	-0.126479000	-0.064327000
C	2.032144000	-0.231935000	3.568895000
H	0.316717000	0.823786000	2.821846000
C	3.264994000	-0.812126000	3.264567000
H	4.696785000	-1.212365000	1.703300000
H	1.652274000	-0.262562000	4.586858000
H	3.851192000	-1.293661000	4.042292000
C	1.357277000	0.587997000	-1.610747000
C	1.978667000	1.406556000	-2.562279000
C	1.205002000	-0.778793000	-1.895381000
C	2.435305000	0.877024000	-3.771682000
H	2.103329000	2.465262000	-2.352376000
C	1.660631000	-1.309505000	-3.099289000
H	0.732037000	-1.428636000	-1.165488000
C	2.276430000	-0.481080000	-4.041680000
H	2.914629000	1.525918000	-4.499531000
H	1.535201000	-2.369156000	-3.305361000

H	2.630591000	-0.895490000	-4.981613000
1			
C	1.328215000	-0.029567000	-3.435859000
C	0.167975000	-0.014033000	-4.213711000
C	-1.086453000	0.010115000	-3.599529000
C	-1.185615000	0.018787000	-2.211967000
C	-0.020916000	0.003196000	-1.421411000
C	1.239650000	-0.021073000	-2.047572000
H	2.303466000	-0.048383000	-3.913245000
H	0.241382000	-0.020713000	-5.297365000
H	-1.988577000	0.022217000	-4.203965000
H	-2.154719000	0.037497000	-1.724391000
H	2.134449000	-0.033048000	-1.433929000
C	-0.118879000	0.011750000	-0.001852000
C	-0.198838000	0.018809000	1.208903000
C	-0.376324000	0.028260000	2.638146000
O	-1.452822000	0.048808000	3.200408000
O	0.815077000	0.011206000	3.276658000
C	0.724865000	0.019114000	4.710684000
H	0.181027000	-0.860240000	5.065654000
H	1.755630000	0.004086000	5.064820000
H	0.209652000	0.918645000	5.057684000
2			
P	0.290270000	0.067288000	0.003113000
C	1.640674000	-0.277361000	1.220368000
C	1.589093000	-1.554203000	2.075530000
H	1.698651000	0.602508000	1.867344000
H	2.548885000	-0.261413000	0.606695000
C	0.642686000	-1.459033000	3.277539000
H	1.331699000	-2.424148000	1.461610000
H	2.603722000	-1.744952000	2.449689000
C	0.598788000	-2.755402000	4.088255000
H	0.965924000	-0.626818000	3.916834000
H	-0.370700000	-1.207403000	2.944300000
H	-0.060458000	-2.660206000	4.957364000
H	0.229316000	-3.588986000	3.478204000
H	1.596484000	-3.028287000	4.451850000
C	0.761550000	-0.766770000	-1.565223000
C	1.510735000	-2.098838000	-1.424730000
H	1.346045000	-0.045916000	-2.143514000
H	-0.163941000	-0.910252000	-2.130908000
C	1.780441000	-2.729715000	-2.795827000
H	2.465470000	-1.944785000	-0.906260000
H	0.937431000	-2.805417000	-0.812550000

C	2.545157000	-4.050791000	-2.693157000
H	0.823711000	-2.891726000	-3.310262000
H	2.341456000	-2.018037000	-3.415162000
H	2.720972000	-4.485752000	-3.682672000
H	3.520831000	-3.906993000	-2.213491000
H	1.988139000	-4.785654000	-2.099011000
C	-1.351868000	-0.619281000	0.469167000
C	-1.543778000	-2.139780000	0.454478000
H	-2.011993000	-0.148274000	-0.270868000
H	-1.623600000	-0.194029000	1.441761000
C	-2.968731000	-2.531134000	0.863444000
H	-1.340192000	-2.525254000	-0.552091000
H	-0.832523000	-2.630911000	1.127612000
C	-3.190391000	-4.044730000	0.838468000
H	-3.172226000	-2.142664000	1.870757000
H	-3.684382000	-2.036949000	0.193162000
H	-2.504484000	-4.555334000	1.525471000
H	-4.212754000	-4.302752000	1.134098000
H	-3.019329000	-4.451705000	-0.165285000
C	0.344730000	3.401015000	3.183862000
C	0.902757000	4.641548000	2.878763000
C	1.172808000	4.961860000	1.544989000
C	0.903607000	4.047045000	0.531476000
C	0.354922000	2.788157000	0.823191000
C	0.070204000	2.487404000	2.164707000
H	0.107723000	3.146204000	4.213603000
H	1.118631000	5.354694000	3.669327000
H	1.600874000	5.929231000	1.295458000
H	1.098686000	4.286477000	-0.508982000
H	-0.400173000	1.540943000	2.422078000
C	0.064378000	1.853358000	-0.299627000
C	-0.410369000	2.250850000	-1.485371000
C	-0.762748000	1.536227000	-2.653348000
O	-0.110018000	1.421229000	-3.690094000
O	-2.055565000	1.008851000	-2.560853000
C	-2.572957000	0.503041000	-3.791821000
H	-2.573931000	1.275530000	-4.566551000
H	-1.983359000	-0.345106000	-4.156791000
H	-3.595386000	0.184783000	-3.575792000
3Z			
P	-1.212123000	-1.746394000	-1.155516000
C	-1.568267000	-3.381410000	-0.423040000
C	-0.728498000	-3.622053000	0.843394000
H	-1.406696000	-4.163567000	-1.173300000

H	-2.636966000	-3.372780000	-0.180978000
C	-1.288363000	-4.761299000	1.700398000
H	0.307552000	-3.846512000	0.558852000
H	-0.684058000	-2.703260000	1.442028000
C	-0.455725000	-5.001201000	2.961116000
H	-2.322864000	-4.518465000	1.979030000
H	-1.337884000	-5.681700000	1.102143000
H	-0.417592000	-4.099244000	3.582774000
H	-0.876756000	-5.810652000	3.566663000
H	0.575796000	-5.272978000	2.707718000
C	0.569235000	-1.662980000	-1.533551000
C	1.036950000	-2.699611000	-2.564433000
H	1.094441000	-1.785201000	-0.585016000
H	0.779427000	-0.646238000	-1.879511000
C	2.548502000	-2.596720000	-2.823268000
H	0.801287000	-3.712947000	-2.212460000
H	0.499247000	-2.559305000	-3.509921000
C	3.409059000	-2.885299000	-1.589561000
H	2.808610000	-3.301685000	-3.622659000
H	2.777098000	-1.593966000	-3.208620000
H	4.472858000	-2.880994000	-1.848394000
H	3.262020000	-2.140459000	-0.799841000
H	3.173399000	-3.870274000	-1.167413000
C	-2.119530000	-1.580686000	-2.733439000
C	-1.789229000	-0.245128000	-3.424365000
H	-3.185569000	-1.632624000	-2.487169000
H	-1.883906000	-2.442848000	-3.365893000
C	-2.745036000	0.083448000	-4.577601000
H	-1.826594000	0.565180000	-2.686971000
H	-0.758327000	-0.273899000	-3.801432000
C	-2.697940000	-0.922079000	-5.730938000
H	-3.768035000	0.152944000	-4.184108000
H	-2.493453000	1.083016000	-4.952824000
H	-3.025259000	-1.919858000	-5.416013000
H	-3.350698000	-0.609221000	-6.552495000
H	-1.680246000	-1.015064000	-6.130548000
P	-2.441140000	2.912928000	-0.254095000
B	-1.593517000	1.824045000	1.318130000
O	-0.483148000	2.465334000	2.000097000
O	-2.607581000	1.541860000	2.299931000
C	-0.804043000	2.604498000	3.388007000
C	-1.981778000	1.576370000	3.587260000
C	0.458451000	2.285195000	4.191649000
C	-1.225243000	4.056112000	3.651629000

C	-3.033531000	2.000073000	4.610352000
C	-1.478496000	0.161051000	3.919769000
H	0.258344000	2.280970000	5.269949000
H	0.873946000	1.317799000	3.901060000
H	1.217125000	3.050245000	3.993043000
H	-2.127629000	4.318115000	3.098190000
H	-1.399018000	4.240177000	4.718147000
H	-0.419820000	4.720139000	3.319641000
H	-3.818395000	1.237497000	4.663629000
H	-2.594588000	2.109126000	5.609164000
H	-3.498818000	2.944780000	4.322678000
H	-2.328038000	-0.528466000	3.879656000
H	-0.725452000	-0.173586000	3.200285000
H	-1.042552000	0.108341000	4.923453000
C	-3.220146000	4.291587000	0.680774000
C	-2.870612000	5.645543000	0.561732000
C	-4.288120000	3.956132000	1.537317000
C	-3.543109000	6.626771000	1.291863000
H	-2.061263000	5.936456000	-0.099560000
C	-4.953409000	4.936782000	2.269288000
H	-4.569486000	2.914696000	1.649700000
C	-4.582164000	6.279132000	2.155123000
H	-3.248317000	7.668338000	1.186945000
H	-5.765325000	4.651490000	2.934319000
H	-5.100478000	7.043701000	2.727777000
C	-0.952053000	3.687416000	-1.027529000
C	0.023217000	4.396056000	-0.304063000
C	-0.742025000	3.492489000	-2.400412000
C	1.161027000	4.893141000	-0.936722000
H	-0.105645000	4.519821000	0.763672000
C	0.406699000	3.970675000	-3.034749000
H	-1.495976000	2.961365000	-2.977279000
C	1.361164000	4.678321000	-2.304095000
H	1.901907000	5.442136000	-0.359932000
H	0.547967000	3.805202000	-4.100385000
H	2.250129000	5.066623000	-2.795255000
C	-5.598304000	-0.171422000	-0.368942000
C	-6.019792000	-0.921021000	0.729196000
C	-5.073182000	-1.504145000	1.573785000
C	-3.714086000	-1.338107000	1.315248000
C	-3.279470000	-0.588868000	0.212667000
C	-4.236835000	-0.010198000	-0.630810000
H	-6.328200000	0.302425000	-1.019072000
H	-7.080094000	-1.042001000	0.932586000

H	-5.392202000	-2.075405000	2.441076000
H	-2.974423000	-1.762535000	1.986377000
H	-3.912422000	0.619596000	-1.450666000
C	-1.804458000	-0.466769000	-0.040625000
C	-1.028027000	0.489191000	0.512464000
C	0.450541000	0.458840000	0.497314000
O	1.109107000	-0.239827000	1.252797000
O	0.983358000	1.325995000	-0.376473000
C	2.380301000	1.611613000	-0.202297000
H	2.981859000	0.708471000	-0.342230000
H	2.610992000	2.362176000	-0.955829000
H	2.544123000	2.009382000	0.801571000

3E

P	-1.169478000	-1.652353000	-1.233008000
C	-1.950190000	-3.201562000	-0.651761000
C	-1.545355000	-3.563590000	0.784565000
H	-1.695310000	-4.002943000	-1.354824000
H	-3.031942000	-3.042829000	-0.716366000
C	-2.449253000	-4.645477000	1.382414000
H	-0.499346000	-3.891968000	0.803559000
H	-1.582574000	-2.668068000	1.413825000
C	-2.070943000	-4.986516000	2.825240000
H	-3.490563000	-4.296657000	1.345228000
H	-2.403290000	-5.549872000	0.759809000
H	-2.163637000	-4.106604000	3.472543000
H	-2.717623000	-5.771333000	3.232136000
H	-1.034283000	-5.336822000	2.890759000
C	0.629872000	-1.863021000	-1.217395000
C	1.154194000	-2.936933000	-2.178654000
H	0.874108000	-2.092718000	-0.176153000
H	1.073129000	-0.880030000	-1.408879000
C	2.663212000	-3.159247000	-1.980877000
H	0.630625000	-3.890560000	-2.022623000
H	0.966394000	-2.639267000	-3.218100000
C	3.031047000	-3.735521000	-0.610286000
H	3.018000000	-3.835659000	-2.769071000
H	3.184690000	-2.204656000	-2.132618000
H	4.105067000	-3.941060000	-0.553037000
H	2.790997000	-3.048240000	0.206894000
H	2.500803000	-4.678839000	-0.426526000
C	-1.689963000	-1.439440000	-2.976182000
C	-1.145804000	-0.141133000	-3.587725000
H	-2.784675000	-1.454880000	-2.999412000
H	-1.342408000	-2.322924000	-3.522615000

C	-1.617270000	0.089867000	-5.029101000
H	-1.448704000	0.703694000	-2.960145000
H	-0.048803000	-0.155533000	-3.560399000
C	-1.111673000	-0.958775000	-6.023701000
H	-2.715583000	0.123134000	-5.050831000
H	-1.274597000	1.083144000	-5.344094000
H	-1.504489000	-1.957601000	-5.801319000
H	-1.414840000	-0.710251000	-7.046175000
H	-0.016424000	-1.019431000	-6.005477000
P	0.976839000	-0.626246000	1.878560000
B	0.435523000	0.953041000	0.643960000
O	0.571460000	2.256884000	1.263933000
O	1.280526000	0.961218000	-0.542657000
C	1.458579000	3.078636000	0.502895000
C	1.553077000	2.330637000	-0.883408000
C	0.842451000	4.477767000	0.417806000
C	2.799888000	3.161518000	1.243623000
C	2.931649000	2.385873000	-1.538741000
C	0.486418000	2.796513000	-1.887069000
H	1.430374000	5.136662000	-0.232528000
H	-0.184776000	4.432506000	0.052383000
H	0.823921000	4.922868000	1.418542000
H	3.275800000	2.184663000	1.327060000
H	3.493050000	3.854099000	0.752456000
H	2.612435000	3.530736000	2.257226000
H	2.913228000	1.831198000	-2.484080000
H	3.221196000	3.419539000	-1.759714000
H	3.691291000	1.938099000	-0.895243000
H	0.522143000	2.143199000	-2.765282000
H	-0.518102000	2.747759000	-1.457400000
H	0.666874000	3.823020000	-2.223685000
C	2.750216000	-0.270006000	2.193580000
C	3.296973000	0.031725000	3.450004000
C	3.630936000	-0.368393000	1.097459000
C	4.667929000	0.242968000	3.602897000
H	2.645430000	0.110129000	4.313876000
C	4.998970000	-0.156613000	1.251368000
H	3.229083000	-0.573497000	0.111270000
C	5.526779000	0.153615000	2.507027000
H	5.065639000	0.482290000	4.586225000
H	5.654628000	-0.227992000	0.386676000
H	6.593335000	0.321483000	2.629082000
C	0.128019000	-0.200093000	3.458671000
C	0.209881000	1.065436000	4.063891000

C	-0.698651000	-1.166966000	4.049182000
C	-0.508801000	1.345415000	5.224678000
H	0.807907000	1.834450000	3.590097000
C	-1.437748000	-0.881982000	5.199299000
H	-0.752590000	-2.156824000	3.603557000
C	-1.340497000	0.376176000	5.793267000
H	-0.430840000	2.328827000	5.682378000
H	-2.075411000	-1.645529000	5.638550000
H	-1.903836000	0.599916000	6.695735000
C	-5.580958000	-0.075830000	-1.119305000
C	-6.159019000	-0.582998000	0.044895000
C	-5.344285000	-0.973552000	1.109694000
C	-3.957752000	-0.876000000	1.003116000
C	-3.365223000	-0.389104000	-0.173388000
C	-4.193274000	0.022240000	-1.226723000
H	-6.209758000	0.257033000	-1.940228000
H	-7.239391000	-0.659224000	0.128147000
H	-5.788353000	-1.347730000	2.027858000
H	-3.321039000	-1.146972000	1.839417000
H	-3.748971000	0.456249000	-2.116975000
C	-1.867391000	-0.303028000	-0.253674000
C	-1.172783000	0.681295000	0.361458000
C	-2.007805000	1.777651000	0.946702000
O	-2.362956000	2.751318000	0.311571000
O	-2.284951000	1.572378000	2.241450000
C	-2.920512000	2.664787000	2.920923000
H	-3.899435000	2.872420000	2.480812000
H	-3.014938000	2.339420000	3.955850000
H	-2.293665000	3.557205000	2.852816000
4R			
P	-1.706359000	-1.277602000	-0.515492000
C	-3.480027000	-1.567044000	-0.956259000
C	-4.262764000	-0.298000000	-1.359529000
H	-3.938102000	-2.034553000	-0.080041000
H	-3.492300000	-2.321473000	-1.749917000
C	-5.655759000	-0.231231000	-0.724604000
H	-3.698437000	0.592783000	-1.067937000
H	-4.356071000	-0.259814000	-2.450961000
C	-6.368987000	1.083494000	-1.042278000
H	-6.261098000	-1.082280000	-1.069393000
H	-5.553614000	-0.332397000	0.360940000
H	-7.367278000	1.115635000	-0.591556000
H	-5.795783000	1.930340000	-0.647942000
H	-6.483651000	1.228024000	-2.124077000

C	-1.143337000	-2.949885000	0.070199000
C	-1.436500000	-4.149688000	-0.837073000
H	-1.593941000	-3.094844000	1.059330000
H	-0.067624000	-2.840770000	0.238351000
C	-0.769862000	-5.435088000	-0.331344000
H	-2.519721000	-4.311090000	-0.910230000
H	-1.088142000	-3.948845000	-1.860011000
C	-1.068447000	-6.648808000	-1.214078000
H	0.315900000	-5.275247000	-0.273857000
H	-1.104022000	-5.632214000	0.696471000
H	-2.146228000	-6.846056000	-1.261230000
H	-0.716915000	-6.486450000	-2.240323000
H	-0.579902000	-7.552197000	-0.832682000
C	-0.767784000	-1.018660000	-2.086145000
C	-1.591584000	-0.523472000	-3.278897000
H	-0.236044000	-1.944499000	-2.336723000
H	-0.014180000	-0.261709000	-1.872717000
C	-0.697364000	-0.158341000	-4.467594000
H	-2.317856000	-1.287151000	-3.586383000
H	-2.151204000	0.363921000	-2.974736000
C	-1.501764000	0.314041000	-5.680438000
H	-0.005187000	0.633884000	-4.153403000
H	-0.076863000	-1.022503000	-4.746745000
H	-0.846563000	0.588781000	-6.514559000
H	-2.182261000	-0.470357000	-6.033779000
H	-2.108983000	1.190870000	-5.426917000
P	-0.040665000	1.685544000	2.357003000
B	1.026362000	0.337425000	0.076416000
O	1.396524000	-0.958857000	0.340246000
O	1.951876000	1.004702000	-0.684136000
C	2.764465000	-1.160231000	-0.116051000
C	3.016995000	0.087739000	-1.058868000
C	3.645208000	-1.180135000	1.132592000
C	2.822889000	-2.513974000	-0.818612000
C	2.845696000	-0.202902000	-2.552875000
C	4.354210000	0.788417000	-0.836717000
H	4.691639000	-1.373378000	0.876214000
H	3.582863000	-0.240896000	1.681854000
H	3.300400000	-1.978990000	1.796460000
H	2.591959000	-3.306797000	-0.100038000
H	2.103655000	-2.578582000	-1.637877000
H	3.824793000	-2.701901000	-1.218649000
H	1.896682000	-0.692465000	-2.774288000
H	2.866311000	0.745955000	-3.096968000

H	3.657560000	-0.833134000	-2.929561000
H	4.472981000	1.118142000	0.194743000
H	5.184341000	0.122297000	-1.096648000
H	4.410189000	1.669032000	-1.484231000
C	-0.500524000	0.243697000	3.409127000
C	-0.105298000	-1.083207000	3.179280000
C	-1.332509000	0.522376000	4.500027000
C	-0.546646000	-2.103379000	4.019356000
H	0.535314000	-1.314298000	2.338524000
C	-1.764556000	-0.497665000	5.349637000
H	-1.670254000	1.541629000	4.663439000
C	-1.377945000	-1.813983000	5.105883000
H	-0.240427000	-3.129185000	3.827496000
H	-2.417377000	-0.264443000	6.186054000
H	-1.721735000	-2.613498000	5.757091000
C	1.794550000	1.738711000	2.617275000
C	2.584549000	2.630072000	1.867327000
C	2.402867000	1.069340000	3.694663000
C	3.932838000	2.817526000	2.164544000
H	2.138133000	3.166980000	1.040047000
C	3.751159000	1.265353000	3.995277000
H	1.819757000	0.387183000	4.301781000
C	4.526725000	2.134751000	3.228444000
H	4.522015000	3.504727000	1.562411000
H	4.195679000	0.729926000	4.830258000
H	5.577216000	2.285975000	3.461026000
C	-4.498585000	-0.316317000	2.921815000
C	-4.927260000	1.004721000	3.067728000
C	-4.239416000	2.011199000	2.385892000
C	-3.159375000	1.704033000	1.561438000
C	-2.702877000	0.375762000	1.398040000
C	-3.404334000	-0.618132000	2.117327000
H	-4.995925000	-1.114588000	3.467502000
H	-5.771005000	1.246675000	3.707553000
H	-4.554736000	3.047198000	2.484203000
H	-2.668082000	2.506785000	1.022469000
H	-3.033012000	-1.638245000	2.101720000
C	-1.544434000	0.051813000	0.553607000
C	-0.346776000	0.984720000	0.526735000
C	-0.571207000	2.175847000	-0.407978000
O	-1.235172000	2.151444000	-1.425646000
O	0.100320000	3.285214000	-0.022118000
C	0.018318000	4.404211000	-0.914571000
H	0.434915000	4.140987000	-1.890369000

H	-1.021246000	4.715614000	-1.041882000
H	0.602766000	5.196221000	-0.445522000
4S			
P	0.135583000	-0.694267000	-0.548000000
C	0.352409000	-2.521566000	-0.385339000
C	-0.923221000	-3.270572000	0.010431000
H	1.146825000	-2.734261000	0.331364000
H	0.710920000	-2.856267000	-1.368054000
C	-0.685931000	-4.772640000	0.190526000
H	-1.310053000	-2.852352000	0.944252000
H	-1.699419000	-3.110919000	-0.749194000
C	-1.962429000	-5.515174000	0.591048000
H	-0.280941000	-5.200311000	-0.737879000
H	0.082160000	-4.919594000	0.961810000
H	-1.779273000	-6.586988000	0.725427000
H	-2.361489000	-5.121124000	1.533158000
H	-2.741249000	-5.401489000	-0.173229000
C	1.843361000	-0.138965000	-1.072336000
C	2.874821000	-0.134877000	0.058454000
H	1.728899000	0.874552000	-1.469335000
H	2.176172000	-0.772383000	-1.905235000
C	4.176247000	0.574320000	-0.333146000
H	2.441868000	0.357353000	0.938657000
H	3.104513000	-1.163597000	0.366662000
C	5.167496000	0.666151000	0.829003000
H	4.639102000	0.050061000	-1.180366000
H	3.939405000	1.584835000	-0.693718000
H	6.091286000	1.173062000	0.529241000
H	4.734426000	1.223917000	1.668422000
H	5.437106000	-0.329918000	1.200272000
C	-0.881276000	-0.550460000	-2.097833000
C	-0.231196000	0.038425000	-3.352362000
H	-1.767175000	0.027384000	-1.837477000
H	-1.236450000	-1.567322000	-2.307478000
C	-1.266902000	0.223655000	-4.468231000
H	0.204517000	1.013991000	-3.113032000
H	0.587197000	-0.599069000	-3.712439000
C	-0.672669000	0.859313000	-5.726703000
H	-1.715414000	-0.748044000	-4.718504000
H	-2.084777000	0.849862000	-4.086874000
H	-0.253234000	1.848801000	-5.506148000
H	0.136148000	0.243128000	-6.137758000
H	-1.429078000	0.983976000	-6.509545000
P	-0.685683000	2.441566000	-0.580918000

B	-2.874370000	0.964739000	0.556788000
O	-3.352721000	0.711412000	-0.709580000
O	-3.826942000	0.756647000	1.519575000
C	-4.628608000	0.033332000	-0.581232000
C	-5.087217000	0.451816000	0.866097000
C	-5.529196000	0.514087000	-1.712872000
C	-4.343969000	-1.465185000	-0.712905000
C	-5.779012000	-0.647547000	1.665053000
C	-5.920307000	1.734380000	0.897107000
H	-6.536709000	0.094398000	-1.617434000
H	-5.596533000	1.603699000	-1.728928000
H	-5.114125000	0.188359000	-2.672066000
H	-3.652728000	-1.801551000	0.064883000
H	-5.262313000	-2.056989000	-0.649512000
H	-3.877858000	-1.655527000	-1.684398000
H	-6.032830000	-0.268323000	2.659534000
H	-6.706065000	-0.962541000	1.173207000
H	-5.132592000	-1.518517000	1.790766000
H	-5.439015000	2.531134000	0.326436000
H	-6.924529000	1.568817000	0.493212000
H	-6.012193000	2.067211000	1.934973000
C	-2.139672000	3.419155000	-1.146365000
C	-2.270602000	3.579281000	-2.533001000
C	-3.121629000	3.965138000	-0.303928000
C	-3.356431000	4.267960000	-3.074479000
H	-1.520800000	3.150171000	-3.192609000
C	-4.206013000	4.654997000	-0.847548000
H	-3.042110000	3.833717000	0.771220000
C	-4.328804000	4.805837000	-2.230853000
H	-3.444964000	4.378941000	-4.151744000
H	-4.959850000	5.074480000	-0.186396000
H	-5.177573000	5.340979000	-2.647921000
C	0.348456000	3.696820000	0.288055000
C	1.662211000	3.321494000	0.613626000
C	-0.079394000	4.987965000	0.624695000
C	2.517815000	4.198343000	1.274421000
H	2.007766000	2.327116000	0.363741000
C	0.781792000	5.873007000	1.275970000
H	-1.086084000	5.306702000	0.381505000
C	2.079207000	5.481739000	1.607564000
H	3.526814000	3.880788000	1.524141000
H	0.432510000	6.870490000	1.528691000
H	2.745342000	6.172720000	2.116766000
C	0.734381000	-2.215761000	3.707962000

C	-0.358874000	-2.281183000	4.570497000
C	-1.506983000	-1.559988000	4.235060000
C	-1.580320000	-0.830267000	3.051962000
C	-0.495225000	-0.769399000	2.142489000
C	0.674197000	-1.455804000	2.541481000
H	1.659206000	-2.731545000	3.957433000
H	-0.311814000	-2.860858000	5.487981000
H	-2.370786000	-1.576620000	4.896162000
H	-2.501120000	-0.309074000	2.825725000
H	1.571607000	-1.361738000	1.944551000
C	-0.592205000	-0.027817000	0.869669000
C	-1.360255000	1.318611000	0.847636000
C	-1.207598000	2.135843000	2.118677000
O	-2.025992000	2.947044000	2.517693000
O	-0.028008000	1.939613000	2.730675000
C	0.217613000	2.769603000	3.871914000
H	-0.535621000	2.586473000	4.642218000
H	1.207744000	2.484553000	4.227667000
H	0.199002000	3.823621000	3.584649000

5R

P	-1.541491000	-0.934187000	-0.739851000
C	-3.383537000	-1.033123000	-0.931838000
C	-4.244107000	0.160017000	-1.339485000
H	-3.721820000	-1.414649000	0.037415000
H	-3.530109000	-1.853414000	-1.644335000
C	-5.731836000	-0.209841000	-1.310318000
H	-4.062404000	1.001463000	-0.667768000
H	-3.962251000	0.510493000	-2.335859000
C	-6.629249000	0.962395000	-1.713332000
H	-5.915413000	-1.062704000	-1.979635000
H	-6.000417000	-0.550675000	-0.300297000
H	-7.689255000	0.686873000	-1.683443000
H	-6.485165000	1.815771000	-1.039852000
H	-6.399204000	1.302225000	-2.730297000
C	-1.335236000	-2.721036000	-0.178760000
C	-1.571021000	-3.818104000	-1.224108000
H	-2.005640000	-2.878880000	0.671205000
H	-0.323908000	-2.830971000	0.226611000
C	-1.331978000	-5.219680000	-0.648662000
H	-2.596751000	-3.766734000	-1.611316000
H	-0.911159000	-3.678422000	-2.089218000
C	-1.552642000	-6.328328000	-1.679942000
H	-0.305995000	-5.276628000	-0.258265000
H	-1.994922000	-5.374520000	0.213159000

H	-2.580324000	-6.311914000	-2.062508000
H	-0.878673000	-6.209104000	-2.537010000
H	-1.372821000	-7.319000000	-1.248432000
C	-0.575467000	-0.962823000	-2.316805000
C	-1.451201000	-0.956001000	-3.573359000
H	0.069193000	-1.844780000	-2.299670000
H	0.067379000	-0.085421000	-2.299281000
C	-0.601950000	-0.954707000	-4.849216000
H	-2.115478000	-1.830579000	-3.588671000
H	-2.086700000	-0.065854000	-3.556681000
C	-1.453522000	-0.940341000	-6.120565000
H	0.060160000	-0.078563000	-4.835779000
H	0.054455000	-1.836429000	-4.852483000
H	-0.829752000	-0.932198000	-7.021126000
H	-2.102585000	-1.823116000	-6.170809000
H	-2.097835000	-0.053621000	-6.150660000
P	-0.167546000	2.616372000	1.913955000
B	0.686914000	-0.643215000	0.865895000
O	1.326385000	-1.225570000	1.926951000
O	1.471286000	-0.617583000	-0.264068000
C	2.709466000	-1.500128000	1.552284000
C	2.669334000	-1.403363000	-0.022498000
C	3.585981000	-0.432001000	2.206110000
C	3.066810000	-2.876795000	2.103666000
C	2.474114000	-2.752732000	-0.722550000
C	3.853720000	-0.676859000	-0.649872000
H	4.643000000	-0.599221000	1.976958000
H	3.313198000	0.571441000	1.877034000
H	3.462363000	-0.483996000	3.291599000
H	3.017226000	-2.852014000	3.196315000
H	2.377556000	-3.647506000	1.751662000
H	4.085371000	-3.158931000	1.815660000
H	1.622125000	-3.306768000	-0.321034000
H	2.293214000	-2.577518000	-1.787131000
H	3.365320000	-3.380209000	-0.625628000
H	3.954123000	0.335283000	-0.259939000
H	4.784247000	-1.224487000	-0.464010000
H	3.706850000	-0.614296000	-1.732897000
C	-0.283406000	1.731753000	3.535822000
C	0.734407000	0.960408000	4.110645000
C	-1.480842000	1.885073000	4.252190000
C	0.556866000	0.345240000	5.349345000
H	1.671042000	0.837826000	3.587189000
C	-1.670271000	1.256471000	5.480424000

H	-2.275204000	2.494288000	3.830269000
C	-0.648930000	0.483383000	6.035582000
H	1.360202000	-0.253310000	5.772310000
H	-2.614304000	1.371829000	6.005779000
H	-0.792038000	-0.002908000	6.996976000
C	1.663291000	2.754213000	1.668498000
C	2.502984000	3.220967000	2.695352000
C	2.212681000	2.594840000	0.387722000
C	3.852555000	3.476793000	2.459157000
H	2.097937000	3.373006000	3.691867000
C	3.558341000	2.875248000	0.144653000
H	1.576746000	2.240463000	-0.416664000
C	4.388962000	3.305215000	1.180453000
H	4.486545000	3.817181000	3.274094000
H	3.959559000	2.753346000	-0.858716000
H	5.438538000	3.514755000	0.992934000
C	-2.429806000	-1.872699000	3.850073000
C	-3.677456000	-1.253834000	3.891029000
C	-3.967746000	-0.243512000	2.971929000
C	-3.016720000	0.132014000	2.028316000
C	-1.768933000	-0.505119000	1.954057000
C	-1.487441000	-1.511539000	2.884530000
H	-2.178918000	-2.640761000	4.576616000
H	-4.409381000	-1.542134000	4.640520000
H	-4.928707000	0.263634000	3.000035000
H	-3.219574000	0.950333000	1.346041000
H	-0.520485000	-1.996624000	2.873297000
C	-0.808205000	-0.088951000	0.826192000
C	-0.732365000	1.430322000	0.666371000
C	-1.223756000	1.927582000	-0.528287000
O	-1.735723000	1.201422000	-1.445544000
O	-1.126772000	3.272859000	-0.751869000
C	-1.777892000	3.760972000	-1.920361000
H	-1.381515000	3.287911000	-2.824158000
H	-2.858704000	3.584536000	-1.880059000
H	-1.577971000	4.833990000	-1.937568000
5S			
P	-1.889937000	-0.062648000	0.052215000
C	-3.174353000	0.039111000	-1.282526000
C	-3.495716000	1.329154000	-2.033273000
H	-2.863731000	-0.732457000	-1.995039000
H	-4.084393000	-0.343097000	-0.805317000
C	-4.534739000	1.070695000	-3.130718000
H	-2.588078000	1.742303000	-2.478624000

H	-3.860317000	2.091964000	-1.340290000
C	-4.882565000	2.339120000	-3.912946000
H	-5.447625000	0.649573000	-2.685420000
H	-4.150165000	0.305723000	-3.820274000
H	-5.618497000	2.137951000	-4.699316000
H	-3.990101000	2.762717000	-4.389005000
H	-5.299969000	3.107817000	-3.251504000
C	-2.096314000	-1.914523000	0.338441000
C	-3.408992000	-2.392619000	0.970560000
H	-1.954783000	-2.415324000	-0.623678000
H	-1.262006000	-2.248840000	0.963711000
C	-3.404644000	-3.906769000	1.216635000
H	-4.259478000	-2.143630000	0.323056000
H	-3.592307000	-1.883076000	1.925104000
C	-4.708859000	-4.412021000	1.836688000
H	-2.560130000	-4.160293000	1.873127000
H	-3.218375000	-4.426077000	0.266863000
H	-5.563853000	-4.199894000	1.183411000
H	-4.901529000	-3.927077000	2.801495000
H	-4.678986000	-5.493812000	2.006593000
C	-2.398744000	0.580523000	1.709777000
C	-3.793687000	1.212711000	1.716632000
H	-2.347446000	-0.248317000	2.419900000
H	-1.647431000	1.310970000	2.002515000
C	-4.173547000	1.722193000	3.111074000
H	-4.548564000	0.486939000	1.384851000
H	-3.808009000	2.043146000	1.004470000
C	-5.563982000	2.360001000	3.145665000
H	-3.421676000	2.451165000	3.442089000
H	-4.130871000	0.889618000	3.827644000
H	-5.814266000	2.721345000	4.149145000
H	-6.335789000	1.639985000	2.847205000
H	-5.622691000	3.212192000	2.458161000
P	2.196971000	1.753145000	-1.182624000
B	0.676812000	-0.690934000	0.858641000
O	1.527326000	-1.761854000	0.919763000
O	0.409500000	-0.167117000	2.103000000
C	2.004141000	-1.907647000	2.290824000
C	0.963987000	-1.052676000	3.112902000
C	3.426755000	-1.351004000	2.345411000
C	2.013629000	-3.398050000	2.614712000
C	-0.198194000	-1.872018000	3.685243000
C	1.569031000	-0.201395000	4.223638000
H	3.850384000	-1.456174000	3.349029000

H	3.459668000	-0.297684000	2.063452000
H	4.057156000	-1.913475000	1.650651000
H	2.731344000	-3.904776000	1.962713000
H	1.033847000	-3.854228000	2.457013000
H	2.317861000	-3.568733000	3.653119000
H	-0.685810000	-2.487502000	2.925302000
H	-0.946006000	-1.188315000	4.097646000
H	0.142373000	-2.530731000	4.489934000
H	2.332462000	0.475886000	3.843210000
H	2.011732000	-0.838280000	4.997539000
H	0.780223000	0.398683000	4.688470000
C	2.877197000	0.230889000	-1.987209000
C	3.553043000	-0.800986000	-1.323821000
C	2.719760000	0.130464000	-3.378454000
C	4.040581000	-1.904978000	-2.022061000
H	3.697316000	-0.744556000	-0.254942000
C	3.187788000	-0.979695000	-4.077343000
H	2.210272000	0.928000000	-3.912176000
C	3.853238000	-2.002973000	-3.400249000
H	4.557451000	-2.695973000	-1.483866000
H	3.035466000	-1.045080000	-5.151163000
H	4.225061000	-2.867152000	-3.944421000
C	3.194342000	1.853352000	0.374818000
C	4.593905000	1.718245000	0.353531000
C	2.590313000	2.283913000	1.565137000
C	5.356542000	1.963062000	1.494155000
H	5.088851000	1.407666000	-0.562249000
C	3.356120000	2.554039000	2.700447000
H	1.511902000	2.397268000	1.595510000
C	4.741049000	2.383245000	2.675964000
H	6.435213000	1.832238000	1.458944000
H	2.866858000	2.895539000	3.609596000
H	5.335674000	2.585127000	3.562745000
C	0.319586000	-2.974352000	-2.997392000
C	-0.147825000	-2.361807000	-4.158319000
C	-0.528603000	-1.019152000	-4.114319000
C	-0.442237000	-0.311218000	-2.919730000
C	-0.005809000	-0.923948000	-1.735534000
C	0.381573000	-2.267294000	-1.794519000
H	0.646449000	-4.010385000	-3.022431000
H	-0.198681000	-2.917792000	-5.090438000
H	-0.878008000	-0.518290000	-5.013467000
H	-0.689855000	0.744373000	-2.893115000
H	0.756075000	-2.756515000	-0.905243000

C	-0.028189000	-0.092612000	-0.440825000
C	0.519331000	1.319353000	-0.655180000
C	-0.403242000	2.338910000	-0.502966000
O	-1.635526000	2.145524000	-0.223993000
O	0.031398000	3.628159000	-0.628129000
C	-0.976385000	4.633813000	-0.599549000
H	-1.535475000	4.610562000	0.341091000
H	-1.683691000	4.516554000	-1.428253000
H	-0.443697000	5.581535000	-0.697954000
6R			
P	1.035677000	-0.521560000	-0.326613000
C	1.276668000	1.164711000	-0.988320000
C	1.749804000	2.212778000	0.034605000
H	0.316178000	1.466492000	-1.407793000
H	1.981593000	1.084990000	-1.824483000
C	1.342417000	3.626738000	-0.396272000
H	1.329849000	2.007144000	1.022614000
H	2.840471000	2.151278000	0.144895000
C	1.834148000	4.696890000	0.578827000
H	1.727503000	3.832327000	-1.404433000
H	0.250116000	3.669350000	-0.470940000
H	2.929189000	4.707861000	0.645005000
H	1.506366000	5.695552000	0.270156000
H	1.445227000	4.513436000	1.587859000
C	0.969573000	-1.631490000	-1.794083000
C	-0.249144000	-1.433489000	-2.702653000
H	0.985423000	-2.657624000	-1.415446000
H	1.903423000	-1.474486000	-2.344564000
C	-0.382277000	-2.541490000	-3.755006000
H	-1.161221000	-1.402908000	-2.100760000
H	-0.174991000	-0.459516000	-3.201978000
C	0.790541000	-2.622190000	-4.736318000
H	-0.504836000	-3.503877000	-3.239767000
H	-1.311792000	-2.371742000	-4.312404000
H	1.728708000	-2.880976000	-4.231550000
H	0.612513000	-3.384018000	-5.502946000
H	0.941972000	-1.663365000	-5.248230000
C	2.596174000	-0.962201000	0.537264000
C	3.868199000	-0.778468000	-0.300132000
H	2.507553000	-1.999130000	0.875678000
H	2.618351000	-0.368786000	1.454208000
C	5.124109000	-1.114718000	0.513206000
H	3.839726000	-1.414334000	-1.194654000
H	3.941045000	0.256630000	-0.656291000

C	6.413845000	-0.929686000	-0.288572000
H	5.148429000	-0.481228000	1.409767000
H	5.054212000	-2.150503000	0.872194000
H	7.295229000	-1.173080000	0.314301000
H	6.426171000	-1.575940000	-1.174640000
H	6.519675000	0.106400000	-0.632097000
P	-2.583695000	0.795620000	-0.947084000
B	-0.211970000	-0.283701000	2.378388000
O	1.051110000	-0.630529000	2.956012000
O	-1.244216000	-0.869650000	3.179730000
C	0.825456000	-1.355484000	4.177379000
C	-0.697367000	-1.077341000	4.483277000
C	1.115650000	-2.837251000	3.909982000
C	1.795843000	-0.829614000	5.234372000
C	-0.914305000	0.195991000	5.318224000
C	-1.440766000	-2.243945000	5.131210000
H	1.070908000	-3.432597000	4.828445000
H	0.405535000	-3.251183000	3.191739000
H	2.124891000	-2.930282000	3.492800000
H	1.617672000	-1.305454000	6.205802000
H	2.825178000	-1.053043000	4.932540000
H	1.706376000	0.252424000	5.351892000
H	-0.585594000	0.067371000	6.355618000
H	-0.388765000	1.048275000	4.881729000
H	-1.984771000	0.426709000	5.321377000
H	-1.433310000	-3.123482000	4.484123000
H	-1.000123000	-2.508901000	6.099527000
H	-2.485172000	-1.960801000	5.298521000
C	-4.153958000	1.212281000	-0.062451000
C	-5.220980000	1.754505000	-0.797298000
C	-4.358278000	0.913840000	1.292939000
C	-6.449013000	2.012155000	-0.191721000
H	-5.083175000	1.990107000	-1.849624000
C	-5.593415000	1.160817000	1.894806000
H	-3.550551000	0.488485000	1.881311000
C	-6.641010000	1.714752000	1.159525000
H	-7.258403000	2.442477000	-0.775931000
H	-5.731645000	0.923215000	2.946490000
H	-7.599548000	1.911208000	1.632112000
C	-2.187546000	2.420075000	-1.761218000
C	-2.554167000	3.680165000	-1.262674000
C	-1.460169000	2.370006000	-2.960662000
C	-2.162878000	4.846433000	-1.918228000
H	-3.140660000	3.740669000	-0.354940000

C	-1.054696000	3.536023000	-3.612374000
H	-1.217333000	1.402936000	-3.392818000
C	-1.399972000	4.780426000	-3.087042000
H	-2.451120000	5.813202000	-1.513151000
H	-0.484013000	3.470596000	-4.535105000
H	-1.091376000	5.692371000	-3.590823000
C	-0.892725000	-4.410487000	0.642804000
C	-2.269904000	-4.575809000	0.498892000
C	-3.080542000	-3.442835000	0.441984000
C	-2.525660000	-2.165005000	0.501430000
C	-1.141931000	-1.977011000	0.613608000
C	-0.345459000	-3.130056000	0.707227000
H	-0.240034000	-5.276267000	0.718913000
H	-2.703944000	-5.570153000	0.446197000
H	-4.158491000	-3.546630000	0.353156000
H	-3.187410000	-1.311219000	0.486323000
H	0.722661000	-3.032340000	0.865965000
C	-0.525760000	-0.593707000	0.723968000
C	-1.394634000	0.625481000	0.406705000
C	-1.173109000	1.563465000	1.387947000
O	-0.367780000	1.275187000	2.380075000
O	-1.731390000	2.782393000	1.378927000
C	-1.624029000	3.554934000	2.579928000
H	-0.578734000	3.765965000	2.817946000
H	-2.159917000	4.481689000	2.371058000
H	-2.086922000	3.029416000	3.419550000
6S			
P	1.010379000	0.426296000	0.311673000
C	1.105622000	-1.331806000	-0.173999000
C	2.454547000	-1.756227000	-0.763902000
H	0.304157000	-1.519753000	-0.892343000
H	0.864876000	-1.881631000	0.739899000
C	2.494696000	-3.267085000	-1.023144000
H	2.636923000	-1.223097000	-1.706384000
H	3.277635000	-1.484963000	-0.088588000
C	3.817515000	-3.726696000	-1.638499000
H	2.319812000	-3.795632000	-0.076543000
H	1.660149000	-3.538771000	-1.682680000
H	4.663289000	-3.490349000	-0.981282000
H	3.820804000	-4.808258000	-1.810965000
H	3.998124000	-3.234585000	-2.601887000
C	2.271856000	0.688961000	1.637516000
C	3.308917000	1.797717000	1.427352000
H	2.771943000	-0.273715000	1.783580000

H	1.695773000	0.883117000	2.543433000
C	4.196289000	1.965716000	2.666373000
H	3.942103000	1.579173000	0.558137000
H	2.805803000	2.749189000	1.219591000
C	5.256060000	3.054229000	2.485135000
H	3.561844000	2.204663000	3.530203000
H	4.683072000	1.008110000	2.898808000
H	4.790515000	4.025326000	2.278850000
H	5.873853000	3.163096000	3.382963000
H	5.922569000	2.820737000	1.646087000
C	1.585927000	1.463933000	-1.092222000
C	0.794743000	1.400498000	-2.398977000
H	2.633182000	1.189491000	-1.266922000
H	1.588001000	2.490628000	-0.713221000
C	1.355918000	2.372236000	-3.441424000
H	0.789255000	0.379546000	-2.797268000
H	-0.250008000	1.647027000	-2.201122000
C	0.549338000	2.355142000	-4.741768000
H	1.354480000	3.386815000	-3.019889000
H	2.406445000	2.125571000	-3.651435000
H	0.536337000	1.352967000	-5.186167000
H	-0.491439000	2.648980000	-4.560052000
H	0.966925000	3.046396000	-5.481960000
P	-2.040304000	-0.424035000	-1.354518000
B	-0.782884000	0.329062000	2.506979000
O	-0.164947000	-0.987212000	2.620274000
O	-0.289661000	1.091174000	3.610928000
C	0.054927000	-1.252023000	4.009341000
C	-0.081741000	0.188510000	4.707141000
C	-0.996423000	-2.271371000	4.471078000
C	1.440990000	-1.891746000	4.147502000
C	1.172486000	0.655085000	5.451915000
C	-1.284691000	0.309361000	5.654286000
H	-0.866838000	-3.195171000	3.896787000
H	-0.894146000	-2.514573000	5.534550000
H	-2.005900000	-1.900967000	4.287484000
H	2.233655000	-1.233137000	3.787617000
H	1.661398000	-2.158252000	5.186855000
H	1.468494000	-2.809302000	3.549715000
H	1.378083000	0.027842000	6.326167000
H	2.057415000	0.650869000	4.810940000
H	1.015155000	1.681544000	5.798284000
H	-2.219147000	0.097868000	5.132577000
H	-1.195047000	-0.360095000	6.516955000

H	-1.335811000	1.338750000	6.022917000
C	-2.555849000	-2.182801000	-1.123117000
C	-3.257095000	-2.848324000	-2.140840000
C	-2.136321000	-2.924690000	-0.006673000
C	-3.549915000	-4.207790000	-2.037678000
H	-3.590195000	-2.294782000	-3.014490000
C	-2.424945000	-4.285772000	0.091425000
H	-1.595641000	-2.432937000	0.796484000
C	-3.135051000	-4.934181000	-0.920114000
H	-4.105124000	-4.699802000	-2.832290000
H	-2.097842000	-4.839349000	0.968374000
H	-3.363373000	-5.993452000	-0.839186000
C	-3.569563000	0.353422000	-2.053523000
C	-3.387852000	1.367721000	-3.005753000
C	-4.878615000	0.008818000	-1.683031000
C	-4.478986000	2.044003000	-3.554036000
H	-2.380449000	1.623662000	-3.324422000
C	-5.969495000	0.674079000	-2.239310000
H	-5.032876000	-0.778187000	-0.955439000
C	-5.774000000	1.697703000	-3.170223000
H	-4.317218000	2.829824000	-4.287312000
H	-6.977881000	0.397543000	-1.941935000
H	-6.627619000	2.216923000	-3.597573000
C	0.064137000	4.662407000	1.423036000
C	-0.677029000	5.236847000	0.389737000
C	-1.463005000	4.416522000	-0.420708000
C	-1.485270000	3.037169000	-0.216217000
C	-0.719214000	2.442243000	0.795732000
C	0.040702000	3.281983000	1.627377000
H	0.654111000	5.290884000	2.085350000
H	-0.657501000	6.311484000	0.230483000
H	-2.066984000	4.847886000	-1.214756000
H	-2.119746000	2.416314000	-0.836781000
H	0.575158000	2.852746000	2.465486000
C	-0.651103000	0.917323000	0.939153000
C	-1.846597000	0.167884000	0.330659000
C	-2.713215000	-0.095341000	1.364286000
O	-2.327729000	0.154367000	2.592988000
O	-3.935319000	-0.614641000	1.181522000
C	-4.570052000	-1.202360000	2.322419000
H	-5.548599000	-1.530224000	1.969322000
H	-3.996028000	-2.063235000	2.678526000
H	-4.679341000	-0.474415000	3.129292000

7Z

P	0.262945000	-1.121388000	2.146122000
B	0.172112000	-0.140047000	-2.098799000
O	0.156555000	1.153258000	-2.563906000
O	0.348193000	-1.078696000	-3.081727000
C	0.632740000	1.110276000	-3.939716000
C	0.322152000	-0.376095000	-4.354910000
C	-0.119754000	2.168988000	-4.737541000
C	2.128489000	1.435015000	-3.903915000
C	1.355166000	-1.011915000	-5.277254000
C	-1.089848000	-0.566385000	-4.917532000
H	0.164089000	2.131535000	-5.795257000
H	-1.201335000	2.038295000	-4.661733000
H	0.131129000	3.162736000	-4.353861000
H	2.262340000	2.414116000	-3.433761000
H	2.676836000	0.700870000	-3.311085000
H	2.550998000	1.476286000	-4.913239000
H	1.413478000	-0.470820000	-6.228494000
H	2.344615000	-1.021289000	-4.816142000
H	1.068784000	-2.046429000	-5.490543000
H	-1.195446000	-0.117306000	-5.910403000
H	-1.295071000	-1.637859000	-4.997755000
H	-1.840991000	-0.130204000	-4.251889000
C	1.585190000	-0.039132000	2.869397000
C	2.163495000	-0.448129000	4.076645000
C	2.018272000	1.160793000	2.285827000
C	3.147860000	0.325414000	4.694362000
H	1.844925000	-1.382902000	4.530590000
C	3.009933000	1.927911000	2.894771000
H	1.591046000	1.492378000	1.344008000
C	3.575471000	1.513783000	4.103138000
H	3.585577000	-0.005285000	5.632426000
H	3.339298000	2.851984000	2.427140000
H	4.346683000	2.113773000	4.578230000
C	-1.213911000	-0.093020000	2.576512000
C	-2.117368000	-0.640701000	3.494662000
C	-1.455719000	1.191622000	2.073071000
C	-3.246176000	0.074463000	3.897745000
H	-1.940137000	-1.639364000	3.885858000
C	-2.586643000	1.902204000	2.464420000
H	-0.772101000	1.626372000	1.351746000
C	-3.485449000	1.345231000	3.377941000
H	-3.940462000	-0.364882000	4.608885000
H	-2.771533000	2.890637000	2.052909000
H	-4.368721000	1.901215000	3.680100000

C	-3.853188000	-1.572970000	0.296145000
C	-4.618391000	-0.562254000	-0.287730000
C	-3.987060000	0.453679000	-1.007367000
C	-2.600891000	0.464612000	-1.136714000
C	-1.817579000	-0.526099000	-0.517976000
C	-2.466622000	-1.555723000	0.181059000
H	-4.336818000	-2.373620000	0.848318000
H	-5.700167000	-0.570869000	-0.188663000
H	-4.576613000	1.240459000	-1.470033000
H	-2.107821000	1.257125000	-1.689743000
H	-1.875725000	-2.349528000	0.627451000
C	-0.347479000	-0.496145000	-0.647687000
C	0.536102000	-0.773683000	0.346606000
C	1.951566000	-0.855198000	-0.111482000
O	2.372738000	-0.341467000	-1.137328000
O	2.727698000	-1.576059000	0.712942000
C	4.128923000	-1.591663000	0.405020000
H	4.295572000	-1.981212000	-0.601804000
H	4.535157000	-0.579194000	0.476370000
H	4.582670000	-2.239365000	1.154474000
7E			
P	-0.444124000	0.959637000	-1.383783000
B	-0.097940000	1.051480000	1.671884000
O	-0.728467000	2.175374000	2.122581000
O	1.264030000	1.083917000	1.815976000
C	0.276703000	2.975499000	2.815622000
C	1.618863000	2.448828000	2.190432000
C	-0.017683000	4.447275000	2.558755000
C	0.132359000	2.646614000	4.303696000
C	2.801112000	2.390952000	3.149006000
C	2.012992000	3.163702000	0.895650000
H	-0.979734000	4.713614000	3.006736000
H	0.755824000	5.079536000	3.008831000
H	-0.068847000	4.662004000	1.489802000
H	-0.894033000	2.860630000	4.615187000
H	0.328188000	1.586868000	4.493794000
H	0.813910000	3.244883000	4.916644000
H	2.592316000	1.751176000	4.009143000
H	3.673614000	1.986347000	2.627110000
H	3.054432000	3.393565000	3.510926000
H	2.809310000	2.597099000	0.405641000
H	1.168908000	3.217801000	0.202626000
H	2.372953000	4.178346000	1.094719000
C	1.344428000	0.558921000	-1.596519000

C	1.995925000	-0.507290000	-0.966628000
C	2.096320000	1.445144000	-2.384001000
C	3.371609000	-0.682058000	-1.121790000
H	1.429226000	-1.196908000	-0.353075000
C	3.467998000	1.263358000	-2.547602000
H	1.603476000	2.285997000	-2.866811000
C	4.111185000	0.199502000	-1.910431000
H	3.865676000	-1.511764000	-0.623432000
H	4.036035000	1.956265000	-3.162418000
H	5.182539000	0.061192000	-2.027179000
C	-1.157973000	0.355061000	-2.974409000
C	-0.479157000	-0.509640000	-3.844329000
C	-2.458755000	0.764794000	-3.299891000
C	-1.093252000	-0.956727000	-5.014118000
H	0.525410000	-0.837287000	-3.599320000
C	-3.075794000	0.308604000	-4.463578000
H	-2.992382000	1.436469000	-2.632675000
C	-2.393256000	-0.552063000	-5.324236000
H	-0.556562000	-1.624558000	-5.682920000
H	-4.087411000	0.626750000	-4.699072000
H	-2.870735000	-0.903571000	-6.234704000
C	-2.791092000	-2.799130000	3.105069000
C	-1.876433000	-3.106683000	4.113402000
C	-0.635208000	-2.468482000	4.135240000
C	-0.313647000	-1.530982000	3.156636000
C	-1.219657000	-1.229642000	2.123548000
C	-2.470774000	-1.869218000	2.117486000
H	-3.765252000	-3.280221000	3.088986000
H	-2.131789000	-3.832458000	4.880445000
H	0.083308000	-2.698620000	4.917260000
H	0.654521000	-1.038683000	3.171877000
H	-3.191470000	-1.623897000	1.346760000
C	-0.840352000	-0.214188000	1.108132000
C	-1.027597000	-0.361312000	-0.220219000
C	-1.674399000	-1.553337000	-0.849441000
O	-2.865724000	-1.697287000	-1.028022000
O	-0.744950000	-2.436676000	-1.271804000
C	-1.260043000	-3.548149000	-2.024468000
H	-1.976478000	-4.115254000	-1.425549000
H	-1.748405000	-3.187751000	-2.933221000
H	-0.391271000	-4.159281000	-2.269605000
8			
P	-0.862868000	-2.376632000	0.504291000
C	-0.346256000	-1.688787000	2.114576000

C	-1.247519000	-0.602346000	2.709969000
H	0.647281000	-1.261518000	1.920402000
H	-0.232120000	-2.535876000	2.803681000
C	-0.716032000	-0.143027000	4.073000000
H	-1.282550000	0.244647000	2.013993000
H	-2.273286000	-0.976187000	2.837071000
C	-1.524047000	1.018714000	4.652632000
H	-0.726224000	-0.990667000	4.773009000
H	0.331606000	0.160270000	3.964144000
H	-1.125981000	1.332232000	5.623676000
H	-1.496811000	1.884805000	3.982308000
H	-2.576645000	0.743080000	4.793247000
C	-2.257308000	-3.535158000	0.750700000
C	-2.643339000	-4.262045000	-0.549870000
H	-3.093967000	-2.937670000	1.123716000
H	-1.991743000	-4.248097000	1.540061000
C	-4.031629000	-4.915412000	-0.484667000
H	-2.631425000	-3.552538000	-1.385980000
H	-1.883142000	-5.021514000	-0.769232000
C	-5.180601000	-3.902303000	-0.467073000
H	-4.143021000	-5.569612000	-1.358485000
H	-4.089690000	-5.568780000	0.397092000
H	-5.154641000	-3.261470000	0.420521000
H	-5.136094000	-3.241524000	-1.340096000
H	-6.149715000	-4.412589000	-0.474502000
C	0.576840000	-3.291305000	-0.141264000
C	1.143365000	-4.363706000	0.795164000
H	1.314768000	-2.510200000	-0.356185000
H	0.282116000	-3.718833000	-1.105900000
C	2.378953000	-5.041611000	0.191229000
H	1.418237000	-3.913905000	1.757025000
H	0.380541000	-5.125228000	1.010379000
C	2.969860000	-6.113714000	1.108665000
H	2.110560000	-5.485755000	-0.776968000
H	3.135705000	-4.274764000	-0.021010000
H	2.240263000	-6.907038000	1.311774000
H	3.852563000	-6.579259000	0.657804000
H	3.272929000	-5.685250000	2.071320000
P	1.910537000	0.743082000	0.560408000
B	0.565209000	1.978871000	-0.315643000
O	-0.728636000	1.857907000	0.302463000
O	0.899802000	3.362313000	-0.372385000
C	-1.429352000	3.088927000	0.055940000
C	-0.259294000	4.154374000	-0.085074000

C	-2.269031000	2.924675000	-1.222160000
C	-2.376415000	3.328206000	1.231608000
C	0.020748000	4.942111000	1.200084000
C	-0.454201000	5.146751000	-1.235969000
H	-2.962242000	2.090439000	-1.086265000
H	-2.854180000	3.825321000	-1.438705000
H	-1.639057000	2.703010000	-2.085521000
H	-3.107229000	2.513293000	1.275416000
H	-1.837780000	3.355118000	2.181488000
H	-2.924743000	4.270101000	1.116972000
H	0.185345000	4.280324000	2.050518000
H	0.938245000	5.521630000	1.058161000
H	-0.793694000	5.635663000	1.439081000
H	-0.530233000	4.631753000	-2.195796000
H	-1.351183000	5.760859000	-1.091568000
H	0.411813000	5.815114000	-1.281320000
C	2.532499000	1.796718000	1.931895000
C	3.890604000	2.053651000	2.169712000
C	1.596145000	2.275985000	2.864539000
C	4.295246000	2.767955000	3.298675000
H	4.635215000	1.698620000	1.463695000
C	1.999359000	2.985154000	3.993636000
H	0.540184000	2.104536000	2.680712000
C	3.355079000	3.235430000	4.218182000
H	5.353404000	2.960765000	3.459282000
H	1.252064000	3.351277000	4.693918000
H	3.673856000	3.789964000	5.096584000
C	3.271913000	0.813900000	-0.685560000
C	3.839658000	-0.380488000	-1.147529000
C	3.696806000	2.024305000	-1.261736000
C	4.802551000	-0.378344000	-2.160204000
H	3.519129000	-1.322102000	-0.707491000
C	4.664445000	2.030557000	-2.264659000
H	3.237948000	2.952253000	-0.935365000
C	5.218230000	0.829412000	-2.719855000
H	5.228113000	-1.316448000	-2.507922000
H	4.981563000	2.973990000	-2.702192000
H	5.968701000	0.837365000	-3.506193000
C	-4.928013000	-0.110141000	-0.258178000
C	-5.352868000	-0.000847000	-1.582386000
C	-4.453380000	-0.266677000	-2.617652000
C	-3.144415000	-0.646739000	-2.330300000
C	-2.708766000	-0.765141000	-1.001513000
C	-3.617948000	-0.492369000	0.029237000

H	-5.612485000	0.114522000	0.555084000
H	-6.373055000	0.296395000	-1.806808000
H	-4.772145000	-0.176765000	-3.652334000
H	-2.437780000	-0.841983000	-3.131395000
H	-3.289578000	-0.530517000	1.060698000
C	-1.291759000	-1.138711000	-0.746409000
C	-0.234132000	-0.649461000	-1.372983000
C	0.197781000	0.332467000	-2.214560000
O	0.555030000	1.511628000	-1.829744000
O	0.405101000	0.017362000	-3.508542000
C	1.319032000	0.871167000	-4.224167000
H	1.376068000	0.442339000	-5.225549000
H	0.943497000	1.895626000	-4.267160000
H	2.302693000	0.865961000	-3.747601000

9

P	0.707109000	-2.037915000	0.820664000
C	0.514247000	-1.489106000	-0.921471000
C	0.805033000	-2.509706000	-2.026681000
H	1.150311000	-0.614474000	-1.055605000
H	-0.516153000	-1.127986000	-1.001630000
C	0.406867000	-1.971861000	-3.410950000
H	1.874028000	-2.759053000	-2.030943000
H	0.264780000	-3.446617000	-1.843040000
C	1.149708000	-0.695325000	-3.820337000
H	0.588397000	-2.759289000	-4.154102000
H	-0.675756000	-1.782929000	-3.418110000
H	0.889751000	0.156116000	-3.183638000
H	2.236724000	-0.842004000	-3.766905000
H	0.905884000	-0.421263000	-4.853349000
C	2.387953000	-2.825908000	0.955024000
C	2.550524000	-4.284823000	0.512920000
H	2.669233000	-2.716284000	2.009205000
H	3.063247000	-2.165209000	0.399464000
C	4.005231000	-4.760021000	0.612927000
H	1.920056000	-4.933353000	1.134301000
H	2.202010000	-4.416886000	-0.518297000
C	4.180250000	-6.221889000	0.195821000
H	4.637204000	-4.117022000	-0.015300000
H	4.358983000	-4.622435000	1.643736000
H	5.226818000	-6.536986000	0.269522000
H	3.585106000	-6.887631000	0.832464000
H	3.855884000	-6.377673000	-0.840357000
C	-0.468453000	-3.452025000	1.017895000
C	-1.933524000	-3.026448000	1.124818000

H	-0.183253000	-4.025976000	1.903006000
H	-0.314921000	-4.114810000	0.158105000
C	-2.857037000	-4.238440000	1.288958000
H	-2.047089000	-2.351400000	1.978632000
H	-2.226680000	-2.452620000	0.237387000
C	-4.332835000	-3.858275000	1.422756000
H	-2.728522000	-4.915529000	0.432201000
H	-2.544587000	-4.805988000	2.176661000
H	-4.683643000	-3.323024000	0.533523000
H	-4.962293000	-4.745539000	1.554188000
H	-4.490692000	-3.203097000	2.287403000
P	-0.690675000	1.790292000	0.722908000
B	0.522483000	2.673391000	-0.697262000
O	0.182459000	2.185803000	-2.007401000
O	0.508837000	4.085595000	-0.701575000
C	0.151294000	3.332307000	-2.884349000
C	-0.188335000	4.495599000	-1.886224000
C	1.543905000	3.480461000	-3.509641000
C	-0.891915000	3.092497000	-3.970436000
C	-1.687677000	4.580688000	-1.561158000
C	0.331857000	5.867860000	-2.302019000
H	1.576958000	4.289629000	-4.247306000
H	2.292991000	3.676818000	-2.737502000
H	1.807066000	2.544467000	-4.012488000
H	-0.588028000	2.247821000	-4.597957000
H	-1.870962000	2.863575000	-3.542671000
H	-0.992482000	3.974037000	-4.613843000
H	-1.816958000	5.213868000	-0.678621000
H	-2.261928000	5.010679000	-2.388737000
H	-2.104298000	3.595404000	-1.331525000
H	1.420006000	5.864873000	-2.393074000
H	-0.103029000	6.179583000	-3.258758000
H	0.057836000	6.609511000	-1.544871000
C	-1.165422000	3.003238000	1.995051000
C	-2.457058000	3.541842000	2.062581000
C	-0.162902000	3.513242000	2.832645000
C	-2.745093000	4.559773000	2.971214000
H	-3.237628000	3.164196000	1.410365000
C	-0.455616000	4.527796000	3.740593000
H	0.839544000	3.099030000	2.778693000
C	-1.747414000	5.052877000	3.813266000
H	-3.751567000	4.965918000	3.021693000
H	0.325799000	4.908935000	4.391782000
H	-1.974678000	5.844467000	4.521656000

C	-2.196270000	0.892757000	0.270873000
C	-3.051768000	0.393291000	1.264444000
C	-2.484784000	0.656268000	-1.082093000
C	-4.205224000	-0.300051000	0.903519000
H	-2.813390000	0.545675000	2.312809000
C	-3.632738000	-0.054788000	-1.434173000
H	-1.803251000	1.029844000	-1.839428000
C	-4.498464000	-0.522938000	-0.443709000
H	-4.867583000	-0.681245000	1.674532000
H	-3.856217000	-0.232070000	-2.482611000
H	-5.398573000	-1.065179000	-0.719781000
C	-0.905457000	-0.025273000	5.345083000
C	-0.790853000	-1.269847000	5.969837000
C	-0.209328000	-2.314948000	5.249353000
C	0.222184000	-2.129229000	3.939491000
C	0.070050000	-0.890814000	3.262124000
C	-0.484048000	0.162760000	4.033451000
H	-1.328859000	0.818796000	5.885496000
H	-1.124245000	-1.415626000	6.993019000
H	-0.068374000	-3.286426000	5.718629000
H	0.727217000	-2.956000000	3.448995000
H	-0.578142000	1.144758000	3.592053000
C	0.427315000	-0.688628000	1.869581000
C	0.589053000	0.639424000	1.255051000
C	1.748967000	1.083602000	0.655260000
O	1.814868000	2.141052000	-0.144047000
O	2.903953000	0.402826000	0.795301000
C	4.045717000	0.889460000	0.078549000
H	3.864124000	0.885859000	-0.999740000
H	4.303611000	1.903907000	0.393074000
H	4.852198000	0.199247000	0.331005000

10Z

P	0.246453000	-0.593557000	-1.943866000
C	-0.516929000	-1.591590000	-3.308197000
C	-1.658562000	-2.460910000	-2.778252000
H	0.270461000	-2.202070000	-3.764294000
H	-0.879869000	-0.914134000	-4.086875000
C	-2.293371000	-3.342688000	-3.856282000
H	-1.287666000	-3.094924000	-1.963134000
H	-2.417616000	-1.809152000	-2.329123000
C	-3.417809000	-4.219474000	-3.299651000
H	-2.683744000	-2.706647000	-4.662698000
H	-1.520703000	-3.978053000	-4.312114000
H	-4.212775000	-3.606108000	-2.859414000

H	-3.867903000	-4.841122000	-4.081446000
H	-3.041951000	-4.888059000	-2.515489000
C	1.412638000	0.568209000	-2.776684000
C	2.337282000	0.033892000	-3.875962000
H	1.987579000	1.006477000	-1.957000000
H	0.790263000	1.379352000	-3.173958000
C	3.293225000	1.117677000	-4.401089000
H	2.932871000	-0.804756000	-3.494509000
H	1.738462000	-0.358954000	-4.706901000
C	4.335161000	1.565831000	-3.370464000
H	3.807323000	0.734449000	-5.292106000
H	2.703578000	1.983362000	-4.734481000
H	3.872354000	1.982701000	-2.470599000
H	4.960860000	0.720106000	-3.058620000
H	4.997235000	2.331264000	-3.790457000
C	1.252164000	-1.775654000	-0.962786000
C	1.852432000	-2.971240000	-1.714273000
H	0.602583000	-2.129899000	-0.159954000
H	2.041004000	-1.183272000	-0.486541000
C	2.815805000	-3.776309000	-0.828293000
H	1.046241000	-3.632247000	-2.055820000
H	2.388772000	-2.641300000	-2.610906000
C	2.159272000	-4.354932000	0.427601000
H	3.238327000	-4.591394000	-1.430303000
H	3.660433000	-3.133716000	-0.542644000
H	2.857795000	-4.999037000	0.973283000
H	1.827086000	-3.571314000	1.115486000
H	1.276906000	-4.953327000	0.174449000
P	-2.376351000	-0.922691000	1.201609000
B	1.324722000	2.077921000	0.476977000
O	0.345805000	2.970898000	0.806978000
O	2.375281000	2.614181000	-0.226933000
C	0.651928000	4.203477000	0.084069000
C	2.199934000	4.061030000	-0.170344000
C	-0.164197000	4.202719000	-1.207457000
C	0.248674000	5.376898000	0.967474000
C	3.053851000	4.556628000	0.999324000
C	2.692521000	4.660301000	-1.480906000
H	-0.002329000	5.127879000	-1.769897000
H	0.096324000	3.353344000	-1.842675000
H	-1.225867000	4.114606000	-0.972837000
H	0.718441000	5.323269000	1.952056000
H	0.523543000	6.327501000	0.497333000
H	-0.836564000	5.367208000	1.105265000

H	3.032391000	5.648011000	1.077588000
H	2.707292000	4.134236000	1.947675000
H	4.089123000	4.239500000	0.843463000
H	3.771428000	4.504044000	-1.576760000
H	2.202984000	4.197859000	-2.340030000
H	2.500352000	5.738349000	-1.507145000
C	-1.847414000	-2.679228000	1.474432000
C	-1.025574000	-3.133194000	2.519949000
C	-2.327908000	-3.618977000	0.549043000
C	-0.690730000	-4.482215000	2.624390000
H	-0.656385000	-2.423719000	3.248868000
C	-1.977505000	-4.967624000	0.641431000
H	-2.995021000	-3.287532000	-0.240896000
C	-1.158794000	-5.403110000	1.682899000
H	-0.056811000	-4.817689000	3.441247000
H	-2.361833000	-5.677732000	-0.086496000
H	-0.892944000	-6.453358000	1.768053000
C	-2.525952000	-0.271515000	2.921058000
C	-2.200396000	1.062816000	3.219337000
C	-3.125825000	-1.046199000	3.926148000
C	-2.449562000	1.594182000	4.484168000
H	-1.726152000	1.685617000	2.467176000
C	-3.369726000	-0.515229000	5.192667000
H	-3.395994000	-2.077914000	3.720742000
C	-3.032129000	0.807941000	5.479564000
H	-2.182731000	2.627534000	4.692150000
H	-3.826488000	-1.139033000	5.956851000
H	-3.223970000	1.222216000	6.465519000
C	-2.949968000	2.385509000	-3.246974000
C	-3.778746000	3.066036000	-2.353671000
C	-3.630881000	2.800799000	-0.989598000
C	-2.678032000	1.898555000	-0.531934000
C	-1.834039000	1.176639000	-1.415937000
C	-2.013603000	1.460550000	-2.794859000
H	-3.036109000	2.567737000	-4.316023000
H	-4.515861000	3.779856000	-2.708933000
H	-4.255578000	3.317197000	-0.264101000
H	-2.562871000	1.763612000	0.534810000
H	-1.406187000	0.958387000	-3.539793000
C	-0.854104000	0.237540000	-0.894515000
C	-0.840268000	-0.114995000	0.543044000
C	0.250880000	0.097470000	1.310432000
O	1.375968000	0.764738000	0.871379000
O	0.429803000	-0.459091000	2.530081000

C	1.088750000	0.342535000	3.516164000
H	1.022518000	-0.225555000	4.444774000
H	2.136123000	0.508498000	3.248660000
H	0.575415000	1.300864000	3.641826000

10E

P	-0.226376000	-1.767018000	0.663487000
C	-0.637179000	-0.975798000	-0.939428000
C	-1.448262000	-1.830346000	-1.925637000
H	0.326521000	-0.687402000	-1.364969000
H	-1.177406000	-0.050687000	-0.720405000
C	-1.275080000	-1.361501000	-3.378909000
H	-1.157093000	-2.888091000	-1.873583000
H	-2.507515000	-1.790822000	-1.645122000
C	0.116928000	-1.650252000	-3.950941000
H	-2.029716000	-1.858137000	-4.002707000
H	-1.482683000	-0.285906000	-3.439939000
H	0.184289000	-1.334455000	-4.997911000
H	0.905566000	-1.126852000	-3.399587000
H	0.341064000	-2.723596000	-3.911786000
C	0.835300000	-3.203671000	0.214119000
C	2.263101000	-2.811859000	-0.172108000
H	0.331837000	-3.703594000	-0.622914000
H	0.836996000	-3.925977000	1.035869000
C	3.109263000	-4.027986000	-0.560199000
H	2.239615000	-2.100480000	-1.005596000
H	2.731417000	-2.284878000	0.664153000
C	4.536801000	-3.646329000	-0.957475000
H	3.137008000	-4.731503000	0.283797000
H	2.625395000	-4.563029000	-1.390060000
H	5.046587000	-3.131407000	-0.134933000
H	5.129127000	-4.529441000	-1.221654000
H	4.535007000	-2.968703000	-1.818669000
C	-1.817997000	-2.527824000	1.228696000
C	-1.718341000	-3.099819000	2.648714000
H	-2.142497000	-3.282451000	0.502087000
H	-2.547742000	-1.710339000	1.214632000
C	-3.087945000	-3.354896000	3.291002000
H	-1.141355000	-4.034950000	2.634801000
H	-1.157443000	-2.394801000	3.270401000
C	-3.940746000	-4.389847000	2.552407000
H	-2.934220000	-3.684724000	4.326956000
H	-3.630123000	-2.400890000	3.345088000
H	-4.888388000	-4.567965000	3.072678000
H	-4.180176000	-4.061974000	1.534464000

H	-3.415453000	-5.350352000	2.477236000
P	0.657452000	2.122875000	0.486441000
B	-2.591607000	2.541970000	0.774613000
O	-3.127663000	3.775105000	0.531789000
O	-2.810927000	1.617234000	-0.221138000
C	-3.499097000	3.775473000	-0.875979000
C	-3.729583000	2.245223000	-1.159798000
C	-4.731685000	4.651701000	-1.054586000
C	-2.305808000	4.352616000	-1.643187000
C	-3.368198000	1.794934000	-2.568317000
C	-5.134617000	1.766111000	-0.786979000
H	-4.480783000	5.689554000	-0.816133000
H	-5.083455000	4.615935000	-2.091751000
H	-5.545639000	4.339472000	-0.397008000
H	-1.413141000	3.735465000	-1.501296000
H	-2.518649000	4.437599000	-2.713719000
H	-2.088005000	5.351002000	-1.253092000
H	-3.557558000	0.722330000	-2.674394000
H	-3.977671000	2.322039000	-3.310457000
H	-2.314055000	1.978635000	-2.785734000
H	-5.409181000	2.095058000	0.219808000
H	-5.885956000	2.135846000	-1.491776000
H	-5.151455000	0.672256000	-0.804070000
C	1.525457000	3.207988000	1.706084000
C	2.799430000	3.731034000	1.433853000
C	0.873038000	3.618515000	2.880821000
C	3.414872000	4.611103000	2.323421000
H	3.321564000	3.437968000	0.529157000
C	1.492747000	4.495792000	3.769586000
H	-0.122689000	3.252597000	3.101494000
C	2.768047000	4.993248000	3.498919000
H	4.406773000	4.993888000	2.097424000
H	0.974291000	4.790948000	4.678142000
H	3.250509000	5.674650000	4.194094000
C	2.070396000	1.271133000	-0.328658000
C	2.077121000	1.230561000	-1.729741000
C	3.143297000	0.692172000	0.367704000
C	3.126330000	0.624024000	-2.426245000
H	1.252894000	1.681538000	-2.276900000
C	4.198328000	0.102168000	-0.325099000
H	3.156106000	0.710146000	1.451349000
C	4.192029000	0.063666000	-1.722013000
H	3.116890000	0.604805000	-3.512705000
H	5.022661000	-0.340156000	0.227247000

H	5.016820000	-0.398454000	-2.257476000
C	2.683869000	-2.391288000	4.263976000
C	3.203171000	-1.321941000	4.996668000
C	2.789091000	-0.033163000	4.653601000
C	1.901842000	0.183291000	3.604181000
C	1.383384000	-0.882891000	2.819539000
C	1.794981000	-2.182868000	3.214403000
H	2.962571000	-3.411518000	4.519566000
H	3.895455000	-1.489581000	5.816227000
H	3.157799000	0.825835000	5.209970000
H	1.601243000	1.198072000	3.377614000
H	1.390538000	-3.053629000	2.713884000
C	0.499434000	-0.595788000	1.705581000
C	-0.087082000	0.761189000	1.547984000
C	-1.294119000	1.040344000	2.074969000
O	-1.911284000	2.269686000	1.932137000
O	-2.033691000	0.170137000	2.812164000
C	-1.895229000	0.344025000	4.232369000
H	-2.233408000	1.342379000	4.532684000
H	-2.530523000	-0.413997000	4.693703000
H	-0.852119000	0.192759000	4.527907000

11R

P	-0.410884000	-0.437621000	1.255857000
C	-1.630005000	-1.671826000	2.082090000
C	-1.410525000	-2.090206000	3.537800000
H	-1.619098000	-2.566318000	1.444289000
H	-2.641714000	-1.260245000	1.969514000
C	-2.282503000	-3.282974000	3.951437000
H	-0.356095000	-2.349215000	3.714827000
H	-1.628391000	-1.248409000	4.207953000
C	-2.090606000	-3.684732000	5.415861000
H	-3.337443000	-3.035931000	3.769433000
H	-2.054741000	-4.138027000	3.299746000
H	-1.048239000	-3.963264000	5.614962000
H	-2.343919000	-2.855824000	6.088257000
H	-2.721663000	-4.538896000	5.686467000
C	1.067447000	-1.559863000	1.202095000
C	1.223792000	-2.300318000	-0.130649000
H	0.971308000	-2.279346000	2.022212000
H	1.946287000	-0.945556000	1.411004000
C	2.481211000	-3.171767000	-0.189569000
H	0.341889000	-2.930095000	-0.304995000
H	1.254550000	-1.576634000	-0.949870000
C	2.623427000	-3.885817000	-1.536055000

H	3.363550000	-2.541448000	-0.014373000
H	2.460566000	-3.909416000	0.624841000
H	3.521689000	-4.512304000	-1.569235000
H	1.757337000	-4.529690000	-1.733340000
H	2.690100000	-3.160667000	-2.356180000
C	-0.271611000	0.708828000	2.724409000
C	-1.545036000	1.528322000	2.959765000
H	0.573930000	1.370510000	2.530917000
H	-0.041938000	0.104297000	3.608429000
C	-1.384399000	2.533723000	4.104637000
H	-1.797423000	2.071426000	2.041654000
H	-2.391611000	0.863338000	3.179833000
C	-2.646622000	3.364560000	4.346564000
H	-1.112309000	1.996727000	5.024455000
H	-0.540602000	3.198276000	3.875030000
H	-2.509330000	4.079097000	5.166108000
H	-2.919794000	3.933136000	3.449126000
H	-3.498498000	2.722314000	4.601929000
P	-0.684878000	0.960990000	-2.850034000
B	2.796748000	1.093391000	0.107302000
O	4.042069000	1.136038000	-0.475729000
O	2.826253000	1.290432000	1.474223000
C	5.009803000	1.155436000	0.604959000
C	4.168161000	1.733729000	1.802455000
C	5.453583000	-0.292743000	0.832128000
C	6.196081000	2.013093000	0.181942000
C	4.129418000	3.264463000	1.828522000
C	4.536279000	1.187792000	3.176219000
H	5.834291000	-0.697174000	-0.110207000
H	6.244844000	-0.360210000	1.585438000
H	4.613876000	-0.916455000	1.153817000
H	5.878165000	3.010682000	-0.127572000
H	6.915750000	2.111497000	1.002317000
H	6.705944000	1.542579000	-0.664270000
H	3.358846000	3.584862000	2.535684000
H	5.088650000	3.688796000	2.141190000
H	3.874395000	3.668875000	0.844069000
H	3.879939000	1.627555000	3.933533000
H	4.423425000	0.102513000	3.219801000
H	5.570665000	1.443679000	3.431059000
C	-1.360427000	-0.582227000	-3.610418000
C	-2.674865000	-0.765150000	-4.053748000
C	-0.447547000	-1.640712000	-3.742342000
C	-3.069632000	-1.983381000	-4.605735000

H	-3.400195000	0.032255000	-3.941719000
C	-0.847072000	-2.863365000	-4.277848000
H	0.580512000	-1.506081000	-3.414204000
C	-2.161502000	-3.036625000	-4.715646000
H	-4.098304000	-2.115397000	-4.929260000
H	-0.130158000	-3.676041000	-4.361054000
H	-2.475707000	-3.986813000	-5.138832000
C	-2.103722000	2.138237000	-2.904283000
C	-2.595335000	2.535551000	-4.159062000
C	-2.634463000	2.744072000	-1.755920000
C	-3.617582000	3.477418000	-4.259395000
H	-2.181406000	2.095663000	-5.062881000
C	-3.644378000	3.701711000	-1.858798000
H	-2.251952000	2.470166000	-0.777995000
C	-4.146731000	4.064882000	-3.108242000
H	-3.995640000	3.759061000	-5.238469000
H	-4.041994000	4.159624000	-0.956853000
H	-4.938658000	4.804390000	-3.186480000
C	-3.785652000	-3.133058000	-1.454940000
C	-4.995324000	-2.438736000	-1.520929000
C	-5.025299000	-1.077919000	-1.216498000
C	-3.854672000	-0.414538000	-0.851261000
C	-2.634714000	-1.103764000	-0.781191000
C	-2.619344000	-2.474547000	-1.079372000
H	-3.748882000	-4.189371000	-1.705484000
H	-5.906366000	-2.954698000	-1.811075000
H	-5.960280000	-0.526672000	-1.269131000
H	-3.877567000	0.646986000	-0.632056000
H	-1.678196000	-3.012702000	-1.054490000
C	-1.404775000	-0.397449000	-0.385562000
C	-0.660529000	0.495105000	-1.069174000
C	0.371445000	0.973070000	-0.072525000
O	1.682305000	0.858251000	-0.625497000
O	0.150820000	2.284737000	0.399999000
C	0.528857000	3.364073000	-0.452902000
H	0.068682000	3.292422000	-1.444229000
H	0.174643000	4.272668000	0.039573000
H	1.616149000	3.422781000	-0.576357000

11S

P	-0.668158000	-1.435828000	0.165452000
C	-2.156049000	-2.121775000	-0.707338000
C	-2.152195000	-1.815534000	-2.210189000
H	-3.033714000	-1.657891000	-0.245111000
H	-2.217733000	-3.201526000	-0.539487000

C	-3.408742000	-2.340358000	-2.911610000
H	-2.080622000	-0.732275000	-2.356918000
H	-1.257440000	-2.242181000	-2.680871000
C	-3.450517000	-1.970969000	-4.396157000
H	-3.464716000	-3.431820000	-2.796271000
H	-4.297498000	-1.934424000	-2.407731000
H	-4.346199000	-2.369505000	-4.885680000
H	-3.452555000	-0.882592000	-4.524200000
H	-2.575019000	-2.366580000	-4.925728000
C	0.409772000	-3.018726000	0.098628000
C	-0.179773000	-4.309040000	0.687843000
H	1.338898000	-2.751144000	0.615428000
H	0.689205000	-3.182609000	-0.949720000
C	0.882366000	-5.284667000	1.222369000
H	-0.878461000	-4.084198000	1.507580000
H	-0.778546000	-4.818408000	-0.077551000
C	1.593402000	-4.779788000	2.482568000
H	0.406127000	-6.249226000	1.444771000
H	1.622862000	-5.479590000	0.434463000
H	2.120927000	-3.836233000	2.302758000
H	0.874177000	-4.608268000	3.293780000
H	2.331807000	-5.505918000	2.840585000
C	-0.891652000	-1.375340000	2.016210000
C	-2.355489000	-1.339706000	2.475875000
H	-0.397739000	-0.447486000	2.316428000
H	-0.357229000	-2.204208000	2.492146000
C	-2.503869000	-0.796385000	3.901013000
H	-2.941288000	-0.700479000	1.810188000
H	-2.792909000	-2.345197000	2.410311000
C	-3.968059000	-0.652015000	4.320384000
H	-1.967971000	-1.447197000	4.606640000
H	-2.016473000	0.186694000	3.949049000
H	-4.491624000	-1.614788000	4.272453000
H	-4.057696000	-0.273395000	5.344854000
H	-4.488506000	0.047270000	3.655322000
P	0.245380000	2.625568000	-1.158516000
B	2.184906000	0.196273000	1.275925000
O	3.310314000	-0.159510000	1.979521000
O	1.377995000	1.090712000	1.942385000
C	3.107211000	0.302022000	3.342218000
C	2.083803000	1.483611000	3.153158000
C	2.524242000	-0.880246000	4.123758000
C	4.453943000	0.708008000	3.927344000
C	2.756689000	2.827226000	2.865580000

C	1.059974000	1.637984000	4.271946000
H	3.203767000	-1.732453000	4.032067000
H	2.405442000	-0.643416000	5.185785000
H	1.550984000	-1.180391000	3.724930000
H	5.100057000	-0.171559000	4.005707000
H	4.959290000	1.444126000	3.299157000
H	4.327714000	1.129245000	4.930752000
H	3.525113000	2.731960000	2.093399000
H	2.000708000	3.532978000	2.509551000
H	3.223880000	3.239837000	3.765289000
H	0.461456000	0.733986000	4.400114000
H	1.555620000	1.868182000	5.221426000
H	0.381368000	2.463221000	4.034570000
C	1.923044000	2.417342000	-1.913975000
C	2.181764000	2.284695000	-3.284152000
C	3.012379000	2.436997000	-1.029238000
C	3.490747000	2.148950000	-3.749902000
H	1.360281000	2.280491000	-3.991547000
C	4.318247000	2.281550000	-1.488876000
H	2.827483000	2.580495000	0.030361000
C	4.562285000	2.136176000	-2.856186000
H	3.671907000	2.046352000	-4.816742000
H	5.143887000	2.281976000	-0.782200000
H	5.579166000	2.023179000	-3.221765000
C	-0.864694000	2.694819000	-2.633464000
C	-1.050342000	1.607240000	-3.503562000
C	-1.572854000	3.878880000	-2.869646000
C	-1.916517000	1.713779000	-4.590345000
H	-0.509564000	0.683445000	-3.323578000
C	-2.448202000	3.982214000	-3.953215000
H	-1.446666000	4.718926000	-2.191928000
C	-2.620194000	2.900510000	-4.815643000
H	-2.042047000	0.870329000	-5.263840000
H	-2.997397000	4.905056000	-4.119051000
H	-3.300656000	2.978310000	-5.659311000
C	-3.450575000	2.804042000	1.984520000
C	-4.685429000	2.683841000	1.341557000
C	-4.789621000	1.889041000	0.197815000
C	-3.678958000	1.201501000	-0.287262000
C	-2.433428000	1.307066000	0.356106000
C	-2.334036000	2.131548000	1.493761000
H	-3.356726000	3.429364000	2.868798000
H	-5.555783000	3.209319000	1.724207000
H	-5.742532000	1.800962000	-0.317525000

H	-3.766100000	0.584325000	-1.176800000
H	-1.369189000	2.221858000	1.983950000
C	-1.279805000	0.507468000	-0.048183000
C	-0.124970000	0.919223000	-0.595969000
C	0.735675000	-0.320983000	-0.675329000
O	1.941644000	-0.352986000	0.057718000
O	1.005891000	-0.705788000	-1.996009000
C	2.319503000	-1.144596000	-2.345859000
H	2.604926000	-2.047239000	-1.795409000
H	2.263153000	-1.368918000	-3.413078000
H	3.062280000	-0.362964000	-2.175979000

12R

P	-0.612996000	-1.789655000	1.063342000
C	-1.297029000	-1.966635000	2.747530000
C	-0.813954000	-3.152115000	3.590332000
H	-2.387467000	-1.962211000	2.646702000
H	-1.028876000	-1.012916000	3.215269000
C	-1.217322000	-2.990469000	5.061021000
H	-1.230442000	-4.088858000	3.201153000
H	0.278096000	-3.251240000	3.529650000
C	-0.770726000	-4.169023000	5.928047000
H	-0.786288000	-2.057403000	5.447869000
H	-2.307617000	-2.873556000	5.124435000
H	0.319321000	-4.287180000	5.902728000
H	-1.066905000	-4.028641000	6.972996000
H	-1.214902000	-5.108699000	5.577890000
C	-0.817330000	-3.283724000	0.031843000
C	-0.072572000	-4.554340000	0.473437000
H	-0.494789000	-2.956003000	-0.961945000
H	-1.895279000	-3.455926000	-0.046303000
C	0.032210000	-5.584015000	-0.663256000
H	0.938390000	-4.310045000	0.822417000
H	-0.591484000	-5.004362000	1.326024000
C	0.949313000	-5.145863000	-1.809868000
H	0.405359000	-6.526790000	-0.243399000
H	-0.973308000	-5.796445000	-1.051434000
H	0.591212000	-4.234794000	-2.301695000
H	1.964293000	-4.947020000	-1.444603000
H	1.017468000	-5.925828000	-2.575593000
C	1.158802000	-1.387859000	1.263603000
C	2.049960000	-1.655488000	0.042987000
H	1.523510000	-1.951652000	2.130914000
H	1.167968000	-0.331351000	1.562761000
C	3.395312000	-0.931108000	0.158380000

H	2.224682000	-2.732890000	-0.063945000
H	1.546409000	-1.343918000	-0.877024000
C	4.349988000	-1.278656000	-0.986237000
H	3.214520000	0.151901000	0.181599000
H	3.862204000	-1.182887000	1.120671000
H	4.575745000	-2.351972000	-0.998466000
H	3.914189000	-1.019962000	-1.957605000
H	5.298158000	-0.738731000	-0.889445000
P	-0.641366000	-0.362765000	-2.301260000
B	-0.870210000	1.671217000	1.445052000
O	-1.487122000	2.888359000	1.874934000
O	0.168302000	1.351722000	2.441734000
C	-1.309548000	2.982778000	3.287647000
C	0.099446000	2.310551000	3.505108000
C	-1.381157000	4.456577000	3.685934000
C	-2.448633000	2.216732000	3.984499000
C	0.257045000	1.572791000	4.835998000
C	1.253168000	3.307628000	3.337758000
H	-1.164017000	4.593308000	4.752109000
H	-0.680660000	5.057911000	3.102743000
H	-2.390145000	4.835777000	3.493131000
H	-3.402075000	2.623674000	3.633146000
H	-2.427877000	1.155486000	3.726119000
H	-2.407962000	2.321594000	5.074863000
H	0.155112000	2.257298000	5.686427000
H	-0.486714000	0.778502000	4.942476000
H	1.251927000	1.115958000	4.888399000
H	1.306022000	4.015045000	4.172762000
H	2.198508000	2.754899000	3.297918000
H	1.146718000	3.869261000	2.407011000
C	-2.236028000	0.008066000	-3.146515000
C	-2.782498000	-0.968074000	-3.989116000
C	-2.909393000	1.228782000	-3.000260000
C	-3.972493000	-0.728591000	-4.678850000
H	-2.271847000	-1.920892000	-4.102263000
C	-4.099226000	1.469469000	-3.685013000
H	-2.506635000	1.981347000	-2.330645000
C	-4.632697000	0.491092000	-4.527528000
H	-4.385064000	-1.495040000	-5.329304000
H	-4.611630000	2.419467000	-3.559553000
H	-5.560755000	0.678395000	-5.060552000
C	0.552275000	0.640870000	-3.280921000
C	1.851974000	0.832076000	-2.786690000
C	0.243364000	1.133448000	-4.555276000

C	2.805858000	1.520724000	-3.527485000
H	2.104496000	0.487446000	-1.792827000
C	1.204566000	1.815885000	-5.303871000
H	-0.752696000	0.997418000	-4.962389000
C	2.485673000	2.016281000	-4.793307000
H	3.792542000	1.687697000	-3.105869000
H	0.943959000	2.198380000	-6.287320000
H	3.227935000	2.558355000	-5.372468000
C	2.630920000	3.835588000	-0.627806000
C	2.275309000	4.562167000	-1.765138000
C	1.031195000	4.343298000	-2.358557000
C	0.157416000	3.396037000	-1.831466000
C	0.508065000	2.647382000	-0.699437000
C	1.750000000	2.898548000	-0.091873000
H	3.593998000	4.002440000	-0.151984000
H	2.959844000	5.294462000	-2.184402000
H	0.745221000	4.900819000	-3.245995000
H	-0.797757000	3.220248000	-2.312433000
H	2.015309000	2.337086000	0.796744000
C	-0.363342000	1.618636000	-0.112277000
C	-0.837384000	0.493893000	-0.694182000
C	-1.617428000	-0.303689000	0.357025000
O	-1.875940000	0.495819000	1.411070000
O	-2.760635000	-0.993252000	-0.131143000
C	-3.953397000	-0.201943000	-0.133626000
H	-4.334606000	-0.070589000	0.882725000
H	-3.777840000	0.780170000	-0.577713000
H	-4.668276000	-0.753876000	-0.746963000
12S			
P	-0.631227000	-2.157815000	1.232004000
C	-1.843954000	-3.371969000	0.566577000
C	-1.590967000	-3.920933000	-0.844287000
H	-2.804966000	-2.848103000	0.584195000
H	-1.896391000	-4.187293000	1.302098000
C	-2.759753000	-4.783109000	-1.329647000
H	-1.440008000	-3.088886000	-1.534020000
H	-0.662780000	-4.503729000	-0.864787000
C	-2.543890000	-5.283921000	-2.759746000
H	-2.907726000	-5.635192000	-0.651208000
H	-3.683573000	-4.189135000	-1.283161000
H	-3.391799000	-5.884856000	-3.106267000
H	-2.418826000	-4.441331000	-3.449676000
H	-1.642682000	-5.904917000	-2.828358000
C	0.764396000	-3.038595000	2.018565000

C	1.678745000	-3.801197000	1.051754000
H	0.342917000	-3.706130000	2.781650000
H	1.336838000	-2.259936000	2.531223000
C	2.877223000	-4.417870000	1.779426000
H	1.113556000	-4.589003000	0.537905000
H	2.028930000	-3.110740000	0.280187000
C	3.814433000	-5.164424000	0.828106000
H	3.430576000	-3.619775000	2.292486000
H	2.521498000	-5.101410000	2.563453000
H	4.207145000	-4.490650000	0.057588000
H	4.667344000	-5.594411000	1.364099000
H	3.291507000	-5.982768000	0.318320000
C	-1.511484000	-1.231481000	2.540589000
C	-0.602513000	-0.418456000	3.479788000
H	-2.134013000	-1.944952000	3.094834000
H	-2.198447000	-0.570429000	2.001650000
C	-1.345436000	0.769753000	4.098995000
H	-0.220666000	-1.076614000	4.271573000
H	0.266069000	-0.025871000	2.946409000
C	-0.437021000	1.588320000	5.017880000
H	-1.704019000	1.413155000	3.283893000
H	-2.235681000	0.423665000	4.643637000
H	-0.960612000	2.461413000	5.422978000
H	-0.084617000	0.986471000	5.864903000
H	0.438379000	1.934536000	4.459779000
P	-2.398987000	-0.182903000	-0.896574000
B	1.339057000	1.068803000	0.741062000
O	2.438309000	1.533288000	-0.074609000
O	1.596376000	1.519814000	2.098015000
C	3.324519000	2.308281000	0.731808000
C	2.995835000	1.810922000	2.186617000
C	4.760000000	2.035823000	0.281477000
C	2.994405000	3.794312000	0.525783000
C	3.212643000	2.851345000	3.282304000
C	3.735198000	0.511581000	2.547324000
H	4.976469000	0.965131000	0.283301000
H	4.900412000	2.406299000	-0.739715000
H	5.484780000	2.544042000	0.929175000
H	1.986695000	4.026462000	0.878249000
H	3.708110000	4.451484000	1.036238000
H	3.031158000	4.011152000	-0.546651000
H	4.259155000	3.176383000	3.316141000
H	2.580509000	3.727729000	3.121763000
H	2.960467000	2.423897000	4.259305000

H	3.606657000	-0.237742000	1.761651000
H	4.806274000	0.677891000	2.707632000
H	3.307253000	0.112203000	3.473694000
C	-3.432214000	1.331287000	-0.805609000
C	-4.069518000	1.876924000	-1.926513000
C	-3.653150000	1.917473000	0.450473000
C	-4.884684000	3.002356000	-1.797343000
H	-3.913807000	1.435627000	-2.905451000
C	-4.449704000	3.050478000	0.574684000
H	-3.167096000	1.508691000	1.331760000
C	-5.067965000	3.599127000	-0.551219000
H	-5.365591000	3.420158000	-2.677920000
H	-4.578169000	3.513097000	1.548822000
H	-5.688089000	4.485830000	-0.454997000
C	-2.143101000	-0.421651000	-2.702293000
C	-1.174408000	0.271704000	-3.439926000
C	-2.951453000	-1.359174000	-3.361031000
C	-1.015223000	0.030649000	-4.803835000
H	-0.533436000	0.988086000	-2.937617000
C	-2.799185000	-1.596430000	-4.727927000
H	-3.701018000	-1.908272000	-2.796559000
C	-1.827098000	-0.903479000	-5.451003000
H	-0.255575000	0.571493000	-5.361592000
H	-3.434308000	-2.324667000	-5.224922000
H	-1.700407000	-1.092262000	-6.513341000
C	-1.651209000	4.688995000	-1.068263000
C	-1.652408000	5.434015000	0.112209000
C	-1.134664000	4.873162000	1.280614000
C	-0.624074000	3.576683000	1.269972000
C	-0.656982000	2.802206000	0.096333000
C	-1.159823000	3.386691000	-1.075263000
H	-2.048911000	5.117411000	-1.983897000
H	-2.047003000	6.446477000	0.118345000
H	-1.117334000	5.450658000	2.201392000
H	-0.186633000	3.142766000	2.162125000
H	-1.177598000	2.810589000	-1.992867000
C	-0.147816000	1.425753000	0.154907000
C	-0.746910000	0.290992000	-0.270187000
C	0.161015000	-0.902337000	0.033684000
O	1.279274000	-0.478547000	0.666148000
O	0.427078000	-1.718376000	-1.109250000
C	1.471972000	-1.193554000	-1.936388000
H	1.404600000	-1.741695000	-2.877957000
H	1.340399000	-0.123685000	-2.116734000

H	2.449374000	-1.341009000	-1.469108000
S1			
P		-1.146301000000	-0.577372000000
B		-2.852010000000	-0.566747000000
O		-2.956806000000	-1.765257000000
O		-2.727030000000	0.543559000000
C		-2.827462000000	-1.442327000000
C		-3.221867000000	0.078071000000
C		-1.378256000000	-1.682360000000
C		-3.761722000000	-2.359401000000
C		-4.741294000000	0.296400000000
C		-2.556729000000	0.894710000000
H		-0.685168000000	-1.011217000000
H		-1.091437000000	-2.707096000000
H		-1.262564000000	-1.541603000000
H		-3.414305000000	-3.394312000000
H		-4.780448000000	-2.313994000000
H		-3.776290000000	-2.088852000000
H		-5.169117000000	0.023349000000
H		-5.239107000000	-0.284696000000
H		-4.948070000000	1.356395000000
H		-1.467531000000	0.856994000000
H		-2.850307000000	0.527157000000
H		-2.867927000000	1.941644000000
C		-0.288735000000	1.017431000000
C		-0.206780000000	1.888804000000
C		0.306967000000	1.371424000000
C		0.481522000000	3.095447000000
H		-0.709363000000	1.626986000000
C		0.990065000000	2.580554000000
H		0.226787000000	0.706511000000
C		1.081611000000	3.441092000000
H		0.540774000000	3.770440000000
H		1.447477000000	2.851917000000
H		1.613610000000	4.383710000000
C		0.067883000000	-1.757757000000
C		1.364601000000	-1.378319000000
C		-0.330461000000	-3.096897000000
C		2.255833000000	-2.330643000000
H		1.675859000000	-0.343868000000
C		0.567688000000	-4.044162000000
H		-1.341776000000	-3.387375000000
C		1.860563000000	-3.663121000000
H		3.259797000000	-2.030757000000

H	0.257289000000	-5.080681000000	-2.874385000000
H	2.557595000000	-4.404052000000	-3.528386000000
C	0.937193000000	-3.151763000000	1.856049000000
C	0.173707000000	-3.907827000000	2.744227000000
C	-1.214158000000	-3.737780000000	2.777363000000
C	-1.828782000000	-2.825727000000	1.927339000000
C	-1.071621000000	-2.066105000000	1.018681000000
C	0.320529000000	-2.239364000000	1.000435000000
H	2.016782000000	-3.270168000000	1.825283000000
H	0.653330000000	-4.621612000000	3.408152000000
H	-1.816910000000	-4.320330000000	3.468920000000
H	-2.904056000000	-2.676877000000	1.950442000000
H	0.929921000000	-1.661135000000	0.314945000000
C	-1.762437000000	-1.103125000000	0.137016000000
C	-2.993050000000	-0.609805000000	0.334480000000
C	-3.780126000000	0.060229000000	-0.569891000000
O	-4.021659000000	-0.409919000000	-1.777149000000
O	-4.415539000000	1.177738000000	-0.206289000000
C	-5.051300000000	1.928760000000	-1.258191000000
H	-4.362993000000	2.083184000000	-2.092428000000
H	-5.942120000000	1.406818000000	-1.616969000000
H	-5.328287000000	2.877840000000	-0.798486000000

S2R

P	1.14880700	-1.41969100	0.28880200
C	-0.18224000	-1.48854100	-0.94927200
C	-0.39245100	-2.81771000	-1.68480000
H	0.03793800	-0.65994700	-1.62543300
H	-1.09396300	-1.20107900	-0.41554600
C	-1.57461100	-2.72253500	-2.66307600
H	0.51243200	-3.10020100	-2.23593600
H	-0.58728700	-3.62260600	-0.96553300
C	-1.38612000	-1.67379800	-3.76347000
H	-1.72684000	-3.70877300	-3.11947300
H	-2.48802700	-2.49738500	-2.09595400
H	-1.35291100	-0.65690800	-3.35870100
H	-0.45301100	-1.84464800	-4.31514600
H	-2.21010400	-1.71197100	-4.48362800
C	2.76503100	-1.09217800	-0.47897600
C	3.05579500	-1.85945000	-1.77348700
H	3.52367500	-1.28394000	0.28836700
H	2.75121600	-0.01438900	-0.65804200
C	4.43888000	-1.51513000	-2.33814600
H	2.99040900	-2.94337200	-1.60618100
H	2.29365400	-1.60852000	-2.52078600

C	4.71654100	-2.21673400	-3.66869300
H	4.51081300	-0.42767100	-2.46999000
H	5.20809800	-1.78697200	-1.60279700
H	5.71105900	-1.96384700	-4.05074700
H	4.66658900	-3.30698700	-3.56022400
H	3.98201100	-1.92311800	-4.42801400
C	1.21650100	-3.00248400	1.20212900
C	-0.05680900	-3.32636100	1.99802100
H	2.08072900	-2.94045000	1.87050700
H	1.42569700	-3.78454900	0.46030100
C	-0.05702900	-4.75208300	2.55485100
H	-0.14948700	-2.60681300	2.81559900
H	-0.94595900	-3.18778300	1.37067500
C	-1.32258100	-5.04103400	3.36607200
H	0.02749400	-5.46969900	1.72635300
H	0.83167700	-4.90041400	3.18345100
H	-2.22206900	-4.90409500	2.75403900
H	-1.32700900	-6.06696900	3.74925200
H	-1.40369900	-4.36027900	4.22124200
P	-1.05376100	3.03399100	0.53585900
B	0.68873700	2.10829600	-0.06845800
O	0.59515900	1.40646300	-1.34925000
O	1.59820200	3.21065000	-0.26687900
C	1.06374500	2.29027100	-2.37818800
C	2.07805400	3.22396900	-1.60760600
C	1.69319300	1.44398600	-3.48517900
C	-0.14209200	3.04978000	-2.95038900
C	2.09175100	4.67104400	-2.10595500
C	3.51972700	2.69061100	-1.60227200
H	2.11353000	2.07748300	-4.27429400
H	2.48999500	0.80299000	-3.10030000
H	0.92899400	0.80370700	-3.94065500
H	-0.87685300	2.32447300	-3.31574100
H	-0.62537800	3.65950900	-2.18250400
H	0.14418400	3.69751400	-3.78570000
H	2.80538700	5.25175400	-1.51243500
H	2.39583400	4.73039400	-3.15812900
H	1.10949200	5.13359700	-1.99398200
H	3.56462300	1.65844500	-1.24720900
H	3.98774600	2.74093100	-2.59240900
H	4.10885500	3.29864400	-0.90926300
C	-0.79456100	3.18034900	2.35375800
C	0.37591000	3.86263800	2.74546100
C	-1.63557000	2.69881600	3.36916900

C	0.69226400	4.03994000	4.08981000
H	1.05180400	4.23174900	1.97878900
C	-1.32238900	2.88546600	4.71687400
H	-2.53481500	2.15463500	3.11162000
C	-0.15542100	3.55353600	5.08922300
H	1.60611100	4.56413800	4.35963200
H	-1.99859400	2.50509200	5.48023000
H	0.08628900	3.70032200	6.13849100
C	-2.55184400	2.00848800	0.26106800
C	-3.77056300	2.25331500	0.92167300
C	-2.56724700	1.07306700	-0.79237200
C	-4.93064700	1.55500400	0.58707500
H	-3.82130900	3.01623700	1.69163500
C	-3.73060500	0.38990000	-1.14052100
H	-1.65121500	0.90464600	-1.34474000
C	-4.91995700	0.61407100	-0.44251100
H	-5.85032400	1.75441900	1.13126000
H	-3.70954000	-0.31833700	-1.96680400
H	-5.82559500	0.07392100	-0.70443400
C	-5.03009100	-2.01007400	2.22457600
C	-5.50742200	-1.63022800	3.48018700
C	-4.71348800	-0.84370200	4.31886100
C	-3.44879800	-0.43645100	3.90744700
C	-2.96600200	-0.80932600	2.63939600
C	-3.76770300	-1.60503100	1.80275700
H	-5.64767600	-2.61514200	1.56708300
H	-6.49521400	-1.94465700	3.80457900
H	-5.08234000	-0.54705700	5.29649300
H	-2.82313900	0.17395600	4.54990400
H	-3.40368400	-1.87101300	0.81693600
C	-1.67051400	-0.40265300	2.21880000
C	-0.56673700	-0.03640200	1.87723800
C	0.84821900	0.05600500	1.48894600
O	1.30593800	1.20621700	0.96138400
O	1.67948000	-0.35787700	2.56436500
C	1.75942400	0.62321400	3.61220500
H	2.21553200	1.54291600	3.24382300
H	0.76281400	0.85042800	4.00534600
H	2.37621600	0.16992800	4.39043900
S2S			
P	-0.48085100	-2.46308100	0.05174100
C	0.87235300	-2.21709800	1.24240100
C	1.76453900	-3.45588300	1.41759700
H	0.40387900	-1.92594700	2.18481800

H	1.44310200	-1.34705400	0.90195500
C	2.92497500	-3.21223400	2.39281400
H	1.16106900	-4.29683500	1.78490900
H	2.17091000	-3.76155000	0.44534600
C	2.47230000	-2.87105100	3.81416300
H	3.54934700	-4.11449100	2.41296800
H	3.55183600	-2.40068300	2.00604900
H	1.78955600	-3.63388200	4.20942500
H	3.33063700	-2.80762200	4.49140900
H	1.96235700	-1.90342400	3.84748000
C	-1.43197400	-3.95201500	0.53335300
C	-2.02795200	-3.94151800	1.95832100
H	-0.73881300	-4.79143800	0.40267400
H	-2.22183800	-4.06896500	-0.21660800
C	-3.46028600	-3.39966800	2.02107600
H	-2.01784600	-4.97086900	2.33777800
H	-1.38967500	-3.36570200	2.63962500
C	-3.98407100	-3.32397200	3.45556100
H	-3.49589000	-2.41171800	1.55626100
H	-4.10818800	-4.04987600	1.41716100
H	-3.37762600	-2.63992900	4.05896900
H	-5.01691400	-2.96021100	3.47980300
H	-3.96506500	-4.30822800	3.94005400
C	0.19593800	-2.75306700	-1.62381500
C	1.45086700	-1.93041200	-1.95981700
H	-0.61850000	-2.51204600	-2.31591200
H	0.39401000	-3.82968400	-1.70807900
C	1.98223800	-2.24646900	-3.36074800
H	1.20780100	-0.86710200	-1.89088000
H	2.24137400	-2.13645600	-1.22640500
C	3.25368400	-1.45253100	-3.66795000
H	2.18070000	-3.32402300	-3.45650200
H	1.20914600	-2.00578400	-4.10233900
H	3.61318500	-1.64852200	-4.68384800
H	3.06754300	-0.37772400	-3.57427600
H	4.05849400	-1.71482600	-2.97006600
P	-0.35581500	2.32831400	0.66788200
B	-0.62151400	1.40855400	-1.11258200
O	-1.77954300	1.97827600	-1.75267100
O	0.46432900	1.45437900	-2.07060400
C	-1.56080000	1.97027100	-3.17061800
C	0.01065300	2.04040200	-3.29463200
C	-2.14857400	0.66953900	-3.74427000
C	-2.29435500	3.16905400	-3.76854500

C	0.55741400	3.47074300	-3.38096500
C	0.58043200	1.22820400	-4.46066000
H	-2.02990900	0.60896300	-4.83150700
H	-1.68170700	-0.20452300	-3.28338100
H	-3.21956800	0.63561100	-3.51997600
H	-3.37301500	3.05133700	-3.61795200
H	-1.98413900	4.09744100	-3.28504200
H	-2.10841300	3.25159900	-4.84586200
H	0.15592100	4.10400200	-2.59170600
H	1.64419600	3.43424600	-3.25667900
H	0.33547800	3.92951400	-4.35138400
H	0.33595700	0.16783600	-4.36807100
H	0.20080800	1.59212700	-5.42285200
H	1.67108600	1.32605900	-4.47361700
C	1.23749500	1.57389400	1.25014700
C	2.26043700	1.14059100	0.38605300
C	1.41672000	1.38548500	2.62952100
C	3.41756700	0.54175200	0.89040800
H	2.13479100	1.28022100	-0.68243800
C	2.57246000	0.78805200	3.13751900
H	0.63554600	1.71644400	3.30804100
C	3.57912100	0.36449500	2.26734000
H	4.19911800	0.21922200	0.20596900
H	2.69386400	0.66578800	4.21135700
H	4.48484900	-0.09103600	2.65960800
C	0.16814400	3.99015200	0.07416100
C	-0.85703600	4.84981500	-0.36351100
C	1.48708900	4.46303200	0.03712000
C	-0.56897600	6.12464400	-0.84535200
H	-1.88497000	4.49874200	-0.34411200
C	1.77470600	5.74424800	-0.43701600
H	2.29731000	3.82275800	0.37053100
C	0.75183100	6.57956200	-0.88604100
H	-1.37702800	6.76652200	-1.18843200
H	2.80639000	6.08759700	-0.46180600
H	0.97869800	7.57494900	-1.25854100
C	-1.01406700	-0.11489300	6.18141400
C	-2.24373200	0.26595100	6.72284800
C	-3.33937700	0.47711100	5.88247600
C	-3.21237200	0.30638000	4.50743500
C	-1.97720300	-0.07924500	3.95518200
C	-0.87652600	-0.28719600	4.80752500
H	-0.15864700	-0.27546100	6.83120100
H	-2.34740800	0.40075000	7.79548500

H	-4.29567000	0.77776700	6.30025800
H	-4.05769700	0.46931700	3.84722800
H	0.07928000	-0.56810600	4.37896800
C	-1.84427900	-0.28096200	2.55325000
C	-1.72293300	-0.42279100	1.35495300
C	-1.51051600	-0.87454800	-0.03099000
O	-0.74736600	-0.11667800	-0.84035000
O	-2.72579500	-1.33445600	-0.60989300
C	-3.75647000	-0.33296500	-0.67674400
H	-4.17769100	-0.15774000	0.32070300
H	-3.36028400	0.59930700	-1.08742700
H	-4.52569000	-0.74497600	-1.33300200

S3

P	-0.68197500	-2.45321300	0.28244700
C	-0.68862700	-1.50040200	1.86713600
C	-2.04795700	-0.85838600	2.18702200
H	0.08383300	-0.73020500	1.80308400
H	-0.39946700	-2.18750800	2.67025000
C	-1.90681800	0.27455800	3.20824400
H	-2.50556500	-0.46546500	1.27380200
H	-2.73776800	-1.61869600	2.57438900
C	-3.25570300	0.87886400	3.60294100
H	-1.39729500	-0.10416500	4.10580000
H	-1.25594300	1.04789500	2.78368300
H	-3.13476100	1.69779100	4.32053600
H	-3.78071300	1.27752900	2.72646200
H	-3.90914000	0.12565100	4.06009200
C	-2.16317400	-3.57810900	0.55688300
C	-2.12387900	-4.48196700	1.79377900
H	-2.24312700	-4.17798400	-0.35767400
H	-3.05556700	-2.94118400	0.58006700
C	-3.36862200	-5.37125600	1.94854700
H	-1.23505800	-5.12719700	1.76151800
H	-2.02216100	-3.86819500	2.69783200
C	-3.53060100	-6.41021600	0.83566100
H	-3.31364800	-5.88737200	2.91650400
H	-4.26190800	-4.73280600	1.98961600
H	-3.67967000	-5.93865500	-0.14143200
H	-2.64132400	-7.04930000	0.76471100
H	-4.39337900	-7.05869900	1.02371200
C	0.66873800	-3.72408600	0.20230200
C	1.49105500	-3.85084100	1.49033300
H	1.31812200	-3.43442800	-0.62691900
H	0.21124000	-4.68785300	-0.05174400

C	2.65352500	-4.83552800	1.32856000
H	1.89058100	-2.86849100	1.76634000
H	0.85662400	-4.17334300	2.32608500
C	3.54872500	-4.90062700	2.56756000
H	2.25410100	-5.83415300	1.10403600
H	3.24929600	-4.53760200	0.45671600
H	2.98044000	-5.20880400	3.45362100
H	4.36943800	-5.61389300	2.43266900
H	3.99013900	-3.91986000	2.78494500
P	1.74141300	0.89649100	0.00891800
B	-0.88327200	2.56303300	0.07192700
O	-1.57647200	3.64965500	-0.39920800
O	-0.17477000	2.84347300	1.21749900
C	-1.14730300	4.81917900	0.34617000
C	-0.51509500	4.18975500	1.64568200
C	-0.13006000	5.55423300	-0.52831100
C	-2.36802500	5.70212900	0.58450700
C	-1.51193500	4.04285400	2.79799500
C	0.76033300	4.86614000	2.13755400
H	-0.59451500	5.78547900	-1.49132200
H	0.19053100	6.49236200	-0.06332700
H	0.74998200	4.93987800	-0.71934300
H	-2.74741700	6.06207800	-0.37662300
H	-3.17202800	5.15378600	1.07949300
H	-2.10693100	6.57300500	1.19609200
H	-2.42213200	3.53047400	2.47437200
H	-1.05396800	3.44528700	3.59136200
H	-1.78991600	5.01638500	3.21414900
H	1.53767200	4.85380200	1.37170600
H	0.56363700	5.90416900	2.42804600
H	1.13870600	4.33162800	3.01434400
C	3.04215200	-0.24181100	-0.65065400
C	3.57238400	-1.17282600	0.25103700
C	3.58775000	-0.17314500	-1.94041300
C	4.58273700	-2.05462000	-0.13707400
H	3.19939700	-1.19332100	1.27101200
C	4.59939300	-1.04711600	-2.33027100
H	3.21662000	0.56638700	-2.64237200
C	5.09316100	-1.99856300	-1.43336600
H	4.98241500	-2.76867300	0.57770900
H	5.00790000	-0.98540600	-3.33572500
H	5.88440300	-2.67767700	-1.73891400
C	2.09735300	2.38447300	-1.03042900
C	3.09740200	3.25276000	-0.56508900

C	1.48510500	2.66919200	-2.25911800
C	3.49064500	4.36052100	-1.31552100
H	3.57129400	3.05263300	0.39264800
C	1.87699400	3.77789200	-3.01127600
H	0.68653000	2.03149200	-2.61981100
C	2.88299000	4.62438600	-2.54509700
H	4.26743500	5.02038900	-0.93864600
H	1.38983400	3.98141000	-3.96102500
H	3.18458700	5.48928000	-3.12919900
C	-4.73015900	0.96847400	-1.02987400
C	-4.85817900	0.38826300	-2.29311300
C	-3.70906600	0.07024400	-3.01731100
C	-2.44827100	0.30990200	-2.47692000
C	-2.29644000	0.86818900	-1.19876400
C	-3.46701100	1.21660300	-0.50022300
H	-5.61543800	1.23495100	-0.45842300
H	-5.84228500	0.19824900	-2.71262100
H	-3.79341900	-0.36627300	-4.00914800
H	-1.56402800	0.07774800	-3.05638700
H	-3.38204500	1.68678200	0.47501300
C	-0.96481400	1.15721700	-0.60553500
C	0.10836900	0.30248300	-0.68429600
C	0.06829200	-1.14774200	-0.94408000
O	-1.29780000	-1.76372900	-1.07805400
O	0.93119400	-1.67912100	-1.88869300
C	0.73784000	-1.25007700	-3.23023800
H	0.79094100	-0.15690600	-3.30784800
H	1.54919800	-1.68992700	-3.81427300
H	-0.22686500	-1.59820000	-3.61760700

S4R

P	1.49369600	-1.31684500	-1.09840000
B	-2.38179700	-0.45929900	-0.62008700
O	-2.70045600	0.56061100	0.24633600
O	-3.46447000	-0.99322300	-1.27213400
C	-4.08839200	0.90402500	-0.02021900
C	-4.64427900	-0.43253400	-0.63652100
C	-4.74103100	1.33353600	1.28706100
C	-4.07167900	2.06446000	-1.01936700
C	-5.72575500	-0.25059300	-1.69397500
C	-5.09768100	-1.43760700	0.42633200
H	-4.27528100	2.25675000	1.64564400
H	-5.80957300	1.52598600	1.14029500
H	-4.62442400	0.57269700	2.06129600
H	-5.08226900	2.42622100	-1.23322200

H	-3.49178900	2.88967900	-0.59560400
H	-3.60012300	1.76675500	-1.96076100
H	-6.03606600	-1.22866300	-2.07396500
H	-6.60519800	0.24427100	-1.26701800
H	-5.36459500	0.34112300	-2.53750800
H	-4.33167800	-1.56798700	1.19701400
H	-6.02826900	-1.12234400	0.90888900
H	-5.26520400	-2.40641000	-0.05281200
C	1.53231000	-0.77724500	-2.86299700
C	2.76173600	-0.57224000	-3.50842900
C	0.35398100	-0.70405600	-3.62330000
C	2.81195300	-0.28014200	-4.87150200
H	3.68645100	-0.63170000	-2.94271600
C	0.40790400	-0.40466100	-4.98343200
H	-0.60480000	-0.87346800	-3.14770900
C	1.63469300	-0.19017800	-5.61376400
H	3.77411400	-0.12051000	-5.35109900
H	-0.51530100	-0.34014000	-5.55332800
H	1.67266000	0.04045000	-6.67487400
C	2.86872300	-0.32926300	-0.36199200
C	3.14162100	1.00372800	-0.70842700
C	3.61639500	-0.92933900	0.65950800
C	4.13015400	1.71971400	-0.03581200
H	2.57086800	1.47353300	-1.50137600
C	4.60949300	-0.21421700	1.33187800
H	3.40878200	-1.95912000	0.93654800
C	4.86470600	1.11340900	0.98741400
H	4.32969700	2.75252400	-0.30906800
H	5.18020500	-0.69349700	2.12259300
H	5.63700600	1.67316900	1.50816100
C	0.28136600	-0.87124300	5.90126700
C	1.50936400	-0.34338100	6.30616600
C	2.38127000	0.19710700	5.35810500
C	2.03297900	0.21238800	4.01086100
C	0.79590200	-0.31742500	3.59715400
C	-0.07772800	-0.85994300	4.55654300
H	-0.39859700	-1.29288600	6.63600100
H	1.78589700	-0.35387700	7.35657400
H	3.33769200	0.60722500	5.67005600
H	2.70645600	0.62226300	3.26569200
H	-1.03004200	-1.26792600	4.23348000
C	0.44778100	-0.29994200	2.21627300
C	0.16860900	-0.25868800	1.03800700
C	0.03649100	-0.24526900	-0.41472000

O	-1.12899400	-0.94946100	-0.84679100
O	0.04054800	1.04041100	-0.98667500
C	-0.04483700	2.17797500	-0.12373200
H	0.85576800	2.27448800	0.49134700
H	-0.11714800	3.03439400	-0.79856500
H	-0.93110600	2.12770000	0.51211000
S4S			
P	-1.68964400	1.83114800	0.51270600
B	-0.06618300	-1.09464500	-1.14951800
O	0.98556100	-1.12726200	-0.26830300
O	-0.27795700	-2.28534500	-1.80389500
C	1.70394700	-2.36298000	-0.53127900
C	0.58789200	-3.26613500	-1.17437700
C	2.83491300	-2.01364000	-1.50336100
C	2.27239700	-2.88510900	0.78191200
C	-0.25689300	-4.00647300	-0.13418000
C	1.08327000	-4.23213900	-2.24370200
H	2.43722000	-1.64344100	-2.45337800
H	3.44924000	-1.22336600	-1.06280600
H	3.47293300	-2.87958600	-1.70684900
H	2.72505800	-3.87274900	0.63958300
H	3.05112600	-2.20604500	1.14314400
H	1.49983600	-2.95181000	1.54920100
H	-0.60810000	-3.32218800	0.64225100
H	-1.12988900	-4.43898200	-0.63205900
H	0.30762900	-4.81541800	0.34077900
H	0.23873300	-4.80117000	-2.64442300
H	1.55920200	-3.70344900	-3.07209000
H	1.80230100	-4.94223100	-1.82010800
C	-1.08445200	0.49140500	1.62801500
C	0.09666700	0.73291100	2.34691400
C	-1.74965500	-0.72834700	1.81084700
C	0.61574200	-0.23187700	3.20736300
H	0.61312500	1.68028200	2.22462500
C	-1.24146100	-1.68557700	2.69023700
H	-2.66980500	-0.92577000	1.27079900
C	-0.05502000	-1.44361400	3.38446600
H	1.53538300	-0.03182800	3.75081100
H	-1.77503800	-2.62149700	2.83416800
H	0.33753800	-2.18968200	4.07025700
C	-3.41979900	1.29075200	0.17561800
C	-3.84260700	0.45072700	-0.86615000
C	-4.38002000	1.79192700	1.06993200
C	-5.19170800	0.11890200	-0.99697000

H	-3.12056800	0.05757800	-1.56901100
C	-5.72473700	1.44641400	0.94532500
H	-4.07004100	2.46068100	1.86957000
C	-6.13461800	0.60855500	-0.09235500
H	-5.50509800	-0.53072400	-1.80997000
H	-6.45140400	1.83942900	1.65115000
H	-7.18300800	0.34340400	-0.19852100
C	4.87932400	1.00373400	1.35185200
C	5.77170200	1.98597700	0.91412200
C	5.35298200	2.94537700	-0.01024900
C	4.04945000	2.92803000	-0.50021900
C	3.14907600	1.94129100	-0.06575000
C	3.57467600	0.97616200	0.86901500
H	5.20207500	0.25749600	2.07267000
H	6.78945400	2.00467000	1.29315800
H	6.04466400	3.71080800	-0.35016000
H	3.71776700	3.67135100	-1.21806100
H	2.86519400	0.22379600	1.19518600
C	1.80804900	1.87342600	-0.53905800
C	0.65973000	1.68527500	-0.87440300
C	-0.74615100	1.33290600	-1.08545200
O	-0.87952300	-0.03900600	-1.44730000
O	-1.37105500	2.09806200	-2.07495200
C	-0.77269200	2.01178300	-3.36775700
H	0.27440100	2.33886900	-3.33582900
H	-0.82535700	0.98959000	-3.75653300
H	-1.34865200	2.68203900	-4.00794000

S5R

P	-0.44453700	-1.59939100	1.62826700
C	0.52974000	-2.04375400	0.14851800
C	1.30043700	-3.36611300	0.23954100
H	1.22488500	-1.20776800	0.00238300
H	-0.16234200	-2.05396000	-0.70003200
C	2.05433400	-3.65001800	-1.06540600
H	2.02057700	-3.32143500	1.06621600
H	0.62303900	-4.20368800	0.45650900
C	2.85893000	-4.94995100	-1.01393200
H	1.33437100	-3.68921600	-1.89451700
H	2.72186000	-2.80490600	-1.27884800
H	3.60693000	-4.91889700	-0.21270400
H	2.20739400	-5.81239600	-0.82745600
H	3.38725100	-5.12806400	-1.95662400
C	0.71552600	-1.63401100	3.03796100
C	0.20134900	-1.01537200	4.34862400

H	1.56539500	-1.05187900	2.65964500
H	1.04701000	-2.66878200	3.17868200
C	1.34673200	-0.72684100	5.32863300
H	-0.31541800	-0.08167900	4.11960900
H	-0.52592100	-1.68628800	4.82033700
C	2.13438100	-1.96733400	5.75899200
H	2.02676400	0.00312700	4.87001800
H	0.92487400	-0.23816600	6.21614300
H	1.47263900	-2.72177100	6.20341100
H	2.65089600	-2.43414000	4.91244500
H	2.89567100	-1.71178700	6.50380400
C	-1.80911900	-2.81603500	1.77324000
C	-2.61109900	-2.78069900	3.08044000
H	-1.37892100	-3.81222200	1.60691500
H	-2.46216900	-2.59329400	0.92059100
C	-3.83923800	-3.69449600	3.01146600
H	-1.97279400	-3.09190000	3.91672100
H	-2.92424200	-1.75206100	3.27996800
C	-4.65043200	-3.67929100	4.30873900
H	-4.47365400	-3.37534300	2.17366300
H	-3.52183500	-4.72206600	2.78424100
H	-4.04736800	-4.02605300	5.15660400
H	-4.99796100	-2.66585800	4.54145100
H	-5.53031000	-4.32766000	4.23693900
P	-2.69520700	-0.18248400	-0.82213600
B	0.89785500	1.46750700	0.79254800
O	1.37291500	2.80903200	0.95620900
O	2.08590400	0.59319000	0.76607100
C	2.73130900	2.75027900	1.39687900
C	3.24976600	1.42327300	0.73393300
C	3.44899000	4.01518400	0.93284600
C	2.73580600	2.67813900	2.93273600
C	4.36808400	0.71762700	1.49969600
C	3.67002100	1.62263000	-0.72945900
H	3.32330200	4.16328900	-0.14204500
H	3.02814900	4.88696100	1.44517300
H	4.52058700	3.97046300	1.16123900
H	2.17164800	3.53111600	3.32263600
H	2.24041100	1.76530600	3.27595800
H	3.74928500	2.71231900	3.34877200
H	4.64818500	-0.20342600	0.97581400
H	5.26108400	1.34946400	1.57228400
H	4.04916300	0.44866900	2.50999200
H	4.62341500	2.15675100	-0.81241800

H	3.78301800	0.63978400	-1.19935000
H	2.90874100	2.17349000	-1.28588900
C	-3.87092500	1.23458600	-0.73140200
C	-3.45877800	2.57494000	-0.77967800
C	-5.23843700	0.95094000	-0.62057800
C	-4.39627700	3.60594600	-0.72548100
H	-2.40098700	2.80536800	-0.85541900
C	-6.17738500	1.98197600	-0.56745100
H	-5.56619200	-0.08426300	-0.57142700
C	-5.75740600	3.31151000	-0.61903700
H	-4.06342500	4.63964300	-0.76442600
H	-7.23478400	1.74734900	-0.48004900
H	-6.48661400	4.11564000	-0.57275300
C	-2.31827500	-0.26441300	-2.62665900
C	-1.84860600	-1.49283000	-3.11543800
C	-2.49304000	0.79427900	-3.52699600
C	-1.51482400	-1.64819600	-4.46036200
H	-1.74816300	-2.33563200	-2.43465900
C	-2.17342300	0.63700200	-4.87354000
H	-2.86044000	1.75028400	-3.17219600
C	-1.67580000	-0.57976500	-5.34296800
H	-1.14238300	-2.60367300	-4.82034600
H	-2.29653100	1.47341900	-5.55545200
H	-1.42082100	-0.69611000	-6.39269000
C	1.12189100	1.21456900	-4.04954400
C	1.07235900	2.57451200	-4.36100700
C	0.63316300	3.48451500	-3.39801000
C	0.24099400	3.03868000	-2.13623500
C	0.24532900	1.66880000	-1.83112100
C	0.71386900	0.76628600	-2.79671500
H	1.46791000	0.49742100	-4.78858400
H	1.38434300	2.92330000	-5.34166400
H	0.61045600	4.54757000	-3.62353200
H	-0.05078400	3.74599500	-1.36636100
H	0.74411400	-0.29177900	-2.56257100
C	-0.11095300	1.22371100	-0.47749300
C	-1.19100100	0.53734800	-0.05645800
C	-1.01380100	0.22772100	1.43353000
O	-0.00801800	0.98754100	1.92992400
O	-2.19430700	0.27604000	2.21316000
C	-2.58294600	1.60755900	2.57403700
H	-1.84557600	2.05797300	3.24307500
H	-2.70185900	2.23723100	1.68820300
H	-3.54602100	1.50359200	3.07720300

S5S

P	-0.63122700	-2.15781500	1.23200400
C	-1.84395400	-3.37196900	0.56657700
C	-1.59096700	-3.92093300	-0.84428700
H	-2.80496600	-2.84810300	0.58419500
H	-1.89639100	-4.18729300	1.30209800
C	-2.75975300	-4.78310900	-1.32964700
H	-1.44000800	-3.08888600	-1.53402000
H	-0.66278000	-4.50372900	-0.86478700
C	-2.54389000	-5.28392100	-2.75974600
H	-2.90772600	-5.63519200	-0.65120800
H	-3.68357300	-4.18913500	-1.28316100
H	-3.39179900	-5.88485600	-3.10626700
H	-2.41882600	-4.44133100	-3.44967600
H	-1.64268200	-5.90491700	-2.82835800
C	0.76439600	-3.03859500	2.01856500
C	1.67874500	-3.80119700	1.05175400
H	0.34291700	-3.70613000	2.78165000
H	1.33683800	-2.25993600	2.53122300
C	2.87722300	-4.41787000	1.77942600
H	1.11355600	-4.58900300	0.53790500
H	2.02893000	-3.11074000	0.28018700
C	3.81443300	-5.16442400	0.82810600
H	3.43057600	-3.61977500	2.29248600
H	2.52149800	-5.10141000	2.56345300
H	4.20714500	-4.49065000	0.05758800
H	4.66734400	-5.59441100	1.36409900
H	3.29150700	-5.98276800	0.31832000
C	-1.51148400	-1.23148100	2.54058900
C	-0.60251300	-0.41845600	3.47978800
H	-2.13401300	-1.94495200	3.09483400
H	-2.19844700	-0.57042900	2.00165000
C	-1.34543600	0.76975300	4.09899500
H	-0.22066600	-1.07661400	4.27157300
H	0.26606900	-0.02587100	2.94640900
C	-0.43702100	1.58832000	5.01788000
H	-1.70401900	1.41315500	3.28389300
H	-2.23568100	0.42366500	4.64363700
H	-0.96061200	2.46141300	5.42297800
H	-0.08461700	0.98647100	5.86490300
H	0.43837900	1.93453600	4.45977900
P	-2.39898700	-0.18290300	-0.89657400
B	1.33905700	1.06880300	0.74106200
O	2.43830900	1.53328800	-0.07460900

O	1.59637600	1.51981400	2.09801500
C	3.32451900	2.30828100	0.73180800
C	2.99583500	1.81092200	2.18661700
C	4.76000000	2.03582300	0.28147700
C	2.99440500	3.79431200	0.52578300
C	3.21264300	2.85134500	3.28230400
C	3.73519800	0.51158100	2.54732400
H	4.97646900	0.96513100	0.28330100
H	4.90041200	2.40629900	-0.73971500
H	5.48478000	2.54404200	0.92917500
H	1.98669500	4.02646200	0.87824900
H	3.70811000	4.45148400	1.03623800
H	3.03115800	4.01115200	-0.54665100
H	4.25915500	3.17638300	3.31614100
H	2.58050900	3.72772900	3.12176300
H	2.96046700	2.42389700	4.25930500
H	3.60665700	-0.23774200	1.76165100
H	4.80627400	0.67789100	2.70763200
H	3.30725300	0.11220300	3.47369400
C	-3.43221400	1.33128700	-0.80560900
C	-4.06951800	1.87692400	-1.92651300
C	-3.65315000	1.91747300	0.45047300
C	-4.88468400	3.00235600	-1.79734300
H	-3.91380700	1.43562700	-2.90545100
C	-4.44970400	3.05047800	0.57468400
H	-3.16709600	1.50869100	1.33176000
C	-5.06796500	3.59912700	-0.55121900
H	-5.36559100	3.42015800	-2.67792000
H	-4.57816900	3.51309700	1.54882200
H	-5.68808900	4.48583000	-0.45499700
C	-2.14310100	-0.42165100	-2.70229300
C	-1.17440800	0.27170400	-3.43992600
C	-2.95145300	-1.35917400	-3.36103100
C	-1.01522300	0.03064900	-4.80383500
H	-0.53343600	0.98808600	-2.93761700
C	-2.79918500	-1.59643000	-4.72792700
H	-3.70101800	-1.90827200	-2.79655900
C	-1.82709800	-0.90347900	-5.45100300
H	-0.25557500	0.57149300	-5.36159200
H	-3.43430800	-2.32466700	-5.22492200
H	-1.70040700	-1.09226200	-6.51334100
C	-1.65120900	4.68899500	-1.06826300
C	-1.65240800	5.43401500	0.11220900
C	-1.13466400	4.87316200	1.28061400

C	-0.62407400	3.57668300	1.26997200
C	-0.65698200	2.80220600	0.09633300
C	-1.15982300	3.38669100	-1.07526300
H	-2.04891100	5.11741100	-1.98389700
H	-2.04700300	6.44647700	0.11834500
H	-1.11733400	5.45065800	2.20139200
H	-0.18663300	3.14276600	2.16212500
H	-1.17759800	2.81058900	-1.99286700
C	-0.14781600	1.42575300	0.15490700
C	-0.74691000	0.29099200	-0.27018700
C	0.16101500	-0.90233700	0.03368400
O	1.27927400	-0.47854700	0.66614800
O	0.42707800	-1.71837600	-1.10925000
C	1.47197200	-1.19355400	-1.93638800
H	1.40460000	-1.74169500	-2.87795700
H	1.34039900	-0.12368500	-2.11673400
H	2.44937400	-1.34100900	-1.46910800

S6

P	0.65238600	-1.36019300	1.94288600
C	-1.03999100	-0.89837800	2.36060400
C	-1.63235900	-1.66799700	3.55239500
H	-1.64720000	-1.07501700	1.46928500
H	-1.06106100	0.18612400	2.51416600
C	-3.12579400	-1.34091400	3.69225500
H	-1.51691900	-2.75072500	3.40342500
H	-1.10642700	-1.42012400	4.48465600
C	-3.78370500	-2.08844700	4.85254500
H	-3.24148900	-0.25800400	3.82679500
H	-3.63278200	-1.57950600	2.74937600
H	-4.84704900	-1.83792800	4.92756400
H	-3.70687800	-3.17463800	4.71892900
H	-3.31263600	-1.83695200	5.81100300
C	0.73262400	-3.13336100	1.53203700
C	-0.31252600	-3.59375500	0.50198800
H	0.62093200	-3.68363100	2.47585100
H	1.74538300	-3.31896000	1.15818500
C	-0.24629500	-5.10163100	0.24755600
H	-1.32005500	-3.32262200	0.83750300
H	-0.14842600	-3.05991200	-0.43702700
C	-1.27677400	-5.53840400	-0.79649400
H	0.76342800	-5.36891000	-0.09270000
H	-0.41197700	-5.64389100	1.18955700
H	-1.11000800	-5.02005000	-1.74749600
H	-1.22353200	-6.61621800	-0.98343900

H	-2.29514600	-5.30281000	-0.46555000
C	1.74072900	-1.00491700	3.35351400
C	3.22934200	-1.25729000	3.07788100
H	1.38432900	-1.60055600	4.20306400
H	1.57297600	0.04827200	3.60905200
C	4.10673400	-0.87596900	4.27475200
H	3.39072200	-2.31455000	2.82900600
H	3.53180200	-0.67681800	2.19938900
C	5.59386400	-1.11588200	4.00683100
H	3.93943000	0.18193200	4.51796300
H	3.78994100	-1.44958600	5.15662000
H	6.20326200	-0.83340200	4.87152500
H	5.79109600	-2.17227800	3.78892900
H	5.93858100	-0.52881600	3.14754200
P	-0.35790200	-0.75643700	-2.99589400
B	-0.57115800	1.78279700	0.17172000
O	0.69514300	2.32123600	-0.14143800
O	-1.19307200	2.58531000	1.14796800
C	0.98480100	3.35984700	0.80245700
C	-0.45098800	3.81708900	1.23458700
C	1.77326400	2.72772200	1.95921200
C	1.82971200	4.42677100	0.11422500
C	-1.07825400	4.80185700	0.24012700
C	-0.56043200	4.35946800	2.65545900
H	1.14814300	2.00572800	2.49330600
H	2.63413200	2.19320900	1.54661800
H	2.12882900	3.47685200	2.67472600
H	1.34585500	4.78264400	-0.79791500
H	2.00515500	5.28178900	0.77717600
H	2.80195700	4.00474600	-0.16228700
H	-0.61188000	5.79141300	0.29349600
H	-0.98983500	4.42601400	-0.78365800
H	-2.14258800	4.90600900	0.47096800
H	-0.25601200	3.61280900	3.39303000
H	0.06271300	5.25212600	2.78290500
H	-1.59848800	4.63604300	2.86593900
C	-1.80579100	0.30311900	-3.41710000
C	-1.81943300	1.69504800	-3.24887300
C	-2.97015400	-0.33597700	-3.85784800
C	-2.97769500	2.42556700	-3.50643200
H	-0.92611300	2.20623900	-2.91135100
C	-4.13110300	0.39297100	-4.11815200
H	-2.97081400	-1.41628600	-3.97577600
C	-4.13676300	1.77531900	-3.93572600

H	-2.97910700	3.50330100	-3.36412900
H	-5.03064400	-0.11911300	-4.44856400
H	-5.04156800	2.34632900	-4.12745700
C	1.02457000	0.21648300	-3.76000700
C	1.57535800	1.38308700	-3.20305000
C	1.53244500	-0.24721000	-4.98134800
C	2.59886200	2.06523400	-3.86246000
H	1.22708700	1.74932900	-2.24267000
C	2.55612800	0.43585900	-5.64037600
H	1.12281500	-1.15595200	-5.41540500
C	3.09268400	1.59607800	-5.08193300
H	3.01205800	2.96783800	-3.41816500
H	2.93701900	0.05858700	-6.58599000
H	3.89105000	2.12952800	-5.59124800
C	-4.09855500	-1.78961200	-0.48344800
C	-5.09318500	-1.01216100	0.10911200
C	-4.76738800	0.29848900	0.48722500
C	-3.49642700	0.81658000	0.28490800
C	-2.45763300	0.04640000	-0.30859200
C	-2.81627400	-1.27993100	-0.67875500
H	-4.31639900	-2.80880400	-0.79843700
H	-6.09267200	-1.40694400	0.26835700
H	-5.52676600	0.93044000	0.94417400
H	-3.27737000	1.83249400	0.59089000
H	-2.06705800	-1.92090500	-1.13261900
C	-1.10273900	0.53245100	-0.44107700
C	-0.13469600	-0.27935100	-1.18375700
C	0.99087600	-0.74462400	-0.61997000
O	1.30942500	-0.49078800	0.76713000
O	1.93803900	-1.52876000	-1.19338400
C	3.25426200	-0.95588100	-1.29719100
H	3.21427400	0.00231900	-1.81996900
H	3.69376200	-0.82340000	-0.30192200
H	3.84693700	-1.66987500	-1.87146800

S7Z

P	6.387625000000	-2.196869000000	0.642733000000
B	8.431729000000	1.119206000000	-1.190577000000
O	9.745239000000	1.443858000000	-0.979401000000
O	7.922834000000	1.599719000000	-2.364513000000
C	10.111092000000	2.409553000000	-2.007461000000
C	9.044375000000	2.129461000000	-3.128992000000
C	9.968415000000	3.793074000000	-1.367785000000
C	11.555299000000	2.151499000000	-2.417346000000
C	9.461060000000	1.027348000000	-4.106140000000

C	8.570524000000	3.363772000000	-3.886521000000
H	8.936211000000	3.972441000000	-1.052796000000
H	10.605588000000	3.839190000000	-0.479672000000
H	10.271907000000	4.589014000000	-2.055198000000
H	11.849913000000	2.814706000000	-3.238362000000
H	12.218866000000	2.344548000000	-1.568715000000
H	11.699342000000	1.116519000000	-2.733814000000
H	9.801534000000	0.133434000000	-3.578517000000
H	8.593752000000	0.745792000000	-4.709785000000
H	10.256652000000	1.366754000000	-4.777684000000
H	9.404247000000	3.833758000000	-4.420197000000
H	7.815360000000	3.073321000000	-4.623219000000
H	8.123993000000	4.100437000000	-3.215477000000
C	7.597545000000	-2.652591000000	1.965635000000
C	8.769837000000	-1.942103000000	2.244255000000
C	7.282355000000	-3.768795000000	2.756324000000
C	9.612750000000	-2.343122000000	3.281838000000
H	9.029682000000	-1.071692000000	1.652414000000
C	8.125575000000	-4.170812000000	3.789847000000
H	6.376363000000	-4.333862000000	2.553361000000
C	9.296230000000	-3.458282000000	4.056948000000
H	10.521122000000	-1.780610000000	3.480993000000
H	7.866541000000	-5.040046000000	4.388375000000
H	9.954190000000	-3.769466000000	4.863536000000
C	6.430118000000	-3.747238000000	-0.368461000000
C	7.554638000000	-4.575242000000	-0.503054000000
C	5.268454000000	-4.066723000000	-1.083335000000
C	7.524276000000	-5.677265000000	-1.352855000000
H	8.458713000000	-4.343157000000	0.049740000000
C	5.235318000000	-5.171272000000	-1.936825000000
H	4.386716000000	-3.439601000000	-0.974105000000
C	6.365970000000	-5.974748000000	-2.076417000000
H	8.406729000000	-6.302526000000	-1.458366000000
H	4.328057000000	-5.404370000000	-2.487733000000
H	6.345318000000	-6.833975000000	-2.741348000000
C	10.119564000000	-2.503061000000	-2.678319000000
C	9.398671000000	-2.852824000000	-3.820035000000
C	8.025800000000	-2.601408000000	-3.875122000000
C	7.375127000000	-2.016576000000	-2.792416000000
C	8.089566000000	-1.671576000000	-1.637939000000
C	9.470237000000	-1.911668000000	-1.594032000000
H	11.188825000000	-2.689540000000	-2.628034000000
H	9.902372000000	-3.316208000000	-4.663605000000
H	7.458635000000	-2.866211000000	-4.762820000000

H	6.307602000000	-1.829777000000	-2.833697000000
H	10.026683000000	-1.639649000000	-0.703201000000
C	7.423505000000	-1.084404000000	-0.442842000000
C	7.605573000000	0.235201000000	-0.195617000000
C	7.029073000000	0.873277000000	1.003840000000
O	6.523872000000	0.308439000000	1.956958000000
O	7.131595000000	2.225323000000	0.919962000000
C	6.610901000000	2.949861000000	2.042345000000
H	6.796447000000	4.001759000000	1.824087000000
H	7.121279000000	2.649381000000	2.961317000000
H	5.539824000000	2.762392000000	2.155030000000
S8S			
P	4.393404000000	0.236746000000	0.284543000000
C	5.283999000000	1.843223000000	0.355367000000
C	5.589615000000	2.397574000000	1.751029000000
H	4.705304000000	2.567609000000	-0.224464000000
H	6.220541000000	1.687068000000	-0.175747000000
C	6.487266000000	3.635751000000	1.660932000000
H	4.661843000000	2.648916000000	2.281490000000
H	6.104343000000	1.638406000000	2.345995000000
C	6.863928000000	4.183999000000	3.038173000000
H	7.398400000000	3.366580000000	1.112169000000
H	5.981149000000	4.413645000000	1.072271000000
H	5.973741000000	4.463051000000	3.615108000000
H	7.415391000000	3.433342000000	3.616870000000
H	7.499537000000	5.071827000000	2.952727000000
C	2.777840000000	0.515032000000	-0.573512000000
C	2.821792000000	1.370559000000	-1.843007000000
H	2.093682000000	0.957692000000	0.163495000000
H	2.409615000000	-0.494863000000	-0.782705000000
C	1.496530000000	1.370510000000	-2.619154000000
H	3.071436000000	2.403181000000	-1.576590000000
H	3.621758000000	1.026944000000	-2.501116000000
C	1.160365000000	0.029076000000	-3.276677000000
H	0.677348000000	1.675389000000	-1.952336000000
H	1.565610000000	2.139482000000	-3.398293000000
H	0.214968000000	0.087325000000	-3.826987000000
H	1.944234000000	-0.264313000000	-3.982896000000
H	1.059231000000	-0.775817000000	-2.539096000000
C	3.789354000000	-0.227751000000	1.973495000000
C	4.790882000000	-0.942893000000	2.888497000000
H	2.935495000000	-0.887896000000	1.789105000000
H	3.396287000000	0.683480000000	2.437214000000
C	4.112794000000	-1.604469000000	4.095787000000

H	5.331869000000	-1.704023000000	2.317250000000
H	5.544770000000	-0.231232000000	3.244455000000
C	3.413398000000	-0.620308000000	5.037577000000
H	3.389790000000	-2.349175000000	3.734301000000
H	4.874408000000	-2.162801000000	4.654411000000
H	2.999007000000	-1.135055000000	5.911091000000
H	4.114965000000	0.141136000000	5.400634000000
H	2.586404000000	-0.099731000000	4.541039000000
P	6.833586000000	-1.030003000000	-2.911668000000
B	7.219566000000	-2.665705000000	-0.610832000000
O	8.001483000000	-3.399115000000	-1.549371000000
O	7.810948000000	-2.805118000000	0.684088000000
C	9.179554000000	-3.873491000000	-0.881758000000
C	8.725515000000	-3.904656000000	0.621916000000
C	9.552003000000	-5.233291000000	-1.467836000000
C	10.308253000000	-2.866581000000	-1.137602000000
C	9.842290000000	-3.659529000000	1.633495000000
C	7.962849000000	-5.188981000000	0.982148000000
H	8.707481000000	-5.925177000000	-1.431553000000
H	9.845839000000	-5.113664000000	-2.516227000000
H	10.396328000000	-5.678193000000	-0.928036000000
H	10.073351000000	-1.895516000000	-0.695421000000
H	11.266995000000	-3.214968000000	-0.737247000000
H	10.412873000000	-2.727362000000	-2.218169000000
H	10.620241000000	-4.428607000000	1.559256000000
H	10.298088000000	-2.678562000000	1.483913000000
H	9.431338000000	-3.689476000000	2.648604000000
H	8.626571000000	-6.058944000000	1.040175000000
H	7.490295000000	-5.049430000000	1.960256000000
H	7.175660000000	-5.391607000000	0.251348000000
C	5.951409000000	0.510192000000	-3.446489000000
C	6.251184000000	1.762107000000	-2.880558000000
C	5.099663000000	0.500680000000	-4.569034000000
C	5.677785000000	2.937777000000	-3.365738000000
H	6.957233000000	1.826140000000	-2.062841000000
C	4.529815000000	1.674726000000	-5.059272000000
H	4.869804000000	-0.439610000000	-5.058111000000
C	4.802324000000	2.901880000000	-4.450703000000
H	5.923214000000	3.885888000000	-2.893306000000
H	3.868301000000	1.628736000000	-5.920663000000
H	4.353432000000	3.816102000000	-4.828810000000
C	5.564116000000	-2.310940000000	-3.317787000000
C	4.183125000000	-2.121914000000	-3.154794000000
C	6.015301000000	-3.553345000000	-3.784607000000

C	3.279164000000	-3.145286000000	-3.436343000000
H	3.812961000000	-1.167984000000	-2.804984000000
C	5.114620000000	-4.581336000000	-4.061887000000
H	7.080817000000	-3.720789000000	-3.886215000000
C	3.744267000000	-4.382547000000	-3.887158000000
H	2.213449000000	-2.974591000000	-3.306044000000
H	5.484563000000	-5.540477000000	-4.414056000000
H	3.042454000000	-5.182440000000	-4.109246000000
C	9.793461000000	1.308309000000	-0.509729000000
C	9.810582000000	1.465821000000	0.873840000000
C	8.854745000000	0.789897000000	1.638255000000
C	7.893206000000	-0.005314000000	1.023844000000
C	7.835138000000	-0.151673000000	-0.375050000000
C	8.824685000000	0.507120000000	-1.121072000000
H	10.536284000000	1.807051000000	-1.126593000000
H	10.560338000000	2.090282000000	1.351481000000
H	8.865559000000	0.873485000000	2.722522000000
H	7.184882000000	-0.552022000000	1.630432000000
H	8.852111000000	0.386389000000	-2.199045000000
C	6.793047000000	-1.065472000000	-0.989928000000
C	5.394851000000	-1.036500000000	-0.371625000000
C	4.940295000000	-2.348725000000	-0.264802000000
O	5.743093000000	-3.312147000000	-0.532129000000
O	3.679216000000	-2.635623000000	0.113609000000
C	3.337997000000	-4.032269000000	0.169153000000
H	3.456636000000	-4.484619000000	-0.817432000000
H	3.971216000000	-4.552447000000	0.891542000000
H	2.294000000000	-4.058891000000	0.483700000000
S9R			
P	-0.126184000000	-0.072619000000	-1.425132000000
C	-1.147492000000	-0.721393000000	-2.854025000000
C	-1.833479000000	-2.090618000000	-2.766147000000
H	-0.454852000000	-0.733820000000	-3.705141000000
H	-1.881761000000	0.058072000000	-3.084412000000
C	-2.827639000000	-2.298565000000	-3.913400000000
H	-1.076432000000	-2.884820000000	-2.798047000000
H	-2.365689000000	-2.205237000000	-1.821399000000
C	-3.548174000000	-3.644582000000	-3.819022000000
H	-3.565893000000	-1.486470000000	-3.887767000000
H	-2.306750000000	-2.216185000000	-4.877847000000
H	-4.258502000000	-3.779278000000	-4.642296000000
H	-2.836550000000	-4.478727000000	-3.851055000000
H	-4.104046000000	-3.716613000000	-2.876904000000
C	0.551351000000	-1.670276000000	-0.791347000000

C	1.489126000000	-1.740870000000	0.413815000000
H	1.024175000000	-2.132220000000	-1.667906000000
H	-0.345203000000	-2.266007000000	-0.590060000000
C	1.924273000000	-3.184751000000	0.685629000000
H	2.363570000000	-1.106526000000	0.252906000000
H	0.978165000000	-1.340849000000	1.294193000000
C	2.851975000000	-3.287056000000	1.898583000000
H	1.036437000000	-3.813212000000	0.845925000000
H	2.429662000000	-3.591526000000	-0.202374000000
H	3.155749000000	-4.322740000000	2.087069000000
H	3.760822000000	-2.692283000000	1.747597000000
H	2.358047000000	-2.910386000000	2.801969000000
C	1.064120000000	0.923823000000	-2.436015000000
C	2.333237000000	0.137194000000	-2.782286000000
H	1.327966000000	1.805232000000	-1.859923000000
H	0.534886000000	1.233708000000	-3.342198000000
C	3.303257000000	0.974358000000	-3.623188000000
H	2.829316000000	-0.168363000000	-1.854505000000
H	2.083767000000	-0.782139000000	-3.331385000000
C	4.588113000000	0.216715000000	-3.965117000000
H	2.802458000000	1.293457000000	-4.547588000000
H	3.548979000000	1.891892000000	-3.072311000000
H	5.271132000000	0.835319000000	-4.557418000000
H	5.117302000000	-0.089495000000	-3.054836000000
H	4.371347000000	-0.689658000000	-4.543606000000
P	-1.602067000000	2.491770000000	-1.221314000000
B	-1.605529000000	0.973522000000	2.437881000000
O	-1.118686000000	0.937880000000	3.739036000000
O	-3.000200000000	1.074705000000	2.446733000000
C	-2.191601000000	1.311514000000	4.624861000000
C	-3.463004000000	0.906418000000	3.802245000000
C	-2.013940000000	0.571022000000	5.946157000000
C	-2.083623000000	2.824898000000	4.851712000000
C	-4.685952000000	1.794218000000	4.009601000000
C	-3.845253000000	-0.568179000000	3.968067000000
H	-1.092089000000	0.906021000000	6.431726000000
H	-2.850706000000	0.773382000000	6.624693000000
H	-1.940120000000	-0.507538000000	5.791301000000
H	-2.814420000000	3.183246000000	5.584512000000
H	-1.078159000000	3.051104000000	5.218091000000
H	-2.230932000000	3.372594000000	3.916260000000
H	-4.473772000000	2.833143000000	3.746924000000
H	-5.505537000000	1.443581000000	3.373451000000
H	-5.024707000000	1.758200000000	5.051163000000

H	-2.971936000000	-1.212719000000	3.831278000000
H	-4.276800000000	-0.767722000000	4.954587000000
H	-4.580753000000	-0.830460000000	3.202140000000
C	-3.294918000000	3.159331000000	-0.895068000000
C	-4.080938000000	2.928343000000	0.242639000000
C	-3.800219000000	3.992016000000	-1.907300000000
C	-5.331226000000	3.533783000000	0.367882000000
H	-3.733426000000	2.261795000000	1.021064000000
C	-5.047464000000	4.603296000000	-1.774872000000
H	-3.208592000000	4.162517000000	-2.803290000000
C	-5.817228000000	4.375513000000	-0.633899000000
H	-5.928179000000	3.341065000000	1.255843000000
H	-5.418286000000	5.250835000000	-2.564979000000
H	-6.791820000000	4.845096000000	-0.530291000000
C	-0.590931000000	3.632420000000	-0.194764000000
C	0.577659000000	4.169749000000	-0.748466000000
C	-0.928988000000	3.970366000000	1.124118000000
C	1.408363000000	5.002421000000	0.002528000000
H	0.839852000000	3.931497000000	-1.775224000000
C	-0.099585000000	4.797305000000	1.878605000000
H	-1.845981000000	3.591421000000	1.557669000000
C	1.074570000000	5.308683000000	1.322296000000
H	2.312407000000	5.409581000000	-0.442119000000
H	-0.367826000000	5.036437000000	2.903736000000
H	1.721900000000	5.951407000000	1.913018000000
C	-4.753048000000	-0.846801000000	-1.143401000000
C	-4.758378000000	-1.964636000000	-0.311223000000
C	-3.680570000000	-2.172736000000	0.552471000000
C	-2.622025000000	-1.269391000000	0.581919000000
C	-2.602099000000	-0.133403000000	-0.246018000000
C	-3.685536000000	0.052140000000	-1.114491000000
H	-5.581748000000	-0.665961000000	-1.822064000000
H	-5.590674000000	-2.662558000000	-0.332297000000
H	-3.664507000000	-3.038494000000	1.208868000000
H	-1.792651000000	-1.429306000000	1.261737000000
H	-3.717415000000	0.906042000000	-1.777270000000
C	-1.369055000000	0.777981000000	-0.206912000000
C	-0.778431000000	0.915925000000	1.174045000000
C	0.605920000000	1.161022000000	1.190472000000
O	1.337812000000	1.076092000000	0.167263000000
O	1.176592000000	1.498600000000	2.376882000000
C	2.564056000000	1.815190000000	2.321749000000
H	2.839219000000	2.084150000000	3.343669000000
H	3.159541000000	0.959248000000	1.987224000000

H	2.746505000000	2.657687000000	1.647784000000
S9S			
P	7.038025000000	-1.866052000000	1.254715000000
C	6.162136000000	-3.472898000000	1.094595000000
C	6.538830000000	-4.560665000000	2.108166000000
H	6.308387000000	-3.822835000000	0.071170000000
H	5.103687000000	-3.229870000000	1.178107000000
C	5.568463000000	-5.751703000000	2.035803000000
H	7.554944000000	-4.919987000000	1.909896000000
H	6.541106000000	-4.164125000000	3.133017000000
C	4.133759000000	-5.417971000000	2.457572000000
H	5.567476000000	-6.148108000000	1.011954000000
H	5.957037000000	-6.551945000000	2.678727000000
H	3.664697000000	-4.692791000000	1.784220000000
H	3.508971000000	-6.317537000000	2.454339000000
H	4.107790000000	-4.998199000000	3.471124000000
C	6.371807000000	-0.998111000000	2.737552000000
C	5.011581000000	-1.493627000000	3.247304000000
H	6.272358000000	0.055461000000	2.467166000000
H	7.131550000000	-1.082820000000	3.524134000000
C	4.557551000000	-0.696924000000	4.473242000000
H	4.274823000000	-1.391208000000	2.444878000000
H	5.054082000000	-2.556951000000	3.509766000000
C	3.158873000000	-1.101374000000	4.943227000000
H	5.279829000000	-0.838550000000	5.289988000000
H	4.572510000000	0.370335000000	4.226500000000
H	2.416546000000	-0.928653000000	4.155198000000
H	3.120368000000	-2.165888000000	5.205191000000
H	2.851556000000	-0.528500000000	5.825098000000
C	8.765212000000	-2.393656000000	1.698703000000
C	9.804325000000	-1.348102000000	2.117413000000
H	9.133399000000	-2.988511000000	0.859184000000
H	8.603926000000	-3.086242000000	2.534391000000
C	10.987844000000	-1.978480000000	2.870438000000
H	10.161020000000	-0.808336000000	1.234849000000
H	9.346169000000	-0.607481000000	2.784808000000
C	11.784126000000	-3.006316000000	2.064347000000
H	11.659075000000	-1.170384000000	3.188761000000
H	10.611914000000	-2.444895000000	3.792515000000
H	11.163972000000	-3.860924000000	1.770905000000
H	12.181888000000	-2.560465000000	1.148107000000
H	12.624033000000	-3.394336000000	2.651035000000
P	7.478367000000	-1.946648000000	-1.748266000000
B	4.326326000000	0.341839000000	0.211770000000

O	4.706141000000	1.132527000000	1.303227000000
O	3.142864000000	0.812345000000	-0.336636000000
C	3.839411000000	2.291930000000	1.338244000000
C	2.571943000000	1.763187000000	0.580871000000
C	3.601016000000	2.691832000000	2.789591000000
C	4.555891000000	3.422086000000	0.595025000000
C	1.812036000000	2.818345000000	-0.214933000000
C	1.609700000000	0.988163000000	1.489652000000
H	3.179879000000	1.870888000000	3.372952000000
H	4.548063000000	2.991036000000	3.251222000000
H	2.913650000000	3.543586000000	2.845911000000
H	4.700870000000	3.167909000000	-0.456800000000
H	3.997621000000	4.362187000000	0.658740000000
H	5.545181000000	3.568832000000	1.037595000000
H	1.418540000000	3.599715000000	0.445632000000
H	2.451219000000	3.284193000000	-0.967798000000
H	0.967477000000	2.350557000000	-0.730716000000
H	1.073315000000	1.649086000000	2.178768000000
H	0.880958000000	0.466472000000	0.862899000000
H	2.148365000000	0.234581000000	2.072018000000
C	9.285006000000	-1.508721000000	-1.585847000000
C	9.892689000000	-0.239211000000	-1.549053000000
C	10.127749000000	-2.633839000000	-1.559109000000
C	11.279588000000	-0.110534000000	-1.466526000000
H	9.293129000000	0.657434000000	-1.609953000000
C	11.515919000000	-2.508993000000	-1.492555000000
H	9.679334000000	-3.623599000000	-1.604492000000
C	12.096666000000	-1.242157000000	-1.438018000000
H	11.721327000000	0.881935000000	-1.436637000000
H	12.139983000000	-3.398367000000	-1.482363000000
H	13.176799000000	-1.136374000000	-1.382945000000
C	7.006971000000	-1.047461000000	-3.293127000000
C	5.681596000000	-1.147501000000	-3.755704000000
C	7.923885000000	-0.312893000000	-4.062942000000
C	5.281250000000	-0.479932000000	-4.911835000000
H	4.979187000000	-1.763759000000	-3.211341000000
C	7.521396000000	0.340663000000	-5.227364000000
H	8.960619000000	-0.243812000000	-3.760839000000
C	6.194028000000	0.275763000000	-5.648833000000
H	4.247967000000	-0.557780000000	-5.239686000000
H	8.250943000000	0.906008000000	-5.801588000000
H	5.877677000000	0.795361000000	-6.549382000000
C	7.296451000000	2.667952000000	-1.533540000000
C	8.180078000000	3.181828000000	-0.580171000000

C	8.517873000000	2.395816000000	0.518620000000
C	8.010119000000	1.100665000000	0.639014000000
C	7.153804000000	0.559124000000	-0.322249000000
C	6.772833000000	1.386492000000	-1.394432000000
H	7.004484000000	3.269747000000	-2.389603000000
H	8.583688000000	4.184802000000	-0.686000000000
H	9.184138000000	2.780864000000	1.285863000000
H	8.303861000000	0.520224000000	1.500583000000
H	6.068877000000	1.012167000000	-2.125197000000
C	6.617254000000	-0.864334000000	-0.317801000000
C	5.102262000000	-0.860589000000	-0.317979000000
C	4.385133000000	-1.982509000000	-0.811007000000
O	4.805580000000	-2.928115000000	-1.501679000000
O	3.066210000000	-2.007432000000	-0.387142000000
C	2.251432000000	-3.000226000000	-0.999613000000
H	2.644505000000	-4.006198000000	-0.821496000000
H	2.179519000000	-2.847146000000	-2.082179000000
H	1.264174000000	-2.892730000000	-0.544512000000

S10R

P	-2.132847000000	-1.062163000000	-0.915484000000
C	-3.863420000000	-0.393341000000	-1.069256000000
C	-3.838359000000	1.086438000000	-1.483122000000
H	-4.361323000000	-0.502459000000	-0.101878000000
H	-4.425439000000	-0.977583000000	-1.803192000000
C	-5.224999000000	1.732784000000	-1.416307000000
H	-3.142456000000	1.643230000000	-0.844719000000
H	-3.440923000000	1.175382000000	-2.503360000000
C	-5.204993000000	3.208346000000	-1.821497000000
H	-5.921001000000	1.178674000000	-2.061580000000
H	-5.613601000000	1.635412000000	-0.393000000000
H	-4.850368000000	3.329383000000	-2.852406000000
H	-6.202440000000	3.657377000000	-1.756150000000
H	-4.533623000000	3.783312000000	-1.172472000000
C	-2.099552000000	-2.755310000000	-0.145911000000
C	-0.674899000000	-3.129905000000	0.285870000000
H	-2.492479000000	-3.493348000000	-0.848158000000
H	-2.765066000000	-2.739847000000	0.720471000000
C	-0.616255000000	-4.449104000000	1.061540000000
H	-0.023366000000	-3.192449000000	-0.596468000000
H	-0.255930000000	-2.329655000000	0.904629000000
C	0.800192000000	-4.785817000000	1.532871000000
H	-1.285566000000	-4.385196000000	1.931018000000
H	-1.006170000000	-5.264810000000	0.437017000000
H	0.826498000000	-5.724107000000	2.098226000000

H	1.485759000000	-4.885834000000	0.682984000000
H	1.191908000000	-3.991010000000	2.179438000000
C	-2.007968000000	-1.646940000000	-2.748605000000
C	-2.925160000000	-2.786101000000	-3.212243000000
H	-0.965049000000	-1.914501000000	-2.949030000000
H	-2.202556000000	-0.751419000000	-3.353444000000
C	-3.120292000000	-2.805337000000	-4.733991000000
H	-2.505864000000	-3.753419000000	-2.904302000000
H	-3.914333000000	-2.727607000000	-2.736046000000
C	-3.984432000000	-3.974257000000	-5.212510000000
H	-3.575310000000	-1.855392000000	-5.047464000000
H	-2.136872000000	-2.846494000000	-5.222296000000
H	-4.114628000000	-3.960528000000	-6.300546000000
H	-3.531392000000	-4.936123000000	-4.942430000000
H	-4.981455000000	-3.940060000000	-4.756172000000
P	-0.484887000000	1.777665000000	2.300499000000
B	1.370934000000	0.376538000000	-0.496235000000
O	2.338815000000	0.863937000000	-1.327818000000
O	1.779837000000	-0.692043000000	0.256125000000
C	3.438695000000	-0.093135000000	-1.319042000000
C	3.205742000000	-0.879970000000	0.026552000000
C	3.253693000000	-0.957387000000	-2.568803000000
C	4.746113000000	0.685990000000	-1.387640000000
C	3.932191000000	-0.268728000000	1.222984000000
C	3.475474000000	-2.378245000000	-0.050087000000
H	4.061383000000	-1.687830000000	-2.679246000000
H	2.298137000000	-1.489871000000	-2.538453000000
H	3.249642000000	-0.308945000000	-3.449776000000
H	4.807156000000	1.425985000000	-0.587357000000
H	5.605479000000	0.010513000000	-1.313253000000
H	4.808501000000	1.212045000000	-2.345304000000
H	5.012862000000	-0.432068000000	1.157151000000
H	3.742448000000	0.801642000000	1.300070000000
H	3.567477000000	-0.739252000000	2.140793000000
H	4.527282000000	-2.571719000000	-0.288000000000
H	3.255434000000	-2.837475000000	0.918017000000
H	2.849460000000	-2.862921000000	-0.801945000000
C	-0.312921000000	0.483294000000	3.608957000000
C	0.448265000000	-0.681028000000	3.412825000000
C	-0.989524000000	0.659281000000	4.819001000000
C	0.515699000000	-1.651564000000	4.409058000000
H	0.969914000000	-0.825606000000	2.472332000000
C	-0.924439000000	-0.316355000000	5.816641000000
H	-1.595506000000	1.548396000000	4.967397000000

C	-0.174834000000	-1.473355000000	5.612433000000
H	1.102964000000	-2.552299000000	4.247528000000
H	-1.468700000000	-0.175587000000	6.746362000000
H	-0.127636000000	-2.235685000000	6.385519000000
C	1.281853000000	2.315582000000	2.124828000000
C	1.702139000000	3.065896000000	1.013531000000
C	2.176846000000	2.167305000000	3.199399000000
C	2.989412000000	3.601006000000	0.956953000000
H	1.018176000000	3.224933000000	0.188828000000
C	3.451767000000	2.729224000000	3.153185000000
H	1.876706000000	1.606968000000	4.077497000000
C	3.870643000000	3.439317000000	2.026405000000
H	3.296843000000	4.155113000000	0.074184000000
H	4.124386000000	2.599232000000	3.996965000000
H	4.868437000000	3.867605000000	1.986657000000
C	-3.649314000000	-1.541550000000	3.908961000000
C	-4.591923000000	-0.540370000000	4.145430000000
C	-4.642366000000	0.566912000000	3.297458000000
C	-3.760785000000	0.666997000000	2.222302000000
C	-2.813450000000	-0.339351000000	1.965293000000
C	-2.773723000000	-1.443774000000	2.830128000000
H	-3.581105000000	-2.396061000000	4.576193000000
H	-5.274451000000	-0.617645000000	4.987145000000
H	-5.364032000000	1.359538000000	3.476088000000
H	-3.788067000000	1.539296000000	1.576297000000
H	-2.011038000000	-2.201185000000	2.693242000000
C	-1.873825000000	-0.177939000000	0.828949000000
C	-0.855396000000	0.688289000000	0.853007000000
C	-0.163389000000	0.810387000000	-0.490027000000
O	-0.723464000000	-0.162471000000	-1.362608000000
O	-0.488736000000	2.115205000000	-0.961231000000
C	-0.133239000000	2.393505000000	-2.314629000000
H	-0.583499000000	1.660296000000	-2.991225000000
H	-0.538958000000	3.385072000000	-2.529185000000
H	0.952437000000	2.395882000000	-2.453457000000
S11			
P	-0.695953000000	-0.625660000000	0.720909000000
B	1.025157000000	1.046758000000	-0.765586000000
O	0.333592000000	1.847984000000	-1.641714000000
O	1.917066000000	1.733763000000	0.012208000000
C	0.654316000000	3.229423000000	-1.319250000000
C	2.005488000000	3.084784000000	-0.523231000000
C	0.754825000000	4.015323000000	-2.621434000000
C	-0.498860000000	3.764045000000	-0.465694000000

C	2.170928000000	4.053550000000	0.641516000000
C	3.243537000000	3.108819000000	-1.423487000000
H	1.061762000000	5.049413000000	-2.428604000000
H	1.466532000000	3.558845000000	-3.311568000000
H	-0.224063000000	4.037074000000	-3.110347000000
H	-0.590612000000	3.215479000000	0.473263000000
H	-0.367320000000	4.826925000000	-0.238637000000
H	-1.434309000000	3.644030000000	-1.020720000000
H	3.123400000000	3.860835000000	1.145025000000
H	2.177457000000	5.089752000000	0.285316000000
H	1.369883000000	3.937967000000	1.374069000000
H	4.113877000000	2.805023000000	-0.834658000000
H	3.135783000000	2.407302000000	-2.256209000000
H	3.429027000000	4.108964000000	-1.828030000000
C	-1.089238000000	0.794686000000	1.761000000000
C	-0.071473000000	1.344205000000	2.557730000000
C	-2.368697000000	1.372386000000	1.764571000000
C	-0.340301000000	2.453982000000	3.355191000000
H	0.919793000000	0.906449000000	2.515916000000
C	-2.625363000000	2.485723000000	2.562195000000
H	-3.154000000000	0.955099000000	1.143479000000
C	-1.613730000000	3.029575000000	3.356759000000
H	0.449591000000	2.876814000000	3.969482000000
H	-3.615811000000	2.931687000000	2.559761000000
H	-1.815881000000	3.901595000000	3.972126000000
C	-2.191964000000	-1.021815000000	-0.267067000000
C	-3.051665000000	-2.042117000000	0.154259000000
C	-2.470879000000	-0.312466000000	-1.445720000000
C	-4.183661000000	-2.357624000000	-0.597790000000
H	-2.828109000000	-2.596119000000	1.061756000000
C	-3.602264000000	-0.634113000000	-2.193961000000
H	-1.801148000000	0.477264000000	-1.774295000000
C	-4.457524000000	-1.655373000000	-1.772179000000
H	-4.846372000000	-3.153684000000	-0.270490000000
H	-3.814432000000	-0.089363000000	-3.109687000000
H	-5.335984000000	-1.904773000000	-2.360737000000
C	3.468811000000	-3.900501000000	0.468389000000
C	3.103244000000	-4.733589000000	1.526832000000
C	1.997029000000	-4.390965000000	2.312264000000
C	1.271715000000	-3.236693000000	2.045223000000
C	1.627696000000	-2.388003000000	0.978140000000
C	2.741656000000	-2.745299000000	0.192378000000
H	4.326316000000	-4.152282000000	-0.150713000000
H	3.668264000000	-5.637029000000	1.737362000000

H	1.697438000000	-5.033053000000	3.136926000000
H	0.405177000000	-2.981978000000	2.650891000000
H	3.041025000000	-2.096425000000	-0.626368000000
C	0.934877000000	-1.149600000000	0.714223000000
C	0.706270000000	-0.476229000000	-0.592041000000
C	0.620084000000	-1.263840000000	-1.874080000000
O	1.027442000000	-0.866546000000	-2.948635000000
O	0.057602000000	-2.476421000000	-1.694134000000
C	-0.057261000000	-3.284668000000	-2.869349000000
H	0.929778000000	-3.481858000000	-3.295638000000
H	-0.526701000000	-4.212131000000	-2.541266000000
H	-0.676715000000	-2.782352000000	-3.617652000000
S12			
P	7.452281000000	-2.104031000000	2.415544000000
C	7.585641000000	-3.895775000000	2.067405000000
C	6.267138000000	-4.686002000000	1.984652000000
H	8.276146000000	-4.333590000000	2.796476000000
H	8.067507000000	-3.902400000000	1.084680000000
C	5.621067000000	-5.036372000000	3.332565000000
H	5.562491000000	-4.146887000000	1.344507000000
H	6.486397000000	-5.617376000000	1.448110000000
C	6.403485000000	-6.072157000000	4.145265000000
H	5.480995000000	-4.131106000000	3.938277000000
H	4.613551000000	-5.423607000000	3.138501000000
H	6.497945000000	-7.012287000000	3.589557000000
H	7.417133000000	-5.730922000000	4.386031000000
H	5.900158000000	-6.292186000000	5.093014000000
C	5.746627000000	-1.478336000000	2.394083000000
C	5.525937000000	-0.090259000000	3.016721000000
H	5.109343000000	-2.234156000000	2.865346000000
H	5.494567000000	-1.442618000000	1.325529000000
C	4.075980000000	0.367889000000	2.815875000000
H	5.762057000000	-0.099984000000	4.087514000000
H	6.193854000000	0.629890000000	2.539250000000
C	3.895179000000	1.846530000000	3.164691000000
H	3.792969000000	0.207294000000	1.768767000000
H	3.403133000000	-0.257072000000	3.420278000000
H	4.517608000000	2.462487000000	2.506825000000
H	2.852295000000	2.158483000000	3.041746000000
H	4.186243000000	2.050564000000	4.202838000000
C	8.312933000000	-1.724125000000	3.981966000000
C	7.908597000000	-2.536041000000	5.223438000000
H	8.209116000000	-0.645220000000	4.144806000000
H	9.369010000000	-1.898614000000	3.741800000000

C	6.557563000000	-2.168430000000	5.845546000000
H	7.919423000000	-3.606680000000	4.984361000000
H	8.691242000000	-2.394183000000	5.979312000000
C	6.229953000000	-3.039840000000	7.059530000000
H	6.570326000000	-1.110085000000	6.136820000000
H	5.756910000000	-2.269356000000	5.103526000000
H	6.169972000000	-4.097944000000	6.778079000000
H	7.000440000000	-2.944702000000	7.833591000000
H	5.270648000000	-2.756210000000	7.504222000000
P	6.705212000000	-2.474870000000	-1.105989000000
B	6.881813000000	1.674538000000	-0.407331000000
O	7.554494000000	2.272065000000	-1.442985000000
O	6.183537000000	2.569323000000	0.369492000000
C	7.094650000000	3.648195000000	-1.530029000000
C	6.516630000000	3.906994000000	-0.085868000000
C	8.282720000000	4.525595000000	-1.908039000000
C	6.034865000000	3.683790000000	-2.634711000000
C	5.248199000000	4.751770000000	-0.050924000000
C	7.552123000000	4.451582000000	0.902223000000
H	9.110369000000	4.407809000000	-1.205108000000
H	8.639820000000	4.244772000000	-2.903522000000
H	7.993189000000	5.582113000000	-1.935633000000
H	5.190846000000	3.029659000000	-2.402680000000
H	5.664430000000	4.700685000000	-2.802596000000
H	6.487457000000	3.323053000000	-3.563158000000
H	5.437056000000	5.756048000000	-0.446562000000
H	4.449590000000	4.288621000000	-0.633913000000
H	4.902265000000	4.853144000000	0.982904000000
H	7.834902000000	5.482781000000	0.667068000000
H	7.122695000000	4.430148000000	1.908420000000
H	8.451497000000	3.829808000000	0.910789000000
C	7.809746000000	-2.558240000000	-2.592778000000
C	8.434424000000	-3.765574000000	-2.945817000000
C	8.159278000000	-1.394893000000	-3.293506000000
C	9.340719000000	-3.821545000000	-4.004172000000
H	8.214073000000	-4.669244000000	-2.380895000000
C	9.075772000000	-1.447369000000	-4.344041000000
H	7.712793000000	-0.448826000000	-2.999831000000
C	9.662380000000	-2.660249000000	-4.710052000000
H	9.804492000000	-4.768092000000	-4.271224000000
H	9.331346000000	-0.536723000000	-4.880256000000
H	10.374414000000	-2.699247000000	-5.530220000000
C	5.176946000000	-3.369705000000	-1.627210000000
C	4.005395000000	-3.167832000000	-0.875556000000

C	5.141756000000	-4.322996000000	-2.654177000000
C	2.848161000000	-3.897744000000	-1.134154000000
H	3.992549000000	-2.398770000000	-0.109037000000
C	3.982064000000	-5.055205000000	-2.913822000000
H	6.018898000000	-4.481808000000	-3.272400000000
C	2.830614000000	-4.851779000000	-2.153838000000
H	1.951837000000	-3.709281000000	-0.548298000000
H	3.978548000000	-5.781981000000	-3.722592000000
H	1.927382000000	-5.419397000000	-2.360344000000
C	3.694724000000	-0.103718000000	-3.732376000000
C	2.864650000000	0.867632000000	-3.163417000000
C	3.126831000000	1.282948000000	-1.857509000000
C	4.192845000000	0.740201000000	-1.140978000000
C	5.069030000000	-0.217920000000	-1.705409000000
C	4.768750000000	-0.631314000000	-3.025017000000
H	3.508941000000	-0.447992000000	-4.747249000000
H	2.027250000000	1.277913000000	-3.720959000000
H	2.482834000000	2.017636000000	-1.377588000000
H	4.351552000000	1.058878000000	-0.118216000000
H	5.400712000000	-1.370407000000	-3.503618000000
C	6.190151000000	-0.768180000000	-0.928599000000
C	6.981964000000	0.131433000000	-0.131940000000
C	7.925031000000	-0.091525000000	0.820437000000
O	8.326384000000	-1.405481000000	1.264237000000
O	8.659448000000	0.885386000000	1.449990000000
C	9.959162000000	1.097089000000	0.870369000000
H	10.563797000000	0.184370000000	0.930381000000
H	10.435316000000	1.891959000000	1.451333000000
H	9.855292000000	1.403037000000	-0.176132000000

TS_{1/2}

P	0.422566000	-0.585064000	-0.293557000
C	0.397389000	-2.167200000	-1.306315000
C	-0.730936000	-3.208665000	-1.131928000
H	1.365996000	-2.655685000	-1.136575000
H	0.424841000	-1.811913000	-2.344213000
C	-0.491848000	-4.238223000	-0.022425000
H	-1.692202000	-2.714850000	-0.966005000
H	-0.835350000	-3.752521000	-2.081825000
C	-1.619853000	-5.269227000	0.060830000
H	0.465043000	-4.747172000	-0.203199000
H	-0.394342000	-3.737159000	0.946378000
H	-1.430623000	-6.006588000	0.848416000
H	-2.578914000	-4.784418000	0.280666000
H	-1.732596000	-5.810860000	-0.886051000

C	-0.934042000	0.469726000	-0.994706000
C	-2.231871000	-0.169721000	-1.498216000
H	-0.454968000	1.013702000	-1.819923000
H	-1.150847000	1.228594000	-0.234523000
C	-3.203296000	0.889229000	-2.034515000
H	-2.018706000	-0.895192000	-2.293742000
H	-2.723047000	-0.725286000	-0.691209000
C	-4.510532000	0.284386000	-2.550962000
H	-3.416442000	1.614403000	-1.238231000
H	-2.712431000	1.454149000	-2.838971000
H	-5.189074000	1.058979000	-2.924823000
H	-4.324504000	-0.420816000	-3.370341000
H	-5.033336000	-0.261906000	-1.756397000
C	-0.008534000	-1.066643000	1.439422000
C	-1.488619000	-1.142376000	1.830487000
H	0.494161000	-0.339742000	2.083434000
H	0.490876000	-2.025816000	1.617234000
C	-1.669781000	-1.533653000	3.300744000
H	-1.954227000	-0.165125000	1.655886000
H	-2.019043000	-1.866054000	1.199456000
C	-3.138430000	-1.551130000	3.729158000
H	-1.221295000	-2.522726000	3.470877000
H	-1.106864000	-0.831468000	3.930007000
H	-3.717114000	-2.260315000	3.124668000
H	-3.246839000	-1.841900000	4.779863000
H	-3.595656000	-0.561976000	3.605605000
C	4.545819000	2.673351000	-1.914503000
C	5.007915000	1.575051000	-2.645810000
C	4.398064000	0.333290000	-2.474516000
C	3.333797000	0.188543000	-1.585324000
C	2.859198000	1.282022000	-0.850438000
C	3.486453000	2.531360000	-1.025755000
H	5.012706000	3.646466000	-2.039948000
H	5.835775000	1.688195000	-3.339954000
H	4.752549000	-0.530103000	-3.030918000
H	2.871180000	-0.782551000	-1.448127000
H	3.120986000	3.377169000	-0.453023000
C	1.758806000	1.202438000	0.101917000
C	1.225226000	1.888818000	1.018088000
C	0.171680000	2.138662000	1.931316000
O	-0.961269000	2.513258000	1.632468000
O	0.549191000	1.938095000	3.231049000
C	-0.473657000	2.205928000	4.196333000
H	-1.344154000	1.562468000	4.037218000

H	-0.019595000	1.996977000	5.166088000
H	-0.797012000	3.249202000	4.142492000
TS_{2/3E}			
P	-1.488408000	-1.204606000	-0.931521000
C	-1.357845000	-2.228462000	0.582125000
C	-0.337485000	-3.369690000	0.589908000
H	-2.371154000	-2.604638000	0.777911000
H	-1.132353000	-1.514676000	1.380856000
C	-0.316958000	-4.085137000	1.945597000
H	-0.553786000	-4.092146000	-0.209338000
H	0.657842000	-2.954746000	0.402133000
C	0.776050000	-5.152084000	2.024449000
H	-0.160399000	-3.338689000	2.734110000
H	-1.299753000	-4.538337000	2.136564000
H	1.766977000	-4.704043000	1.884180000
H	0.771447000	-5.655233000	2.997462000
H	0.643874000	-5.918686000	1.250773000
C	0.160481000	-0.833793000	-1.635866000
C	0.819283000	-1.960925000	-2.443104000
H	0.785451000	-0.518363000	-0.801062000
H	0.015591000	0.058396000	-2.254621000
C	2.206006000	-1.562060000	-2.972875000
H	0.920930000	-2.860965000	-1.826241000
H	0.181424000	-2.234767000	-3.291961000
C	3.250383000	-1.338182000	-1.874886000
H	2.550673000	-2.353106000	-3.651720000
H	2.109886000	-0.652914000	-3.582697000
H	4.241344000	-1.169180000	-2.311341000
H	3.011224000	-0.472125000	-1.252033000
H	3.319547000	-2.218453000	-1.223002000
C	-2.406840000	-2.183395000	-2.180025000
C	-2.662623000	-1.406664000	-3.481358000
H	-3.360427000	-2.478314000	-1.730208000
H	-1.837507000	-3.100986000	-2.362952000
C	-3.496574000	-2.202250000	-4.494781000
H	-3.183164000	-0.474229000	-3.241430000
H	-1.706047000	-1.124576000	-3.940377000
C	-2.809587000	-3.469327000	-5.011990000
H	-4.461722000	-2.460332000	-4.038038000
H	-3.725973000	-1.544013000	-5.342104000
H	-2.639608000	-4.199165000	-4.212219000
H	-3.417290000	-3.962084000	-5.778424000
H	-1.835842000	-3.233153000	-5.459198000
P	1.546479000	-0.434590000	1.855618000

B	1.544566000	1.350685000	1.095124000
O	1.228833000	2.541289000	1.680460000
O	2.242914000	1.467672000	-0.077657000
C	1.989861000	3.572804000	0.968544000
C	2.314655000	2.886132000	-0.412781000
C	1.138674000	4.830704000	0.867455000
C	3.234215000	3.827923000	1.824036000
C	3.717322000	3.162756000	-0.944700000
C	1.275306000	3.142648000	-1.503274000
H	1.667708000	5.601038000	0.294159000
H	0.176320000	4.628249000	0.395238000
H	0.957401000	5.226829000	1.872500000
H	3.840558000	2.923616000	1.928480000
H	3.855648000	4.623381000	1.400419000
H	2.915053000	4.134186000	2.824742000
H	3.860470000	2.628066000	-1.889082000
H	3.853480000	4.232732000	-1.137069000
H	4.487288000	2.829342000	-0.245895000
H	1.488434000	2.476193000	-2.346325000
H	0.258297000	2.955677000	-1.155609000
H	1.331533000	4.175475000	-1.862894000
C	3.260549000	-0.258865000	2.540556000
C	3.547925000	0.549330000	3.651990000
C	4.317653000	-0.897390000	1.878642000
C	4.861462000	0.709012000	4.090192000
H	2.737552000	1.055114000	4.167616000
C	5.634225000	-0.727742000	2.310146000
H	4.106014000	-1.526509000	1.018895000
C	5.909045000	0.074566000	3.417700000
H	5.069565000	1.337656000	4.952048000
H	6.443582000	-1.227124000	1.784111000
H	6.932930000	0.203754000	3.757693000
C	0.503115000	-0.352443000	3.364646000
C	-0.630990000	0.467652000	3.424083000
C	0.756041000	-1.238469000	4.426480000
C	-1.495189000	0.398644000	4.517979000
H	-0.847071000	1.160678000	2.622922000
C	-0.101287000	-1.293965000	5.523687000
H	1.634677000	-1.878104000	4.396493000
C	-1.235117000	-0.477884000	5.570989000
H	-2.372020000	1.040214000	4.537259000
H	0.112909000	-1.978055000	6.340808000
H	-1.907142000	-0.527352000	6.423547000
C	-5.544278000	1.839304000	-1.804905000

C	-6.478569000	0.858737000	-1.464332000
C	-6.055654000	-0.290421000	-0.795172000
C	-4.707711000	-0.458901000	-0.480326000
C	-3.755391000	0.510423000	-0.832797000
C	-4.195689000	1.668087000	-1.497274000
H	-5.865801000	2.740826000	-2.319497000
H	-7.527995000	0.992470000	-1.711288000
H	-6.776758000	-1.050405000	-0.505962000
H	-4.395281000	-1.339118000	0.076677000
H	-3.468954000	2.430725000	-1.756086000
C	-2.309327000	0.345074000	-0.515648000
C	-1.468091000	1.211081000	0.078147000
C	-1.873560000	2.531158000	0.477555000
O	-1.743763000	3.551856000	-0.200523000
O	-2.330286000	2.582634000	1.767034000
C	-2.518871000	3.898879000	2.295528000
H	-3.178007000	4.488191000	1.653314000
H	-2.969348000	3.757345000	3.279516000
H	-1.559303000	4.414833000	2.392735000

TS_{3Z/4R}

P	-1.228997000000	-1.669591000000	-0.914609000000
C	-0.633614000000	-3.406107000000	-0.895676000000
C	0.725535000000	-3.637573000000	-0.228583000000
H	-0.633085000000	-3.761679000000	-1.934383000000
H	-1.417470000000	-3.966301000000	-0.369270000000
C	1.073668000000	-5.127242000000	-0.151276000000
H	1.506150000000	-3.097774000000	-0.775859000000
H	0.718890000000	-3.196155000000	0.772895000000
C	2.426273000000	-5.372530000000	0.521206000000
H	0.284413000000	-5.655853000000	0.401942000000
H	1.078951000000	-5.558546000000	-1.162532000000
H	2.433260000000	-4.976552000000	1.543282000000
H	2.659189000000	-6.441685000000	0.572223000000
H	3.234832000000	-4.877667000000	-0.029549000000
C	-0.195372000000	-0.640312000000	-2.016274000000
C	-0.182785000000	-1.067521000000	-3.491140000000
H	0.814813000000	-0.641787000000	-1.612220000000
H	-0.579655000000	0.380284000000	-1.905861000000
C	0.404626000000	0.036466000000	-4.385909000000
H	0.411424000000	-1.984753000000	-3.598405000000
H	-1.192116000000	-1.302946000000	-3.845633000000
C	1.806356000000	0.497258000000	-3.976190000000
H	0.423147000000	-0.330228000000	-5.420018000000
H	-0.277153000000	0.897781000000	-4.374526000000

H	2.216518000000	1.194662000000	-4.714259000000
H	1.793159000000	1.015564000000	-3.011578000000
H	2.496979000000	-0.351613000000	-3.897941000000
C	-2.871964000000	-1.789887000000	-1.728648000000
C	-3.461998000000	-0.429456000000	-2.134856000000
H	-3.530201000000	-2.293816000000	-1.014037000000
H	-2.761867000000	-2.456766000000	-2.590512000000
C	-4.971661000000	-0.498972000000	-2.394327000000
H	-3.266897000000	0.312653000000	-1.351703000000
H	-2.951723000000	-0.065846000000	-3.037084000000
C	-5.364241000000	-1.425567000000	-3.548142000000
H	-5.471572000000	-0.822394000000	-1.471425000000
H	-5.331828000000	0.516503000000	-2.600287000000
H	-5.090113000000	-2.467187000000	-3.343678000000
H	-6.444887000000	-1.400993000000	-3.725159000000
H	-4.866774000000	-1.127086000000	-4.479679000000
P	-2.323643000000	2.247403000000	0.599108000000
B	-1.178050000000	0.904184000000	2.493013000000
O	-0.212534000000	1.569156000000	3.259254000000
O	-2.313496000000	0.618532000000	3.264407000000
C	-0.771399000000	1.837698000000	4.561708000000
C	-1.943328000000	0.792097000000	4.648417000000
C	0.333453000000	1.636989000000	5.597130000000
C	-1.245989000000	3.293552000000	4.589980000000
C	-3.164643000000	1.254116000000	5.434149000000
C	-1.487005000000	-0.585721000000	5.147823000000
H	-0.059230000000	1.748919000000	6.614393000000
H	0.795129000000	0.651477000000	5.505703000000
H	1.113703000000	2.390792000000	5.449775000000
H	-2.046065000000	3.469729000000	3.871085000000
H	-1.599177000000	3.580968000000	5.586444000000
H	-0.402094000000	3.939714000000	4.326400000000
H	-3.940308000000	0.482318000000	5.386911000000
H	-2.908098000000	1.416508000000	6.487491000000
H	-3.576509000000	2.177830000000	5.025696000000
H	-2.291419000000	-1.304261000000	4.964444000000
H	-0.603040000000	-0.925255000000	4.598579000000
H	-1.253720000000	-0.580801000000	6.217839000000
C	-3.218270000000	3.499819000000	1.589473000000
C	-3.033172000000	4.894162000000	1.531646000000
C	-4.232978000000	3.010230000000	2.441719000000
C	-3.809586000000	5.755717000000	2.305414000000
H	-2.279168000000	5.309365000000	0.871964000000
C	-5.006579000000	3.873446000000	3.212587000000

H	-4.389662000000	1.938939000000	2.515098000000
C	-4.797290000000	5.253942000000	3.154520000000
H	-3.642339000000	6.828403000000	2.241341000000
H	-5.775539000000	3.466503000000	3.865177000000
H	-5.399487000000	5.928118000000	3.757363000000
C	-1.039146000000	3.228796000000	-0.273658000000
C	-0.117936000000	4.062185000000	0.388240000000
C	-0.883193000000	3.053244000000	-1.659029000000
C	0.899086000000	4.706879000000	-0.311633000000
H	-0.189401000000	4.173164000000	1.465408000000
C	0.156007000000	3.670902000000	-2.359494000000
H	-1.601391000000	2.436859000000	-2.195504000000
C	1.048451000000	4.506772000000	-1.688444000000
H	1.591764000000	5.355555000000	0.219782000000
H	0.253872000000	3.516348000000	-3.431560000000
H	1.849772000000	5.001736000000	-2.230485000000
C	-5.061268000000	-1.499028000000	1.934292000000
C	-4.934112000000	-2.679779000000	2.670756000000
C	-3.689387000000	-3.300397000000	2.769879000000
C	-2.578664000000	-2.741197000000	2.133641000000
C	-2.694927000000	-1.555722000000	1.396538000000
C	-3.953165000000	-0.942779000000	1.300343000000
H	-6.025566000000	-1.003238000000	1.862272000000
H	-5.799692000000	-3.110149000000	3.166777000000
H	-3.578601000000	-4.215441000000	3.345436000000
H	-1.602292000000	-3.209535000000	2.228091000000
H	-4.042183000000	-0.008493000000	0.757135000000
C	-1.475282000000	-0.998846000000	0.726523000000
C	-0.708616000000	-0.002738000000	1.286453000000
C	0.685084000000	0.189753000000	0.810329000000
O	1.412103000000	-0.736709000000	0.458682000000
O	1.115642000000	1.452243000000	0.852023000000
C	2.485943000000	1.661438000000	0.497769000000
H	2.664878000000	1.360544000000	-0.538520000000
H	2.647666000000	2.731693000000	0.610296000000
H	3.142815000000	1.088102000000	1.156739000000

TS_{3Z/4S}

P	-1.19262400	-1.75535700	-0.89607900
C	-0.59067500	-1.36071700	-2.59239100
C	-1.43897300	-0.28566000	-3.28296400
H	-0.61730000	-2.29817900	-3.15895900
H	0.44844500	-1.04195600	-2.51468100
C	-0.95063600	0.01563500	-4.70329900
H	-2.49128700	-0.60025000	-3.31814600

H	-1.41744900	0.63457800	-2.68807300
C	-1.78172900	1.10590000	-5.38327800
H	0.10268700	0.32423900	-4.66056000
H	-0.97813100	-0.90393100	-5.30416500
H	-1.74703200	2.04019700	-4.81081400
H	-1.41354700	1.31651000	-6.39296800
H	-2.83355100	0.80669800	-5.46604500
C	-2.61078600	-2.89328200	-1.18484700
C	-2.27237500	-4.16287100	-1.97801600
H	-3.39850100	-2.32480200	-1.68759900
H	-3.01855600	-3.15014300	-0.20262200
C	-3.44479400	-5.15099400	-1.98748400
H	-2.01571500	-3.90513700	-3.01317500
H	-1.39002300	-4.66140600	-1.55670100
C	-3.14060500	-6.41665300	-2.79128000
H	-3.69513700	-5.41852900	-0.95201700
H	-4.33324000	-4.65229200	-2.39742300
H	-3.98924000	-7.10866800	-2.77970600
H	-2.91893100	-6.17694500	-3.83818500
H	-2.27206500	-6.94541500	-2.38055400
C	0.06685000	-2.77370800	-0.02546700
C	-0.50604000	-3.64261800	1.10091200
H	0.80506400	-2.06602800	0.35519500
H	0.56151200	-3.38302600	-0.79163100
C	0.59300700	-4.35228900	1.90407200
H	-1.09100000	-3.01552500	1.77973300
H	-1.18903600	-4.39776800	0.69243400
C	1.41703700	-5.35003200	1.08553100
H	1.25689500	-3.60000000	2.34973800
H	0.11772600	-4.87842600	2.74153800
H	1.99080200	-4.85465800	0.29414300
H	2.13220300	-5.88333600	1.72057000
H	0.76957400	-6.09837400	0.61084700
P	0.01497400	1.41259600	2.71722700
B	-1.73337600	2.02548900	1.15590500
O	-3.01109500	1.90232900	1.74120700
O	-1.50677000	3.37676000	0.79177400
C	-3.62511000	3.20127300	1.81319200
C	-2.78602200	4.02969600	0.77281000
C	-5.10372700	3.03749800	1.46021500
C	-3.51133500	3.73856400	3.24422600
C	-2.59189700	5.50061700	1.12750600
C	-3.32762600	3.90348800	-0.66003400
H	-5.61648400	4.00672300	1.46065300

H	-5.23744600	2.56470800	0.48660500
H	-5.58224300	2.39450000	2.20577900
H	-2.47292300	3.86023500	3.55257200
H	-4.02238400	4.70196800	3.34756800
H	-3.99332700	3.03066500	3.92647000
H	-1.97870700	5.98407200	0.35929700
H	-3.55493700	6.02263300	1.17213400
H	-2.08302400	5.61103600	2.08631600
H	-2.58907800	4.32428100	-1.34957200
H	-3.47951100	2.85215500	-0.92512200
H	-4.27529000	4.43618900	-0.79467600
C	-0.08327100	2.92779000	3.74031700
C	-0.34879800	2.94267600	5.12251700
C	0.23429500	4.15351700	3.11987300
C	-0.32916900	4.13431200	5.84574900
H	-0.57320600	2.01420900	5.63681400
C	0.25383100	5.34208300	3.84634000
H	0.43040000	4.17099500	2.05382500
C	-0.03476300	5.34339100	5.21308200
H	-0.54324100	4.11609800	6.91187000
H	0.49028200	6.27502200	3.33976100
H	-0.02337000	6.27171800	5.77775900
C	-0.93424900	0.16124500	3.66916100
C	-2.15107700	0.41085400	4.33293300
C	-0.44684700	-1.15813400	3.68267700
C	-2.83479200	-0.60713200	4.99328600
H	-2.56491600	1.40926500	4.31962100
C	-1.13508900	-2.18368700	4.33593700
H	0.49967000	-1.37110200	3.19159100
C	-2.33363700	-1.91215000	4.99735600
H	-3.77185900	-0.38377400	5.49743500
H	-0.72434000	-3.19018400	4.34393600
H	-2.86680700	-2.70500600	5.51530400
C	-5.66804600	-0.31477300	-0.09317400
C	-5.98833800	-0.92228500	1.12236200
C	-4.96589200	-1.33323500	1.97886500
C	-3.63181000	-1.14368000	1.62315400
C	-3.30258400	-0.52583400	0.41272400
C	-4.33282600	-0.12023700	-0.44475000
H	-6.45733200	0.01609300	-0.76287000
H	-7.02814500	-1.06940000	1.40091200
H	-5.20001300	-1.79278800	2.93487400
H	-2.84229300	-1.44122600	2.30183400
H	-4.07995900	0.36679200	-1.38315800

C	-1.87307500	-0.33653900	0.00865800
C	-1.20921700	0.84474600	0.22845300
C	0.18355100	0.95529000	-0.29882400
O	0.88135000	-0.00943200	-0.60356900
O	0.60839900	2.20822100	-0.45400200
C	1.98283800	2.35877000	-0.83316800
H	2.16954000	1.89396700	-1.80534800
H	2.15002800	3.43439000	-0.88133600
H	2.63010200	1.90022800	-0.08155400

TS_{3E/4R}

P	-1.134430000	-2.010791000	0.191816000
C	-0.698824000	-2.666364000	-1.470796000
C	0.112780000	-1.684323000	-2.322340000
H	-0.160694000	-3.612221000	-1.334214000
H	-1.644362000	-2.910171000	-1.969866000
C	0.519631000	-2.299012000	-3.665830000
H	1.003063000	-1.363451000	-1.769822000
H	-0.486192000	-0.781037000	-2.485777000
C	1.313275000	-1.332519000	-4.547698000
H	-0.382975000	-2.627457000	-4.199973000
H	1.114444000	-3.205441000	-3.484865000
H	0.731567000	-0.430450000	-4.768005000
H	1.586211000	-1.798760000	-5.500659000
H	2.238621000	-1.014955000	-4.053458000
C	0.358724000	-2.050580000	1.232096000
C	1.159281000	-3.357994000	1.131258000
H	0.964266000	-1.187159000	0.953067000
H	0.016205000	-1.881349000	2.255572000
C	2.339681000	-3.381126000	2.114056000
H	1.545797000	-3.481846000	0.111408000
H	0.512256000	-4.222194000	1.332211000
C	3.400331000	-2.319063000	1.815735000
H	2.799291000	-4.377445000	2.080622000
H	1.956871000	-3.243159000	3.132264000
H	4.234692000	-2.389485000	2.522183000
H	2.986555000	-1.309359000	1.887504000
H	3.806832000	-2.444837000	0.804499000
C	-2.292900000	-3.254061000	0.878636000
C	-2.783405000	-2.940065000	2.298004000
H	-3.142697000	-3.328049000	0.194358000
H	-1.765844000	-4.214020000	0.843046000
C	-3.901686000	-3.885572000	2.755193000
H	-3.151535000	-1.910614000	2.330338000
H	-1.941722000	-2.993664000	2.997010000

C	-3.481672000	-5.355652000	2.839958000
H	-4.758008000	-3.779228000	2.075406000
H	-4.250320000	-3.551491000	3.740609000
H	-3.215725000	-5.762462000	1.857377000
H	-4.291760000	-5.974780000	3.239876000
H	-2.611828000	-5.478268000	3.497417000
P	-0.866323000	2.037608000	2.216907000
B	0.160942000	1.342339000	0.038447000
O	1.338425000	0.560564000	0.128034000
O	0.456547000	2.555618000	-0.622643000
C	2.457724000	1.362915000	-0.332258000
C	1.751397000	2.443153000	-1.227738000
C	3.425583000	0.449777000	-1.079732000
C	3.159880000	1.969212000	0.884589000
C	2.421671000	3.813622000	-1.222165000
C	1.527862000	1.975924000	-2.672156000
H	4.249268000	1.032625000	-1.506786000
H	2.931419000	-0.091904000	-1.888971000
H	3.853562000	-0.283736000	-0.389477000
H	2.489590000	2.621746000	1.447101000
H	4.039551000	2.547892000	0.585083000
H	3.497291000	1.162089000	1.542279000
H	1.848721000	4.498760000	-1.855426000
H	3.440140000	3.751810000	-1.623114000
H	2.455893000	4.236385000	-0.217475000
H	0.865260000	2.691236000	-3.168531000
H	1.039655000	0.999387000	-2.694440000
H	2.462430000	1.914472000	-3.239925000
C	0.254538000	3.457844000	2.516545000
C	1.079217000	3.617026000	3.646604000
C	0.193661000	4.520399000	1.590893000
C	1.841859000	4.771015000	3.822930000
H	1.120105000	2.836906000	4.399045000
C	0.955647000	5.672243000	1.773186000
H	-0.446910000	4.426073000	0.721574000
C	1.793324000	5.802346000	2.883625000
H	2.473297000	4.865492000	4.703342000
H	0.896566000	6.473357000	1.040200000
H	2.390772000	6.699648000	3.020722000
C	-0.197001000	0.698474000	3.284947000
C	1.163828000	0.427774000	3.528871000
C	-1.142961000	-0.148998000	3.893987000
C	1.556058000	-0.614975000	4.364753000
H	1.918027000	1.047418000	3.063053000

C	-0.753592000	-1.205117000	4.720873000
H	-2.199970000	0.047046000	3.734738000
C	0.600086000	-1.440620000	4.965676000
H	2.613645000	-0.791844000	4.543428000
H	-1.509520000	-1.830072000	5.190085000
H	0.908204000	-2.249398000	5.622790000
C	-5.548895000	0.313532000	0.933377000
C	-6.256734000	-0.498962000	0.045671000
C	-5.558358000	-1.281593000	-0.875517000
C	-4.164507000	-1.257779000	-0.898594000
C	-3.438228000	-0.472429000	0.011354000
C	-4.154942000	0.324927000	0.921584000
H	-6.082101000	0.939026000	1.643795000
H	-7.342809000	-0.513130000	0.062333000
H	-6.098880000	-1.896569000	-1.590165000
H	-3.633683000	-1.832175000	-1.653137000
H	-3.602019000	0.960479000	1.607524000
C	-1.944523000	-0.430249000	0.036104000
C	-1.287406000	0.769434000	-0.165417000
C	-2.131839000	1.850080000	-0.803040000
O	-2.516045000	2.896364000	-0.335716000
O	-2.366422000	1.487275000	-2.093614000
C	-3.122237000	2.442076000	-2.851071000
H	-4.106788000	2.592194000	-2.400079000
H	-3.218173000	2.013388000	-3.849450000
H	-2.599051000	3.401074000	-2.890458000

TS_{3E/4S}

P	-1.062575000	-2.049675000	-0.114235000
C	-0.646919000	-2.680660000	1.563313000
C	0.131208000	-1.674782000	2.418148000
H	-0.089057000	-3.617769000	1.446433000
H	-1.596743000	-2.936740000	2.047705000
C	0.526175000	-2.266892000	3.775213000
H	1.024828000	-1.343500000	1.877391000
H	-0.486801000	-0.780977000	2.561589000
C	1.283951000	-1.274596000	4.660025000
H	-0.378984000	-2.607931000	4.297004000
H	1.142385000	-3.162814000	3.614747000
H	0.679850000	-0.382541000	4.859959000
H	1.549564000	-1.724566000	5.622830000
H	2.211122000	-0.943051000	4.178512000
C	0.454753000	-2.068850000	-1.120199000
C	1.273494000	-3.363049000	-0.997183000
H	1.040226000	-1.195570000	-0.829146000

H	0.135039000	-1.906583000	-2.152028000
C	2.470172000	-3.373824000	-1.960080000
H	1.644520000	-3.474085000	0.029847000
H	0.644145000	-4.238804000	-1.203456000
C	3.507134000	-2.290506000	-1.654452000
H	2.946518000	-4.361553000	-1.910287000
H	2.101646000	-3.251190000	-2.985512000
H	4.355273000	-2.354231000	-2.344951000
H	3.077700000	-1.288833000	-1.745084000
H	3.897327000	-2.398215000	-0.634712000
C	-2.178913000	-3.324691000	-0.812038000
C	-2.641788000	-3.040454000	-2.246521000
H	-3.042889000	-3.409938000	-0.146968000
H	-1.630738000	-4.271488000	-0.751651000
C	-3.689489000	-4.047822000	-2.738050000
H	-3.065780000	-2.033035000	-2.292436000
H	-1.777497000	-3.047453000	-2.919214000
C	-3.181997000	-5.490544000	-2.814763000
H	-4.570717000	-3.995500000	-2.084273000
H	-4.027601000	-3.730292000	-3.732549000
H	-2.924446000	-5.886922000	-1.825791000
H	-3.941583000	-6.153392000	-3.242717000
H	-2.285950000	-5.558868000	-3.444347000
P	-0.836704000	1.983178000	-2.178220000
B	0.161551000	1.331825000	0.025135000
O	1.355078000	0.571750000	-0.031372000
O	0.421876000	2.558803000	0.676103000
C	2.449853000	1.400364000	0.440149000
C	1.706384000	2.477868000	1.307794000
C	3.419581000	0.513945000	1.217050000
C	3.164373000	2.003485000	-0.771116000
C	2.352150000	3.859968000	1.298327000
C	1.462501000	2.023697000	2.753052000
H	4.225830000	1.115803000	1.650991000
H	2.920141000	-0.026005000	2.024220000
H	3.871908000	-0.220700000	0.543747000
H	2.492950000	2.634742000	-1.356122000
H	4.026846000	2.603228000	-0.463162000
H	3.529633000	1.193657000	-1.410360000
H	1.753517000	4.542983000	1.909729000
H	3.362487000	3.821209000	1.722174000
H	2.401283000	4.270221000	0.289079000
H	0.777909000	2.732926000	3.227830000
H	0.990623000	1.039160000	2.776860000

H	2.386568000	1.984859000	3.339705000
C	0.259416000	3.424326000	-2.469903000
C	1.104472000	3.589912000	-3.583855000
C	0.156203000	4.494563000	-1.556872000
C	1.846169000	4.758130000	-3.755983000
H	1.177462000	2.803662000	-4.327449000
C	0.897334000	5.660532000	-1.735005000
H	-0.501064000	4.395766000	-0.700613000
C	1.755737000	5.797455000	-2.828648000
H	2.493996000	4.857391000	-4.623872000
H	0.805519000	6.467511000	-1.011892000
H	2.336776000	6.705969000	-2.962420000
C	-0.120218000	0.647845000	-3.220256000
C	1.250092000	0.403439000	-3.437335000
C	-1.037201000	-0.225954000	-3.836491000
C	1.679107000	-0.639990000	-4.254056000
H	1.982580000	1.044258000	-2.965802000
C	-0.610946000	-1.281887000	-4.645253000
H	-2.100776000	-0.051111000	-3.697542000
C	0.751553000	-1.491829000	-4.862852000
H	2.743219000	-0.796547000	-4.411752000
H	-1.344981000	-1.927235000	-5.121598000
H	1.088252000	-2.300999000	-5.505292000
C	-5.508728000	0.172951000	-0.958671000
C	-6.215092000	-0.643784000	-0.073707000
C	-5.517150000	-1.400948000	0.868823000
C	-4.124723000	-1.347878000	0.915858000
C	-3.399025000	-0.557734000	0.009592000
C	-4.115732000	0.213791000	-0.922602000
H	-6.042220000	0.778838000	-1.685673000
H	-7.300181000	-0.680854000	-0.109147000
H	-6.057461000	-2.018793000	1.581149000
H	-3.595441000	-1.901989000	1.686453000
H	-3.563826000	0.853220000	-1.605695000
C	-1.906312000	-0.483987000	0.011046000
C	-1.278188000	0.731208000	0.210714000
C	-2.156268000	1.801782000	0.818957000
O	-2.551043000	2.834953000	0.331546000
O	-2.409451000	1.449631000	2.109004000
C	-3.199704000	2.397967000	2.839007000
H	-4.176929000	2.523824000	2.365244000
H	-3.308965000	1.978728000	3.840019000
H	-2.696054000	3.367382000	2.878298000

TS_{4R/5R}

P	-1.526614000	-1.661311000	-0.652798000
C	-3.353189000	-1.416281000	-0.960668000
C	-3.904075000	0.010544000	-0.913644000
H	-3.823877000	-2.010335000	-0.166772000
H	-3.617633000	-1.902080000	-1.906673000
C	-5.432696000	0.029505000	-0.811468000
H	-3.474686000	0.546537000	-0.058580000
H	-3.579883000	0.566882000	-1.796954000
C	-5.996207000	1.451693000	-0.767085000
H	-5.865683000	-0.514944000	-1.662711000
H	-5.743273000	-0.518335000	0.089954000
H	-7.088921000	1.449746000	-0.685753000
H	-5.595750000	2.004587000	0.091042000
H	-5.728031000	2.009210000	-1.672602000
C	-1.512680000	-3.453093000	-0.188831000
C	-2.140638000	-4.401145000	-1.217427000
H	-2.013009000	-3.560357000	0.777413000
H	-0.459994000	-3.711911000	-0.022365000
C	-1.989370000	-5.871573000	-0.810337000
H	-3.207063000	-4.172357000	-1.337276000
H	-1.682590000	-4.256636000	-2.205049000
C	-2.619673000	-6.832291000	-1.820867000
H	-0.922068000	-6.104187000	-0.692865000
H	-2.444649000	-6.020102000	0.178164000
H	-3.693306000	-6.638288000	-1.932746000
H	-2.158924000	-6.722549000	-2.810200000
H	-2.499362000	-7.875839000	-1.510135000
C	-0.605315000	-1.665043000	-2.254533000
C	-1.441527000	-1.432674000	-3.514849000
H	-0.097932000	-2.636485000	-2.308629000
H	0.176911000	-0.914421000	-2.170591000
C	-0.558646000	-1.361432000	-4.765405000
H	-2.183499000	-2.232266000	-3.644509000
H	-1.994710000	-0.493835000	-3.411488000
C	-1.363860000	-1.118498000	-6.043638000
H	0.178523000	-0.558147000	-4.632361000
H	0.016767000	-2.293098000	-4.861121000
H	-0.713335000	-1.062653000	-6.923527000
H	-2.088169000	-1.924459000	-6.214190000
H	-1.924486000	-0.178069000	-5.981013000
P	-0.698047000	1.755557000	2.125302000
B	1.150384000	-0.150506000	0.478640000
O	2.084605000	-0.500522000	1.459144000
O	1.708868000	-0.299651000	-0.806085000

C	3.135231000	-1.248809000	0.803430000
C	3.088697000	-0.684280000	-0.663723000
C	4.437775000	-0.991997000	1.551942000
C	2.766557000	-2.734471000	0.877507000
C	3.425711000	-1.700171000	-1.752431000
C	3.931002000	0.582685000	-0.855334000
H	5.278474000	-1.490258000	1.056152000
H	4.655320000	0.076191000	1.619732000
H	4.359299000	-1.386871000	2.569794000
H	2.679295000	-3.029920000	1.927316000
H	1.803675000	-2.919377000	0.392243000
H	3.527690000	-3.364925000	0.407212000
H	2.738676000	-2.548947000	-1.733344000
H	3.345350000	-1.223359000	-2.734623000
H	4.449637000	-2.074226000	-1.639345000
H	3.696313000	1.333062000	-0.095962000
H	5.004406000	0.368726000	-0.821235000
H	3.694438000	1.014563000	-1.832455000
C	-0.213335000	0.949234000	3.725032000
C	1.091607000	0.615102000	4.117360000
C	-1.250376000	0.791626000	4.654576000
C	1.341828000	0.117312000	5.393618000
H	1.910107000	0.717986000	3.420330000
C	-1.000414000	0.294671000	5.933990000
H	-2.264688000	1.047655000	4.365230000
C	0.297945000	-0.045748000	6.307110000
H	2.358597000	-0.142810000	5.677547000
H	-1.822166000	0.169907000	6.633950000
H	0.497639000	-0.433154000	7.302854000
C	0.600850000	3.074317000	2.064008000
C	0.173630000	4.381978000	2.326033000
C	1.960637000	2.855290000	1.798599000
C	1.078958000	5.445666000	2.332250000
H	-0.879405000	4.567666000	2.521821000
C	2.864231000	3.915071000	1.796895000
H	2.311195000	1.852569000	1.589787000
C	2.427455000	5.215143000	2.064804000
H	0.728160000	6.453068000	2.540839000
H	3.914298000	3.726811000	1.586188000
H	3.134322000	6.040595000	2.063987000
C	-0.891045000	-2.700383000	4.033151000
C	-2.237965000	-2.578403000	4.379432000
C	-3.093838000	-1.850003000	3.554749000
C	-2.601271000	-1.255475000	2.392313000

C	-1.255496000	-1.396188000	2.006913000
C	-0.411098000	-2.125167000	2.858847000
H	-0.210946000	-3.245462000	4.681967000
H	-2.612202000	-3.035278000	5.291575000
H	-4.141144000	-1.731130000	3.821069000
H	-3.265683000	-0.661266000	1.773394000
H	0.634765000	-2.210559000	2.596295000
C	-0.762642000	-0.843140000	0.695277000
C	-0.203291000	0.610836000	0.666117000
C	-0.535520000	1.357186000	-0.591903000
O	-1.238903000	0.943403000	-1.502289000
O	0.071441000	2.553568000	-0.663141000
C	-0.157833000	3.307151000	-1.858742000
H	0.221368000	2.763752000	-2.728626000
H	-1.225146000	3.499981000	-1.995278000
H	0.387313000	4.240461000	-1.718180000

TS_{4R/5S}

P	-1.17476100	0.85472800	1.45571600
C	-2.91567000	1.40264800	1.69845500
C	-3.97910300	0.31784100	1.47682400
H	-3.07898500	2.23456800	1.00682200
H	-2.98468200	1.80823800	2.71512500
C	-5.36622500	0.90985300	1.21143600
H	-3.69776600	-0.30422200	0.62447300
H	-4.02064600	-0.34754500	2.34877900
C	-6.41994900	-0.17266600	0.97194400
H	-5.66641800	1.54692700	2.05525500
H	-5.30260400	1.56137600	0.33060100
H	-7.40560500	0.26378700	0.77715800
H	-6.15055500	-0.79083100	0.10705400
H	-6.51270300	-0.83768200	1.83927900
C	-0.21001900	2.23974800	2.24055000
C	-0.05028700	3.48501600	1.36695400
H	0.77362500	1.84350400	2.50184100
H	-0.71657300	2.48342900	3.18427900
C	0.71615000	4.60661000	2.07685100
H	0.47977000	3.20674200	0.44897300
H	-1.03149100	3.86480700	1.05729100
C	1.03956200	5.76914600	1.13572300
H	0.12952600	4.96549900	2.93369500
H	1.64904200	4.20640500	2.49688000
H	1.56953600	6.57357500	1.65757800
H	1.67153700	5.42956900	0.30654900
H	0.12534400	6.19511800	0.70496000

C	-0.93946100	-0.60515600	2.56780800
C	0.02279700	-0.46769200	3.75041700
H	-0.61087700	-1.41322100	1.91051400
H	-1.93914600	-0.87897700	2.92492200
C	0.21667300	-1.81545500	4.45513200
H	0.99667200	-0.12349200	3.38734800
H	-0.33764500	0.27869600	4.47139000
C	1.19671800	-1.73217700	5.62695600
H	-0.75422500	-2.19072800	4.80795800
H	0.57963300	-2.54483200	3.71840700
H	2.18333600	-1.39158900	5.28969700
H	0.84536100	-1.02519300	6.38843400
H	1.32694200	-2.70669400	6.11026700
P	1.81226800	-0.09811100	0.47507100
B	-0.46397600	-1.25038200	-0.84325400
O	-0.30121300	-2.30248600	0.08879500
O	-1.16552800	-1.70601600	-1.97314400
C	-1.17016700	-3.37869500	-0.30244300
C	-1.35308900	-3.12611800	-1.84768000
C	-0.47741400	-4.69057500	0.05710000
C	-2.47944500	-3.24499300	0.48484200
C	-2.73541000	-3.48368600	-2.39221500
C	-0.27602300	-3.80517100	-2.70105600
H	-1.05096700	-5.55219100	-0.30355100
H	0.52967700	-4.73047700	-0.36191100
H	-0.39000800	-4.77206000	1.14581500
H	-2.97321100	-2.29497400	0.26587400
H	-3.17566200	-4.05960100	0.26073400
H	-2.25758500	-3.27048400	1.55634100
H	-2.77874600	-3.24147200	-3.45863500
H	-2.93821700	-4.55471900	-2.27659900
H	-3.52780200	-2.92519500	-1.88819300
H	0.72141200	-3.58507700	-2.31762800
H	-0.40759100	-4.89229800	-2.73500600
H	-0.34159700	-3.41196900	-3.71981300
C	2.61880400	-1.71336700	0.12392100
C	3.14794100	-2.39630900	1.22691500
C	2.71512000	-2.29687500	-1.14779700
C	3.76755900	-3.63647000	1.06865000
H	3.06114800	-1.95903400	2.21894600
C	3.33597100	-3.53600100	-1.30444000
H	2.28859800	-1.78904800	-2.00731800
C	3.86171100	-4.20984200	-0.19941600
H	4.16778500	-4.15674200	1.93474700

H	3.40298800	-3.98003200	-2.29424300
H	4.33939300	-5.17752200	-0.32679900
C	3.08981200	1.10249500	-0.11874200
C	3.19793500	2.32404000	0.56085300
C	3.94912200	0.86415500	-1.20216400
C	4.10208400	3.30245400	0.14847500
H	2.57454500	2.50673100	1.42830400
C	4.86063000	1.83710200	-1.61176200
H	3.90286400	-0.07977600	-1.73126800
C	4.93343500	3.06260200	-0.94586000
H	4.16392100	4.24344600	0.68867200
H	5.51678000	1.63580100	-2.45436300
H	5.64348400	3.81874600	-1.26935000
C	-2.85313500	3.24090200	-2.17077900
C	-3.94370900	2.53119100	-2.67525700
C	-4.02570000	1.15902000	-2.44155500
C	-3.03733500	0.51159000	-1.69894000
C	-1.93911500	1.20601000	-1.16341900
C	-1.86722100	2.58494800	-1.43421900
H	-2.76841200	4.31021700	-2.34818400
H	-4.71506900	3.04033200	-3.24694100
H	-4.86151600	0.58618900	-2.83514700
H	-3.09909800	-0.55535800	-1.54138600
H	-1.02525200	3.14837700	-1.06095200
C	-0.96248300	0.48915900	-0.25331200
C	0.43613400	0.02166600	-0.80481300
C	0.93590900	0.64571300	-2.06634100
O	1.43558300	0.04672800	-3.00119600
O	0.87095200	1.99794500	-2.03440700
C	1.40810700	2.67269700	-3.17775400
H	0.92110800	2.32441500	-4.09163000
H	1.20407600	3.73158200	-3.01344100
H	2.48420200	2.49609900	-3.24756500
TS_{4S/5R}			
P	1.32253700	0.65549400	1.56995000
C	0.42867000	1.92226900	2.59395000
C	0.30132300	3.28994000	1.92166200
H	-0.56294100	1.51542200	2.81001200
H	0.96940300	1.99900700	3.54734900
C	-0.43912000	4.31317400	2.78917200
H	-0.22929000	3.16637700	0.97032500
H	1.29444400	3.68418000	1.67172000
C	-0.70461700	5.62100100	2.04007300
H	0.14319000	4.51128200	3.69945500

H	-1.39183700	3.88381400	3.12881000
H	-1.22411300	6.34854000	2.67325300
H	-1.32332300	5.44085400	1.15298800
H	0.23268200	6.07963000	1.70256300
C	1.24899900	-0.85844000	2.63049800
C	-0.09861200	-1.45667300	3.03515000
H	1.83724800	-1.60955800	2.10168800
H	1.81563900	-0.57603000	3.52951500
C	0.07687900	-2.69331100	3.92316800
H	-0.63738700	-1.75215800	2.13688300
H	-0.71145200	-0.71234600	3.55797300
C	-1.26431700	-3.35260500	4.25415700
H	0.60380900	-2.42435800	4.85001300
H	0.71883800	-3.41773900	3.40285000
H	-1.13268500	-4.24338700	4.87847400
H	-1.78401800	-3.65288600	3.33693100
H	-1.92092300	-2.65947000	4.79476700
C	3.09272400	1.13691400	1.73917600
C	4.09010100	0.04548400	1.31986700
H	3.24157900	2.03304300	1.13146500
H	3.24890500	1.42422200	2.78585800
C	5.47162500	0.61874000	0.99293100
H	3.71349700	-0.47513400	0.43563600
H	4.17495300	-0.70588100	2.11511900
C	6.45267800	-0.46250500	0.53623600
H	5.87297600	1.14501300	1.87041300
H	5.35783400	1.36825600	0.19934700
H	6.08179200	-0.96371600	-0.36592200
H	6.59123100	-1.22807400	1.30942200
H	7.43589000	-0.03926700	0.30344100
P	-1.84605400	0.15409300	0.54620200
B	0.35170900	-1.18115200	-0.83385600
O	0.96742400	-1.61877500	-2.01963200
O	0.18000000	-2.25966600	0.05761300
C	1.04631300	-3.05315900	-1.99196600
C	0.89844800	-3.39420600	-0.45760800
C	2.37650500	-3.47269100	-2.61752200
C	-0.10586000	-3.59253000	-2.84693800
C	0.06918700	-4.63944400	-0.14991700
C	2.25028500	-3.48167000	0.26119800
H	2.50093500	-4.56128400	-2.58870600
H	3.22793600	-3.01220700	-2.11056700
H	2.39705900	-3.15563800	-3.66485300
H	-1.07133300	-3.32518600	-2.41658100

H	-0.05856800	-4.68201700	-2.95205700
H	-0.04206200	-3.14031600	-3.84089100
H	0.01423600	-4.77978700	0.93511000
H	0.52116300	-5.53708400	-0.58714000
H	-0.95096400	-4.53366400	-0.52326200
H	2.83750400	-2.57135600	0.10991200
H	2.84097500	-4.33578300	-0.08511900
H	2.08034300	-3.60700300	1.33511300
C	-2.77836000	-1.38303200	0.15237700
C	-3.40104900	-2.02874500	1.22936300
C	-2.88815200	-1.94110900	-1.12937100
C	-4.11774900	-3.21058900	1.03680100
H	-3.31129900	-1.60986800	2.22831900
C	-3.60917600	-3.11994900	-1.32140900
H	-2.40040000	-1.45712800	-1.96988800
C	-4.22124200	-3.76021300	-0.24120000
H	-4.58855600	-3.70240100	1.88383600
H	-3.68790400	-3.54341200	-2.31934900
H	-4.77523700	-4.68214100	-0.39576200
C	-3.01052200	1.46094600	-0.05307900
C	-3.02866100	2.67385400	0.65035500
C	-3.87647400	1.31078500	-1.14703400
C	-3.85321100	3.72624000	0.25383800
H	-2.39853000	2.78843100	1.52466400
C	-4.70802200	2.35899100	-1.54109800
H	-3.89855100	0.37790100	-1.69719300
C	-4.69296800	3.57226200	-0.84950100
H	-3.84829600	4.65769400	0.81373600
H	-5.37103600	2.22608000	-2.39187600
H	-5.34212000	4.38615700	-1.16061500
C	2.98113800	3.32957700	-1.83076000
C	3.94574000	2.61416200	-2.54333400
C	3.91317500	1.22103500	-2.51769300
C	2.94050000	0.55162600	-1.77201100
C	1.97103700	1.24808400	-1.03218900
C	2.00760800	2.65365300	-1.09743600
H	2.98496300	4.41666800	-1.84659000
H	4.70734500	3.13730300	-3.11548500
H	4.64911700	0.64730400	-3.07529300
H	2.91105400	-0.52875300	-1.77332300
H	1.25723300	3.22123700	-0.56487500
C	0.99465200	0.49850100	-0.14895800
C	-0.43668800	0.15735800	-0.70576600
C	-0.86662000	0.87031400	-1.94959700

O	-1.40608700	0.34934900	-2.90881600
O	-0.68806900	2.20856300	-1.86407200
C	-1.14939600	2.97030100	-2.98524200
H	-0.67560500	2.62080800	-3.90571900
H	-0.86311800	4.00126000	-2.77375400
H	-2.23478200	2.88469400	-3.07791900
TS_{4S/5S}			
P	-1.64569400	-1.56862600	0.62661200
C	-1.77991900	-3.38246600	0.27482500
C	-2.86677300	-3.85710400	-0.70071700
H	-0.79059700	-3.68476100	-0.08433500
H	-1.91853000	-3.86875000	1.24885300
C	-2.62804300	-5.29691000	-1.16555800
H	-2.90345200	-3.21213700	-1.58011200
H	-3.85172100	-3.78772400	-0.22185200
C	-3.66976600	-5.75254000	-2.18869600
H	-2.62472900	-5.97496600	-0.30013900
H	-1.62790800	-5.35637000	-1.61440600
H	-3.48778900	-6.78196500	-2.51694400
H	-3.64389700	-5.10521100	-3.07307900
H	-4.68318300	-5.70864900	-1.77095900
C	-0.72261400	-1.54881900	2.22561900
C	-1.50265600	-1.21270700	3.49845400
H	-0.26342400	-2.54267900	2.30994700
H	0.10317600	-0.85100800	2.09283500
C	-0.56162000	-1.03005500	4.69454800
H	-2.22851100	-2.00239600	3.72877600
H	-2.06567500	-0.28708700	3.34292600
C	-1.31031100	-0.70313800	5.98830400
H	0.15050700	-0.22639300	4.46325100
H	0.03804300	-1.94075500	4.83268300
H	-2.00824600	-1.50638100	6.25456200
H	-1.89335500	0.21955300	5.88138800
H	-0.62044900	-0.56801800	6.82875000
C	-3.42179700	-1.05969900	0.80536100
C	-4.32062600	-1.82602600	1.78861000
H	-3.42151200	0.01014500	1.01798100
H	-3.80471100	-1.18108400	-0.21642600
C	-5.80553900	-1.67823300	1.43544700
H	-4.15404800	-1.45686700	2.80533900
H	-4.06821400	-2.89384100	1.80563900
C	-6.72389000	-2.39130000	2.43001900
H	-5.97336100	-2.07506400	0.42447000
H	-6.06160400	-0.61095400	1.39165300

H	-7.77796900	-2.28103100	2.15264300
H	-6.59998800	-1.98632000	3.44165500
H	-6.49995500	-3.46430500	2.47345000
P	-0.66764400	1.87759700	-2.07356800
B	1.13598800	-0.13441300	-0.47397500
O	1.69843200	-0.25891300	0.81348000
O	2.07216200	-0.49474700	-1.45110300
C	3.10953600	-0.49554100	0.65654700
C	3.18198500	-1.13222100	-0.77638000
C	3.58165300	-1.40464100	1.78694600
C	3.80814300	0.86713600	0.74584500
C	4.45499000	-0.82189800	-1.55467300
C	2.91823100	-2.64132500	-0.76578200
H	4.63532700	-1.67718700	1.65799100
H	2.98618500	-2.31882300	1.83944900
H	3.48194800	-0.88143800	2.74347800
H	3.53883400	1.33331400	1.69842600
H	3.47801400	1.53378700	-0.05522900
H	4.89849600	0.77137000	0.70332800
H	4.58745100	0.25399700	-1.68709000
H	4.40349100	-1.28279100	-2.54639600
H	5.33481100	-1.22222100	-1.03839400
H	1.99781500	-2.86765900	-0.21905700
H	3.74413600	-3.19563200	-0.30863800
H	2.80018000	-2.98875500	-1.79659700
C	-0.36545700	1.14499100	-3.74747300
C	0.61593600	0.21672800	-4.12149600
C	-1.22036800	1.65475000	-4.73783600
C	0.72192100	-0.19644500	-5.44855700
H	1.27602500	-0.20662700	-3.37611700
C	-1.10069500	1.25363100	-6.06805600
H	-1.99411600	2.36530600	-4.45773600
C	-0.13042900	0.31889000	-6.42631200
H	1.47488800	-0.93260800	-5.71831300
H	-1.77248100	1.66166900	-6.81880300
H	-0.04127300	-0.00970500	-7.45845700
C	0.76833900	3.04855000	-2.00487700
C	0.49244500	4.38856100	-1.70515700
C	2.09583700	2.67404000	-2.25505800
C	1.51725300	5.33436700	-1.64143600
H	-0.53448400	4.68851400	-1.51320700
C	3.12112400	3.61664200	-2.18897000
H	2.32946700	1.64207400	-2.48582300
C	2.83629800	4.94890800	-1.88012700

H	1.28505000	6.37031400	-1.40792600
H	4.14657100	3.31090300	-2.38216800
H	3.63729800	5.68181100	-1.83195400
C	-0.78090300	-3.13744300	-3.73324400
C	-1.89605600	-2.68063200	-4.43718500
C	-2.62811100	-1.60171400	-3.93800500
C	-2.25230100	-0.99889300	-2.73906500
C	-1.12940000	-1.43972400	-2.01543000
C	-0.40034200	-2.51602700	-2.54431500
H	-0.19811600	-3.97030700	-4.11852600
H	-2.18635800	-3.15327100	-5.37134900
H	-3.49054200	-1.22885000	-4.48320400
H	-2.82814300	-0.16286800	-2.35161200
H	0.47879700	-2.85579800	-2.01098400
C	-0.75641300	-0.83044100	-0.69725400
C	-0.21063700	0.62788400	-0.67593700
C	-0.54738200	1.39186100	0.57577900
O	-1.41841200	1.11255500	1.38710800
O	0.25558800	2.45613800	0.74033300
C	0.01187600	3.26578300	1.89454500
H	0.25061500	2.70803300	2.80485400
H	-1.03335400	3.58267900	1.93302500
H	0.67235700	4.12596900	1.78478200

TS_{4R/10Z}

P	-0.802476000	0.262683000	-1.473780000
C	-2.068673000	-0.764110000	-2.373202000
C	-1.480574000	-1.565132000	-3.537651000
H	-2.876797000	-0.107213000	-2.720217000
H	-2.495442000	-1.437577000	-1.625250000
C	-2.482196000	-2.551906000	-4.145096000
H	-1.125097000	-0.885359000	-4.323822000
H	-0.606751000	-2.122541000	-3.185815000
C	-1.888649000	-3.337592000	-5.316915000
H	-2.815572000	-3.247148000	-3.361866000
H	-3.380284000	-2.011571000	-4.475541000
H	-1.589865000	-2.664908000	-6.129976000
H	-0.996200000	-3.891307000	-5.003019000
H	-2.607486000	-4.056589000	-5.725149000
C	-0.083295000	1.341366000	-2.778202000
C	-1.120896000	2.103510000	-3.612438000
H	0.547080000	0.731378000	-3.426758000
H	0.592089000	2.035053000	-2.267293000
C	-0.457926000	3.070392000	-4.600124000
H	-1.747409000	1.396143000	-4.170652000

H	-1.800890000	2.669326000	-2.963058000
C	-1.475631000	3.831025000	-5.452702000
H	0.165520000	3.782205000	-4.042369000
H	0.226558000	2.508761000	-5.250185000
H	-0.980447000	4.514988000	-6.150325000
H	-2.091804000	3.140665000	-6.041481000
H	-2.151133000	4.424678000	-4.824881000
C	-1.847342000	1.404103000	-0.456960000
C	-1.132959000	2.705321000	-0.079354000
H	-2.115830000	0.871436000	0.456715000
H	-2.776309000	1.593434000	-1.005875000
C	-1.889888000	3.502061000	0.990344000
H	-0.139165000	2.450863000	0.297260000
H	-0.993439000	3.333202000	-0.968930000
C	-3.267626000	3.995750000	0.539673000
H	-1.984152000	2.873705000	1.882840000
H	-1.276492000	4.365961000	1.280900000
H	-3.945559000	3.162326000	0.321752000
H	-3.741641000	4.608502000	1.314442000
H	-3.191792000	4.606937000	-0.368863000
P	1.529467000	-2.488092000	1.146880000
B	0.053679000	-0.340439000	2.637333000
O	-0.347263000	1.010922000	2.702511000
O	1.189215000	-0.565182000	3.420863000
C	0.639628000	1.723684000	3.481766000
C	1.332687000	0.567701000	4.298374000
C	1.600629000	2.437858000	2.527230000
C	-0.079801000	2.754315000	4.349472000
C	0.589989000	0.225081000	5.596472000
C	2.816456000	0.775105000	4.579039000
H	1.039843000	3.151540000	1.917960000
H	2.369361000	2.993417000	3.073776000
H	2.090914000	1.731309000	1.855070000
H	-0.881355000	2.293625000	4.930165000
H	0.621123000	3.237151000	5.040091000
H	-0.520214000	3.531213000	3.717433000
H	0.706120000	1.006549000	6.354764000
H	-0.477186000	0.074011000	5.408485000
H	0.994827000	-0.710189000	5.994301000
H	3.206876000	-0.082971000	5.135547000
H	3.385925000	0.861824000	3.651371000
H	2.981038000	1.675137000	5.182397000
C	1.305467000	-3.531759000	-0.370392000
C	0.093623000	-3.725804000	-1.048198000

C	2.455972000	-4.158609000	-0.864666000
C	0.029811000	-4.554369000	-2.167896000
H	-0.802579000	-3.220950000	-0.704217000
C	2.398531000	-4.979416000	-1.992531000
H	3.408041000	-3.983599000	-0.370632000
C	1.183185000	-5.182345000	-2.645176000
H	-0.920645000	-4.709357000	-2.671443000
H	3.303480000	-5.452611000	-2.363945000
H	1.132520000	-5.821610000	-3.522619000
C	0.713459000	-3.586318000	2.405931000
C	1.251591000	-3.557838000	3.700307000
C	-0.344344000	-4.468887000	2.143276000
C	0.733600000	-4.369485000	4.709872000
H	2.064323000	-2.874310000	3.916527000
C	-0.864737000	-5.279781000	3.150350000
H	-0.759754000	-4.535741000	1.144224000
C	-0.329291000	-5.230276000	4.439099000
H	1.161725000	-4.328870000	5.708118000
H	-1.684429000	-5.958178000	2.926838000
H	-0.733531000	-5.864985000	5.223317000
C	3.440265000	-0.925474000	-2.914185000
C	4.489215000	-0.494199000	-2.101264000
C	4.208262000	-0.090076000	-0.794300000
C	2.898676000	-0.088548000	-0.321508000
C	1.817789000	-0.509311000	-1.125769000
C	2.135717000	-0.954386000	-2.425159000
H	3.640915000	-1.277864000	-3.923063000
H	5.509804000	-0.487237000	-2.473819000
H	5.012561000	0.237556000	-0.140268000
H	2.694987000	0.226837000	0.695053000
H	1.349584000	-1.372453000	-3.044888000
C	0.440474000	-0.521901000	-0.577927000
C	0.215797000	-1.130002000	0.758147000
C	-1.036384000	-1.408439000	1.326761000
O	-1.060243000	-1.326841000	2.651780000
O	-2.207919000	-1.515746000	0.681624000
C	-3.405323000	-1.449687000	1.480665000
H	-4.228995000	-1.428261000	0.766286000
H	-3.476569000	-2.330951000	2.121593000
H	-3.400330000	-0.548661000	2.098294000
TS_{4S/10Z}			
P	-0.454385000	-1.240870000	-1.311213000
C	-1.961563000	-1.906275000	-2.130875000
C	-2.436243000	-3.235326000	-1.527951000

H	-1.741265000	-2.023718000	-3.197154000
H	-2.740831000	-1.147808000	-2.046985000
C	-3.821152000	-3.660158000	-2.038631000
H	-1.704858000	-4.019174000	-1.762765000
H	-2.466326000	-3.145513000	-0.437283000
C	-4.953875000	-2.745627000	-1.561827000
H	-3.811582000	-3.705504000	-3.137379000
H	-4.016168000	-4.683777000	-1.692549000
H	-5.927794000	-3.122769000	-1.893814000
H	-4.966354000	-2.674252000	-0.469124000
H	-4.847835000	-1.725215000	-1.944127000
C	0.824254000	-2.533109000	-1.594453000
C	1.133701000	-2.850765000	-3.062008000
H	0.475043000	-3.427761000	-1.070065000
H	1.722962000	-2.172905000	-1.094485000
C	2.228209000	-3.919915000	-3.208330000
H	0.226595000	-3.196346000	-3.573049000
H	1.459059000	-1.939935000	-3.580475000
C	3.606017000	-3.461338000	-2.721614000
H	1.923897000	-4.823572000	-2.661993000
H	2.298918000	-4.209651000	-4.264743000
H	4.358976000	-4.242861000	-2.870587000
H	3.935568000	-2.570099000	-3.269595000
H	3.598679000	-3.204087000	-1.657137000
C	0.093866000	0.213171000	-2.350111000
C	-0.457025000	0.344246000	-3.773723000
H	1.186414000	0.178026000	-2.351696000
H	-0.182226000	1.093203000	-1.758060000
C	0.110645000	1.573504000	-4.493870000
H	-0.223188000	-0.552844000	-4.361363000
H	-1.552154000	0.417565000	-3.747846000
C	-0.439441000	1.738433000	-5.912182000
H	-0.112896000	2.471206000	-3.901258000
H	1.206370000	1.495256000	-4.527498000
H	-0.017176000	2.620628000	-6.405687000
H	-0.203543000	0.863962000	-6.530800000
H	-1.530205000	1.851443000	-5.900998000
P	0.155677000	0.279965000	2.913252000
B	2.197244000	-0.200682000	1.012891000
O	2.557933000	-0.386371000	-0.357469000
O	2.725170000	1.013108000	1.470217000
C	3.772526000	0.376909000	-0.537823000
C	3.521219000	1.597935000	0.416018000
C	4.953367000	-0.495867000	-0.089947000

C	3.929414000	0.727344000	-2.013227000
C	2.713696000	2.711910000	-0.257283000
C	4.780021000	2.185161000	1.049032000
H	4.871737000	-0.763193000	0.966758000
H	4.952839000	-1.419790000	-0.676735000
H	5.910953000	0.010302000	-0.248615000
H	4.824366000	1.339635000	-2.169509000
H	4.041519000	-0.190383000	-2.600156000
H	3.067456000	1.275433000	-2.397697000
H	2.379222000	3.420218000	0.505969000
H	3.318242000	3.257122000	-0.989972000
H	1.832673000	2.310890000	-0.765989000
H	5.307882000	1.439736000	1.646996000
H	5.461368000	2.573028000	0.282637000
H	4.503327000	3.012166000	1.710215000
C	-1.003001000	1.578475000	2.316804000
C	-0.511687000	2.406728000	1.296084000
C	-2.281582000	1.828828000	2.827625000
C	-1.284844000	3.445753000	0.784746000
H	0.481459000	2.225678000	0.909320000
C	-3.047299000	2.881946000	2.329218000
H	-2.704148000	1.176936000	3.581892000
C	-2.557711000	3.691454000	1.304196000
H	-0.888499000	4.070056000	-0.012690000
H	-4.043993000	3.050755000	2.727414000
H	-3.162448000	4.504905000	0.912336000
C	-0.819519000	-0.705731000	4.133491000
C	-1.296781000	-0.035132000	5.274629000
C	-0.909902000	-2.105555000	4.112946000
C	-1.903420000	-0.730341000	6.319115000
H	-1.189217000	1.043571000	5.349319000
C	-1.503677000	-2.803608000	5.164418000
H	-0.530058000	-2.662763000	3.264496000
C	-2.015394000	-2.120507000	6.267841000
H	-2.279912000	-0.183779000	7.179841000
H	-1.570876000	-3.887599000	5.115814000
H	-2.482660000	-2.664761000	7.083704000
C	-4.251624000	-1.055741000	1.936940000
C	-4.945453000	-0.092108000	1.202625000
C	-4.275172000	0.595435000	0.189021000
C	-2.930280000	0.340278000	-0.062886000
C	-2.206360000	-0.632588000	0.658717000
C	-2.916446000	-1.334852000	1.651063000
H	-4.754821000	-1.609657000	2.725841000

H	-5.988951000	0.121189000	1.417246000
H	-4.789446000	1.366015000	-0.379664000
H	-2.407234000	0.948480000	-0.795145000
H	-2.408651000	-2.115292000	2.200648000
C	-0.784798000	-0.935412000	0.359889000
C	0.313888000	-0.787537000	1.345806000
C	1.222146000	-1.850097000	1.635953000
O	2.445993000	-1.428027000	1.872151000
O	1.000747000	-3.145695000	1.466358000
C	2.151915000	-4.011876000	1.452053000
H	1.772024000	-4.990215000	1.158005000
H	2.888434000	-3.647669000	0.732421000
H	2.603571000	-4.059732000	2.445367000
TS_{SR/TE}			
P	0.561196000	-1.958269000	-0.065127000
C	-0.116972000	-3.150826000	1.185331000
C	-1.300055000	-3.973328000	0.669651000
H	-0.437844000	-2.545718000	2.037923000
H	0.685958000	-3.813134000	1.530872000
C	-1.854775000	-4.931116000	1.728718000
H	-2.096996000	-3.290413000	0.356872000
H	-1.007206000	-4.546928000	-0.220256000
C	-3.081444000	-5.703208000	1.238295000
H	-1.067611000	-5.635181000	2.031210000
H	-2.115480000	-4.356624000	2.627705000
H	-3.463409000	-6.382170000	2.008409000
H	-3.893797000	-5.018429000	0.964422000
H	-2.843096000	-6.302471000	0.351282000
C	2.046813000	-1.200323000	0.728120000
C	2.582537000	-1.823808000	2.019048000
H	1.789028000	-0.153058000	0.918269000
H	2.816003000	-1.176201000	-0.049987000
C	3.897152000	-1.159925000	2.446292000
H	1.841435000	-1.705799000	2.819536000
H	2.745754000	-2.903162000	1.900162000
C	4.364298000	-1.610363000	3.830836000
H	4.669910000	-1.385374000	1.698089000
H	3.767038000	-0.071804000	2.441381000
H	3.627837000	-1.336300000	4.595966000
H	4.499870000	-2.698202000	3.874019000
H	5.317481000	-1.143477000	4.103148000
C	1.240849000	-2.997616000	-1.430484000
C	2.247307000	-4.076580000	-1.018633000
H	1.690800000	-2.271340000	-2.115961000

H	0.395501000	-3.441881000	-1.966935000
C	2.809688000	-4.834165000	-2.227149000
H	3.077287000	-3.622498000	-0.461322000
H	1.772804000	-4.794328000	-0.335616000
C	3.808638000	-5.923616000	-1.830926000
H	1.978487000	-5.279697000	-2.790932000
H	3.290166000	-4.117667000	-2.906539000
H	4.197911000	-6.449169000	-2.709882000
H	4.662977000	-5.497741000	-1.290819000
H	3.341474000	-6.669039000	-1.175493000
P	-0.400962000	2.145226000	0.562554000
B	-1.971326000	-0.136599000	-0.022364000
O	-3.175255000	0.325186000	-0.477696000
O	-2.060935000	-0.752793000	1.208376000
C	-4.205497000	-0.111548000	0.446865000
C	-3.385710000	-0.464938000	1.745562000
C	-5.210357000	1.022358000	0.613217000
C	-4.879432000	-1.325186000	-0.200984000
C	-3.873146000	-1.697844000	2.499095000
C	-3.235644000	0.711992000	2.711486000
H	-5.705436000	1.212620000	-0.343693000
H	-5.978175000	0.759074000	1.349284000
H	-4.719150000	1.944447000	0.929120000
H	-5.721248000	-1.687246000	0.398021000
H	-5.250994000	-1.035376000	-1.187800000
H	-4.171777000	-2.147600000	-0.341426000
H	-4.883054000	-1.535018000	2.891206000
H	-3.885457000	-2.587955000	1.867628000
H	-3.209213000	-1.892127000	3.347359000
H	-2.823609000	1.584652000	2.200764000
H	-4.194576000	0.974566000	3.169045000
H	-2.541846000	0.431252000	3.510133000
C	0.901116000	2.157269000	1.875430000
C	2.054516000	2.955194000	1.874248000
C	0.701257000	1.267034000	2.944086000
C	2.978183000	2.866612000	2.916354000
H	2.221940000	3.645516000	1.055988000
C	1.627633000	1.172660000	3.982387000
H	-0.185562000	0.638419000	2.947463000
C	2.768198000	1.977588000	3.973256000
H	3.866882000	3.492549000	2.903032000
H	1.456845000	0.478331000	4.801048000
H	3.489642000	1.911410000	4.783101000
C	-0.308890000	3.824729000	-0.173316000

C	-0.462396000	4.004850000	-1.555209000
C	-0.230336000	4.961047000	0.646209000
C	-0.517977000	5.284370000	-2.104241000
H	-0.532901000	3.132284000	-2.196969000
C	-0.276929000	6.241546000	0.095388000
H	-0.121619000	4.845010000	1.721136000
C	-0.419958000	6.409032000	-1.282756000
H	-0.631426000	5.403618000	-3.178778000
H	-0.203003000	7.109662000	0.745440000
H	-0.457562000	7.406444000	-1.712204000
C	-0.923268000	-0.476252000	-4.736783000
C	-1.656319000	-1.655624000	-4.863909000
C	-2.049171000	-2.340694000	-3.712666000
C	-1.697194000	-1.850027000	-2.459013000
C	-0.943052000	-0.674806000	-2.313463000
C	-0.576600000	0.011708000	-3.477453000
H	-0.619180000	0.073435000	-5.623412000
H	-1.925132000	-2.033292000	-5.846448000
H	-2.632823000	-3.254217000	-3.789932000
H	-2.005158000	-2.395860000	-1.572225000
H	-0.020020000	0.935828000	-3.397016000
C	-0.670274000	-0.115953000	-0.938994000
C	0.171076000	1.015168000	-0.730280000
C	1.471878000	1.076887000	-1.352035000
O	2.013111000	0.169531000	-1.989285000
O	2.129135000	2.253305000	-1.121349000
C	3.470704000	2.309493000	-1.601797000
H	4.096618000	1.566249000	-1.097572000
H	3.510785000	2.126942000	-2.679173000
H	3.821949000	3.316867000	-1.372337000

TS_{SS/7E}

P	0.310750000	-1.959188000	-0.019047000
C	-0.785362000	-3.209311000	-0.851155000
C	-0.178576000	-4.554963000	-1.265566000
H	-1.627204000	-3.391607000	-0.172725000
H	-1.197738000	-2.688939000	-1.720692000
C	-1.180666000	-5.414432000	-2.046874000
H	0.149882000	-5.106337000	-0.376364000
H	0.714938000	-4.398992000	-1.883488000
C	-0.601947000	-6.769151000	-2.460999000
H	-1.508658000	-4.862110000	-2.938382000
H	-2.079749000	-5.567118000	-1.433574000
H	-1.333737000	-7.364274000	-3.018153000
H	-0.295121000	-7.351389000	-1.583817000

H	0.280994000	-6.641430000	-3.098813000
C	1.563937000	-1.596280000	-1.334340000
C	2.717108000	-0.662044000	-0.944205000
H	1.964976000	-2.559892000	-1.674742000
H	0.999802000	-1.171545000	-2.172927000
C	3.864219000	-0.714510000	-1.955815000
H	3.092425000	-0.910287000	0.052606000
H	2.345189000	0.362347000	-0.879646000
C	5.001479000	0.237664000	-1.581150000
H	3.482726000	-0.455186000	-2.951876000
H	4.245857000	-1.744060000	-2.024112000
H	5.413660000	-0.012737000	-0.595533000
H	4.640517000	1.270964000	-1.544081000
H	5.821047000	0.192498000	-2.307567000
C	1.162087000	-2.867864000	1.350395000
C	2.402043000	-3.698891000	0.993032000
H	1.429696000	-2.091400000	2.071780000
H	0.397053000	-3.495629000	1.823880000
C	3.015276000	-4.357295000	2.234319000
H	3.156456000	-3.055264000	0.525781000
H	2.158818000	-4.473569000	0.256334000
C	4.271702000	-5.168813000	1.910848000
H	2.265829000	-5.006250000	2.708505000
H	3.254681000	-3.577519000	2.969312000
H	4.696901000	-5.625473000	2.811453000
H	5.044654000	-4.533865000	1.461066000
H	4.050735000	-5.974649000	1.200007000
P	-0.429080000	2.372669000	-0.335634000
B	-1.973797000	0.031571000	-0.170811000
O	-1.859512000	-0.357617000	-1.493041000
O	-3.263627000	0.308660000	0.188776000
C	-3.132524000	-0.076423000	-2.145023000
C	-4.128996000	-0.037911000	-0.925095000
C	-3.399678000	-1.183904000	-3.159758000
C	-3.001164000	1.267225000	-2.864839000
C	-5.226173000	1.014789000	-1.024790000
C	-4.735090000	-1.404812000	-0.591270000
H	-2.628477000	-1.158275000	-3.936118000
H	-4.371328000	-1.038143000	-3.644345000
H	-3.386473000	-2.174279000	-2.699790000
H	-3.925467000	1.520828000	-3.393384000
H	-2.193851000	1.202916000	-3.600560000
H	-2.750546000	2.067192000	-2.165695000
H	-5.868890000	0.826212000	-1.891811000

H	-4.805321000	2.018352000	-1.108249000
H	-5.847433000	0.980857000	-0.124691000
H	-3.963852000	-2.179051000	-0.534082000
H	-5.476222000	-1.710365000	-1.336782000
H	-5.225481000	-1.343522000	0.384305000
C	0.941899000	2.599420000	-1.554328000
C	2.025146000	3.476247000	-1.401609000
C	0.886138000	1.794779000	-2.703741000
C	3.026840000	3.540713000	-2.370299000
H	2.081938000	4.103056000	-0.519569000
C	1.892419000	1.851077000	-3.668206000
H	0.051335000	1.110277000	-2.825472000
C	2.966703000	2.726968000	-3.504085000
H	3.861412000	4.224672000	-2.237667000
H	1.834016000	1.218930000	-4.550654000
H	3.750847000	2.777006000	-4.254558000
C	-0.410907000	3.934980000	0.630769000
C	-0.529221000	3.928583000	2.027015000
C	-0.417187000	5.169864000	-0.036835000
C	-0.632708000	5.123349000	2.737784000
H	-0.536647000	2.979206000	2.552572000
C	-0.510240000	6.365169000	0.674772000
H	-0.337592000	5.197024000	-1.120513000
C	-0.617811000	6.347052000	2.066520000
H	-0.718650000	5.098207000	3.821167000
H	-0.501844000	7.311865000	0.140563000
H	-0.692963000	7.277996000	2.621852000
C	-1.045542000	-0.821141000	4.621946000
C	-1.928529000	-1.900211000	4.626038000
C	-2.439437000	-2.364458000	3.412912000
C	-2.054184000	-1.760426000	2.220055000
C	-1.142751000	-0.690366000	2.193842000
C	-0.661948000	-0.220533000	3.423474000
H	-0.649396000	-0.438903000	5.558788000
H	-2.224228000	-2.366387000	5.561693000
H	-3.146855000	-3.189216000	3.394939000
H	-2.481217000	-2.118590000	1.290309000
H	0.022162000	0.615400000	3.446108000
C	-0.779339000	-0.041561000	0.882274000
C	0.106689000	1.077747000	0.805679000
C	1.397345000	1.060873000	1.443427000
O	1.934566000	0.092257000	1.989320000
O	2.065214000	2.249669000	1.337735000
C	3.409738000	2.245374000	1.812941000

H	4.031179000	1.570132000	1.216690000
H	3.455843000	1.933842000	2.859990000
H	3.761094000	3.272815000	1.704293000
TS_{SR/GR}			
P	-2.180053000000	-1.458132000000	-0.368408000000
C	-3.853170000000	-0.705854000000	-0.186132000000
C	-3.961705000000	0.824736000000	-0.246544000000
H	-4.254091000000	-1.076394000000	0.763207000000
H	-4.463384000000	-1.159851000000	-0.976979000000
C	-5.422403000000	1.282512000000	-0.274766000000
H	-3.450938000000	1.264730000000	0.612926000000
H	-3.440035000000	1.211384000000	-1.126694000000
C	-5.540248000000	2.808107000000	-0.294004000000
H	-5.926222000000	0.856957000000	-1.155047000000
H	-5.948856000000	0.881621000000	0.603473000000
H	-6.587402000000	3.130106000000	-0.308643000000
H	-5.060894000000	3.246482000000	0.588616000000
H	-5.044910000000	3.227336000000	-1.177638000000
C	-2.401359000000	-3.215619000000	0.159305000000
C	-3.608918000000	-3.942797000000	-0.446006000000
H	-2.467707000000	-3.240505000000	1.248692000000
H	-1.464079000000	-3.714668000000	-0.113824000000
C	-3.635368000000	-5.423634000000	-0.048454000000
H	-4.536819000000	-3.465033000000	-0.107081000000
H	-3.605988000000	-3.867885000000	-1.541312000000
C	-4.847433000000	-6.165180000000	-0.616052000000
H	-2.709901000000	-5.904439000000	-0.393617000000
H	-3.630976000000	-5.501535000000	1.047092000000
H	-5.784454000000	-5.721248000000	-0.258950000000
H	-4.857942000000	-6.124645000000	-1.711992000000
H	-4.843872000000	-7.219953000000	-0.320831000000
C	-1.830627000000	-1.643537000000	-2.180144000000
C	-2.536747000000	-0.664847000000	-3.119800000000
H	-2.100341000000	-2.676053000000	-2.435329000000
H	-0.751840000000	-1.548281000000	-2.280243000000
C	-2.083343000000	-0.866684000000	-4.569545000000
H	-3.627083000000	-0.785493000000	-3.062099000000
H	-2.287940000000	0.351649000000	-2.809525000000
C	-2.767721000000	0.104575000000	-5.533700000000
H	-0.994849000000	-0.729529000000	-4.618219000000
H	-2.280720000000	-1.902068000000	-4.882678000000
H	-2.423810000000	-0.042791000000	-6.563454000000
H	-3.856566000000	-0.027970000000	-5.522311000000
H	-2.557584000000	1.143802000000	-5.254553000000

P	-1.098659000000	1.930106000000	2.364456000000
B	0.526179000000	-1.112523000000	0.258882000000
O	1.719851000000	-0.492687000000	0.510640000000
O	0.668143000000	-2.234903000000	-0.529620000000
C	2.694387000000	-1.019174000000	-0.429085000000
C	2.087953000000	-2.428281000000	-0.789183000000
C	2.727879000000	-0.043670000000	-1.609436000000
C	4.050043000000	-1.065229000000	0.265781000000
C	2.549617000000	-3.550957000000	0.142731000000
C	2.253958000000	-2.844364000000	-2.245507000000
H	3.438577000000	-0.365515000000	-2.377540000000
H	1.732856000000	0.079500000000	-2.044276000000
H	3.043640000000	0.936779000000	-1.239399000000
H	4.365571000000	-0.046765000000	0.510840000000
H	4.009757000000	-1.638365000000	1.194566000000
H	4.808331000000	-1.508185000000	-0.389454000000
H	2.435825000000	-3.267188000000	1.193005000000
H	1.935680000000	-4.438522000000	-0.038270000000
H	3.597580000000	-3.813471000000	-0.032408000000
H	1.803837000000	-2.114053000000	-2.920907000000
H	3.314209000000	-2.949078000000	-2.500489000000
H	1.767508000000	-3.811094000000	-2.410580000000
C	-0.087225000000	1.068926000000	3.681419000000
C	1.225422000000	0.618720000000	3.480270000000
C	-0.661068000000	0.907930000000	4.946700000000
C	1.936228000000	0.014702000000	4.514352000000
H	1.684904000000	0.720618000000	2.505866000000
C	0.048003000000	0.301595000000	5.986329000000
H	-1.679652000000	1.248766000000	5.112793000000
C	1.349735000000	-0.147915000000	5.772270000000
H	2.952174000000	-0.331860000000	4.338556000000
H	-0.419217000000	0.178178000000	6.960186000000
H	1.904836000000	-0.620471000000	6.578729000000
C	0.136389000000	3.280961000000	2.016036000000
C	-0.103051000000	4.528996000000	2.599238000000
C	1.305995000000	3.104991000000	1.262062000000
C	0.804362000000	5.580325000000	2.442850000000
H	-1.012029000000	4.679916000000	3.176737000000
C	2.209955000000	4.151814000000	1.101049000000
H	1.494981000000	2.146078000000	0.790320000000
C	1.963729000000	5.394991000000	1.692140000000
H	0.600479000000	6.544008000000	2.902948000000
H	3.111896000000	4.000007000000	0.512090000000
H	2.669890000000	6.211328000000	1.564070000000

C	-0.773829000000	-2.884078000000	4.012754000000
C	-1.994036000000	-2.575869000000	4.612969000000
C	-2.826228000000	-1.623030000000	4.023826000000
C	-2.438708000000	-0.990688000000	2.845801000000
C	-1.224576000000	-1.309345000000	2.217333000000
C	-0.400855000000	-2.264958000000	2.820194000000
H	-0.106077000000	-3.606026000000	4.473919000000
H	-2.285991000000	-3.061356000000	5.539681000000
H	-3.769075000000	-1.355674000000	4.492808000000
H	-3.067231000000	-0.214839000000	2.423802000000
H	0.553234000000	-2.513124000000	2.367559000000
C	-0.856156000000	-0.656905000000	0.893008000000
C	-0.905562000000	0.850443000000	0.896734000000
C	-0.774003000000	1.373574000000	-0.380939000000
O	-0.512263000000	0.667586000000	-1.401918000000
O	-1.047840000000	2.716138000000	-0.529939000000
C	-0.510128000000	3.342408000000	-1.688107000000
H	0.577132000000	3.456236000000	-1.596356000000
H	-0.736271000000	2.768656000000	-2.590683000000
H	-0.971696000000	4.330789000000	-1.736939000000
TS_{55/65}			
P	-2.169434000000	-0.940167000000	0.051189000000
C	-3.133807000000	-0.248907000000	-1.352566000000
C	-3.018113000000	1.265276000000	-1.592946000000
H	-2.836374000000	-0.808519000000	-2.244651000000
H	-4.176190000000	-0.522888000000	-1.147872000000
C	-4.171590000000	1.797087000000	-2.446613000000
H	-2.064364000000	1.476811000000	-2.078924000000
H	-2.986771000000	1.801772000000	-0.638585000000
C	-4.034813000000	3.297123000000	-2.716512000000
H	-5.128431000000	1.594308000000	-1.942694000000
H	-4.205100000000	1.250490000000	-3.399728000000
H	-4.856527000000	3.671010000000	-3.337276000000
H	-3.092173000000	3.515610000000	-3.230777000000
H	-4.035260000000	3.864450000000	-1.778067000000
C	-2.565944000000	-2.743831000000	0.078445000000
C	-4.005664000000	-3.126178000000	0.441035000000
H	-2.301933000000	-3.155893000000	-0.898988000000
H	-1.866002000000	-3.182413000000	0.799329000000
C	-4.212876000000	-4.644939000000	0.392416000000
H	-4.713476000000	-2.647155000000	-0.248242000000
H	-4.254731000000	-2.764695000000	1.445673000000
C	-5.640182000000	-5.055802000000	0.759960000000
H	-3.499543000000	-5.126127000000	1.075282000000

H	-3.967140000000	-5.010371000000	-0.613704000000
H	-6.368931000000	-4.609600000000	0.072517000000
H	-5.896977000000	-4.727201000000	1.774285000000
H	-5.765237000000	-6.143148000000	0.719319000000
C	-2.908801000000	-0.308906000000	1.626859000000
C	-4.369296000000	0.151941000000	1.532481000000
H	-2.797833000000	-1.120946000000	2.351590000000
H	-2.274912000000	0.514878000000	1.942937000000
C	-4.899358000000	0.568504000000	2.909738000000
H	-5.015678000000	-0.634100000000	1.124643000000
H	-4.445025000000	1.005333000000	0.849182000000
C	-6.343167000000	1.072189000000	2.855891000000
H	-4.246807000000	1.349107000000	3.322433000000
H	-4.829629000000	-0.286144000000	3.597203000000
H	-6.701784000000	1.363544000000	3.849057000000
H	-7.017844000000	0.298088000000	2.470272000000
H	-6.430751000000	1.945731000000	2.198936000000
P	1.138687000000	0.753417000000	-2.458222000000
B	0.393093000000	-0.805076000000	1.191654000000
O	1.630098000000	-0.300770000000	1.490626000000
O	-0.201908000000	-1.424347000000	2.271331000000
C	1.959267000000	-0.685774000000	2.849119000000
C	0.546996000000	-1.015596000000	3.456881000000
C	2.685322000000	0.481968000000	3.506607000000
C	2.884747000000	-1.902077000000	2.753111000000
C	0.526090000000	-2.162956000000	4.457215000000
C	-0.160383000000	0.217669000000	4.025129000000
H	2.887571000000	0.272381000000	4.562914000000
H	2.100871000000	1.400804000000	3.432629000000
H	3.642353000000	0.646379000000	3.001843000000
H	3.750298000000	-1.639369000000	2.138052000000
H	2.382715000000	-2.750724000000	2.279409000000
H	3.241781000000	-2.215575000000	3.739277000000
H	0.899188000000	-3.089888000000	4.016201000000
H	-0.499879000000	-2.335615000000	4.797399000000
H	1.137214000000	-1.921419000000	5.333812000000
H	-0.189195000000	1.022799000000	3.286038000000
H	0.333261000000	0.573011000000	4.935220000000
H	-1.190889000000	-0.049284000000	4.279197000000
C	2.412203000000	-0.616254000000	-2.414134000000
C	3.173398000000	-0.935834000000	-1.281100000000
C	2.656444000000	-1.315739000000	-3.600592000000
C	4.140465000000	-1.936572000000	-1.333536000000
H	2.994767000000	-0.410894000000	-0.351605000000

C	3.627503000000	-2.318070000000	-3.658461000000
H	2.069877000000	-1.078245000000	-4.484610000000
C	4.371378000000	-2.633236000000	-2.522678000000
H	4.718237000000	-2.175543000000	-0.443195000000
H	3.798408000000	-2.853690000000	-4.589028000000
H	5.126689000000	-3.414048000000	-2.562471000000
C	2.320329000000	2.109105000000	-1.963694000000
C	2.828992000000	2.913595000000	-2.987868000000
C	2.767400000000	2.327087000000	-0.652207000000
C	3.769103000000	3.911566000000	-2.716947000000
H	2.480994000000	2.760141000000	-4.006687000000
C	3.700604000000	3.324100000000	-0.379004000000
H	2.369215000000	1.720978000000	0.154961000000
C	4.207249000000	4.120678000000	-1.410656000000
H	4.152400000000	4.527993000000	-3.526388000000
H	4.036067000000	3.482320000000	0.643675000000
H	4.934556000000	4.899087000000	-1.194598000000
C	0.850560000000	-4.325461000000	-1.310967000000
C	0.414223000000	-4.376650000000	-2.633928000000
C	-0.198375000000	-3.255879000000	-3.196990000000
C	-0.368170000000	-2.099062000000	-2.441915000000
C	0.055048000000	-2.037231000000	-1.104888000000
C	0.660730000000	-3.170347000000	-0.552795000000
H	1.341193000000	-5.185785000000	-0.864615000000
H	0.560781000000	-5.276383000000	-3.224454000000
H	-0.526709000000	-3.274899000000	-4.232404000000
H	-0.803203000000	-1.217921000000	-2.901323000000
H	0.989445000000	-3.152695000000	0.481145000000
C	-0.221420000000	-0.792728000000	-0.270811000000
C	0.154046000000	0.518040000000	-0.927369000000
C	-0.272776000000	1.617204000000	-0.191623000000
O	-0.812503000000	1.545380000000	0.951341000000
O	-0.173749000000	2.840276000000	-0.820334000000
C	-0.233689000000	3.985700000000	0.019936000000
H	0.687709000000	4.083104000000	0.607065000000
H	-1.088998000000	3.932459000000	0.698403000000
H	-0.326591000000	4.843607000000	-0.649187000000

TS_{6R/7Z}

P	-0.923254000	-1.045645000	1.819961000
C	-1.343785000	-2.822412000	1.470167000
C	-1.810111000	-3.170424000	0.051626000
H	-2.100475000	-3.118833000	2.212281000
H	-0.426591000	-3.372119000	1.696702000
C	-2.271777000	-4.630061000	-0.073880000

H	-2.632091000	-2.513344000	-0.250851000
H	-0.986685000	-2.973888000	-0.636840000
C	-1.168572000	-5.658275000	0.194900000
H	-3.115845000	-4.810115000	0.607782000
H	-2.662377000	-4.781987000	-1.088961000
H	-0.803149000	-5.602000000	1.226478000
H	-1.531158000	-6.679191000	0.030806000
H	-0.311656000	-5.492993000	-0.467874000
C	-0.120126000	-1.175004000	3.484021000
C	1.332824000	-1.660056000	3.409041000
H	-0.726887000	-1.827056000	4.127796000
H	-0.146574000	-0.172723000	3.922709000
C	2.093612000	-1.450732000	4.721089000
H	1.358992000	-2.720449000	3.126344000
H	1.850623000	-1.121221000	2.612282000
C	3.565263000	-1.853221000	4.604850000
H	2.027935000	-0.390128000	4.998284000
H	1.609892000	-2.016662000	5.529908000
H	4.099790000	-1.702489000	5.549450000
H	3.668152000	-2.909247000	4.326414000
H	4.067090000	-1.256153000	3.834412000
C	-2.546278000	-0.243647000	2.229702000
C	-3.640349000	-0.374022000	1.162009000
H	-2.334640000	0.819079000	2.392758000
H	-2.903047000	-0.652805000	3.185050000
C	-4.885801000	0.447130000	1.509478000
H	-3.259019000	-0.046790000	0.188786000
H	-3.926844000	-1.426550000	1.050654000
C	-5.970935000	0.340673000	0.435612000
H	-5.284447000	0.114908000	2.478291000
H	-4.593198000	1.497254000	1.643412000
H	-5.594993000	0.686949000	-0.534017000
H	-6.302118000	-0.697685000	0.312632000
H	-6.849534000	0.943352000	0.691627000
P	-1.471284000	2.796764000	0.122240000
B	0.843244000	-0.666796000	-0.596357000
O	1.958983000	-0.226817000	-1.385858000
O	1.150611000	-1.974307000	-0.096086000
C	2.641132000	-1.403540000	-1.841434000
C	2.390591000	-2.425064000	-0.665554000
C	2.011032000	-1.848621000	-3.171319000
C	4.107873000	-1.047355000	-2.074091000
C	3.460874000	-2.364972000	0.432282000
C	2.221430000	-3.876334000	-1.116081000

H	2.055972000	-1.008165000	-3.871330000
H	2.546966000	-2.695722000	-3.613341000
H	0.961396000	-2.120477000	-3.043026000
H	4.686964000	-1.930148000	-2.368620000
H	4.180258000	-0.308932000	-2.879127000
H	4.562718000	-0.615751000	-1.179472000
H	3.132164000	-2.975559000	1.278534000
H	4.424929000	-2.751435000	0.084789000
H	3.603393000	-1.344526000	0.794686000
H	3.128139000	-4.246954000	-1.608403000
H	2.026960000	-4.509810000	-0.244185000
H	1.381369000	-3.984291000	-1.805459000
C	-0.031554000	3.913595000	-0.210085000
C	1.110663000	3.524141000	-0.922169000
C	-0.096745000	5.215391000	0.306138000
C	2.159973000	4.422906000	-1.117140000
H	1.187766000	2.513627000	-1.311171000
C	0.947394000	6.116284000	0.102733000
H	-0.971727000	5.521697000	0.875222000
C	2.081344000	5.720101000	-0.608914000
H	3.042832000	4.104870000	-1.665527000
H	0.881069000	7.122958000	0.507144000
H	2.901654000	6.416749000	-0.759805000
C	-2.562917000	3.215790000	-1.309007000
C	-2.078111000	3.650885000	-2.549460000
C	-3.945256000	3.080502000	-1.133492000
C	-2.956718000	3.908616000	-3.599661000
H	-1.009560000	3.775405000	-2.693491000
C	-4.827023000	3.329077000	-2.185975000
H	-4.331326000	2.774376000	-0.165962000
C	-4.332857000	3.739534000	-3.424318000
H	-2.568373000	4.240805000	-4.559088000
H	-5.896963000	3.211463000	-2.035216000
H	-5.015954000	3.940549000	-4.245324000
C	3.296595000	1.832673000	2.178690000
C	2.746324000	2.505822000	3.269196000
C	1.359573000	2.535994000	3.423519000
C	0.537665000	1.887507000	2.504811000
C	1.076776000	1.179349000	1.418189000
C	2.472827000	1.176912000	1.265294000
H	4.373306000	1.820459000	2.032406000
H	3.388262000	3.013721000	3.983394000
H	0.913830000	3.072918000	4.256276000
H	-0.537298000	1.938540000	2.632910000

H	2.892462000	0.688432000	0.396017000
C	0.234773000	0.470181000	0.408092000
C	-0.775178000	1.171017000	-0.342336000
C	-1.115326000	0.338232000	-1.418186000
O	-0.455913000	-0.764852000	-1.568979000
O	-2.130377000	0.589975000	-2.242279000
C	-2.300726000	-0.286273000	-3.364598000
H	-3.142005000	0.130199000	-3.918434000
H	-1.400300000	-0.297467000	-3.984251000
H	-2.521525000	-1.303438000	-3.031063000

TS_{6S/7Z}

P	0.798471000	1.494050000	0.323701000
C	1.272028000	0.525099000	-1.172905000
C	2.222946000	-0.645668000	-0.873024000
H	1.691507000	1.195154000	-1.931775000
H	0.336294000	0.132536000	-1.581615000
C	2.213312000	-1.713949000	-1.976812000
H	3.244160000	-0.263711000	-0.740623000
H	1.946058000	-1.112131000	0.077656000
C	2.691788000	-1.202029000	-3.337290000
H	2.852146000	-2.549955000	-1.659743000
H	1.197125000	-2.115617000	-2.076569000
H	3.709683000	-0.796853000	-3.271472000
H	2.695201000	-2.005909000	-4.081262000
H	2.035812000	-0.412691000	-3.717387000
C	2.399428000	1.949765000	1.139683000
C	3.445112000	2.652966000	0.268009000
H	2.790204000	1.019522000	1.562403000
H	2.137324000	2.568783000	2.006024000
C	4.756124000	2.899326000	1.024571000
H	3.654244000	2.050688000	-0.625868000
H	3.053692000	3.612826000	-0.093296000
C	5.811918000	3.603873000	0.169861000
H	4.546940000	3.496541000	1.922812000
H	5.149282000	1.937913000	1.382370000
H	6.061167000	3.010050000	-0.718015000
H	5.452457000	4.580693000	-0.175938000
H	6.737724000	3.768548000	0.732072000
C	0.148092000	3.095868000	-0.340820000
C	-1.126801000	2.910741000	-1.179379000
H	0.919948000	3.627074000	-0.911090000
H	-0.078989000	3.709560000	0.538831000
C	-2.030187000	4.146868000	-1.175171000
H	-0.849941000	2.653704000	-2.210489000

H	-1.713634000	2.067559000	-0.802148000
C	-3.313545000	3.922474000	-1.977267000
H	-2.287518000	4.382022000	-0.134107000
H	-1.481421000	5.014319000	-1.568742000
H	-3.091733000	3.696978000	-3.027845000
H	-3.877397000	3.076451000	-1.567869000
H	-3.961675000	4.805750000	-1.954533000
P	-2.662925000	-0.610433000	-0.924274000
B	-0.194215000	-0.520684000	2.530857000
O	0.949450000	0.129617000	3.068054000
O	-0.974713000	-1.049538000	3.602460000
C	1.150240000	-0.395305000	4.392338000
C	-0.316550000	-0.758151000	4.842765000
C	2.066686000	-1.622538000	4.281214000
C	1.832517000	0.681335000	5.231490000
C	-1.054471000	0.415050000	5.500835000
C	-0.413331000	-1.988224000	5.745221000
H	2.315182000	-2.037110000	5.264101000
H	1.604600000	-2.404468000	3.674118000
H	2.997425000	-1.320461000	3.789366000
H	1.260168000	1.611822000	5.224933000
H	1.954315000	0.353813000	6.270221000
H	2.827093000	0.890990000	4.823116000
H	-2.112524000	0.151030000	5.592402000
H	-0.663979000	0.637212000	6.500380000
H	-0.992337000	1.316827000	4.888273000
H	-0.022602000	-2.877804000	5.246504000
H	0.136605000	-1.838051000	6.681902000
H	-1.463067000	-2.175164000	5.994252000
C	-1.874921000	-1.288410000	-2.459390000
C	-1.744263000	-2.650260000	-2.770921000
C	-1.409722000	-0.345074000	-3.389022000
C	-1.128712000	-3.052126000	-3.955384000
H	-2.126467000	-3.392821000	-2.081505000
C	-0.784594000	-0.744927000	-4.570956000
H	-1.545512000	0.713033000	-3.183920000
C	-0.636321000	-2.102313000	-4.853887000
H	-1.032042000	-4.111464000	-4.179133000
H	-0.425311000	0.002472000	-5.273232000
H	-0.153374000	-2.419470000	-5.773994000
C	-3.838760000	-1.951976000	-0.454194000
C	-4.739757000	-2.450215000	-1.409981000
C	-3.947918000	-2.402667000	0.870012000
C	-5.704685000	-3.391337000	-1.058004000

H	-4.675870000	-2.108028000	-2.439628000
C	-4.923422000	-3.336934000	1.222345000
H	-3.266538000	-2.027031000	1.627898000
C	-5.801021000	-3.838821000	0.261762000
H	-6.385150000	-3.773551000	-1.814495000
H	-4.990340000	-3.676416000	2.252620000
H	-6.555864000	-4.570063000	0.537432000
C	-2.143787000	3.496789000	2.975936000
C	-3.517999000	3.517586000	2.719190000
C	-4.098409000	2.451366000	2.035518000
C	-3.314905000	1.387431000	1.585100000
C	-1.927321000	1.372193000	1.794592000
C	-1.366210000	2.434949000	2.527956000
H	-1.679736000	4.306616000	3.532501000
H	-4.128026000	4.348288000	3.062520000
H	-5.169146000	2.437713000	1.852476000
H	-3.797793000	0.554636000	1.091298000
H	-0.303862000	2.407597000	2.748236000
C	-1.071015000	0.234461000	1.375708000
C	-1.415220000	-0.744376000	0.398478000
C	-0.593504000	-1.872411000	0.646725000
O	0.238585000	-1.835020000	1.620959000
O	-0.655089000	-2.960553000	-0.111357000
C	0.188914000	-4.063399000	0.255209000
H	1.240858000	-3.776447000	0.192615000
H	-0.040340000	-4.396818000	1.269696000
H	-0.036876000	-4.845146000	-0.469817000
TS₂₈			
P	-0.900223000	-2.176260000	0.524383000
C	-0.696146000	-1.363832000	2.151975000
C	-1.874602000	-0.527147000	2.653876000
H	0.192673000	-0.734177000	2.026699000
H	-0.443472000	-2.149555000	2.875573000
C	-1.550093000	0.135663000	3.997556000
H	-2.094690000	0.249794000	1.916912000
H	-2.770274000	-1.155025000	2.764337000
C	-2.751481000	0.858209000	4.609165000
H	-1.182814000	-0.624106000	4.701693000
H	-0.724446000	0.842328000	3.845057000
H	-2.487485000	1.332976000	5.560475000
H	-3.126990000	1.639219000	3.939703000
H	-3.575003000	0.159611000	4.801714000
C	-2.213851000	-3.449441000	0.661675000
C	-2.358740000	-4.257936000	-0.638830000

H	-3.143712000	-2.924371000	0.893473000
H	-1.989435000	-4.104127000	1.512300000
C	-3.640624000	-5.101710000	-0.686465000
H	-2.357228000	-3.574716000	-1.496135000
H	-1.482203000	-4.907452000	-0.753413000
C	-4.920204000	-4.263805000	-0.777291000
H	-3.582133000	-5.762216000	-1.560886000
H	-3.682943000	-5.759826000	0.192846000
H	-5.079130000	-3.655582000	0.119805000
H	-4.881138000	-3.576572000	-1.629855000
H	-5.799316000	-4.906576000	-0.895583000
C	0.688013000	-3.027898000	0.220457000
C	1.013762000	-4.173054000	1.184963000
H	1.439786000	-2.233687000	0.270034000
H	0.665893000	-3.372050000	-0.818675000
C	2.395463000	-4.772185000	0.896451000
H	0.991807000	-3.815195000	2.222548000
H	0.254781000	-4.963768000	1.111366000
C	2.749339000	-5.922586000	1.840807000
H	2.424253000	-5.122500000	-0.144269000
H	3.150547000	-3.979018000	0.974986000
H	2.021857000	-6.739389000	1.759337000
H	3.739188000	-6.332801000	1.614196000
H	2.757795000	-5.587664000	2.885024000
P	2.063850000	0.700836000	0.642867000
B	0.718284000	2.092885000	0.372983000
O	-0.549269000	1.940455000	0.879250000
O	1.018973000	3.374840000	0.018405000
C	-1.287628000	3.166377000	0.592154000
C	-0.134399000	4.210989000	0.290453000
C	-2.198939000	2.871019000	-0.601274000
C	-2.134548000	3.498780000	1.816851000
C	0.248686000	5.078103000	1.492852000
C	-0.376932000	5.079967000	-0.939724000
H	-2.874681000	2.051975000	-0.338333000
H	-2.804850000	3.745995000	-0.859872000
H	-1.616374000	2.557867000	-1.467898000
H	-2.894120000	2.723075000	1.953423000
H	-1.532742000	3.552349000	2.726903000
H	-2.653112000	4.454360000	1.683451000
H	0.499027000	4.463211000	2.361773000
H	1.138018000	5.660909000	1.235626000
H	-0.553685000	5.771092000	1.766131000
H	-0.490762000	4.463394000	-1.832751000

H	-1.270213000	5.702207000	-0.814181000
H	0.481902000	5.741893000	-1.089021000
C	3.045759000	1.662215000	1.892513000
C	4.434664000	1.832184000	1.817613000
C	2.375926000	2.159540000	3.024067000
C	5.128857000	2.489025000	2.835224000
H	4.974716000	1.460514000	0.952417000
C	3.067423000	2.818328000	4.038123000
H	1.297322000	2.037192000	3.104886000
C	4.450907000	2.987386000	3.947948000
H	6.205646000	2.615488000	2.753764000
H	2.525657000	3.202799000	4.898878000
H	4.993151000	3.501860000	4.736464000
C	3.094226000	0.856446000	-0.880180000
C	3.456857000	-0.314812000	-1.556230000
C	3.505757000	2.093065000	-1.400659000
C	4.217601000	-0.259316000	-2.725399000
H	3.120761000	-1.273995000	-1.175093000
C	4.272839000	2.149327000	-2.562813000
H	3.204125000	3.007072000	-0.902243000
C	4.630767000	0.973927000	-3.228956000
H	4.484237000	-1.177692000	-3.241717000
H	4.583514000	3.113661000	-2.956633000
H	5.225386000	1.021021000	-4.137662000
C	-4.972694000	-0.437135000	-0.979396000
C	-5.188298000	-0.373408000	-2.355593000
C	-4.105458000	-0.526838000	-3.225304000
C	-2.824665000	-0.750751000	-2.726421000
C	-2.593156000	-0.821135000	-1.341534000
C	-3.689357000	-0.660142000	-0.479906000
H	-5.802486000	-0.306258000	-0.289829000
H	-6.186957000	-0.202071000	-2.747039000
H	-4.260691000	-0.478273000	-4.299827000
H	-1.984893000	-0.872397000	-3.402895000
H	-3.537661000	-0.677195000	0.593529000
C	-1.205082000	-1.057882000	-0.857319000
C	-0.051992000	-0.581138000	-1.344266000
C	0.186603000	0.395378000	-2.339958000
O	0.319760000	1.606204000	-2.111609000
O	0.437962000	-0.123927000	-3.581682000
C	0.973784000	0.814262000	-4.523551000
H	1.161527000	0.237827000	-5.431505000
H	0.259949000	1.618011000	-4.727062000
H	1.903392000	1.249332000	-4.149380000

TS_{8/9}

P	-0.512690000	-2.602568000	0.866045000
C	-0.066911000	-2.080002000	2.567014000
C	-1.228238000	-1.569215000	3.428084000
H	0.668440000	-1.278015000	2.429212000
H	0.446920000	-2.920848000	3.052321000
C	-0.748408000	-1.132731000	4.815730000
H	-1.701860000	-0.719746000	2.927049000
H	-1.997019000	-2.346816000	3.535434000
C	-1.885935000	-0.578194000	5.673704000
H	-0.276778000	-1.985719000	5.324772000
H	0.025155000	-0.366125000	4.696447000
H	-1.522052000	-0.263879000	6.658042000
H	-2.341080000	0.293654000	5.191841000
H	-2.671886000	-1.327748000	5.829848000
C	-1.554491000	-4.116518000	0.995098000
C	-2.303217000	-4.454021000	-0.305285000
H	-2.249441000	-3.972733000	1.827011000
H	-0.887988000	-4.938295000	1.287035000
C	-3.361759000	-5.550842000	-0.119084000
H	-2.784621000	-3.550328000	-0.695129000
H	-1.576792000	-4.767275000	-1.062371000
C	-4.550243000	-5.119521000	0.746635000
H	-3.729754000	-5.840018000	-1.111301000
H	-2.893900000	-6.448799000	0.308262000
H	-4.252196000	-4.906685000	1.780045000
H	-5.018434000	-4.213831000	0.344048000
H	-5.311657000	-5.905605000	0.786263000
C	1.072731000	-3.069879000	0.095986000
C	0.986308000	-3.519969000	-1.374861000
H	1.533590000	-3.836205000	0.731580000
H	1.675821000	-2.160614000	0.181806000
C	2.256406000	-3.161179000	-2.152617000
H	0.809712000	-4.602681000	-1.420543000
H	0.140567000	-3.034664000	-1.869089000
C	2.163894000	-3.557769000	-3.626434000
H	2.409533000	-2.077412000	-2.075902000
H	3.129747000	-3.637625000	-1.684938000
H	1.316108000	-3.052012000	-4.101987000
H	3.072756000	-3.280693000	-4.171283000
H	2.019950000	-4.639241000	-3.741937000
P	1.405758000	0.854423000	0.404947000
B	0.868741000	1.996379000	-1.193414000
O	-0.447144000	2.544092000	-0.983024000

O	1.745661000	3.044723000	-1.582086000
C	-0.448735000	3.870631000	-1.528597000
C	1.057296000	4.286896000	-1.382975000
C	-0.894090000	3.781342000	-2.995771000
C	-1.436667000	4.715334000	-0.729142000
C	1.383643000	4.810543000	0.023421000
C	1.548941000	5.283355000	-2.430210000
H	-1.865885000	3.277648000	-3.037659000
H	-0.999194000	4.770235000	-3.455595000
H	-0.178174000	3.195516000	-3.578658000
H	-2.455119000	4.345923000	-0.893908000
H	-1.227549000	4.655200000	0.341091000
H	-1.402773000	5.766062000	-1.040044000
H	1.027585000	4.121068000	0.794068000
H	2.470219000	4.902563000	0.116986000
H	0.941090000	5.795990000	0.205928000
H	1.451356000	4.877404000	-3.439332000
H	0.990191000	6.225066000	-2.371801000
H	2.607458000	5.503716000	-2.257500000
C	0.771115000	1.558690000	1.957497000
C	1.551502000	1.705523000	3.119652000
C	-0.600358000	1.879254000	2.030913000
C	0.988412000	2.187096000	4.301369000
H	2.607632000	1.456580000	3.093054000
C	-1.157065000	2.353584000	3.217102000
H	-1.218117000	1.784877000	1.146811000
C	-0.367943000	2.515349000	4.358492000
H	1.614614000	2.306104000	5.182189000
H	-2.215007000	2.602373000	3.244400000
H	-0.804260000	2.888126000	5.280866000
C	3.236836000	0.949829000	0.485148000
C	4.009936000	-0.161104000	0.119891000
C	3.900638000	2.139950000	0.829414000
C	5.403769000	-0.091549000	0.096581000
H	3.517331000	-1.088365000	-0.156704000
C	5.292108000	2.205066000	0.826046000
H	3.321150000	3.014970000	1.098782000
C	6.049292000	1.090690000	0.456190000
H	5.983212000	-0.963466000	-0.195736000
H	5.787787000	3.133209000	1.098694000
H	7.134419000	1.146494000	0.445866000
C	-4.809211000	-0.832821000	1.040840000
C	-5.147688000	0.378152000	0.440204000
C	-4.181461000	1.049462000	-0.314853000

C	-2.906696000	0.519290000	-0.478856000
C	-2.549854000	-0.707251000	0.117605000
C	-3.529395000	-1.363767000	0.884467000
H	-5.538439000	-1.370252000	1.641622000
H	-6.142459000	0.796289000	0.564019000
H	-4.418880000	2.004552000	-0.776730000
H	-2.159231000	1.076593000	-1.031477000
H	-3.302481000	-2.298244000	1.380636000
C	-1.186312000	-1.245829000	-0.090912000
C	-0.221184000	-0.663180000	-0.838038000
C	0.101083000	-0.130901000	-2.037548000
O	0.860252000	0.911474000	-2.277034000
O	-0.342313000	-0.810445000	-3.132943000
C	-0.187265000	-0.148588000	-4.395205000
H	-0.625035000	-0.831381000	-5.125490000
H	-0.720958000	0.806141000	-4.404791000
H	0.866586000	0.027525000	-4.623495000

TS_{9/10E}

P	-0.402131000	-2.015835000	1.019607000
C	-1.129027000	-1.333200000	-0.520996000
C	-1.875103000	-2.313149000	-1.433459000
H	-0.287348000	-0.871274000	-1.043901000
H	-1.795328000	-0.512459000	-0.255431000
C	-2.344775000	-1.630295000	-2.728842000
H	-1.243138000	-3.173747000	-1.691793000
H	-2.749117000	-2.713303000	-0.905936000
C	-1.199559000	-1.222181000	-3.659762000
H	-3.017205000	-2.314437000	-3.262242000
H	-2.936272000	-0.744899000	-2.463532000
H	-1.584060000	-0.785530000	-4.588083000
H	-0.544497000	-0.479424000	-3.194801000
H	-0.582991000	-2.089188000	-3.928733000
C	0.802168000	-3.284279000	0.429372000
C	2.084732000	-2.708774000	-0.173583000
H	0.259001000	-3.884685000	-0.311847000
H	1.036847000	-3.967003000	1.250494000
C	3.034348000	-3.816654000	-0.640755000
H	1.841029000	-2.050571000	-1.015872000
H	2.583086000	-2.079803000	0.569616000
C	4.331202000	-3.277551000	-1.247382000
H	3.272367000	-4.466595000	0.213199000
H	2.520974000	-4.453339000	-1.375527000
H	4.872641000	-2.656392000	-0.524802000
H	4.995375000	-4.092379000	-1.556374000

H	4.125784000	-2.656480000	-2.126253000
C	-1.736375000	-3.049392000	1.783154000
C	-1.277165000	-3.784620000	3.052035000
H	-2.114154000	-3.755577000	1.035034000
H	-2.547370000	-2.350213000	2.019041000
C	-2.441274000	-4.358654000	3.871090000
H	-0.594940000	-4.600143000	2.776597000
H	-0.697000000	-3.102375000	3.683547000
C	-3.268388000	-5.408131000	3.123912000
H	-2.036030000	-4.801976000	4.789817000
H	-3.093862000	-3.533499000	4.188426000
H	-4.040468000	-5.836715000	3.772018000
H	-3.773086000	-4.980397000	2.250423000
H	-2.633247000	-6.230740000	2.771763000
P	0.205311000	1.974220000	0.753652000
B	-2.125348000	2.429249000	0.237994000
O	-2.363151000	3.786743000	0.132693000
O	-2.297700000	1.759064000	-0.984553000
C	-2.396487000	4.101987000	-1.275703000
C	-2.840231000	2.731720000	-1.913795000
C	-3.380458000	5.248628000	-1.484879000
C	-0.989224000	4.541316000	-1.696418000
C	-2.275212000	2.463931000	-3.303832000
C	-4.360615000	2.538663000	-1.916965000
H	-3.000059000	6.150498000	-0.995423000
H	-3.504825000	5.465928000	-2.551821000
H	-4.357573000	5.018080000	-1.055828000
H	-0.263013000	3.734414000	-1.575084000
H	-0.968631000	4.880062000	-2.737418000
H	-0.676384000	5.369711000	-1.054175000
H	-2.602367000	1.480718000	-3.655601000
H	-2.632528000	3.215371000	-4.016962000
H	-1.183385000	2.479994000	-3.306658000
H	-4.778812000	2.733273000	-0.925243000
H	-4.853940000	3.194625000	-2.641804000
H	-4.584579000	1.500718000	-2.182294000
C	0.996891000	3.168109000	1.891139000
C	2.229430000	3.780177000	1.624394000
C	0.267727000	3.577897000	3.020283000
C	2.738429000	4.750144000	2.488095000
H	2.799417000	3.491270000	0.747576000
C	0.780776000	4.544153000	3.881828000
H	-0.702360000	3.134216000	3.223543000
C	2.021279000	5.130922000	3.622541000

H	3.701526000	5.205812000	2.273813000
H	0.208677000	4.842318000	4.756223000
H	2.421318000	5.884031000	4.295510000
C	1.549905000	1.277238000	-0.260222000
C	1.344145000	1.161797000	-1.642816000
C	2.770408000	0.852420000	0.287549000
C	2.343386000	0.644960000	-2.469293000
H	0.393791000	1.472830000	-2.065040000
C	3.774187000	0.355955000	-0.542488000
H	2.931488000	0.910877000	1.358753000
C	3.565016000	0.253589000	-1.919837000
H	2.171122000	0.560944000	-3.538780000
H	4.717958000	0.035484000	-0.110536000
H	4.351376000	-0.134126000	-2.561046000
C	3.053540000	-2.079278000	4.158240000
C	3.472693000	-0.928220000	4.828723000
C	2.778935000	0.259166000	4.586584000
C	1.716848000	0.301217000	3.689134000
C	1.299940000	-0.841777000	2.958079000
C	1.995389000	-2.042226000	3.255804000
H	3.551731000	-3.028491000	4.343877000
H	4.301206000	-0.960887000	5.529876000
H	3.058726000	1.172217000	5.107431000
H	1.187274000	1.233487000	3.549574000
H	1.695693000	-2.972860000	2.791365000
C	0.223111000	-0.716862000	1.989829000
C	-0.456786000	0.573523000	1.753095000
C	-1.777699000	0.800590000	2.008591000
O	-2.476528000	1.823981000	1.478484000
O	-2.585840000	0.056170000	2.801634000
C	-2.055506000	-0.297691000	4.088467000
H	-1.726339000	0.602763000	4.617279000
H	-2.881958000	-0.766775000	4.625286000
H	-1.213119000	-0.983852000	3.997219000
TS_{10E/11R}			
P	1.933054000	1.350710000	-0.771118000
C	3.669209000	1.098196000	-1.457202000
C	3.732565000	0.403673000	-2.823454000
H	4.224583000	0.514960000	-0.712457000
H	4.163699000	2.076496000	-1.515236000
C	5.125081000	-0.137731000	-3.163425000
H	3.010067000	-0.421925000	-2.862612000
H	3.420487000	1.103290000	-3.609542000
C	5.155577000	-0.877209000	-4.502833000

H	5.845335000	0.691812000	-3.175254000
H	5.452393000	-0.813095000	-2.361315000
H	4.465857000	-1.730469000	-4.492811000
H	4.853560000	-0.218178000	-5.325936000
H	6.157105000	-1.258715000	-4.730232000
C	1.080865000	2.074807000	-2.249571000
C	0.340749000	1.065943000	-3.134297000
H	1.846857000	2.604622000	-2.831365000
H	0.370893000	2.810959000	-1.870436000
C	-0.614161000	1.751046000	-4.115726000
H	1.060811000	0.445506000	-3.680380000
H	-0.245863000	0.393573000	-2.506001000
C	-1.378277000	0.735658000	-4.968055000
H	-1.327105000	2.355090000	-3.540931000
H	-0.056907000	2.442809000	-4.763508000
H	-1.972506000	0.069215000	-4.331784000
H	-2.062860000	1.230811000	-5.665589000
H	-0.692118000	0.113663000	-5.556810000
C	2.386502000	2.637748000	0.492366000
C	2.437357000	4.069794000	-0.053327000
H	3.373051000	2.347803000	0.877729000
H	1.676148000	2.536128000	1.312015000
C	2.958938000	5.091941000	0.968636000
H	3.079774000	4.104920000	-0.943278000
H	1.435629000	4.371559000	-0.385616000
C	2.068418000	5.251177000	2.203993000
H	3.971645000	4.800930000	1.280292000
H	3.059002000	6.064487000	0.468714000
H	2.464575000	6.019223000	2.877157000
H	1.051596000	5.547859000	1.919798000
H	1.993859000	4.318765000	2.773648000
P	-1.051699000	-1.704437000	-0.430594000
B	-2.818874000	1.157999000	-0.292425000
O	-3.893010000	1.503286000	-1.080508000
O	-3.173135000	0.542379000	0.884921000
C	-5.079254000	1.309794000	-0.265705000
C	-4.594407000	0.256540000	0.801481000
C	-5.420741000	2.671047000	0.348456000
C	-6.213263000	0.837412000	-1.166986000
C	-4.750051000	-1.190743000	0.329367000
C	-5.187618000	0.417694000	2.196244000
H	-6.345124000	2.630854000	0.933493000
H	-4.613612000	3.022131000	0.999433000
H	-5.549028000	3.400913000	-0.456338000

H	-7.110885000	0.616945000	-0.578473000
H	-6.461758000	1.623723000	-1.886684000
H	-5.931316000	-0.057048000	-1.725703000
H	-4.292789000	-1.336304000	-0.653302000
H	-4.244553000	-1.853258000	1.035050000
H	-5.805170000	-1.478117000	0.275910000
H	-6.272247000	0.262268000	2.179065000
H	-4.742874000	-0.328525000	2.861711000
H	-4.980806000	1.407299000	2.609365000
C	0.106461000	-2.961004000	-1.117143000
C	0.629563000	-4.052544000	-0.412785000
C	0.498754000	-2.770765000	-2.452520000
C	1.524798000	-4.927789000	-1.025912000
H	0.360993000	-4.201821000	0.626509000
C	1.411937000	-3.632456000	-3.057796000
H	0.088557000	-1.937866000	-3.017114000
C	1.925345000	-4.718478000	-2.346067000
H	1.929374000	-5.762493000	-0.460284000
H	1.711337000	-3.464150000	-4.089312000
H	2.631508000	-5.396543000	-2.817557000
C	-1.499691000	-2.331142000	1.236553000
C	-2.083695000	-3.603320000	1.352960000
C	-1.425772000	-1.515742000	2.376797000
C	-2.552194000	-4.064396000	2.582649000
H	-2.174411000	-4.237967000	0.475324000
C	-1.909062000	-1.976091000	3.601961000
H	-1.024614000	-0.510726000	2.302677000
C	-2.468224000	-3.250246000	3.713612000
H	-2.990687000	-5.056277000	2.654200000
H	-1.846883000	-1.331497000	4.475009000
H	-2.838941000	-3.604761000	4.671476000
C	2.883275000	-2.805924000	2.190637000
C	3.893775000	-3.418879000	1.448670000
C	4.120555000	-3.015062000	0.132003000
C	3.349865000	-2.005292000	-0.437756000
C	2.334435000	-1.372764000	0.295275000
C	2.118148000	-1.790845000	1.621598000
H	2.690772000	-3.115438000	3.214340000
H	4.494910000	-4.209390000	1.889585000
H	4.886598000	-3.503346000	-0.463980000
H	3.495536000	-1.753775000	-1.478046000
H	1.334169000	-1.309615000	2.195667000
C	1.452137000	-0.307230000	-0.232276000
C	0.071302000	-0.281537000	-0.086611000

C	-0.377854000	1.088702000	0.046227000
O	-1.547694000	1.465284000	-0.665602000
O	-0.418040000	1.518443000	1.398088000
C	-0.831708000	2.859580000	1.586740000
H	-0.354497000	3.541498000	0.871136000
H	-1.919825000	2.960004000	1.493071000
H	-0.539950000	3.136706000	2.603577000

TS_{10E/11S}

P	-1.001267000	-0.985769000	1.755111000
C	-2.217569000	-2.357615000	2.129550000
C	-1.579045000	-3.751227000	2.237500000
H	-2.964620000	-2.359768000	1.331427000
H	-2.755225000	-2.112776000	3.052382000
C	-2.610383000	-4.882065000	2.175992000
H	-0.859098000	-3.897331000	1.424861000
H	-1.006614000	-3.827551000	3.171539000
C	-1.963302000	-6.268201000	2.200679000
H	-3.319092000	-4.780919000	3.010182000
H	-3.194881000	-4.771131000	1.253398000
H	-1.296309000	-6.396837000	1.339767000
H	-1.367022000	-6.413476000	3.110015000
H	-2.715524000	-7.064196000	2.163871000
C	0.046657000	-1.129060000	3.305003000
C	-0.709295000	-1.225784000	4.635891000
H	0.712493000	-0.264716000	3.301903000
H	0.695932000	-2.002487000	3.168402000
C	0.245695000	-1.168171000	5.835606000
H	-1.433747000	-0.404289000	4.723447000
H	-1.288076000	-2.155109000	4.691072000
C	-0.483790000	-1.266353000	7.177458000
H	0.977417000	-1.983369000	5.750730000
H	0.822079000	-0.234508000	5.792903000
H	-1.042024000	-2.207311000	7.256111000
H	0.217024000	-1.222518000	8.018490000
H	-1.201138000	-0.445283000	7.297389000
C	-2.028851000	0.536124000	1.942238000
C	-3.036675000	0.741065000	0.806098000
H	-1.351733000	1.390756000	2.016884000
H	-2.546483000	0.431548000	2.902790000
C	-3.754543000	2.095839000	0.872497000
H	-2.513161000	0.657526000	-0.148681000
H	-3.780424000	-0.067683000	0.820916000
C	-4.621765000	2.284206000	2.120104000
H	-3.006459000	2.899195000	0.820829000

H	-4.379599000	2.200888000	-0.024111000
H	-5.161481000	3.236929000	2.087393000
H	-5.364774000	1.481361000	2.206307000
H	-4.019871000	2.279355000	3.035678000
P	0.493528000	0.212933000	-2.172435000
B	2.081299000	2.387098000	0.372170000
O	2.477430000	3.639217000	0.772277000
O	2.923241000	1.809449000	-0.553752000
C	3.554518000	4.038581000	-0.115043000
C	4.095708000	2.653972000	-0.641651000
C	2.926578000	4.892868000	-1.217862000
C	4.561983000	4.856077000	0.684521000
C	5.153940000	2.031205000	0.273904000
C	4.573104000	2.659178000	-2.088875000
H	3.685277000	5.293971000	-1.898100000
H	2.204010000	4.317677000	-1.799655000
H	2.396106000	5.730973000	-0.756283000
H	5.430074000	5.112150000	0.066600000
H	4.095134000	5.787862000	1.018532000
H	4.906977000	4.314488000	1.567788000
H	4.806657000	2.006282000	1.311176000
H	5.334365000	1.000769000	-0.046615000
H	6.100749000	2.579155000	0.232288000
H	5.419994000	3.342309000	-2.219043000
H	4.899253000	1.652659000	-2.369073000
H	3.770738000	2.955148000	-2.767533000
C	-1.012444000	-0.423276000	-3.046474000
C	-2.290256000	0.139274000	-2.921034000
C	-0.849034000	-1.536578000	-3.881898000
C	-3.381257000	-0.418582000	-3.585652000
H	-2.431271000	1.030250000	-2.318233000
C	-1.937706000	-2.096215000	-4.549020000
H	0.136305000	-1.980487000	-3.988939000
C	-3.208704000	-1.541645000	-4.397576000
H	-4.366282000	0.028075000	-3.475912000
H	-1.794103000	-2.968842000	-5.179921000
H	-4.059616000	-1.976695000	-4.914951000
C	0.158301000	2.021997000	-2.337249000
C	0.674192000	2.637592000	-3.488441000
C	-0.641200000	2.782481000	-1.472578000
C	0.383542000	3.970489000	-3.779135000
H	1.303082000	2.061534000	-4.162509000
C	-0.917873000	4.120749000	-1.753291000
H	-1.027365000	2.333938000	-0.567488000

C	-0.413949000	4.716995000	-2.909892000
H	0.787750000	4.428414000	-4.677933000
H	-1.531540000	4.696384000	-1.065565000
H	-0.633248000	5.758415000	-3.128162000
C	-2.493607000	-4.040010000	-1.774696000
C	-1.458328000	-4.887182000	-2.175078000
C	-0.137659000	-4.545275000	-1.882208000
C	0.141246000	-3.375239000	-1.176987000
C	-0.890273000	-2.525895000	-0.743198000
C	-2.210952000	-2.875002000	-1.067643000
H	-3.522330000	-4.278100000	-2.029810000
H	-1.678827000	-5.798961000	-2.723180000
H	0.676543000	-5.190099000	-2.202190000
H	1.168678000	-3.107939000	-0.953390000
H	-3.013675000	-2.195367000	-0.804579000
C	-0.586583000	-1.294513000	0.026374000
C	0.195437000	-0.207611000	-0.388186000
C	0.789577000	0.407229000	0.757864000
O	0.936456000	1.806796000	0.826510000
O	1.914180000	-0.164721000	1.397918000
C	2.666682000	-1.126563000	0.682352000
H	2.165213000	-2.104990000	0.677155000
H	2.846688000	-0.805554000	-0.348905000
H	3.619037000	-1.226746000	1.212527000
TS_{11R/10Z}			
P	1.725924000	1.270074000	0.511451000
C	3.570274000	1.030647000	0.675424000
C	4.351079000	1.215319000	-0.634781000
H	3.734443000	0.018117000	1.052166000
H	3.947687000	1.713268000	1.445609000
C	5.779814000	0.669402000	-0.546410000
H	3.836539000	0.702440000	-1.453578000
H	4.379820000	2.277709000	-0.909508000
C	6.529742000	0.770758000	-1.876070000
H	6.331054000	1.204057000	0.240190000
H	5.732322000	-0.382640000	-0.236014000
H	6.013640000	0.194488000	-2.653231000
H	6.594337000	1.810792000	-2.218997000
H	7.550975000	0.382322000	-1.792514000
C	1.716304000	3.067058000	-0.015171000
C	2.634837000	4.018113000	0.760908000
H	0.674554000	3.383029000	0.069771000
H	1.941223000	3.086373000	-1.085931000
C	2.401283000	5.480196000	0.357361000

H	2.465732000	3.920138000	1.842544000
H	3.688342000	3.769016000	0.590215000
C	3.310501000	6.453780000	1.110811000
H	2.561420000	5.583200000	-0.724321000
H	1.349236000	5.740199000	0.535822000
H	4.368153000	6.235116000	0.919390000
H	3.123916000	7.490367000	0.809196000
H	3.149634000	6.386757000	2.193817000
C	1.178838000	1.209170000	2.274830000
C	1.428983000	-0.141976000	2.957758000
H	0.117786000	1.464501000	2.297743000
H	1.720716000	2.010614000	2.789618000
C	0.791368000	-0.242214000	4.350530000
H	1.033678000	-0.939899000	2.322894000
H	2.509694000	-0.316942000	3.042771000
C	1.341274000	0.764789000	5.364119000
H	-0.295743000	-0.116206000	4.257389000
H	0.947509000	-1.260799000	4.728791000
H	0.900333000	0.609831000	6.354817000
H	2.429634000	0.667453000	5.463652000
H	1.126277000	1.797401000	5.067070000
P	-1.239957000	-1.718539000	-0.737409000
B	-0.902021000	1.598157000	-2.747665000
O	-0.493532000	2.212294000	-3.915804000
O	-1.886977000	0.657834000	-2.946280000
C	-1.430747000	1.802573000	-4.944693000
C	-1.982661000	0.444559000	-4.373080000
C	-2.505043000	2.891204000	-5.031848000
C	-0.683500000	1.685835000	-6.267465000
C	-1.093118000	-0.757889000	-4.705262000
C	-3.434556000	0.135352000	-4.717647000
H	-3.220269000	2.690913000	-5.836234000
H	-3.055515000	2.973096000	-4.089580000
H	-2.020389000	3.852231000	-5.228398000
H	-1.345390000	1.307220000	-7.054499000
H	-0.318452000	2.671262000	-6.573555000
H	0.175865000	1.017677000	-6.181601000
H	-0.040472000	-0.532831000	-4.510149000
H	-1.384171000	-1.591011000	-4.059597000
H	-1.193378000	-1.061356000	-5.752625000
H	-3.566268000	0.035513000	-5.801074000
H	-3.725070000	-0.809185000	-4.247728000
H	-4.105780000	0.914778000	-4.351307000
C	-0.168635000	-3.125244000	-0.185983000

C	0.135300000	-3.409590000	1.152668000
C	0.369949000	-3.947952000	-1.185183000
C	0.980676000	-4.469419000	1.479464000
H	-0.303806000	-2.810713000	1.943851000
C	1.217794000	-5.005831000	-0.861983000
H	0.138537000	-3.739713000	-2.226028000
C	1.528729000	-5.266926000	0.472878000
H	1.207442000	-4.677033000	2.522305000
H	1.639742000	-5.620967000	-1.651699000
H	2.188742000	-6.091522000	0.728672000
C	-2.403400000	-1.641620000	0.694946000
C	-3.588503000	-2.380454000	0.588098000
C	-2.152356000	-0.945434000	1.885659000
C	-4.494839000	-2.435869000	1.648293000
H	-3.803762000	-2.913178000	-0.334669000
C	-3.057284000	-0.994687000	2.943438000
H	-1.251362000	-0.352379000	1.974403000
C	-4.231493000	-1.742755000	2.829422000
H	-5.408749000	-3.015188000	1.547764000
H	-2.848212000	-0.445573000	3.858350000
H	-4.937845000	-1.779993000	3.654279000
C	3.902677000	-2.896836000	-0.922112000
C	3.934209000	-2.937778000	-2.317668000
C	3.069445000	-2.124742000	-3.052167000
C	2.188627000	-1.271364000	-2.390501000
C	2.155442000	-1.209752000	-0.987615000
C	3.025195000	-2.038702000	-0.264530000
H	4.552561000	-3.547516000	-0.343940000
H	4.622765000	-3.605324000	-2.828185000
H	3.082090000	-2.153664000	-4.138413000
H	1.524028000	-0.622720000	-2.952175000
H	2.972870000	-2.045023000	0.818646000
C	1.225523000	-0.258023000	-0.334049000
C	-0.157207000	-0.239617000	-0.455212000
C	-0.639300000	1.116073000	-0.378575000
O	-0.336071000	1.918558000	-1.555450000
O	-1.988765000	1.258126000	-0.056452000
C	-2.321114000	2.510344000	0.505343000
H	-1.748147000	2.704782000	1.425184000
H	-2.134095000	3.330811000	-0.200649000
H	-3.387252000	2.477806000	0.745397000
TS_{11S/10Z}			
P	1.193972000	0.368485000	-0.312024000
C	2.674201000	-0.759361000	-0.588922000

C	2.385812000	-1.941923000	-1.533508000
H	2.980882000	-1.131031000	0.395430000
H	3.508373000	-0.154531000	-0.959496000
C	3.147766000	-3.222362000	-1.167787000
H	1.314081000	-2.166825000	-1.537242000
H	2.637226000	-1.654100000	-2.562778000
C	4.669371000	-3.067395000	-1.234216000
H	2.848349000	-3.535995000	-0.160333000
H	2.833996000	-4.026841000	-1.846140000
H	4.992371000	-2.765780000	-2.238848000
H	5.025792000	-2.305652000	-0.530997000
H	5.176673000	-4.007124000	-0.988311000
C	2.087480000	1.750503000	0.590524000
C	1.678750000	3.167790000	0.165980000
H	3.167113000	1.601203000	0.477573000
H	1.856387000	1.609200000	1.651480000
C	1.908960000	4.198564000	1.276113000
H	2.241186000	3.458711000	-0.731326000
H	0.621511000	3.182402000	-0.110466000
C	1.476735000	5.606536000	0.862075000
H	1.347231000	3.883776000	2.163785000
H	2.971207000	4.204664000	1.559742000
H	2.034026000	5.952935000	-0.017364000
H	0.410003000	5.625801000	0.606496000
H	1.639807000	6.330752000	1.668117000
C	0.780850000	0.890605000	-2.037254000
C	1.976223000	1.257961000	-2.925121000
H	0.093563000	1.735652000	-1.967452000
H	0.217639000	0.060986000	-2.475652000
C	1.508074000	1.770623000	-4.292456000
H	2.585384000	2.032565000	-2.442170000
H	2.631972000	0.393923000	-3.072673000
C	2.671628000	2.135691000	-5.216739000
H	0.881917000	1.002660000	-4.767455000
H	0.860767000	2.645928000	-4.146298000
H	3.314915000	1.267238000	-5.403064000
H	2.314153000	2.501098000	-6.185790000
H	3.295629000	2.920792000	-4.772743000
P	-2.815756000	-1.065360000	0.164729000
B	-0.670436000	1.438088000	2.785148000
O	-1.126242000	0.205463000	3.199464000
O	-0.111328000	2.183425000	3.805268000
C	-1.055656000	0.196743000	4.651678000
C	0.038732000	1.290819000	4.937142000

C	-2.438117000	0.591753000	5.180022000
C	-0.700002000	-1.213873000	5.103351000
C	1.465831000	0.736644000	4.878604000
C	-0.164720000	2.088769000	6.219330000
H	-3.181868000	-0.120342000	4.811207000
H	-2.465929000	0.577328000	6.273907000
H	-2.720420000	1.592712000	4.838242000
H	-0.565169000	-1.249515000	6.190286000
H	-1.510479000	-1.898068000	4.834952000
H	0.208014000	-1.574782000	4.618347000
H	2.170828000	1.573010000	4.873215000
H	1.688772000	0.096920000	5.738165000
H	1.620860000	0.154468000	3.965442000
H	-0.134834000	1.430809000	7.094932000
H	0.635180000	2.828634000	6.321644000
H	-1.117871000	2.621259000	6.211694000
C	-4.073828000	0.226256000	0.523152000
C	-4.983034000	0.740930000	-0.409121000
C	-4.167044000	0.648033000	1.859905000
C	-5.946193000	1.672468000	-0.016985000
H	-4.932931000	0.423969000	-1.445414000
C	-5.125897000	1.580993000	2.249460000
H	-3.467332000	0.250775000	2.586328000
C	-6.020532000	2.098697000	1.309843000
H	-6.640328000	2.068168000	-0.753953000
H	-5.176146000	1.901170000	3.287224000
H	-6.772131000	2.823616000	1.609977000
C	-2.910880000	-1.288884000	-1.666434000
C	-3.246675000	-2.557368000	-2.158892000
C	-2.604207000	-0.266002000	-2.579950000
C	-3.270321000	-2.806415000	-3.533276000
H	-3.485052000	-3.353938000	-1.458586000
C	-2.627562000	-0.515508000	-3.951173000
H	-2.348361000	0.718735000	-2.202904000
C	-2.957512000	-1.786363000	-4.431025000
H	-3.530000000	-3.795789000	-3.900117000
H	-2.384813000	0.282856000	-4.648078000
H	-2.969726000	-1.979035000	-5.500413000
C	1.503134000	-3.523526000	2.501465000
C	0.922922000	-4.678293000	1.973746000
C	0.025419000	-4.567095000	0.909982000
C	-0.287167000	-3.318979000	0.374782000
C	0.281264000	-2.145963000	0.900917000
C	1.180665000	-2.275088000	1.972718000

H	2.202406000	-3.592815000	3.330750000
H	1.169553000	-5.653248000	2.384168000
H	-0.427973000	-5.458921000	0.485808000
H	-0.958281000	-3.248397000	-0.474503000
H	1.622096000	-1.379460000	2.399889000
C	-0.015347000	-0.814709000	0.340381000
C	-1.234998000	-0.139803000	0.324657000
C	-0.974400000	1.279396000	0.321019000
O	-0.686782000	1.948764000	1.533750000
O	-1.750609000	2.090131000	-0.507540000
C	-2.490466000	3.174242000	0.057133000
H	-3.109250000	3.560865000	-0.755198000
H	-3.134117000	2.845339000	0.875324000
H	-1.818804000	3.961876000	0.416195000

TS_{10Z/6R}

P	0.931741000	-0.433106000	-0.554008000
C	1.191898000	1.279233000	-1.149463000
C	1.733708000	2.289845000	-0.124679000
H	0.222953000	1.614743000	-1.524856000
H	1.859990000	1.212135000	-2.016063000
C	1.328407000	3.722142000	-0.492330000
H	1.363743000	2.065186000	0.877699000
H	2.827662000	2.210196000	-0.071914000
C	1.818177000	4.746041000	0.532108000
H	1.714228000	3.972036000	-1.490366000
H	0.235970000	3.769713000	-0.563511000
H	2.912171000	4.741369000	0.615288000
H	1.506806000	5.760854000	0.260863000
H	1.409774000	4.523727000	1.525554000
C	0.936188000	-1.453864000	-2.102466000
C	-0.340179000	-1.277411000	-2.934625000
H	1.047335000	-2.502859000	-1.814668000
H	1.830823000	-1.183362000	-2.673585000
C	-0.526997000	-2.382214000	-3.981381000
H	-1.210878000	-1.261908000	-2.270506000
H	-0.310170000	-0.300495000	-3.432999000
C	0.593845000	-2.453778000	-5.022208000
H	-0.614881000	-3.345884000	-3.461387000
H	-1.486128000	-2.219579000	-4.489014000
H	1.559276000	-2.696228000	-4.562727000
H	0.387058000	-3.222115000	-5.775188000
H	0.706957000	-1.495744000	-5.545534000
C	2.470698000	-0.922490000	0.323834000
C	3.769299000	-0.783879000	-0.479044000

H	2.339639000	-1.957040000	0.657172000
H	2.501760000	-0.325270000	1.240427000
C	4.998360000	-1.131558000	0.369105000
H	3.744613000	-1.436959000	-1.361090000
H	3.873562000	0.241849000	-0.855817000
C	6.310980000	-0.998383000	-0.405477000
H	5.019276000	-0.478393000	1.251822000
H	4.893809000	-2.156874000	0.749892000
H	7.172281000	-1.248259000	0.223436000
H	6.327265000	-1.666268000	-1.275292000
H	6.450477000	0.025992000	-0.771476000
P	-2.750760000	0.901431000	-0.822209000
B	-0.078128000	0.036879000	2.733898000
O	1.157071000	-0.358887000	3.205913000
O	-1.132101000	-0.639755000	3.312353000
C	0.958044000	-1.511751000	4.062943000
C	-0.603197000	-1.481070000	4.360856000
C	1.408942000	-2.754761000	3.295726000
C	1.845423000	-1.326335000	5.292403000
C	-0.957142000	-0.786817000	5.680635000
C	-1.291633000	-2.840614000	4.284140000
H	1.335236000	-3.652343000	3.917930000
H	0.806342000	-2.907174000	2.400160000
H	2.455642000	-2.629059000	3.000246000
H	1.700377000	-2.144840000	6.006019000
H	2.895875000	-1.326888000	4.984184000
H	1.643704000	-0.380159000	5.798455000
H	-0.626101000	-1.365046000	6.549341000
H	-0.512812000	0.211681000	5.733514000
H	-2.044051000	-0.674032000	5.734679000
H	-1.173649000	-3.300509000	3.302388000
H	-0.899077000	-3.519270000	5.050175000
H	-2.363717000	-2.710746000	4.460195000
C	-4.182380000	1.447161000	0.214235000
C	-5.281034000	2.040730000	-0.429479000
C	-4.276926000	1.199792000	1.592076000
C	-6.424880000	2.397134000	0.282009000
H	-5.234316000	2.238430000	-1.497300000
C	-5.426867000	1.547606000	2.302760000
H	-3.449479000	0.735690000	2.118771000
C	-6.503561000	2.151932000	1.654510000
H	-7.257509000	2.864694000	-0.237218000
H	-5.475871000	1.346777000	3.370070000
H	-7.396175000	2.425917000	2.210126000

C	-2.351531000	2.476824000	-1.726817000
C	-2.598160000	3.772436000	-1.244903000
C	-1.745713000	2.345071000	-2.986370000
C	-2.209842000	4.891525000	-1.979364000
H	-3.091579000	3.898773000	-0.290038000
C	-1.340607000	3.463696000	-3.716788000
H	-1.599506000	1.352163000	-3.401156000
C	-1.566138000	4.742912000	-3.210580000
H	-2.405757000	5.886204000	-1.586813000
H	-0.864614000	3.334366000	-4.685370000
H	-1.257968000	5.618223000	-3.775852000
C	-1.112660000	-4.328989000	0.467144000
C	-2.463838000	-4.410583000	0.800797000
C	-3.161495000	-3.220318000	1.020410000
C	-2.531804000	-1.986887000	0.901806000
C	-1.169128000	-1.869655000	0.544445000
C	-0.483252000	-3.091116000	0.344361000
H	-0.533247000	-5.234749000	0.303919000
H	-2.957375000	-5.373300000	0.894479000
H	-4.213202000	-3.248281000	1.294684000
H	-3.100819000	-1.091728000	1.107875000
H	0.575696000	-3.089826000	0.110281000
C	-0.532678000	-0.545559000	0.437858000
C	-1.387214000	0.692506000	0.396199000
C	-1.111040000	1.620465000	1.348258000
O	-0.224816000	1.392799000	2.334857000
O	-1.629843000	2.859539000	1.349145000
C	-1.752098000	3.530077000	2.608381000
H	-0.775185000	3.673071000	3.075063000
H	-2.205752000	4.494097000	2.374762000
H	-2.407168000	2.967059000	3.280421000
TS_{10Z/6S}			
P	-0.926780000	-1.160175000	0.741273000
C	0.090072000	-2.531568000	1.423816000
C	-0.565347000	-3.364336000	2.530510000
H	1.015297000	-2.061045000	1.771041000
H	0.379321000	-3.176861000	0.590615000
C	0.410194000	-4.390221000	3.118620000
H	-0.928952000	-2.713716000	3.336628000
H	-1.445381000	-3.889067000	2.136084000
C	-0.222198000	-5.248991000	4.215785000
H	0.783609000	-5.034794000	2.310968000
H	1.286040000	-3.861032000	3.517626000
H	-0.576868000	-4.628182000	5.047465000

H	-1.082274000	-5.810297000	3.831006000
H	0.494422000	-5.971661000	4.620772000
C	-1.271883000	-0.060786000	2.165167000
C	-0.060010000	0.238534000	3.066384000
H	-2.075451000	-0.517716000	2.748469000
H	-1.677114000	0.861635000	1.745555000
C	-0.203825000	1.590569000	3.773198000
H	0.050888000	-0.561327000	3.810452000
H	0.863922000	0.254196000	2.486413000
C	1.010725000	1.918915000	4.642528000
H	-0.330230000	2.368906000	3.010938000
H	-1.120268000	1.599210000	4.379799000
H	0.900950000	2.892109000	5.134073000
H	1.158864000	1.164080000	5.424750000
H	1.921692000	1.948497000	4.032955000
C	-2.548221000	-1.942521000	0.243577000
C	-3.667645000	-1.979305000	1.292333000
H	-2.326814000	-2.961102000	-0.095899000
H	-2.863450000	-1.385198000	-0.643802000
C	-4.912465000	-2.736980000	0.801819000
H	-3.306125000	-2.458483000	2.209879000
H	-3.951470000	-0.955771000	1.559909000
C	-5.613328000	-2.086316000	-0.394113000
H	-4.628913000	-3.767441000	0.545331000
H	-5.621621000	-2.813221000	1.636577000
H	-5.926466000	-1.063024000	-0.156496000
H	-4.962957000	-2.039160000	-1.273980000
H	-6.508584000	-2.650087000	-0.677742000
P	-1.793122000	1.901017000	-1.382342000
B	2.278743000	0.307043000	0.050509000
O	2.879427000	-0.686482000	0.792329000
O	2.768630000	0.425971000	-1.226988000
C	3.741145000	-1.435743000	-0.109026000
C	3.914102000	-0.451138000	-1.339201000
C	5.031053000	-1.750993000	0.643671000
C	3.030880000	-2.738233000	-0.478563000
C	3.880613000	-1.126597000	-2.705881000
C	5.149483000	0.448256000	-1.223762000
H	4.805707000	-2.407059000	1.490509000
H	5.744301000	-2.268923000	-0.006936000
H	5.503766000	-0.847208000	1.033362000
H	2.092243000	-2.548261000	-1.001528000
H	3.663330000	-3.359353000	-1.120686000
H	2.818261000	-3.301220000	0.435363000

H	2.946494000	-1.664368000	-2.869839000
H	3.963974000	-0.364456000	-3.486659000
H	4.721922000	-1.820534000	-2.815329000
H	5.107690000	1.203332000	-2.014262000
H	5.170332000	0.968139000	-0.261022000
H	6.078853000	-0.119407000	-1.335600000
C	-2.959851000	2.271518000	0.012106000
C	-4.120957000	1.489816000	0.087793000
C	-2.715978000	3.208137000	1.032708000
C	-5.003938000	1.613369000	1.164268000
H	-4.331080000	0.778372000	-0.706206000
C	-3.595161000	3.331902000	2.106571000
H	-1.825408000	3.822636000	0.985265000
C	-4.738235000	2.529846000	2.180296000
H	-5.899316000	0.998364000	1.204739000
H	-3.387559000	4.053579000	2.892446000
H	-5.420255000	2.627576000	3.020540000
C	-1.248019000	3.586196000	-1.896919000
C	-2.137537000	4.670313000	-1.885304000
C	0.028433000	3.781035000	-2.449943000
C	-1.756112000	5.915538000	-2.386726000
H	-3.133274000	4.544652000	-1.470828000
C	0.408825000	5.023849000	-2.951921000
H	0.740018000	2.961084000	-2.464568000
C	-0.480710000	6.100003000	-2.920200000
H	-2.459759000	6.743639000	-2.358033000
H	1.405344000	5.152483000	-3.367148000
H	-0.183516000	7.069556000	-3.310222000
C	-0.020810000	-2.892590000	-3.351048000
C	0.339492000	-2.114940000	-4.450807000
C	0.533461000	-0.744895000	-4.254424000
C	0.382338000	-0.172901000	-2.997656000
C	0.010836000	-0.933453000	-1.862720000
C	-0.188578000	-2.315874000	-2.093353000
H	-0.184121000	-3.961564000	-3.467615000
H	0.462902000	-2.561683000	-5.432878000
H	0.818370000	-0.110922000	-5.090742000
H	0.578186000	0.883211000	-2.872093000
H	-0.483225000	-2.969619000	-1.279782000
C	-0.114875000	-0.280701000	-0.553611000
C	-0.332378000	1.199702000	-0.503428000
C	0.560939000	1.930966000	0.206025000
O	1.694653000	1.401016000	0.717616000
O	0.370167000	3.220064000	0.551629000

C	1.533512000	4.053062000	0.639870000
H	2.082034000	4.046987000	-0.306694000
H	1.153875000	5.056494000	0.834522000
H	2.187037000	3.725935000	1.451825000
TS_{11R/12R}			
P	-0.917498000	-0.875490000	1.363331000
C	-2.449104000	-0.615367000	2.358917000
C	-2.274528000	0.438723000	3.462329000
H	-2.782197000	-1.571997000	2.778138000
H	-3.211610000	-0.286248000	1.645370000
C	-3.611209000	0.976475000	3.980019000
H	-1.705513000	0.007156000	4.295791000
H	-1.672487000	1.274033000	3.088731000
C	-3.435910000	2.018570000	5.086475000
H	-4.164121000	1.417471000	3.139495000
H	-4.223716000	0.141402000	4.347416000
H	-4.402222000	2.396139000	5.437752000
H	-2.908060000	1.594585000	5.949183000
H	-2.851386000	2.875005000	4.729180000
C	-1.166703000	-2.495033000	0.536927000
C	-2.273219000	-2.516278000	-0.519413000
H	-1.378809000	-3.205944000	1.345292000
H	-0.206087000	-2.765316000	0.091255000
C	-2.327621000	-3.838305000	-1.295825000
H	-3.247371000	-2.320530000	-0.052521000
H	-2.099526000	-1.706476000	-1.226010000
C	-2.657971000	-5.059641000	-0.434157000
H	-3.079342000	-3.730195000	-2.086609000
H	-1.364394000	-3.987553000	-1.801475000
H	-1.882388000	-5.250889000	0.316680000
H	-3.608752000	-4.922047000	0.096683000
H	-2.746575000	-5.963311000	-1.047078000
C	0.438900000	-1.092025000	2.575430000
C	0.226508000	-2.237388000	3.573613000
H	0.558663000	-0.134779000	3.090868000
H	1.348003000	-1.232099000	1.988638000
C	1.367782000	-2.311169000	4.595234000
H	-0.725240000	-2.117542000	4.108319000
H	0.163654000	-3.194221000	3.039685000
C	1.192002000	-3.459367000	5.591004000
H	2.320201000	-2.422113000	4.060502000
H	1.429170000	-1.356015000	5.134216000
H	1.159086000	-4.426912000	5.075821000
H	2.016623000	-3.492272000	6.311176000

H	0.258204000	-3.352780000	6.156481000
P	-0.818066000	0.825243000	-2.714084000
B	1.618311000	1.298346000	0.600603000
O	2.578948000	0.766823000	1.448719000
O	2.161082000	2.211384000	-0.286682000
C	3.811479000	1.499735000	1.244671000
C	3.597620000	2.202827000	-0.158252000
C	3.914088000	2.488364000	2.411888000
C	4.977044000	0.517453000	1.291727000
C	4.169569000	1.433827000	-1.350792000
C	4.076011000	3.653428000	-0.218936000
H	4.837466000	3.075205000	2.372384000
H	3.062708000	3.175436000	2.418499000
H	3.900359000	1.926308000	3.350735000
H	4.877891000	-0.261204000	0.533239000
H	5.928685000	1.036716000	1.133146000
H	5.011070000	0.035951000	2.274264000
H	3.852622000	1.932213000	-2.271934000
H	5.264304000	1.415676000	-1.328972000
H	3.798641000	0.410307000	-1.389715000
H	3.844095000	4.066938000	-1.205315000
H	3.582482000	4.274344000	0.531325000
H	5.160057000	3.716498000	-0.071795000
C	-2.499764000	0.063693000	-2.895577000
C	-3.587336000	0.280723000	-2.031266000
C	-2.658836000	-0.852000000	-3.946814000
C	-4.786139000	-0.406475000	-2.209617000
H	-3.471229000	0.967930000	-1.202600000
C	-3.856789000	-1.548824000	-4.121525000
H	-1.830341000	-1.021712000	-4.629716000
C	-4.923912000	-1.328414000	-3.251307000
H	-5.615664000	-0.229069000	-1.529390000
H	-3.956329000	-2.257536000	-4.939374000
H	-5.857931000	-1.867702000	-3.384010000
C	-1.200896000	2.613801000	-2.475638000
C	-0.146282000	3.450548000	-2.069303000
C	-2.429153000	3.204976000	-2.806544000
C	-0.330765000	4.827306000	-1.956522000
H	0.813781000	3.019383000	-1.808048000
C	-2.609594000	4.585412000	-2.697074000
H	-3.253575000	2.588313000	-3.147483000
C	-1.565508000	5.403115000	-2.264747000
H	0.495512000	5.450721000	-1.623758000
H	-3.572645000	5.020965000	-2.952064000

H	-1.709144000	6.476789000	-2.178221000
C	3.487298000	-2.829438000	-2.151214000
C	2.842509000	-3.428900000	-3.237330000
C	1.521458000	-3.078169000	-3.524604000
C	0.863621000	-2.114677000	-2.763491000
C	1.505839000	-1.469590000	-1.680060000
C	2.819191000	-1.890783000	-1.372360000
H	4.504378000	-3.117361000	-1.896322000
H	3.354986000	-4.176660000	-3.836240000
H	1.000204000	-3.556552000	-4.350457000
H	-0.167695000	-1.868784000	-2.988577000
H	3.288444000	-1.476146000	-0.485690000
C	0.823974000	-0.553424000	-0.789504000
C	-0.206666000	0.274097000	-1.051794000
C	-0.711930000	0.778046000	0.312109000
O	0.271387000	1.470888000	1.005669000
O	-1.928070000	1.452423000	0.338132000
C	-1.955794000	2.828093000	0.738159000
H	-1.146674000	3.392270000	0.278971000
H	-2.912830000	3.208448000	0.377662000
H	-1.903868000	2.924043000	1.827742000
TS_{1/7E}			
P	-0.151398000	-0.142104000	-1.074028000
B	-0.073506000	1.044233000	0.458606000
O	-1.114319000	1.821796000	0.858742000
O	1.095483000	1.248817000	1.114940000
C	-0.673560000	2.525207000	2.073335000
C	0.898363000	2.409193000	1.986509000
C	-1.216218000	3.947647000	2.003425000
C	-1.279305000	1.781457000	3.260750000
C	1.591783000	2.127237000	3.312757000
C	1.562860000	3.583041000	1.264054000
H	-2.309348000	3.921373000	2.038751000
H	-0.863053000	4.534274000	2.858417000
H	-0.915813000	4.454696000	1.083998000
H	-2.365046000	1.737848000	3.135441000
H	-0.910262000	0.758974000	3.333596000
H	-1.060588000	2.301796000	4.198586000
H	1.244205000	1.190270000	3.750834000
H	2.670985000	2.049009000	3.149102000
H	1.412376000	2.943159000	4.021471000
H	2.612784000	3.336661000	1.082314000
H	1.087756000	3.774147000	0.296767000
H	1.518682000	4.498867000	1.861604000

C	1.593340000	-0.532019000	-1.466979000
C	2.170823000	-1.732783000	-1.036411000
C	2.378603000	0.396500000	-2.165770000
C	3.511701000	-2.003014000	-1.308807000
H	1.576341000	-2.450536000	-0.482488000
C	3.717935000	0.123092000	-2.435033000
H	1.941120000	1.330348000	-2.504378000
C	4.287083000	-1.078161000	-2.008153000
H	3.948453000	-2.939074000	-0.972997000
H	4.317128000	0.849312000	-2.977017000
H	5.331247000	-1.290983000	-2.219114000
C	-0.760023000	0.773806000	-2.535090000
C	-0.497474000	0.305498000	-3.834894000
C	-1.625852000	1.866567000	-2.358775000
C	-1.072955000	0.934101000	-4.934701000
H	0.163902000	-0.542520000	-3.977197000
C	-2.196642000	2.491543000	-3.467018000
H	-1.849155000	2.224135000	-1.358654000
C	-1.922651000	2.029806000	-4.755020000
H	-0.857127000	0.572000000	-5.936223000
H	-2.856359000	3.342630000	-3.322538000
H	-2.369677000	2.518524000	-5.615958000
C	-1.652877000	-1.695261000	4.691614000
C	-0.397959000	-1.647613000	5.307990000
C	0.745211000	-1.631713000	4.500530000
C	0.649332000	-1.635216000	3.115336000
C	-0.622457000	-1.692807000	2.474632000
C	-1.776061000	-1.735941000	3.309337000
H	-2.554100000	-1.717591000	5.299935000
H	-0.312062000	-1.629143000	6.389968000
H	1.731228000	-1.597232000	4.958631000
H	1.542908000	-1.577440000	2.501856000
H	-2.755618000	-1.790923000	2.845452000
C	-0.735138000	-1.657800000	1.091093000
C	-0.862958000	-1.709561000	-0.189997000
C	-1.287953000	-2.800943000	-1.099922000
O	-1.757939000	-3.867664000	-0.774864000
O	-1.072063000	-2.448743000	-2.401482000
C	-1.456888000	-3.422945000	-3.375540000
H	-0.862889000	-4.334074000	-3.261812000
H	-2.514985000	-3.674581000	-3.266766000
H	-1.270377000	-2.960253000	-4.345364000
TS_{1/S1}			
P		-0.082992000000	-0.439359000000
			0.273776000000

B	-0.905669000000	1.295172000000	0.207466000000
O	-0.190744000000	2.412251000000	0.486554000000
O	-2.175130000000	1.503393000000	-0.234830000000
C	-1.115059000000	3.547252000000	0.347226000000
C	-2.282468000000	2.943154000000	-0.521170000000
C	-1.534765000000	3.915312000000	1.771154000000
C	-0.369320000000	4.695104000000	-0.318369000000
C	-2.074489000000	3.092992000000	-2.028219000000
C	-3.679123000000	3.398440000000	-0.119602000000
H	-2.066242000000	3.091365000000	2.257319000000
H	-0.637596000000	4.132729000000	2.357598000000
H	-2.178421000000	4.800457000000	1.780619000000
H	0.116075000000	4.363317000000	-1.237040000000
H	-1.059117000000	5.516487000000	-0.542268000000
H	0.397715000000	5.077852000000	0.362705000000
H	-1.079199000000	2.760979000000	-2.336005000000
H	-2.824950000000	2.487003000000	-2.545415000000
H	-2.205894000000	4.135044000000	-2.337198000000
H	-3.904544000000	3.155463000000	0.920829000000
H	-3.781346000000	4.480346000000	-0.257396000000
H	-4.420444000000	2.905395000000	-0.755512000000
C	1.061816000000	-0.441175000000	1.693938000000
C	0.687417000000	-0.964944000000	2.940863000000
C	2.339755000000	0.115693000000	1.532147000000
C	1.583126000000	-0.940884000000	4.008168000000
H	-0.299803000000	-1.394662000000	3.074360000000
C	3.225003000000	0.144418000000	2.609368000000
H	2.642673000000	0.529614000000	0.576506000000
C	2.853622000000	-0.385441000000	3.845582000000
H	1.285337000000	-1.352388000000	4.968602000000
H	4.211994000000	0.578201000000	2.475771000000
H	3.550334000000	-0.366997000000	4.678974000000
C	-1.316114000000	-1.738949000000	0.549760000000
C	-2.669966000000	-1.546007000000	0.227392000000
C	-0.872952000000	-3.024574000000	0.910032000000
C	-3.558846000000	-2.618908000000	0.280352000000
H	-3.021348000000	-0.563825000000	-0.067231000000
C	-1.768223000000	-4.087962000000	0.961283000000
H	0.175536000000	-3.195474000000	1.128093000000
C	-3.114496000000	-3.889759000000	0.646988000000
H	-4.604748000000	-2.458187000000	0.033780000000
H	-1.410079000000	-5.076051000000	1.235079000000
H	-3.811150000000	-4.722475000000	0.682475000000
C	-0.205338000000	-4.120472000000	-2.521478000000

C	0.774718000000	-4.955296000000	-1.981143000000
C	1.873377000000	-4.399586000000	-1.322936000000
C	1.989250000000	-3.015402000000	-1.199680000000
C	1.008611000000	-2.170823000000	-1.740741000000
C	-0.091883000000	-2.737564000000	-2.398910000000
H	-1.064452000000	-4.547513000000	-3.030961000000
H	0.682359000000	-6.033980000000	-2.072285000000
H	2.641228000000	-5.044347000000	-0.904026000000
H	2.835335000000	-2.573868000000	-0.682147000000
H	-0.860427000000	-2.084216000000	-2.799993000000
C	1.097864000000	-0.719974000000	-1.534102000000
C	1.683906000000	0.290476000000	-2.042480000000
C	1.849465000000	1.687735000000	-1.917962000000
O	1.165523000000	2.564990000000	-2.444384000000
O	2.958526000000	1.985876000000	-1.158402000000
C	3.178429000000	3.377311000000	-0.920736000000
H	3.142996000000	3.944649000000	-1.853916000000
H	2.423267000000	3.769841000000	-0.233469000000
H	4.169164000000	3.446203000000	-0.467539000000
TS_{1/82S}			
P	1.720691000000	-0.179884000000	2.075687000000
C	1.742451000000	-0.962397000000	3.745620000000
C	1.744790000000	-2.496570000000	3.689118000000
H	0.836955000000	-0.618518000000	4.259392000000
H	2.601617000000	-0.585976000000	4.317636000000
C	1.605433000000	-3.124018000000	5.079844000000
H	0.925480000000	-2.837923000000	3.046329000000
H	2.672327000000	-2.852190000000	3.221210000000
C	1.562356000000	-4.652823000000	5.035793000000
H	2.437909000000	-2.792219000000	5.715664000000
H	0.690609000000	-2.741091000000	5.553934000000
H	2.476957000000	-5.060205000000	4.588747000000
H	1.462532000000	-5.079376000000	6.039773000000
H	0.715601000000	-5.005122000000	4.434739000000
C	3.356294000000	-0.562987000000	1.313570000000
C	3.595713000000	0.187952000000	-0.006002000000
H	3.370752000000	-1.645770000000	1.138832000000
H	4.153336000000	-0.348065000000	2.039060000000
C	4.817603000000	-0.344724000000	-0.761390000000
H	2.713558000000	0.109965000000	-0.648901000000
H	3.723310000000	1.259420000000	0.189364000000
C	5.002668000000	0.336667000000	-2.118242000000
H	5.717375000000	-0.214704000000	-0.143125000000
H	4.701311000000	-1.428126000000	-0.909074000000

H	5.108924000000	1.421170000000	-2.005431000000
H	5.891628000000	-0.042899000000	-2.634369000000
H	4.130893000000	0.159898000000	-2.756788000000
C	1.762186000000	1.640088000000	2.390507000000
C	0.515076000000	2.208467000000	3.094156000000
H	1.905191000000	2.130516000000	1.421494000000
H	2.666683000000	1.830387000000	2.984495000000
C	-0.648371000000	2.515699000000	2.145676000000
H	0.173384000000	1.525129000000	3.882905000000
H	0.807017000000	3.132291000000	3.610795000000
C	-1.904116000000	2.957156000000	2.897260000000
H	-0.338873000000	3.306234000000	1.450724000000
H	-0.872233000000	1.643001000000	1.526439000000
H	-2.721527000000	3.177890000000	2.202573000000
H	-2.248505000000	2.172983000000	3.581166000000
H	-1.718086000000	3.859567000000	3.493143000000
P	0.699129000000	0.301248000000	-2.836321000000
B	-0.862040000000	0.041675000000	-1.610972000000
O	-1.767214000000	1.124774000000	-1.543973000000
O	-1.578078000000	-1.169928000000	-1.787629000000
C	-3.109470000000	0.621584000000	-1.455000000000
C	-2.975975000000	-0.874209000000	-1.961166000000
C	-3.565217000000	0.745849000000	0.004833000000
C	-3.998460000000	1.507707000000	-2.328696000000
C	-3.300817000000	-1.041374000000	-3.449769000000
C	-3.773598000000	-1.891044000000	-1.143871000000
H	-2.942983000000	0.147120000000	0.669873000000
H	-3.470870000000	1.794099000000	0.306866000000
H	-4.610300000000	0.441885000000	0.134407000000
H	-3.995884000000	2.526341000000	-1.926390000000
H	-3.631019000000	1.550744000000	-3.355115000000
H	-5.033640000000	1.147006000000	-2.335681000000
H	-3.026730000000	-2.056231000000	-3.755292000000
H	-4.368329000000	-0.897107000000	-3.649050000000
H	-2.730349000000	-0.343245000000	-4.064072000000
H	-3.462413000000	-1.892857000000	-0.096479000000
H	-4.849155000000	-1.685380000000	-1.193240000000
H	-3.601784000000	-2.894315000000	-1.547442000000
C	1.363288000000	1.966605000000	-2.373192000000
C	0.948565000000	2.689595000000	-1.242661000000
C	2.406233000000	2.501366000000	-3.149213000000
C	1.579281000000	3.884673000000	-0.887095000000
H	0.115722000000	2.327760000000	-0.655148000000
C	3.024877000000	3.701799000000	-2.805329000000

H	2.739577000000	1.961635000000	-4.031978000000
C	2.621874000000	4.394761000000	-1.661342000000
H	1.239007000000	4.430148000000	-0.009308000000
H	3.827319000000	4.093161000000	-3.425741000000
H	3.107886000000	5.326588000000	-1.384462000000
C	-0.216605000000	0.714919000000	-4.385783000000
C	-0.249477000000	-0.226092000000	-5.424058000000
C	-0.947419000000	1.904755000000	-4.536021000000
C	-1.000823000000	0.004336000000	-6.578306000000
H	0.314428000000	-1.149598000000	-5.319781000000
C	-1.689862000000	2.141261000000	-5.691707000000
H	-0.945639000000	2.631481000000	-3.731048000000
C	-1.723034000000	1.189726000000	-6.715276000000
H	-1.019122000000	-0.740041000000	-7.370354000000
H	-2.251679000000	3.066788000000	-5.792275000000
H	-2.306207000000	1.374065000000	-7.613696000000
C	-3.324616000000	-1.840605000000	6.059591000000
C	-4.441379000000	-1.001782000000	6.044967000000
C	-4.677490000000	-0.173312000000	4.945384000000
C	-3.801760000000	-0.174579000000	3.863876000000
C	-2.671112000000	-1.012969000000	3.875453000000
C	-2.443208000000	-1.850805000000	4.983046000000
H	-3.141701000000	-2.489518000000	6.911084000000
H	-5.127635000000	-0.996212000000	6.886699000000
H	-5.548305000000	0.475386000000	4.929643000000
H	-3.979851000000	0.462063000000	3.004113000000
H	-1.578215000000	-2.506463000000	4.981424000000
C	-1.762158000000	-1.014458000000	2.780238000000
C	-0.996273000000	-1.013242000000	1.839755000000
C	-0.012403000000	-0.981138000000	0.770363000000
O	-0.050062000000	-0.069711000000	-0.137548000000
O	0.373436000000	-2.260713000000	0.506072000000
C	1.029174000000	-2.528637000000	-0.746637000000
H	1.815021000000	-1.800956000000	-0.950570000000
H	1.452088000000	-3.528082000000	-0.633855000000
H	0.294294000000	-2.501278000000	-1.551469000000
TS_{1/84S}			
P	-0.936592000000	-0.589876000000	-0.106186000000
B	-0.569434000000	1.197345000000	0.846439000000
O	0.619257000000	1.833588000000	0.374599000000
O	-1.625121000000	2.142439000000	0.886276000000
C	0.229446000000	3.112894000000	-0.157890000000
C	-1.037142000000	3.447090000000	0.703594000000
C	1.396754000000	4.079861000000	0.013362000000

C	-0.100967000000	2.945147000000	-1.646931000000
C	-2.061730000000	4.348213000000	0.023318000000
C	-0.677585000000	3.999143000000	2.088608000000
H	1.744310000000	4.101420000000	1.048456000000
H	2.232674000000	3.764244000000	-0.620861000000
H	1.113224000000	5.095624000000	-0.285576000000
H	-0.329703000000	3.906075000000	-2.119952000000
H	0.758828000000	2.503191000000	-2.158074000000
H	-0.953758000000	2.275255000000	-1.788270000000
H	-1.627267000000	5.326098000000	-0.214298000000
H	-2.436027000000	3.897924000000	-0.898817000000
H	-2.912958000000	4.509308000000	0.692920000000
H	0.072298000000	3.368308000000	2.574374000000
H	-0.295252000000	5.024269000000	2.033262000000
H	-1.577052000000	3.998841000000	2.711946000000
C	-2.688772000000	-1.080261000000	-0.186731000000
C	-3.054083000000	-2.421077000000	-0.403106000000
C	-3.692730000000	-0.127442000000	0.059101000000
C	-4.395555000000	-2.797080000000	-0.399625000000
H	-2.282849000000	-3.168850000000	-0.566875000000
C	-5.033317000000	-0.514614000000	0.074402000000
H	-3.411054000000	0.903723000000	0.246894000000
C	-5.388442000000	-1.843826000000	-0.159425000000
H	-4.666360000000	-3.834914000000	-0.573424000000
H	-5.803524000000	0.227863000000	0.265191000000
H	-6.434016000000	-2.138992000000	-0.149440000000
C	-0.200491000000	-0.854603000000	-1.741441000000
C	-0.842183000000	-1.521124000000	-2.799189000000
C	1.119824000000	-0.399288000000	-1.925839000000
C	-0.175329000000	-1.732609000000	-4.004092000000
H	-1.864632000000	-1.864722000000	-2.682716000000
C	1.782882000000	-0.622635000000	-3.129531000000
H	1.606364000000	0.151388000000	-1.133328000000
C	1.139891000000	-1.292278000000	-4.172150000000
H	-0.685858000000	-2.242905000000	-4.816533000000
H	2.803963000000	-0.269894000000	-3.247576000000
H	1.656741000000	-1.466563000000	-5.111775000000
C	5.931663000000	-1.461919000000	-0.400194000000
C	6.196280000000	-0.195164000000	-0.926623000000
C	5.271826000000	0.839862000000	-0.757761000000
C	4.086619000000	0.614664000000	-0.066228000000
C	3.813015000000	-0.665514000000	0.460198000000
C	4.746976000000	-1.702557000000	0.289136000000
H	6.650063000000	-2.265872000000	-0.531384000000

H	7.121173000000	-0.014713000000	-1.466813000000
H	5.477663000000	1.825610000000	-1.165116000000
H	3.351173000000	1.400910000000	0.074206000000
H	4.529701000000	-2.685894000000	0.693247000000
C	2.572186000000	-0.864337000000	1.117849000000
C	1.472605000000	-0.914454000000	1.632926000000
C	0.127949000000	-0.744218000000	2.066015000000
O	-0.376190000000	0.469942000000	2.189049000000
O	-0.332173000000	-1.702698000000	2.877299000000
C	-1.671782000000	-1.525891000000	3.372580000000
H	-1.744228000000	-0.615132000000	3.969557000000
H	-2.376132000000	-1.477106000000	2.538101000000
H	-1.865252000000	-2.407655000000	3.983134000000
TS_{7Z/S5S}			
P	-1.340685000000	-0.866047000000	-0.932107000000
C	-2.738560000000	-0.344125000000	-2.023560000000
C	-4.110248000000	-0.846074000000	-1.549957000000
H	-2.534062000000	-0.695196000000	-3.044006000000
H	-2.708539000000	0.750306000000	-2.051218000000
C	-5.264389000000	-0.240784000000	-2.355220000000
H	-4.152020000000	-1.939831000000	-1.629323000000
H	-4.242547000000	-0.614868000000	-0.487731000000
C	-6.632080000000	-0.738555000000	-1.883122000000
H	-5.222951000000	0.854607000000	-2.278094000000
H	-5.129376000000	-0.476170000000	-3.420024000000
H	-6.798329000000	-0.487232000000	-0.828530000000
H	-7.444989000000	-0.292105000000	-2.465879000000
H	-6.709996000000	-1.828237000000	-1.979438000000
C	0.141923000000	-0.474368000000	-1.963826000000
C	1.506987000000	-0.666307000000	-1.290342000000
H	0.036089000000	0.581639000000	-2.229410000000
H	0.069009000000	-1.064674000000	-2.887854000000
C	2.664755000000	-0.247018000000	-2.198513000000
H	1.541565000000	-0.056579000000	-0.386876000000
H	1.647593000000	-1.707429000000	-0.982883000000
C	4.023577000000	-0.495254000000	-1.538984000000
H	2.608980000000	-0.793213000000	-3.151428000000
H	2.549878000000	0.817802000000	-2.426931000000
H	4.175391000000	-1.563098000000	-1.334994000000
H	4.848231000000	-0.157100000000	-2.176254000000
H	4.096373000000	0.036127000000	-0.583323000000
C	-1.536930000000	-2.717856000000	-0.936924000000
C	-0.263781000000	-3.549301000000	-0.748904000000
H	-1.995383000000	-2.956855000000	-1.904724000000

H	-2.268864000000	-2.968248000000	-0.163775000000
C	-0.531782000000	-5.061272000000	-0.799641000000
H	0.458680000000	-3.301607000000	-1.534902000000
H	0.204236000000	-3.293821000000	0.207478000000
C	-0.995271000000	-5.565058000000	-2.169949000000
H	0.392771000000	-5.582707000000	-0.519488000000
H	-1.277217000000	-5.320692000000	-0.039887000000
H	-0.274691000000	-5.298692000000	-2.953353000000
H	-1.101595000000	-6.655329000000	-2.172047000000
H	-1.966016000000	-5.143169000000	-2.453779000000
P	-0.782218000000	-0.578883000000	3.109400000000
B	0.247385000000	2.406537000000	0.242999000000
O	1.185422000000	2.409875000000	-0.848627000000
O	-0.036379000000	3.769014000000	0.587558000000
C	1.139145000000	3.714001000000	-1.447615000000
C	0.759754000000	4.632572000000	-0.228728000000
C	2.499807000000	4.009198000000	-2.072889000000
C	0.058380000000	3.700937000000	-2.540113000000
C	-0.073521000000	5.860259000000	-0.597271000000
C	1.980804000000	5.071290000000	0.592319000000
H	2.684347000000	3.321632000000	-2.905843000000
H	2.539569000000	5.032226000000	-2.464602000000
H	3.304463000000	3.883269000000	-1.345108000000
H	-0.925824000000	3.492882000000	-2.112437000000
H	0.013330000000	4.650453000000	-3.084433000000
H	0.293743000000	2.907608000000	-3.258283000000
H	0.469385000000	6.516868000000	-1.287806000000
H	-1.021441000000	5.572493000000	-1.057642000000
H	-0.299297000000	6.433032000000	0.308214000000
H	2.607315000000	4.216579000000	0.857741000000
H	2.592878000000	5.807942000000	0.059457000000
H	1.626729000000	5.524215000000	1.523609000000
C	-1.794998000000	-2.030961000000	2.535867000000
C	-3.176715000000	-1.868719000000	2.325266000000
C	-1.280288000000	-3.337075000000	2.537562000000
C	-3.998525000000	-2.963414000000	2.065177000000
H	-3.605467000000	-0.876401000000	2.361997000000
C	-2.111780000000	-4.437093000000	2.316125000000
H	-0.226573000000	-3.502239000000	2.728586000000
C	-3.470632000000	-4.256918000000	2.062214000000
H	-5.059444000000	-2.806994000000	1.888293000000
H	-1.689779000000	-5.438018000000	2.341400000000
H	-4.114444000000	-5.113154000000	1.881553000000
C	0.853532000000	-1.389017000000	3.368206000000

C	1.772416000000	-1.627842000000	2.338395000000
C	1.185041000000	-1.776908000000	4.672421000000
C	3.001265000000	-2.225483000000	2.607513000000
H	1.535638000000	-1.316619000000	1.329506000000
C	2.409845000000	-2.387803000000	4.942997000000
H	0.484174000000	-1.585662000000	5.481096000000
C	3.323377000000	-2.607084000000	3.911663000000
H	3.710691000000	-2.383206000000	1.799632000000
H	2.655811000000	-2.679109000000	5.960483000000
H	4.284434000000	-3.067450000000	4.123417000000
C	2.938231000000	1.669130000000	4.438727000000
C	4.164065000000	1.768392000000	3.777867000000
C	4.193952000000	1.793393000000	2.382567000000
C	3.008984000000	1.708608000000	1.655001000000
C	1.772427000000	1.559867000000	2.308913000000
C	1.755231000000	1.564702000000	3.711982000000
H	2.903907000000	1.664740000000	5.524745000000
H	5.087260000000	1.835975000000	4.346885000000
H	5.141775000000	1.887242000000	1.858835000000
H	3.018078000000	1.752590000000	0.571619000000
H	0.806015000000	1.491074000000	4.233789000000
C	0.563019000000	1.406435000000	1.489466000000
C	-0.448975000000	0.517161000000	1.664171000000
C	-1.468829000000	0.779062000000	0.597965000000
O	-1.155062000000	1.757978000000	-0.204907000000
O	-2.780763000000	0.732838000000	1.009357000000
C	-3.587820000000	1.869741000000	0.664405000000
H	-3.834387000000	1.880148000000	-0.400551000000
H	-4.499651000000	1.753332000000	1.252672000000
H	-3.074203000000	2.797675000000	0.923210000000
TS_{10z/sss}			
P	0.694594000000	-1.550582000000	0.483571000000
C	-0.750719000000	-2.322784000000	1.309584000000
C	-1.896472000000	-2.739777000000	0.388489000000
H	-1.103752000000	-1.593912000000	2.040423000000
H	-0.360435000000	-3.186861000000	1.864448000000
C	-3.087452000000	-3.273944000000	1.191035000000
H	-2.217222000000	-1.878932000000	-0.201452000000
H	-1.559602000000	-3.498469000000	-0.330734000000
C	-4.263907000000	-3.672910000000	0.299569000000
H	-2.766351000000	-4.133328000000	1.797215000000
H	-3.407904000000	-2.495981000000	1.896408000000
H	-5.098573000000	-4.060270000000	0.894645000000
H	-4.624160000000	-2.815559000000	-0.277146000000

H	-3.973277000000	-4.448098000000	-0.419550000000
C	1.423791000000	-2.874959000000	-0.578220000000
C	1.578843000000	-4.257291000000	0.066903000000
H	2.393644000000	-2.487307000000	-0.910797000000
H	0.798354000000	-2.938161000000	-1.475191000000
C	2.257425000000	-5.279916000000	-0.858356000000
H	2.157212000000	-4.179656000000	0.997930000000
H	0.589750000000	-4.637887000000	0.346732000000
C	3.709394000000	-4.940955000000	-1.206807000000
H	2.224267000000	-6.262282000000	-0.370020000000
H	1.668291000000	-5.375466000000	-1.780811000000
H	3.786163000000	-4.013213000000	-1.784409000000
H	4.313686000000	-4.819312000000	-0.299258000000
H	4.164609000000	-5.736561000000	-1.806097000000
C	1.958154000000	-1.226225000000	1.781364000000
C	1.387151000000	-0.831844000000	3.148177000000
H	2.582049000000	-0.417108000000	1.392012000000
H	2.584451000000	-2.123717000000	1.861647000000
C	2.483151000000	-0.361471000000	4.106512000000
H	0.660523000000	-0.029778000000	2.995950000000
H	0.851072000000	-1.681616000000	3.591361000000
C	1.916639000000	0.077864000000	5.458119000000
H	3.221301000000	-1.162837000000	4.256219000000
H	3.013140000000	0.474257000000	3.635824000000
H	1.391788000000	-0.746430000000	5.956251000000
H	2.707916000000	0.425583000000	6.132000000000
H	1.199231000000	0.896862000000	5.331030000000
P	-2.172242000000	1.093723000000	-1.637223000000
B	1.191183000000	1.853383000000	0.555742000000
O	1.867538000000	1.916317000000	1.763973000000
O	0.802678000000	3.105038000000	0.114975000000
C	2.095371000000	3.309487000000	2.086519000000
C	1.087004000000	4.082275000000	1.137145000000
C	1.842538000000	3.516346000000	3.576504000000
C	3.569354000000	3.581472000000	1.766704000000
C	1.684409000000	5.311058000000	0.451947000000
C	-0.240349000000	4.468632000000	1.792620000000
H	2.548072000000	2.915661000000	4.158582000000
H	1.983967000000	4.567410000000	3.851509000000
H	0.830154000000	3.219695000000	3.857245000000
H	4.189362000000	2.904365000000	2.362466000000
H	3.783737000000	3.392057000000	0.710863000000
H	3.856900000000	4.610980000000	2.003105000000
H	2.559284000000	5.055236000000	-0.149186000000

H	0.935334000000	5.753072000000	-0.212120000000
H	1.972388000000	6.068160000000	1.189751000000
H	-0.741187000000	3.608216000000	2.234243000000
H	-0.101618000000	5.234740000000	2.562681000000
H	-0.904008000000	4.871870000000	1.021865000000
C	-1.139790000000	1.643151000000	-3.069631000000
C	-1.284237000000	1.150989000000	-4.374712000000
C	-0.238242000000	2.699026000000	-2.850876000000
C	-0.525293000000	1.674540000000	-5.423272000000
H	-1.984537000000	0.348307000000	-4.577602000000
C	0.523699000000	3.214371000000	-3.898289000000
H	-0.111902000000	3.102513000000	-1.852449000000
C	0.387421000000	2.703423000000	-5.191068000000
H	-0.650164000000	1.273331000000	-6.426162000000
H	1.225027000000	4.021473000000	-3.700671000000
H	0.978703000000	3.107862000000	-6.008285000000
C	-2.960935000000	-0.447378000000	-2.304668000000
C	-2.262410000000	-1.552440000000	-2.821069000000
C	-4.362692000000	-0.494496000000	-2.286655000000
C	-2.948571000000	-2.666421000000	-3.301105000000
H	-1.179235000000	-1.522732000000	-2.843993000000
C	-5.052233000000	-1.609380000000	-2.770250000000
H	-4.914381000000	0.355078000000	-1.892222000000
C	-4.345384000000	-2.698438000000	-3.278615000000
H	-2.393307000000	-3.513046000000	-3.697701000000
H	-6.138669000000	-1.625022000000	-2.750389000000
H	-4.877883000000	-3.568295000000	-3.653366000000
C	-2.930059000000	1.758347000000	3.948501000000
C	-4.225612000000	1.368113000000	3.597588000000
C	-4.443130000000	0.760379000000	2.358855000000
C	-3.389334000000	0.574397000000	1.467341000000
C	-2.073728000000	0.988154000000	1.786421000000
C	-1.873481000000	1.546434000000	3.069134000000
H	-2.741221000000	2.204911000000	4.921657000000
H	-5.050093000000	1.514751000000	4.289768000000
H	-5.442015000000	0.430112000000	2.083996000000
H	-3.574895000000	0.081060000000	0.519708000000
H	-0.858326000000	1.791452000000	3.365719000000
C	-0.933253000000	0.698030000000	0.939877000000
C	-0.914980000000	0.534510000000	-0.398681000000
C	0.466517000000	-0.020005000000	-0.757710000000
O	1.483431000000	0.849367000000	-0.400040000000
O	0.610976000000	-0.484596000000	-2.054664000000
C	1.788625000000	-0.141547000000	-2.786019000000

H	2.686761000000	-0.579034000000	-2.334174000000
H	1.631903000000	-0.558606000000	-3.781731000000
H	1.899244000000	0.940839000000	-2.855159000000
TS_{SU/SZ}			
P	6.143175000000	-0.522682000000	-0.248194000000
B	8.401524000000	-4.433432000000	-0.748013000000
O	9.751519000000	-4.750179000000	-0.691597000000
O	7.875614000000	-4.515037000000	-2.027978000000
C	10.149276000000	-5.154247000000	-2.024882000000
C	8.996522000000	-4.577404000000	-2.940617000000
C	11.531631000000	-4.575244000000	-2.309715000000
C	10.206097000000	-6.685685000000	-2.018963000000
C	8.602528000000	-5.474899000000	-4.110619000000
C	9.268054000000	-3.158435000000	-3.448401000000
H	11.542196000000	-3.491242000000	-2.178396000000
H	12.260135000000	-5.010122000000	-1.617933000000
H	11.850407000000	-4.809603000000	-3.331799000000
H	9.222452000000	-7.113589000000	-1.803097000000
H	10.560593000000	-7.086114000000	-2.974592000000
H	10.894471000000	-7.007893000000	-1.231839000000
H	9.445341000000	-5.611232000000	-4.797542000000
H	8.264497000000	-6.455680000000	-3.770263000000
H	7.783653000000	-5.007908000000	-4.666848000000
H	10.047213000000	-3.151165000000	-4.217775000000
H	8.347106000000	-2.760910000000	-3.886207000000
H	9.569796000000	-2.491044000000	-2.640937000000
C	6.364844000000	0.523879000000	1.253279000000
C	6.912445000000	0.029587000000	2.447925000000
C	5.983041000000	1.869778000000	1.185205000000
C	7.069672000000	0.868707000000	3.548940000000
H	7.207608000000	-1.012539000000	2.512906000000
C	6.140951000000	2.710116000000	2.288881000000
H	5.562519000000	2.258645000000	0.261687000000
C	6.685551000000	2.210157000000	3.471225000000
H	7.495527000000	0.477680000000	4.469113000000
H	5.841078000000	3.752341000000	2.223511000000
H	6.812725000000	2.862854000000	4.330541000000
C	5.003001000000	-1.848502000000	0.312683000000
C	4.214099000000	-1.742130000000	1.465142000000
C	4.870438000000	-2.989919000000	-0.496907000000
C	3.328444000000	-2.762968000000	1.813359000000
H	4.302831000000	-0.868242000000	2.101896000000
C	4.000290000000	-4.017037000000	-0.136419000000
H	5.476609000000	-3.097347000000	-1.392343000000

C	3.224631000000	-3.906610000000	1.020292000000
H	2.724396000000	-2.666301000000	2.711729000000
H	3.931847000000	-4.903641000000	-0.760099000000
H	2.539674000000	-4.703606000000	1.296942000000
C	9.844911000000	1.112006000000	-2.228128000000
C	11.140466000000	0.682067000000	-1.944307000000
C	11.333805000000	-0.424268000000	-1.110474000000
C	10.241449000000	-1.089067000000	-0.566532000000
C	8.925738000000	-0.668517000000	-0.848290000000
C	8.747237000000	0.444633000000	-1.685635000000
H	9.684742000000	1.965988000000	-2.880285000000
H	11.994523000000	1.203151000000	-2.367880000000
H	12.339862000000	-0.765278000000	-0.882006000000
H	10.380824000000	-1.957708000000	0.068433000000
H	7.743318000000	0.773623000000	-1.932836000000
C	7.793324000000	-1.412385000000	-0.252449000000
C	7.975735000000	-2.675917000000	0.160150000000
C	7.356584000000	-3.646908000000	0.910358000000
O	7.468547000000	-4.842094000000	0.349322000000
O	6.916692000000	-3.545450000000	2.151661000000
C	6.524757000000	-4.761322000000	2.822754000000
H	5.609238000000	-5.145692000000	2.369508000000
H	7.320894000000	-5.505919000000	2.757609000000
H	6.345696000000	-4.471126000000	3.857576000000
TS_{S1/S8S}			
P	3.981649000000	0.287565000000	0.350194000000
C	4.450291000000	2.068277000000	0.593091000000
C	5.652434000000	2.300822000000	1.513093000000
H	3.569262000000	2.616451000000	0.957107000000
H	4.675249000000	2.456623000000	-0.404204000000
C	6.207039000000	3.725390000000	1.409784000000
H	5.374446000000	2.093860000000	2.555564000000
H	6.451863000000	1.596775000000	1.264238000000
C	7.444815000000	3.933702000000	2.285740000000
H	6.465314000000	3.928085000000	0.360679000000
H	5.426160000000	4.450725000000	1.679559000000
H	7.211502000000	3.761803000000	3.343970000000
H	8.241388000000	3.235860000000	2.003550000000
H	7.835217000000	4.953393000000	2.191851000000
C	2.391274000000	0.435591000000	-0.605775000000
C	2.513445000000	1.335601000000	-1.842964000000
H	1.596422000000	0.807704000000	0.056493000000
H	2.128273000000	-0.589506000000	-0.886200000000
C	1.300565000000	1.267112000000	-2.781876000000

H	2.650774000000	2.372412000000	-1.518480000000
H	3.415202000000	1.079231000000	-2.408671000000
C	1.168395000000	-0.062478000000	-3.529724000000
H	0.382507000000	1.466602000000	-2.210918000000
H	1.391606000000	2.078070000000	-3.515778000000
H	0.288603000000	-0.063921000000	-4.182899000000
H	2.050148000000	-0.246345000000	-4.153451000000
H	1.066957000000	-0.909371000000	-2.840942000000
C	3.375049000000	-0.241380000000	2.028697000000
C	4.464526000000	-0.885499000000	2.896369000000
H	2.569511000000	-0.964363000000	1.855403000000
H	2.926777000000	0.625952000000	2.529953000000
C	3.941826000000	-1.431761000000	4.232066000000
H	4.930936000000	-1.697966000000	2.328491000000
H	5.262390000000	-0.157819000000	3.090551000000
C	3.398397000000	-0.354856000000	5.175865000000
H	3.157848000000	-2.177273000000	4.034988000000
H	4.757720000000	-1.970169000000	4.731890000000
H	3.098714000000	-0.785076000000	6.137801000000
H	4.159013000000	0.410610000000	5.374269000000
H	2.522379000000	0.150009000000	4.753991000000
P	6.963352000000	-0.610434000000	-2.943546000000
B	6.936740000000	-3.829674000000	-0.499719000000
O	7.648955000000	-4.621697000000	-1.355525000000
O	7.628551000000	-3.407972000000	0.601163000000
C	9.040314000000	-4.515417000000	-0.934585000000
C	8.907689000000	-4.105121000000	0.579510000000
C	9.723267000000	-5.854265000000	-1.181118000000
C	9.675698000000	-3.420097000000	-1.794716000000
C	9.995113000000	-3.164357000000	1.081219000000
C	8.759291000000	-5.304470000000	1.519490000000
H	9.192387000000	-6.673888000000	-0.692319000000
H	9.749474000000	-6.059179000000	-2.255746000000
H	10.754966000000	-5.833659000000	-0.813175000000
H	9.190256000000	-2.454581000000	-1.631395000000
H	10.744087000000	-3.314434000000	-1.582282000000
H	9.558171000000	-3.685810000000	-2.849247000000
H	10.974009000000	-3.654404000000	1.025857000000
H	10.027348000000	-2.237198000000	0.509095000000
H	9.802239000000	-2.902656000000	2.125460000000
H	9.696846000000	-5.861444000000	1.613242000000
H	8.472105000000	-4.941910000000	2.511024000000
H	7.981024000000	-5.989350000000	1.168110000000
C	6.005752000000	0.921288000000	-3.335748000000

C	6.158875000000	2.060531000000	-2.528820000000
C	5.219732000000	1.028924000000	-4.494623000000
C	5.526975000000	3.259929000000	-2.856969000000
H	6.772019000000	2.003243000000	-1.634220000000
C	4.576710000000	2.224989000000	-4.815021000000
H	5.094449000000	0.164793000000	-5.140037000000
C	4.724133000000	3.345848000000	-3.995891000000
H	5.655740000000	4.127804000000	-2.214774000000
H	3.958220000000	2.279885000000	-5.707188000000
H	4.224105000000	4.277360000000	-4.245704000000
C	5.817641000000	-1.942619000000	-3.489669000000
C	4.423236000000	-1.888790000000	-3.337808000000
C	6.390241000000	-3.111464000000	-4.007469000000
C	3.627412000000	-2.979153000000	-3.679063000000
H	3.962438000000	-0.996239000000	-2.934642000000
C	5.596646000000	-4.208186000000	-4.344860000000
H	7.467553000000	-3.166528000000	-4.130016000000
C	4.214153000000	-4.144802000000	-4.178094000000
H	2.550320000000	-2.920840000000	-3.548537000000
H	6.060077000000	-5.111888000000	-4.730405000000
H	3.593866000000	-4.998575000000	-4.438056000000
C	10.026667000000	1.017363000000	-0.008632000000
C	9.976127000000	0.857646000000	1.378042000000
C	8.900344000000	0.160319000000	1.935672000000
C	7.898064000000	-0.361538000000	1.126377000000
C	7.921916000000	-0.200552000000	-0.278302000000
C	9.018941000000	0.502693000000	-0.821883000000
H	10.855145000000	1.553986000000	-0.464138000000
H	10.760216000000	1.264161000000	2.010384000000
H	8.845024000000	0.016328000000	3.012182000000
H	7.086017000000	-0.927218000000	1.565228000000
H	9.081596000000	0.643372000000	-1.896899000000
C	6.830533000000	-0.731135000000	-1.102544000000
C	5.690107000000	-1.220124000000	-0.539197000000
C	5.031840000000	-2.374297000000	-0.432068000000
O	5.596362000000	-3.582138000000	-0.717888000000
O	3.710452000000	-2.472635000000	-0.122411000000
C	3.298487000000	-3.660144000000	0.560321000000
H	3.405698000000	-4.535611000000	-0.084058000000
H	3.875072000000	-3.807626000000	1.480771000000
H	2.247077000000	-3.501933000000	0.806748000000
TS_{S7Z/S9R}			
P	-0.075888000000	-0.137225000000	-1.325354000000
C	-1.008906000000	-0.835778000000	-2.782800000000

C	-1.632073000000	-2.225437000000	-2.621867000000
H	-0.331358000000	-0.830255000000	-3.645961000000
H	-1.792970000000	-0.101515000000	-3.003211000000
C	-2.564767000000	-2.577117000000	-3.784945000000
H	-0.839898000000	-2.982485000000	-2.549019000000
H	-2.201867000000	-2.279755000000	-1.691859000000
C	-3.222433000000	-3.947232000000	-3.609373000000
H	-3.342062000000	-1.804891000000	-3.857697000000
H	-2.006686000000	-2.546345000000	-4.731363000000
H	-3.893422000000	-4.181406000000	-4.443377000000
H	-2.470419000000	-4.743684000000	-3.551123000000
H	-3.810293000000	-3.976308000000	-2.684426000000
C	0.582860000000	-1.626248000000	-0.443508000000
C	1.367608000000	-1.334740000000	0.840297000000
H	1.192231000000	-2.204500000000	-1.150047000000
H	-0.291085000000	-2.243876000000	-0.213462000000
C	1.942598000000	-2.608976000000	1.464136000000
H	2.171379000000	-0.619157000000	0.637552000000
H	0.708069000000	-0.843129000000	1.562246000000
C	2.680379000000	-2.325859000000	2.774805000000
H	1.128501000000	-3.325070000000	1.647270000000
H	2.622329000000	-3.095809000000	0.749844000000
H	3.081891000000	-3.243704000000	3.218767000000
H	3.518262000000	-1.637091000000	2.611947000000
H	2.009112000000	-1.860859000000	3.506426000000
C	1.347305000000	0.683235000000	-2.187421000000
C	2.409909000000	-0.267502000000	-2.749341000000
H	1.785340000000	1.387010000000	-1.480066000000
H	0.891610000000	1.267318000000	-2.996808000000
C	3.472737000000	0.477340000000	-3.566672000000
H	2.901741000000	-0.796518000000	-1.923098000000
H	1.948106000000	-1.039447000000	-3.381165000000
C	4.564632000000	-0.453017000000	-4.099733000000
H	2.985869000000	0.996460000000	-4.403722000000
H	3.922596000000	1.259186000000	-2.940361000000
H	5.310067000000	0.097519000000	-4.684063000000
H	5.088481000000	-0.956451000000	-3.278204000000
H	4.139612000000	-1.230146000000	-4.746779000000
P	-1.766623000000	2.438072000000	-1.287237000000
B	-1.907338000000	0.923726000000	2.593122000000
O	-1.352328000000	0.489378000000	3.784822000000
O	-3.281747000000	1.094437000000	2.714902000000
C	-2.336481000000	0.700826000000	4.822426000000
C	-3.684486000000	0.622036000000	4.020933000000

C	-2.160693000000	-0.369156000000	5.893431000000
C	-2.068317000000	2.090934000000	5.410601000000
C	-4.798598000000	1.527724000000	4.534391000000
C	-4.203954000000	-0.808375000000	3.851393000000
H	-1.188831000000	-0.244544000000	6.381146000000
H	-2.940080000000	-0.284885000000	6.659297000000
H	-2.197778000000	-1.373465000000	5.465905000000
H	-2.730868000000	2.310787000000	6.254298000000
H	-1.031943000000	2.129963000000	5.757632000000
H	-2.194619000000	2.868042000000	4.650916000000
H	-4.498236000000	2.577538000000	4.515366000000
H	-5.684169000000	1.415960000000	3.900217000000
H	-5.078063000000	1.260881000000	5.559853000000
H	-3.407256000000	-1.480491000000	3.523299000000
H	-4.626875000000	-1.195635000000	4.784348000000
H	-4.981802000000	-0.813746000000	3.082784000000
C	-3.406050000000	3.209506000000	-0.898764000000
C	-4.091967000000	3.073093000000	0.316807000000
C	-3.980222000000	3.985800000000	-1.917218000000
C	-5.319877000000	3.708388000000	0.504699000000
H	-3.688361000000	2.463828000000	1.115433000000
C	-5.202705000000	4.628459000000	-1.722219000000
H	-3.464110000000	4.085810000000	-2.869300000000
C	-5.877455000000	4.489540000000	-0.508389000000
H	-5.840735000000	3.587451000000	1.451217000000
H	-5.630252000000	5.230813000000	-2.519428000000
H	-6.833640000000	4.983043000000	-0.356195000000
C	-0.669135000000	3.754077000000	-0.612813000000
C	0.442995000000	4.131780000000	-1.375291000000
C	-0.916184000000	4.414540000000	0.598589000000
C	1.310869000000	5.126275000000	-0.927520000000
H	0.633851000000	3.633256000000	-2.320880000000
C	-0.046413000000	5.405372000000	1.050953000000
H	-1.782467000000	4.147309000000	1.192161000000
C	1.070472000000	5.761137000000	0.291806000000
H	2.172790000000	5.404672000000	-1.527907000000
H	-0.241902000000	5.901026000000	1.997975000000
H	1.744820000000	6.536768000000	0.645162000000
C	-4.740479000000	-0.962352000000	-1.170616000000
C	-4.665944000000	-2.086475000000	-0.350151000000
C	-3.620188000000	-2.187316000000	0.570645000000
C	-2.672789000000	-1.173936000000	0.666625000000
C	-2.743339000000	-0.018641000000	-0.135839000000
C	-3.791896000000	0.056243000000	-1.067027000000

H	-5.544770000000	-0.867275000000	-1.894491000000
H	-5.407925000000	-2.875892000000	-0.429377000000
H	-3.537652000000	-3.061251000000	1.210740000000
H	-1.853700000000	-1.271460000000	1.370705000000
H	-3.893944000000	0.919942000000	-1.710202000000
C	-1.657521000000	1.022828000000	-0.006954000000
C	-1.131860000000	1.241593000000	1.311891000000
C	0.206521000000	1.749476000000	1.424176000000
O	1.070957000000	1.687199000000	0.539923000000
O	0.510992000000	2.281027000000	2.643185000000
C	1.862789000000	2.708338000000	2.796690000000
H	1.931525000000	3.098671000000	3.814010000000
H	2.559043000000	1.873826000000	2.666004000000
H	2.106219000000	3.489393000000	2.070784000000
TS_{S7Z/S9S}			
P	7.039187000000	-1.745881000000	1.286943000000
C	6.097646000000	-3.312702000000	1.036637000000
C	6.312229000000	-4.422228000000	2.073842000000
H	6.334665000000	-3.676171000000	0.033801000000
H	5.048912000000	-3.019973000000	1.009897000000
C	5.311592000000	-5.574679000000	1.887457000000
H	7.331381000000	-4.816567000000	1.987736000000
H	6.217189000000	-4.029966000000	3.095309000000
C	3.857990000000	-5.190343000000	2.181820000000
H	5.390719000000	-5.954031000000	0.860001000000
H	5.606359000000	-6.401141000000	2.547248000000
H	3.489783000000	-4.420408000000	1.495670000000
H	3.197421000000	-6.058668000000	2.084466000000
H	3.752175000000	-4.803318000000	3.203052000000
C	6.230435000000	-0.854831000000	2.698547000000
C	4.815824000000	-1.314988000000	3.075863000000
H	6.176764000000	0.199523000000	2.417029000000
H	6.903019000000	-0.940766000000	3.561332000000
C	4.262689000000	-0.503318000000	4.250090000000
H	4.159527000000	-1.195756000000	2.209134000000
H	4.805142000000	-2.378607000000	3.340113000000
C	2.804113000000	-0.846860000000	4.558229000000
H	4.883048000000	-0.677618000000	5.140917000000
H	4.349249000000	0.562477000000	4.013091000000
H	2.163389000000	-0.636482000000	3.693395000000
H	2.688682000000	-1.910193000000	4.802055000000
H	2.424818000000	-0.266020000000	5.406435000000
C	8.661685000000	-2.353249000000	1.990065000000
C	9.696976000000	-1.286703000000	2.358966000000

H	9.075783000000	-3.050595000000	1.257819000000
H	8.394852000000	-2.936026000000	2.881990000000
C	10.832510000000	-1.838958000000	3.235875000000
H	10.106016000000	-0.844450000000	1.444257000000
H	9.212704000000	-0.474721000000	2.917289000000
C	11.670007000000	-2.937940000000	2.578198000000
H	11.488975000000	-1.004124000000	3.514085000000
H	10.403432000000	-2.216541000000	4.175027000000
H	11.063742000000	-3.816371000000	2.329321000000
H	12.124270000000	-2.577690000000	1.650292000000
H	12.472524000000	-3.269833000000	3.246226000000
P	7.410754000000	-1.797479000000	-1.776423000000
B	4.322980000000	0.625849000000	0.055730000000
O	4.596741000000	1.324994000000	1.227304000000
O	3.265132000000	1.195994000000	-0.628222000000
C	3.801059000000	2.537726000000	1.218868000000
C	2.628270000000	2.145167000000	0.253646000000
C	3.375297000000	2.862209000000	2.645878000000
C	4.689200000000	3.655917000000	0.667911000000
C	2.070608000000	3.293070000000	-0.579606000000
C	1.491569000000	1.397035000000	0.960259000000
H	2.828998000000	2.035984000000	3.104410000000
H	4.260166000000	3.069259000000	3.256751000000
H	2.737111000000	3.752956000000	2.663688000000
H	4.982814000000	3.451442000000	-0.363359000000
H	4.183965000000	4.626714000000	0.707754000000
H	5.603637000000	3.711771000000	1.265476000000
H	1.646761000000	4.072690000000	0.063748000000
H	2.842566000000	3.739783000000	-1.209836000000
H	1.274999000000	2.920431000000	-1.232401000000
H	0.905123000000	2.058630000000	1.606387000000
H	0.828843000000	0.970780000000	0.201741000000
H	1.884382000000	0.570880000000	1.560409000000
C	9.212898000000	-1.462528000000	-1.451850000000
C	9.884703000000	-0.225817000000	-1.464403000000
C	9.977509000000	-2.619432000000	-1.226165000000
C	11.258291000000	-0.155263000000	-1.234090000000
H	9.344373000000	0.686174000000	-1.676328000000
C	11.354180000000	-2.554231000000	-1.005841000000
H	9.479676000000	-3.586099000000	-1.238164000000
C	11.997688000000	-1.317060000000	-1.001801000000
H	11.752293000000	0.812583000000	-1.244687000000
H	11.920416000000	-3.466525000000	-0.840745000000
H	13.069109000000	-1.258031000000	-0.829895000000

C	7.115875000000	-0.895136000000	-3.362985000000
C	5.802169000000	-0.832474000000	-3.864177000000
C	8.146204000000	-0.329831000000	-4.130094000000
C	5.528818000000	-0.170260000000	-5.059204000000
H	5.004277000000	-1.319299000000	-3.319977000000
C	7.869490000000	0.319512000000	-5.333918000000
H	9.173942000000	-0.392194000000	-3.795080000000
C	6.558443000000	0.417400000000	-5.796652000000
H	4.504180000000	-0.120344000000	-5.418153000000
H	8.685279000000	0.753204000000	-5.906610000000
H	6.342102000000	0.932585000000	-6.728687000000
C	7.451287000000	2.872731000000	-1.565034000000
C	8.320455000000	3.312095000000	-0.563126000000
C	8.578399000000	2.477472000000	0.522019000000
C	7.999825000000	1.209261000000	0.586289000000
C	7.147782000000	0.744390000000	-0.417587000000
C	6.857603000000	1.615710000000	-1.484521000000
H	7.226255000000	3.512899000000	-2.413545000000
H	8.777812000000	4.295650000000	-0.622782000000
H	9.237476000000	2.804446000000	1.321686000000
H	8.232806000000	0.579932000000	1.432248000000
H	6.173807000000	1.292289000000	-2.258288000000
C	6.535856000000	-0.639217000000	-0.477795000000
C	5.084818000000	-0.607175000000	-0.458826000000
C	4.303850000000	-1.713987000000	-0.930316000000
O	4.642192000000	-2.650172000000	-1.661605000000
O	3.019220000000	-1.685647000000	-0.417443000000
C	2.125058000000	-2.652524000000	-0.963272000000
H	2.478833000000	-3.670729000000	-0.774306000000
H	2.013902000000	-2.521222000000	-2.044505000000
H	1.168506000000	-2.484333000000	-0.464391000000
TS_{4R/S10R}			
P	-2.378235000000	-1.404363000000	-0.265257000000
C	-3.407310000000	-0.262766000000	-1.278074000000
C	-4.118262000000	0.800172000000	-0.413806000000
H	-4.116782000000	-0.856129000000	-1.863167000000
H	-2.710051000000	0.204362000000	-1.975543000000
C	-4.099502000000	2.185480000000	-1.069763000000
H	-5.151295000000	0.490230000000	-0.208200000000
H	-3.618580000000	0.880452000000	0.559123000000
C	-4.730123000000	3.257348000000	-0.179358000000
H	-3.055377000000	2.452566000000	-1.277440000000
H	-4.614392000000	2.146411000000	-2.040135000000
H	-4.708203000000	4.241300000000	-0.661567000000

H	-5.776727000000	3.022144000000	0.051996000000
H	-4.185751000000	3.334765000000	0.769471000000
C	-3.605552000000	-2.441509000000	0.643077000000
C	-4.573650000000	-3.225248000000	-0.249672000000
H	-4.156449000000	-1.776290000000	1.317230000000
H	-3.040524000000	-3.125760000000	1.284433000000
C	-5.527816000000	-4.102383000000	0.569108000000
H	-5.164388000000	-2.535721000000	-0.866808000000
H	-4.014509000000	-3.861441000000	-0.948512000000
C	-6.504421000000	-4.890225000000	-0.306600000000
H	-4.939275000000	-4.795109000000	1.185940000000
H	-6.086519000000	-3.468245000000	1.270752000000
H	-7.128313000000	-4.216925000000	-0.906745000000
H	-5.968490000000	-5.550368000000	-0.999503000000
H	-7.171986000000	-5.512677000000	0.299122000000
C	-1.483042000000	-2.616384000000	-1.343572000000
C	-1.872809000000	-2.623187000000	-2.824802000000
H	-1.632575000000	-3.608871000000	-0.897264000000
H	-0.431552000000	-2.347832000000	-1.236657000000
C	-1.043306000000	-3.633092000000	-3.625020000000
H	-2.939916000000	-2.856919000000	-2.944198000000
H	-1.712988000000	-1.619198000000	-3.229339000000
C	-1.408947000000	-3.652301000000	-5.110789000000
H	0.021082000000	-3.387059000000	-3.509165000000
H	-1.175793000000	-4.637339000000	-3.197715000000
H	-0.798677000000	-4.373791000000	-5.665495000000
H	-2.461767000000	-3.924647000000	-5.254606000000
H	-1.257499000000	-2.665648000000	-5.564502000000
P	-0.861324000000	2.084341000000	1.833897000000
B	1.098926000000	0.306950000000	-0.035460000000
O	1.413354000000	-1.010539000000	0.194087000000
O	2.187856000000	1.089356000000	-0.298893000000
C	2.764999000000	-1.202604000000	-0.318572000000
C	3.376462000000	0.243424000000	-0.199495000000
C	3.451336000000	-2.263178000000	0.530715000000
C	2.610456000000	-1.677050000000	-1.766504000000
C	4.324051000000	0.636153000000	-1.326038000000
C	4.019816000000	0.532411000000	1.157758000000
H	4.492798000000	-2.397517000000	0.217892000000
H	3.434697000000	-2.000289000000	1.590502000000
H	2.934331000000	-3.220146000000	0.409656000000
H	2.058470000000	-2.622105000000	-1.770605000000
H	2.034579000000	-0.955544000000	-2.353143000000
H	3.581077000000	-1.842537000000	-2.244262000000

H	3.833665000000	0.576006000000	-2.299667000000
H	4.659781000000	1.666756000000	-1.176666000000
H	5.206526000000	-0.013633000000	-1.335662000000
H	3.351981000000	0.276142000000	1.983769000000
H	4.955852000000	-0.022406000000	1.278709000000
H	4.239131000000	1.601620000000	1.221836000000
C	-0.063886000000	1.450097000000	3.374526000000
C	0.877570000000	0.413709000000	3.426798000000
C	-0.437486000000	2.076605000000	4.571128000000
C	1.419132000000	0.005617000000	4.644072000000
H	1.153874000000	-0.111624000000	2.521450000000
C	0.113976000000	1.679723000000	5.789226000000
H	-1.175642000000	2.874713000000	4.547690000000
C	1.041314000000	0.638440000000	5.829429000000
H	2.126012000000	-0.819312000000	4.666543000000
H	-0.189622000000	2.175820000000	6.707271000000
H	1.460411000000	0.316029000000	6.778660000000
C	0.390820000000	3.377679000000	1.388662000000
C	-0.066450000000	4.498062000000	0.677497000000
C	1.725351000000	3.350947000000	1.807912000000
C	0.796033000000	5.544571000000	0.361230000000
H	-1.103759000000	4.535765000000	0.358429000000
C	2.591718000000	4.398705000000	1.493641000000
H	2.091778000000	2.513253000000	2.388622000000
C	2.132653000000	5.495190000000	0.765198000000
H	0.425302000000	6.402259000000	-0.194018000000
H	3.626656000000	4.358561000000	1.824526000000
H	2.806677000000	6.312915000000	0.524011000000
C	-0.512502000000	-3.056332000000	3.680986000000
C	-1.254491000000	-2.596179000000	4.769852000000
C	-2.075980000000	-1.477674000000	4.620103000000
C	-2.154513000000	-0.827469000000	3.389822000000
C	-1.392861000000	-1.254613000000	2.291018000000
C	-0.579429000000	-2.388577000000	2.457824000000
H	0.129820000000	-3.927038000000	3.788703000000
H	-1.193393000000	-3.104676000000	5.728290000000
H	-2.655658000000	-1.110824000000	5.462719000000
H	-2.795272000000	0.041676000000	3.273740000000
H	0.030552000000	-2.711890000000	1.620114000000
C	-1.458882000000	-0.560807000000	0.969911000000
C	-0.780189000000	0.649684000000	0.637572000000
C	-0.448675000000	0.897915000000	-0.762323000000
O	-0.569081000000	0.046252000000	-1.717481000000
O	-0.419429000000	2.250643000000	-1.080478000000

C	0.244075000000	2.586389000000	-2.295236000000
H	1.315243000000	2.376096000000	-2.215593000000
H	-0.182376000000	2.032452000000	-3.135663000000
H	0.091869000000	3.659685000000	-2.424621000000
TS_{4R/S11}			
P	-1.928313000000	-1.440102000000	-0.693780000000
C	-3.745887000000	-1.452949000000	-0.312456000000
C	-4.027665000000	-1.495459000000	1.194295000000
H	-4.241251000000	-2.287766000000	-0.824972000000
H	-4.155373000000	-0.529413000000	-0.736117000000
C	-5.496754000000	-1.221707000000	1.527665000000
H	-3.737374000000	-2.474801000000	1.600666000000
H	-3.397253000000	-0.755113000000	1.698629000000
C	-5.771169000000	-1.243127000000	3.032893000000
H	-5.771999000000	-0.242253000000	1.114344000000
H	-6.133456000000	-1.961608000000	1.022064000000
H	-5.167771000000	-0.487622000000	3.550794000000
H	-6.825116000000	-1.040591000000	3.254602000000
H	-5.519193000000	-2.218760000000	3.466683000000
C	-1.364889000000	-3.099921000000	-0.068727000000
C	-2.238119000000	-4.320870000000	-0.370059000000
H	-1.222108000000	-2.979369000000	1.008922000000
H	-0.360439000000	-3.246476000000	-0.475252000000
C	-1.604342000000	-5.634625000000	0.116057000000
H	-3.223072000000	-4.205163000000	0.100013000000
H	-2.417899000000	-4.393465000000	-1.450227000000
C	-1.389215000000	-5.696581000000	1.631929000000
H	-2.245304000000	-6.471500000000	-0.191598000000
H	-0.642119000000	-5.780818000000	-0.395518000000
H	-1.014508000000	-6.679738000000	1.937437000000
H	-0.663502000000	-4.948505000000	1.969688000000
H	-2.328623000000	-5.515285000000	2.169272000000
C	-1.939579000000	-1.656097000000	-2.545786000000
C	-0.521735000000	-1.616418000000	-3.131217000000
H	-2.528985000000	-0.818472000000	-2.940564000000
H	-2.466724000000	-2.576486000000	-2.827053000000
C	-0.484059000000	-1.572837000000	-4.664873000000
H	0.008377000000	-0.742139000000	-2.732500000000
H	0.037426000000	-2.496371000000	-2.785709000000
C	-1.068200000000	-2.817309000000	-5.339565000000
H	-1.022888000000	-0.679511000000	-5.010920000000
H	0.558167000000	-1.443694000000	-4.985087000000
H	-2.134523000000	-2.935639000000	-5.117376000000
H	-0.962440000000	-2.765314000000	-6.428991000000

H	-0.555812000000	-3.725464000000	-4.997224000000
P	-0.401476000000	1.697964000000	2.172914000000
B	1.238607000000	-0.099076000000	0.571306000000
O	2.555010000000	0.246343000000	0.757242000000
O	1.051995000000	-1.448978000000	0.483730000000
C	3.308821000000	-0.970090000000	1.011474000000
C	2.363006000000	-2.079043000000	0.416843000000
C	4.662633000000	-0.842367000000	0.323030000000
C	3.488672000000	-1.074360000000	2.526516000000
C	2.309359000000	-3.374029000000	1.220114000000
C	2.630115000000	-2.369860000000	-1.062009000000
H	5.239418000000	-1.768169000000	0.426388000000
H	4.552482000000	-0.611089000000	-0.738088000000
H	5.233291000000	-0.033671000000	0.789924000000
H	2.530072000000	-1.162439000000	3.038644000000
H	4.112008000000	-1.933866000000	2.793826000000
H	3.979865000000	-0.166377000000	2.888844000000
H	1.625105000000	-4.079455000000	0.738624000000
H	3.299097000000	-3.841145000000	1.268669000000
H	1.952265000000	-3.194989000000	2.236111000000
H	1.849767000000	-3.033986000000	-1.443809000000
H	2.607343000000	-1.449202000000	-1.652120000000
H	3.597218000000	-2.861695000000	-1.205521000000
C	0.133109000000	0.400138000000	3.360920000000
C	-0.379576000000	-0.903846000000	3.253703000000
C	0.964557000000	0.708188000000	4.449225000000
C	-0.046018000000	-1.877302000000	4.193071000000
H	-1.031564000000	-1.134929000000	2.421254000000
C	1.284898000000	-0.265818000000	5.395528000000
H	1.368548000000	1.708748000000	4.554379000000
C	0.789258000000	-1.564017000000	5.268088000000
H	-0.445246000000	-2.882953000000	4.086018000000
H	1.933381000000	-0.009412000000	6.228945000000
H	1.047863000000	-2.323163000000	6.001123000000
C	0.785797000000	3.094750000000	2.518292000000
C	0.237501000000	4.253069000000	3.082040000000
C	2.157148000000	3.059439000000	2.224160000000
C	1.043531000000	5.358101000000	3.362353000000
H	-0.828076000000	4.289561000000	3.294300000000
C	2.958813000000	4.167095000000	2.497151000000
H	2.591004000000	2.170031000000	1.780834000000
C	2.406072000000	5.316799000000	3.067680000000
H	0.606533000000	6.250115000000	3.803327000000
H	4.019915000000	4.133885000000	2.262754000000

H	3.035470000000	6.177394000000	3.278079000000
C	-3.487968000000	2.255518000000	-2.053669000000
C	-4.585142000000	2.683035000000	-1.306207000000
C	-4.575470000000	2.510339000000	0.081768000000
C	-3.492163000000	1.899968000000	0.706433000000
C	-2.376346000000	1.459209000000	-0.028612000000
C	-2.393097000000	1.664124000000	-1.421879000000
H	-3.480636000000	2.381016000000	-3.133599000000
H	-5.437876000000	3.144691000000	-1.796039000000
H	-5.421855000000	2.842632000000	0.677209000000
H	-3.490461000000	1.752777000000	1.781560000000
H	-1.550030000000	1.329705000000	-2.016955000000
C	-1.327246000000	0.649288000000	0.657986000000
C	0.121340000000	1.005711000000	0.468774000000
C	0.492370000000	1.965180000000	-0.639079000000
O	1.023549000000	1.605716000000	-1.677267000000
O	0.108323000000	3.229698000000	-0.405442000000
C	0.302398000000	4.158100000000	-1.479526000000
H	-0.354391000000	3.903273000000	-2.315900000000
H	0.038871000000	5.133333000000	-1.070694000000
H	1.341768000000	4.143572000000	-1.815273000000
TS_{S7S/S12}			
P	1.148796000000	-0.249752000000	-0.934789000000
C	-0.474324000000	-1.098075000000	-0.980392000000
C	-0.689834000000	-2.080529000000	0.182746000000
H	-0.582111000000	-1.610307000000	-1.944742000000
H	-1.219552000000	-0.301159000000	-0.941898000000
C	-2.161742000000	-2.491026000000	0.291494000000
H	-0.065287000000	-2.972253000000	0.030583000000
H	-0.374629000000	-1.630397000000	1.129029000000
C	-2.389814000000	-3.516662000000	1.401525000000
H	-2.756167000000	-1.594983000000	0.502168000000
H	-2.506263000000	-2.894312000000	-0.671851000000
H	-1.823993000000	-4.439141000000	1.219181000000
H	-2.073160000000	-3.106275000000	2.365249000000
H	-3.449152000000	-3.784428000000	1.484214000000
C	1.507487000000	0.654695000000	-2.484669000000
C	0.658002000000	0.267163000000	-3.703656000000
H	2.576291000000	0.524352000000	-2.696277000000
H	1.334602000000	1.706070000000	-2.232655000000
C	0.960219000000	1.133715000000	-4.935745000000
H	0.820259000000	-0.789931000000	-3.950772000000
H	-0.399351000000	0.379265000000	-3.439225000000
C	0.563456000000	2.604599000000	-4.771997000000

H	2.029527000000	1.059676000000	-5.179756000000
H	0.421307000000	0.708825000000	-5.792727000000
H	-0.501066000000	2.698070000000	-4.530058000000
H	1.124314000000	3.095505000000	-3.970240000000
H	0.752102000000	3.162789000000	-5.695765000000
C	2.447289000000	-1.537781000000	-0.740205000000
C	2.512743000000	-2.573245000000	-1.875124000000
H	2.263114000000	-2.028544000000	0.222142000000
H	3.403575000000	-1.008050000000	-0.645397000000
C	3.604536000000	-3.624497000000	-1.641503000000
H	1.541337000000	-3.075485000000	-1.971230000000
H	2.694910000000	-2.064192000000	-2.830699000000
C	3.677582000000	-4.657802000000	-2.767916000000
H	4.574350000000	-3.119255000000	-1.537072000000
H	3.416508000000	-4.130104000000	-0.684701000000
H	3.895572000000	-4.178623000000	-3.729903000000
H	4.461610000000	-5.398727000000	-2.578415000000
H	2.727584000000	-5.195428000000	-2.872496000000
P	-1.141021000000	2.540247000000	-1.164343000000
B	-1.806658000000	0.864855000000	2.700688000000
O	-2.617415000000	-0.246567000000	2.752239000000
O	-1.719920000000	1.523749000000	3.902170000000
C	-3.315709000000	-0.208211000000	4.026717000000
C	-2.359199000000	0.682506000000	4.898859000000
C	-4.676915000000	0.439770000000	3.759206000000
C	-3.498967000000	-1.634002000000	4.531560000000
C	-1.238712000000	-0.117600000000	5.570578000000
C	-3.065377000000	1.579580000000	5.907193000000
H	-5.302024000000	0.446989000000	4.658539000000
H	-4.566793000000	1.463587000000	3.395649000000
H	-5.191704000000	-0.132496000000	2.982291000000
H	-4.151812000000	-2.185000000000	3.847783000000
H	-2.547368000000	-2.165791000000	4.594297000000
H	-3.966768000000	-1.634245000000	5.522719000000
H	-0.725501000000	-0.749582000000	4.840053000000
H	-0.507279000000	0.582361000000	5.985954000000
H	-1.617249000000	-0.746360000000	6.383159000000
H	-2.326363000000	2.175508000000	6.452039000000
H	-3.754632000000	2.263703000000	5.408433000000
H	-3.625878000000	0.981619000000	6.634714000000
C	-2.627462000000	3.135883000000	-2.076239000000
C	-3.290192000000	4.335771000000	-1.777960000000
C	-3.145510000000	2.317141000000	-3.088665000000
C	-4.447374000000	4.695870000000	-2.463705000000

H	-2.905013000000	4.975764000000	-0.991552000000
C	-4.307482000000	2.672927000000	-3.775480000000
H	-2.638305000000	1.385889000000	-3.331524000000
C	-4.961542000000	3.864097000000	-3.461706000000
H	-4.956734000000	5.622386000000	-2.212651000000
H	-4.698387000000	2.023818000000	-4.554749000000
H	-5.866647000000	4.145661000000	-3.993160000000
C	-0.299473000000	4.137348000000	-0.765663000000
C	-0.003555000000	5.043474000000	-1.797745000000
C	0.159442000000	4.416564000000	0.529031000000
C	0.714404000000	6.209284000000	-1.538010000000
H	-0.359966000000	4.845470000000	-2.805255000000
C	0.887975000000	5.579869000000	0.784403000000
H	-0.046414000000	3.715592000000	1.330287000000
C	1.165396000000	6.480872000000	-0.243797000000
H	0.919091000000	6.908617000000	-2.344904000000
H	1.236079000000	5.783474000000	1.794019000000
H	1.727861000000	7.388245000000	-0.040417000000
C	-4.709286000000	3.867609000000	2.068919000000
C	-5.821010000000	3.289930000000	1.453830000000
C	-5.634635000000	2.269507000000	0.518182000000
C	-4.349900000000	1.837055000000	0.199820000000
C	-3.217035000000	2.415734000000	0.796062000000
C	-3.422824000000	3.435800000000	1.741570000000
H	-4.841415000000	4.661796000000	2.799674000000
H	-6.823135000000	3.629091000000	1.702215000000
H	-6.493418000000	1.808343000000	0.037326000000
H	-4.207717000000	1.044742000000	-0.528408000000
H	-2.557632000000	3.891758000000	2.211903000000
C	-1.835382000000	1.995455000000	0.434821000000
C	-1.082396000000	1.315627000000	1.387583000000
C	0.286316000000	0.993687000000	1.408191000000
O	1.139381000000	1.084358000000	0.376988000000
O	0.652039000000	0.034358000000	2.363377000000
C	1.784157000000	0.402336000000	3.146311000000
H	1.555149000000	1.287157000000	3.752354000000
H	2.008608000000	-0.445934000000	3.799477000000
H	2.650551000000	0.613811000000	2.508482000000
5'R			
P	-1.484591000000	-0.981202000000	-0.887296000000
C	-3.323497000000	-1.209828000000	-1.049812000000
C	-4.325077000000	-0.066818000000	-0.876727000000
H	-3.545419000000	-2.001336000000	-0.324687000000
H	-3.457650000000	-1.666129000000	-2.038001000000

C	-5.756795000000	-0.607469000000	-0.776587000000
H	-4.091203000000	0.515622000000	0.020059000000
H	-4.242164000000	0.629913000000	-1.712526000000
C	-6.791387000000	0.511359000000	-0.635675000000
H	-5.985605000000	-1.211065000000	-1.666829000000
H	-5.833086000000	-1.290130000000	0.081996000000
H	-7.808791000000	0.111715000000	-0.560793000000
H	-6.599705000000	1.112212000000	0.261408000000
H	-6.758606000000	1.187451000000	-1.498372000000
C	-1.120032000000	-2.807821000000	-0.644217000000
C	-1.465356000000	-3.724729000000	-1.827330000000
H	-1.651237000000	-3.155619000000	0.243579000000
H	-0.054966000000	-2.897040000000	-0.438540000000
C	-1.032583000000	-5.173720000000	-1.569631000000
H	-2.544057000000	-3.709112000000	-2.026681000000
H	-0.977524000000	-3.371765000000	-2.744413000000
C	-1.372799000000	-6.109655000000	-2.731391000000
H	0.049428000000	-5.196979000000	-1.380083000000
H	-1.511852000000	-5.534957000000	-0.649301000000
H	-2.453012000000	-6.127184000000	-2.920201000000
H	-0.880799000000	-5.784876000000	-3.656300000000
H	-1.052982000000	-7.137078000000	-2.525807000000
C	-0.481211000000	-0.700167000000	-2.415698000000
C	-1.303394000000	-0.587308000000	-3.703241000000
H	0.245894000000	-1.514744000000	-2.483418000000
H	0.079694000000	0.220208000000	-2.244969000000
C	-0.416785000000	-0.296854000000	-4.918930000000
H	-1.862234000000	-1.516003000000	-3.882826000000
H	-2.037326000000	0.214311000000	-3.581803000000
C	-1.218932000000	-0.181830000000	-6.216976000000
H	0.136750000000	0.635209000000	-4.741563000000
H	0.339100000000	-1.088480000000	-5.019511000000
H	-0.569174000000	0.033995000000	-7.072235000000
H	-1.757238000000	-1.112996000000	-6.432403000000
H	-1.961998000000	0.621677000000	-6.148995000000
P	-0.002890000000	2.574712000000	1.664332000000
B	0.642514000000	-0.792186000000	0.946455000000
O	1.174434000000	-1.112091000000	2.164236000000
O	1.492531000000	-1.092874000000	-0.092613000000
C	2.539130000000	-1.592276000000	1.987831000000
C	2.634313000000	-1.834069000000	0.425939000000
C	3.489782000000	-0.510454000000	2.497811000000
C	2.686825000000	-2.846463000000	2.846667000000
C	2.452585000000	-3.300104000000	0.018346000000

C	3.895117000000	-1.288771000000	-0.236218000000
H	4.532025000000	-0.825565000000	2.386966000000
H	3.350996000000	0.432987000000	1.971157000000
H	3.300812000000	-0.341497000000	3.561407000000
H	2.551681000000	-2.576522000000	3.898069000000
H	1.940893000000	-3.603980000000	2.597395000000
H	3.684410000000	-3.283885000000	2.732240000000
H	1.568448000000	-3.751202000000	0.473866000000
H	2.342956000000	-3.357646000000	-1.069130000000
H	3.324089000000	-3.896218000000	0.306075000000
H	4.022087000000	-0.223746000000	-0.047973000000
H	4.781374000000	-1.821514000000	0.125214000000
H	3.826196000000	-1.440398000000	-1.318294000000
C	-0.184795000000	2.032897000000	3.418647000000
C	0.807831000000	1.427267000000	4.200016000000
C	-1.405678000000	2.355046000000	4.034890000000
C	0.584477000000	1.137919000000	5.546531000000
H	1.757758000000	1.173134000000	3.751050000000
C	-1.638654000000	2.053363000000	5.374966000000
H	-2.178416000000	2.846971000000	3.449082000000
C	-0.641428000000	1.442316000000	6.138853000000
H	1.368974000000	0.664321000000	6.132055000000
H	-2.593700000000	2.306804000000	5.828271000000
H	-0.815719000000	1.215328000000	7.187117000000
C	1.817080000000	2.531757000000	1.365106000000
C	2.719394000000	3.126845000000	2.266867000000
C	2.308595000000	2.132198000000	0.113052000000
C	4.067672000000	3.269558000000	1.946351000000
H	2.361854000000	3.479327000000	3.229949000000
C	3.653928000000	2.298198000000	-0.218683000000
H	1.622251000000	1.687465000000	-0.600535000000
C	4.544980000000	2.853986000000	0.700314000000
H	4.747460000000	3.715808000000	2.667875000000
H	4.007328000000	1.986817000000	-1.198787000000
H	5.594192000000	2.975299000000	0.445603000000
C	-0.822827000000	-0.195501000000	0.726964000000
C	-0.744485000000	1.341314000000	0.578202000000
C	-1.407579000000	1.860814000000	-0.530703000000
O	-1.994028000000	1.139831000000	-1.401068000000
O	-1.403241000000	3.211558000000	-0.730458000000
C	-2.104546000000	3.676885000000	-1.878385000000
H	-1.682738000000	3.263704000000	-2.800768000000
H	-3.167128000000	3.415180000000	-1.833779000000
H	-1.987405000000	4.762216000000	-1.867228000000

C	-1.864957000000	-0.619419000000	1.781487000000
C	-1.941282000000	-1.995043000000	2.423936000000
C	-1.606679000000	-0.793230000000	3.256397000000
H	-2.832247000000	-0.167761000000	1.575917000000
H	-1.122886000000	-2.685538000000	2.246363000000
H	-2.914756000000	-2.470999000000	2.517116000000
H	-2.354015000000	-0.389498000000	3.930312000000
H	-0.590878000000	-0.712407000000	3.613679000000
5'S			
P	-1.918037000000	-0.006026000000	-0.099821000000
C	-3.372011000000	-0.040317000000	-1.266585000000
C	-3.883438000000	1.172207000000	-2.039777000000
H	-3.120941000000	-0.842734000000	-1.967044000000
H	-4.182166000000	-0.439402000000	-0.644512000000
C	-5.111004000000	0.800044000000	-2.881003000000
H	-3.095786000000	1.564979000000	-2.686234000000
H	-4.138649000000	1.983603000000	-1.352623000000
C	-5.650869000000	1.989114000000	-3.679071000000
H	-5.902311000000	0.405763000000	-2.227025000000
H	-4.849290000000	-0.016699000000	-3.568873000000
H	-6.525731000000	1.709206000000	-4.276311000000
H	-4.888617000000	2.380657000000	-4.363164000000
H	-5.947691000000	2.807635000000	-3.012238000000
C	-2.178403000000	-1.824373000000	0.389759000000
C	-3.342905000000	-2.144266000000	1.335718000000
H	-2.311819000000	-2.383090000000	-0.544331000000
H	-1.259963000000	-2.222618000000	0.824775000000
C	-3.473613000000	-3.648959000000	1.603358000000
H	-4.293546000000	-1.775763000000	0.928888000000
H	-3.205636000000	-1.629054000000	2.294523000000
C	-4.608500000000	-3.982784000000	2.573710000000
H	-2.522284000000	-4.027165000000	2.004115000000
H	-3.630766000000	-4.172974000000	0.650837000000
H	-5.574515000000	-3.640262000000	2.183419000000
H	-4.452663000000	-3.496303000000	3.544267000000
H	-4.682545000000	-5.061650000000	2.748496000000
C	-2.178969000000	0.847995000000	1.514009000000
C	-3.520466000000	1.575798000000	1.632431000000
H	-2.066180000000	0.110905000000	2.311885000000
H	-1.349744000000	1.550676000000	1.614788000000
C	-3.672709000000	2.268544000000	2.990556000000
H	-4.352054000000	0.871161000000	1.494345000000
H	-3.590896000000	2.317557000000	0.831244000000
C	-5.003080000000	3.012336000000	3.125789000000

H	-2.839267000000	2.970677000000	3.128855000000
H	-3.581545000000	1.522935000000	3.792960000000
H	-5.090266000000	3.504397000000	4.100677000000
H	-5.851721000000	2.325404000000	3.020521000000
H	-5.102874000000	3.782342000000	2.351446000000
P	2.228487000000	1.814779000000	-0.934085000000
B	0.598316000000	-0.858373000000	0.608386000000
O	1.170108000000	-2.104176000000	0.535503000000
O	0.585414000000	-0.355160000000	1.879764000000
C	1.734924000000	-2.437343000000	1.837665000000
C	1.060553000000	-1.377587000000	2.799864000000
C	3.252698000000	-2.284804000000	1.722941000000
C	1.380433000000	-3.891306000000	2.134999000000
C	-0.166913000000	-1.902687000000	3.552118000000
C	2.016686000000	-0.730247000000	3.793421000000
H	3.747321000000	-2.571902000000	2.656096000000
H	3.539067000000	-1.259745000000	1.480292000000
H	3.617386000000	-2.939683000000	0.925797000000
H	1.852958000000	-4.539209000000	1.390731000000
H	0.302400000000	-4.063948000000	2.096532000000
H	1.746468000000	-4.185513000000	3.124442000000
H	-0.899645000000	-2.359931000000	2.884871000000
H	-0.650215000000	-1.064090000000	4.062316000000
H	0.118387000000	-2.642540000000	4.306296000000
H	2.852120000000	-0.240361000000	3.297414000000
H	2.404028000000	-1.480347000000	4.492324000000
H	1.482430000000	0.030486000000	4.369215000000
C	3.294385000000	0.570378000000	-1.800873000000
C	3.372947000000	-0.804666000000	-1.532316000000
C	4.126904000000	1.094794000000	-2.802062000000
C	4.246906000000	-1.624722000000	-2.243374000000
H	2.734271000000	-1.250743000000	-0.784898000000
C	5.006949000000	0.277248000000	-3.514929000000
H	4.077905000000	2.157800000000	-3.021954000000
C	5.068856000000	-1.087198000000	-3.236812000000
H	4.283185000000	-2.688912000000	-2.022825000000
H	5.640892000000	0.707375000000	-4.285831000000
H	5.750229000000	-1.728479000000	-3.789725000000
C	2.903558000000	1.741758000000	0.788687000000
C	4.211477000000	1.324468000000	1.080447000000
C	2.168309000000	2.372590000000	1.807501000000
C	4.766436000000	1.536145000000	2.346056000000
H	4.805828000000	0.842144000000	0.310449000000
C	2.722852000000	2.592344000000	3.064142000000

H	1.154271000000	2.700294000000	1.596260000000
C	4.029207000000	2.177477000000	3.341271000000
H	5.781157000000	1.202341000000	2.549311000000
H	2.135194000000	3.086492000000	3.834150000000
H	4.464033000000	2.350358000000	4.321974000000
C	-0.083006000000	-0.125603000000	-0.631724000000
C	0.505879000000	1.268675000000	-0.850205000000
C	-0.451658000000	2.268435000000	-0.938352000000
O	-1.703544000000	2.038072000000	-0.793374000000
O	-0.072324000000	3.561566000000	-1.139251000000
C	-1.121027000000	4.524527000000	-1.181959000000
H	-1.675601000000	4.554744000000	-0.237947000000
H	-1.825777000000	4.315202000000	-1.993254000000
H	-0.625709000000	5.481854000000	-1.354616000000
C	-0.104924000000	-1.034238000000	-1.884066000000
C	-0.827429000000	-0.623421000000	-3.154518000000
C	0.666334000000	-0.725184000000	-3.141701000000
H	-0.161153000000	-2.093430000000	-1.647682000000
H	-1.235809000000	0.382424000000	-3.184819000000
H	-1.416433000000	-1.368242000000	-3.684129000000
H	1.155092000000	-1.553687000000	-3.645282000000
H	1.211909000000	0.207780000000	-3.177424000000

TS_{S/R7E}

P	0.537175000000	-1.963589000000	-0.052693000000
C	-0.194466000000	-3.180385000000	1.142369000000
C	-1.387477000000	-3.926101000000	0.536956000000
H	-0.528070000000	-2.598897000000	2.006864000000
H	0.566140000000	-3.889919000000	1.489570000000
C	-2.055006000000	-4.882716000000	1.530000000000
H	-2.124525000000	-3.192410000000	0.188197000000
H	-1.070602000000	-4.493206000000	-0.348870000000
C	-3.305350000000	-5.551866000000	0.954943000000
H	-1.330374000000	-5.648969000000	1.837793000000
H	-2.318345000000	-4.328300000000	2.440478000000
H	-3.762333000000	-6.238225000000	1.676187000000
H	-4.060217000000	-4.804452000000	0.680271000000
H	-3.066699000000	-6.125585000000	0.051241000000
C	2.024239000000	-1.244033000000	0.782955000000
C	2.489497000000	-1.862551000000	2.103311000000
H	1.797398000000	-0.184780000000	0.945623000000
H	2.824162000000	-1.259203000000	0.035734000000
C	3.807839000000	-1.236381000000	2.572909000000
H	1.720999000000	-1.709430000000	2.872028000000
H	2.620665000000	-2.948177000000	2.006068000000

C	4.217463000000	-1.694731000000	3.973250000000
H	4.597772000000	-1.487700000000	1.851307000000
H	3.710297000000	-0.144784000000	2.559475000000
H	3.465454000000	-1.398468000000	4.714892000000
H	4.320507000000	-2.785842000000	4.023382000000
H	5.174424000000	-1.254426000000	4.275175000000
C	1.233206000000	-3.006846000000	-1.413350000000
C	2.209200000000	-4.110345000000	-0.992420000000
H	1.714479000000	-2.287410000000	-2.083464000000
H	0.389577000000	-3.435045000000	-1.968937000000
C	2.784391000000	-4.870989000000	-2.193081000000
H	3.035329000000	-3.673174000000	-0.415913000000
H	1.709097000000	-4.823099000000	-0.322578000000
C	3.764690000000	-5.972139000000	-1.782722000000
H	1.958801000000	-5.307003000000	-2.772746000000
H	3.284670000000	-4.158037000000	-2.862087000000
H	4.162741000000	-6.500841000000	-2.655892000000
H	4.614348000000	-5.555976000000	-1.227931000000
H	3.278569000000	-6.712990000000	-1.136085000000
P	-0.391421000000	2.218680000000	0.456709000000
B	-1.966496000000	-0.074048000000	-0.018439000000
O	-3.198050000000	0.321347000000	-0.469552000000
O	-2.010638000000	-0.628971000000	1.244160000000
C	-4.191873000000	-0.088701000000	0.505115000000
C	-3.330183000000	-0.354198000000	1.798642000000
C	-5.220197000000	1.028546000000	0.640319000000
C	-4.853048000000	-1.349255000000	-0.061440000000
C	-3.764741000000	-1.564295000000	2.618048000000
C	-3.195826000000	0.870190000000	2.706817000000
H	-5.743022000000	1.159858000000	-0.311876000000
H	-5.963401000000	0.784261000000	1.407558000000
H	-4.744456000000	1.976311000000	0.898681000000
H	-5.660729000000	-1.709161000000	0.584000000000
H	-5.272025000000	-1.114631000000	-1.044192000000
H	-4.125109000000	-2.155837000000	-0.191405000000
H	-4.769787000000	-1.412279000000	3.026742000000
H	-3.765866000000	-2.480177000000	2.025123000000
H	-3.076181000000	-1.702782000000	3.457641000000
H	-2.824532000000	1.733833000000	2.151268000000
H	-4.151857000000	1.122475000000	3.176286000000
H	-2.474888000000	0.647410000000	3.499556000000
C	0.912892000000	2.270837000000	1.765340000000
C	2.040685000000	3.103746000000	1.754303000000
C	0.741880000000	1.383028000000	2.841070000000

C	2.972640000000	3.047282000000	2.791128000000
H	2.182096000000	3.795420000000	0.931968000000
C	1.675108000000	1.323699000000	3.875660000000
H	-0.125818000000	0.728550000000	2.852231000000
C	2.793697000000	2.159001000000	3.854181000000
H	3.843013000000	3.698230000000	2.769294000000
H	1.528127000000	0.630443000000	4.699844000000
H	3.520823000000	2.118217000000	4.660652000000
C	-0.296435000000	3.882655000000	-0.313217000000
C	-0.309165000000	4.052142000000	-1.704293000000
C	-0.349888000000	5.024720000000	0.501601000000
C	-0.364431000000	5.327219000000	-2.265396000000
H	-0.260013000000	3.177991000000	-2.344975000000
C	-0.393586000000	6.300179000000	-0.059330000000
H	-0.347237000000	4.915084000000	1.583089000000
C	-0.402516000000	6.456890000000	-1.446617000000
H	-0.368582000000	5.438505000000	-3.346716000000
H	-0.423718000000	7.172630000000	0.588344000000
H	-0.440070000000	7.450428000000	-1.884924000000
C	-0.695269000000	-0.066028000000	-0.971501000000
C	0.176240000000	1.041183000000	-0.801871000000
C	1.500347000000	1.063216000000	-1.380866000000
O	2.075996000000	0.121765000000	-1.933510000000
O	2.147929000000	2.251696000000	-1.192806000000
C	3.515574000000	2.276294000000	-1.596422000000
H	4.104014000000	1.554029000000	-1.022056000000
H	3.615497000000	2.042623000000	-2.660013000000
H	3.861546000000	3.291303000000	-1.394723000000
C	-1.032324000000	-0.698270000000	-2.294710000000
C	-1.653552000000	0.199848000000	-3.355750000000
C	-0.334342000000	-0.473981000000	-3.610129000000
H	-1.529264000000	-1.661516000000	-2.191369000000
H	-1.648248000000	1.264892000000	-3.148120000000
H	-2.547166000000	-0.157744000000	-3.859492000000
H	-0.313965000000	-1.315899000000	-4.297836000000
H	0.566796000000	0.122904000000	-3.614579000000
TS^{S/S77E}			
P	0.322876000000	-1.965519000000	0.001231000000
C	-0.837965000000	-3.213132000000	-0.741819000000
C	-0.297827000000	-4.600015000000	-1.107705000000
H	-1.669015000000	-3.320540000000	-0.030783000000
H	-1.255951000000	-2.721659000000	-1.625626000000
C	-1.354716000000	-5.462593000000	-1.808597000000
H	0.046641000000	-5.117906000000	-0.204000000000

H	0.577793000000	-4.503243000000	-1.762626000000
C	-0.837824000000	-6.856529000000	-2.171211000000
H	-1.695796000000	-4.945585000000	-2.716436000000
H	-2.236186000000	-5.551754000000	-1.158278000000
H	-1.608990000000	-7.452783000000	-2.671159000000
H	-0.519731000000	-7.403960000000	-1.275748000000
H	0.025518000000	-6.793601000000	-2.844561000000
C	1.563223000000	-1.687224000000	-1.345114000000
C	2.683474000000	-0.699556000000	-0.991163000000
H	1.989832000000	-2.655138000000	-1.639289000000
H	0.988947000000	-1.314015000000	-2.201720000000
C	3.796748000000	-0.681411000000	-2.040119000000
H	3.106263000000	-0.937573000000	-0.009808000000
H	2.261794000000	0.304230000000	-0.900624000000
C	4.901189000000	0.315879000000	-1.684526000000
H	3.370240000000	-0.421667000000	-3.017802000000
H	4.221908000000	-1.690784000000	-2.142262000000
H	5.362062000000	0.062761000000	-0.721346000000
H	4.494594000000	1.329908000000	-1.608880000000
H	5.693800000000	0.326806000000	-2.441556000000
C	1.179895000000	-2.880723000000	1.369699000000
C	2.403253000000	-3.729700000000	0.999377000000
H	1.464711000000	-2.109565000000	2.089207000000
H	0.412737000000	-3.504822000000	1.847620000000
C	2.993633000000	-4.442848000000	2.221271000000
H	3.173747000000	-3.086877000000	0.557473000000
H	2.148305000000	-4.474458000000	0.235978000000
C	4.237252000000	-5.266841000000	1.879917000000
H	2.227963000000	-5.094668000000	2.665164000000
H	3.241112000000	-3.695247000000	2.986575000000
H	4.642010000000	-5.768336000000	2.765975000000
H	5.028490000000	-4.630859000000	1.464921000000
H	4.007908000000	-6.038282000000	1.134454000000
P	-0.442071000000	2.440190000000	-0.319692000000
B	-1.957950000000	0.034367000000	-0.250021000000
O	-1.764115000000	-0.291684000000	-1.579244000000
O	-3.279360000000	0.193943000000	0.069380000000
C	-3.028143000000	-0.072520000000	-2.270835000000
C	-4.072165000000	-0.163563000000	-1.094475000000
C	-3.177413000000	-1.144249000000	-3.345403000000
C	-2.961726000000	1.311771000000	-2.919828000000
C	-5.240165000000	0.810181000000	-1.197002000000
C	-4.587120000000	-1.584126000000	-0.842981000000
H	-2.376498000000	-1.033921000000	-4.083212000000

H	-4.134832000000	-1.036287000000	-3.866817000000
H	-3.121810000000	-2.152852000000	-2.930443000000
H	-3.874764000000	1.527736000000	-3.483667000000
H	-2.115636000000	1.341399000000	-3.612862000000
H	-2.802524000000	2.090671000000	-2.171572000000
H	-5.833622000000	0.613128000000	-2.096769000000
H	-4.893605000000	1.844831000000	-1.223070000000
H	-5.891632000000	0.691962000000	-0.325825000000
H	-3.760888000000	-2.295896000000	-0.757348000000
H	-5.254786000000	-1.920039000000	-1.642862000000
H	-5.142228000000	-1.595223000000	0.099498000000
C	0.945825000000	2.711868000000	-1.509014000000
C	1.975130000000	3.649762000000	-1.349137000000
C	0.947522000000	1.899295000000	-2.654479000000
C	2.977937000000	3.772237000000	-2.311290000000
H	1.987617000000	4.281203000000	-0.468052000000
C	1.954875000000	2.014940000000	-3.612291000000
H	0.155857000000	1.165642000000	-2.781164000000
C	2.972719000000	2.955506000000	-3.444480000000
H	3.769912000000	4.504255000000	-2.174105000000
H	1.940687000000	1.378460000000	-4.493403000000
H	3.756206000000	3.052136000000	-4.191079000000
C	-0.458667000000	3.989788000000	0.668875000000
C	-0.440064000000	3.990493000000	2.069756000000
C	-0.623154000000	5.214631000000	0.001478000000
C	-0.575589000000	5.181240000000	2.783493000000
H	-0.304940000000	3.053798000000	2.598950000000
C	-0.744224000000	6.406396000000	0.713634000000
H	-0.647313000000	5.235173000000	-1.085417000000
C	-0.723603000000	6.394160000000	2.109978000000
H	-0.555643000000	5.161011000000	3.870180000000
H	-0.860281000000	7.345138000000	0.178048000000
H	-0.823661000000	7.321818000000	2.666854000000
C	-0.814749000000	0.020306000000	0.852176000000
C	0.077406000000	1.127105000000	0.811676000000
C	1.366687000000	1.087624000000	1.454625000000
O	1.903904000000	0.102048000000	1.968827000000
O	2.042063000000	2.273472000000	1.370198000000
C	3.394644000000	2.246753000000	1.821090000000
H	3.993349000000	1.559271000000	1.215977000000
H	3.454030000000	1.937111000000	2.868290000000
H	3.761238000000	3.267684000000	1.703089000000
C	-1.271414000000	-0.635146000000	2.125206000000
C	-0.667613000000	-0.437047000000	3.490179000000

C	-1.958480000000	0.254922000000	3.153338000000
H	-1.776012000000	-1.587766000000	1.970057000000
H	0.236957000000	0.150458000000	3.565706000000
H	-0.703710000000	-1.287043000000	4.167035000000
H	-2.888230000000	-0.103338000000	3.585964000000
H	-1.928246000000	1.322924000000	2.964416000000
TS_{5'R/6'R}			
P	-1.729587000000	-1.226054000000	0.321190000000
C	-3.199729000000	-0.287771000000	0.909740000000
C	-3.727027000000	0.945870000000	0.165105000000
H	-2.959708000000	-0.014006000000	1.943818000000
H	-3.995144000000	-1.040287000000	0.962367000000
C	-5.132373000000	1.316369000000	0.649137000000
H	-3.050595000000	1.783762000000	0.328585000000
H	-3.747025000000	0.774738000000	-0.913136000000
C	-5.636797000000	2.609013000000	0.004728000000
H	-5.827871000000	0.493188000000	0.429625000000
H	-5.122717000000	1.426054000000	1.741981000000
H	-6.642593000000	2.867632000000	0.353676000000
H	-4.970965000000	3.447801000000	0.239413000000
H	-5.673822000000	2.515040000000	-1.087424000000
C	-1.705869000000	-2.661681000000	1.485762000000
C	-2.984662000000	-3.508952000000	1.534384000000
H	-1.465052000000	-2.286231000000	2.484252000000
H	-0.856061000000	-3.278651000000	1.173994000000
C	-2.790658000000	-4.786911000000	2.359724000000
H	-3.804311000000	-2.925824000000	1.971031000000
H	-3.305780000000	-3.784305000000	0.521180000000
C	-4.063413000000	-5.631853000000	2.444621000000
H	-1.979046000000	-5.380648000000	1.917442000000
H	-2.456483000000	-4.515839000000	3.370386000000
H	-4.879652000000	-5.069899000000	2.914169000000
H	-4.401815000000	-5.937006000000	1.447037000000
H	-3.900521000000	-6.540144000000	3.034592000000
C	-2.065435000000	-2.047058000000	-1.306882000000
C	-3.416873000000	-1.746379000000	-1.959480000000
H	-1.953375000000	-3.123886000000	-1.132955000000
H	-1.263296000000	-1.742071000000	-1.972116000000
C	-3.641360000000	-2.622645000000	-3.196735000000
H	-4.247371000000	-1.897412000000	-1.257093000000
H	-3.430102000000	-0.694594000000	-2.258210000000
C	-4.959905000000	-2.307722000000	-3.906448000000
H	-2.802731000000	-2.480873000000	-3.891690000000
H	-3.621598000000	-3.681710000000	-2.902981000000

H	-5.102168000000	-2.943098000000	-4.787407000000
H	-5.815424000000	-2.465405000000	-3.238353000000
H	-4.987089000000	-1.263119000000	-4.238414000000
P	-0.360694000000	2.596288000000	1.626078000000
B	0.831584000000	-0.596707000000	-0.691653000000
O	0.865962000000	-1.844253000000	-1.283781000000
O	1.866359000000	0.204140000000	-1.107423000000
C	2.046656000000	-1.909517000000	-2.132656000000
C	2.427645000000	-0.391555000000	-2.304413000000
C	3.094490000000	-2.717180000000	-1.362617000000
C	1.668055000000	-2.626146000000	-3.423265000000
C	1.740609000000	0.282300000000	-3.496340000000
C	3.924665000000	-0.104550000000	-2.322616000000
H	4.002895000000	-2.865142000000	-1.954971000000
H	3.365865000000	-2.222464000000	-0.425830000000
H	2.678023000000	-3.699942000000	-1.120388000000
H	1.380274000000	-3.658642000000	-3.200623000000
H	0.827549000000	-2.135758000000	-3.918620000000
H	2.516022000000	-2.651268000000	-4.116575000000
H	0.657212000000	0.151272000000	-3.448916000000
H	1.941815000000	1.356819000000	-3.448481000000
H	2.122345000000	-0.099155000000	-4.449020000000
H	4.413823000000	-0.451159000000	-1.409783000000
H	4.403244000000	-0.585393000000	-3.183112000000
H	4.085026000000	0.974732000000	-2.403623000000
C	-1.232837000000	1.997056000000	3.158661000000
C	-0.650129000000	1.329170000000	4.248431000000
C	-2.611958000000	2.260675000000	3.220980000000
C	-1.421023000000	0.900034000000	5.329611000000
H	0.419819000000	1.148431000000	4.252814000000
C	-3.390590000000	1.822593000000	4.292939000000
H	-3.075196000000	2.823863000000	2.415435000000
C	-2.797719000000	1.132223000000	5.351389000000
H	-0.944042000000	0.381649000000	6.157900000000
H	-4.456440000000	2.036474000000	4.309370000000
H	-3.397607000000	0.796493000000	6.192864000000
C	1.397759000000	2.729211000000	2.168858000000
C	1.754808000000	3.275538000000	3.412722000000
C	2.419647000000	2.465191000000	1.243000000000
C	3.092545000000	3.499602000000	3.740408000000
H	0.982815000000	3.527448000000	4.134377000000
C	3.755094000000	2.697276000000	1.568112000000
H	2.161113000000	2.054516000000	0.272800000000
C	4.101353000000	3.205678000000	2.821732000000

H	3.345619000000	3.909057000000	4.715431000000
H	4.530145000000	2.473348000000	0.838533000000
H	5.143293000000	3.380287000000	3.076645000000
C	-0.098618000000	-0.218228000000	0.544761000000
C	-0.444070000000	1.266519000000	0.431718000000
C	-0.880524000000	1.537502000000	-0.872164000000
O	-1.023734000000	0.616243000000	-1.734198000000
O	-1.205485000000	2.822415000000	-1.208492000000
C	-1.689543000000	3.007744000000	-2.533752000000
H	-0.946633000000	2.702720000000	-3.277554000000
H	-2.608256000000	2.437162000000	-2.708766000000
H	-1.892231000000	4.077022000000	-2.622400000000
C	0.515130000000	-0.643968000000	1.873159000000
C	1.337112000000	-1.906293000000	2.028909000000
C	2.002651000000	-0.560288000000	2.108728000000
H	-0.089350000000	-0.391133000000	2.735539000000
H	1.516731000000	-2.511312000000	1.145875000000
H	1.209504000000	-2.481330000000	2.942498000000
H	2.337882000000	-0.188240000000	3.071989000000
H	2.622095000000	-0.241954000000	1.279375000000
TS_{5'S/6'S}			
P	1.253241000000	0.115904000000	-0.031235000000
C	0.963046000000	-1.222525000000	-1.255009000000
C	1.520196000000	-2.615200000000	-0.930580000000
H	1.326129000000	-0.878766000000	-2.227509000000
H	-0.128602000000	-1.275631000000	-1.324403000000
C	0.833538000000	-3.681090000000	-1.792682000000
H	2.606588000000	-2.641897000000	-1.095510000000
H	1.334507000000	-2.838136000000	0.122416000000
C	1.339528000000	-5.092879000000	-1.493611000000
H	-0.248413000000	-3.630080000000	-1.618195000000
H	0.975161000000	-3.450843000000	-2.857532000000
H	1.173232000000	-5.353127000000	-0.440994000000
H	0.822908000000	-5.838349000000	-2.108254000000
H	2.415151000000	-5.183174000000	-1.690342000000
C	2.453660000000	-0.401137000000	1.265056000000
C	3.201452000000	0.745071000000	1.959949000000
H	3.161438000000	-1.077833000000	0.769719000000
H	1.874408000000	-0.980411000000	1.980782000000
C	3.926802000000	0.246148000000	3.213581000000
H	3.928791000000	1.206273000000	1.280306000000
H	2.494989000000	1.525980000000	2.256651000000
C	4.640049000000	1.369915000000	3.967142000000
H	3.192001000000	-0.233208000000	3.871669000000

H	4.648877000000	-0.533763000000	2.934298000000
H	3.926453000000	2.138189000000	4.289191000000
H	5.150025000000	0.992629000000	4.860310000000
H	5.391043000000	1.859377000000	3.335034000000
C	2.227708000000	1.420403000000	-0.924759000000
C	1.876074000000	1.754005000000	-2.379880000000
H	3.270251000000	1.080111000000	-0.886244000000
H	2.176511000000	2.324758000000	-0.311325000000
C	2.681907000000	2.953865000000	-2.891839000000
H	2.082556000000	0.888728000000	-3.021488000000
H	0.810141000000	1.970788000000	-2.485929000000
C	2.373582000000	3.287687000000	-4.352800000000
H	2.466146000000	3.825568000000	-2.259015000000
H	3.755244000000	2.748453000000	-2.775698000000
H	2.610999000000	2.442401000000	-5.009811000000
H	1.311082000000	3.523232000000	-4.486839000000
H	2.953650000000	4.151061000000	-4.695906000000
P	-2.941328000000	-0.015413000000	-0.709072000000
B	-0.522872000000	1.052012000000	2.114498000000
O	0.404020000000	0.665244000000	3.051655000000
O	-1.611982000000	1.667740000000	2.698188000000
C	-0.249691000000	0.718789000000	4.350959000000
C	-1.330809000000	1.826112000000	4.113151000000
C	-0.850789000000	-0.668093000000	4.597964000000
C	0.793014000000	1.049923000000	5.409922000000
C	-0.791165000000	3.246647000000	4.303232000000
C	-2.629995000000	1.638812000000	4.886422000000
H	-0.062312000000	-1.417710000000	4.496689000000
H	-1.284925000000	-0.738679000000	5.600637000000
H	-1.621725000000	-0.904861000000	3.860196000000
H	1.355914000000	1.950280000000	5.153460000000
H	0.316761000000	1.200706000000	6.384948000000
H	1.500927000000	0.221097000000	5.504881000000
H	-0.613992000000	3.473340000000	5.359328000000
H	0.146171000000	3.387446000000	3.755699000000
H	-1.523040000000	3.960365000000	3.914066000000
H	-3.096669000000	0.678974000000	4.657589000000
H	-2.448656000000	1.693336000000	5.965685000000
H	-3.335499000000	2.430623000000	4.617176000000
C	-2.878794000000	-1.475062000000	-1.858025000000
C	-2.165124000000	-1.290821000000	-3.053574000000
C	-3.429601000000	-2.741123000000	-1.606396000000
C	-1.972650000000	-2.339442000000	-3.953191000000
H	-1.754236000000	-0.307893000000	-3.276552000000

C	-3.247654000000	-3.789818000000	-2.508536000000
H	-3.995501000000	-2.901021000000	-0.697053000000
C	-2.512335000000	-3.597094000000	-3.680527000000
H	-1.412120000000	-2.172683000000	-4.869745000000
H	-3.678503000000	-4.764769000000	-2.293392000000
H	-2.369672000000	-4.417619000000	-4.378689000000
C	-4.420665000000	-0.374936000000	0.329865000000
C	-4.384861000000	-0.161860000000	1.715031000000
C	-5.643449000000	-0.729709000000	-0.260591000000
C	-5.533816000000	-0.314814000000	2.489089000000
H	-3.447609000000	0.131284000000	2.174361000000
C	-6.790230000000	-0.895900000000	0.515929000000
H	-5.697192000000	-0.888150000000	-1.334706000000
C	-6.740808000000	-0.689924000000	1.895862000000
H	-5.485873000000	-0.145852000000	3.562762000000
H	-7.724985000000	-1.184230000000	0.041280000000
H	-7.634802000000	-0.816238000000	2.500852000000
C	-0.459562000000	0.799202000000	0.549397000000
C	-1.526952000000	-0.287319000000	0.371278000000
C	-1.221696000000	-1.508443000000	1.000732000000
O	-0.104104000000	-1.785744000000	1.502932000000
O	-2.222160000000	-2.444967000000	1.027692000000
C	-1.838399000000	-3.745176000000	1.460452000000
H	-2.758047000000	-4.333600000000	1.469557000000
H	-1.117748000000	-4.196779000000	0.769175000000
H	-1.394499000000	-3.717367000000	2.459359000000
C	-0.739572000000	2.037957000000	-0.296805000000
C	-1.687348000000	3.133641000000	0.115961000000
C	-0.205627000000	3.406287000000	0.058481000000
H	-0.802689000000	1.815922000000	-1.358041000000
H	-2.158790000000	3.064749000000	1.086735000000
H	-2.315592000000	3.537606000000	-0.671711000000
H	0.187003000000	4.037321000000	-0.735195000000
H	0.318967000000	3.513160000000	1.006445000000

10. DFT-optimized cartesian coordinates of all species involved in the phosphine-catalyzed hydroboration reaction.

PMe₃

P	0.00000000	0.00009200	0.60049900
C	0.00000000	1.63569000	-0.28015800
H	-0.88602300	2.21019100	0.01003100
H	0.88602300	2.21019100	0.01003100
H	0.00000000	1.50592600	-1.36938500
C	-1.41628900	-0.81795000	-0.28046000
H	-1.47122500	-1.87234100	0.01020200
H	-2.35698200	-0.33742000	0.00842700
H	-1.30231100	-0.75333600	-1.36951400
C	1.41628900	-0.81795000	-0.28046000
H	2.35698200	-0.33742000	0.00842700
H	1.47122500	-1.87234100	0.01020200
H	1.30231100	-0.75333600	-1.36951400

I

C	-6.04097900	-3.24889500	-3.22291900
C	-4.83519500	-3.34241600	-3.13172700
C	-3.42930100	-3.45324700	-3.02699700
C	-2.78502400	-4.64993300	-3.38994500
C	-2.66836600	-2.36638100	-2.55934700
C	-1.40522000	-4.75062500	-3.28503300
H	-3.37681400	-5.48561200	-3.75014500
C	-1.28935400	-2.48155100	-2.45872700
H	-3.17047300	-1.44526200	-2.28045300
C	-0.65592300	-3.67007800	-2.82053300
H	-0.91061800	-5.67555800	-3.56648000
H	-0.70466500	-1.64101900	-2.09682000
H	0.42395400	-3.75452500	-2.74003600
C	-7.45455900	-3.05071700	-3.30972300
O	-8.01419100	-2.00629400	-3.02664100
O	-8.08062600	-4.16004500	-3.74178500
C	-9.52256000	-4.04858900	-3.86193400
H	-9.77963800	-3.27076700	-4.58554800
H	-9.85510100	-5.02567900	-4.21018800
H	-9.96301900	-3.81195000	-2.89008900

HBpin

O	-1.07307900	1.20721300	-0.40789700
O	1.07294900	1.20734000	0.40779100
C	-0.78212900	-0.19268200	-0.05055000
C	0.78213200	-0.19260900	0.05054700
C	-1.34927500	-1.10011800	-1.12655000

H	-1.06481400	-2.13883200	-0.92748500
H	-2.44175100	-1.03834000	-1.11942700
H	-0.99147100	-0.82252700	-2.12015100
C	-1.47328200	-0.44855500	1.28460300
H	-2.54307900	-0.24841400	1.17294500
H	-1.34823100	-1.48996100	1.59584500
H	-1.07917900	0.20392000	2.07008300
C	1.34934900	-1.09990900	1.12662400
H	1.06499100	-2.13866500	0.92763500
H	2.44181900	-1.03802700	1.11951000
H	0.99150600	-0.82227400	2.12019900
C	1.47332500	-0.44851300	-1.28457900
H	2.54310200	-0.24826400	-1.17292200
H	1.34837600	-1.48995200	-1.59574900
H	1.07917200	0.20386900	-2.07011100
B	-0.00008000	1.94923400	-0.00012600
H	-0.00016000	3.14058100	-0.00011500

S13

C	-0.26852800	-1.55343400	-0.12308000
C	0.40711700	-0.39560600	-0.10333300
C	-0.14723700	0.98614500	-0.11206700
C	-1.09702400	1.35056900	-1.07658000
C	0.22051800	1.93107200	0.85510600
C	-1.66477000	2.62069900	-1.06801800
H	-1.38385000	0.62705400	-1.83393900
C	-0.34789500	3.20172800	0.86220500
H	0.93729200	1.66237000	1.62799200
C	-1.29205000	3.55214400	-0.10030000
H	-2.39742500	2.88647100	-1.82542600
H	-0.05903200	3.91675200	1.62792900
H	-1.73536100	4.54394900	-0.09570400
C	-1.69041600	-1.65521400	-0.18800500
O	-2.34987200	-1.88034500	-1.20664800
O	-2.27826500	-1.61074000	1.05346700
C	-3.69106100	-1.89719800	1.08126600
H	-3.89313000	-2.89904600	0.68954000
H	-3.97954400	-1.83937800	2.13203400
H	-4.25132200	-1.16146100	0.49635500
P	2.20339400	-0.61321400	-0.02942200
C	2.76112200	-1.07808700	1.63365100
H	2.53331600	-0.27196700	2.33707600
H	2.22718800	-1.98414600	1.93584700
H	3.83925100	-1.26744500	1.62540600
C	3.11953800	0.87220400	-0.52974500

H	2.74470600	1.21582100	-1.49894000
H	2.99173300	1.66880500	0.20725000
H	4.18207300	0.62406800	-0.61552500
C	2.69651800	-1.94500900	-1.15023600
H	2.12648200	-2.84237300	-0.89768300
H	2.46867900	-1.64965200	-2.17865800
H	3.76977700	-2.13133600	-1.04320400
S14			
C	1.26167400	-0.41285500	1.51102400
C	1.97701000	-0.24914000	0.38174300
C	2.26416400	1.09103300	-0.20987300
C	1.64957100	1.49306100	-1.40050900
C	3.13300000	1.97462100	0.43897800
C	1.89289200	2.75791400	-1.92709400
H	0.96045200	0.81855700	-1.90324800
C	3.37392300	3.24023900	-0.08855200
H	3.61743100	1.66279300	1.36060200
C	2.75567000	3.63491200	-1.27270400
H	1.39981700	3.06288400	-2.84602200
H	4.04867000	3.91847400	0.42656000
H	2.94365500	4.62288800	-1.68348300
C	0.70002400	0.80735900	2.14688500
O	-0.26372000	1.42267400	1.72918700
O	1.34009200	1.10526900	3.29260700
C	0.79683000	2.22131900	4.04034100
H	-0.23739900	2.01410400	4.32764200
H	1.42951900	2.31274600	4.92298300
H	0.83784800	3.13514100	3.44131900
P	2.72937200	-1.64912200	-0.49648300
C	3.44820800	-2.89571600	0.60028400
H	4.11047700	-2.40296200	1.31758000
H	2.65866600	-3.43295000	1.12701900
H	4.02597100	-3.58629400	-0.02349200
C	4.11832800	-0.98488300	-1.45659800
H	3.76022600	-0.28347100	-2.21461400
H	4.81311900	-0.46734600	-0.78830400
H	4.62975100	-1.82120700	-1.94288000
C	1.63123600	-2.47955000	-1.67530800
H	0.86595500	-3.01550300	-1.11003800
H	1.16634600	-1.73884400	-2.33248100
H	2.22659900	-3.17824800	-2.27295700
O	-0.37284600	-1.53658500	3.10235500
O	0.42791500	-2.86854300	1.32769700
C	-1.32226900	-2.57497200	2.84586300

C	-1.00656500	-2.95434800	1.36143900
C	-2.72741500	-2.03262500	3.07567300
H	-3.48331300	-2.76780600	2.77650500
H	-2.86804900	-1.81546400	4.14025100
H	-2.89204700	-1.10933700	2.51428900
C	-1.05880300	-3.74308300	3.80397600
H	-1.09396000	-3.36717700	4.83212000
H	-1.81171500	-4.53249200	3.70214000
H	-0.06868500	-4.17607100	3.62925200
C	-1.42285500	-4.36352800	0.95989900
H	-2.50282800	-4.49886500	1.08792600
H	-1.18336300	-4.53324000	-0.09613200
H	-0.90120000	-5.11721600	1.55509200
C	-1.60686300	-1.94071800	0.37964500
H	-1.20997600	-2.13156400	-0.62275600
H	-2.69769900	-2.02792300	0.33215500
H	-1.34854700	-0.91580600	0.66361600
B	0.82767300	-1.81105400	2.28469100
H	1.81321600	-2.16200600	2.95403000

S15

C	1.86860200	-0.69450300	1.36783000
C	1.93704900	-0.04975500	-0.00316600
C	2.61025300	1.22756700	-0.13554800
C	2.30765800	2.16313800	-1.15726600
C	3.61448400	1.62830800	0.78480100
C	2.99067100	3.36543100	-1.28487600
H	1.48808500	1.95944200	-1.84192800
C	4.27908500	2.84171400	0.66490900
H	3.89597400	0.96053900	1.59459900
C	3.98796200	3.72443300	-0.37665800
H	2.71646600	4.04727600	-2.08701500
H	5.04689900	3.09666800	1.39236400
H	4.51044900	4.67202500	-0.46754300
C	1.51994900	0.32997600	2.44694300
O	0.69056900	1.21161600	2.35407800
O	2.22583400	0.10204600	3.57710600
C	1.91733700	0.97362900	4.68995800
H	0.86613500	0.87099200	4.97353300
H	2.56716800	0.64771900	5.50220500
H	2.12608800	2.01361000	4.42454100
P	1.40424500	-0.87511400	-1.41926800
C	1.36230900	-2.68607500	-1.18252000
H	0.41206400	-2.98823000	-0.73944100
H	1.45223200	-3.15742900	-2.16622500

H	2.19402000	-3.01345300	-0.55159500
C	2.54507400	-0.64333000	-2.83014400
H	2.67324900	0.41243600	-3.07306900
H	3.51772500	-1.06987400	-2.56741000
H	2.13704000	-1.16633900	-3.70079500
C	-0.25530200	-0.52215600	-2.13770100
H	-0.44924700	-1.18663800	-2.98754000
H	-1.01066500	-0.68282000	-1.36306700
H	-0.30326600	0.51737400	-2.47497500
O	-0.55335700	-1.65552500	1.14604700
O	0.85751000	-2.73140900	2.60066900
C	-1.42107500	-2.50438300	1.97804000
C	-0.39746300	-3.49684800	2.64332300
C	-2.45486300	-3.16164300	1.08330100
H	-3.07117600	-3.85560600	1.66436200
H	-3.11042000	-2.39454200	0.65985800
H	-1.98689000	-3.71095900	0.26295300
C	-2.08982600	-1.56766300	2.97785500
H	-2.64757400	-0.80413400	2.42735100
H	-2.78853600	-2.11108800	3.62080200
H	-1.34935400	-1.06345000	3.60752600
C	-0.70284500	-3.83923800	4.09128300
H	-1.67544400	-4.33754700	4.16130600
H	0.05999600	-4.52519200	4.47191400
H	-0.71690800	-2.94960800	4.72437900
C	-0.16301200	-4.77320100	1.84375200
H	0.67784800	-5.31520300	2.28675600
H	-1.04413000	-5.42119800	1.87436200
H	0.07801200	-4.56170600	0.79876000
B	0.71029500	-1.74180500	1.66569700
H	2.81563800	-1.16075000	1.68586900

S16

C	2.19099500	-0.75983500	1.87698700
C	1.76651800	-0.59912800	0.39694000
C	1.55258700	0.75390000	-0.21225800
C	2.50429400	1.77275700	-0.08058200
C	0.40886100	1.00108000	-0.97952500
C	2.31902300	3.00245500	-0.70075900
H	3.38989500	1.59556300	0.52419200
C	0.22340500	2.23170500	-1.60529900
H	-0.34369000	0.22194700	-1.06871800
C	1.17754500	3.23676200	-1.46798800
H	3.06580900	3.78363400	-0.58497900
H	-0.67309900	2.40792000	-2.19387300

H	1.03184100	4.19922300	-1.95082700
C	2.16889500	0.31614700	2.82918000
O	1.60761900	1.40392900	2.75120700
O	2.82955500	-0.06089200	3.98512200
C	2.72535000	0.86631400	5.07847300
H	1.68039200	1.01304900	5.37089600
H	3.28329700	0.41495100	5.90081600
H	3.16189400	1.83533600	4.81619800
P	2.65525000	-1.64223400	-0.74910300
C	3.18946400	-3.21727500	-0.03056500
H	2.33357900	-3.72323000	0.42140600
H	3.61090300	-3.82594300	-0.83703300
H	3.96099300	-3.04119800	0.72410500
C	4.15545400	-0.85156500	-1.39972300
H	3.88957400	0.05680800	-1.94699200
H	4.81736400	-0.59202200	-0.56756500
H	4.66782900	-1.54951700	-2.06957300
C	1.58926400	-2.02093300	-2.16178900
H	2.13576300	-2.65131000	-2.86988000
H	0.70024400	-2.54745100	-1.80195000
H	1.28921600	-1.09185500	-2.65454100
O	-0.52989400	-0.62383700	1.65519200
O	0.44509600	-2.72989900	1.38027600
C	-1.38473600	-1.59273300	2.29916200
C	-0.97561300	-2.91578500	1.57278500
C	-2.83458500	-1.18151400	2.09877000
H	-3.50951600	-1.95706000	2.47763900
H	-3.03528900	-0.25645700	2.64938400
H	-3.05586500	-1.00753000	1.04287200
C	-1.04309400	-1.61861300	3.79111900
H	-1.15609200	-0.60663200	4.19365000
H	-1.70775900	-2.28815800	4.34688300
H	-0.00752600	-1.93800900	3.94949200
C	-1.20587100	-4.18263300	2.38236700
H	-2.26746200	-4.28906100	2.63220900
H	-0.90609500	-5.05738100	1.79523900
H	-0.62619500	-4.17476700	3.30857500
C	-1.62812000	-3.04734500	0.19479300
H	-1.14737900	-3.87023200	-0.34489000
H	-2.69820800	-3.26648900	0.27215800
H	-1.49844300	-2.12749700	-0.38511600
B	0.67940600	-1.31012300	1.33926900
H	2.89997500	-1.54981800	2.10745900

S17

C	2.05444700	-0.81845900	1.39858000
C	1.62093300	-0.60700400	-0.04531500
C	1.67755400	0.81109100	-0.59450100
C	2.60949100	1.73340300	-0.10956300
C	0.82213100	1.20276200	-1.62910300
C	2.69612400	3.00714900	-0.65884600
H	3.25677300	1.43896000	0.71148700
C	0.90501600	2.48014700	-2.17795400
H	0.07495200	0.50592900	-2.00252700
C	1.84489600	3.38753400	-1.69619500
H	3.42484000	3.71270900	-0.26834700
H	0.22808900	2.76701600	-2.97815100
H	1.90732000	4.38712000	-2.11756200
C	1.65772200	0.02514400	2.43436400
O	1.04390300	1.10762200	2.39274800
O	2.06530500	-0.48500500	3.68983800
C	1.69194100	0.31372600	4.81304500
H	0.60342800	0.42380700	4.88902800
H	2.06775500	-0.21547400	5.69267400
H	2.13933100	1.31380600	4.76843400
P	2.73224000	-1.59048500	-1.12334700
C	3.03177900	-3.26717500	-0.50074000
H	2.08206200	-3.76313400	-0.28989200
H	3.57913000	-3.81627500	-1.27378100
H	3.64012400	-3.22330700	0.40614700
C	4.35401800	-0.79917700	-1.27063800
H	4.26641100	0.13613400	-1.82890600
H	4.74553600	-0.59323300	-0.26980600
H	5.02851800	-1.48335500	-1.79488000
C	2.03271700	-1.75299600	-2.78489100
H	2.72130400	-2.34078700	-3.39969200
H	1.06702800	-2.26447200	-2.72666900
H	1.89967900	-0.76392800	-3.23089000
O	-0.94932400	-0.53939000	0.34328100
O	-0.03486100	-2.62024600	-0.02290200
C	-1.94704900	-1.51378700	0.79901500
C	-1.48537600	-2.81661300	0.06469400
C	-3.32765200	-1.01990700	0.40977500
H	-4.08052800	-1.77660300	0.65536300
H	-3.56283600	-0.10981900	0.97020000
H	-3.38938500	-0.79550800	-0.65748100
C	-1.81047500	-1.60423100	2.31601400
H	-1.96511300	-0.60861000	2.74255000
H	-2.55517000	-2.28384600	2.74144500

H	-0.80991400	-1.94734000	2.60075200
C	-1.76061600	-4.10330600	0.82161400
H	-2.83720300	-4.22022500	0.98551400
H	-1.40991600	-4.95818600	0.23481900
H	-1.25460200	-4.11385700	1.78932600
C	-2.00234500	-2.91225900	-1.36714900
H	-1.48546300	-3.73148400	-1.87671500
H	-3.07674900	-3.11915100	-1.38578200
H	-1.81296200	-1.98525600	-1.91825600
B	0.19317600	-1.25692700	0.07499700
H	2.48049800	-1.77602200	1.67169800
S18			
O	-0.68812800	1.28818400	-1.03018100
O	-1.20069900	0.59965500	1.12699000
C	-1.15221100	2.45126800	-0.31720000
C	-1.91791900	1.83270300	0.90706700
C	-2.02904000	3.28431600	-1.24708200
H	-2.47850700	4.12466600	-0.70571600
H	-1.41596300	3.69191500	-2.05808600
H	-2.82711100	2.68324300	-1.68908400
C	0.05624800	3.28755500	0.10556000
H	0.67004100	3.49047300	-0.77834100
H	-0.25284000	4.24526900	0.53874200
H	0.67416700	2.75740400	0.83312100
C	-1.86078900	2.66660200	2.17984200
H	-2.30193700	3.65530500	2.01209800
H	-2.43291600	2.16977500	2.97097800
H	-0.83303600	2.79685500	2.52783400
C	-3.37898000	1.50329200	0.58361200
H	-3.79151400	0.90183600	1.40081700
H	-3.98104100	2.41320100	0.48918200
H	-3.46307200	0.92781800	-0.34178700
B	-0.75019200	0.13502100	-0.16477100
H	0.88280700	-2.75564000	-1.42112200
C	0.24054200	-1.96501000	-1.05371900
C	0.64385700	-0.84400900	-0.13436000
C	1.92052800	-0.11966700	-0.49949600
C	2.50559300	0.82507300	0.35348200
C	2.53107200	-0.33988900	-1.74010000
C	3.65724000	1.51463900	-0.01090300
H	2.03953500	1.05556800	1.30451400
C	3.68020600	0.35453400	-2.11146500
H	2.08783000	-1.05441900	-2.42663300
C	4.25567100	1.28161000	-1.24719700

H	4.08183600	2.24627100	0.67182300
H	4.12795300	0.16522200	-3.08379300
H	5.15479900	1.81976900	-1.53420000
C	-1.09081900	-1.89160400	-1.30262400
O	-1.77085400	-0.88464000	-0.79285000
O	-1.76086600	-2.81587100	-2.02279300
C	-3.13324900	-2.51684600	-2.34720800
H	-3.20334000	-1.59869200	-2.93906300
H	-3.48102500	-3.36705600	-2.93560500
H	-3.73801000	-2.41538300	-1.44143600
P	0.79114600	-1.66197700	1.51305500
C	1.16114100	-0.64156200	2.98094800
H	2.22327500	-0.38781000	3.01575800
H	0.55146800	0.26482800	2.95468200
H	0.90652600	-1.23003800	3.86876500
C	2.10637400	-2.91413400	1.44964800
H	1.87851300	-3.65528500	0.67925800
H	3.05784700	-2.42581400	1.21618300
H	2.18240900	-3.40980600	2.42238700
C	-0.75201200	-2.52398400	1.92138200
H	-1.54426400	-1.78664900	2.07387300
H	-1.02564700	-3.20293000	1.11083300
H	-0.59027000	-3.09315800	2.84216000

S19Z

O	0.04680300	-1.67298000	-0.25215800
O	1.35486600	0.07012200	0.47157800
C	1.29295000	-2.28140300	0.24131200
C	2.27301800	-1.05893400	0.25599400
C	1.69373100	-3.40728200	-0.69386900
H	2.66841700	-3.80817600	-0.39648400
H	0.95816000	-4.21482000	-0.63137700
H	1.75386700	-3.06998300	-1.73078600
C	0.98555700	-2.82272300	1.63311000
H	0.15886600	-3.53569400	1.56065600
H	1.85366800	-3.34244200	2.04945400
H	0.69302000	-2.02047300	2.31808800
C	3.29624200	-1.07733000	1.37604500
H	3.93408200	-1.96309300	1.28663200
H	3.93301100	-0.19017000	1.30567500
H	2.81892400	-1.08610600	2.35817500
C	2.94951600	-0.81606400	-1.08874800
H	3.45546000	0.15356400	-1.06081400
H	3.69608400	-1.58856700	-1.29604100
H	2.22023100	-0.80351000	-1.90509100

B	0.12126600	-0.33588800	0.03237400
H	-0.00282300	2.17793700	0.82168000
C	-0.94292300	1.89766100	0.35170500
C	-1.09854200	0.63950700	-0.10849600
C	-2.36383300	0.10387700	-0.65787500
C	-2.37764300	-0.52766800	-1.90719500
C	-3.55063100	0.16469500	0.08215700
C	-3.56104300	-1.04688700	-2.42256500
H	-1.45915700	-0.59585400	-2.48458200
C	-4.72730500	-0.37334400	-0.42465200
H	-3.54293600	0.63157900	1.06376200
C	-4.73910200	-0.97388600	-1.68270200
H	-3.56052800	-1.51726500	-3.40199400
H	-5.63934800	-0.32400200	0.16389600
H	-5.66026100	-1.39062000	-2.08030200
C	-1.93089400	2.99353000	0.24885500
O	-2.84146800	3.08586600	-0.55184500
O	-1.64903000	3.94817900	1.16482800
C	-2.52515700	5.09894200	1.15658400
H	-3.55705700	4.79160700	1.34739300
H	-2.16298400	5.74499700	1.95599000
H	-2.46774100	5.61062500	0.19197300

S19E

O	0.85145400	-0.79364200	-1.12736900
O	0.80922200	-0.66922600	1.16775800
C	1.69136400	-1.90699500	-0.65490300
C	1.96435700	-1.52188900	0.84530200
C	2.93155800	-1.97561200	-1.52770200
H	3.61610000	-2.74345300	-1.15188300
H	2.64388800	-2.24547700	-2.54850500
H	3.45660400	-1.01855200	-1.55528000
C	0.86193000	-3.17683600	-0.81195500
H	0.54845400	-3.26768600	-1.85656100
H	1.45052000	-4.06174100	-0.55115100
H	-0.03236200	-3.15644300	-0.18182200
C	1.97571000	-2.69747400	1.80699100
H	2.77086800	-3.39829500	1.53197600
H	2.17461800	-2.33687200	2.82082800
H	1.02217200	-3.22967800	1.80828400
C	3.21469200	-0.67158300	1.03754900
H	3.23171200	-0.30066700	2.06705000
H	4.11688000	-1.26862700	0.87256200
H	3.22371700	0.18702000	0.36269500
B	0.32548400	-0.18441400	-0.01870100

H	-1.58193100	2.83326200	-0.20672700
C	-0.74630900	2.13931200	-0.15931700
C	-0.91036100	0.80462200	-0.06094600
C	-2.25329000	0.20772000	0.04444200
C	-2.49833900	-1.06279100	-0.50069200
C	-3.30744700	0.87422000	0.69047600
C	-3.76286700	-1.63587300	-0.42748900
H	-1.69694200	-1.59045500	-1.01075100
C	-4.56633500	0.29362000	0.77216600
H	-3.12876500	1.83939300	1.15579600
C	-4.80100700	-0.96085800	0.20982400
H	-3.93681200	-2.61386100	-0.86738200
H	-5.36770600	0.81767700	1.28554900
H	-5.78665000	-1.41266200	0.27675900
C	0.60267400	2.70211300	-0.23768500
O	1.63418700	2.04469400	-0.21263200
O	0.58227000	4.04446200	-0.34623200
C	1.87706500	4.68379100	-0.43937200
H	2.41334900	4.32384800	-1.32149000
H	1.66841400	5.74986600	-0.52515600
H	2.46635400	4.47777500	0.45817500
S20			
O	2.98292700	0.51560500	1.55183200
O	1.59599800	0.64215000	-0.32846600
C	3.67573200	1.26300600	0.54169000
C	2.95887400	0.79854100	-0.76944800
C	5.16098900	0.93120600	0.60358500
H	5.69892100	1.40310300	-0.22665500
H	5.58398600	1.30925300	1.54063100
H	5.32937100	-0.14776000	0.56308800
C	3.47170400	2.75793700	0.81381300
H	3.81247900	2.97754100	1.83103100
H	4.04404400	3.38098200	0.11796100
H	2.41320700	3.02702800	0.73915800
C	2.99425600	1.81124700	-1.90669100
H	4.02798600	2.03895200	-2.19090700
H	2.48450700	1.39830400	-2.78473400
H	2.49475600	2.74218800	-1.62666700
C	3.48998000	-0.54907800	-1.26885800
H	2.85076900	-0.90484200	-2.08394900
H	4.51030300	-0.46065300	-1.65750500
H	3.48066800	-1.29466500	-0.46825400
B	1.62258300	0.29770300	1.09251900
H	0.73468000	0.85948700	1.72952300

C	-0.96767100	-1.00575600	0.97644900
C	-1.85531400	-0.52929300	0.12542900
C	-3.01512300	0.32557300	0.51763600
C	-4.33380700	-0.04529900	0.23507600
C	-2.77603200	1.52840700	1.19132800
C	-5.39335000	0.77173800	0.62198500
H	-4.53732200	-0.99177100	-0.25843800
C	-3.83544700	2.34596200	1.57131100
H	-1.75037100	1.81159900	1.41295600
C	-5.14709900	1.97134700	1.28530600
H	-6.41413500	0.46499700	0.41104700
H	-3.63637700	3.27875100	2.09184500
H	-5.97445400	2.60929800	1.58329200
C	0.17629200	-1.72518400	1.14326600
O	1.36912300	-1.24065900	1.29426500
O	0.03564000	-3.06443700	1.29553300
C	1.18164100	-3.78588900	1.80096600
H	1.47405200	-3.40909000	2.78544500
H	0.84896500	-4.82163700	1.87782200
H	2.02663400	-3.70946600	1.11131800
P	-1.54453500	-0.66259000	-1.66738400
C	-0.18044600	-1.80267500	-1.96523300
H	0.70963800	-1.42085500	-1.45711500
H	-0.43906600	-2.79539800	-1.58564700
H	0.00072800	-1.85196400	-3.04375400
C	-1.09230100	0.97573000	-2.29088800
H	-1.90766000	1.67608200	-2.08356300
H	-0.18165100	1.28991200	-1.76954300
H	-0.91662000	0.92456800	-3.37033400
C	-2.97356500	-1.23458700	-2.63040500
H	-3.31044100	-2.20589800	-2.25700300
H	-3.78758100	-0.50834100	-2.55966100
H	-2.66576700	-1.33007600	-3.67721600

S21Z

O	2.26328600	-0.30747600	0.31481600
O	3.51242600	1.22455100	-0.87959800
C	3.48410200	-0.07464500	1.09639600
C	4.44921100	0.54311900	0.02334200
C	3.94766400	-1.39489100	1.68214900
H	4.90794700	-1.26200000	2.19147900
H	3.21694600	-1.74622500	2.41724200
H	4.06062600	-2.16021800	0.91131800
C	3.11248100	0.90627200	2.20378900
H	2.29212700	0.48076200	2.78950700

H	3.95966000	1.08400700	2.87297000
H	2.78347300	1.86565300	1.79126900
C	5.43266500	1.56032200	0.57071600
H	6.07662300	1.08967700	1.32110100
H	6.06736200	1.93103000	-0.23995800
H	4.92064300	2.40919600	1.02872700
C	5.17103400	-0.51253300	-0.80675900
H	5.66930400	-0.02114000	-1.64783300
H	5.92950300	-1.02953200	-0.21133900
H	4.47090100	-1.25478300	-1.20438700
B	2.30988100	0.57880300	-0.73288100
H	-0.34573400	1.72010100	0.08486400
C	-0.77753400	0.84672900	-0.40252700
C	-2.09239900	0.35964200	0.01750800
C	-2.40673500	-1.05003200	0.13687100
C	-3.72578300	-1.56871100	0.08625000
C	-1.37847400	-2.00698600	0.33872500
C	-3.99448000	-2.92087300	0.26655400
H	-4.56232300	-0.90857500	-0.12697300
C	-1.65179600	-3.35510900	0.50518400
H	-0.34981200	-1.66138500	0.38165300
C	-2.96461500	-3.83672600	0.47804600
H	-5.02548100	-3.26467800	0.21680800
H	-0.82545000	-4.04481200	0.66617300
H	-3.17482000	-4.89465400	0.60392900
C	0.00872700	0.32363800	-1.35939000
O	1.28451500	0.81914200	-1.60752900
O	-0.38405300	-0.64547600	-2.21991800
C	0.58943300	-1.66830900	-2.52177200
H	0.96604700	-2.13157700	-1.60262100
H	0.06119800	-2.41400500	-3.11780600
H	1.42360200	-1.25709100	-3.09981900
P	-3.29640700	1.57016900	0.31549200
C	-2.51009300	3.19633500	0.53293300
H	-1.77235400	3.15383100	1.33898300
H	-2.02166700	3.50892800	-0.39391800
H	-3.28820300	3.92137300	0.79033000
C	-4.25953700	1.29183700	1.84183000
H	-4.66952400	0.27973600	1.86308100
H	-3.59230900	1.42091700	2.69922500
H	-5.07953900	2.01439400	1.90060300
C	-4.55784800	1.89563500	-0.98660200
H	-4.03719700	2.13897900	-1.91827000
H	-5.17935600	1.01144600	-1.15112000

H	-5.19730200	2.73588400	-0.69375500
S21E			
O	1.64858600	-0.88845000	1.56756200
O	1.76125400	-0.27564000	-0.65512800
C	2.39530000	0.37806300	1.53037900
C	2.82810000	0.46789000	0.02283000
C	3.54619300	0.29255500	2.51598900
H	4.17375000	1.18671300	2.43804500
H	3.15218500	0.24068600	3.53568900
H	4.16605400	-0.58845500	2.33648300
C	1.42206800	1.47920500	1.93437600
H	1.02561100	1.25433400	2.92906500
H	1.92761500	2.44883800	1.97647700
H	0.58424600	1.54998900	1.23217800
C	2.87270300	1.87718000	-0.53904800
H	3.60212500	2.47973700	0.01273400
H	3.18239300	1.84180500	-1.58826600
H	1.89587400	2.36357400	-0.48379200
C	4.12923100	-0.27150400	-0.27167200
H	4.26350800	-0.32939500	-1.35601000
H	4.98772500	0.25628800	0.15464800
H	4.10692700	-1.28964700	0.13026000
B	1.21520000	-1.10843100	0.28505200
H	-1.76373400	-1.27853000	-2.36813100
C	-1.26533300	-1.20893000	-1.39822800
C	-1.60361600	-0.12872300	-0.45289700
C	-1.42441900	1.24874200	-0.83647700
C	-0.82729400	1.57484800	-2.08509400
C	-1.78557100	2.35834100	-0.02387300
C	-0.62521800	2.88825800	-2.48331700
H	-0.49978700	0.76666300	-2.73275300
C	-1.57449000	3.66885700	-0.42947200
H	-2.22172500	2.19881200	0.95798300
C	-0.99502600	3.95938800	-1.66648400
H	-0.16079700	3.07968900	-3.44879100
H	-1.86521600	4.47853900	0.23667600
H	-0.83200200	4.98606100	-1.98025000
C	-0.35673100	-2.16013300	-1.14647200
O	0.40551100	-2.18899300	0.00052900
O	-0.21138900	-3.25963200	-1.92861200
C	1.15628700	-3.64066000	-2.19975800
H	1.65705000	-3.98557100	-1.28996800
H	1.09939400	-4.45560900	-2.92256600
H	1.70815000	-2.79659800	-2.63085200

P	-2.52394100	-0.57955300	0.94921800
C	-1.81094700	-0.15824900	2.58384700
H	-0.82828600	-0.63224300	2.66799900
H	-1.68769900	0.92211200	2.69287200
H	-2.47319100	-0.52411800	3.37578500
C	-2.74761500	-2.38027300	1.01081200
H	-3.22998600	-2.72764900	0.09376600
H	-1.78159100	-2.87750600	1.12517400
H	-3.38233400	-2.61361700	1.87158200
C	-4.23593700	0.08480200	1.02914100
H	-4.23434400	1.17558700	0.96522000
H	-4.80129400	-0.31753600	0.18287900
H	-4.71081400	-0.22039700	1.96760700

S22

C	3.02720300	1.49391900	0.19328000
C	3.88172900	0.56088400	-0.73317100
C	3.80154300	2.16193100	1.31386100
H	4.59235000	2.79529700	0.89825200
H	3.12724200	2.79539100	1.89828700
H	4.25535500	1.42666800	1.98189900
C	2.20947900	2.52052000	-0.58411900
H	1.49566100	2.99319000	0.09751900
H	2.85320900	3.29912900	-1.00467200
H	1.65008100	2.04936100	-1.39916100
C	4.41141000	1.22838000	-1.98900600
H	5.06685300	2.06426200	-1.72241300
H	4.99638300	0.50752800	-2.56846900
H	3.60093400	1.60374000	-2.61763100
C	5.00611700	-0.14892400	0.01444500
H	5.42923600	-0.92154600	-0.63449600
H	5.80271700	0.55163800	0.28224400
H	4.63622400	-0.62648300	0.92772700
B	1.96042600	-0.49054600	-0.11734200
H	-0.29125800	0.54819700	1.75932100
C	-0.72489300	-0.16051300	1.05873300
C	-1.84856600	-0.06893700	0.32790900
C	-2.73798300	1.08490000	0.20281900
C	-4.07701200	0.92143700	-0.19182800
C	-2.27385100	2.39471900	0.42710600
C	-4.92440400	2.01656700	-0.32693200
H	-4.45863900	-0.07581600	-0.39286800
C	-3.11873400	3.48820500	0.28551900
H	-1.23321900	2.54783100	0.70227900
C	-4.45051100	3.30457800	-0.08804600

H	-5.95789800	1.86401100	-0.62639200
H	-2.73749800	4.49075700	0.46158600
H	-5.11029200	4.16034500	-0.20070300
C	-0.15314300	-1.50335900	0.71451100
O	1.04872000	-1.50187200	-0.07847600
O	-0.01703900	-2.43915100	1.74504000
C	0.98401900	-2.10967800	2.72424300
H	0.77670800	-1.13908400	3.19143000
H	0.94114900	-2.89460600	3.48188300
H	1.98500200	-2.09457300	2.27613500
P	-1.67839000	-1.91839400	-0.43151100
C	-3.15244200	-2.64482600	0.39884000
H	-2.78960900	-3.24846700	1.23765600
H	-3.83171800	-1.88079500	0.78032500
H	-3.67626900	-3.30777800	-0.29699600
C	-0.96112400	-3.60954400	-0.96965300
H	-0.06252200	-3.45620900	-1.57774000
H	-0.68216500	-4.19888600	-0.08948600
H	-1.68843800	-4.17596200	-1.56214100
C	-1.98449100	-1.36898200	-2.17262200
H	-2.71432000	-0.55609000	-2.20005500
H	-1.03021200	-0.98589500	-2.55557100
H	-2.30183500	-2.20098700	-2.80790900
O	2.07060700	0.54835300	0.77889300
O	2.90918600	-0.46588000	-1.11608800

S23

O	-0.95021300	1.28300400	1.29198600
O	-0.59718800	1.22606900	-1.01246000
C	-1.78768300	2.28910600	0.70372200
C	-1.11411300	2.52855100	-0.69232800
C	-1.80286000	3.51730300	1.60803600
H	-2.35977500	4.33768400	1.14032400
H	-2.29607300	3.27016500	2.55451200
H	-0.78980900	3.86197100	1.82959300
C	-3.21046200	1.73591500	0.58554600
H	-3.54506600	1.41973600	1.57956900
H	-3.91155200	2.49081000	0.21278100
H	-3.24218400	0.86593900	-0.07605700
C	-2.07532500	2.96401900	-1.79124000
H	-2.56930100	3.90521400	-1.52402600
H	-1.52251600	3.12423600	-2.72354800
H	-2.84146200	2.20560700	-1.97232200
C	0.05456300	3.51871500	-0.61511300
H	0.60664300	3.48016200	-1.56069900

H	-0.29311800	4.54625800	-0.46201600
H	0.74056800	3.25260200	0.19394500
B	-0.21819700	0.57873300	0.24183500
H	1.14725100	-2.63642900	0.51571500
C	0.87607100	-1.58230600	0.45877600
C	-0.33287500	-1.05334600	0.22325900
C	-1.54265600	-1.85837400	0.01946600
C	-1.82405600	-2.98235200	0.81248400
C	-2.45086600	-1.51599000	-0.99490000
C	-2.97024300	-3.74011300	0.59496900
H	-1.14114400	-3.24756600	1.61607100
C	-3.58987500	-2.28252100	-1.21961600
H	-2.23967100	-0.64631600	-1.61090400
C	-3.85723100	-3.39551600	-0.42419500
H	-3.17481300	-4.60139800	1.22575700
H	-4.27571100	-2.00762300	-2.01695600
H	-4.75215000	-3.98799300	-0.59368400
C	1.92003200	-0.50843700	0.60438800
O	1.29916700	0.71234200	0.54179000
O	2.78532100	-0.65833700	1.72964000
C	2.08207300	-0.63609800	2.98419000
H	1.42602600	-1.50966300	3.08460800
H	2.84950300	-0.66073700	3.76030100
H	1.48714700	0.27929300	3.08057900
P	3.12966200	-0.54142300	-0.83682700
C	4.12167900	-2.05392300	-0.89159600
H	4.72403800	-2.12295500	0.01852200
H	3.45731200	-2.92052300	-0.95940700
H	4.77880100	-2.02927400	-1.76702100
C	4.22546000	0.88703900	-0.67794800
H	3.61366600	1.79261300	-0.63694200
H	4.80824400	0.79509400	0.24251000
H	4.89754000	0.92971400	-1.54070500
C	2.15238900	-0.38376400	-2.34452300
H	2.81001400	-0.13867700	-3.18395400
H	1.63279800	-1.32524000	-2.54383600
H	1.41351600	0.41172200	-2.19111700
TS_{1/S13}			
C	-0.85391700	-1.16306500	0.01840800
C	0.24487900	-0.59025800	-0.04370300
C	1.68307700	-0.70401700	-0.07943500
C	2.27291200	-1.79070700	0.58929600
C	2.50351000	0.18818500	-0.78035000
C	3.65020000	-1.97096400	0.55427300

H	1.63858600	-2.48360400	1.13389800
C	3.87893500	-0.00551100	-0.82065900
H	2.05199900	1.03302300	-1.29127600
C	4.45880400	-1.08108800	-0.15021400
H	4.09372200	-2.80954700	1.08382300
H	4.50205500	0.69055300	-1.37509600
H	5.53545600	-1.22313600	-0.17417700
C	-2.23115800	-1.42180400	0.18803800
O	-2.79792100	-1.51370000	1.27309300
O	-2.87014900	-1.58999600	-1.00056700
C	-4.28548700	-1.87048700	-0.90255300
H	-4.80685600	-1.04261100	-0.41371200
H	-4.62789200	-1.98209000	-1.93146000
H	-4.45473900	-2.79279900	-0.34005600
P	-0.27539500	1.87091200	0.09643000
C	-1.67285300	2.02471700	-1.09324900
H	-1.27879900	2.22865000	-2.09407900
H	-2.23638500	1.08712300	-1.12866900
H	-2.34777000	2.83647000	-0.79927900
C	0.43223900	3.58442600	0.06807200
H	1.21645600	3.66641700	0.82732600
H	0.87781300	3.77918200	-0.91259900
H	-0.34275900	4.33434400	0.26772200
C	-1.14845300	1.85096200	1.71826200
H	-1.73372600	0.93068500	1.80706800
H	-0.41405900	1.87363800	2.52992800
H	-1.81606400	2.71503900	1.81200100
TS_{SI3/SI4}			
C	1.15425500	-0.45695300	0.92577100
C	2.12856000	-0.07476400	0.08645000
C	2.54771200	1.31992200	-0.23091200
C	1.59242900	2.25818800	-0.64516900
C	3.87578700	1.74037800	-0.07985400
C	1.95539800	3.57816200	-0.89391700
H	0.56118800	1.94120700	-0.77039800
C	4.23800100	3.06094200	-0.33000800
H	4.63102700	1.03607700	0.26188800
C	3.27935200	3.98524700	-0.73881700
H	1.20113900	4.29091400	-1.21654700
H	5.27104100	3.37051000	-0.19544200
H	3.56182400	5.01589100	-0.93425100
C	0.32226900	0.45627000	1.64418500
O	-0.83196400	0.76220000	1.33276400
O	0.88663800	0.87452600	2.81871200

C	0.00370400	1.58320800	3.71117700
H	-0.85962000	0.96269300	3.97092700
H	0.59697700	1.79487400	4.60211800
H	-0.34325600	2.51712000	3.25863600
P	3.00863500	-1.43953300	-0.71297900
C	4.24450500	-2.20106500	0.37671300
H	5.00505300	-1.46362300	0.64851300
H	3.74127500	-2.55298400	1.28210100
H	4.71710100	-3.04525100	-0.13565300
C	3.86004800	-0.90885500	-2.22511400
H	3.14201500	-0.41479500	-2.88714600
H	4.66463500	-0.20988100	-1.98335900
H	4.27837900	-1.78637200	-2.72772300
C	1.83471100	-2.73302000	-1.17075300
H	1.29834400	-3.05561500	-0.27319600
H	1.12009000	-2.32807100	-1.89361300
H	2.37946700	-3.57321400	-1.61339000
O	-0.28964900	-2.03111400	3.31950300
O	0.23499700	-3.61869800	1.73934200
C	-1.50761300	-2.81691700	3.11780700
C	-1.23001200	-3.53571800	1.75200700
C	-2.70227200	-1.87891200	3.10794600
H	-3.61764600	-2.43263000	2.87210500
H	-2.82141600	-1.43040500	4.09961800
H	-2.57070700	-1.07631300	2.37902000
C	-1.59981700	-3.78345500	4.29619000
H	-1.60363800	-3.20584300	5.22565700
H	-2.52042000	-4.37403700	4.25409400
H	-0.74350700	-4.46503300	4.31622200
C	-1.79457500	-4.94233600	1.64800600
H	-2.88547000	-4.91721900	1.74395200
H	-1.54885400	-5.36177600	0.66721800
H	-1.38939800	-5.60172400	2.41882600
C	-1.64946600	-2.70587400	0.54312700
H	-1.28731200	-3.19779000	-0.36565800
H	-2.73955700	-2.63194800	0.47939000
H	-1.22084900	-1.70019500	0.58982100
B	0.70148100	-2.60187300	2.54978400
H	1.86178500	-2.45452900	2.77596600
TS_{S14/S15}			
C	0.83395200	-0.11323300	0.94970700
C	1.71211300	0.03022900	-0.13604500
C	2.70774400	1.13481700	-0.13076700
C	2.84819600	2.03907200	-1.19532200

C	3.50600900	1.33713300	1.00742500
C	3.76218400	3.08597600	-1.13278100
H	2.20810800	1.93943900	-2.06702900
C	4.41088500	2.39196800	1.07677400
H	3.40836400	0.65063700	1.84532200
C	4.54943700	3.26928700	0.00315200
H	3.84414500	3.77700200	-1.96786400
H	5.01629600	2.52398300	1.97001000
H	5.25632500	4.09273500	0.05374500
C	0.42589300	1.16612500	1.61221200
O	-0.17691800	2.03733200	1.00961700
O	0.73878100	1.26113300	2.91714600
C	0.24874700	2.44637700	3.58760700
H	-0.84270500	2.48780400	3.53697100
H	0.58137800	2.35039400	4.62122600
H	0.67324900	3.34384600	3.12929200
P	1.88365800	-1.26200100	-1.31550000
C	2.84383100	-2.69446300	-0.71700300
H	2.35684500	-3.10957400	0.16856300
H	2.90378500	-3.45635900	-1.50137300
H	3.85202200	-2.35270200	-0.46103400
C	2.78533200	-0.72233400	-2.79719400
H	2.20481500	0.01687200	-3.35382700
H	3.75368600	-0.29666700	-2.52135400
H	2.94392900	-1.60482400	-3.42560600
C	0.28140700	-1.88293900	-1.89049600
H	0.43998900	-2.71300700	-2.58669800
H	-0.29347700	-2.23113000	-1.03088400
H	-0.25241400	-1.07059600	-2.39224000
O	-0.99288300	-1.19170600	2.42929600
O	0.30563800	-2.71168000	1.23812400
C	-1.27734400	-2.50263000	2.97333100
C	-0.81563100	-3.44170500	1.80726700
C	-2.75804600	-2.58566800	3.30742200
H	-3.02477700	-3.60432500	3.60938200
H	-2.98383900	-1.91299100	4.14123800
H	-3.37716700	-2.29705500	2.45478300
C	-0.44268200	-2.68536400	4.24197000
H	-0.67644300	-1.86983600	4.93385300
H	-0.66796800	-3.63464700	4.73837500
H	0.62911700	-2.65147600	4.02065700
C	-0.33117000	-4.81317500	2.25210500
H	-1.13430400	-5.35181600	2.76720800
H	-0.03399700	-5.40063400	1.37695700

H	0.52701500	-4.73606800	2.92362200
C	-1.88226100	-3.59084200	0.72325400
H	-1.44741100	-4.10736300	-0.13876200
H	-2.72934400	-4.18467500	1.08136100
H	-2.25256800	-2.61317000	0.39817900
B	0.18089600	-1.34981900	1.64202000
H	1.32476600	-0.91821700	2.24244700
TS_{S15/S16}			
C	2.14179200	-0.72384500	1.84501400
C	1.62055200	-0.47526600	0.40195900
C	1.54775200	0.91471600	-0.12221400
C	2.56319000	1.86413500	0.11366100
C	0.46713500	1.32858900	-0.92179600
C	2.49944000	3.14821700	-0.41260900
H	3.42641400	1.57980700	0.71314300
C	0.41064700	2.60714000	-1.47102900
H	-0.34429400	0.62672200	-1.09795400
C	1.42266800	3.52975900	-1.21502800
H	3.30234600	3.85317700	-0.20975600
H	-0.44132000	2.89093700	-2.08440100
H	1.37337000	4.53271400	-1.62991300
C	2.20910200	0.48006500	2.73843300
O	1.40003200	1.38221300	2.81157400
O	3.29038300	0.40398100	3.55961100
C	3.38706500	1.44943000	4.55383400
H	2.51172600	1.43624000	5.20957500
H	4.29196900	1.22875900	5.12053300
H	3.46646500	2.42771400	4.07163900
P	2.25954800	-1.54812300	-0.78666800
C	2.18729800	-3.30815000	-0.33566900
H	1.14759600	-3.61951200	-0.21564200
H	2.66038900	-3.88965400	-1.13354700
H	2.71882900	-3.48358500	0.60301300
C	4.03975100	-1.31162700	-1.22182000
H	4.18391300	-0.28906500	-1.58569900
H	4.64980900	-1.45556300	-0.32372600
H	4.36076300	-2.02116900	-1.99196200
C	1.41871000	-1.40262900	-2.39332900
H	1.87976300	-2.10939500	-3.09106500
H	0.35588300	-1.63226600	-2.28132100
H	1.52926400	-0.38707800	-2.78252000
O	-0.18757900	-1.18214200	2.93730600
O	1.17862300	-3.00583500	2.67164600
C	-0.80892900	-2.26273400	3.70539800

C	-0.12517700	-3.53534800	3.10035900
C	-2.31381800	-2.19651800	3.51656500
H	-2.79412500	-3.05087500	4.00536300
H	-2.69903100	-1.28036900	3.97458600
H	-2.58724100	-2.19627900	2.45915100
C	-0.44186300	-2.02468600	5.16739600
H	-0.78934500	-1.02941000	5.46037400
H	-0.91809700	-2.76345700	5.81925100
H	0.64199900	-2.07001400	5.31587700
C	0.11068800	-4.66373400	4.08786900
H	-0.84406600	-5.00805100	4.49944500
H	0.58550100	-5.50674700	3.57633300
H	0.75477200	-4.34925000	4.91185200
C	-0.83001900	-4.05428500	1.85274200
H	-0.21292300	-4.83123800	1.39148800
H	-1.79917600	-4.49347800	2.10777500
H	-0.98769600	-3.25248500	1.12345800
B	1.02190900	-1.65331800	2.48339900
H	3.11966800	-1.22407300	1.89788900

TS_{S15/S21E}

C	2.60445800	-0.64882200	2.17854800
C	3.01938900	-0.53650800	0.74869900
C	2.70197800	0.61188800	-0.07526800
C	2.45794400	0.51144600	-1.46824400
C	2.64639300	1.92485900	0.46224500
C	2.25385300	1.63107600	-2.26722800
H	2.40120500	-0.46857300	-1.93406300
C	2.42673700	3.03625500	-0.33537600
H	2.81780700	2.07713200	1.52503300
C	2.23590300	2.91030900	-1.71526900
H	2.07603600	1.49522500	-3.33178400
H	2.41067400	4.02152100	0.12536000
H	2.05609600	3.78383500	-2.33470900
C	1.78416200	0.32105400	2.79360400
O	0.57379800	0.39328300	2.28562800
O	2.07885500	0.88403000	3.95137900
C	0.96942700	1.44178600	4.71667500
H	0.19578600	0.68227100	4.85297000
H	1.40411100	1.73240400	5.67230300
H	0.56084000	2.31203800	4.19935300
P	3.73030000	-1.95209400	0.04549700
C	4.45740800	-2.97715300	1.36282500
H	3.67395400	-3.37700600	2.01213700
H	4.98971300	-3.81193700	0.89682300

H	5.15752400	-2.38470300	1.95827600
C	5.11442100	-1.50841300	-1.05705500
H	4.78094500	-0.80613500	-1.82425100
H	5.90294000	-1.03946900	-0.46191200
H	5.50064300	-2.41192600	-1.53900200
C	2.75576800	-3.18096400	-0.92173400
H	3.39926400	-4.02046800	-1.20841400
H	1.93387300	-3.53348800	-0.29517700
H	2.33734600	-2.72223900	-1.82165400
O	0.26955600	-1.84963100	3.28006300
O	0.35265200	-1.77042200	0.95529700
C	-0.42458900	-3.01986300	2.78334200
C	-0.79817000	-2.58044000	1.32889500
C	-1.61767000	-3.30819700	3.68153100
H	-2.21963900	-4.12367600	3.26550500
H	-1.26828800	-3.61500500	4.67289800
H	-2.25165400	-2.42612100	3.79662300
C	0.54764500	-4.19867500	2.80820300
H	0.94375700	-4.30784800	3.82291400
H	0.05215600	-5.13435700	2.52922900
H	1.38635800	-4.02958800	2.12540400
C	-0.95639900	-3.72172800	0.33848900
H	-1.79011400	-4.36549900	0.63993300
H	-1.17918700	-3.31989900	-0.65554600
H	-0.05572900	-4.33506200	0.27033300
C	-2.03744000	-1.68423400	1.28857100
H	-2.11625400	-1.23815100	0.29211700
H	-2.95014700	-2.25673700	1.48289100
H	-1.96660400	-0.87743700	2.02452000
B	0.79045300	-1.15453800	2.14892600
H	3.31202600	-1.10955800	2.87126100
TS_{S16/S17}			
C	2.30707700	-0.77234800	1.73025700
C	1.75858500	-0.64723100	0.30913700
C	1.61598400	0.71736100	-0.31934100
C	2.58329800	1.70782600	-0.12072000
C	0.52980700	0.99574000	-1.15506200
C	2.47377000	2.94050100	-0.75263800
H	3.41684000	1.50412100	0.54597600
C	0.41860500	2.23122500	-1.78867200
H	-0.24171000	0.24260700	-1.29584900
C	1.39096100	3.20808800	-1.59067100
H	3.23176000	3.70117200	-0.58496200
H	-0.43500800	2.43265600	-2.43040000

H	1.30224000	4.17526100	-2.07782600
C	2.14241000	0.20891800	2.71997300
O	1.54883800	1.29537100	2.66638100
O	2.74255200	-0.19795100	3.92428600
C	2.50863200	0.67020500	5.03729700
H	1.43823200	0.76190400	5.25560700
H	3.01885700	0.20818400	5.88574900
H	2.91766200	1.67149200	4.86149100
P	2.66180000	-1.69554000	-0.86495600
C	3.19418400	-3.27557400	-0.15623900
H	2.34081600	-3.78404800	0.29703000
H	3.60828000	-3.88175100	-0.96854600
H	3.97080200	-3.10342700	0.59380300
C	4.15814100	-0.87705300	-1.47674600
H	3.88869000	0.00232300	-2.06726000
H	4.77609400	-0.56984400	-0.62733300
H	4.71686500	-1.58424600	-2.09792200
C	1.59956400	-2.06181300	-2.28253400
H	2.14783700	-2.69552000	-2.98625000
H	0.70463000	-2.58525300	-1.93198800
H	1.31085600	-1.13059900	-2.77759900
O	-0.62215600	-0.65482200	1.35572900
O	0.33543100	-2.73884300	1.02525300
C	-1.45822500	-1.62058500	2.05762900
C	-1.06920600	-2.95842100	1.34498600
C	-2.91328800	-1.21756800	1.89458300
H	-3.56927600	-1.98767000	2.31499600
H	-3.09874900	-0.28119100	2.43022200
H	-3.17245400	-1.07169100	0.84322400
C	-1.05554800	-1.59713600	3.53045900
H	-1.18051800	-0.57903800	3.91235600
H	-1.68107200	-2.26992400	4.12547700
H	-0.00595100	-1.88382900	3.65493600
C	-1.19117200	-4.19925700	2.21315200
H	-2.22604700	-4.32652100	2.54947500
H	-0.91095300	-5.08494900	1.63354500
H	-0.54209400	-4.13849700	3.08958100
C	-1.80581300	-3.16007400	0.02213100
H	-1.34248500	-3.99392200	-0.51516700
H	-2.86145400	-3.40008400	0.18425500
H	-1.74087400	-2.26410400	-0.60432200
B	0.52835000	-1.34443200	0.97439300
H	2.88647800	-1.65003000	1.98748400

TS_{S17/S19Z}

C	1.58854500	-0.20370500	1.87899100
C	1.26886300	-0.36592400	0.51826700
C	1.35491500	0.78809600	-0.45230600
C	1.60747700	0.62767000	-1.81944500
C	0.99604800	2.06546300	0.00105800
C	1.53524200	1.70557000	-2.69706000
H	1.86161000	-0.35337200	-2.20864300
C	0.92325900	3.14362600	-0.87405300
H	0.77009600	2.20456000	1.05370500
C	1.19797400	2.97286400	-2.22900500
H	1.74440400	1.55071400	-3.75223500
H	0.65076200	4.12400900	-0.49215900
H	1.14639500	3.81610100	-2.91223700
C	2.60537000	0.66154800	2.38149900
O	3.38294500	1.38171000	1.75102800
O	2.65240100	0.61698300	3.76509500
C	3.64736200	1.45487700	4.37207700
H	3.47547700	2.50919700	4.13159400
H	3.55002800	1.29642900	5.44765600
H	4.65317400	1.17498400	4.04152700
P	2.78331200	-1.95464200	-0.25556900
C	2.39569500	-3.36365500	0.85070200
H	1.54662000	-3.91981800	0.44119900
H	3.25906400	-4.03235800	0.92941800
H	2.13727500	-2.99366000	1.84802100
C	4.43948700	-1.40350400	0.29994600
H	4.80655400	-0.61663200	-0.36556900
H	4.37453100	-1.00157700	1.31381500
H	5.13455800	-2.25046100	0.28547200
C	3.14009100	-2.80191900	-1.86170900
H	3.84842300	-3.62490400	-1.70838100
H	2.20828900	-3.19694700	-2.27715300
H	3.57037200	-2.08635700	-2.56892800
O	-1.13890800	-1.17249700	1.01135300
O	-0.18289200	-1.99305800	-0.90463700
C	-2.08808200	-2.16586400	0.48244200
C	-1.61337600	-2.31678500	-1.00366900
C	-3.49794200	-1.62965200	0.64526800
H	-4.21280300	-2.30804000	0.16747600
H	-3.74578200	-1.56618400	1.70914900
H	-3.60587400	-0.63700500	0.20296400
C	-1.89658700	-3.43170700	1.31008700
H	-2.06466200	-3.19309700	2.36451900
H	-2.61126400	-4.20504200	1.01279900

H	-0.88266200	-3.82948100	1.20302800
C	-1.75821400	-3.71258100	-1.58045600
H	-2.81200600	-4.01060200	-1.58351100
H	-1.39799000	-3.72065000	-2.61374600
H	-1.18797900	-4.44662300	-1.00662300
C	-2.22243500	-1.27811500	-1.93965200
H	-1.70481500	-1.32428100	-2.90262800
H	-3.28523800	-1.47532700	-2.10840600
H	-2.11071600	-0.26627800	-1.53640800
B	-0.02820300	-1.20900200	0.21101300
H	1.10077500	-0.84474400	2.60726900

TS_{S21E/S18}

O	1.51877500	-0.57209100	-0.97444600
O	1.83257800	0.21617800	1.17460100
C	1.95998800	-1.71785800	-0.17887900
C	2.60992400	-1.02006600	1.06768600
C	2.92397500	-2.54030000	-1.01755000
H	3.35931600	-3.34204200	-0.41134400
H	2.38150100	-2.99916000	-1.85029800
H	3.73166400	-1.92759700	-1.42417000
C	0.73855000	-2.55137600	0.18604800
H	0.20196200	-2.82064100	-0.72840900
H	1.03728300	-3.46960800	0.70199800
H	0.04934800	-1.99075000	0.82137600
C	2.49300100	-1.79736000	2.36652200
H	3.01336100	-2.75719800	2.27905000
H	2.96085300	-1.22926700	3.17702300
H	1.45125100	-1.98895300	2.63177800
C	4.05942000	-0.60465300	0.82796500
H	4.38686000	0.03262800	1.65517700
H	4.71893700	-1.47690800	0.78281400
H	4.15990800	-0.04014000	-0.10474400
B	1.34011100	0.47763300	-0.09475800
H	-1.79719500	2.13728100	-1.69851300
C	-0.99519200	1.74575800	-1.07134500
C	-1.21939400	0.64993000	-0.09658200
C	-1.84036000	-0.56718700	-0.60977800
C	-1.68347900	-0.90043500	-1.97735300
C	-2.59915400	-1.47857900	0.16252300
C	-2.20565800	-2.06826900	-2.51474800
H	-1.11516400	-0.22616900	-2.61122000
C	-3.11500100	-2.65031600	-0.37817200
H	-2.79930800	-1.28152100	1.21092200
C	-2.92267500	-2.96697300	-1.72248400

H	-2.04720400	-2.28275100	-3.56955400
H	-3.68685400	-3.31938800	0.26110700
H	-3.33165900	-3.88056600	-2.14393200
C	0.22962100	2.26735600	-1.22543700
O	1.30391900	1.81602100	-0.53388000
O	0.47627900	3.35945500	-1.98598800
C	1.73045000	3.35175700	-2.70323600
H	1.82121700	2.44074000	-3.30647900
H	1.70037900	4.22595700	-3.35502300
H	2.57834300	3.42744500	-2.01668000
P	-1.60003200	1.21044500	1.52228500
C	-1.04780800	0.11188600	2.87051600
H	0.04111800	0.03393300	2.81364500
H	-1.34147900	0.55656600	3.82699300
H	-1.48163400	-0.88676400	2.79437300
C	-3.36549800	1.57695700	1.88350100
H	-3.70704900	2.34983000	1.18731100
H	-3.97720700	0.68153000	1.74405100
H	-3.47739300	1.93630600	2.91198000
C	-0.75423600	2.78248200	1.85334800
H	-1.08976100	3.54212600	1.14303200
H	-1.00169600	3.09726800	2.87198700
H	0.32717600	2.65358300	1.76193300

TS_{S18/S19E}

O	1.30590100	-1.13542700	-1.26030900
O	1.13684300	-0.55980300	0.97788400
C	1.98347000	-2.17441800	-0.51599200
C	2.23498100	-1.49963700	0.88014600
C	3.25384200	-2.56772100	-1.25984800
H	3.83108700	-3.29649800	-0.67944500
H	2.98863200	-3.03021800	-2.21643200
H	3.88545600	-1.69949900	-1.46143600
C	1.04900400	-3.38301200	-0.44065500
H	0.77440100	-3.67532900	-1.45946000
H	1.53487700	-4.23695400	0.04309800
H	0.13103900	-3.14539600	0.10326700
C	2.16090300	-2.45122700	2.06556600
H	2.92230600	-3.23398700	1.97702800
H	2.34852300	-1.89769900	2.99182400
H	1.17819800	-2.92331600	2.13861600
C	3.54896700	-0.71634600	0.93562500
H	3.56062000	-0.11782900	1.85268500
H	4.41253500	-1.38934900	0.95414400
H	3.64734300	-0.04020600	0.08293900

B	0.80311700	-0.15969300	-0.34217900
H	-1.28271600	2.20194500	-1.91765400
C	-0.51870900	1.60207100	-1.43641600
C	-0.67121700	0.43633500	-0.70099900
C	-1.89271500	-0.38769400	-0.74518900
C	-2.07806800	-1.42258500	0.18588600
C	-2.87551400	-0.19377000	-1.72520400
C	-3.20724200	-2.22756600	0.14433200
H	-1.32842000	-1.56623800	0.95951800
C	-4.01007300	-1.00094100	-1.76702800
H	-2.74544100	0.58312900	-2.47287600
C	-4.18249300	-2.01803300	-0.83290300
H	-3.33276200	-3.02069000	0.87663700
H	-4.75964700	-0.83492200	-2.53611300
H	-5.06837100	-2.64628700	-0.86531800
C	0.82875100	2.02182400	-1.36247800
O	1.66118500	1.28881000	-0.73724800
O	1.20519200	3.16567800	-1.92213400
C	2.60522000	3.52240300	-1.79240100
H	3.23381500	2.75988400	-2.25902500
H	2.70605600	4.47454000	-2.31217500
H	2.86978400	3.62957200	-0.73725200
P	-1.13762800	1.43960500	1.65716000
C	-1.27307700	0.83954900	3.40150200
H	-1.99327000	0.01571200	3.44327900
H	-0.29818400	0.46344900	3.72724400
H	-1.60052600	1.63755200	4.07869900
C	-2.78776900	2.21419400	1.38413300
H	-2.80834900	2.68315700	0.39409100
H	-3.56115300	1.43901600	1.41114700
H	-3.00978500	2.97228400	2.14370000
C	-0.04657700	2.91494300	1.83298000
H	0.95024700	2.59479900	2.15186000
H	0.04390800	3.42054100	0.86514700
H	-0.45359600	3.62426400	2.56282400
TS_{S13/S20}			
C	1.18424100	-0.77950000	1.31183200
C	2.01302400	-0.39906700	0.33744300
C	2.11145800	0.95706100	-0.28330300
C	1.01605900	1.48412200	-0.97886500
C	3.26921300	1.73352200	-0.15231900
C	1.08055800	2.76118700	-1.52874100
H	0.11343300	0.88452900	-1.07347300
C	3.32928000	3.01191000	-0.70186800

H	4.11752800	1.34653900	0.40656900
C	2.23693300	3.52806600	-1.39533400
H	0.22346800	3.15864900	-2.06651800
H	4.22943400	3.60867500	-0.58089400
H	2.28485900	4.52470900	-1.82529900
C	0.23207200	0.02349400	1.97295300
O	-0.99590100	0.06243200	1.72932800
O	0.73059300	0.68875000	3.05537900
C	-0.24059200	1.33884600	3.90275200
H	-0.95318400	0.61238400	4.30473300
H	0.33825800	1.78668700	4.71169500
H	-0.78247500	2.11366600	3.35260800
P	2.99016500	-1.70240600	-0.44191600
C	2.79623100	-3.25664700	0.45376800
H	3.16138400	-3.13410700	1.47685600
H	1.73799500	-3.52709900	0.48174900
H	3.37315400	-4.03164900	-0.06107400
C	4.76572600	-1.33799800	-0.55792400
H	4.92122000	-0.44896900	-1.17548600
H	5.17032100	-1.16414500	0.44346700
H	5.27500900	-2.19061500	-1.01853800
C	2.39763700	-1.93591800	-2.14092900
H	1.34197500	-2.22341100	-2.11223500
H	2.49894300	-0.99253500	-2.68677700
H	2.98341100	-2.71299500	-2.64141800
O	-3.18193800	-1.21307500	0.86987100
O	-1.82659200	-0.49277100	-0.85181300
C	-4.05988500	-0.61635100	-0.12557300
C	-3.07308400	0.25274400	-0.97699300
C	-5.15198500	0.17060800	0.58158000
H	-5.77856400	0.69535000	-0.14825000
H	-5.79081000	-0.51663300	1.14566600
H	-4.73406800	0.90274300	1.27631500
C	-4.67649500	-1.76602300	-0.92252700
H	-5.19478300	-2.43577100	-0.22904200
H	-5.40246400	-1.40244400	-1.65709600
H	-3.90422300	-2.34050500	-1.44400700
C	-3.42552600	0.35517400	-2.45265600
H	-4.40993400	0.81901600	-2.57877400
H	-2.68606500	0.98286100	-2.96137300
H	-3.43517600	-0.62570100	-2.93329700
C	-2.86246800	1.65050600	-0.39638500
H	-2.03171500	2.13156900	-0.92267700
H	-3.75572600	2.26858000	-0.53282700

H	-2.61377500	1.60542100	0.66628000
B	-1.88190000	-1.19037900	0.35776700
H	-1.10305800	-2.07410100	0.57518500
TS_{s20/s21z}			
O	-2.08301500	-0.12106300	0.63197300
O	-2.65938700	-0.63845800	-1.57160700
C	-3.12034800	-1.12147700	0.67806100
C	-3.78954900	-0.96698400	-0.72869400
C	-4.03904500	-0.82436300	1.85420800
H	-4.89573200	-1.50762600	1.85861200
H	-3.48999200	-0.96276700	2.79199800
H	-4.40954000	0.20298800	1.82107900
C	-2.46751000	-2.49385900	0.86221900
H	-1.87137400	-2.48159500	1.78058800
H	-3.21641300	-3.28742000	0.95382700
H	-1.80550900	-2.73017800	0.02287200
C	-4.45551200	-2.22750300	-1.25906100
H	-5.24543900	-2.56237000	-0.57724600
H	-4.91247000	-2.02169200	-2.23286300
H	-3.73261700	-3.03746200	-1.38305900
C	-4.77211900	0.20529300	-0.77625400
H	-5.04421300	0.39557800	-1.81947500
H	-5.68780900	-0.01405700	-0.21674400
H	-4.31670000	1.11250500	-0.36660700
B	-1.67757500	0.00035600	-0.75082600
H	-0.45543900	-0.45136800	-0.93853100
C	0.75108500	0.70786400	-0.71796000
C	1.81075100	0.33786200	0.03957900
C	2.94618000	-0.43586400	-0.50318000
C	3.74642600	-1.29459400	0.26763100
C	3.24481700	-0.32658900	-1.87397700
C	4.80462400	-1.99922900	-0.30150100
H	3.54153000	-1.44759900	1.32271000
C	4.29528300	-1.03348600	-2.44079700
H	2.63200400	0.33111300	-2.48479900
C	5.08858000	-1.87410200	-1.65774500
H	5.40176800	-2.65916000	0.32219700
H	4.50320500	-0.92356700	-3.50207000
H	5.91292500	-2.42508200	-2.10120100
C	-0.15253200	1.69774000	-0.93380300
O	-1.42786600	1.45063400	-1.13380400
O	0.26857700	2.97375400	-1.03402200
C	-0.70759100	3.94827600	-1.46722200
H	-1.54549800	3.99595800	-0.76608600

H	-0.17047900	4.89720200	-1.48103600
H	-1.07594400	3.70907700	-2.46887900
P	1.65307400	0.62664200	1.80427400
C	3.19335800	1.20398400	2.58151400
H	3.97961900	0.44926700	2.51648600
H	3.52278600	2.11265700	2.06852600
H	2.99404700	1.42862800	3.63418200
C	1.05123900	-0.82189800	2.73093700
H	0.08129000	-1.09978000	2.30487500
H	1.73900600	-1.66626800	2.64612600
H	0.92682800	-0.55451800	3.78558500
C	0.41474700	1.90899300	2.11082700
H	0.69317700	2.83334300	1.59887100
H	-0.56200400	1.56335200	1.75931800
H	0.37414600	2.08086500	3.19144000

TS_{s21z/s22}

O	3.51777400	-0.91210200	-0.78240300
O	2.33988700	0.62729800	0.47138800
C	4.48582300	0.09341400	-0.34423800
C	3.55982600	1.30315600	0.02346100
C	5.46438300	0.36568800	-1.47218900
H	6.13154700	1.18964100	-1.19772300
H	6.07581500	-0.52413600	-1.65134400
H	4.94850000	0.62526100	-2.39931200
C	5.21114800	-0.48595500	0.86713800
H	5.66818500	-1.43839800	0.58230700
H	6.00184900	0.18600200	1.21477900
H	4.51713500	-0.66812100	1.69448200
C	4.07632800	2.18120500	1.14880700
H	5.04405400	2.61383200	0.87364800
H	3.37347500	3.00108700	1.32651400
H	4.19444500	1.61735000	2.07668300
C	3.17632100	2.15023200	-1.18602400
H	2.37966500	2.84113900	-0.89345200
H	4.02778500	2.73720800	-1.54354800
H	2.80959700	1.52612100	-2.00756300
B	2.32865700	-0.60754000	-0.14735000
H	-0.04169000	0.96319400	-0.10407000
C	-0.60400400	0.04117800	0.07139700
C	-1.96799400	-0.02572800	-0.06197900
C	-2.91834100	1.08832500	0.04996800
C	-4.04375400	1.02103500	0.88485400
C	-2.71193900	2.26349900	-0.69274300
C	-4.94073900	2.08231900	0.96143800

H	-4.20545300	0.13457800	1.49287500
C	-3.60431100	3.32519900	-0.60655900
H	-1.84840800	2.33194200	-1.34969600
C	-4.72812500	3.23958600	0.21596100
H	-5.80500600	2.00742700	1.61631300
H	-3.42741000	4.22287100	-1.19333400
H	-5.42760600	4.06840000	0.27722100
C	-0.02840300	-1.24536100	0.31967100
O	1.29551000	-1.48773900	-0.17781200
O	-0.17227300	-1.81183600	1.59499700
C	0.53512300	-1.11745300	2.64242000
H	0.21134600	-0.06978300	2.69802000
H	0.29415100	-1.63104200	3.57736600
H	1.62063200	-1.15339600	2.48362200
P	-2.36684600	-1.73667600	-0.48527400
C	-1.55132900	-2.21596200	-2.05389200
H	-2.31041100	-2.44122700	-2.81140900
H	-0.92181000	-1.39310300	-2.39650500
H	-0.92732800	-3.09693100	-1.88743400
C	-4.15192800	-1.63602100	-0.98763500
H	-4.80759200	-1.52288800	-0.12008200
H	-4.30609800	-0.78389800	-1.65774300
H	-4.42522100	-2.55807500	-1.51023500
C	-2.50245900	-3.22249900	0.59849800
H	-1.51237000	-3.62593800	0.81246700
H	-2.98144000	-2.93721700	1.54048100
H	-3.12619200	-3.96784400	0.09222000

TS_{S22/S21E}

O	-1.64997900	0.31235100	-0.66601300
O	-2.68160000	-0.62999500	1.17130700
C	-2.80410100	1.15974300	-0.36039700
C	-3.11726300	0.76536700	1.12435800
C	-3.91505900	0.76525000	-1.32871100
H	-4.79438300	1.40393100	-1.20134700
H	-3.54874600	0.88169800	-2.35323400
H	-4.21418400	-0.27799800	-1.18338900
C	-2.40575500	2.61052400	-0.56294900
H	-2.21161500	2.79224400	-1.62469100
H	-3.21732100	3.27395100	-0.24542100
H	-1.50379900	2.86133700	0.00069000
C	-2.26398100	1.52961700	2.13319700
H	-2.57246900	2.57744700	2.20016700
H	-2.38564500	1.06980200	3.11865100
H	-1.20331000	1.49352400	1.86222200

C	-4.58513300	0.84087700	1.50311800
H	-4.70890500	0.55918300	2.55349900
H	-4.95246500	1.86514200	1.37882200
H	-5.19302100	0.17215500	0.88989000
B	-1.72087200	-0.77158800	0.18568600
H	0.59205500	-0.59212900	-2.37981800
C	0.73078200	-0.93098500	-1.34762100
C	1.60039400	-0.32954800	-0.48105000
C	2.08587700	1.05485600	-0.55143800
C	2.72206200	1.52363700	-1.71240600
C	1.91019800	1.94730900	0.51673500
C	3.16845800	2.83746700	-1.79680200
H	2.87080500	0.84358800	-2.54754600
C	2.36635900	3.25931300	0.43278100
H	1.39312500	1.61187000	1.41244900
C	2.99796300	3.71227000	-0.72345500
H	3.66075400	3.17923300	-2.70357600
H	2.21710100	3.93392500	1.27191500
H	3.35189700	4.73714200	-0.78984100
C	0.12557800	-2.10334300	-0.78391300
O	-0.96295200	-1.89697800	0.14566800
O	-0.21170600	-3.12183100	-1.67841500
C	-1.42859100	-2.90068900	-2.42255500
H	-1.41172100	-1.91998000	-2.91755900
H	-1.48658400	-3.68971200	-3.17633000
H	-2.30796600	-2.95783100	-1.76938000
P	2.01866300	-1.56463900	0.77646900
C	3.37834100	-0.71875300	1.71790200
H	4.09715600	-0.27207100	1.02299500
H	2.98347500	0.06829700	2.36647000
H	3.89315100	-1.45609400	2.34200300
C	2.89908700	-2.98453600	0.02732600
H	2.85749300	-2.89875600	-1.05954400
H	3.94251400	-2.99612800	0.36138800
H	2.40798800	-3.91273500	0.32997300
C	1.04599900	-2.13975500	2.23724000
H	0.48513000	-1.29453100	2.65006800
H	0.34117000	-2.91711700	1.94129000
H	1.74068900	-2.51161000	2.99824200
TS_{S22/S23}			
O	0.51417500	-2.52676300	-1.03351600
O	1.02259500	-1.34029300	0.87738900
C	1.96835200	-2.62209600	-0.86388200
C	2.14522500	-2.26109500	0.64999900

C	2.41970200	-4.02120800	-1.23952500
H	3.48689400	-4.13998000	-1.02434800
H	2.26824500	-4.18042100	-2.31156100
H	1.86369700	-4.78527800	-0.69184500
C	2.58710900	-1.58579700	-1.79668000
H	2.25414300	-1.78786500	-2.81920800
H	3.67977900	-1.63776000	-1.77256800
H	2.27536400	-0.57135200	-1.52459500
C	3.44347100	-1.55134000	0.98636200
H	4.29405300	-2.20324400	0.76010200
H	3.46708400	-1.31708600	2.05511900
H	3.55550600	-0.62281600	0.42346900
C	1.93085400	-3.45177900	1.57885300
H	1.87108900	-3.08909600	2.60960300
H	2.76324100	-4.15890800	1.51074600
H	1.00158700	-3.98100300	1.34322400
B	0.07498700	-1.65373700	-0.06498800
H	-0.47656200	1.28897000	1.69028800
C	-0.73688900	1.04677500	0.64831500
C	-0.26996800	1.68533200	-0.43264100
C	0.73924600	2.70718700	-0.27509200
C	2.03659700	2.40095400	0.20130700
C	0.50054900	4.05005500	-0.65207700
C	3.02663300	3.37375900	0.29092600
H	2.25224900	1.37612800	0.49400000
C	1.48403100	5.02312800	-0.53159100
H	-0.48064800	4.31668100	-1.04018600
C	2.76209400	4.69596700	-0.06860100
H	4.01374600	3.09945800	0.65808300
H	1.25830400	6.04919500	-0.81444600
H	3.53484200	5.45579800	0.00532600
C	-1.74180200	-0.06001700	0.50727400
O	-1.24523200	-1.27610300	-0.06992500
O	-2.47915400	-0.33542500	1.67481600
C	-1.73496400	-0.94229100	2.74659400
H	-0.89244800	-0.31756400	3.06089600
H	-2.44176600	-1.04679500	3.57175600
H	-1.36632500	-1.93111500	2.45176700
P	-3.09307800	0.43110700	-0.72403700
C	-3.70325300	2.09417800	-0.37569300
H	-3.93699500	2.17081800	0.69066400
H	-2.93274900	2.82240900	-0.63729600
H	-4.61029900	2.26700000	-0.96414500
C	-4.46317400	-0.73267000	-0.49061900

H	-4.08843600	-1.75418200	-0.60476700
H	-4.88946400	-0.61084000	0.50753700
H	-5.22818500	-0.53822300	-1.24892000
C	-2.57012900	0.28089200	-2.44648500
H	-3.44483000	0.44424900	-3.08634300
H	-1.78668500	1.01554300	-2.64028700
H	-2.17879600	-0.72776200	-2.60707500

TS_{S23/S19Z}

O	0.98727700	-1.63752000	1.23136400
O	0.14681500	-1.10615000	-0.87131000
C	1.34094800	-2.71893600	0.34143600
C	0.33264900	-2.53804000	-0.84491300
C	1.20487200	-4.03794200	1.09180700
H	1.37351000	-4.88492200	0.41690900
H	1.95411000	-4.08515200	1.88934900
H	0.21540500	-4.13993300	1.54375200
C	2.79424400	-2.53616500	-0.10071900
H	3.42909500	-2.46068200	0.78849900
H	3.13938600	-3.38830100	-0.69603600
H	2.91676700	-1.62281100	-0.69002800
C	0.86032100	-2.98732700	-2.20103100
H	1.11835900	-4.05211600	-2.17960300
H	0.08679900	-2.84087100	-2.96268800
H	1.74512800	-2.41802400	-2.49539200
C	-1.01187800	-3.22129300	-0.57590200
H	-1.72059900	-2.92771000	-1.35673100
H	-0.91399900	-4.31167600	-0.60249600
H	-1.42289100	-2.92641000	0.39294000
B	0.26791500	-0.63487500	0.49070400
H	-0.46465000	2.72909700	1.16659900
C	-0.37953600	1.65609200	1.01206600
C	0.68571700	0.94213000	0.60682600
C	1.97321600	1.54399900	0.25646600
C	3.17127800	0.90393200	0.60976100
C	2.04952100	2.76608500	-0.43284900
C	4.40156600	1.47088300	0.29487000
H	3.12139600	-0.03473900	1.15169400
C	3.28016000	3.32497100	-0.75819700
H	1.13177000	3.26722300	-0.72898400
C	4.46225900	2.68077200	-0.39440600
H	5.31812500	0.96481100	0.58676100
H	3.31866400	4.26572200	-1.30117100
H	5.42367000	3.11845500	-0.64870600
C	-1.51980900	0.75734300	1.24375700

O	-1.21492200	-0.50424600	1.15953400
O	-2.42748900	1.16418800	2.16021500
C	-3.47460000	0.22209300	2.45657000
H	-3.06431400	-0.69386100	2.88972500
H	-4.13164200	0.72186900	3.16863500
H	-4.02957900	-0.02171400	1.54158300
P	-2.69233900	1.21404000	-0.78220900
C	-3.96031300	2.53662700	-0.67756300
H	-4.76578100	2.21751900	-0.00875200
H	-3.50385800	3.44290600	-0.26722300
H	-4.37696200	2.75743000	-1.66690700
C	-3.54687800	-0.19217700	-1.59522200
H	-4.33369700	-0.58504700	-0.94472500
H	-3.98541000	0.12825500	-2.54735000
H	-2.81595600	-0.98371200	-1.78293100
C	-1.52368400	1.79772200	-2.06545500
H	-2.03181900	1.89352700	-3.03160600
H	-1.11318100	2.76807700	-1.77157500
H	-0.70178400	1.07895100	-2.14899000

11. DFT-optimized cartesian coordinates of all species involved in the Fe(II) complex mediated C-H borylation reaction.

PEt₃

P	-0.5483870000000000	0.2100590000000000	-1.3727580000000000
C	1.1494930000000000	-0.0630580000000000	-2.0813480000000000
H	1.7140290000000000	-0.6354380000000000	-1.3264140000000000
H	1.0738910000000000	-0.7088630000000000	-2.9747040000000000
C	1.8854510000000000	1.2296140000000000	-2.4036780000000000
H	2.9020630000000000	1.0271880000000000	-2.7752480000000000
H	1.3662340000000000	1.8143630000000000	-3.1792330000000000
H	1.9742540000000000	1.8704700000000000	-1.5126650000000000
C	-1.0771020000000000	-1.5590720000000000	-1.1492860000000000
H	-0.8405390000000000	-2.1303980000000000	-2.0649800000000000
H	-2.1763490000000000	-1.5471510000000000	-1.0612990000000000
C	-0.4693820000000000	-2.2213070000000000	0.0790250000000000
H	-0.7136550000000000	-1.6617890000000000	0.9954280000000000
H	-0.8429170000000000	-3.2497290000000000	0.2029810000000000
H	0.6283840000000000	-2.2799530000000000	0.0120260000000000
C	-1.4732050000000000	0.6128970000000000	-2.9354880000000000
H	-0.9885350000000000	1.5064530000000000	-3.3631500000000000
H	-1.3302150000000000	-0.2033160000000000	-3.6663970000000000
C	-2.9527370000000000	0.8887290000000000	-2.7085100000000000
H	-3.4542560000000000	1.1695630000000000	-3.6477410000000000
H	-3.4778810000000000	0.0060710000000000	-2.3108150000000000
H	-3.0993550000000000	1.7102250000000000	-1.9900490000000000

C₆H₆

C	2.7963220000000000	-2.0666540000000000	-0.3246150000000000
C	2.7210910000000000	-0.6759120000000000	-0.2465890000000000
C	3.4378900000000000	0.0074560000000000	0.7361680000000000
C	4.2302460000000000	-0.6998580000000000	1.6405220000000000
C	4.3057040000000000	-2.0908490000000000	1.5623090000000000
C	3.5888410000000000	-2.7741310000000000	0.5798510000000000
H	2.2352340000000000	-2.6022040000000000	-1.0944960000000000
H	2.1005250000000000	-0.1212290000000000	-0.9548830000000000
H	3.3788360000000000	1.0970530000000000	0.7967200000000000
H	4.7918150000000000	-0.1645850000000000	2.4102530000000000
H	4.9263670000000000	-2.6452680000000000	2.2706690000000000
H	3.6480860000000000	-3.8636980000000000	0.5186660000000000

Ph-Bpin

B	1.7984360000000000	-1.6512490000000000	-0.1529720000000000
O	2.8314770000000000	-2.2705050000000000	0.4937360000000000
O	2.2202180000000000	-0.7488100000000000	-1.0892560000000000
C	4.0413960000000000	-1.5833650000000000	0.1237090000000000

C	3.640802000000000	-0.924980000000000	-1.243790000000000
C	4.320209000000000	-0.557692000000000	1.215808000000000
C	5.174957000000000	-2.586768000000000	0.040269000000000
C	3.844710000000000	-1.856865000000000	-2.432301000000000
C	4.280295000000000	0.422997000000000	-1.513776000000000
H	3.514443000000000	0.188506000000000	1.276006000000000
H	4.375714000000000	-1.076917000000000	2.183307000000000
H	5.271854000000000	-0.033625000000000	1.048317000000000
H	6.095015000000000	-2.105314000000000	-0.323522000000000
H	5.378005000000000	-2.998148000000000	1.039617000000000
H	4.926694000000000	-3.422378000000000	-0.626241000000000
H	3.401459000000000	-2.845544000000000	-2.243271000000000
H	3.346520000000000	-1.423464000000000	-3.311335000000000
H	4.910224000000000	-1.989537000000000	-2.667668000000000
H	3.937488000000000	0.806235000000000	-2.485791000000000
H	4.011187000000000	1.158696000000000	-0.745376000000000
H	5.376385000000000	0.333933000000000	-1.549675000000000
C	-0.712870000000000	-1.331052000000000	-0.608545000000000
C	0.301355000000000	-1.942317000000000	0.144895000000000
C	-0.068667000000000	-2.822177000000000	1.173905000000000
C	-1.410045000000000	-3.084866000000000	1.443284000000000
C	-2.404992000000000	-2.466802000000000	0.684248000000000
C	-2.055979000000000	-1.588642000000000	-0.342955000000000
H	-0.436903000000000	-0.644909000000000	-1.413802000000000
H	0.712463000000000	-3.304157000000000	1.767984000000000
H	-1.684113000000000	-3.772520000000000	2.247373000000000
H	-3.458223000000000	-2.670774000000000	0.894217000000000
H	-2.835661000000000	-1.105384000000000	-0.937186000000000
HBpin			
B	2.313689000000000	0.755771000000000	-1.936970000000000
O	2.389622000000000	-0.100982000000000	-0.883533000000000
O	3.467591000000000	0.847667000000000	-2.650982000000000
C	3.639989000000000	-0.812913000000000	-0.999799000000000
C	4.488109000000000	0.148251000000000	-1.907132000000000
C	4.206367000000000	-1.043854000000000	0.387610000000000
C	3.326101000000000	-2.143946000000000	-1.671567000000000
C	5.416436000000000	-0.550457000000000	-2.881297000000000
C	5.250235000000000	1.201111000000000	-1.112092000000000
H	3.544682000000000	-1.719613000000000	0.948397000000000
H	5.200714000000000	-1.511059000000000	0.329045000000000
H	4.290273000000000	-0.106501000000000	0.951762000000000
H	4.216477000000000	-2.785100000000000	-1.737419000000000
H	2.563403000000000	-2.668800000000000	-1.078827000000000
H	2.925885000000000	-1.995046000000000	-2.684992000000000

H	5.960666000000000	0.198520000000000	-3.474379000000000
H	6.155625000000000	-1.162439000000000	-2.343141000000000
H	4.863328000000000	-1.195743000000000	-3.575283000000000
H	4.594042000000000	1.708975000000000	-0.390386000000000
H	6.098003000000000	0.762928000000000	-0.566701000000000
H	5.639051000000000	1.957628000000000	-1.808477000000000
H	1.319819000000000	1.373913000000000	-2.211198000000000

12

Fe	-1.429380000000000	1.482030000000000	0.411632000000000
P	-0.777513000000000	0.551421000000000	-1.435397000000000
P	-0.048213000000000	0.626515000000000	1.867021000000000
C	0.377674000000000	1.879130000000000	3.193168000000000
H	0.169339000000000	2.851684000000000	2.729169000000000
H	-0.380060000000000	1.746820000000000	3.983665000000000
C	1.772124000000000	1.891066000000000	3.795122000000000
H	2.534643000000000	2.071968000000000	3.023215000000000
H	1.859581000000000	2.698775000000000	4.539682000000000
H	2.025192000000000	0.948985000000000	4.304501000000000
C	-0.779408000000000	-0.742763000000000	2.894718000000000
H	-1.771911000000000	-0.387943000000000	3.210690000000000
H	-0.978021000000000	-1.572182000000000	2.196197000000000
C	0.009659000000000	-1.222895000000000	4.103302000000000
H	0.130785000000000	-0.424894000000000	4.851370000000000
H	-0.507317000000000	-2.058266000000000	4.601957000000000
H	1.016381000000000	-1.577033000000000	3.833811000000000
C	1.591946000000000	-0.128235000000000	1.440791000000000
H	2.046699000000000	0.552445000000000	0.708642000000000
H	2.239722000000000	-0.102938000000000	2.328896000000000
C	1.510189000000000	-1.556507000000000	0.918606000000000
H	0.717490000000000	-1.685378000000000	0.167647000000000
H	2.460374000000000	-1.858635000000000	0.451127000000000
H	1.303324000000000	-2.274029000000000	1.726019000000000
C	1.033384000000000	0.435079000000000	-1.853257000000000
H	1.489287000000000	1.284637000000000	-1.323930000000000
H	1.412744000000000	-0.462483000000000	-1.346506000000000
C	1.484334000000000	0.432891000000000	-3.306215000000000
H	2.585195000000000	0.430571000000000	-3.353658000000000
H	1.133381000000000	-0.448784000000000	-3.859811000000000
H	1.141849000000000	1.326695000000000	-3.848025000000000
C	-1.402522000000000	-1.198169000000000	-1.639603000000000
H	-2.476650000000000	-1.096601000000000	-1.869151000000000
H	-1.371004000000000	-1.611005000000000	-0.618878000000000
C	-0.727488000000000	-2.155861000000000	-2.609239000000000
H	0.337258000000000	-2.294453000000000	-2.366604000000000

H	-1.200702000000000	-3.149696000000000	-2.560452000000000
H	-0.789258000000000	-1.814422000000000	-3.651408000000000
C	-1.481228000000000	1.450647000000000	-2.907261000000000
H	-2.420372000000000	1.889318000000000	-2.546164000000000
H	-0.814709000000000	2.314439000000000	-3.060133000000000
C	-1.747226000000000	0.713536000000000	-4.211111000000000
H	-2.199765000000000	1.399050000000000	-4.945468000000000
H	-0.837633000000000	0.301620000000000	-4.667666000000000
H	-2.455680000000000	-0.116811000000000	-4.069953000000000
B	-0.106567000000000	2.856465000000000	0.001410000000000
O	1.261732000000000	2.886171000000000	0.334778000000000
O	-0.399621000000000	4.048122000000000	-0.677063000000000
C	1.788322000000000	4.195168000000000	0.105971000000000
C	0.803186000000000	4.756681000000000	-0.970375000000000
C	1.712180000000000	4.960488000000000	1.423679000000000
C	3.233978000000000	4.078578000000000	-0.342204000000000
C	1.218524000000000	4.397861000000000	-2.394541000000000
C	0.536967000000000	6.249122000000000	-0.877541000000000
H	2.259549000000000	4.400811000000000	2.195495000000000
H	2.157162000000000	5.962985000000000	1.343936000000000
H	0.668872000000000	5.066397000000000	1.755391000000000
H	3.646763000000000	5.063772000000000	-0.608246000000000
H	3.842628000000000	3.665340000000000	0.475986000000000
H	3.335495000000000	3.411285000000000	-1.208101000000000
H	0.383857000000000	4.625914000000000	-3.073614000000000
H	2.098801000000000	4.968189000000000	-2.725457000000000
H	1.444967000000000	3.326080000000000	-2.482722000000000
H	1.464397000000000	6.827284000000000	-1.010129000000000
H	-0.166111000000000	6.547215000000000	-1.669338000000000
H	0.088573000000000	6.517779000000000	0.087476000000000
C	-2.771024000000000	1.817636000000000	1.961805000000000
C	-2.608153000000000	2.991078000000000	1.177273000000000
H	-2.567117000000000	1.744502000000000	3.029282000000000
C	-3.290657000000000	0.774914000000000	1.132422000000000
C	-3.021904000000000	2.683032000000000	-0.152394000000000
H	-2.264411000000000	3.960595000000000	1.532498000000000
H	-3.552114000000000	-0.234743000000000	1.444022000000000
C	-3.427788000000000	1.316805000000000	-0.171212000000000
H	-3.004542000000000	3.373715000000000	-0.992311000000000
H	-3.810935000000000	0.780175000000000	-1.039302000000000
13			
Fe	0.376422000000000	-0.357193000000000	-1.345969000000000
P	-0.373407000000000	-1.125074000000000	0.540533000000000
C	-0.877059000000000	-2.911568000000000	0.497963000000000

H	-1.485379000000000	-3.037878000000000	-0.410892000000000
H	0.059418000000000	-3.460177000000000	0.301247000000000
C	-1.604179000000000	-3.483450000000000	1.704507000000000
H	-2.591605000000000	-3.018365000000000	1.844007000000000
H	-1.769307000000000	-4.565003000000000	1.579508000000000
H	-1.037893000000000	-3.348505000000000	2.638887000000000
C	0.844370000000000	-1.133390000000000	1.936439000000000
H	1.732382000000000	-1.659244000000000	1.546412000000000
H	0.437915000000000	-1.764020000000000	2.744500000000000
C	1.231250000000000	0.237075000000000	2.473339000000000
H	1.596621000000000	0.902217000000000	1.677902000000000
H	0.375019000000000	0.736474000000000	2.952753000000000
H	2.018921000000000	0.142551000000000	3.236794000000000
C	-1.840648000000000	-0.298842000000000	1.294555000000000
H	-2.101501000000000	-0.809318000000000	2.236441000000000
H	-1.514164000000000	0.717633000000000	1.558414000000000
C	-3.026218000000000	-0.220249000000000	0.346561000000000
H	-3.373654000000000	-1.218350000000000	0.034971000000000
H	-3.877070000000000	0.289565000000000	0.824558000000000
H	-2.752326000000000	0.348840000000000	-0.553579000000000
B	0.151368000000000	1.492541000000000	-0.736800000000000
O	1.215172000000000	2.240973000000000	-0.221598000000000
O	-0.962015000000000	2.316876000000000	-0.869323000000000
C	0.878740000000000	3.631884000000000	-0.307952000000000
C	-0.683187000000000	3.587753000000000	-0.269431000000000
C	1.529068000000000	4.377954000000000	0.841998000000000
C	1.418045000000000	4.144347000000000	-1.639737000000000
C	-1.373984000000000	4.675776000000000	-1.070991000000000
C	-1.233795000000000	3.558090000000000	1.152564000000000
H	2.623127000000000	4.345696000000000	0.732413000000000
H	1.219225000000000	5.434289000000000	0.850626000000000
H	1.273945000000000	3.929300000000000	1.810728000000000
H	2.496811000000000	3.936252000000000	-1.687309000000000
H	0.934727000000000	3.626357000000000	-2.481078000000000
H	1.267358000000000	5.227328000000000	-1.758445000000000
H	-1.104701000000000	5.674780000000000	-0.695016000000000
H	-1.112132000000000	4.617339000000000	-2.135228000000000
H	-2.464810000000000	4.562214000000000	-0.985128000000000
H	-0.703964000000000	2.812806000000000	1.763215000000000
H	-1.149035000000000	4.536367000000000	1.647865000000000
H	-2.296876000000000	3.278630000000000	1.115068000000000
C	-0.728083000000000	0.054907000000000	-2.998590000000000
C	0.661794000000000	0.166005000000000	-3.321064000000000
H	-1.464131000000000	0.855509000000000	-3.045163000000000

C	-0.977869000000000	-1.278971000000000	-2.576324000000000
C	1.247622000000000	-1.112007000000000	-3.080399000000000
H	1.173789000000000	1.050100000000000	-3.697322000000000
H	-1.949612000000000	-1.666499000000000	-2.272570000000000
C	0.248622000000000	-2.017830000000000	-2.644832000000000
H	2.308888000000000	-1.345867000000000	-3.181393000000000
H	0.387811000000000	-3.073492000000000	-2.418928000000000
14			
Fe	0.438401000000000	-0.246926000000000	-1.455720000000000
P	0.603565000000000	1.862535000000000	-0.759828000000000
C	-0.218177000000000	2.966120000000000	-2.006791000000000
H	0.182772000000000	2.684947000000000	-2.991194000000000
H	-1.272384000000000	2.646505000000000	-2.009016000000000
C	-0.111115000000000	4.471803000000000	-1.820919000000000
H	0.931710000000000	4.820713000000000	-1.866068000000000
H	-0.661974000000000	4.991752000000000	-2.620104000000000
H	-0.536817000000000	4.810809000000000	-0.865168000000000
C	-0.262895000000000	2.434097000000000	0.772330000000000
H	-1.312583000000000	2.128244000000000	0.643701000000000
H	-0.242248000000000	3.535049000000000	0.736492000000000
C	0.263851000000000	1.959278000000000	2.115295000000000
H	0.240265000000000	0.866550000000000	2.195108000000000
H	1.302387000000000	2.277407000000000	2.286799000000000
H	-0.356484000000000	2.378791000000000	2.922746000000000
C	2.258487000000000	2.660417000000000	-0.545932000000000
H	2.089277000000000	3.708748000000000	-0.250236000000000
H	2.710493000000000	2.149378000000000	0.315075000000000
C	3.176955000000000	2.577307000000000	-1.752318000000000
H	2.761712000000000	3.099891000000000	-2.628937000000000
H	4.153805000000000	3.035457000000000	-1.532796000000000
H	3.357378000000000	1.531556000000000	-2.041361000000000
B	1.887717000000000	-0.758469000000000	-0.097114000000000
O	2.773509000000000	-1.811718000000000	-0.288022000000000
O	2.284934000000000	-0.002201000000000	0.992973000000000
C	3.925800000000000	-1.586172000000000	0.529650000000000
C	3.339812000000000	-0.694667000000000	1.673429000000000
C	4.479853000000000	-2.923400000000000	0.983752000000000
C	4.956387000000000	-0.850182000000000	-0.320637000000000
C	4.305818000000000	0.318452000000000	2.257700000000000
C	2.691797000000000	-1.510371000000000	2.786596000000000
H	4.861855000000000	-3.479493000000000	0.115224000000000
H	5.310874000000000	-2.783432000000000	1.691518000000000
H	3.706557000000000	-3.536340000000000	1.463919000000000
H	5.164294000000000	-1.445875000000000	-1.221509000000000

H	4.577486000000000	0.131340000000000	-0.640072000000000
H	5.902949000000000	-0.701450000000000	0.218394000000000
H	5.167450000000000	-0.185925000000000	2.720509000000000
H	4.677549000000000	1.013701000000000	1.493932000000000
H	3.798667000000000	0.907110000000000	3.036213000000000
H	1.999915000000000	-2.259325000000000	2.374068000000000
H	3.439539000000000	-2.026377000000000	3.405780000000000
H	2.114865000000000	-0.832856000000000	3.432482000000000
C	1.831397000000000	-0.931722000000000	-2.880576000000000
C	0.837075000000000	-1.927535000000000	-2.634551000000000
H	2.900942000000000	-1.048430000000000	-2.728511000000000
C	1.167229000000000	0.218073000000000	-3.373907000000000
C	-0.425415000000000	-1.387278000000000	-2.970933000000000
H	1.022929000000000	-2.913855000000000	-2.213503000000000
H	1.650161000000000	1.147302000000000	-3.669221000000000
C	-0.228115000000000	-0.051711000000000	-3.428886000000000
H	-1.383770000000000	-1.892179000000000	-2.866602000000000
H	-0.997455000000000	0.630592000000000	-3.782692000000000
C	-2.483595000000000	0.329648000000000	-1.172512000000000
C	-1.328266000000000	-0.196495000000000	-0.554967000000000
C	-1.534235000000000	-0.692174000000000	0.751670000000000
C	-2.770285000000000	-0.641964000000000	1.398512000000000
C	-3.880841000000000	-0.092285000000000	0.760667000000000
C	-3.726279000000000	0.388905000000000	-0.538364000000000
H	-2.425236000000000	0.720490000000000	-2.191680000000000
H	0.614232000000000	-1.123253000000000	-0.212095000000000
H	-0.696972000000000	-1.129128000000000	1.304554000000000
H	-2.862281000000000	-1.038197000000000	2.414364000000000
H	-4.850279000000000	-0.046785000000000	1.263349000000000
H	-4.582367000000000	0.815848000000000	-1.069846000000000

15

Fe	0.275883000000000	-0.002142000000000	-1.494313000000000
P	0.522040000000000	2.215338000000000	-1.131376000000000
C	-0.058280000000000	3.291153000000000	-2.530404000000000
H	0.202200000000000	2.791354000000000	-3.472768000000000
H	-1.159677000000000	3.258853000000000	-2.472544000000000
C	0.438859000000000	4.728599000000000	-2.561931000000000
H	1.528670000000000	4.780522000000000	-2.702419000000000
H	-0.024639000000000	5.273039000000000	-3.399028000000000
H	0.196404000000000	5.283706000000000	-1.643486000000000
C	-0.296088000000000	3.128744000000000	0.267070000000000
H	-1.353492000000000	2.815315000000000	0.256461000000000
H	-0.298704000000000	4.192930000000000	-0.016011000000000
C	0.311195000000000	2.970671000000000	1.654109000000000

H	0.450323000000000	1.918427000000000	1.936933000000000
H	1.304624000000000	3.440307000000000	1.705317000000000
H	-0.327022000000000	3.464376000000000	2.403016000000000
C	2.286818000000000	2.689352000000000	-0.891810000000000
H	2.341398000000000	3.766563000000000	-0.663868000000000
H	2.585189000000000	2.143143000000000	0.017928000000000
C	3.197627000000000	2.327539000000000	-2.053390000000000
H	2.928745000000000	2.864596000000000	-2.976860000000000
H	4.243411000000000	2.579545000000000	-1.820076000000000
H	3.154357000000000	1.250006000000000	-2.268190000000000
B	1.351681000000000	-0.745122000000000	0.428484000000000
O	2.221338000000000	-1.877848000000000	0.443600000000000
O	1.864550000000000	0.221261000000000	1.366813000000000
C	3.420941000000000	-1.487332000000000	1.088266000000000
C	2.910326000000000	-0.401209000000000	2.096813000000000
C	4.054157000000000	-2.706677000000000	1.735906000000000
C	4.372520000000000	-0.902475000000000	0.044560000000000
C	3.942709000000000	0.644091000000000	2.482890000000000
C	2.303159000000000	-1.026937000000000	3.351293000000000
H	4.388805000000000	-3.407966000000000	0.956771000000000
H	4.929836000000000	-2.426075000000000	2.341273000000000
H	3.334889000000000	-3.233390000000000	2.376328000000000
H	4.505988000000000	-1.640324000000000	-0.760610000000000
H	3.957492000000000	0.013155000000000	-0.399869000000000
H	5.360846000000000	-0.668110000000000	0.466657000000000
H	4.808062000000000	0.181496000000000	2.982231000000000
H	4.300924000000000	1.198155000000000	1.605007000000000
H	3.495184000000000	1.368273000000000	3.180374000000000
H	1.580925000000000	-1.810866000000000	3.080736000000000
H	3.066092000000000	-1.461647000000000	4.014177000000000
H	1.764030000000000	-0.246486000000000	3.908276000000000
C	1.235299000000000	-0.969226000000000	-3.059465000000000
C	0.197843000000000	-1.797338000000000	-2.564558000000000
H	2.297431000000000	-1.209774000000000	-3.056828000000000
C	0.660204000000000	0.247924000000000	-3.504421000000000
C	-1.029642000000000	-1.083451000000000	-2.706824000000000
H	0.321763000000000	-2.785956000000000	-2.131409000000000
H	1.209537000000000	1.067128000000000	-3.963232000000000
C	-0.759796000000000	0.172013000000000	-3.294994000000000
H	-2.003832000000000	-1.429873000000000	-2.364861000000000
H	-1.496584000000000	0.931474000000000	-3.548615000000000
C	-1.200351000000000	-0.087863000000000	0.347225000000000
C	-0.198307000000000	-1.082495000000000	0.360690000000000
C	-0.631839000000000	-2.439171000000000	0.288863000000000

C	-1.965134000000000	-2.771897000000000	0.210028000000000
C	-2.950076000000000	-1.756360000000000	0.155288000000000
C	-2.571598000000000	-0.434485000000000	0.228678000000000
H	-0.964501000000000	0.920861000000000	0.669538000000000
H	1.649071000000000	-0.067233000000000	-0.799685000000000
H	0.134308000000000	-3.218006000000000	0.332375000000000
H	-2.270671000000000	-3.821705000000000	0.200336000000000
H	-4.007432000000000	-2.025547000000000	0.086998000000000
H	-3.327398000000000	0.355725000000000	0.236745000000000
16			
Fe	1.070803000000000	1.495486000000000	-1.638142000000000
P	0.087784000000000	1.992540000000000	0.241564000000000
C	0.951120000000000	1.256274000000000	1.708191000000000
H	0.640305000000000	0.197317000000000	1.729738000000000
H	2.016625000000000	1.250084000000000	1.427963000000000
C	0.775717000000000	1.903695000000000	3.074458000000000
H	1.153225000000000	2.936757000000000	3.084124000000000
H	-0.273750000000000	1.932287000000000	3.397713000000000
H	1.341191000000000	1.345059000000000	3.836540000000000
C	-0.049996000000000	3.794075000000000	0.619039000000000
H	-0.538950000000000	3.918924000000000	1.598944000000000
H	-0.752569000000000	4.189523000000000	-0.133990000000000
C	1.264927000000000	4.553816000000000	0.562590000000000
H	1.747138000000000	4.416802000000000	-0.414909000000000
H	1.102761000000000	5.628716000000000	0.736912000000000
H	1.975831000000000	4.195935000000000	1.323389000000000
C	-1.669747000000000	1.426735000000000	0.382552000000000
H	-2.178754000000000	1.898562000000000	-0.475012000000000
H	-1.638389000000000	0.350823000000000	0.143581000000000
C	-2.449467000000000	1.669803000000000	1.665361000000000
H	-2.458353000000000	2.731714000000000	1.953865000000000
H	-3.498318000000000	1.357620000000000	1.542001000000000
H	-2.038778000000000	1.095255000000000	2.508224000000000
C	-0.358044000000000	2.238115000000000	-2.881061000000000
C	0.943192000000000	2.587539000000000	-3.339507000000000
H	-1.139676000000000	2.946647000000000	-2.606502000000000
C	-0.471998000000000	0.809423000000000	-2.879935000000000
C	1.659730000000000	1.381254000000000	-3.611648000000000
H	1.325343000000000	3.601870000000000	-3.443278000000000
H	-1.350289000000000	0.225755000000000	-2.609509000000000
C	0.782191000000000	0.300421000000000	-3.305583000000000
H	2.679113000000000	1.300999000000000	-3.983908000000000
H	1.045814000000000	-0.757613000000000	-3.355455000000000
H	2.283045000000000	2.254807000000000	-1.076005000000000

17

Fe	-1.427050000000000	1.171452000000000	0.257146000000000
P	-0.738558000000000	0.002758000000000	-1.426018000000000
P	-0.177880000000000	0.445009000000000	1.872857000000000
C	0.439836000000000	1.893738000000000	2.880251000000000
H	0.477183000000000	2.721038000000000	2.156391000000000
H	-0.385492000000000	2.138546000000000	3.570157000000000
C	1.756946000000000	1.803389000000000	3.635926000000000
H	2.608463000000000	1.666715000000000	2.952471000000000
H	1.939182000000000	2.735479000000000	4.194249000000000
H	1.778698000000000	0.978270000000000	4.362680000000000
C	-1.056152000000000	-0.589196000000000	3.143844000000000
H	-1.984702000000000	-0.045959000000000	3.376851000000000
H	-1.381332000000000	-1.494518000000000	2.604731000000000
C	-0.326129000000000	-0.950601000000000	4.427649000000000
H	-0.097326000000000	-0.058222000000000	5.028966000000000
H	-0.944408000000000	-1.613266000000000	5.053924000000000
H	0.622878000000000	-1.475366000000000	4.237692000000000
C	1.364373000000000	-0.554490000000000	1.632123000000000
H	1.946293000000000	-0.041953000000000	0.850405000000000
H	1.973163000000000	-0.504160000000000	2.546971000000000
C	1.108950000000000	-2.010369000000000	1.269369000000000
H	2.035079000000000	-2.505645000000000	0.938701000000000
H	0.725788000000000	-2.577746000000000	2.130425000000000
H	0.369597000000000	-2.113034000000000	0.462354000000000
C	1.062374000000000	-0.249738000000000	-1.785676000000000
H	1.472554000000000	-0.892902000000000	-0.996220000000000
H	1.145363000000000	-0.830179000000000	-2.717207000000000
C	1.862391000000000	1.038378000000000	-1.891023000000000
H	2.931410000000000	0.823934000000000	-2.045601000000000
H	1.524441000000000	1.658947000000000	-2.735477000000000
H	1.751251000000000	1.645965000000000	-0.981242000000000
C	-1.439121000000000	-1.726763000000000	-1.565217000000000
H	-2.435326000000000	-1.595639000000000	-2.021394000000000
H	-1.637721000000000	-2.031522000000000	-0.525619000000000
C	-0.657120000000000	-2.813542000000000	-2.288451000000000
H	0.307579000000000	-3.014924000000000	-1.798803000000000
H	-1.223066000000000	-3.758698000000000	-2.289699000000000
H	-0.445978000000000	-2.556436000000000	-3.336022000000000
C	-1.283493000000000	0.775617000000000	-3.028385000000000
H	-2.375342000000000	0.886990000000000	-2.944460000000000
H	-0.882920000000000	1.801901000000000	-2.996860000000000
C	-0.931624000000000	0.096702000000000	-4.342056000000000
H	-1.297191000000000	0.693612000000000	-5.192674000000000

H	0.154358000000000	-0.022349000000000	-4.475577000000000
H	-1.391574000000000	-0.899289000000000	-4.426241000000000
C	-2.773334000000000	1.944047000000000	1.637603000000000
C	-2.477169000000000	2.912797000000000	0.645484000000000
H	-2.620926000000000	2.073205000000000	2.708471000000000
C	-3.352440000000000	0.798051000000000	0.999656000000000
C	-2.862181000000000	2.383462000000000	-0.619085000000000
H	-2.030456000000000	3.889544000000000	0.823156000000000
H	-3.719133000000000	-0.102372000000000	1.489380000000000
C	-3.391973000000000	1.074636000000000	-0.390152000000000
H	-2.782211000000000	2.890177000000000	-1.578429000000000
H	-3.795207000000000	0.407073000000000	-1.151875000000000
H	-0.191969000000000	1.987229000000000	-0.046368000000000

S24

Fe	0.5102490000000	-0.4223730000000	0.6494830000000
P	0.0763020000000	1.7910520000000	0.7305890000000
C	1.5481360000000	2.9155080000000	0.6120260000000
H	1.9523900000000	2.8122310000000	-0.4070510000000
H	1.2157340000000	3.9627270000000	0.6997300000000
C	2.6138330000000	2.5828830000000	1.6441850000000
H	3.5335920000000	3.1630450000000	1.4733920000000
H	2.2740640000000	2.8036070000000	2.6676650000000
H	2.8629960000000	1.5113480000000	1.6044160000000
C	-1.1489200000000	2.6326360000000	-0.3814160000000
H	-1.2173230000000	3.6730980000000	-0.0275570000000
H	-2.1126160000000	2.1545500000000	-0.1425020000000
C	-0.9386790000000	2.6235400000000	-1.8856230000000
H	-0.0112870000000	3.1398160000000	-2.1757500000000
H	-0.9106080000000	1.6020090000000	-2.2870010000000
H	-1.7711110000000	3.1526860000000	-2.3752230000000
C	-0.6350410000000	2.3215090000000	2.3670900000000
H	-1.4922240000000	1.6549560000000	2.5526290000000
H	0.1183910000000	2.0504910000000	3.1194190000000
C	-1.0396610000000	3.7754840000000	2.5558230000000
H	-0.2173440000000	4.4703800000000	2.3247060000000
H	-1.9011760000000	4.0562820000000	1.9336570000000
H	-1.3273130000000	3.9528920000000	3.6038480000000
B	2.1939190000000	0.7188850000000	-1.7620940000000
O	2.3159130000000	-0.1437430000000	-0.6936170000000
O	3.3189190000000	0.8105740000000	-2.5102290000000
C	3.5580840000000	-0.8928810000000	-0.9244750000000
C	4.3641180000000	0.1133430000000	-1.8093980000000
C	4.2629080000000	-1.2282310000000	0.3710130000000
C	3.1909330000000	-2.1628740000000	-1.6758350000000

C	5.289631000000	-0.537570000000	-2.818226000000
C	5.118100000000	1.156217000000	-0.992658000000
H	3.770205000000	-2.062291000000	0.882785000000
H	5.293451000000	-1.541170000000	0.146454000000
H	4.302180000000	-0.367886000000	1.049900000000
H	4.064284000000	-2.821991000000	-1.777475000000
H	2.410841000000	-2.698288000000	-1.120223000000
H	2.802987000000	-1.944675000000	-2.680395000000
H	5.817006000000	0.242016000000	-3.386151000000
H	6.043479000000	-1.158414000000	-2.311745000000
H	4.738081000000	-1.162403000000	-3.531435000000
H	4.472552000000	1.604932000000	-0.225133000000
H	6.001941000000	0.728065000000	-0.500174000000
H	5.452668000000	1.955652000000	-1.668673000000
C	1.590503000000	-1.368235000000	2.248814000000
C	0.533227000000	-0.606097000000	2.774899000000
H	2.638549000000	-1.237694000000	2.503367000000
C	1.032229000000	-2.341015000000	1.357681000000
C	-0.695707000000	-1.081313000000	2.217097000000
H	0.643048000000	0.189228000000	3.507714000000
H	1.574718000000	-3.103837000000	0.802453000000
C	-0.371899000000	-2.166723000000	1.356062000000
H	-1.697169000000	-0.724114000000	2.449631000000
H	-1.082175000000	-2.745953000000	0.769775000000
C	-2.085023000000	-0.458273000000	-0.759412000000
C	-0.689801000000	-0.642518000000	-0.887949000000
C	-0.273488000000	-1.070280000000	-2.164446000000
C	-1.152318000000	-1.245444000000	-3.237450000000
C	-2.516955000000	-1.015747000000	-3.075663000000
C	-2.979248000000	-0.629915000000	-1.816036000000
H	-2.496064000000	-0.157147000000	0.210787000000
H	1.215054000000	1.344881000000	-2.001281000000
H	0.782260000000	-1.284416000000	-2.345412000000
H	-0.763148000000	-1.568134000000	-4.208445000000
H	-3.209989000000	-1.145265000000	-3.911064000000
H	-4.048609000000	-0.458970000000	-1.655633000000
S25			
Fe	0.104448000000	0.018415000000	-0.163208000000
P	0.249451000000	2.150283000000	0.629016000000
C	0.306040000000	2.287439000000	2.475466000000
H	0.189263000000	3.353574000000	2.730169000000
H	-0.597886000000	1.785763000000	2.854001000000
C	1.541988000000	1.711254000000	3.137832000000
H	2.453083000000	2.251894000000	2.841363000000

H	1.462749000000	1.774293000000	4.233551000000
H	1.678201000000	0.656820000000	2.866103000000
C	1.689200000000	3.169895000000	0.101538000000
H	1.651401000000	3.224966000000	-0.997032000000
H	2.570242000000	2.542721000000	0.305492000000
C	1.823156000000	4.556042000000	0.709188000000
H	2.715566000000	5.060005000000	0.307856000000
H	0.958144000000	5.197072000000	0.479628000000
H	1.934444000000	4.523246000000	1.803510000000
C	-1.213062000000	3.250905000000	0.348523000000
H	-2.071006000000	2.740722000000	0.816007000000
H	-1.044955000000	4.164899000000	0.941506000000
C	-1.536753000000	3.606726000000	-1.091381000000
H	-0.689840000000	4.096819000000	-1.596119000000
H	-1.805872000000	2.716000000000	-1.673240000000
H	-2.388180000000	4.302820000000	-1.131931000000
B	2.527203000000	0.142980000000	-1.550670000000
O	3.554179000000	-0.853925000000	-1.817605000000
O	2.128536000000	-0.137380000000	-0.104424000000
C	3.749099000000	-1.703843000000	-0.719669000000
C	3.198587000000	-0.873783000000	0.492777000000
C	2.969553000000	-3.003888000000	-0.934100000000
C	5.232080000000	-2.038596000000	-0.607362000000
C	4.225578000000	0.145673000000	0.983319000000
C	2.726754000000	-1.730237000000	1.651395000000
H	3.287611000000	-3.444477000000	-1.890601000000
H	3.151451000000	-3.745055000000	-0.141174000000
H	1.892627000000	-2.804489000000	-0.997916000000
H	5.533460000000	-2.637877000000	-1.479374000000
H	5.844604000000	-1.128179000000	-0.602557000000
H	5.451316000000	-2.623623000000	0.299831000000
H	5.075107000000	-0.337401000000	1.486658000000
H	4.604859000000	0.742691000000	0.142341000000
H	3.746949000000	0.824095000000	1.701488000000
H	2.387247000000	-1.107425000000	2.490376000000
H	1.907709000000	-2.397829000000	1.364334000000
H	3.560541000000	-2.348440000000	2.017025000000
C	-1.952305000000	-0.255476000000	-0.333206000000
C	-1.277321000000	-1.389933000000	-0.868470000000
H	-2.638693000000	0.397852000000	-0.867665000000
C	-1.570814000000	-0.154515000000	1.033033000000
C	-0.489435000000	-1.973544000000	0.144778000000
H	-1.312165000000	-1.711233000000	-1.907606000000
H	-1.929526000000	0.593272000000	1.738179000000

C	-0.649541000000	-1.193179000000	1.332436000000
H	0.145969000000	-2.847757000000	0.026917000000
H	-0.182137000000	-1.372362000000	2.298287000000
C	0.221469000000	0.988511000000	-2.597152000000
C	1.175614000000	-0.034175000000	-2.449741000000
C	0.992023000000	-1.191539000000	-3.242571000000
C	-0.080496000000	-1.327169000000	-4.110411000000
C	-1.042996000000	-0.308196000000	-4.202678000000
C	-0.888879000000	0.845849000000	-3.450737000000
H	0.410960000000	1.965714000000	-2.149940000000
H	2.963670000000	1.297940000000	-1.684934000000
H	1.754345000000	-1.971496000000	-3.189742000000
H	-0.175487000000	-2.221501000000	-4.732658000000
H	-1.889466000000	-0.411257000000	-4.886582000000
H	-1.607078000000	1.663268000000	-3.557224000000
S26			
Fe	-0.033495000000	-0.486815000000	1.039583000000
P	-0.325842000000	1.701319000000	0.991040000000
C	1.052575000000	2.547596000000	0.103133000000
H	1.004729000000	2.188328000000	-0.936977000000
H	0.869411000000	3.633963000000	0.071900000000
C	2.408148000000	2.227785000000	0.715846000000
H	3.225709000000	2.666943000000	0.124365000000
H	2.496032000000	2.616197000000	1.742519000000
H	2.572152000000	1.139529000000	0.767725000000
C	-1.856396000000	2.376741000000	0.193552000000
H	-2.128208000000	3.311843000000	0.709878000000
H	-2.643679000000	1.641785000000	0.426992000000
C	-1.786365000000	2.608662000000	-1.309083000000
H	-1.071557000000	3.405200000000	-1.564303000000
H	-1.494227000000	1.697610000000	-1.849631000000
H	-2.772014000000	2.919250000000	-1.688458000000
C	-0.360399000000	2.537223000000	2.642018000000
H	-1.314995000000	2.232337000000	3.102345000000
H	0.427245000000	2.063078000000	3.247550000000
C	-0.214742000000	4.050386000000	2.658020000000
H	0.776052000000	4.369129000000	2.301082000000
H	-0.969335000000	4.549284000000	2.030616000000
H	-0.333809000000	4.439338000000	3.680988000000
C	1.071128000000	-1.850240000000	2.148959000000
C	0.603522000000	-0.828871000000	3.015835000000
H	2.120442000000	-2.077888000000	1.954233000000
C	-0.037620000000	-2.492844000000	1.529141000000
C	-0.823398000000	-0.810377000000	2.898840000000

H	1.216670000000	-0.188281000000	3.647081000000
H	0.007276000000	-3.310265000000	0.812066000000
C	-1.215651000000	-1.835282000000	1.993728000000
H	-1.503354000000	-0.139962000000	3.422706000000
H	-2.238064000000	-2.060556000000	1.694205000000
C	-2.037500000000	-0.932677000000	-1.195074000000
C	-0.747098000000	-0.623683000000	-0.731919000000
C	0.247801000000	-0.458064000000	-1.719240000000
C	-0.022654000000	-0.590252000000	-3.082460000000
C	-1.318698000000	-0.882574000000	-3.510307000000
C	-2.323351000000	-1.054015000000	-2.556527000000
H	-2.852795000000	-1.068583000000	-0.476580000000
H	1.276479000000	-0.205409000000	-1.424111000000
H	0.778979000000	-0.455089000000	-3.815007000000
H	-1.543027000000	-0.975086000000	-4.575992000000
H	-3.343603000000	-1.284382000000	-2.878677000000

TS_{13/14}

Fe	0.5404850000000000	0.1202640000000000	-1.4235210000000000
P	0.6029310000000000	2.2489580000000000	-0.8623160000000000
C	-0.2438310000000000	3.3454410000000000	-2.0979570000000000
H	0.2554740000000000	3.1547020000000000	-3.0612100000000000
H	-1.2588450000000000	2.9299140000000000	-2.2107000000000000
C	-0.3025880000000000	4.8389750000000000	-1.8193670000000000
H	0.7006390000000000	5.2841260000000000	-1.7386190000000000
H	-0.8240410000000000	5.3620090000000000	-2.6361330000000000
H	-0.8453580000000000	5.0659190000000000	-0.8897370000000000
C	-0.1967590000000000	2.8047660000000000	0.7168090000000000
H	-1.2864650000000000	2.7772140000000000	0.5633520000000000
H	0.0715280000000000	3.8650680000000000	0.8542050000000000
C	0.1801310000000000	2.0055160000000000	1.9531660000000000
H	-0.1695060000000000	0.9654080000000000	1.8832740000000000
H	1.2675570000000000	1.9786440000000000	2.1037930000000000
H	-0.2787180000000000	2.4476240000000000	2.8509630000000000
C	2.2491410000000000	3.0675100000000000	-0.6512020000000000
H	2.0716850000000000	4.1410030000000000	-0.4750490000000000
H	2.6523580000000000	2.6386910000000000	0.2767370000000000
C	3.2456250000000000	2.8542830000000000	-1.7756930000000000
H	2.8865100000000000	3.2562150000000000	-2.7366950000000000
H	4.1979980000000000	3.3581940000000000	-1.5485840000000000
H	3.4572880000000000	1.7837930000000000	-1.9077680000000000
B	1.9314400000000000	-0.3891650000000000	-0.1121110000000000
O	2.2037440000000000	-1.7328870000000000	0.1380570000000000
O	2.8249940000000000	0.3928510000000000	0.6122300000000000
C	3.4622190000000000	-1.8394040000000000	0.8107490000000000

C	3.576926000000000	-0.442956000000000	1.503668000000000
C	3.421024000000000	-3.025186000000000	1.756508000000000
C	4.531877000000000	-2.057280000000000	-0.254875000000000
C	4.988303000000000	0.102341000000000	1.618900000000000
C	2.888754000000000	-0.405572000000000	2.863554000000000
H	3.336379000000000	-3.956124000000000	1.176816000000000
H	4.340469000000000	-3.081850000000000	2.358936000000000
H	2.558604000000000	-2.969454000000000	2.433007000000000
H	4.255632000000000	-2.933181000000000	-0.859658000000000
H	4.605542000000000	-1.188869000000000	-0.925690000000000
H	5.522094000000000	-2.239010000000000	0.187379000000000
H	5.619728000000000	-0.566953000000000	2.222822000000000
H	5.453142000000000	0.229813000000000	0.632907000000000
H	4.966813000000000	1.085197000000000	2.112566000000000
H	1.861728000000000	-0.793009000000000	2.798132000000000
H	3.439279000000000	-0.991760000000000	3.613338000000000
H	2.838187000000000	0.635175000000000	3.214169000000000
C	1.893483000000000	-0.656478000000000	-2.782819000000000
C	0.873980000000000	-1.627344000000000	-2.532871000000000
H	2.963174000000000	-0.795225000000000	-2.636743000000000
C	1.269676000000000	0.496263000000000	-3.331862000000000
C	-0.362207000000000	-1.056267000000000	-2.929740000000000
H	1.023414000000000	-2.608939000000000	-2.090235000000000
H	1.783941000000000	1.398929000000000	-3.654364000000000
C	-0.136128000000000	0.248382000000000	-3.428618000000000
H	-1.337105000000000	-1.529105000000000	-2.822091000000000
H	-0.889422000000000	0.928834000000000	-3.820206000000000
C	-2.247647000000000	0.356425000000000	-0.367585000000000
C	-1.088587000000000	-0.437436000000000	-0.313464000000000
C	-1.228868000000000	-1.744540000000000	0.189677000000000
C	-2.467990000000000	-2.250308000000000	0.579155000000000
C	-3.609201000000000	-1.454087000000000	0.490019000000000
C	-3.490280000000000	-0.147629000000000	0.014944000000000
H	-2.196479000000000	1.374577000000000	-0.756224000000000
H	0.194799000000000	-0.152038000000000	0.020754000000000
H	-0.334142000000000	-2.368474000000000	0.272713000000000
H	-2.541160000000000	-3.273346000000000	0.958340000000000
H	-4.583602000000000	-1.845666000000000	0.792437000000000
H	-4.377177000000000	0.487153000000000	-0.066145000000000
TS_{14/15}			
Fe	1.051750000000000	0.508524000000000	-1.470411000000000
P	0.188642000000000	2.372808000000000	-0.644975000000000
C	-0.853122000000000	3.341028000000000	-1.823292000000000
H	-0.261896000000000	3.440578000000000	-2.747021000000000

H	-1.693183000000000	2.673534000000000	-2.072366000000000
C	-1.358376000000000	4.701107000000000	-1.368245000000000
H	-0.533864000000000	5.400304000000000	-1.162536000000000
H	-1.983389000000000	5.156712000000000	-2.151670000000000
H	-1.975840000000000	4.632886000000000	-0.460521000000000
C	-0.890419000000000	2.232796000000000	0.843432000000000
H	-1.736297000000000	1.596536000000000	0.542144000000000
H	-1.290455000000000	3.234975000000000	1.067589000000000
C	-0.196708000000000	1.648440000000000	2.064927000000000
H	0.258282000000000	0.673373000000000	1.844015000000000
H	0.589988000000000	2.315289000000000	2.450492000000000
H	-0.923461000000000	1.497966000000000	2.877611000000000
C	1.422980000000000	3.613162000000000	-0.037074000000000
H	0.864132000000000	4.456921000000000	0.401181000000000
H	1.945405000000000	3.122635000000000	0.800167000000000
C	2.436173000000000	4.104240000000000	-1.056245000000000
H	1.952775000000000	4.582659000000000	-1.922768000000000
H	3.109231000000000	4.849483000000000	-0.605490000000000
H	3.055934000000000	3.276154000000000	-1.428255000000000
B	2.282064000000000	-0.427865000000000	-0.023874000000000
O	1.940848000000000	-1.075611000000000	1.144634000000000
O	3.622462000000000	-0.636680000000000	-0.306474000000000
C	2.988095000000000	-2.000329000000000	1.471389000000000
C	4.224302000000000	-1.316565000000000	0.802595000000000
C	3.067995000000000	-2.141292000000000	2.978859000000000
C	2.629231000000000	-3.336457000000000	0.831013000000000
C	5.281035000000000	-2.273119000000000	0.284654000000000
C	4.860200000000000	-0.251560000000000	1.689110000000000
H	2.153875000000000	-2.623341000000000	3.354658000000000
H	3.926172000000000	-2.767245000000000	3.266234000000000
H	3.162934000000000	-1.164830000000000	3.470556000000000
H	1.639350000000000	-3.650916000000000	1.191317000000000
H	2.574987000000000	-3.250508000000000	-0.264046000000000
H	3.357018000000000	-4.119385000000000	1.087552000000000
H	5.698671000000000	-2.875920000000000	1.105130000000000
H	4.872784000000000	-2.949978000000000	-0.476743000000000
H	6.103621000000000	-1.704389000000000	-0.172962000000000
H	4.099086000000000	0.434759000000000	2.088676000000000
H	5.410185000000000	-0.694467000000000	2.531789000000000
H	5.566394000000000	0.336169000000000	1.084970000000000
C	2.755481000000000	0.530086000000000	-2.728955000000000
C	2.139611000000000	-0.765357000000000	-2.720074000000000
H	3.763538000000000	0.747049000000000	-2.383464000000000
C	1.809310000000000	1.459602000000000	-3.200757000000000

C	0.8180620000000000	-0.6154360000000000	-3.2117700000000000
H	2.6217840000000000	-1.6996310000000000	-2.4450000000000000
H	1.9759800000000000	2.5262990000000000	-3.3361180000000000
C	0.5996370000000000	0.7561260000000000	-3.4971850000000000
H	0.0821710000000000	-1.4105910000000000	-3.3088590000000000
H	-0.3117930000000000	1.1898820000000000	-3.9021960000000000
C	-1.8217540000000000	-0.1006770000000000	-1.6145020000000000
C	-0.6539160000000000	-0.3610170000000000	-0.8564090000000000
C	-0.8673080000000000	-1.2157460000000000	0.2442280000000000
C	-2.1227740000000000	-1.7344200000000000	0.5770810000000000
C	-3.2483740000000000	-1.4328790000000000	-0.1850280000000000
C	-3.0821510000000000	-0.6094170000000000	-1.2975410000000000
H	-1.7615030000000000	0.5352580000000000	-2.5016980000000000
H	1.7903490000000000	0.7930950000000000	-0.1368450000000000
H	-0.0270270000000000	-1.4850510000000000	0.8812560000000000
H	-2.2152840000000000	-2.3870480000000000	1.4513940000000000
H	-4.2311090000000000	-1.8343810000000000	0.0762270000000000
H	-3.9399350000000000	-0.3576890000000000	-1.9292970000000000
TS_{S24/S25a}			
Fe	0.1210430000000000	-0.0465730000000000	0.0047790000000000
P	0.2188450000000000	2.1507890000000000	0.5858010000000000
C	0.5228780000000000	2.4166460000000000	2.3999690000000000
H	0.5775820000000000	3.5021890000000000	2.5829840000000000
H	-0.3837350000000000	2.0710980000000000	2.9198870000000000
C	1.7457070000000000	1.7128070000000000	2.9556550000000000
H	2.6717230000000000	2.0868680000000000	2.4942190000000000
H	1.8307510000000000	1.8682930000000000	4.0421310000000000
H	1.6921690000000000	0.6328950000000000	2.7611950000000000
C	1.4794760000000000	3.3035240000000000	-0.1355350000000000
H	1.4595970000000000	3.1648500000000000	-1.2257950000000000
H	2.4507560000000000	2.8932470000000000	0.1837730000000000
C	1.3719230000000000	4.7788280000000000	0.2151410000000000
H	2.2090150000000000	5.3370910000000000	-0.2318830000000000
H	0.4427870000000000	5.2270510000000000	-0.1676070000000000
H	1.4074470000000000	4.9590550000000000	1.3002580000000000
C	-1.3652410000000000	3.1094240000000000	0.4833510000000000
H	-2.0888410000000000	2.5366340000000000	1.0853190000000000
H	-1.2066360000000000	4.0564730000000000	1.0250650000000000
C	-1.9361050000000000	3.3790200000000000	-0.8980380000000000
H	-1.2552080000000000	3.9886250000000000	-1.5121120000000000
H	-2.1302630000000000	2.4483500000000000	-1.4492870000000000
H	-2.8849200000000000	3.9315850000000000	-0.8171450000000000
B	2.5476820000000000	0.1915680000000000	-1.1365100000000000
O	3.3941920000000000	-0.7428450000000000	-1.6799930000000000

O	2.255981000000000	-0.132518000000000	0.209927000000000
C	3.681455000000000	-1.760939000000000	-0.720084000000000
C	3.287320000000000	-1.068195000000000	0.630088000000000
C	2.845945000000000	-2.995703000000000	-1.026587000000000
C	5.156346000000000	-2.112395000000000	-0.832145000000000
C	4.417707000000000	-0.210045000000000	1.188873000000000
C	2.788767000000000	-2.016680000000000	1.696278000000000
H	2.994317000000000	-3.271112000000000	-2.080249000000000
H	3.145449000000000	-3.846975000000000	-0.398556000000000
H	1.779660000000000	-2.800890000000000	-0.868689000000000
H	5.338471000000000	-2.604768000000000	-1.798265000000000
H	5.790086000000000	-1.218029000000000	-0.785791000000000
H	5.458805000000000	-2.806609000000000	-0.033607000000000
H	5.249505000000000	-0.829576000000000	1.551113000000000
H	4.804144000000000	0.482908000000000	0.427404000000000
H	4.038667000000000	0.382413000000000	2.031139000000000
H	2.519798000000000	-1.462668000000000	2.606469000000000
H	1.919267000000000	-2.593093000000000	1.366719000000000
H	3.592039000000000	-2.721220000000000	1.958622000000000
C	-1.962603000000000	-0.214119000000000	0.214120000000000
C	-1.465476000000000	-1.340111000000000	-0.484810000000000
H	-2.696305000000000	0.496513000000000	-0.159982000000000
C	-1.358219000000000	-0.224700000000000	1.512407000000000
C	-0.547316000000000	-2.030227000000000	0.343956000000000
H	-1.723435000000000	-1.605844000000000	-1.507168000000000
H	-1.553782000000000	0.480480000000000	2.317689000000000
C	-0.486447000000000	-1.328181000000000	1.589878000000000
H	-0.035114000000000	-2.957383000000000	0.094830000000000
H	0.111638000000000	-1.596906000000000	2.457637000000000
C	0.087120000000000	1.262190000000000	-2.748783000000000
C	0.378729000000000	0.092244000000000	-2.013487000000000
C	0.487301000000000	-1.069579000000000	-2.809324000000000
C	0.324899000000000	-1.075076000000000	-4.195678000000000
C	0.023787000000000	0.105623000000000	-4.870768000000000
C	-0.096323000000000	1.281803000000000	-4.130232000000000
H	0.006905000000000	2.216441000000000	-2.227553000000000
H	2.558997000000000	1.307749000000000	-1.565503000000000
H	0.711370000000000	-2.025824000000000	-2.332636000000000
H	0.430426000000000	-2.012734000000000	-4.749677000000000
H	-0.109899000000000	0.111677000000000	-5.955777000000000
H	-0.330024000000000	2.225202000000000	-4.633174000000000
TS_{S24/S25b}			
Fe	-0.002353000000	-0.278953000000	-0.561248000000
P	0.192747000000	1.132536000000	1.244001000000

C	1.397146000000	2.541709000000	1.404521000000
H	2.405035000000	2.103069000000	1.370158000000
H	1.299177000000	3.137402000000	0.487236000000
C	1.265513000000	3.435047000000	2.629516000000
H	2.042045000000	4.215417000000	2.605526000000
H	0.294637000000	3.950741000000	2.667089000000
H	1.390344000000	2.883946000000	3.573196000000
C	-1.383684000000	2.095755000000	1.455135000000
H	-1.366771000000	2.562352000000	2.453318000000
H	-2.220257000000	1.384305000000	1.467923000000
C	-1.600353000000	3.143978000000	0.373226000000
H	-1.508630000000	2.709526000000	-0.632638000000
H	-2.599948000000	3.595745000000	0.465873000000
H	-0.864438000000	3.959121000000	0.439942000000
C	0.439239000000	0.391272000000	2.942224000000
H	1.518383000000	0.497993000000	3.142621000000
H	-0.066210000000	1.047470000000	3.668828000000
C	0.034906000000	-1.054964000000	3.163515000000
H	0.530603000000	-1.723020000000	2.444759000000
H	0.320343000000	-1.377727000000	4.176720000000
H	-1.048888000000	-1.210013000000	3.067916000000
B	1.811816000000	-0.535393000000	-2.228241000000
O	1.773691000000	-1.219193000000	-0.971216000000
O	3.145283000000	-0.187899000000	-2.473079000000
C	3.099743000000	-1.394897000000	-0.444665000000
C	3.987564000000	-1.027011000000	-1.695380000000
C	3.313163000000	-0.472083000000	0.738214000000
C	3.216288000000	-2.836974000000	0.022763000000
C	4.332220000000	-2.247676000000	-2.548225000000
C	5.260607000000	-0.270523000000	-1.355214000000
H	4.292616000000	-0.647731000000	1.204329000000
H	3.256282000000	0.580573000000	0.442015000000
H	2.536520000000	-0.666234000000	1.489587000000
H	2.927889000000	-3.541901000000	-0.766479000000
H	4.243861000000	-3.065138000000	0.342704000000
H	2.548462000000	-2.998114000000	0.882256000000
H	5.033096000000	-2.926725000000	-2.041488000000
H	3.428016000000	-2.811783000000	-2.819006000000
H	4.798770000000	-1.898308000000	-3.480237000000
H	5.807096000000	-0.048385000000	-2.283019000000
H	5.043681000000	0.683944000000	-0.858996000000
H	5.917526000000	-0.867728000000	-0.705000000000
C	-1.459687000000	-0.993681000000	-1.916263000000
C	-0.802404000000	-2.092689000000	-1.334342000000

H	-1.454292000000	-0.762284000000	-2.978812000000
C	-2.076842000000	-0.233117000000	-0.880587000000
C	-1.001649000000	-2.048384000000	0.073943000000
H	-0.181185000000	-2.809675000000	-1.867165000000
H	-2.685710000000	0.660257000000	-1.003126000000
C	-1.795226000000	-0.907633000000	0.343200000000
H	-0.623548000000	-2.761588000000	0.802240000000
H	-2.152562000000	-0.614460000000	1.327320000000
C	-0.099337000000	2.986351000000	-3.428417000000
C	-0.237803000000	1.746950000000	-2.808613000000
C	0.673502000000	1.250475000000	-1.843540000000
C	1.769832000000	2.104688000000	-1.609114000000
C	1.942847000000	3.342254000000	-2.229804000000
C	0.995140000000	3.802450000000	-3.138903000000
H	-0.851805000000	3.315639000000	-4.150845000000
H	-1.108581000000	1.155663000000	-3.094110000000
H	1.120043000000	-0.909155000000	-3.149600000000
H	2.558161000000	1.778039000000	-0.930113000000
H	2.826469000000	3.944951000000	-2.000728000000
H	1.114439000000	4.772043000000	-3.629362000000

12. DFT-optimized cartesian coordinates of all species involved in the SET-triggered deaminative cross-coupling reaction

18

C	-3.2749890000000000	-0.0944610000000000	-0.1215220000000000
C	-4.2211800000000000	-0.8365070000000000	-0.8595620000000000
C	-5.5647030000000000	-0.4786210000000000	-0.8918530000000000
C	-6.0213390000000000	0.6257290000000000	-0.1603940000000000
C	-5.1091370000000000	1.3484810000000000	0.6106080000000000
C	-3.7590080000000000	0.9903660000000000	0.6362250000000000
H	-3.8581670000000000	-1.7028530000000000	-1.4020130000000000
H	-6.2651990000000000	-1.0625940000000000	-1.4851000000000000
H	-7.0714720000000000	0.9048690000000000	-0.1793810000000000
H	-5.4511090000000000	2.1867080000000000	1.2136720000000000
H	-3.0911320000000000	1.5332610000000000	1.2973070000000000
C	-1.8544400000000000	-0.5529490000000000	-0.1775730000000000
O	-1.6456820000000000	-1.8118150000000000	-0.4167490000000000
C	-0.8364940000000000	0.3679460000000000	0.0142690000000000
S	-0.9522740000000000	2.1642020000000000	0.1439940000000000
N	0.5577550000000000	0.0414060000000000	-0.0531770000000000
C	0.7718120000000000	2.3330210000000000	-0.3251560000000000
C	1.3920500000000000	1.1331630000000000	-0.3381440000000000
C	1.0656860000000000	-1.2726510000000000	0.1841530000000000
C	1.3019000000000000	3.7220090000000000	-0.5277300000000000
C	2.8625550000000000	0.9317920000000000	-0.6121400000000000
C	1.1906160000000000	-1.7767700000000000	1.4981650000000000
C	1.4943330000000000	-2.0355890000000000	-0.9279550000000000
C	2.8350100000000000	3.8675900000000000	-0.4831500000000000
H	0.8833730000000000	4.3561670000000000	0.2713330000000000
H	0.9182260000000000	4.1526120000000000	-1.4661690000000000
C	3.8218200000000000	1.6434590000000000	0.3630910000000000
H	3.0954600000000000	-0.1335240000000000	-0.6012010000000000
H	3.0708310000000000	1.2725900000000000	-1.6326270000000000
C	1.7251790000000000	-3.0641240000000000	1.6590860000000000
C	0.7730980000000000	-1.0539790000000000	2.7780430000000000
C	2.0381520000000000	-3.3039660000000000	-0.7115110000000000
C	1.3032040000000000	-1.5400990000000000	-2.3551430000000000
C	3.4630340000000000	3.1043190000000000	0.6940160000000000
H	3.2792680000000000	3.5333560000000000	-1.4288090000000000
H	3.0635560000000000	4.9370440000000000	-0.4043740000000000
H	3.8857600000000000	1.0690070000000000	1.2944540000000000
H	4.8216200000000000	1.6072900000000000	-0.0890980000000000
C	2.1496900000000000	-3.8258280000000000	0.5751530000000000
H	1.8219840000000000	-3.4653160000000000	2.6654580000000000

C	-0.738710000000000	-1.166794000000000	3.047069000000000
C	1.246717000000000	0.401769000000000	2.904471000000000
H	1.272500000000000	-1.605814000000000	3.585831000000000
H	2.361221000000000	-3.898627000000000	-1.561532000000000
C	0.141520000000000	-2.300294000000000	-3.019261000000000
C	2.583585000000000	-1.633296000000000	-3.199619000000000
H	1.011991000000000	-0.488192000000000	-2.305220000000000
H	4.371035000000000	3.615909000000000	1.035736000000000
H	2.761332000000000	3.127626000000000	1.537074000000000
H	2.570282000000000	-4.815633000000000	0.732307000000000
H	-0.972391000000000	-0.766747000000000	4.041741000000000
H	-1.304855000000000	-0.607751000000000	2.299100000000000
H	-1.065177000000000	-2.212245000000000	3.014183000000000
H	0.721636000000000	1.069331000000000	2.220433000000000
H	1.066628000000000	0.753559000000000	3.927862000000000
H	2.319909000000000	0.486570000000000	2.705237000000000
H	-0.067832000000000	-1.889031000000000	-4.015239000000000
H	0.393000000000000	-3.362036000000000	-3.141374000000000
H	-0.746780000000000	-2.217801000000000	-2.384060000000000
H	3.415404000000000	-1.090556000000000	-2.738101000000000
H	2.899054000000000	-2.673422000000000	-3.342153000000000
H	2.409649000000000	-1.205604000000000	-4.194139000000000

19

C	0.304470000000000	1.325968000000000	0.429607000000000
C	-1.029942000000000	1.607340000000000	0.190765000000000
C	-1.953483000000000	0.600955000000000	-0.128137000000000
C	-1.478675000000000	-0.716488000000000	-0.057913000000000
C	-0.141191000000000	-0.993368000000000	0.156101000000000
N	0.769287000000000	0.038822000000000	0.262174000000000
H	-1.360012000000000	2.625733000000000	0.348809000000000
H	-2.149905000000000	-1.557705000000000	-0.169944000000000
C	0.304543000000000	-2.391227000000000	0.316993000000000
C	-0.104199000000000	-3.371409000000000	-0.600810000000000
C	1.069668000000000	-2.761281000000000	1.434478000000000
C	0.282359000000000	-4.696878000000000	-0.422938000000000
H	-0.698080000000000	-3.085211000000000	-1.462599000000000
C	1.445462000000000	-4.089647000000000	1.611484000000000
H	1.349721000000000	-2.014936000000000	2.171031000000000
C	1.061694000000000	-5.056569000000000	0.679428000000000
H	-0.022206000000000	-5.447288000000000	-1.145285000000000
H	2.033893000000000	-4.370148000000000	2.479053000000000
H	1.363888000000000	-6.090269000000000	0.815280000000000
C	1.164852000000000	2.369714000000000	1.015599000000000
C	1.875469000000000	2.091346000000000	2.194410000000000

C	1.2050570000000000	3.6573670000000000	0.4637650000000000
C	2.6366160000000000	3.0884490000000000	2.7979830000000000
H	1.8211790000000000	1.1024930000000000	2.6391920000000000
C	1.9753310000000000	4.6479900000000000	1.0680940000000000
H	0.6609500000000000	3.8689680000000000	-0.4513030000000000
C	2.6937200000000000	4.3651330000000000	2.2323150000000000
H	3.1817810000000000	2.8702710000000000	3.7107020000000000
H	2.0185300000000000	5.6389200000000000	0.6276530000000000
H	3.2935140000000000	5.1390800000000000	2.7009250000000000
C	-3.3578480000000000	0.9126030000000000	-0.4286910000000000
C	-3.6911330000000000	2.1378560000000000	-1.0336810000000000
C	-4.3844440000000000	-0.0001280000000000	-0.1277730000000000
C	-5.0159610000000000	2.4382310000000000	-1.3355950000000000
H	-2.9083300000000000	2.8417720000000000	-1.2968800000000000
C	-5.7093930000000000	0.3087730000000000	-0.4211670000000000
H	-4.1535070000000000	-0.9373530000000000	0.3671750000000000
C	-6.0285260000000000	1.5261490000000000	-1.0278470000000000
H	-5.2579130000000000	3.3817480000000000	-1.8144630000000000
H	-6.4938490000000000	-0.3985880000000000	-0.1715030000000000
H	-7.0623930000000000	1.7633100000000000	-1.2592770000000000
C	2.2302100000000000	-0.2594200000000000	-0.0163650000000000
H	2.6935560000000000	-0.6448100000000000	0.8891950000000000
C	3.0497640000000000	0.9193420000000000	-0.5760860000000000
H	3.3469250000000000	1.6304410000000000	0.1886500000000000
H	3.9622960000000000	0.4939130000000000	-1.0036280000000000
H	2.5072630000000000	1.4343160000000000	-1.3717310000000000
C	2.3754030000000000	-1.3430290000000000	-1.0958040000000000
O	3.2339250000000000	-2.1950100000000000	-1.0508910000000000
O	1.5622850000000000	-1.1170030000000000	-2.1325970000000000
C	1.7079390000000000	-2.0208250000000000	-3.2506490000000000
H	1.5308580000000000	-3.0467030000000000	-2.9221670000000000
H	0.9548400000000000	-1.7094130000000000	-3.9719660000000000
H	2.7114050000000000	-1.9325610000000000	-3.6709550000000000
20			
C	-1.9097730000000000	0.0743550000000000	0.5585290000000000
S	-2.3487960000000000	1.7197890000000000	0.2385680000000000
N	-0.6289590000000000	-0.0293030000000000	0.1461030000000000
C	-0.7989760000000000	2.1745400000000000	-0.4666420000000000
C	0.0216750000000000	1.0945710000000000	-0.4390940000000000
C	0.0402210000000000	-1.3101850000000000	0.2500930000000000
C	-0.5529730000000000	3.5694680000000000	-0.9734820000000000
C	1.4139330000000000	0.9956210000000000	-1.0042660000000000
C	0.6331150000000000	-1.7012370000000000	1.4635640000000000
C	0.0646170000000000	-2.1196390000000000	-0.9020930000000000

C	0.909345000000000	3.891906000000000	-1.331881000000000
H	-0.878284000000000	4.271537000000000	-0.193842000000000
H	-1.201700000000000	3.763078000000000	-1.838441000000000
C	2.434452000000000	2.010711000000000	-0.445193000000000
H	1.799367000000000	-0.014039000000000	-0.848509000000000
H	1.342339000000000	1.121598000000000	-2.090898000000000
C	1.275227000000000	-2.948127000000000	1.485209000000000
C	0.569501000000000	-0.927669000000000	2.778566000000000
C	0.714702000000000	-3.354987000000000	-0.823831000000000
C	-0.658108000000000	-1.693648000000000	-2.172970000000000
C	1.899799000000000	3.440430000000000	-0.244888000000000
H	1.173554000000000	3.440432000000000	-2.295648000000000
H	0.976248000000000	4.975736000000000	-1.476921000000000
H	2.835757000000000	1.643205000000000	0.505301000000000
H	3.277008000000000	2.030886000000000	-1.147046000000000
C	1.321219000000000	-3.766002000000000	0.360665000000000
H	1.742717000000000	-3.277185000000000	2.409326000000000
C	-0.781570000000000	-1.165793000000000	3.480361000000000
C	0.900873000000000	0.570867000000000	2.710398000000000
H	1.342272000000000	-1.381015000000000	3.412002000000000
H	0.746499000000000	-4.001313000000000	-1.694279000000000
C	-2.105996000000000	-2.218794000000000	-2.141947000000000
C	0.063361000000000	-2.120584000000000	-3.458024000000000
H	-0.712824000000000	-0.601216000000000	-2.184873000000000
H	2.754851000000000	4.124861000000000	-0.206302000000000
H	1.406622000000000	3.514491000000000	0.732860000000000
H	1.828451000000000	-4.725425000000000	0.407162000000000
H	-0.792837000000000	-0.669991000000000	4.458282000000000
H	-1.600501000000000	-0.770693000000000	2.871687000000000
H	-0.955894000000000	-2.236227000000000	3.636212000000000
H	0.110545000000000	1.157693000000000	2.237768000000000
H	1.031710000000000	0.953979000000000	3.728723000000000
H	1.832308000000000	0.747594000000000	2.164628000000000
H	-2.655923000000000	-1.882399000000000	-3.028541000000000
H	-2.117404000000000	-3.315104000000000	-2.126784000000000
H	-2.626515000000000	-1.855581000000000	-1.249807000000000
H	1.105486000000000	-1.782802000000000	-3.461018000000000
H	0.057465000000000	-3.207994000000000	-3.590927000000000
H	-0.440450000000000	-1.683682000000000	-4.326944000000000
21			
C	-0.632017000000000	1.160767000000000	-0.000355000000000
C	0.767814000000000	1.194468000000000	-0.016873000000000
C	1.490225000000000	-0.003815000000000	0.000076000000000
C	0.761386000000000	-1.198212000000000	0.017028000000000

C	-0.638257000000000	-1.157021000000000	0.000365000000000
N	-1.316130000000000	0.003707000000000	-0.000050000000000
H	1.292322000000000	2.141817000000000	-0.034667000000000
H	1.280835000000000	-2.148344000000000	0.034877000000000
C	-1.451969000000000	-2.400346000000000	0.000672000000000
C	-0.939449000000000	-3.615822000000000	-0.479683000000000
C	-2.768856000000000	-2.371400000000000	0.486744000000000
C	-1.719260000000000	-4.771574000000000	-0.465469000000000
H	0.063908000000000	-3.658729000000000	-0.891095000000000
C	-3.546283000000000	-3.527032000000000	0.504044000000000
H	-3.166893000000000	-1.431920000000000	0.853301000000000
C	-3.024423000000000	-4.732986000000000	0.028989000000000
H	-1.308362000000000	-5.701126000000000	-0.848639000000000
H	-4.560544000000000	-3.487872000000000	0.891164000000000
H	-3.630926000000000	-5.633908000000000	0.040987000000000
C	-1.439031000000000	2.408435000000000	-0.000707000000000
C	-0.920340000000000	3.621024000000000	0.480302000000000
C	-2.755756000000000	2.386578000000000	-0.487532000000000
C	-1.694065000000000	4.780860000000000	0.466060000000000
H	0.083020000000000	3.658496000000000	0.892255000000000
C	-3.527107000000000	3.546269000000000	-0.504858000000000
H	-3.158351000000000	1.449285000000000	-0.854677000000000
C	-2.999162000000000	4.749288000000000	-0.029085000000000
H	-1.278501000000000	5.708118000000000	0.849751000000000
H	-4.541344000000000	3.512577000000000	-0.892555000000000
H	-3.600922000000000	5.653386000000000	-0.041076000000000
C	2.972055000000000	-0.007774000000000	0.000051000000000
C	3.686008000000000	-0.985035000000000	0.711981000000000
C	3.691183000000000	0.965670000000000	-0.711903000000000
C	5.079796000000000	-0.987352000000000	0.713333000000000
H	3.146910000000000	-1.731237000000000	1.287521000000000
C	5.084963000000000	0.960542000000000	-0.713313000000000
H	3.156057000000000	1.714758000000000	-1.287406000000000
C	5.784358000000000	-0.015276000000000	-0.000003000000000
H	5.615575000000000	-1.745192000000000	1.277340000000000
H	5.624760000000000	1.715513000000000	-1.277338000000000
H	6.870332000000000	-0.018168000000000	-0.000033000000000

22R

C	-0.738643000000000	-0.178807000000000	0.731542000000000
C	-1.240010000000000	-0.113165000000000	-0.578498000000000
C	-2.561028000000000	0.268424000000000	-0.807589000000000
C	-3.395551000000000	0.585569000000000	0.265641000000000
C	-2.905750000000000	0.521888000000000	1.574006000000000
C	-1.587754000000000	0.143153000000000	1.803516000000000

H	-0.614151000000000	-0.353835000000000	-1.429202000000000
H	-2.937272000000000	0.317154000000000	-1.824684000000000
H	-4.424491000000000	0.881740000000000	0.084139000000000
H	-3.552715000000000	0.768531000000000	2.410425000000000
H	-1.190075000000000	0.090045000000000	2.810835000000000
C	0.665406000000000	-0.569645000000000	1.054575000000000
O	1.060243000000000	-0.590828000000000	2.213288000000000
C	1.627445000000000	-1.007516000000000	-0.061687000000000
C	1.281049000000000	-2.396521000000000	-0.615855000000000
C	1.769943000000000	0.035556000000000	-1.160196000000000
H	1.276889000000000	-3.128367000000000	0.196721000000000
H	0.300337000000000	-2.410939000000000	-1.097046000000000
H	2.028476000000000	-2.697347000000000	-1.353993000000000
O	1.792808000000000	-0.193719000000000	-2.353082000000000
O	1.886772000000000	1.264092000000000	-0.629976000000000
C	2.009470000000000	2.350427000000000	-1.570647000000000
H	2.095465000000000	3.250889000000000	-0.964470000000000
H	2.898227000000000	2.216019000000000	-2.190642000000000
H	1.121986000000000	2.396954000000000	-2.205895000000000
H	2.603911000000000	-1.056959000000000	0.433383000000000
22S			
C	1.122412000000000	-0.819499000000000	0.023692000000000
C	1.279860000000000	0.521738000000000	-0.361138000000000
C	2.537577000000000	1.121599000000000	-0.322168000000000
C	3.650397000000000	0.390640000000000	0.097502000000000
C	3.503908000000000	-0.946185000000000	0.481271000000000
C	2.249514000000000	-1.544833000000000	0.444857000000000
H	0.433328000000000	1.111699000000000	-0.690697000000000
H	2.646911000000000	2.159670000000000	-0.620305000000000
H	4.629165000000000	0.860282000000000	0.125907000000000
H	4.367896000000000	-1.516746000000000	0.808343000000000
H	2.116466000000000	-2.579506000000000	0.740612000000000
C	-0.192311000000000	-1.526385000000000	0.017389000000000
O	-0.280832000000000	-2.690150000000000	0.387317000000000
C	-1.452707000000000	-0.820978000000000	-0.508880000000000
C	-1.434762000000000	-0.661250000000000	-2.035499000000000
C	-1.738457000000000	0.490570000000000	0.207584000000000
H	-0.619217000000000	-0.015131000000000	-2.368548000000000
H	-2.377357000000000	-0.223445000000000	-2.372867000000000
H	-1.314096000000000	-1.639945000000000	-2.508271000000000
O	-2.093578000000000	1.523276000000000	-0.324810000000000
O	-1.561138000000000	0.351686000000000	1.531738000000000
C	-1.785881000000000	1.533240000000000	2.327730000000000
H	-1.097806000000000	2.325559000000000	2.024335000000000

H	-1.594322000000000	1.231027000000000	3.356159000000000
H	-2.815776000000000	1.877301000000000	2.212152000000000
H	-2.269811000000000	-1.497062000000000	-0.232838000000000
23			
C	-0.487007000000000	1.338203000000000	0.035315000000000
C	-1.798444000000000	0.947029000000000	-0.080018000000000
C	-2.196623000000000	-0.413845000000000	-0.146144000000000
C	-1.152616000000000	-1.358123000000000	0.061675000000000
C	0.159113000000000	-0.988036000000000	0.181765000000000
N	0.548619000000000	0.367605000000000	0.044455000000000
H	-2.555491000000000	1.719841000000000	-0.018698000000000
H	-1.379319000000000	-2.411542000000000	0.178543000000000
C	1.203123000000000	-1.981329000000000	0.503797000000000
C	2.090349000000000	-1.770535000000000	1.572862000000000
C	1.291590000000000	-3.182101000000000	-0.220268000000000
C	3.046237000000000	-2.730444000000000	1.898831000000000
H	2.022879000000000	-0.852145000000000	2.144456000000000
C	2.249015000000000	-4.140581000000000	0.107182000000000
H	0.614577000000000	-3.349507000000000	-1.052815000000000
C	3.132855000000000	-3.917036000000000	1.165379000000000
H	3.719950000000000	-2.555222000000000	2.732844000000000
H	2.310237000000000	-5.058807000000000	-0.469739000000000
H	3.882611000000000	-4.661075000000000	1.417544000000000
C	-0.112554000000000	2.748093000000000	0.229957000000000
C	0.991343000000000	3.102339000000000	1.030226000000000
C	-0.867506000000000	3.779466000000000	-0.361970000000000
C	1.311721000000000	4.441296000000000	1.243692000000000
H	1.599164000000000	2.320902000000000	1.471585000000000
C	-0.547178000000000	5.115716000000000	-0.139191000000000
H	-1.696667000000000	3.527723000000000	-1.015878000000000
C	0.543706000000000	5.455408000000000	0.666330000000000
H	2.164136000000000	4.693227000000000	1.868605000000000
H	-1.142023000000000	5.894594000000000	-0.607858000000000
H	0.796974000000000	6.498193000000000	0.833486000000000
C	-3.594053000000000	-0.804354000000000	-0.317693000000000
C	-4.533306000000000	0.089180000000000	-0.881796000000000
C	-4.064771000000000	-2.081872000000000	0.061647000000000
C	-5.866654000000000	-0.272210000000000	-1.048973000000000
H	-4.206770000000000	1.067766000000000	-1.219134000000000
C	-5.398124000000000	-2.441093000000000	-0.110175000000000
H	-3.386944000000000	-2.794080000000000	0.520494000000000
C	-6.312270000000000	-1.540476000000000	-0.665283000000000
H	-6.560393000000000	0.437456000000000	-1.491758000000000
H	-5.727997000000000	-3.429112000000000	0.199646000000000

H	-7.352355000000000	-1.822882000000000	-0.798422000000000
C	1.677897000000000	0.636026000000000	-0.896303000000000
H	1.676321000000000	1.718472000000000	-1.038809000000000
C	1.456666000000000	-0.028657000000000	-2.254920000000000
H	1.511266000000000	-1.116733000000000	-2.187920000000000
H	0.469088000000000	0.254029000000000	-2.632056000000000
H	2.212972000000000	0.309971000000000	-2.967835000000000
C	3.037427000000000	0.363850000000000	-0.244912000000000
O	3.412433000000000	0.899189000000000	0.780810000000000
O	3.792914000000000	-0.471216000000000	-0.967060000000000
C	5.103234000000000	-0.750705000000000	-0.435682000000000
H	5.570124000000000	-1.421829000000000	-1.155123000000000
H	5.677398000000000	0.173162000000000	-0.338245000000000
H	5.010325000000000	-1.234346000000000	0.538455000000000
24			
C	3.211090000000000	0.098675000000000	0.010497000000000
C	3.590657000000000	-0.682314000000000	1.112386000000000
C	4.926887000000000	-1.039293000000000	1.301281000000000
C	5.900382000000000	-0.622291000000000	0.391831000000000
C	5.533662000000000	0.170618000000000	-0.700177000000000
C	4.202402000000000	0.537325000000000	-0.881199000000000
H	2.846133000000000	-0.989156000000000	1.839862000000000
H	5.207336000000000	-1.635157000000000	2.165236000000000
H	6.939225000000000	-0.904569000000000	0.536676000000000
H	6.287646000000000	0.504759000000000	-1.407462000000000
H	3.910817000000000	1.166844000000000	-1.716023000000000
C	1.805855000000000	0.572025000000000	-0.215472000000000
O	1.616116000000000	1.776147000000000	-0.535563000000000
C	0.743251000000000	-0.370072000000000	-0.103811000000000
S	0.940067000000000	-2.101370000000000	0.117114000000000
N	-0.608331000000000	-0.077115000000000	-0.215527000000000
C	-0.806017000000000	-2.337993000000000	0.190611000000000
C	-1.466805000000000	-1.163761000000000	0.018433000000000
C	-1.113637000000000	1.270207000000000	-0.333078000000000
C	-1.349022000000000	-3.722761000000000	0.414408000000000
C	-2.953557000000000	-0.943658000000000	0.140851000000000
C	-1.443139000000000	1.788078000000000	-1.599583000000000
C	-1.303749000000000	1.994828000000000	0.855957000000000
C	-2.758298000000000	-3.918197000000000	-0.166714000000000
H	-1.343871000000000	-3.965134000000000	1.487140000000000
H	-0.664814000000000	-4.438473000000000	-0.057037000000000
C	-3.600836000000000	-1.872294000000000	1.182224000000000
H	-3.120849000000000	0.097022000000000	0.426821000000000
H	-3.443321000000000	-1.066442000000000	-0.832142000000000

C	-1.9830360000000000	3.0797450000000000	-1.6344490000000000
C	-1.2342540000000000	1.0744760000000000	-2.9343530000000000
C	-1.8434140000000000	3.2823430000000000	0.7631620000000000
C	-0.9089940000000000	1.4316740000000000	2.2131210000000000
C	-3.8829990000000000	-3.2953010000000000	0.6738030000000000
H	-2.7727520000000000	-3.5019490000000000	-1.1816000000000000
H	-2.9508370000000000	-4.9919340000000000	-0.2723480000000000
H	-2.9509860000000000	-1.9090390000000000	2.0647450000000000
H	-4.5439720000000000	-1.4235220000000000	1.5140600000000000
C	-2.1842790000000000	3.8222270000000000	-0.4724380000000000
H	-2.2453180000000000	3.5103620000000000	-2.5969280000000000
C	-2.1139910000000000	-0.1716620000000000	-3.1326680000000000
C	0.2360960000000000	0.7516660000000000	-3.2514540000000000
H	-1.5609830000000000	1.8006060000000000	-3.6889890000000000
H	-1.9947030000000000	3.8647690000000000	1.6670300000000000
C	-2.0891500000000000	1.4183230000000000	3.1981880000000000
C	0.2912630000000000	2.2066600000000000	2.7859230000000000
H	-0.5903280000000000	0.3950990000000000	2.0768260000000000
H	-4.7987380000000000	-3.2885240000000000	0.0689010000000000
H	-4.0881280000000000	-3.9374720000000000	1.5398400000000000
H	-2.6047290000000000	4.8219780000000000	-0.5332980000000000
H	-1.7809710000000000	-1.0066550000000000	-2.5100840000000000
H	-3.1635520000000000	0.0389060000000000	-2.9022560000000000
H	-2.0561060000000000	-0.4975320000000000	-4.1774820000000000
H	0.6078150000000000	-0.0761000000000000	-2.6423760000000000
H	0.3232950000000000	0.4589250000000000	-4.3042880000000000
H	0.8822730000000000	1.6138210000000000	-3.0705820000000000
H	-2.4468040000000000	2.4315410000000000	3.4124090000000000
H	-2.9315890000000000	0.8401670000000000	2.8030960000000000
H	-1.7820370000000000	0.9656410000000000	4.1476090000000000
H	0.6325070000000000	1.7462700000000000	3.7201880000000000
H	1.1210050000000000	2.2144650000000000	2.0734520000000000
H	0.0188170000000000	3.2464260000000000	3.0021790000000000

25

C	-1.3896130000000000	-0.4845200000000000	-0.0004680000000000
H	-1.8402560000000000	-1.4718500000000000	-0.0029060000000000
C	-2.2584420000000000	0.7192290000000000	-0.0001070000000000
H	-2.9054940000000000	0.7293990000000000	-0.8895910000000000
H	-2.9361410000000000	0.7069700000000000	0.8657220000000000
H	-1.6779340000000000	1.6426960000000000	0.0205270000000000
C	0.0562810000000000	-0.4802080000000000	-0.0016030000000000
O	0.7460600000000000	-1.4986710000000000	-0.0031490000000000
O	0.5902860000000000	0.7682420000000000	-0.0004520000000000
C	2.0242720000000000	0.8247000000000000	-0.0006190000000000

H	2.428720000000000	0.338522000000000	-0.892429000000000
H	2.276054000000000	1.884984000000000	0.001597000000000
H	2.429103000000000	0.334658000000000	0.888888000000000
26R			
C	2.921224000000000	0.083434000000000	-0.686708000000000
C	3.274264000000000	-0.801016000000000	0.339881000000000
C	4.286544000000000	-0.473090000000000	1.243832000000000
C	4.961718000000000	0.744254000000000	1.132755000000000
C	4.598643000000000	1.640737000000000	0.125194000000000
C	3.577930000000000	1.313296000000000	-0.768977000000000
H	2.774038000000000	-1.759379000000000	0.434123000000000
H	4.545548000000000	-1.169987000000000	2.036605000000000
H	5.753087000000000	0.996603000000000	1.833083000000000
H	5.107967000000000	2.597268000000000	0.038787000000000
H	3.263536000000000	1.993976000000000	-1.552201000000000
C	1.909596000000000	-0.237118000000000	-1.823533000000000
O	1.436100000000000	0.818888000000000	-2.446196000000000
C	0.700419000000000	-1.053187000000000	-1.217981000000000
S	0.510287000000000	-2.760344000000000	-1.178507000000000
N	-0.427607000000000	-0.471955000000000	-0.775105000000000
C	-1.113394000000000	-2.649249000000000	-0.556340000000000
C	-1.465077000000000	-1.346055000000000	-0.389020000000000
C	-0.616232000000000	0.966989000000000	-0.639528000000000
C	-1.929056000000000	-3.894958000000000	-0.331681000000000
C	-2.778712000000000	-0.820799000000000	0.122494000000000
C	-1.275229000000000	1.686471000000000	-1.652566000000000
C	-0.221600000000000	1.543722000000000	0.583349000000000
C	-3.426430000000000	-3.676021000000000	-0.608340000000000
H	-1.779401000000000	-4.261115000000000	0.692897000000000
H	-1.546615000000000	-4.679794000000000	-0.992896000000000
C	-3.433502000000000	-1.765362000000000	1.145460000000000
H	-2.616105000000000	0.161725000000000	0.568823000000000
H	-3.462519000000000	-0.654376000000000	-0.718090000000000
C	-1.472077000000000	3.053531000000000	-1.415835000000000
C	-1.815316000000000	1.177584000000000	-2.996793000000000
C	-0.466714000000000	2.909735000000000	0.764730000000000
C	0.399490000000000	0.742866000000000	1.723268000000000
C	-4.177247000000000	-2.958431000000000	0.524400000000000
H	-3.524910000000000	-3.112497000000000	-1.544183000000000
H	-3.897940000000000	-4.648997000000000	-0.784986000000000
H	-2.660910000000000	-2.124540000000000	1.835816000000000
H	-4.139577000000000	-1.186679000000000	1.750682000000000
C	-1.076984000000000	3.664097000000000	-0.230396000000000
H	-1.945941000000000	3.649973000000000	-2.190584000000000

C	-3.356902000000000	1.236799000000000	-3.014728000000000
C	-1.332425000000000	-0.173735000000000	-3.535085000000000
H	-1.468465000000000	1.927078000000000	-3.720947000000000
H	-0.176444000000000	3.383286000000000	1.696241000000000
C	-0.646128000000000	0.412203000000000	2.805216000000000
C	1.592097000000000	1.469912000000000	2.362577000000000
H	0.776192000000000	-0.200646000000000	1.322287000000000
H	-5.144976000000000	-2.618685000000000	0.134583000000000
H	-4.398702000000000	-3.676023000000000	1.324252000000000
H	-1.249103000000000	4.726245000000000	-0.082274000000000
H	-3.789703000000000	0.484931000000000	-2.347134000000000
H	-3.734845000000000	2.215785000000000	-2.705105000000000
H	-3.724927000000000	1.032997000000000	-4.026451000000000
H	-1.724588000000000	-1.021298000000000	-2.963379000000000
H	-1.696219000000000	-0.286943000000000	-4.562820000000000
H	-0.241957000000000	-0.199198000000000	-3.535970000000000
H	-1.076634000000000	1.330965000000000	3.219994000000000
H	-1.465228000000000	-0.198332000000000	2.418796000000000
H	-0.174394000000000	-0.141363000000000	3.624976000000000
H	2.101426000000000	0.798293000000000	3.060544000000000
H	2.314883000000000	1.787404000000000	1.609386000000000
H	1.267924000000000	2.349780000000000	2.929609000000000
C	2.697860000000000	-1.219636000000000	-2.899433000000000
H	1.920875000000000	-1.806685000000000	-3.399157000000000
C	3.392436000000000	-0.331264000000000	-3.928484000000000
H	3.865487000000000	-0.939457000000000	-4.707221000000000
H	2.649327000000000	0.328691000000000	-4.374830000000000
H	4.163844000000000	0.285284000000000	-3.459914000000000
C	3.633326000000000	-2.207792000000000	-2.256287000000000
O	3.295984000000000	-3.277351000000000	-1.766221000000000
O	4.911487000000000	-1.784143000000000	-2.227375000000000
C	5.833200000000000	-2.616845000000000	-1.505388000000000
H	5.852284000000000	-3.625742000000000	-1.923709000000000
H	6.805935000000000	-2.138143000000000	-1.615757000000000
H	5.548879000000000	-2.661683000000000	-0.451374000000000

26S

C	3.037959000000000	0.381180000000000	0.097032000000000
C	3.320847000000000	-0.987216000000000	0.020555000000000
C	4.333400000000000	-1.463484000000000	-0.818156000000000
C	5.088624000000000	-0.576911000000000	-1.585528000000000
C	4.814535000000000	0.791477000000000	-1.514795000000000
C	3.794544000000000	1.259130000000000	-0.688284000000000
H	2.763577000000000	-1.704842000000000	0.610755000000000
H	4.526074000000000	-2.531855000000000	-0.869760000000000

H	5.876634000000000	-0.947509000000000	-2.235199000000000
H	5.391523000000000	1.493692000000000	-2.111193000000000
H	3.540637000000000	2.311715000000000	-0.641371000000000
C	1.982700000000000	1.064488000000000	1.028861000000000
O	1.547663000000000	2.212086000000000	0.563041000000000
C	0.765129000000000	0.092963000000000	1.247084000000000
S	0.707253000000000	-1.343881000000000	2.193049000000000
N	-0.445971000000000	0.320790000000000	0.716894000000000
C	-0.970826000000000	-1.620362000000000	1.824646000000000
C	-1.449493000000000	-0.625044000000000	1.031824000000000
C	-0.859219000000000	1.500064000000000	-0.041714000000000
C	-1.664573000000000	-2.856117000000000	2.334277000000000
C	-2.859298000000000	-0.462813000000000	0.526207000000000
C	-0.928701000000000	1.445414000000000	-1.440332000000000
C	-1.425075000000000	2.545734000000000	0.713934000000000
C	-2.701350000000000	-3.394841000000000	1.333552000000000
H	-2.137597000000000	-2.650662000000000	3.303714000000000
H	-0.905463000000000	-3.622322000000000	2.523155000000000
C	-3.903662000000000	-1.101839000000000	1.456128000000000
H	-3.074019000000000	0.602220000000000	0.427758000000000
H	-2.944813000000000	-0.876270000000000	-0.487923000000000
C	-1.567860000000000	2.521073000000000	-2.079664000000000
C	-0.296665000000000	0.409762000000000	-2.372758000000000
C	-2.035189000000000	3.592638000000000	0.023086000000000
C	-1.371921000000000	2.576239000000000	2.234729000000000
C	-4.033125000000000	-2.627751000000000	1.341499000000000
H	-2.256139000000000	-3.371357000000000	0.331369000000000
H	-2.895903000000000	-4.449221000000000	1.558471000000000
H	-3.664607000000000	-0.821002000000000	2.489210000000000
H	-4.877618000000000	-0.651070000000000	1.236408000000000
C	-2.113679000000000	3.581994000000000	-1.368989000000000
H	-1.632434000000000	2.510768000000000	-3.164565000000000
C	-0.063184000000000	-1.018770000000000	-1.861885000000000
C	1.021454000000000	0.996220000000000	-2.917663000000000
H	-0.993247000000000	0.322417000000000	-3.216793000000000
H	-2.464169000000000	4.419448000000000	0.580890000000000
C	-2.776012000000000	2.641189000000000	2.857764000000000
C	-0.483331000000000	3.736057000000000	2.712744000000000
H	-0.904554000000000	1.653390000000000	2.587592000000000
H	-4.582946000000000	-2.877723000000000	0.425480000000000
H	-4.648543000000000	-2.979432000000000	2.179055000000000
H	-2.606346000000000	4.394779000000000	-1.894595000000000
H	0.747028000000000	-1.074002000000000	-1.131506000000000
H	-0.961491000000000	-1.463437000000000	-1.426065000000000

H	0.2310660000000000	-1.6433900000000000	-2.7123720000000000
H	1.6911660000000000	1.2322550000000000	-2.0893200000000000
H	1.5191930000000000	0.2791060000000000	-3.5809850000000000
H	0.8383500000000000	1.9169190000000000	-3.4816000000000000
H	-3.2985650000000000	3.5607930000000000	2.5719100000000000
H	-3.3952460000000000	1.7928060000000000	2.5466610000000000
H	-2.7036390000000000	2.6246720000000000	3.9510290000000000
H	-0.3692100000000000	3.7065590000000000	3.8028670000000000
H	0.4970970000000000	3.6436240000000000	2.2403550000000000
H	-0.9198010000000000	4.7058190000000000	2.4455790000000000
C	2.7132460000000000	1.2661450000000000	2.5075930000000000
H	1.9092620000000000	1.2572940000000000	3.2499720000000000
C	3.4085350000000000	2.6243960000000000	2.5207890000000000
H	4.2091140000000000	2.6636210000000000	1.7783230000000000
H	2.6816420000000000	3.3999580000000000	2.2833300000000000
H	3.8461580000000000	2.8214290000000000	3.5057560000000000
C	3.6400340000000000	0.1346080000000000	2.8579950000000000
O	3.2906250000000000	-0.9391330000000000	3.3306190000000000
O	4.9262980000000000	0.3896990000000000	2.5506070000000000
C	5.8385430000000000	-0.7088610000000000	2.7097800000000000
H	5.5580100000000000	-1.5257970000000000	2.0405180000000000
H	6.8181360000000000	-0.3153920000000000	2.4393850000000000
H	5.8397120000000000	-1.0648900000000000	3.7425320000000000
TSI			
C	-0.5069100000000000	1.3316360000000000	0.2380000000000000
C	-1.8135610000000000	0.9418130000000000	-0.0178950000000000
C	-2.1642120000000000	-0.4164340000000000	-0.1355220000000000
C	-1.1347110000000000	-1.3481370000000000	0.0942590000000000
C	0.1607150000000000	-0.9302290000000000	0.3524280000000000
N	0.5132060000000000	0.4029270000000000	0.3387050000000000
H	-2.5927530000000000	1.6941830000000000	-0.0392150000000000
H	-1.3525440000000000	-2.4096880000000000	0.1124160000000000
C	1.2284040000000000	-1.8924750000000000	0.6888950000000000
C	2.2055670000000000	-1.5481820000000000	1.6367180000000000
C	1.2733950000000000	-3.1685430000000000	0.1039120000000000
C	3.1929090000000000	-2.4616720000000000	1.9996410000000000
H	2.1764800000000000	-0.5619090000000000	2.0858120000000000
C	2.2673920000000000	-4.0772260000000000	0.4607340000000000
H	0.5409590000000000	-3.4395060000000000	-0.6506060000000000
C	3.2291170000000000	-3.7290050000000000	1.4125380000000000
H	3.9348460000000000	-2.1846630000000000	2.7433000000000000
H	2.2953360000000000	-5.0560540000000000	-0.0092050000000000
H	4.0028670000000000	-4.4382280000000000	1.6914720000000000
C	-0.1332790000000000	2.7451730000000000	0.4457080000000000

C	1.0460800000000000	3.0673170000000000	1.1427460000000000
C	-0.9302560000000000	3.7974930000000000	-0.0413140000000000
C	1.4025840000000000	4.3961440000000000	1.3615040000000000
H	1.6839700000000000	2.2648540000000000	1.4937590000000000
C	-0.5733210000000000	5.1246040000000000	0.1831520000000000
H	-1.8229530000000000	3.5801060000000000	-0.6186280000000000
C	0.5931470000000000	5.4315720000000000	0.8890580000000000
H	2.3156960000000000	4.6232910000000000	1.9045810000000000
H	-1.2015980000000000	5.9214050000000000	-0.2044200000000000
H	0.8719730000000000	6.4672090000000000	1.0602130000000000
C	-3.5480320000000000	-0.8325250000000000	-0.4219300000000000
C	-4.3987510000000000	-0.0129500000000000	-1.1875310000000000
C	-4.0594520000000000	-2.0532850000000000	0.0571930000000000
C	-5.7094950000000000	-0.3977950000000000	-1.4609290000000000
H	-4.0203890000000000	0.9201230000000000	-1.5936360000000000
C	-5.3696900000000000	-2.4374510000000000	-0.2179240000000000
H	-3.4363400000000000	-2.6938810000000000	0.6733220000000000
C	-6.2025480000000000	-1.6122700000000000	-0.9781240000000000
H	-6.3442780000000000	0.2485460000000000	-2.0603850000000000
H	-5.7444100000000000	-3.3802680000000000	0.1703450000000000
H	-7.2239140000000000	-1.9128970000000000	-1.1921200000000000
C	1.7522180000000000	0.7545510000000000	-1.1036000000000000
H	1.6083370000000000	1.8286350000000000	-1.0867960000000000
C	1.1735180000000000	0.0436600000000000	-2.2914220000000000
H	1.2153870000000000	-1.0415550000000000	-2.1720990000000000
H	0.1322170000000000	0.3455760000000000	-2.4421180000000000
H	1.7338990000000000	0.2993070000000000	-3.2003330000000000
C	3.1043610000000000	0.4143340000000000	-0.6206280000000000
O	3.7252280000000000	1.0657000000000000	0.2104210000000000
O	3.6038950000000000	-0.6978190000000000	-1.2082050000000000
C	4.9207770000000000	-1.0837740000000000	-0.7881840000000000
H	5.1467410000000000	-1.9975240000000000	-1.3374570000000000
H	5.6446840000000000	-0.3015040000000000	-1.0319820000000000
H	4.9346940000000000	-1.2738640000000000	0.2862850000000000

TSIR

C	3.45096500	0.84750600	-0.02755600
C	3.80382900	0.16293300	1.14461900
C	5.14568200	0.00007200	1.49323600
C	6.15060800	0.52131500	0.67694400
C	5.80665500	1.22267100	-0.48406500
C	4.46806500	1.39145500	-0.82707200
H	3.03075500	-0.21828700	1.80437400
H	5.40374700	-0.52553400	2.40809500
H	7.19476400	0.39081100	0.94602100

H	6.58441600	1.63621400	-1.11992000
H	4.18840200	1.93718700	-1.72210400
C	2.03553600	1.05701800	-0.46141800
O	1.70460800	2.14303100	-1.00676000
C	1.11484400	-0.02284300	-0.31768000
S	1.54843000	-1.68785900	0.01308900
N	-0.23242000	0.05412400	-0.64563500
C	-0.05318900	-2.24058600	-0.46956300
C	-0.87318600	-1.19202300	-0.74362200
C	-0.97960900	1.27617600	-0.44079700
C	-0.31234200	-3.71884700	-0.57840000
C	-2.33976300	-1.25361600	-1.07360800
C	-1.44145700	2.00952000	-1.54537800
C	-1.24992600	1.65950500	0.88564000
C	-1.39123800	-4.05581800	-1.61995000
H	-0.58057100	-4.13991100	0.40115900
H	0.62540100	-4.19883600	-0.87858500
C	-3.04744400	-2.45612800	-0.42941800
H	-2.80398400	-0.32902800	-0.71945600
H	-2.48111300	-1.26406100	-2.16274400
C	-2.17370900	3.17413800	-1.29227900
C	-1.15188100	1.59198700	-2.97643000
C	-1.97315400	2.84063200	1.08811200
C	-0.79409700	0.83644800	2.08206500
C	-2.83220000	-3.79158200	-1.15865600
H	-1.17666500	-3.48151400	-2.52990000
H	-1.29739300	-5.11254400	-1.89546900
H	-2.70705500	-2.53562600	0.61024600
H	-4.12252800	-2.24865300	-0.38589800
C	-2.43111200	3.59395800	0.01057000
H	-2.53878200	3.76423100	-2.12748300
C	-0.24728700	2.62431100	-3.67060900
C	-2.44433500	1.36878600	-3.77962100
H	-0.60963300	0.64332800	-2.94221500
H	-2.18796100	3.16682100	2.10131700
C	-1.97809300	0.44356800	2.98096700
C	0.29547300	1.57645200	2.87648900
H	-0.35502500	-0.09403000	1.71617700
H	-3.48727100	-3.83343400	-2.03839400
H	-3.15523000	-4.60250400	-0.49336200
H	-2.99481400	4.50583300	0.18598800
H	-0.74825500	3.59689000	-3.74182100
H	0.68061900	2.75078400	-3.10806800
H	-0.00665900	2.29813000	-4.68890900

H	-3.00662700	2.30221900	-3.89614000
H	-2.20511900	0.99730500	-4.78252600
H	-3.10194100	0.64118400	-3.29346200
H	-2.45840400	1.32128300	3.42720200
H	-2.73682100	-0.10451300	2.41137100
H	-1.63274300	-0.19954300	3.79821200
H	0.65516900	0.95357000	3.70340600
H	1.14829000	1.82263500	2.23571900
H	-0.09094800	2.51073000	3.30000800
C	1.70118800	-1.62477100	-3.65935900
H	0.80345100	-2.17294400	-3.92265600
C	1.86823400	-0.19802900	-4.03959400
H	1.12347500	0.10422300	-4.77930700
H	1.76225800	0.46308600	-3.16726100
H	2.87076600	-0.00991600	-4.44243500
C	2.68978500	-2.37485400	-2.91793300
O	2.59258100	-3.56849100	-2.63432400
O	3.75066700	-1.61175000	-2.55788100
C	4.75036300	-2.25791200	-1.75831700
H	5.23987400	-3.05443700	-2.32587100
H	5.46104200	-1.47589900	-1.49502000
H	4.30125400	-2.67816800	-0.85580600

TSIIS

C	2.43123900	1.83664300	-0.33241300
C	2.70866800	1.85831200	-1.70707400
C	3.99659200	2.14093400	-2.16543400
C	5.02164600	2.40791200	-1.25663100
C	4.74887200	2.40750400	0.11585400
C	3.46245700	2.13337000	0.57195800
H	1.91270300	1.68452100	-2.42437000
H	4.19495400	2.16203700	-3.23316300
H	6.02467000	2.62355800	-1.61322300
H	5.54131700	2.62092400	0.82770600
H	3.23709400	2.13512400	1.63329300
C	1.07629500	1.54217700	0.22763100
O	0.67213200	2.16944000	1.24254600
C	0.31317400	0.49183600	-0.36275200
S	0.93648400	-0.71014800	-1.47494300
N	-0.96961500	0.13950300	0.03577400
C	-0.48442800	-1.72390500	-1.23728800
C	-1.40135600	-1.10737800	-0.44635300
C	-1.90897200	1.13924800	0.49486500
C	-0.50808500	-3.10015600	-1.84530700
C	-2.78115200	-1.60218600	-0.10706400

C	-2.30381100	1.16330400	1.84184800
C	-2.42646900	2.03427700	-0.45935000
C	-1.36429200	-4.08897700	-1.03811400
H	-0.85234500	-3.05831800	-2.88861600
H	0.52272800	-3.46965100	-1.87176500
C	-3.38985400	-2.48038900	-1.21167500
H	-3.42153900	-0.73095100	0.05598500
H	-2.76284200	-2.14539700	0.84735800
C	-3.22905500	2.13769200	2.23063000
C	-1.74392600	0.19574200	2.86968300
C	-3.33780400	3.00103000	-0.01909000
C	-2.03404000	1.97613500	-1.92867000
C	-2.87970700	-3.92990800	-1.23137700
H	-1.10653600	-3.97502700	0.02227300
H	-1.07884100	-5.11041600	-1.31480300
H	-3.19380700	-1.99895700	-2.17752900
H	-4.47877800	-2.49271200	-1.08984200
C	-3.73649200	3.05523700	1.31380300
H	-3.54840800	2.18358800	3.26740700
C	-0.90330600	0.94551000	3.91715300
C	-2.85299800	-0.62864900	3.54442500
H	-1.08140800	-0.49853400	2.34597400
H	-3.74617500	3.71192300	-0.73111400
C	-3.26519000	1.82601200	-2.83737000
C	-1.18993300	3.20081500	-2.32066700
H	-1.41581600	1.09007400	-2.08774100
H	-3.38803400	-4.50327000	-0.44544600
H	-3.17403600	-4.38476800	-2.18585100
H	-4.44813500	3.80942900	1.63753600
H	-1.52415500	1.64798200	4.48555900
H	-0.10362800	1.50557400	3.42682500
H	-0.46138500	0.23940500	4.62946500
H	-3.52101000	0.00961000	4.13382500
H	-2.41273100	-1.36666800	4.22452100
H	-3.46358600	-1.16265400	2.80934500
H	-3.92698800	2.69660000	-2.77230400
H	-3.84636600	0.93791100	-2.56536500
H	-2.95123100	1.72287900	-3.88212800
H	-0.86555100	3.12344200	-3.36467000
H	-0.29934500	3.28059800	-1.68909600
H	-1.76581700	4.12730300	-2.21302600
C	1.63594200	-2.33783100	1.73164400
H	0.87696800	-3.11200700	1.75204300
C	1.64107600	-1.24230900	2.73543200

H	0.98605300	-1.47441300	3.57828300
H	1.29661900	-0.29566700	2.29430200
H	2.65413700	-1.05149300	3.10912000
C	2.60413300	-2.44639900	0.66319700
O	2.64286000	-3.36618000	-0.15345300
O	3.47623100	-1.40885200	0.65333800
C	4.42694800	-1.39378800	-0.41996500
H	5.10460300	-2.24889700	-0.34463400
H	4.97088100	-0.45652100	-0.31239400
H	3.91234400	-1.42194100	-1.38299600

TSIHR

C	3.0478030000000000	0.3660350000000000	-0.7049320000000000
C	3.3626150000000000	-0.5127700000000000	0.3397830000000000
C	4.2920330000000000	-0.1545990000000000	1.3151010000000000
C	4.9180420000000000	1.0939830000000000	1.2671350000000000
C	4.5892970000000000	1.9875990000000000	0.2470680000000000
C	3.6574650000000000	1.6245230000000000	-0.7280390000000000
H	2.8816130000000000	-1.4829430000000000	0.3925410000000000
H	4.5223230000000000	-0.8491750000000000	2.1183780000000000
H	5.6433310000000000	1.3713700000000000	2.0268630000000000
H	5.0589120000000000	2.9669060000000000	0.2076270000000000
H	3.3919640000000000	2.3059690000000000	-1.5289640000000000
C	2.1627500000000000	0.0123670000000000	-1.9011010000000000
O	1.6410090000000000	0.9593940000000000	-2.5432300000000000
C	0.6461220000000000	-0.9875600000000000	-1.0302280000000000
S	0.3244190000000000	-2.6743040000000000	-0.9623110000000000
N	-0.4837330000000000	-0.3416510000000000	-0.7069030000000000
C	-1.3455510000000000	-2.4520490000000000	-0.4820860000000000
C	-1.6194150000000000	-1.1249860000000000	-0.3835090000000000
C	-0.5491450000000000	1.1082300000000000	-0.6320370000000000
C	-2.2652770000000000	-3.6281260000000000	-0.2876540000000000
C	-2.9205890000000000	-0.4842690000000000	0.0156260000000000
C	-1.0706440000000000	1.8466680000000000	-1.7075910000000000
C	-0.1086350000000000	1.7041500000000000	0.5681730000000000
C	-3.7172090000000000	-3.3132680000000000	-0.6875960000000000
H	-2.2237030000000000	-3.9719390000000000	0.7550600000000000
H	-1.8929380000000000	-4.4603010000000000	-0.8949130000000000
C	-3.7243960000000000	-1.3448940000000000	1.0054900000000000
H	-2.7099980000000000	0.4934320000000000	0.4556620000000000
H	-3.5282580000000000	-0.2840400000000000	-0.8747950000000000
C	-1.1286910000000000	3.2387180000000000	-1.5418030000000000
C	-1.5840130000000000	1.3356980000000000	-3.0609320000000000
C	-0.2077380000000000	3.0944040000000000	0.6769310000000000
C	0.4231840000000000	0.8871400000000000	1.7416640000000000

C	-4.500197000000000	-2.503557000000000	0.358550000000000
H	-3.700641000000000	-2.776857000000000	-1.644339000000000
H	-4.246390000000000	-4.254859000000000	-0.872705000000000
H	-3.039214000000000	-1.735552000000000	1.767421000000000
H	-4.433876000000000	-0.698949000000000	1.534253000000000
C	-0.711177000000000	3.858950000000000	-0.371437000000000
H	-1.502419000000000	3.843798000000000	-2.363292000000000
C	-3.109074000000000	1.538501000000000	-3.174696000000000
C	-1.201149000000000	-0.075090000000000	-3.522829000000000
H	-1.127150000000000	2.018970000000000	-3.789228000000000
H	0.118329000000000	3.584271000000000	1.587290000000000
C	-0.707799000000000	0.493093000000000	2.710142000000000
C	1.535230000000000	1.614289000000000	2.510364000000000
H	0.859152000000000	-0.032279000000000	1.344322000000000
H	-5.406363000000000	-2.109963000000000	-0.119261000000000
H	-4.837871000000000	-3.175292000000000	1.157884000000000
H	-0.770523000000000	4.939542000000000	-0.277612000000000
H	-3.651175000000000	0.860854000000000	-2.507910000000000
H	-3.405602000000000	2.561523000000000	-2.924012000000000
H	-3.437123000000000	1.329576000000000	-4.199091000000000
H	-1.686065000000000	-0.861419000000000	-2.936853000000000
H	-1.530833000000000	-0.198198000000000	-4.560994000000000
H	-0.119191000000000	-0.203907000000000	-3.484919000000000
H	-1.219651000000000	1.384858000000000	3.090442000000000
H	-1.452424000000000	-0.148802000000000	2.235077000000000
H	-0.295261000000000	-0.053153000000000	3.566052000000000
H	2.009936000000000	0.920231000000000	3.211075000000000
H	2.305730000000000	1.992400000000000	1.835499000000000
H	1.140520000000000	2.452090000000000	3.096556000000000
C	2.775267000000000	-1.130311000000000	-2.836718000000000
H	1.927521000000000	-1.656085000000000	-3.282715000000000
C	3.581023000000000	-0.438391000000000	-3.944478000000000
H	4.001546000000000	-1.173004000000000	-4.638783000000000
H	2.918588000000000	0.235557000000000	-4.489494000000000
H	4.404410000000000	0.146785000000000	-3.525643000000000
C	3.584120000000000	-2.169903000000000	-2.101312000000000
O	3.127389000000000	-3.181447000000000	-1.591210000000000
O	4.891552000000000	-1.858614000000000	-2.031910000000000
C	5.707936000000000	-2.742049000000000	-1.244775000000000
H	5.639214000000000	-3.765799000000000	-1.618861000000000
H	6.725050000000000	-2.364183000000000	-1.343418000000000
H	5.390314000000000	-2.711385000000000	-0.199579000000000
TSIHS			
C	3.157917000000000	0.633501000000000	-0.247116000000000

C	3.559829000000000	-0.706315000000000	-0.191634000000000
C	4.468885000000000	-1.221664000000000	-1.115279000000000
C	5.003550000000000	-0.399823000000000	-2.110382000000000
C	4.618701000000000	0.940336000000000	-2.169891000000000
C	3.703793000000000	1.447259000000000	-1.246015000000000
H	3.167688000000000	-1.369264000000000	0.570489000000000
H	4.757722000000000	-2.267553000000000	-1.056879000000000
H	5.711547000000000	-0.801183000000000	-2.830075000000000
H	5.028164000000000	1.591750000000000	-2.937543000000000
H	3.385080000000000	2.482588000000000	-1.286927000000000
C	2.208159000000000	1.321209000000000	0.745272000000000
O	1.674130000000000	2.399142000000000	0.370737000000000
C	0.741960000000000	0.004506000000000	0.972818000000000
S	0.768674000000000	-1.588224000000000	1.606804000000000
N	-0.542436000000000	0.339941000000000	0.764909000000000
C	-0.968614000000000	-1.761255000000000	1.591692000000000
C	-1.531880000000000	-0.614045000000000	1.128956000000000
C	-0.989948000000000	1.633482000000000	0.261866000000000
C	-1.628513000000000	-3.040701000000000	2.032427000000000
C	-3.001476000000000	-0.296615000000000	1.036449000000000
C	-1.241120000000000	1.799048000000000	-1.111785000000000
C	-1.282044000000000	2.622188000000000	1.215641000000000
C	-2.962211000000000	-3.298432000000000	1.311793000000000
H	-1.779553000000000	-3.030009000000000	3.120612000000000
H	-0.939848000000000	-3.868496000000000	1.830944000000000
C	-3.820955000000000	-0.994878000000000	2.135539000000000
H	-3.130306000000000	0.784190000000000	1.114976000000000
H	-3.389153000000000	-0.569627000000000	0.048196000000000
C	-1.802425000000000	3.021519000000000	-1.505800000000000
C	-0.926088000000000	0.792544000000000	-2.218870000000000
C	-1.849850000000000	3.818394000000000	0.765408000000000
C	-0.988501000000000	2.446436000000000	2.698471000000000
C	-4.139347000000000	-2.471398000000000	1.851792000000000
H	-2.820262000000000	-3.099071000000000	0.242482000000000
H	-3.209427000000000	-4.362655000000000	1.395371000000000
H	-3.279944000000000	-0.902712000000000	3.085061000000000
H	-4.763391000000000	-0.451388000000000	2.266110000000000
C	-2.111711000000000	4.019180000000000	-0.585481000000000
H	-2.001097000000000	3.186231000000000	-2.561030000000000
C	-1.743332000000000	-0.509254000000000	-2.175536000000000
C	0.572461000000000	0.490011000000000	-2.351744000000000
H	-1.223988000000000	1.302086000000000	-3.143249000000000
H	-2.084347000000000	4.599177000000000	1.482252000000000
C	-2.274123000000000	2.428221000000000	3.542747000000000

C	-0.0253000000000000	3.5420040000000000	3.1860680000000000
H	-0.4871670000000000	1.4853930000000000	2.8406090000000000
H	-4.9622960000000000	-2.5315500000000000	1.1283410000000000
H	-4.5075070000000000	-2.9272680000000000	2.7796260000000000
H	-2.5539550000000000	4.9520260000000000	-0.9231500000000000
H	-1.4527000000000000	-1.1509530000000000	-1.3392180000000000
H	-2.8167220000000000	-0.3063110000000000	-2.1041980000000000
H	-1.5692090000000000	-1.0752090000000000	-3.0976380000000000
H	0.9303140000000000	-0.1490070000000000	-1.5419220000000000
H	0.7631210000000000	-0.0305200000000000	-3.2976560000000000
H	1.1663610000000000	1.4052960000000000	-2.3279020000000000
H	-2.8254890000000000	3.3698570000000000	3.4413440000000000
H	-2.9432180000000000	1.6136350000000000	3.2490390000000000
H	-2.0268420000000000	2.2964570000000000	4.6021180000000000
H	0.3093410000000000	3.3289980000000000	4.2078420000000000
H	0.8431700000000000	3.5895490000000000	2.5264040000000000
H	-0.5119770000000000	4.5240020000000000	3.1923170000000000
C	2.7975860000000000	1.3883730000000000	2.2360430000000000
H	1.9381810000000000	1.4644340000000000	2.9051890000000000
C	3.6399130000000000	2.6696560000000000	2.3292390000000000
H	4.4805080000000000	2.6345320000000000	1.6309500000000000
H	3.0171540000000000	3.5275650000000000	2.0750600000000000
H	4.0398220000000000	2.8013670000000000	3.3400340000000000
C	3.5794010000000000	0.1812730000000000	2.6947530000000000
O	3.1107720000000000	-0.7765330000000000	3.2889980000000000
O	4.8864110000000000	0.2555440000000000	2.3719920000000000
C	5.6790810000000000	-0.8987260000000000	2.6913800000000000
H	5.3295160000000000	-1.7648070000000000	2.1233670000000000
H	6.6977950000000000	-0.6428180000000000	2.4017250000000000
H	5.6263740000000000	-1.1190990000000000	3.7598560000000000