

Supporting Information for

Insights into NHC-catalyzed oxidative α -C(sp³)-H activation of aliphatic aldehydes and cascade [2 + 3] cycloaddition with azomethine imines

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

^aThe College of Chemistry and Molecular Engineering, Zhengzhou University, 100 Science Avenue, Zhengzhou, Henan 450001, P.R. China

^bDepartment of Material and Chemical Engineering, Zhengzhou University of Light Industry, 136 Science Avenue, Zhengzhou, Henan 450002, P.R. China

E-mail: lizhongjun@zzu.edu.cn; donghuiwei@zzu.edu.cn

Table of Contents

1. Computational details	S1
2. Test results of computational methods	S2
3. Test results of basis sets	S3
4. Optimized geometries of the stationary points	S5
5. Different conformers and configurations of TS1 and M1	S5
6. The direct/DBU-assisted proton transfer for the formation of Re/Si-M2	S7
7. The possible pathways during the oxidation process	S7
8. The possible intermolecular SET processes	S10
9. The possibilities for the α -C(sp ³)-H deprotonations	S10
10. Distortion/interaction analysis for [2 + 3] cycloaddition step	S12
11. IRC results of the reaction	S14
12. The global and local reactivity index analyses	S18
13. Absolute SPE and GFE of the optimized structures by M06-2X	S19
14. Absolute SPE and GFE of the optimized structures by other DFT methods	S22
15. The Cartesian coordinates of all the stationary points	S22

1. Computational details

All structures were completely optimized by the M06-2X functional¹ at the 6-31G(d, p) basis set and employed the integral equation formalism polarizable continuum model (IEF-PCM)² with chloroform solvent in all the computations. Frequency calculations were carried out at the same level to confirm the characteristics of all of the optimized structures as minima (no imaginary frequency) or transition states (only one imaginary frequency) and provided the thermal relative Gibbs free energy correction. All the energies discussed in the main text are the relative Gibbs free energies (GFE) and obtained by the addition of the thermal Gibbs free energy corrections (GFEC) at the M06-2X/6-31G(d, p)/IEF-PCM_{chloroform} level and the single-point energies (SPE) at a higher computational level of M06-2X/6-311++G(2df, 2pd)/IEF-PCM_{chloroform}.

To check whether the selected method is reliable, different DFT methods including M06-2X, ω B97X-D, and CAM-B3LYP at different levels (**Table S1**) have been performed additionally for the key transition states involved in the selectivity-determining step, and the computed results were summarized as **Table S2**. As shown in **Table S1**, we have denoted the seven computational levels “M06-2X/6-311++G(2df, 2pd)/IEF-PCM_{chloroform}//M06-2X/6-31G(d, p)/IEF-PCM_{chloroform}”, “M06-2X-D3/6-311++G(2df, 2pd)/IEF-PCM_{chloroform}//M06-2X/6-31G(d, p)/IEF-PCM_{chloroform}”, “M06-2X/6-311++G(2df, 2pd)/SMD_{chloroform}//M06-2X/6-31G(d, p)/SMD_{chloroform}”, “M06-2X/6-311++G(d, p)/SMD_{chloroform}//M06-2X/6-31G(d, p)/SMD_{chloroform}”, “M06-2X/6-31++G(d, p)/SMD_{chloroform}//M06-2X/6-31G(d, p)/SMD_{chloroform}”, “ ω B97X-D/6-311++G(2df, 2pd)/IEF-PCM_{chloroform}// ω B97X-D/6-31G(d, p)/IEF-PCM_{chloroform}”, and “CAM-B3LYP/6-311++G(2df, 2pd)/IEF-PCM_{chloroform}//CAM-B3LYP/6-31G(d, p)/IEF-PCM_{chloroform}” as “L1-7”, respectively.

In the distortion/interaction theory, the activation energy ($\Delta E^\ddagger$) is divided into two main components: the distortion ($\Delta E^\ddagger_{\text{dist}}$) and interaction ($\Delta E^\ddagger_{\text{int}}$) energies. The distortion energy involves geometric and electronic changes to deform the reactants to their transition state geometry. The interaction energy is obtained by the relationship: $\Delta E^\ddagger_{\text{int}} = \Delta E^\ddagger - \Delta E^\ddagger_{\text{dist}}$.

For the global reactivity index (GRI) analysis, the relevant parameters of GRI, *i.e.*, electrophilicity index ω ,³ electronic chemical potential μ , chemical hardness η , one-electron energies of the frontier molecular orbital HOMO (E_L) and LUMO (E_H), were computed to determine what is the role (Lewis base or nucleophile) of the catalyst NHC. The HOMO energies obtained within the Kohn–Sham scheme,⁴ nucleophilicity index N ⁵ was generally utilized to judge the nucleophilicity character by using the equations $N = E_{\text{H(SR)}} - E_{\text{H(TCNE)}}$ ($E_{\text{H(TCNE)}} = -0.37872$ au), $\omega = \mu^2/2\eta$, $\mu = (E_H + E_L)/2$, and $\eta = (E_L - E_H)$.

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

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

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

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

2. Test results of computational methods

To check whether the aforementioned calculation methods (*i.e.*, L1) can obtain reliable results, we also performed additional calculations for the key transition states involved in the selectivity determining step using different functions including M06-2X, ω B97X-D, and CAM-B3LYP at different levels (**Table S1**), and the results are shown as **Table S2**. Apparently, there are small differences between the results calculated by those methods, and all the results calculated by the various levels lead to the same trend and conclusion. Thus, the selected computational method should be reliable for the systems studied in this work.

In addition, we have additionally performed frequency calculations at 40 °C (313.15 K) to compare with those performed at 25 °C (298.15 K) for the first step. As summarized in **Table S3**, there are small differences (≤ 1.1 kcal/mol) between the free energies of **Re/Si-TS1** and **Re/Si-M1** at 25 °C (298.15 K) and those at 40 °C (313.15 K), suggesting that the energies discussed in the manuscript should be reasonable and reliable.

Table S1. Different Levels

Level	Optimization			Refinement		
	Functional	Basis set	Solvent model	Functional	Basis set	Solvent model
L1	M06-2X	6-31G(d, p)	IEFPCM	M06-2X	6-311++G (2df, 2pd)	IEF-PCM
L2	M06-2X	6-31G(d, p)	IEFPCM	M06-2X-D3	6-311++G (2df, 2pd)	IEF-PCM
L3	M06-2X	6-31G(d, p)	SMD	M06-2X	6-311++G (2df, 2pd)	SMD

L4	M06-2X	6-31G(d, p)	SMD	M06-2X	6-311++G(d, p)	SMD
L5	M06-2X	6-31G(d, p)	SMD	M06-2X	6-31++G(d, p)	SMD
L6	ω B97X-D	6-31G(d, p)	IEFPCM	ω B97X-D	6-311++G(2df, 2pd)	IEF-PCM
L7	CAM-B3LYP	6-31G(d, p)	IEFPCM	CAM-B3LYP	6-311++G(2df, 2pd)	IEF-PCM

Table S2. Comparisons of Relative Gibbs Free Energies for Selected Stationary Points with Different Levels $L_n = L1 \sim L7$ (Unit: kcal/mol)

	L1	L2	L3	L4	L5	L6	L7
TS5RR_{L_n}	5.1	4.9	5.6	6.4	5.7	6.1	5.5
TS5RS_{L_n}	3.8	3.6	3.5	4.1	3.3	0.7	1.1
TS5SR_{L_n}	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TS5SS_{L_n}	9.5	9.6	8.4	8.7	8.2	9.3	5.9

Table S3. The Relative Gibbs Free Energies for the First Step at Different Temperatures Computed at L1 Level (Unit: kcal/mol)

	25 °C (298.15 K)	40 °C (313.15 K)
Re-TS1	13.1	13.9
Si-TS1	14.2	15.3
Re-M1	7.4	8.1
Si-M1	8.6	9.3

3. Test results of basis sets

To test the accuracy of the selected basis set, we also performed the single-point energy calculations using the other two different basis sets including 6-311++G(d, p) and 6-31++G(d, p) for the key transition states **TS5RR/RS/SR/SS** optimized at the M06-2X/6-31G(d, p)/IEF-PCM_{chloroform} level. As summarized in **Table S4**, the relative Gibbs free energies of **TS5RR/RS/SR/SS** calculated by 6-311++G(d, p) and 6-31++G(d, p) basis sets are close to those

calculated by the selected basis set 6-311++G(2df, 2pd). Thus, the calculated results should be reliable and the selected basis set is suitable for the systems studied in this work.

Table S4. The Relative Gibbs Free Energies (kcal/mol) of **TS5RR/RS/SR/SS** Related to That of **TS5SR** Calculated by Three Different Basis Sets as Below

Basis set	6-311++G(2df, 2pd)	6-311++G(d, p)	6-31++G(d, p)
TS5RR	5.1 ^a	6.0	5.3
TS5RS	3.8	4.4	3.6
TS5SR	0.0	0.0	0.0
TS5SS	9.5	10.0	9.5

^a All the energies were gained at the above three different basis sets by using M06-2X method, and the geometries were obtained at the M06-2X/6-31G(d, p)/IEF-PCM_{chloroform} level of theory.

4. Optimized geometries of the stationary points

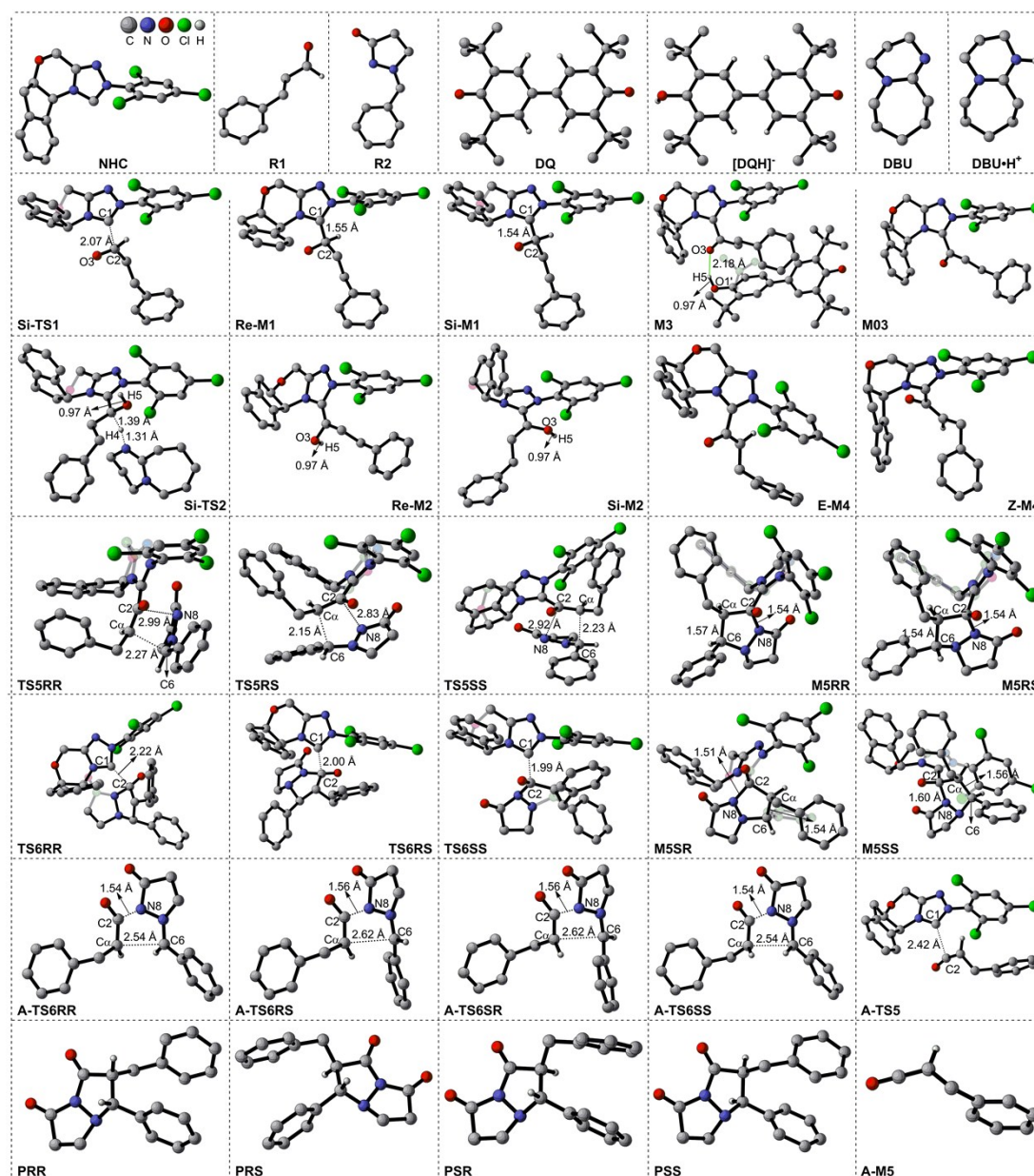


Figure S1. Optimized geometries of the stationary points involved in the catalytic cycle. Most of the hydrogen atoms are omitted for the sake of clarity.

5. Different conformers and configurations of TS1 and M1

To ensure the selected configuration of the stationary point with the lowest energy, we have considered and investigated sixteen (4×4) possible conformations for the transition state **Re/Si-TS1** and intermediate **Re/Si-M1** by rotating 90° per time of dihedral angle $\Phi(\text{N-C1-C2-O3})$ involved in the first step. The computed results (*i.e.*, the relative Gibbs free energies and their related dihedral Φ angles) and optimized conformational structures are provided in **Figure S2** and

Table S5. As shown in **Figure S2**, after rotating three times of the Φ with regard to those ($-4^\circ/22^\circ/-15^\circ/-23^\circ$) in the initial structures of **Re-TS1/Re-M1/Si-TS1/Si-M1**, the relevant dihedral angles Φ of **Re-TS1/Re-M1/Si-TS1/Si-M1** change to $-87^\circ/-104^\circ/-82^\circ/-93^\circ$, $174^\circ/-164^\circ/149^\circ/168^\circ$, and $82^\circ/84^\circ/31^\circ/34^\circ$, respectively, after the optimization. As revealed by these data, the dihedral angle $\Phi(\text{N-C1-C2-O3})$ is $-4^\circ/22^\circ/-15^\circ/-23^\circ$ in the most stable conformation of **Re-TS1/Re-M1/Si-TS1/Si-M1**, separately.

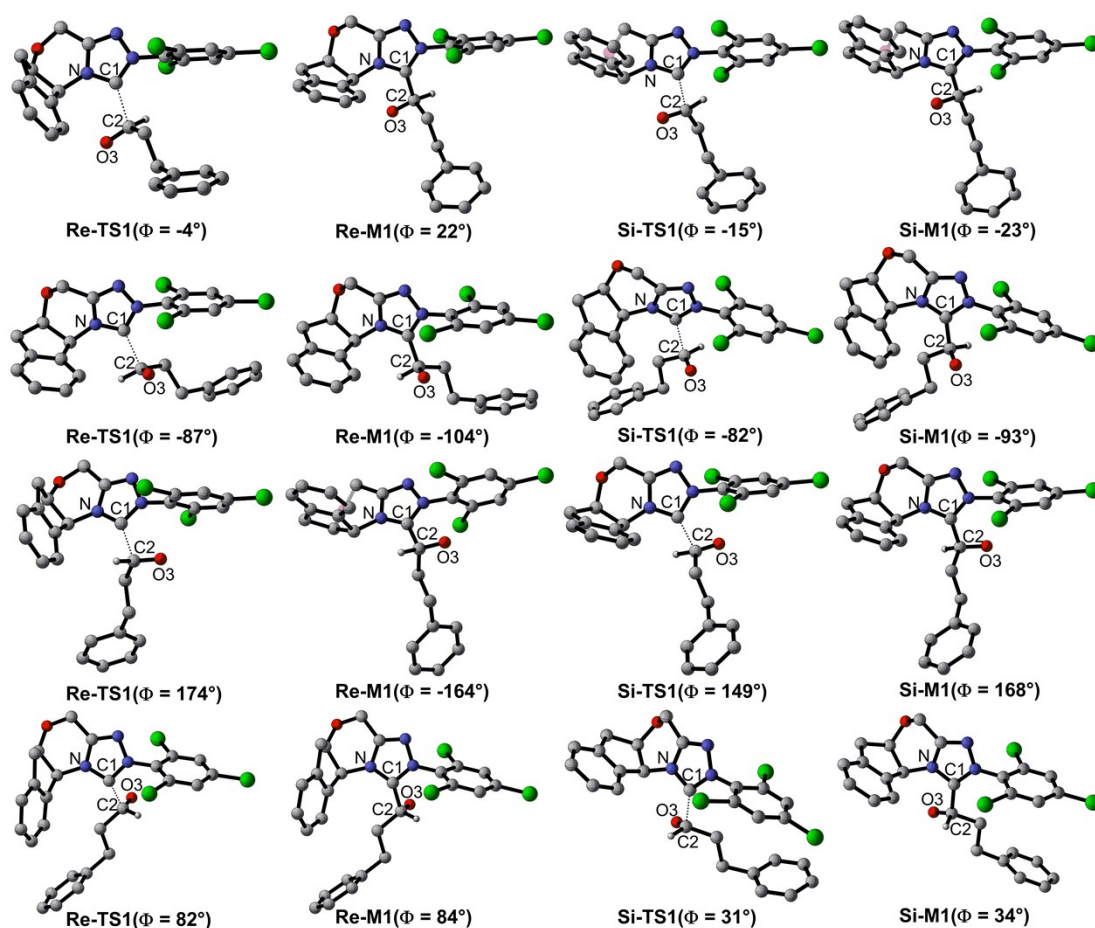


Figure S2. Different configurations of the stationary points **TS1** and **M1** with different Φ optimized at the L1 computational theory level.

Table S5. The Relative Gibbs Free Energies (kcal/mol) of Different Conformers of **TS1** and **M1**

Re-TS1	Re-M1	Si-TS1	Si-M1
13.1 ($\Phi=-4^\circ$)	7.4 ($\Phi=22^\circ$)	14.2 ($\Phi=-15^\circ$)	8.6 ($\Phi=-23^\circ$)
16.6 ($\Phi=-87^\circ$)	10.7 ($\Phi=-104^\circ$)	17.1 ($\Phi=-82^\circ$)	12.5 ($\Phi=-93^\circ$)
17.0 ($\Phi=174^\circ$)	9.7 ($\Phi=-164^\circ$)	16.2 ($\Phi=149^\circ$)	11.1 ($\Phi=168^\circ$)
22.4 ($\Phi=82^\circ$)	20.6 ($\Phi=84^\circ$)	14.9 ($\Phi=31^\circ$)	9.8 ($\Phi=34^\circ$)

6. The direct/DBU-assisted proton transfer for the formation of Re/Si-M2

As shown in **Figure S3**, we also considered and studied the direct/DBU-assisted [1,2]-proton transfer pathways *via* the relevant transition states **Re/Si-TS2a** ($\Delta G^\ddagger = 41.9/42.6$ kcal/mol) or **Re/Si-TS2b** ($\Delta G^\ddagger = 26.1/27.1$ kcal/mol). The energy barriers of the direct/DBU-assisted [1,2]-proton transfer pathways are much higher than that of the DBU·H⁺ assisted pathway *via* **Re/Si-TS2** ($\Delta G^\ddagger = 7.6/9.4$ kcal/mol, **Figure 1**), so the direct and DBU-assisted [1,2]-proton transfer pathways can be safely excluded.

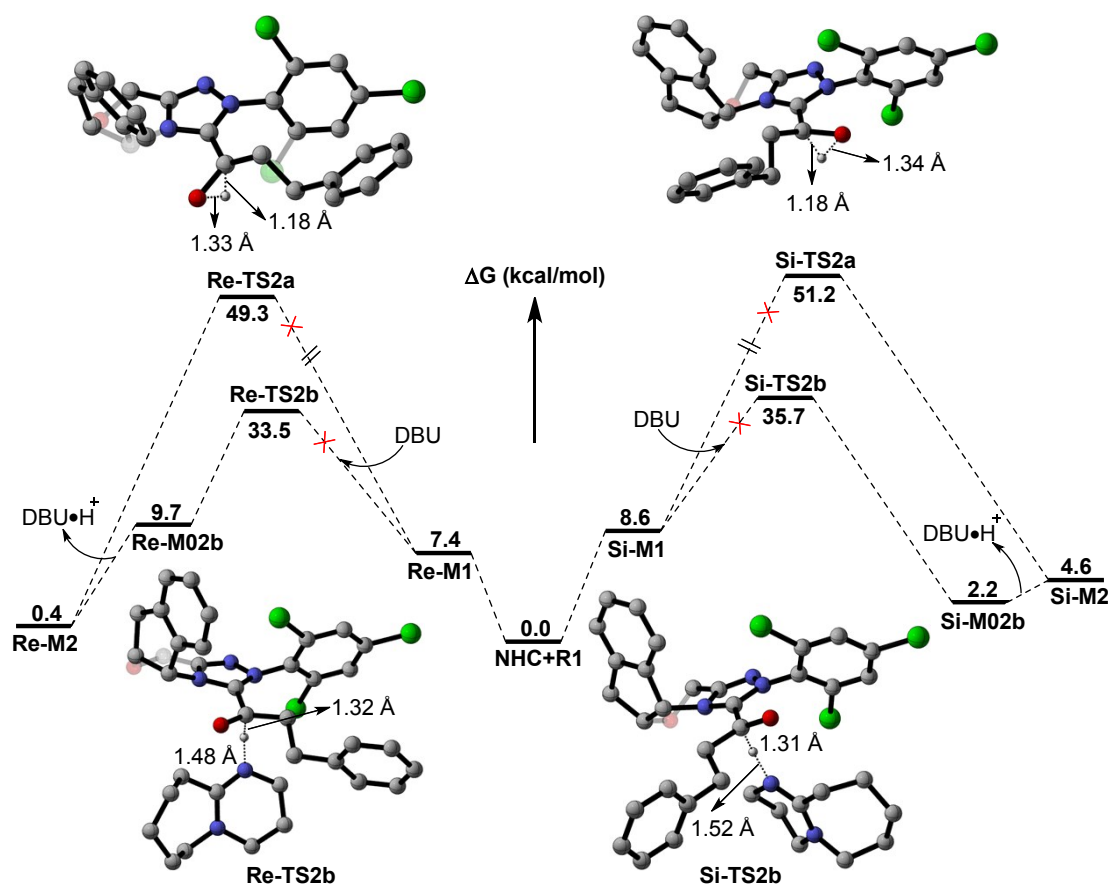


Figure S3. Relative Gibbs free energy profiles of the direct/DBU-assisted proton transfer pathway for the formation of Breslow intermediate **Re/Si-M2** (energy: kcal/mol; distance: Å).

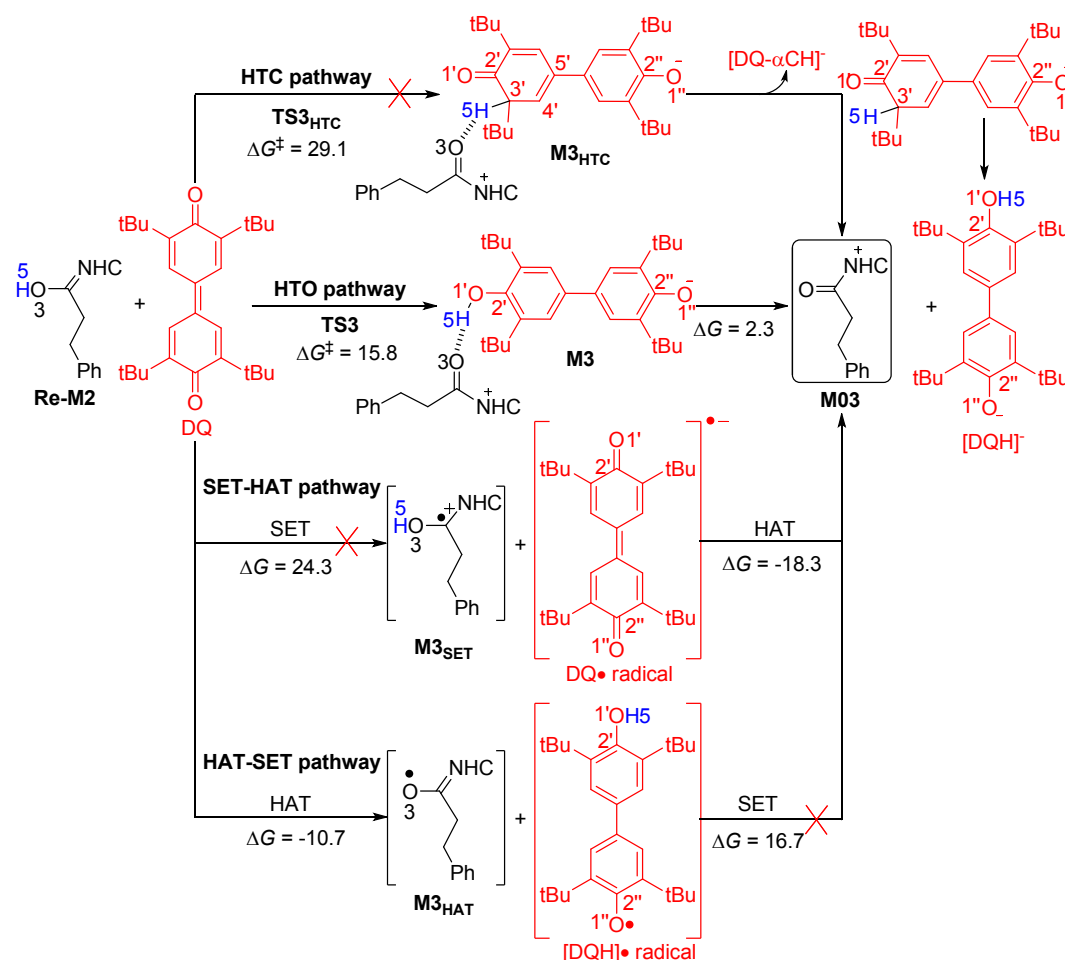
7. The possible pathways during the oxidation process

As discussed in the introduction, we have considered and investigated the other three possible pathways (*i.e.*, the HTC, SET-HAT, and HAT-SET pathways). As presented in **Schemes S1-2**, in the HTC pathway, the hydride H5 can transfer from the O3 atom in **Re-M2** to four different types of carbon (*i.e.*, C2', C3', C4', and C5') atom of DQ to give the intermediate **M3_{HTC}** *via* the

corresponding transition states $\text{TS3}_{\text{HTC}}^{\text{C2'}}$ ($\Delta G^\ddagger = 47.4$ kcal/mol, **Figure S4**), TS3_{HTC} ($\Delta G^\ddagger = 29.1$ kcal/mol, **Figure S4**), $\text{TS3}_{\text{HTC}}^{\text{C4'}}$ ($\Delta G^\ddagger = 39.2$ kcal/mol, **Figure S4**), and $\text{TS3}_{\text{HTC}}^{\text{C5'}}$ ($\Delta G^\ddagger = 27.5$ kcal/mol, **Figure S4**), respectively. Therefore, all the four HTC pathways are unlikely to occur under these experimental conditions and can be safely excluded.

For the SET-HAT and HAT-SET pathways, each of them contains two processes. In the SET-HAT pathway, the first process is a single electron transfer from **Re-M2** to DQ in forming the intermediate radical M3_{SET} and the $\text{DQ}\cdot^-$ radical, which needs to overcome a high relative Gibbs free energy (24.3 kcal/mol) to accomplish the SET process. So it is unnecessary to consider and investigate the following HAT process, and the SET-HAT pathway can be ignored. In the HAT-SET pathway, the first process is a HAT process releasing 10.7 kcal/mol Gibbs free energy to render the radical intermediate M3_{HAT} and the $[\text{DQH}]\cdot$ radical, which is followed by a single electron transfer from the radical M3_{HAT} to the $[\text{DQH}]\cdot$ radical. The HAT process is exothermic, indicating this process is easy to happen. Whereas, the SET process needs to absorb a high relative Gibbs free energy (16.7 kcal/mol), which is higher than the energy barrier *via* **TS3** ($\Delta G^\ddagger = 15.8$ kcal/mol, **Scheme S1**). Hence, the HAT-SET pathway can be neglected.

Scheme S1. Four possible pathways for the oxidation process (energy unit in kcal/mol)



Scheme S2. The other possible HTC pathways for the oxidation process (energy unit in kcal/mol)

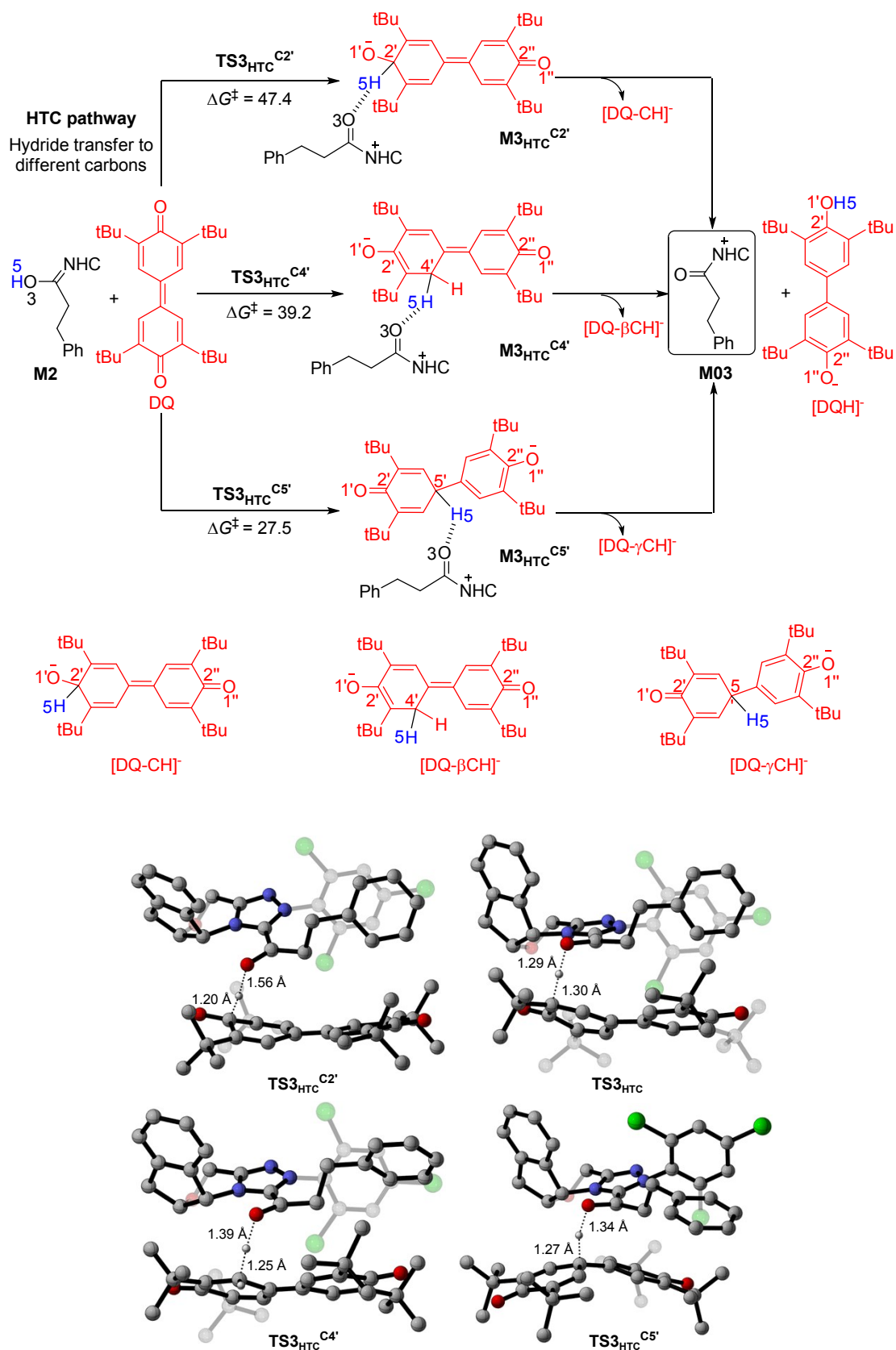


Figure S4. Optimized geometries of the transition states for the possible HTC pathways of the oxidation process calculated at the L1 level of theory. Most of the hydrogen atoms are omitted for the sake of clarity.

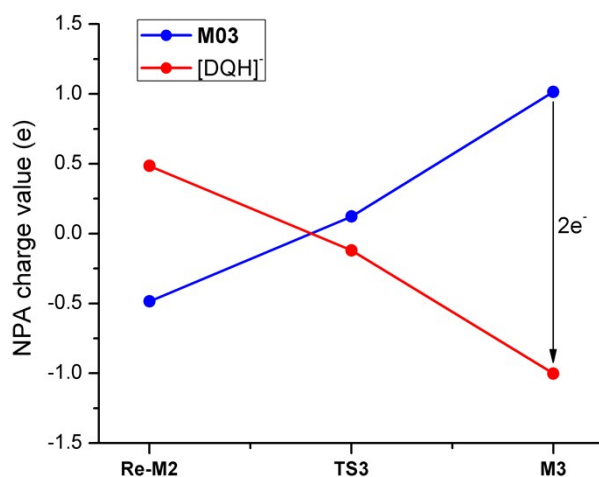
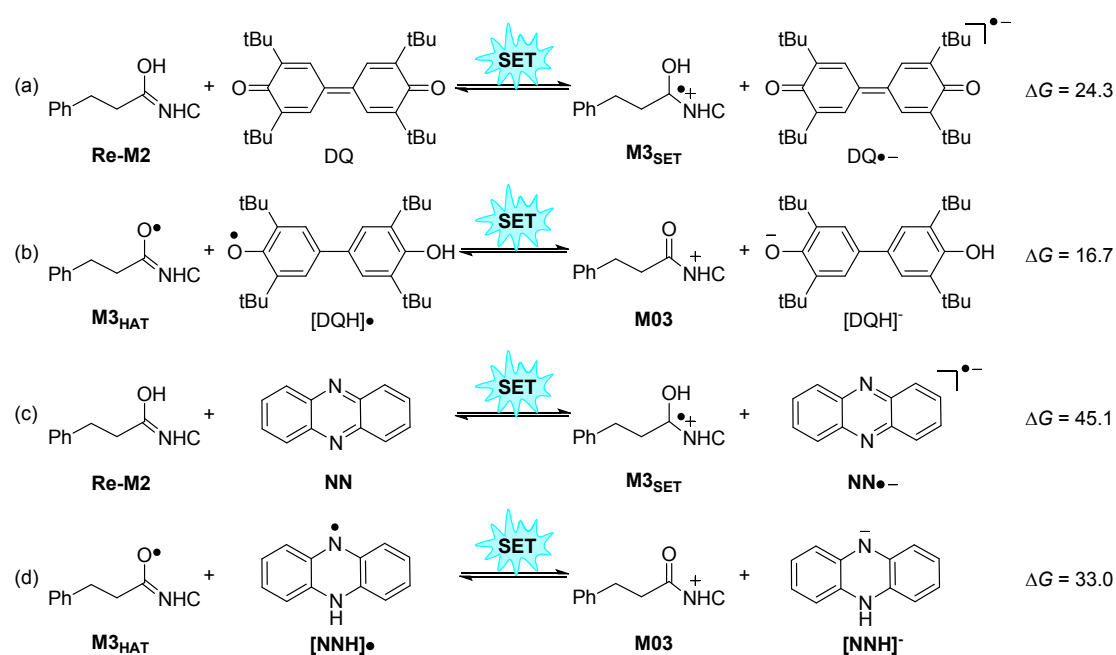


Figure S5. The NPA charge evolution during the oxidation process by DQ (**M03** and **[DQH]•** refer to the fragments of **TS3** and **M3**, respectively.)

8. The possible intermolecular SET processes



Scheme S3. The possible intermolecular single electron transfer processes for intermediates **Re-M2** and **M3_{HAT}** associated with the related thermodynamic data (energy: kcal/mol)

9. The possibilities for the α -C(sp³)-H deprotonations

As shown in **Figures S6-7**, three possible pathways including the DBU-assisted with the presence of **[DQH]⁻**, DBU-assisted without the presence of **[DQH]⁻**, **[DQH]⁻**-assisted α -C(sp³)-H

deprotonation pathways were taken into account and investigated *via* the related transition states **E/Z-TS4a** ($\Delta G^\ddagger = 23.4/30.3$ kcal/mol), **E/Z-TS4b** ($\Delta G^\ddagger = 27.4/33.2$ kcal/mol), and **E/Z-TS4** ($\Delta G^\ddagger = 7.9/14.7$ kcal/mol) in generating the corresponding *E/Z*-configured intermediates **E/Z-M4**, respectively. Evidently, the [DQH]⁻-assisted pathway *via E*-configured transition state **E-TS4** with an energy barrier of 7.9 kcal/mol is revealed to be the most energetically favorable among all the possible deprotonation pathways, so the remaining proton media-assisted α -C(sp³)-H deprotonation pathways can be safely excluded.

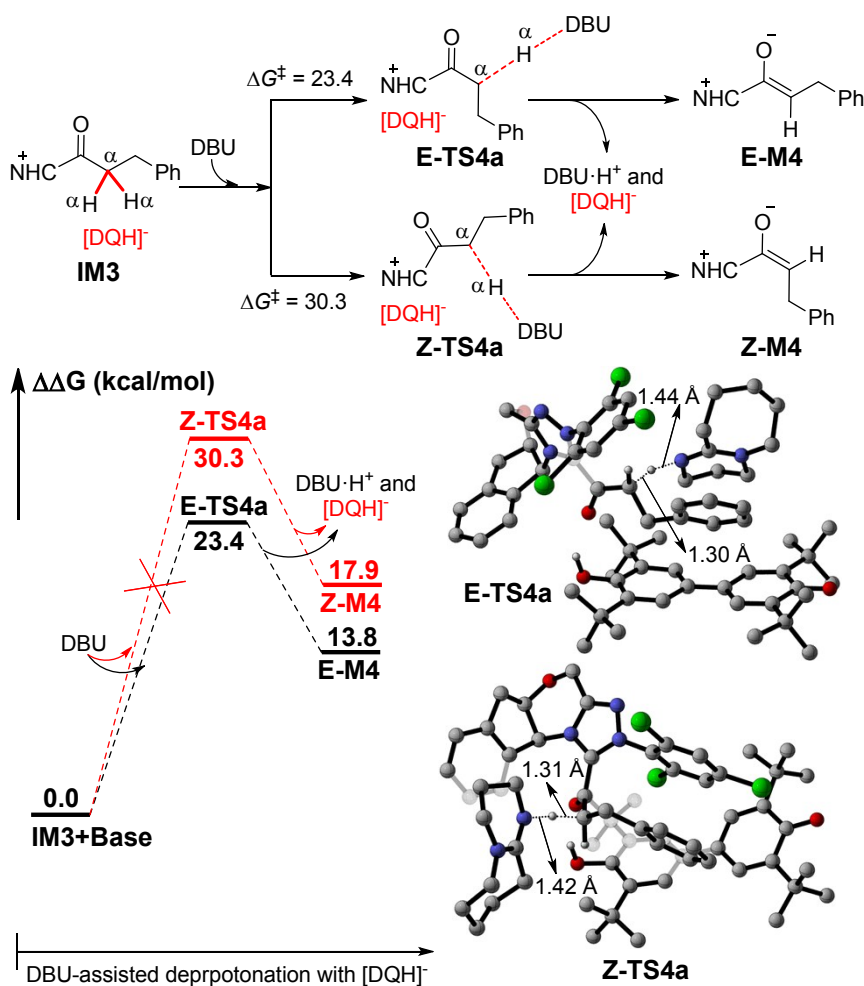


Figure S6. The relative Gibbs free energy profiles of the DBU-assisted α -C(sp³)-H deprotonation pathway with the presence of [DQH]⁻ anion, and the energy of **IM3**+DBU is set as 0.0 kcal/mol as the reference (Unit in kcal/mol). Most of the hydrogen atoms for the optimized geometries of **TS4** are omitted for the sake of clarity.

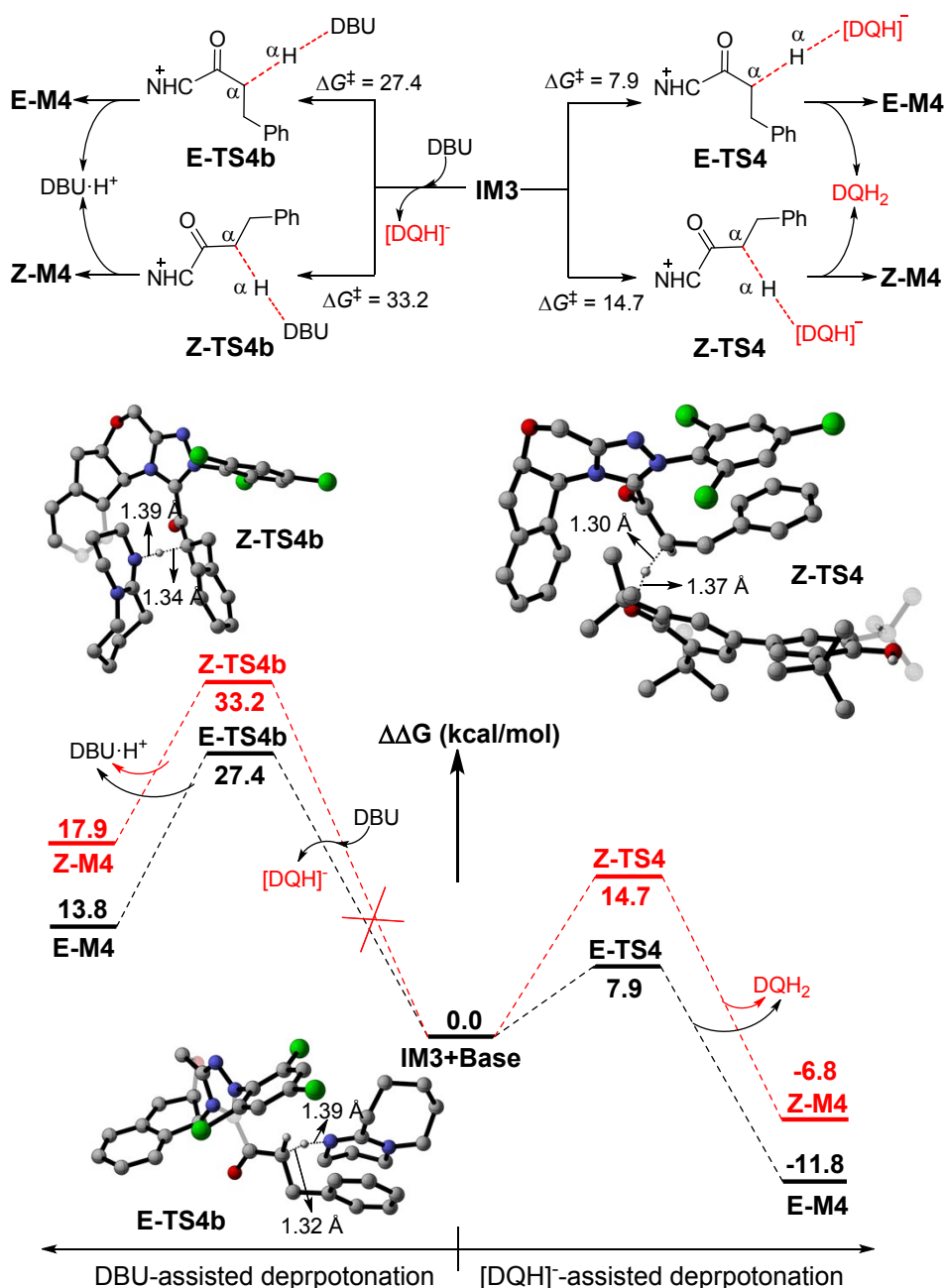


Figure S7. The relative Gibbs free energy profiles of the DBU/[DQH]⁻-assisted α -C(sp³)-H deprotonation pathways, and the energy of **IM3+Base** is set as 0.0 kcal/mol as the reference (Unit in kcal/mol). Most of the hydrogen atoms for the optimized geometries of **TS4** are omitted for the sake of clarity.

10. Distortion/interaction analysis for [2 + 3] cycloaddition step

As summarized in **Table S6**, the much higher energy barriers *via* **A-TS6RR/RS/SR/SS** are mainly due to their extremely larger distortion energies ($\Delta E_{\text{dist_total}}^\ddagger = 68.8/56.2/68.8/56.2$ kcal/mol) than those of **TS5RR/RS/SR/SS** ($\Delta E_{\text{dist_total}}^\ddagger = 25.7/31.9/24.8/29.4$ kcal/mol).

Table S6. Distortion/interaction analysis for the NHC-catalyzed or uncatalyzed [2 + 3] cycloaddition step (All values are in kcal/mol)

	$\Delta E_{\text{dist_E-M4}}^{\ddagger}$	$\Delta E_{\text{dist_R2}}^{\ddagger}$	$\Delta E_{\text{dist_total}}^{\ddagger}$
TS5RR	12.5	13.2	25.7
TS5RS	14.4	17.5	31.9
TS5SR	8.3	16.5	24.8
TS5SS	10.7	18.7	29.4
	$\Delta E_{\text{dist_A-M5}}^{\ddagger}$	$\Delta E_{\text{dist_R2}}^{\ddagger}$	$\Delta E_{\text{dist_total}}^{\ddagger}$
A-TS6RR/SS	45.4	23.4	68.8
A-TS6RS/SR	37.6	18.6	56.2

11. IRC results of the reaction

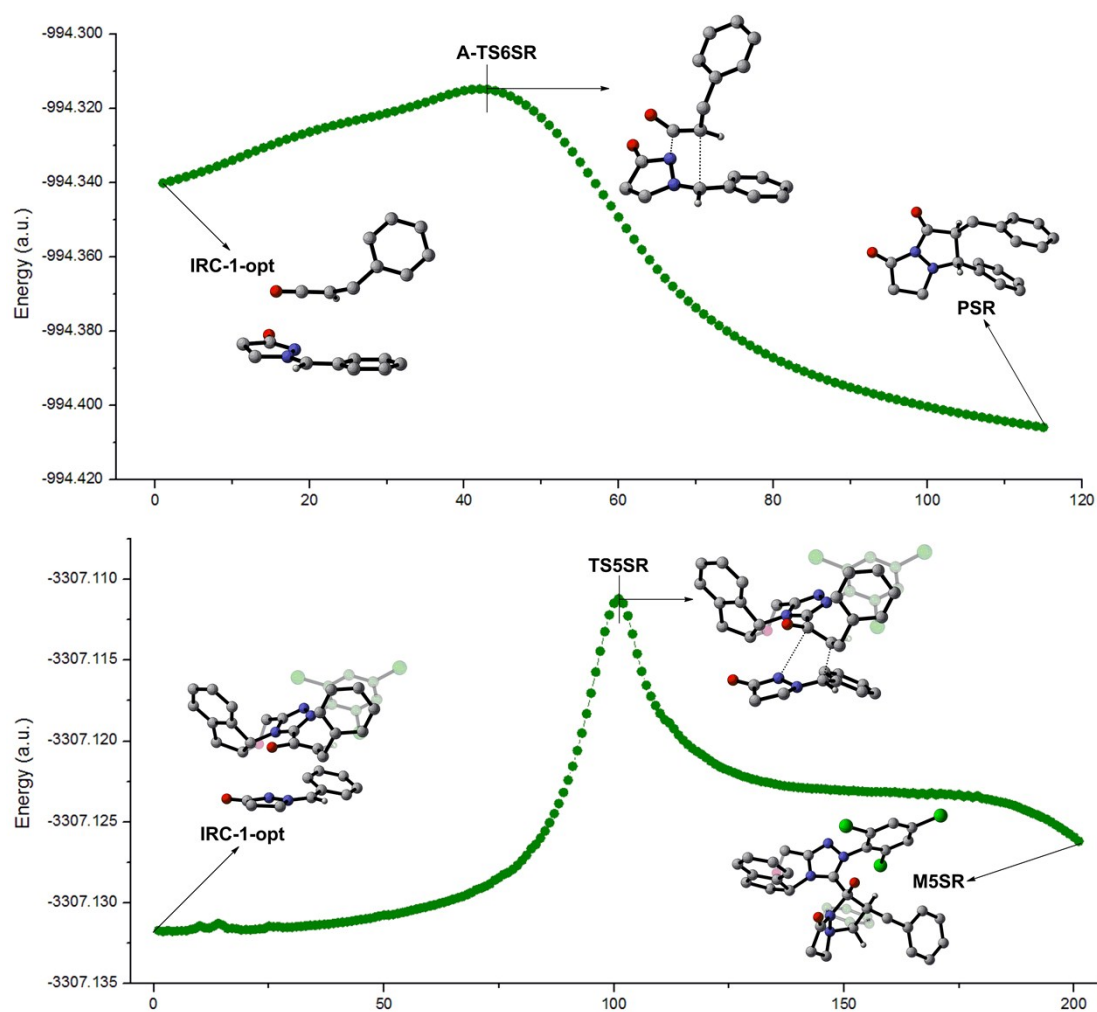


Figure S8. The tracking IRC results of TS5SR and A-TS6SR calculated at the M06-2X/6-31G(d, p)/IEF-PCM_{chloroform} level (unit: a.u.)

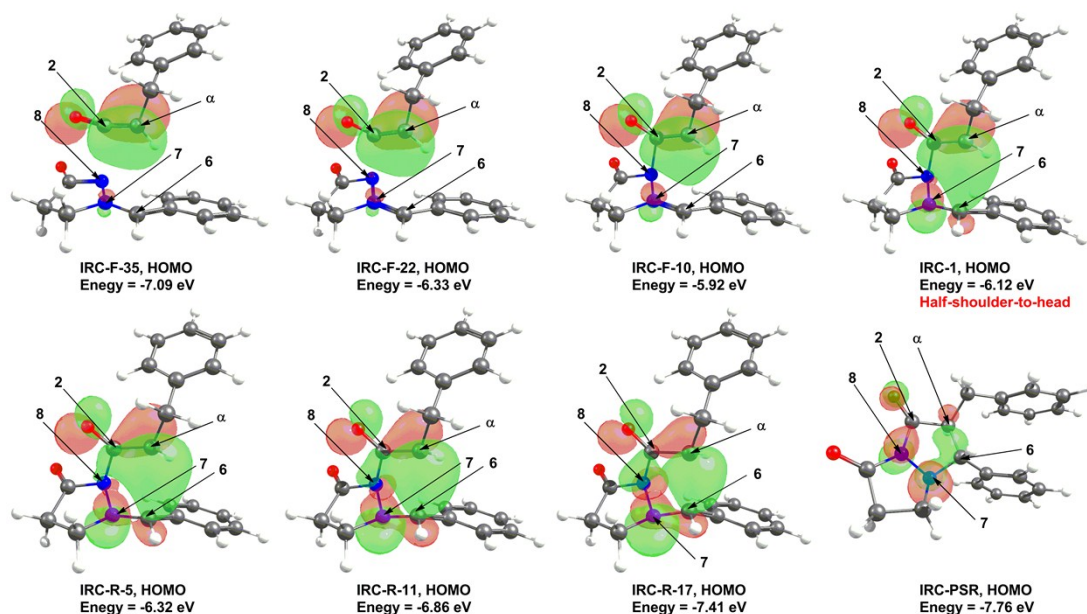


Figure S9. The HOMOs of several representative IRC points of **A-TS6SR** calculated at the M06-2X/6-31G(d, p)/IEF-PCM_{chloroform} level (“F” and “R” represent forward and reverse, respectively; IRC-1 is the structure of **A-TS6SR**.)

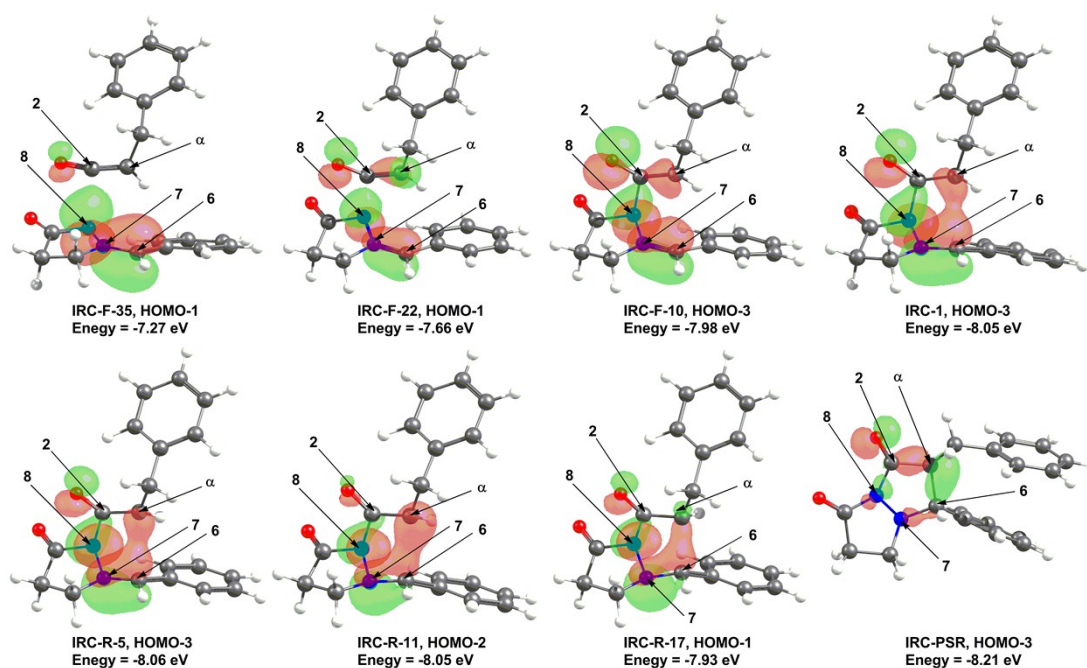


Figure S10. The other HOMOs of several representative IRC points of **A-TS6SR** calculated at the M06-2X/6-31G(d, p)/IEF-PCM_{chloroform} level (“F” and “R” represent forward and reverse, respectively; IRC-1 is the structure of **A-TS6SR**).

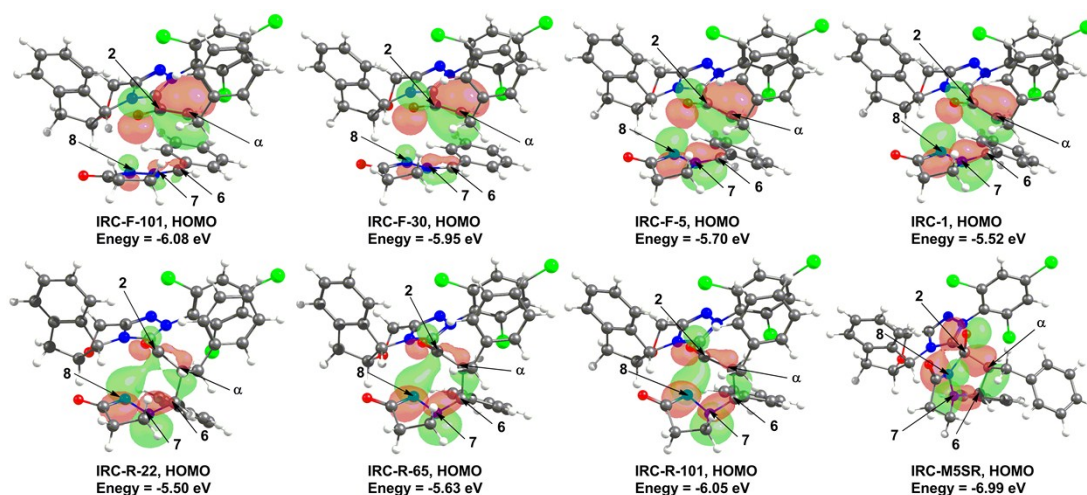


Figure S11. The HOMOs of several representative IRC points of **TS5SR** calculated at the M06-2X/6-31G(d, p)/IEF-PCM_{chloroform} level (“F” and “R” represent forward and reverse, respectively; IRC-1 is the structure of **TS5SR**.)

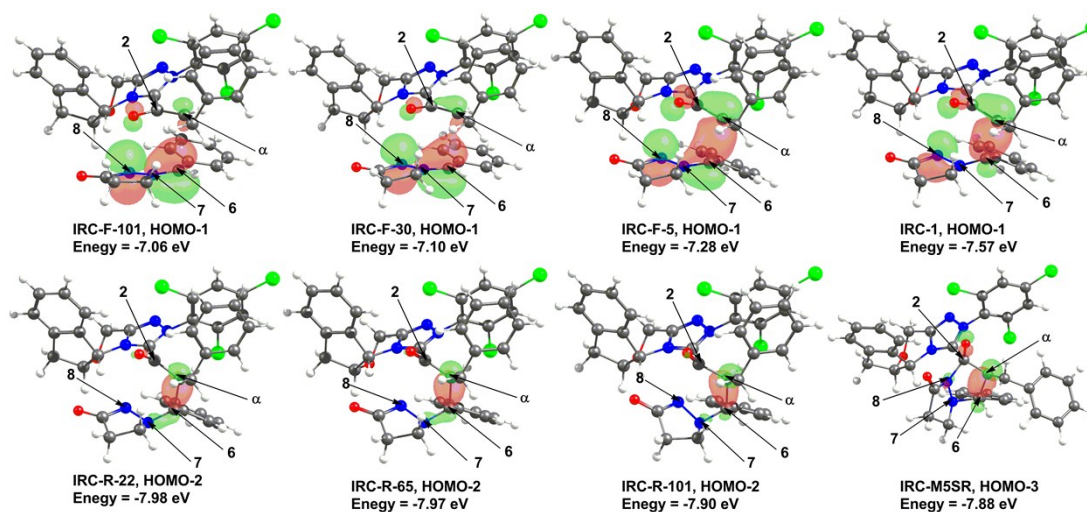


Figure S12. The other HOMOs of several representative IRC points of **TS5SR** calculated at the M06-2X/6-31G(d, p)/IEF-PCM_{chloroform} level (“F” and “R” represent forward and reverse, respectively; IRC-1 is the structure of **TS5SR**).

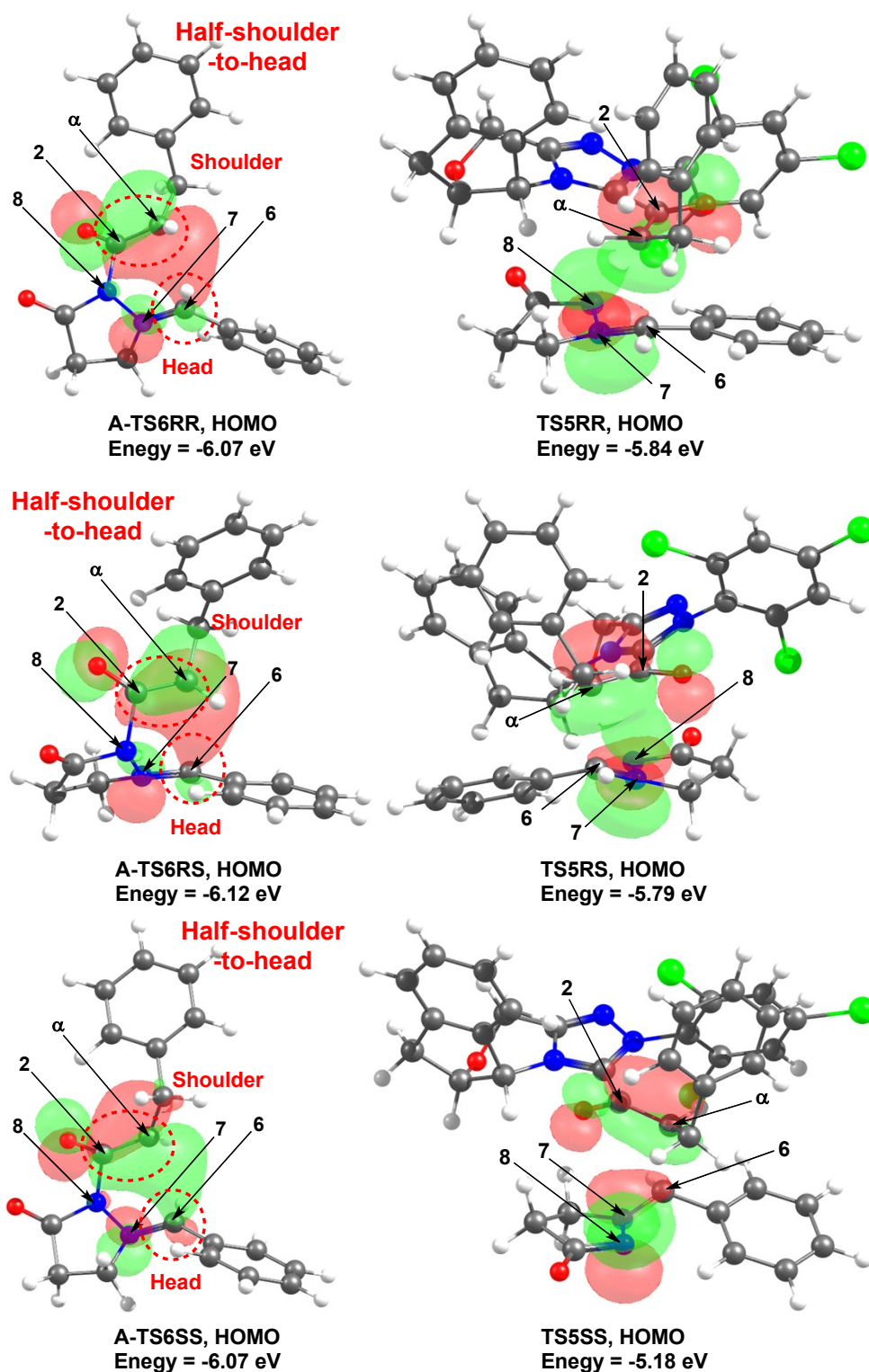


Figure S13. The representative FMO overlap mode involved in the key transition states of uncatalyzed/NHC-catalyzed [2 + 3] cycloadditions

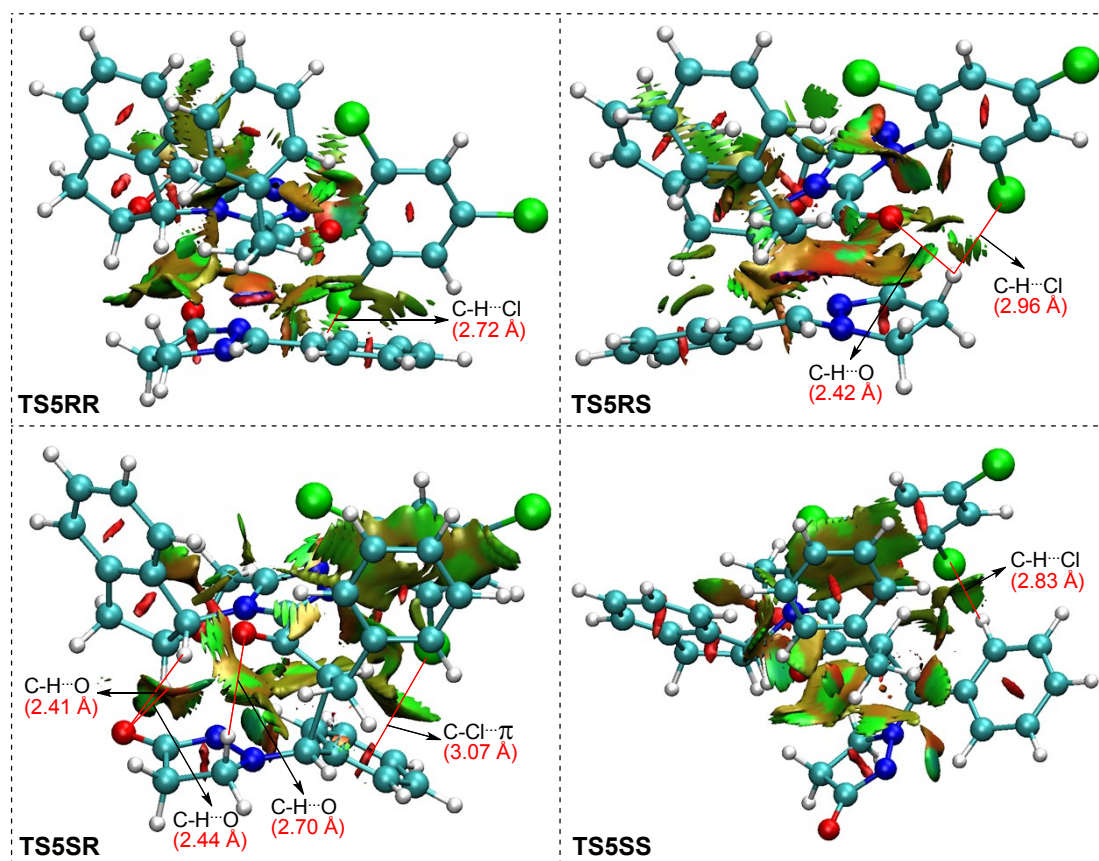


Figure S14. Interaction analysis for the diastereoisomeric transition states **TS5RR/RS/SR/SS** (Blue, green, and red represent the strong attraction, weak interaction, and steric effect, respectively; the δ value of isosurface is set to 0.6.)

12. The global and local reactivity index analyses

In the view of molecular level, the catalyst NHC could also work as a Lewis base to improve the nucleophilicity of aldehyde **R1** as summarized in **Table S7**, and thus facilitates the following [2 + 3] cycloaddition process. These data were obtained by performing the global reactivity index (GRI) analysis.³⁻⁵ In the view of atomic level, the $C\alpha$ atom of **E-M4** with the highest the P_k^- value (0.60, **Table S8**) would be the most nucleophilic site after analyzing the local reactivity indexes (electrophilic (P_k^+) and nucleophilic (P_k^-) Parr functions)^{5c} on the potential sites (*i.e.*, C2 and $C\alpha$ atoms) of some intermediates (**Re-M2**, **M3**, **E-M4**, and **A-M5**). Hence, the catalyst NHC can enhance the nucleophilicity of enal **R1**, and thus facilitates the following [2 + 3] cycloaddition of **E-M4** with **R2** by strengthening the nucleophilicity of the $C\alpha$ atom in **E-M4**.

Table S7. Energies of HOMO (E_H) and LUMO (E_L), Electronic Potential (μ), Chemical Hardness (η), Global Electrophilicity (ω), and Global Nucleophilicity (N) of Some

Intermediates

	E_H (a.u.)	E_L (a.u.)	μ (a.u.)	η (a.u.)	ω (eV)	N (eV)
R1	-0.304	-0.002	-0.153	0.302	1.049	2.025
R2	-0.271	-0.050	-0.160	0.221	1.577	2.927
Re-M1	-0.259	-0.036	-0.148	0.223	1.331	3.232
Re-M2	-0.229	-0.024	-0.127	0.205	1.061	4.055
E-M4	-0.234	-0.032	-0.133	0.203	1.187	3.919
A-M5	-0.290	-0.007	-0.148	0.283	1.057	2.394

Table S8. Electrophilic and Nucleophilic Parr Functions (P_k^+ and P_k^-) For the Atoms (C2 and C α) of Some Intermediates

Parr	Re-M2		M3		E-M4		A-M5	
function	C2	C α	C2	C α	C2	C α	C2	C α
P_k^+	0.0	0.0	0.21	-0.02	-0.01	0.03	0.66	0.01
P_k^-	0.55	-0.02	0.0	0.0	-0.09	0.60	0.02	0.57

As summarized in **Table S9**, the values of ΔG , ΔH , $-T\Delta S$ are all positive during the uncatalyzed [2 + 3] cycloaddition process, indicating that this process is much endothermic and unfavorable to occur under the experimental condition. In contrast, the values of ΔG , $-T\Delta S$ are positive and the value of ΔH is negative during the NHC-catalyzed [2 + 3] cycloaddition process, indicating that this catalytic process is spontaneous and favorable to happen at such condition. By comparing these thermodynamic data of the uncatalyzed and NHC-catalyzed cycloaddition processes, it can be found that smaller entropic cost is favorable for driving the uncatalyzed process and more negative enthalpic cost is favorable for driving the NHC-catalyzed process. Hence, the NHC-catalyzed cycloaddition is an enthalpically-derived process.

Table S9. Thermodynamic Parameters (unit of kcal/mol) of the Uncatalyzed and NHC-Catalyzed [2 + 3] Cycloaddition Processes

[2 + 3] cycloaddition process	ΔG	ΔH	$-T\Delta S$
A-M5 + R2 $\rightarrow$ A-TS6RR/SS	31.4	16.3	15.1
A-M5 + R2 $\rightarrow$ A-TS6RS/SR	35.7	20.1	15.6
A-M5 + NHC + R2 $\rightarrow$ TS5RR	11.0	-21.2	32.2
A-M5 + NHC + R2 $\rightarrow$ TS5RS	9.6	-22.3	31.9
A-M5 + NHC + R2 $\rightarrow$ TS5SR	5.8	-27.4	33.2
A-M5 + NHC + R2 $\rightarrow$ TS5SS	15.4	-15.5	30.9

13. Absolute SPE and GFE of the optimized structures by M06-2X

Table S10. The SPE and GFE (=SPE+GFEC) of the Stationary Points Involved in the Catalytic Cycle and Substituent Effects Computed at the L1 Computational Level (unit: a.u.)

	SPE	GEE		SPE	GEE
NHC	-2313.106127	-2312.885672	IM3	-3978.7024056	-3977.7311516
R1	-424.1519129	-424.0197529	E-TS4a	-4440.724619	-4439.521358
R2	-571.7338176	-571.5842136	Z-TS4a	-4440.719743	-4439.510510
DBU	-462.0407314	-461.8275194	E-TS4b	-3198.576858	-3197.974039
DBU·H⁺	-462.5032841	-462.2749681	Z-TS4b	-3198.570842	-3197.963185
NN	-571.551247	-571.4143420	E-TS4	-3978.682151	-3977.718571
[NNH]⁻	-572.2526968	-572.1080988	Z-TS4	-3978.677701	-3977.707825
NN⁻	-571.6554141	-571.5230081	E-M4	-2736.0823806	-2735.7222696
[NNH]·	-572.1469850	-572.0001700	Z-M4	-2736.07441	-2735.714253
NNH₂	-572.7679593	-572.6090893	TS5RR	-3307.804417	-3307.269977
DQ	-1241.363115	-1240.802666	TS5RS	-3307.806728	-3307.272069
DQ⁻	-1241.503428	-1240.9445409	TS5SR	-3307.815262	-3307.278173
[DQH]·	-1241.979191	-1241.4070793	TS5SS	-3307.7955893	-3307.2628603
[DQH]⁻	-1242.112841	-1241.541030	M5RR	-3307.835096	-3307.293016
DQH₂	-1242.613316	-1242.027792	M5RS	-3307.843914	-3307.301978
Re-TS1	-2737.258987	-2736.884593	M5SR	-3307.841727	-3307.301468
Si-TS1	-2737.257712	-2736.882826	M5SS	-3307.832255	-3307.291635
Re-M1	-2737.269592	-2736.893594	TS6RR	-3307.817612	-3307.281162
Si-M1	-2737.270897	-2736.891799	TS6RS	-3307.835098	-3307.296361
Re-TS2	-3199.782044	-3199.156557	TS6SR	-3307.8365823	-3307.2964343
Si-TS2	-3199.778270	-3199.151659	TS6SS	-3307.822012	-3307.282869
Re-TS2a	-2737.201610	-2736.826920	A-TS5	-2736.045261	-2735.691042
Si-TS2a	-2737.196981	-2736.823903	A-M5	-422.926801	-422.817545
Re-TS2b	-3199.292205	-3198.679599	A-TS6RR	-994.6358071	-994.3516821
Si-TS2b	-3199.286637	-3198.676049	A-TS6RS	-994.6295273	-994.3449733
Re-M2	-2737.283117	-2736.904852	A-TS6SR	-994.6295262	-994.3449722
Si-M2	-2737.277781	-2736.898165	A-TS6SS	-994.6358071	-994.3516811
M3_{SET}	-2737.104623	-2736.7243200	PRR	-994.7342197	-994.4449757
M3_{HAT}	-2736.683926	-2736.3175667	PRS	-994.7370903	-994.4456373
TS3	-3978.651302	-3977.682203	PSR	-994.7370903	-994.4456373
TS3_{HTC}	-3978.629593	-3977.661075	PSS	-994.7342197	-994.4449757
TS3_{HTC}^{C2'}	-3978.601865	-3977.632532			
TS3_{HTC}^{C4'}	-3978.614593	-3977.645633			
TS3_{HTC}^{C5'}	-3978.630471	-3977.664295			
M3	-3978.675206	-3977.701656			
M03	-2736.527993	-2736.157065			
TS3N	-3308.816683	-3308.278231			
M3N	-3308.828941	-3308.287225			

Table S11. The SPE and GFE (=SPE+GFEC) of the Stationary Points for the First Step at the Temperature of 40 °C (313.15 K) Computed at the L1 Theory Level

	SPE (a.u.)	GEE (a.u.)
NHC (313.15 K)	-2313.106127	-2312.889319
R1 (313.15 K)	-424.1519129	-424.0220879
Re-TS1 (313.15 K)	-2737.258987	-2736.889298
Si-TS1 (313.15 K)	-2737.257712	-2736.887099
Re-M1 (313.15 K)	-2737.269592	-2736.898502
Si-M1 (313.15 K)	-2737.270897	-2736.896598

Table S12. The SPE and GFE (=E+GFEC) of Different Conformers of **Re/Si-TS1** and **Re/Si-M1** Calculated at the L1 Theory Level

	SPE (a.u.)	GEE (a.u.)
Re-TS1 ($\Phi = -4^\circ$)	-2737.258987	-2736.884593
Re-TS1 ($\Phi = -87^\circ$)	-2737.256866	-2736.878993
Re-TS1 ($\Phi = 174^\circ$)	-2737.255646	-2736.878316
Re-TS1 ($\Phi = 82^\circ$)	-2737.249081	-2736.869779
Si-TS1 ($\Phi = -15^\circ$)	-2737.257712	-2736.882826
Si-TS1 ($\Phi = -82^\circ$)	-2737.255969	-2736.878193
Si-TS1 ($\Phi = 149^\circ$)	-2737.255415	-2736.879559
Si-TS1 ($\Phi = 31^\circ$)	-2737.259395	-2736.881743
Re-M1 ($\Phi = 22^\circ$)	-2737.269592	-2736.893594
Re-M1 ($\Phi = -104^\circ$)	-2737.267017	-2736.888398
Re-M1 ($\Phi = -164^\circ$)	-2737.266711	-2736.889892
Re-M1 ($\Phi = 84^\circ$)	-2737.252681	-2736.872659
Si-M1 ($\Phi = -23^\circ$)	-2737.270897	-2736.891799
Si-M1 ($\Phi = -93^\circ$)	-2737.265458	-2736.885461
Si-M1 ($\Phi = 168^\circ$)	-2737.266261	-2736.887761
Si-M1 ($\Phi = 34^\circ$)	-2737.267391	-2736.889872

Table S13. The SPE and GFE (=E+GFEC) of the Stationary Points Refined the Energies by Different Basis Sets as Below Based on the Geometries Calculated at the M06-2X/6-31G(d, p)/IEF-PCM_{chloroform} Level of Theory

	6-311++G(d, p)		6-31++G(d, p)	
	SPE (a.u.)	GEE (a.u.)	SPE (a.u.)	GEE (a.u.)
TS5RR	-3307.6680275	-3307.1335875	-3307.1563910	-3306.6219510
TS5RS	-3307.6708316	-3307.1361726	-3307.1593836	-3306.6247246
TS5SR	-3307.6803077	-3307.1432187	-3307.1675329	-3306.6304439
TS5SS	-3307.6975388	-3307.1643998	-3307.1855399	-3306.6524009

Table S14. The GFE(=E+GFEC), Enthalpy (H=E+HC), and TS of the Stationary Points for Other Reaction Models Computed at the L1 Computational Level (Temperature T=298.15 K)

	GFE (a.u.)	H (a.u.)	TS (kcal/mol)
NHC	-2312.8856716	-2312.8141306	44.89333995
R2	-571.5842136	-571.5351986	30.75745215
A-M5	-422.8175450	-422.7727330	28.12001725
A-TS6RR	-994.3516821	-994.2819401	43.7636496
A-TS6RS	-994.3449733	-994.2758863	43.35309705
A-TS6SR	-994.3449722	-994.2758852	43.3527989
A-TS6SS	-994.3516811	-994.2819401	43.7636496
TS5RR	-3307.2699765	-3307.1558765	71.59923175
TS5RS	-3307.2720688	-3307.1575678	71.8505722
TS5SR	-3307.2781730	-3307.1657700	70.53364365
TS5SS	-3307.2628603	-3307.1468043	72.826119

Table S15. The SPE and GFE (=E+GFEC) of the Stationary Points for Other Reaction Models Calculated at the M06-2X/6-311++G(2df, 2pd)/IEF-PCM_{DCE}//M06-2X/6-31G(d, p)/IEF-PCM_{DCE} Level of Theory

	SPE (a.u.)	GEE (a.u.)
R2_{DCE}	-571.7373242	-571.5876692
M4_{NHC1}	-2736.085954	-2735.725963
TS5SR_{NHC1}	-3307.820042	-3307.282908
M4_{NHC2}	-1475.21417	-1474.739374
TS5SR_{NHC2}	-2046.948858	-2046.29791
M4_{NHC3}	-2737.284514	-2736.904719
TS5SR_{NHC3}	-3309.012625	-3308.454559

14. Absolute SPE and GFE of the optimized structures by other DFT methods

Table S16. The SPE and GFE (=E+GFEC) of the Stereochemical Transition States for the Reaction Calculated at the Different Computational Levels (L2-7) (unit: a.u.)

	SPE (a.u.)	GEE (a.u.)		SPE (a.u.)	GEE (a.u.)
L2	M06-2X-D3/6-311++G(2df, 2pd)/IEF-PCM _{chloroform} //M06-2X/6-31G(d, p)/IEF-PCM _{chloroform}		L3	M06-2X/6-311++G(2df, 2pd)/SMD _{chloroform} //M06-2X/6-31G(d, p)/SMD _{chloroform}	
TS5RR_{L2}	-3307.815987	-3307.281547	TS5RR_{L3}	-3307.838918	-3307.303755
TS5RS_{L2}	-3307.81832	-3307.283661	TS5RS_{L3}	-3307.840705	-3307.306968
TS5SR_{L2}	-3307.826454	-3307.289365	TS5SR_{L3}	-3307.848165	-3307.312606
TS5SS_{L2}	-3307.806764	-3307.274035	TS5SS_{L3}	-3307.832364	-3307.299225

L4	M06-2X/6-311++G(d, p)/SMD _{chloroform} //M06-2X/6- 31G(d, p)/SMD _{chloroform}		L5	M06-2X/6-31++G(d, p)/SMD _{chloroform} //M06-2X/6-31G(d, p)/SMD _{chloroform}	
TS5RR_{L4}	-3307.703353	-3307.16819	TS5RR_{L5}	-3307.191567	-3306.656404
TS5RS_{L4}	-3307.705552	-3307.171815	TS5RS_{L5}	-3307.194041	-3306.660304
TS5SR_{L4}	-3307.713891	-3307.178332	TS5SR_{L5}	-3307.201059	-3306.6655
TS5SS_{L4}	-3307.697539	-3307.164400	TS5SS_{L5}	-3307.185540	-3306.652401
L6	ω B97X-D /6-311++G(2df, 2pd)/IEF-PCM _{chloroform} // ω B97X- D/6-31G(d, p)/IEF-PCM _{chloroform}		L7	CAM-B3LYP/6-311++G(2df, 2pd)/IEF-PCM _{chloroform} //CAM- B3LYP/6-31G(d, p)/IEF- PCM _{chloroform}	
TS5RR_{L6}	-3307.951381	-3307.413572	TS5RR_{L7}	-3307.625725	-3307.09036
TS5RS_{L6}	-3307.959192	-3307.422102	TS5RS_{L7}	-3307.630948	-3307.097498
TS5SR_{L6}	-3307.962400	-3307.423250	TS5SR_{L7}	-3307.635134	-3307.099195
TS5SS_{L6}	-3307.944149	-3307.408430	TS5SS_{L7}	-3307.621599	-3307.089731

15. The Cartesian coordinates of all the stationary points

NHC

0 1

C	0.34639600	0.20360000	0.79136200
C	1.05317100	1.60646100	-0.83664900
C	2.77198600	0.87474900	0.83232900
H	2.72793200	1.37693700	1.80156700
N	-0.20769300	1.44954500	-1.09645600
N	-0.60311000	0.58939900	-0.08883600
N	1.41739000	0.87690700	0.26777600
C	2.04529000	2.43344100	-1.59479200
H	1.59952300	3.39162600	-1.86619900
H	2.33127600	1.91781900	-2.52064600
C	3.73652400	1.58621800	-0.15143800
O	3.17122700	2.71291500	-0.78776300
C	4.22369600	-0.73680400	-0.16749800
C	3.35477300	-0.51502400	0.90294800
C	3.11416700	-1.49901700	1.85391500
C	3.77187400	-2.72117300	1.72727700
C	4.65028500	-2.94469800	0.66517200
C	4.88216200	-1.95575400	-0.29020200
C	4.28190100	0.47062100	-1.07040000
H	2.42249400	-1.31676900	2.66998200

H	5.15939800	-3.89984100	0.58274400
H	5.56639300	-2.13543300	-1.11412900
H	3.63640500	0.31726700	-1.94365600
H	5.28405800	0.69943400	-1.43956700
C	-1.95461400	0.17416200	-0.05290600
C	-2.37310200	-0.94878100	-0.76967300
C	-2.90352100	0.88316800	0.68622200
C	-3.69645700	-1.37012800	-0.74849000
C	-4.23396700	0.48508800	0.72773000
C	-4.60827300	-0.64114800	0.00494700
H	-4.00433200	-2.24522100	-1.30688500
H	-4.95813500	1.04294100	1.30826800
H	4.56519300	1.98149600	0.44136700
H	3.60379300	-3.50321000	2.46039700
Cl	-1.21716000	-1.84352800	-1.69926700
Cl	-6.26912400	-1.15288400	0.04228500
Cl	-2.41510800	2.28751900	1.57417900

R1

0 1

C	3.28924900	-0.29276500	-0.07706100
O	4.18208700	0.46801400	-0.36688700
H	3.50228100	-1.21310200	0.50786300
C	1.84368600	-0.09435300	-0.44599000
C	0.93411200	-0.18277200	0.79267700
H	1.56275200	-0.89167200	-1.14694000
H	1.73296700	0.86672400	-0.95499900
H	1.11578500	-1.13354800	1.30674600
H	1.19775600	0.61808200	1.49144500
C	-0.52308900	-0.07537000	0.41466900
C	-1.27187000	-1.21882900	0.12648100
C	-1.13535500	1.17499300	0.30074600
C	-2.60468400	-1.11626000	-0.26376800
H	-0.80608800	-2.19751400	0.21476800
C	-2.46756100	1.28218300	-0.08940100
H	-0.56167100	2.07113100	0.52477500
C	-3.20628000	0.13536900	-0.37232700
H	-3.17437900	-2.01456600	-0.48023300

H	-2.92975600	2.26102700	-0.17038600
H	-4.24559300	0.21614600	-0.67409000

R2

0 1

C	2.33685900	-1.54379800	-0.07539000
C	2.79965000	0.79696900	0.01233500
C	3.48262600	-0.57567500	0.11475800
H	2.22210000	-2.28867600	0.71103000
H	2.34010700	-2.03452800	-1.04957700
H	4.25436300	-0.66003500	-0.65010100
H	3.95523500	-0.66146600	1.09517000
N	1.43943400	0.67291800	-0.05128800
N	1.13784900	-0.63331400	-0.03700200
O	3.40101600	1.85773600	0.00865000
C	-0.06098400	-1.13236300	-0.02083500
H	-0.09135500	-2.21725300	-0.01899300
C	-1.32898000	-0.42153900	-0.00857900
C	-2.48269900	-1.22641800	0.02516500
C	-1.47369200	0.97667700	-0.02766100
C	-3.74657100	-0.65629300	0.03972900
H	-2.37717700	-2.30788500	0.04070700
C	-2.74671900	1.53771300	-0.01280000
H	-0.59158800	1.60092500	-0.05364100
C	-3.88201000	0.73172200	0.02077300
H	-4.62572800	-1.29135400	0.06514800
H	-2.85033200	2.61774500	-0.02809200
H	-4.86963300	1.18144300	0.03221500

DBU

0 1

C	2.75292000	0.00010600	0.38708500
C	1.90081300	-1.24995300	0.61435300
C	0.88920200	-1.54884800	-0.50635100
C	1.96639200	1.30773600	0.29549000
C	-0.40336000	-0.77778300	-0.36424100
C	0.90544000	1.29064000	-0.80888700
H	3.31799000	-0.13073200	-0.54640000

H	2.57198500	-2.10983700	0.70906600
H	1.35142700	-1.35917000	-1.48363400
H	1.47067700	1.52420800	1.25086000
H	0.61336300	2.31404400	-1.06248900
C	-2.69860900	-0.67483400	0.01479900
H	-3.44123700	-1.28972100	0.53239100
C	-1.42012500	1.44126700	0.01183600
C	-2.44527900	0.62192100	0.77885000
H	-2.05359800	0.37434200	1.77159200
H	-3.36186400	1.20258400	0.91213200
H	-1.00588800	2.23139000	0.65101600
N	-0.32083200	0.59290900	-0.44434800
N	-1.47710300	-1.45210400	-0.14120200
H	1.32630600	0.85741600	-1.72399700
H	2.66479900	2.13006000	0.10365700
H	3.49441000	0.08064700	1.18939400
H	1.36102700	-1.16979700	1.56664500
H	0.60112800	-2.60045200	-0.48349900
H	-3.11935400	-0.43534900	-0.97413400
H	-1.88999900	1.93323000	-0.85135400

DBU·H⁺

1 1

C	-2.79140500	-0.01617500	-0.38825100
C	-1.94232300	-1.27396000	-0.57200500
C	-0.91637900	-1.51050900	0.55392600
C	-2.00433600	1.29429400	-0.36157600
C	0.33068000	-0.69389100	0.37182900
C	-0.95513000	1.34949600	0.74783100
H	-3.35325000	-0.10708200	0.55033800
H	-2.60238300	-2.14456200	-0.59784200
H	-1.35816500	-1.27663200	1.52874500
H	-1.50997400	1.47170300	-1.32435200
H	-0.65078900	2.37881000	0.94244900
C	2.74462700	-0.66822500	-0.09693500
H	3.34659900	-1.30957500	-0.74030600
C	1.46305100	1.45214100	0.09046500
C	2.46550300	0.67667600	-0.74850100

H	2.06424900	0.51965900	-1.75364900
H	3.38811200	1.25220900	-0.83491400
H	1.10152800	2.32460300	-0.45841300
N	0.28450800	0.62515800	0.40811900
N	1.46412300	-1.33579700	0.13229000
H	-1.35394100	0.95387100	1.68710200
H	-2.70144100	2.12263600	-0.20450100
H	-3.53222600	0.02901200	-1.19172400
H	-1.41921200	-1.24630900	-1.53507100
H	-0.62527700	-2.56238800	0.58446300
H	3.26595300	-0.54508700	0.85757200
H	1.90713100	1.79896900	1.02938400
H	1.42694800	-2.34444600	0.09715600

NN

0 1

C	3.56024600	0.71537800	0.00005000
C	2.38983600	1.41361700	0.00002200
C	1.13944500	0.71918200	-0.00008200
C	1.13944400	-0.71917500	-0.00019900
C	2.38983200	-1.41361800	0.00012200
C	3.56024600	-0.71538600	0.00017200
C	-1.13945000	-0.71917200	-0.00008600
C	-1.13944900	0.71917700	-0.00002500
C	-2.38983200	1.41361400	0.00007700
H	-2.36310400	2.49802900	0.00007100
C	-3.56024700	0.71537600	0.00011900
C	-3.56024700	-0.71538200	0.00008900
C	-2.38983000	-1.41361500	0.00003600
H	4.50821500	1.24300700	0.00004300
H	2.36310700	2.49803100	-0.00003200
H	2.36308800	-2.49803200	0.00017100
H	4.50821600	-1.24301200	0.00026500
H	-4.50821400	1.24300800	0.00019500
H	-4.50821400	-1.24301400	0.00006200
H	-2.36308700	-2.49802900	-0.00001500
N	0.00000200	1.41931400	-0.00015500
N	0.00000100	-1.41930900	-0.00020700

[NNH]-

-1 1

C	3.65211900	0.67339300	0.00029200
C	2.42616600	1.36759900	0.00009800
C	1.22240400	0.68712000	-0.00015600
C	1.16606400	-0.74546300	-0.00008100
C	2.41011000	-1.40082400	0.00019800
C	3.62919700	-0.71072000	0.00033500
C	-1.16606400	-0.74546300	-0.00026100
C	-1.22240300	0.68712000	-0.00018700
C	-2.42616700	1.36759900	0.00026000
H	-2.41177600	2.45629700	0.00035600
C	-3.65211800	0.67339200	0.00046300
C	-3.62919700	-0.71072100	0.00026500
C	-2.41011000	-1.40082400	-0.00008000
H	4.58771600	1.22331000	0.00035600
H	2.41177400	2.45629700	0.00006200
H	2.39105600	-2.48709900	0.00029900
H	4.55913800	-1.27409000	0.00047700
H	-4.58771500	1.22331200	0.00076400
H	-4.55914000	-1.27408900	0.00036600
H	-2.39105600	-2.48709900	-0.00018200
N	0.00000000	1.36291100	-0.00065900
N	0.00000000	-1.45729500	-0.00052100
H	0.00000100	2.37058500	-0.00110600

NN--

-1 2

C	3.59546300	0.70210200	-0.00021300
C	2.39472500	1.39226100	-0.00019500
C	1.15044900	0.72017900	0.00012600
C	1.15044900	-0.72017900	0.00028400
C	2.39472600	-1.39226100	0.00022400
C	3.59546300	-0.70210100	0.00000300
C	-1.15044900	-0.72017900	-0.00012000
C	-1.15044900	0.72017900	-0.00003700
C	-2.39472500	1.39226100	0.00017600

H	-2.36940900	2.47854800	0.00037400
C	-3.59546300	0.70210100	0.00010400
C	-3.59546300	-0.70210200	-0.00015900
C	-2.39472500	-1.39226100	-0.00024800
H	4.53513300	1.24724800	-0.00045200
H	2.36940800	2.47854800	-0.00039400
H	2.36940600	-2.47854800	0.00037200
H	4.53513100	-1.24725100	-0.00002300
H	-4.53513200	1.24725000	0.00025400
H	-4.53513200	-1.24724900	-0.00028000
H	-2.36940800	-2.47854800	-0.00039900
N	0.00000000	1.44483100	0.00006000
N	0.00000000	-1.44483100	0.00006600

[NNH]•

0 2

C	3.61187400	0.66818900	-0.00002100
C	2.42328500	1.38084900	0.00007200
C	1.20402800	0.69631800	0.00007500
C	1.16059600	-0.72827000	0.00010700
C	2.39556700	-1.41677500	-0.00004800
C	3.59638600	-0.73591600	-0.00010500
C	-1.16059600	-0.72827000	0.00003700
C	-1.20402800	0.69631800	0.00000600
C	-2.42328400	1.38084900	-0.00003600
H	-2.42552600	2.46721700	-0.00005700
C	-3.61187400	0.66818900	-0.00005500
C	-3.59638600	-0.73591600	-0.00002200
C	-2.39556700	-1.41677500	0.00002300
H	4.55591100	1.20220000	-0.00005700
H	2.42552600	2.46721700	0.00013100
H	2.35562600	-2.50100600	-0.00009200
H	4.53125200	-1.28602900	-0.00021100
H	-4.55591000	1.20220300	-0.00008600
H	-4.53125300	-1.28602700	-0.00005100
H	-2.35562800	-2.50100600	0.00006000
N	0.00000000	1.36426500	0.00002100
N	0.00000000	-1.43750400	0.00004300

H	0.00000000	2.37516300	-0.00028600
---	------------	------------	-------------

NNH₂

0 1

C	3.64762200	0.69252400	0.00075000
C	2.43329500	1.38900900	0.00027000
C	1.22536900	0.70586500	-0.00039500
C	1.22536900	-0.70586600	-0.00040300
C	2.43329600	-1.38900900	0.00023500
C	3.64762200	-0.69252300	0.00072900
C	-1.22536900	-0.70586500	-0.00040200
C	-1.22536900	0.70586500	-0.00041400
C	-2.43329500	1.38900900	0.00022600
H	-2.42254000	2.47542100	0.00025600
C	-3.64762200	0.69252400	0.00073700
C	-3.64762200	-0.69252300	0.00075500
C	-2.43329600	-1.38900900	0.00026300
H	4.58040100	1.24574800	0.00115800
H	2.42253900	2.47542100	0.00033500
H	2.42254100	-2.47542100	0.00028400
H	4.58039900	-1.24575100	0.00111600
H	-4.58040000	1.24575000	0.00114200
H	-4.58040000	-1.24574900	0.00116500
H	-2.42254200	-2.47542100	0.00034200
N	0.00000000	1.36972300	-0.00115700
N	0.00000000	-1.36972400	-0.00114300
H	0.00000100	2.37726500	-0.00185600
H	0.00000000	-2.37726600	-0.00195200

DQ

0 1

C	-2.80819100	-1.28080400	-0.07213500
C	-1.45862600	-1.23396200	-0.06272200
C	-0.69383600	0.00000800	-0.00033600
C	-1.45859400	1.23400000	0.06206200
C	-2.80816500	1.28084900	0.07153200
C	-3.57274800	0.00004800	-0.00047400
H	-0.91471000	-2.16368800	-0.13515700

H	-0.91464800	2.16369000	0.13457900
C	0.69381300	-0.00000600	-0.00023500
C	1.45859500	1.23398300	-0.06233600
C	1.45857700	-1.23400100	0.06205000
C	2.80816200	1.28083900	-0.07151100
H	0.91467100	2.16370300	-0.13476200
C	2.80814700	-1.28083400	0.07173600
H	0.91463700	-2.16371600	0.13428500
C	3.57272300	0.00000500	0.00022100
O	-4.79999400	0.00015100	-0.00047400
O	4.79996900	-0.00004800	0.00022300
C	-3.58431400	2.59487000	0.15925200
C	-4.47092100	2.76371300	-1.08984700
C	-4.45610200	2.60592500	1.42970100
C	-2.64157800	3.80255000	0.22896900
H	-3.85838800	2.76390200	-1.99723600
H	-5.21096300	1.96745900	-1.16351500
H	-4.99392800	3.72405500	-1.03451700
H	-3.83274300	2.49698500	2.32305200
H	-4.98229900	3.56360300	1.49896600
H	-5.19341900	1.80389300	1.41387300
H	-3.23945200	4.71621700	0.28710800
H	-1.99984100	3.76845800	1.11546500
H	-2.00704400	3.87634600	-0.66041800
C	-3.58420900	-2.59494100	-0.15960400
C	-4.47075600	-2.76381600	1.08957200
C	-4.45594900	-2.60647800	-1.43008500
C	-2.64119000	-3.80237800	-0.22907700
H	-3.85818100	-2.76356900	1.99693400
H	-5.21107000	-1.96781400	1.16309600
H	-4.99335800	-3.72438100	1.03445800
H	-3.83257400	-2.49748200	-2.32341200
H	-4.98184100	-3.56433800	-1.49919300
H	-5.19353300	-1.80469500	-1.41441300
H	-3.23878400	-4.71623800	-0.28712200
H	-1.99943500	-3.76833900	-1.11557300
H	-2.00662800	-3.87586800	0.66031500
C	3.58427300	-2.59488000	0.15931400

C	4.45593400	-2.60617500	1.42984900
C	2.64148800	-3.80253300	0.22874800
C	4.47098600	-2.76356400	-1.08973200
H	5.19329400	-1.80417900	1.41421900
H	3.83249200	-2.49734300	2.32315600
H	4.98207400	-3.56389100	1.49901600
H	2.00702800	-3.87615600	-0.66070800
H	3.23931900	-4.71623500	0.28679100
H	1.99967000	-3.76856200	1.11519100
H	4.99390000	-3.72396500	-1.03453500
H	3.85854000	-2.76354000	-1.99718100
H	5.21110600	-1.96736500	-1.16318600
C	3.58424900	2.59495100	-0.15869700
C	4.47071600	2.76349300	1.09057500
C	4.45612300	2.60660500	-1.42908000
C	2.64136000	3.80250300	-0.22804800
H	3.85807000	2.76321600	1.99788800
H	5.21088200	1.96734300	1.16403600
H	4.99350000	3.72397000	1.03564300
H	3.83282900	2.49784400	-2.32249200
H	4.98214400	3.56440900	-1.49796300
H	5.19360200	1.80472100	-1.41347000
H	3.23905800	4.71630500	-0.28594100
H	1.99964500	3.76865800	-1.11458100
H	2.00676700	3.87594900	0.66132300

DQ--

-1 2

C	2.83906100	1.23660100	0.20160600
C	1.46821100	1.19432100	0.19065800
C	0.71858100	0.00000700	-0.00014200
C	1.46818500	-1.19430800	-0.19105700
C	2.83903400	-1.23658000	-0.20225100
C	3.60185700	0.00001300	-0.00040000
H	0.91792900	2.10753800	0.38134900
H	0.91786400	-2.10753200	-0.38160300
C	-0.71860100	-0.00000400	0.00000900
C	-1.46818800	-1.19429200	0.19114600

C	-1.46824900	1.19427100	-0.19098200
C	-2.83903500	-1.23657100	0.20238500
H	-0.91785700	-2.10747900	0.38185200
C	-2.83909700	1.23654400	-0.20188200
H	-0.91797500	2.10745600	-0.38184800
C	-3.60187700	-0.00000100	0.00042800
O	4.86005000	-0.00002500	-0.00031300
O	-4.86006900	-0.00001900	0.00043900
C	3.60040700	-2.54601800	-0.43135500
C	4.48610100	-2.43117400	-1.68538700
C	4.47802600	-2.85844000	0.79475400
C	2.65665100	-3.73644300	-0.63977000
H	3.86940700	-2.23153300	-2.56849800
H	5.20999800	-1.62485900	-1.57138100
H	5.02155900	-3.37344100	-1.85184400
H	3.85430600	-2.98279400	1.68677000
H	5.02742200	-3.79335800	0.63212100
H	5.18976600	-2.05235300	0.97106000
H	3.25114800	-4.64397800	-0.78758400
H	2.00795400	-3.90010800	0.22747300
H	2.02383700	-3.60490600	-1.52389200
C	3.60044400	2.54605200	0.43060300
C	4.48608700	2.43137200	1.68469100
C	4.47810800	2.85833300	-0.79550700
C	2.65669000	3.73650800	0.63881900
H	3.86936500	2.23175100	2.56778700
H	5.21004000	1.62510400	1.57077200
H	5.02146700	3.37369200	1.85110800
H	3.85442700	2.98269900	-1.68754800
H	5.02758900	3.79320700	-0.63290700
H	5.18978400	2.05217800	-0.97176600
H	3.25118300	4.64407700	0.78643900
H	2.00796500	3.89998700	-0.22843800
H	2.02390200	3.60515200	1.52298800
C	-3.60049800	2.54595300	-0.43105000
C	-4.47799700	2.85848900	0.79512000
C	-2.65674800	3.73634900	-0.63966200
C	-4.48631300	2.43101300	-1.68498700

H	-5.18970800	2.05240600	0.97157100
H	-3.85418800	2.98294100	1.68706000
H	-5.02742500	3.79338200	0.63245200
H	-2.02401700	3.60471900	-1.52383000
H	-3.25125000	4.64387600	-0.78750600
H	-2.00796900	3.90008700	0.22750500
H	-5.02173100	3.37329200	-1.85149800
H	-3.86971800	2.23123500	-2.56813500
H	-5.21024200	1.62475200	-1.57082300
C	-3.60035400	-2.54598300	0.43181500
C	-4.48594000	-2.43091700	1.68591000
C	-4.47806100	-2.85874600	-0.79414500
C	-2.65651100	-3.73630600	0.64038500
H	-3.86916900	-2.23108800	2.56892400
H	-5.20985000	-1.62462700	1.57180700
H	-5.02137200	-3.37315700	1.85260400
H	-3.85442700	-2.98330100	-1.68619600
H	-5.02738400	-3.79365500	-0.63121600
H	-5.18988100	-2.05276400	-0.97059200
H	-3.25093600	-4.64387100	0.78830500
H	-2.00780100	-3.90000700	-0.22684200
H	-2.02370700	-3.60462900	1.52449500

[DQH]·

0 2

C	2.85028500	-1.22745100	-0.32216600
C	1.47859700	-1.17923100	-0.30975100
C	0.75907700	-0.00033200	0.00068600
C	1.48039600	1.17731200	0.31160700
C	2.85212700	1.22361000	0.32403100
C	3.60235400	-0.00243800	0.00096100
H	0.90914200	-2.05944500	-0.58186500
H	0.91217700	2.05850500	0.58282800
C	-0.70876400	0.00219300	-0.00088400
C	-1.42796600	1.16529900	-0.30766300
C	-1.43210700	-1.15592000	0.30492200
C	-2.81687200	1.20580200	-0.32198400
H	-0.87311900	2.05435500	-0.57769500

C	-2.82362800	-1.18814100	0.31540200
H	-0.88200100	-2.04700800	0.57753200
C	-3.50150500	0.01007500	-0.00544700
O	4.85186500	-0.00342500	0.00095600
O	-4.86161200	0.07621300	-0.02734700
C	3.61581300	2.49974000	0.67366900
C	4.48977900	2.26584400	1.92040200
C	4.50111300	2.92019200	-0.51579900
C	2.66490500	3.66322500	0.98187100
H	3.87035600	1.96826600	2.77276100
H	5.23583100	1.49285400	1.73959000
H	5.00309300	3.19687600	2.18366200
H	3.88757000	3.10432100	-1.40386400
H	5.02515300	3.84943800	-0.26777400
H	5.23793000	2.15185300	-0.74809700
H	3.25652900	4.55288300	1.21605800
H	2.02449900	3.90442100	0.12706100
H	2.02762200	3.45075200	1.84634400
C	3.61246900	-2.50403200	-0.67343700
C	4.48536100	-2.26972700	-1.92087900
C	4.49867200	-2.92653900	0.51460000
C	2.66020300	-3.66630500	-0.98191000
H	3.86537200	-1.97047500	-2.77223100
H	5.23237000	-1.49770100	-1.73995500
H	4.99749200	-3.20096800	-2.18572600
H	3.88600700	-3.11102600	1.40321200
H	5.02169500	-3.85595100	0.26504500
H	5.23634800	-2.15903200	0.74684200
H	3.25072700	-4.55642000	-1.21711900
H	2.02013700	-3.90735800	-0.12677300
H	2.02265000	-3.45244400	-1.84584400
C	-3.58124100	-2.48058500	0.67042700
C	-4.43603800	-2.95539100	-0.52549500
C	-2.61662500	-3.63360300	0.98545400
C	-4.43631700	-2.28311400	1.94099000
H	-5.17076700	-2.22999100	-0.88541800
H	-3.78549600	-3.18766200	-1.37334600
H	-4.98022400	-3.86446900	-0.25205900

H	-1.98312800	-3.40706600	1.84787300
H	-3.19895900	-4.52768900	1.22497600
H	-1.97583400	-3.87164200	0.13127300
H	-4.96917500	-3.21001600	2.17387900
H	-3.78747700	-2.03928500	2.78687800
H	-5.18174100	-1.48564700	1.87826300
C	-3.57204500	2.49776300	-0.67301000
C	-4.43888100	2.29039700	-1.92845700
C	-4.44841800	2.94169000	0.51355400
C	-2.60360000	3.64959500	-0.97662100
H	-3.81471700	1.99331100	-2.77726800
H	-5.20302400	1.52920700	-1.77458600
H	-4.93595500	3.23148000	-2.18723300
H	-3.82876400	3.11818800	1.39869400
H	-4.95402300	3.88018200	0.26213800
H	-5.20560700	2.19788800	0.76036700
H	-3.18435700	4.54580500	-1.21260600
H	-1.96431700	3.88400100	-0.11929500
H	-1.96594000	3.43069600	-1.83893800
H	-5.24298100	-0.77586500	0.20311100

[DQH]⁻

-1 1

C	-2.87967600	-1.19275600	0.31871900
C	-1.49504800	-1.15390800	0.31926900
C	-0.75771200	0.00412400	0.02566200
C	-1.48987500	1.16290100	-0.27760500
C	-2.87431200	1.20221100	-0.29772200
C	-3.64140800	0.00457900	0.00342400
H	-0.94102200	-2.04851600	0.58989000
H	-0.93196600	2.05666600	-0.54278700
C	0.71595300	0.00045800	0.02736100
C	1.45226700	1.15363500	0.33006900
C	1.44295600	-1.15579100	-0.28701000
C	2.84737300	1.18366100	0.32962500
H	0.89917800	2.04546400	0.59587200
C	2.83737600	-1.19952500	-0.28262500
H	0.88147600	-2.03696400	-0.56952100

C	3.52492400	-0.01569700	0.04340100
O	-4.91573600	0.00404500	-0.00952500
O	4.92263000	-0.01577000	0.03164400
C	-3.62907200	2.48950800	-0.64894200
C	-4.49578500	2.26462800	-1.90062600
C	-4.53048000	2.90177100	0.52918500
C	-2.68671200	3.66289600	-0.94221800
H	-3.86122800	2.02378300	-2.76112300
H	-5.18487300	1.43813000	-1.72704200
H	-5.06494500	3.17244300	-2.13999000
H	-3.91954600	3.12754300	1.41082700
H	-5.10518000	3.80158600	0.27317800
H	-5.21547800	2.08847800	0.76964100
H	-3.27919700	4.55499900	-1.17507400
H	-2.05055600	3.89794500	-0.08165600
H	-2.03804000	3.45850700	-1.80098500
C	-3.64050100	-2.48165800	0.65059700
C	-4.53956500	-2.26127800	1.87994300
C	-4.51118900	-2.89331400	-0.55072700
C	-2.70324400	-3.65358600	0.96572700
H	-3.92822200	-2.01320700	2.75505400
H	-5.23131900	-1.44112200	1.68763000
H	-5.10646800	-3.17360000	2.10732900
H	-3.87798000	-3.11570600	-1.41731100
H	-5.09042000	-3.79474900	-0.31111900
H	-5.19135800	-2.08053000	-0.80626000
H	-3.29944500	-4.54686600	1.18428000
H	-2.04644600	-3.88736000	0.12049100
H	-2.07545200	-3.44802800	1.83970100
C	3.58471800	-2.48929200	-0.66591200
C	4.49619300	-2.96632500	0.48045200
C	2.61252600	-3.63883700	-0.96803500
C	4.42383800	-2.25093900	-1.93336100
H	5.34885900	-2.30199500	0.62812200
H	3.93583900	-3.03948000	1.41804000
H	4.89666800	-3.95921900	0.24727900
H	1.95171400	-3.40033600	-1.80623100
H	3.18719000	-4.53013900	-1.23888000

H	1.99285500	-3.88727700	-0.10056300
H	4.94779900	-3.17265500	-2.21291600
H	3.77616700	-1.96179900	-2.76691100
H	5.16065200	-1.46317700	-1.77554900
C	3.60730500	2.48847900	0.62588900
C	4.50457100	2.34035200	1.86782000
C	4.46316300	2.87876200	-0.59281700
C	2.64848600	3.65442900	0.90506900
H	3.92277400	1.98858700	2.72582700
H	5.33004900	1.64930100	1.69356200
H	4.93950100	3.31170600	2.12929000
H	3.82458600	3.03500500	-1.46812600
H	4.99627000	3.81502300	-0.38929900
H	5.19280500	2.10302400	-0.82677200
H	3.23368500	4.56301900	1.07917700
H	1.98087000	3.84282200	0.05905400
H	2.03592300	3.47463600	1.79407300
H	5.22671200	-0.28905500	0.90515800

DQH₂

0 1

C	2.84822700	-1.18617100	-0.38444600
C	1.45556600	-1.14269500	-0.37056000
C	0.74205900	-0.00293200	0.00543100
C	1.46373400	1.12982700	0.37849700
C	2.85929600	1.16261800	0.38126900
C	3.53533200	-0.01313800	-0.00698500
H	0.89225500	-2.01356100	-0.68351700
H	0.90837900	2.00382900	0.69641300
C	-0.74207200	0.00283600	0.00540400
C	-1.45554200	1.14262000	-0.37060500
C	-1.46377900	-1.12991200	0.37843500
C	-2.84820000	1.18611300	-0.38455700
H	-0.89220000	2.01349100	-0.68349900
C	-2.85934900	-1.16265300	0.38118400
H	-0.90846200	-2.00393700	0.69636600
C	-3.53533100	0.01310500	-0.00709700
O	4.90283100	-0.07931400	-0.03785200

O	-4.90284200	0.07927300	-0.03811400
C	3.61683900	2.43494600	0.80396900
C	4.48144100	2.16789200	2.05513400
C	4.46261500	2.98053500	-0.36756500
C	2.65271000	3.56648000	1.19059800
H	3.83820800	1.88007000	2.89150400
H	5.22179700	1.37172800	1.94130400
H	5.01947300	3.07910700	2.33448100
H	3.80554900	3.26124400	-1.19560100
H	5.00944300	3.87259100	-0.04643800
H	5.19368900	2.27701700	-0.77536600
H	3.23452500	4.44701600	1.47814400
H	2.00648500	3.85001100	0.35476600
H	2.02328300	3.28854600	2.04078400
C	3.59961400	-2.45914500	-0.80679400
C	4.45962800	-2.18718000	-2.05464100
C	4.48288500	-2.96716000	0.34800200
C	2.62839600	-3.59284000	-1.16535800
H	3.83002400	-1.84674800	-2.88310900
H	5.22273600	-1.43294300	-1.86473700
H	4.95648400	-3.11273700	-2.36563900
H	3.86791200	-3.19249000	1.22534700
H	4.98889700	-3.88996100	0.04369500
H	5.23921800	-2.23557400	0.63146600
H	3.20599600	-4.47752000	-1.44909900
H	1.99152500	-3.86740900	-0.31832500
H	1.98702600	-3.32820700	-2.01184400
C	-3.61694800	-2.43489600	0.80399900
C	-4.46276500	-2.98058800	-0.36746100
C	-2.65286200	-3.56644300	1.19070200
C	-4.48147000	-2.16761800	2.05516300
H	-5.19370400	-2.27706700	-0.77551800
H	-3.80568800	-3.26155600	-1.19540300
H	-5.00973800	-3.87250000	-0.04618700
H	-2.02347800	-3.28849300	2.04091500
H	-3.23471400	-4.44695600	1.47824400
H	-2.00660200	-3.84999700	0.35490600
H	-5.01971300	-3.07868800	2.33457400

H	-3.83814400	-1.87993900	2.89152000
H	-5.22160600	-1.37125000	1.94131600
C	-3.59953000	2.45913200	-0.80680700
C	-4.45943000	2.18738300	-2.05477200
C	-4.48287400	2.96696600	0.34800600
C	-2.62822300	3.59284200	-1.16511400
H	-3.82974700	1.84710100	-2.88324100
H	-5.22256500	1.43311800	-1.86509300
H	-4.95625600	3.11299800	-2.36564700
H	-3.86796700	3.19206500	1.22545600
H	-4.98878800	3.88987200	0.04385100
H	-5.23929800	2.23538200	0.63123800
H	-3.20576200	4.47770800	-1.44839500
H	-1.99114300	3.86697900	-0.31809600
H	-1.98705900	3.32845500	-2.01183200
H	-5.28083800	-0.76563600	0.21984100
H	5.28084000	0.76563000	0.21999600

Re-TS1

0 1

C	0.90274500	-0.72170500	-0.38902300
C	2.42159500	-2.26219000	0.13543700
C	3.31191000	-0.12983100	-0.87338800
H	3.16586900	-0.02575200	-1.95010200
N	1.29377800	-2.81119200	0.47072000
N	0.37961000	-1.83880000	0.13710700
N	2.22678600	-1.00026800	-0.37650000
C	3.78960100	-2.86186500	0.24570300
H	3.75814200	-3.90149900	-0.08390200
H	4.12392900	-2.84617700	1.29053700
C	4.66373200	-0.77419100	-0.47396900
O	4.68718100	-2.18092900	-0.60333700
C	4.31789400	1.14209900	0.88002600
C	3.36648300	1.19085500	-0.14253900
C	2.64576400	2.34979700	-0.40651000
C	2.86882500	3.46400100	0.40213400
C	3.80418900	3.41615500	1.43737700
C	4.54207400	2.25755200	1.67894800

C	4.99057700	-0.20658300	0.92562100
H	1.94262700	2.36225100	-1.23468300
H	3.97031500	4.29512000	2.05252800
H	5.28352700	2.23072500	2.47211300
H	4.55772600	-0.82050600	1.72433000
H	6.06718100	-0.15417600	1.10188600
C	-1.00414000	-2.06993900	0.32881700
C	-1.68165500	-1.48919200	1.40400700
C	-1.71792000	-2.87267300	-0.56422700
C	-3.04305200	-1.69413900	1.58822500
C	-3.07783100	-3.09980300	-0.39682200
C	-3.71932300	-2.50170800	0.68154900
H	-3.55966100	-1.23461200	2.42160700
H	-3.62231400	-3.72289300	-1.09539200
H	5.41124200	-0.40941500	-1.18207300
H	2.31984900	4.38208400	0.21698700
Cl	-0.81854900	-0.49118400	2.52424000
Cl	-5.42086000	-2.77000900	0.90158000
Cl	-0.89788700	-3.58589800	-1.91156200
C	0.05268900	0.44705100	-1.81230600
O	0.95386200	0.88165100	-2.55624500
H	-0.53007500	-0.44615300	-2.13896200
C	-0.77493400	1.39645500	-0.95437800
C	-1.54340800	2.36250600	-1.86819700
H	-0.11744900	1.96478500	-0.28882700
H	-1.47461800	0.82726400	-0.32946300
H	-0.81415500	2.89587400	-2.48687600
H	-2.18504100	1.78972300	-2.54886200
C	-2.37753600	3.33838600	-1.07791100
C	-1.79632500	4.48684900	-0.53185100
C	-3.73113900	3.09572200	-0.83300200
C	-2.54792700	5.37262700	0.23465900
H	-0.74279100	4.68613600	-0.71649200
C	-4.48839500	3.97898000	-0.06698600
H	-4.19488100	2.20599400	-1.25223500
C	-3.89870200	5.12104300	0.46909100
H	-2.08149900	6.26217200	0.64680700
H	-5.54048200	3.77656300	0.10889600

H	-4.48774200	5.81150900	1.06424700
---	-------------	------------	------------

Si-TS1

0 1

C	-0.68856900	-0.08679400	0.08255600
C	-2.09937600	-0.75082600	1.67067800
C	-2.83889800	1.22559800	0.37064200
H	-2.28191300	2.05800500	-0.06274200
N	-1.14144100	-1.62301700	1.73136700
N	-0.29007400	-1.18921900	0.73548200
N	-1.85582800	0.18953700	0.70037500
C	-3.30364000	-0.54894600	2.52872800
H	-3.19393400	-1.07129100	3.47864200
H	-4.20950700	-0.91007300	2.02190600
C	-3.65537500	1.63882800	1.65306000
O	-3.36875500	0.84054200	2.79345400
C	-5.16736900	0.85912000	-0.08437900
C	-3.88045700	0.69409400	-0.58726000
C	-3.65022100	0.10158000	-1.82525700
C	-4.74759300	-0.34859600	-2.55436200
C	-6.04356200	-0.19822500	-2.05138700
C	-6.26376300	0.41102700	-0.81834000
C	-5.14858600	1.56179500	1.24870300
H	-2.63633700	0.02839300	-2.20906000
H	-6.88823000	-0.55612500	-2.63154100
H	-7.27271300	0.53215900	-0.43539500
H	-5.71810200	1.03781800	2.02323000
H	-5.57293400	2.56723200	1.16637200
C	0.89648300	-1.90853400	0.45462500
C	0.94235700	-2.81214000	-0.60971400
C	2.04298100	-1.72020500	1.22996100
C	2.10333600	-3.51567600	-0.90408500
C	3.21526900	-2.41388500	0.95848600
C	3.22397600	-3.30393000	-0.10938000
H	2.12913700	-4.21285200	-1.73216400
H	4.09947800	-2.25836200	1.56381500
H	-3.37503000	2.64689000	1.95822300
H	-4.59831800	-0.81448900	-3.52293300

Cl	-0.46912200	-3.06240000	-1.58046000
Cl	4.68249100	-4.17642300	-0.46461500
Cl	2.00810400	-0.58876200	2.53815900
C	0.01307100	1.06423000	-1.49023000
O	-0.92910500	1.76265000	-1.90402100
H	0.32134500	0.15726700	-2.05524600
C	1.17298800	1.70605500	-0.73596200
C	1.97236000	2.59613500	-1.70087800
H	1.82467500	0.93426400	-0.30765700
H	0.78139900	2.31740200	0.08468600
H	2.31451100	1.99131000	-2.54966000
H	1.29936900	3.36150900	-2.09925400
C	3.15552600	3.23650900	-1.01956800
C	4.38636100	2.57733200	-0.95651100
C	3.03086200	4.47795900	-0.39027000
C	5.46708200	3.14415700	-0.28610700
H	4.49602000	1.61072100	-1.44277400
C	4.10836200	5.04925800	0.28205000
H	2.07839100	5.00068200	-0.43276900
C	5.33099200	4.38351000	0.33588800
H	6.41720500	2.62005400	-0.25209200
H	3.99434100	6.01663500	0.76134700
H	6.17279300	4.82857700	0.85648500

Re-M1

0 1

C	-0.34367200	0.83823600	-0.63347700
C	-1.58359400	2.30460800	0.43280100
C	-2.86993900	0.67988100	-0.89523800
H	-2.59298300	0.05469300	-1.75499300
N	-0.37081900	2.60584200	0.78674100
N	0.38582800	1.67178200	0.12072200
N	-1.60329900	1.23430300	-0.42178100
C	-2.89573400	2.98378400	0.66251800
H	-2.73967000	3.99866800	1.02750700
H	-3.49894400	2.42500400	1.38928500
C	-3.85292100	1.83985600	-1.24928100
O	-3.52482500	3.07155600	-0.60444600

C	-4.93359700	0.28255500	0.23960200
C	-3.58550100	-0.07271900	0.20699000
C	-3.05742600	-0.98367700	1.11429600
C	-3.91120900	-1.55766300	2.05532800
C	-5.26498200	-1.21862600	2.08133700
C	-5.78503600	-0.29413200	1.17551700
C	-5.23736300	1.31539200	-0.81777100
H	-1.99918500	-1.23132800	1.10575300
H	-5.91737100	-1.67036600	2.82167400
H	-6.83498900	-0.01905100	1.21030200
H	-5.86165100	2.13954500	-0.46242200
H	-5.74653500	0.85770200	-1.67309100
C	1.79461500	1.64691900	0.28235700
C	2.36007400	0.99963500	1.38298400
C	2.62672200	2.29102100	-0.63567100
C	3.73584900	0.97753100	1.56651600
C	4.00585900	2.27673500	-0.47508700
C	4.53760900	1.61755700	0.62775500
H	4.16973900	0.47488000	2.42191000
H	4.64788900	2.77297900	-1.19226500
H	-3.81090000	2.07244500	-2.31385400
H	-3.51901000	-2.26874500	2.77474800
Cl	1.33003900	0.22100700	2.53549400
Cl	6.25882400	1.59766000	0.84377300
Cl	1.92844000	3.11960000	-1.98196200
C	0.09651700	-0.25139300	-1.64802000
O	-0.82274800	-0.40995100	-2.58422600
H	1.09146200	0.14920800	-1.99390700
C	0.43314700	-1.53053200	-0.83222200
C	0.94657600	-2.60990200	-1.78750200
H	-0.49129300	-1.88686700	-0.35943200
H	1.17031800	-1.33890700	-0.03903500
H	0.22769800	-2.67245200	-2.60951300
H	1.90534400	-2.28567000	-2.21131900
C	1.10459300	-3.94694600	-1.11032800
C	0.03209600	-4.84186100	-1.05330600
C	2.30242400	-4.30437900	-0.48547800
C	0.15221900	-6.06210500	-0.39373400

H	-0.90456300	-4.57479500	-1.53700900
C	2.42872600	-5.52400800	0.17556800
H	3.14569800	-3.61845100	-0.52345900
C	1.35294100	-6.40777300	0.22294200
H	-0.69064000	-6.74599500	-0.36563200
H	3.36919900	-5.78655900	0.65060900
H	1.45085800	-7.36077800	0.73317400

Si-M1

0 1

C	-0.57996600	-0.08844400	0.06138400
C	-1.94410700	-0.70403500	1.66054600
C	-2.77594600	1.19676800	0.29172800
H	-2.24686400	2.00417900	-0.21444400
N	-0.96583500	-1.55332900	1.74181500
N	-0.12644200	-1.15419200	0.73251700
N	-1.74390100	0.20644400	0.65412900
C	-3.13754100	-0.50029800	2.53411600
H	-2.99009900	-0.98361800	3.49950900
H	-4.04167300	-0.90702700	2.06014200
C	-3.56988500	1.63660400	1.57786700
O	-3.22999400	0.89510700	2.74371000
C	-5.09494500	0.70131400	-0.06610000
C	-3.81792800	0.56457500	-0.60222800
C	-3.59506900	-0.07508100	-1.81840800
C	-4.69326000	-0.61543600	-2.48252500
C	-5.97829900	-0.50286700	-1.94254300
C	-6.19072600	0.16360200	-0.73784000
C	-5.06830300	1.49057900	1.21757500
H	-2.58503000	-0.09092800	-2.22340100
H	-6.82239500	-0.93218200	-2.47345100
H	-7.19237700	0.26146000	-0.32970100
H	-5.60445000	1.00685000	2.04053100
H	-5.52220600	2.47652600	1.07676100
C	1.04416400	-1.89930000	0.43799800
C	1.04948400	-2.79773500	-0.63268000
C	2.18792800	-1.76903500	1.22736700
C	2.18330800	-3.53989900	-0.93256300

C	3.33106700	-2.50728000	0.94906600
C	3.30943600	-3.38017300	-0.13274600
H	2.18387900	-4.22849600	-1.76810700
H	4.21665000	-2.40169100	1.56324700
H	-3.31435400	2.66458300	1.83425600
H	-4.55417500	-1.11990500	-3.43342300
Cl	-0.37594400	-2.98973600	-1.59505700
Cl	4.73162500	-4.30446000	-0.49341000
Cl	2.18341500	-0.67602000	2.56732100
C	0.05020300	0.68047200	-1.11906000
O	-0.87323800	1.33796200	-1.80344300
H	0.60922100	-0.12202900	-1.67542100
C	1.15201600	1.57738400	-0.47841500
C	1.84324600	2.38353000	-1.57906600
H	1.88970100	0.98252700	0.07950100
H	0.67233200	2.26589600	0.23041100
H	2.34944400	1.69045400	-2.26303600
H	1.05735000	2.88776600	-2.14780500
C	2.83287800	3.37537300	-1.02381300
C	4.15901700	3.00700900	-0.77971800
C	2.43307100	4.67427200	-0.69647400
C	5.06338400	3.91050600	-0.22754100
H	4.48370800	1.99997500	-1.03177700
C	3.33266400	5.58206400	-0.14354000
H	1.40438400	4.97346500	-0.88334500
C	4.65235600	5.20273700	0.09244000
H	6.09084300	3.60733700	-0.05002200
H	3.00474200	6.58822400	0.09950400
H	5.35635300	5.91004800	0.51921300

Re-TS2

1 1

C	0.24060700	-1.05374600	-0.05910000
C	1.45260200	-2.35319100	-1.36754200
C	2.77134600	-1.16778500	0.35592500
H	2.65449400	-0.19653600	0.83688200
N	0.24586900	-2.51909900	-1.80219800
N	-0.51025100	-1.71925600	-0.96709400

N	1.50529600	-1.47626300	-0.31220500
C	2.76297300	-2.81482000	-1.91510600
H	2.64149900	-3.18610800	-2.93177600
H	3.19625500	-3.60503000	-1.28771000
C	3.94994800	-1.14382900	-0.68667200
O	3.58773700	-1.66192300	-1.95910400
C	4.46152700	-2.67989400	1.12336800
C	3.15592500	-2.24875800	1.33977800
C	2.36910000	-2.79191300	2.34918900
C	2.91631700	-3.78474100	3.15676200
C	4.22912900	-4.21707400	2.95068200
C	5.00968800	-3.67006100	1.93492500
C	5.09789700	-1.94489400	-0.02918300
H	1.34864400	-2.45111400	2.49728800
H	4.64264800	-4.99271400	3.58692800
H	6.02607500	-4.01635800	1.77435600
H	5.55313000	-2.61262500	-0.76721300
H	5.88350300	-1.26803600	0.32113500
C	-1.91897300	-1.86574900	-0.96127000
C	-2.55431200	-2.53332500	0.08972300
C	-2.69359000	-1.35955800	-2.00679200
C	-3.93334100	-2.68670600	0.11130400
C	-4.07320700	-1.51157600	-2.01393200
C	-4.67344800	-2.17366900	-0.94817000
H	-4.41717100	-3.19992800	0.93293700
H	-4.66553300	-1.11190200	-2.82773100
H	4.23712800	-0.11039600	-0.89037400
H	2.32191400	-4.22686800	3.94928500
Cl	-1.61326100	-3.17261000	1.39970400
Cl	-6.39609000	-2.35969100	-0.93633600
Cl	-1.92681600	-0.48832400	-3.28912300
C	-0.08329600	0.07509800	0.77752800
O	0.65260000	0.07761400	1.99088700
H	0.65849000	0.97935700	0.01361300
C	-1.51465900	0.54274600	0.92239300
C	-1.55493500	1.97733900	1.47318500
H	-2.10250800	-0.11270500	1.58588600
H	-2.01326900	0.53550200	-0.05342800

H	-1.01942400	2.01039500	2.42807000
H	-1.01420600	2.62990000	0.77656400
C	-2.97026300	2.46639900	1.64954500
C	-3.64645500	2.27342400	2.85657500
C	-3.64909000	3.07557800	0.59096100
C	-4.96876200	2.68352600	3.00597500
H	-3.12807300	1.80169500	3.68803000
C	-4.97085700	3.48821500	0.73557800
H	-3.13283000	3.23165900	-0.35364200
C	-5.63457500	3.29303600	1.94491800
H	-5.47750500	2.53126800	3.95264100
H	-5.48172000	3.96674300	-0.09404600
H	-6.66346700	3.61777200	2.06084900
C	2.20633500	5.66753600	1.14217600
C	1.29378000	4.45044800	1.29926600
C	2.00604400	3.09679600	1.11541600
C	2.84096300	5.81676900	-0.24043400
C	2.14197300	2.70840100	-0.33489100
C	3.67984900	4.60714900	-0.65530000
H	3.00715000	5.60270400	1.89077600
H	0.85625800	4.46503200	2.30211000
H	2.99727300	3.13089900	1.58345200
H	2.07017800	5.98514400	-1.00281400
H	4.35517600	4.87515700	-1.47046800
C	1.52239400	1.25081200	-2.14243300
H	0.59711400	0.70026800	-2.35241100
C	2.87371100	3.27161700	-2.60350800
C	1.64872100	2.47977400	-3.03249500
H	0.75231100	3.09889400	-2.92431800
H	1.74305200	2.19700600	-4.08282300
H	2.87562400	4.25801600	-3.07641800
N	2.87972200	3.48003500	-1.14945400
N	1.49264300	1.64991400	-0.74092600
H	4.31031300	4.27382000	0.17607900
H	3.48872400	6.69912300	-0.24087100
H	1.63574600	6.57202200	1.37432300
H	0.45677300	4.51776000	0.59264600
H	1.44969300	2.29720800	1.61102100

H	2.35619000	0.55674900	-2.32071600
H	3.79605300	2.75639800	-2.89834900
H	0.15709100	-0.42263300	2.65688900

Si-TS2

1 1

C	-1.00986900	-0.87720000	0.09444000
C	-2.22504200	-1.98436800	1.57074900
C	-3.23275000	0.14929600	0.90733400
H	-2.86422500	1.13764900	0.63817000
N	-1.27736000	-2.80716900	1.27259100
N	-0.52908600	-2.11966000	0.34422700
N	-2.10565800	-0.78926100	0.89255500
C	-3.34991100	-2.10842400	2.54662800
H	-3.11169300	-2.85482500	3.30407400
H	-4.27780100	-2.39962500	2.03540700
C	-3.89063200	0.20293600	2.33591200
O	-3.46511800	-0.85156800	3.18376600
C	-5.57131900	-0.28028200	0.65071700
C	-4.34488900	-0.31268400	-0.00746200
C	-4.23834900	-0.73891300	-1.32741700
C	-5.39817000	-1.11938600	-1.99747400
C	-6.63419200	-1.07424200	-1.34837600
C	-6.73011100	-0.65873800	-0.02184600
C	-5.41501500	0.18550200	2.07622100
H	-3.27257400	-0.79241900	-1.82537600
H	-7.52928700	-1.37619800	-1.88218600
H	-7.69185400	-0.63950400	0.48149800
H	-5.90818100	-0.47019900	2.80043300
H	-5.83359400	1.18785400	2.20998500
C	0.70750400	-2.67028700	-0.07724500
C	0.79636400	-3.41953500	-1.25088100
C	1.84933900	-2.49562400	0.70412200
C	1.99882900	-3.97789300	-1.65533500
C	3.06605100	-3.05081500	0.32542600
C	3.12059000	-3.77960300	-0.85652300
H	2.05991100	-4.55089800	-2.57207600
H	3.94787900	-2.92024700	0.94106600

H	-3.57888700	1.10861400	2.85679400
H	-5.34165800	-1.45803600	-3.02635900
Cl	-0.61442800	-3.62408600	-2.23433400
Cl	4.63748400	-4.45815400	-1.35486100
Cl	1.75026800	-1.57848300	2.17016000
C	-0.34684500	0.10551700	-0.72780700
O	0.35846900	-0.49536900	-1.79763900
H	0.63384100	0.66043500	0.08267900
C	-1.06894600	1.39653200	-1.09741500
C	-0.19829800	2.24316100	-2.04947100
H	-1.22284300	1.98204900	-0.18218300
H	-2.05916600	1.24432900	-1.55305900
H	0.85656800	2.07231300	-1.81645600
H	-0.35021000	1.90820800	-3.07977800
C	-0.50901300	3.71208400	-1.91483700
C	0.27134000	4.51635000	-1.07858200
C	-1.60394800	4.28511600	-2.56571500
C	-0.03376300	5.86264500	-0.89570800
H	1.13356300	4.07852000	-0.57706900
C	-1.91330600	5.63104700	-2.38503500
H	-2.21577500	3.67106300	-3.22221800
C	-1.12963700	6.42310000	-1.54826200
H	0.58686500	6.47592800	-0.24968800
H	-2.76464600	6.06398000	-2.90084600
H	-1.36798400	7.47265700	-1.41020800
C	5.76987800	0.81728600	-0.15009900
C	4.43375300	0.07815000	-0.23653400
C	3.24976700	0.94806000	-0.70186300
C	5.80506700	1.96134500	0.86285100
C	2.64160900	1.73701800	0.43083800
C	4.73754100	3.02465100	0.60643000
H	6.00914200	1.22080000	-1.14311400
H	4.53684900	-0.75115800	-0.94381600
H	3.57397100	1.62707600	-1.50020100
H	5.67931300	1.57765000	1.88313900
H	4.98685400	3.94807200	1.13368100
C	0.78775400	2.12494500	1.90286300
H	0.01697300	1.45218600	2.29617000

C	2.94080000	3.26769600	2.32051600
C	1.83620500	2.44223500	2.96029000
H	2.25239500	1.50597200	3.34677600
H	1.39986000	2.99274700	3.79607200
H	3.80164700	3.33977600	2.99181000
N	3.40171200	2.64073400	1.07563700
N	1.41173900	1.46466200	0.76637800
H	4.69332400	3.27639600	-0.45864900
H	6.78717700	2.44320600	0.82108800
H	6.55897400	0.09836900	0.09181200
H	4.18574400	-0.36670400	0.73671900
H	2.45865700	0.31865400	-1.11875200
H	0.28687400	3.04653000	1.57231200
H	2.59490100	4.28718300	2.10791400
H	-0.26396000	-0.73581600	-2.49938300

Re-TS2a

0 1

C	1.08778400	-0.39456200	-0.57894000
C	2.57012600	-1.95730600	-0.07952500
C	3.51891100	0.17540700	-1.03541800
H	3.35815700	0.47240300	-2.07145500
N	1.46741300	-2.42032100	0.40877900
N	0.54156200	-1.43046700	0.12987100
N	2.41007200	-0.72489800	-0.66951900
C	3.90918700	-2.63173800	-0.08743500
H	3.79483500	-3.65501800	-0.44972800
H	4.31693100	-2.67687900	0.92935400
C	4.86230200	-0.57142700	-0.78764000
O	4.77443100	-1.97050400	-0.98260700
C	4.65569800	1.19127800	0.81590000
C	3.61387700	1.35870500	-0.09710700
C	2.80818500	2.49248700	-0.08023500
C	3.06019500	3.46608900	0.88471800
C	4.10045800	3.30586300	1.80254300
C	4.90877400	2.17027100	1.77197400
C	5.36750600	-0.11949800	0.60247300
H	2.02804500	2.59858900	-0.83342300

H	4.28556600	4.07614000	2.54485600
H	5.72145000	2.05261100	2.48269700
H	5.09384000	-0.83368900	1.38700900
H	6.45622600	-0.02951400	0.62010800
C	-0.83293900	-1.68797600	0.31314200
C	-1.43553900	-1.49562000	1.56086400
C	-1.62679200	-2.13260100	-0.74920200
C	-2.79487000	-1.70764600	1.74765400
C	-2.99201400	-2.34049500	-0.59298200
C	-3.55505100	-2.11984700	0.65880300
H	-3.24966800	-1.54290800	2.71654200
H	-3.59744300	-2.67220700	-1.42760800
H	5.56406600	-0.22587200	-1.54930600
H	2.44777400	4.36175100	0.91833600
Cl	-0.47440600	-0.94331700	2.88869600
Cl	-5.26388300	-2.34720500	0.86567500
Cl	-0.90056600	-2.44888400	-2.28842700
C	0.41453600	0.64429900	-1.26778000
O	1.16635800	1.38376400	-2.24360900
H	0.36522000	0.33854800	-2.41141300
C	-0.75160300	1.36662000	-0.63580800
C	-1.90544200	1.58926300	-1.62285200
H	-0.38420400	2.34269800	-0.28737000
H	-1.12752700	0.84141100	0.24883300
H	-1.52389200	2.15545900	-2.47857200
H	-2.23584300	0.61162500	-1.99806700
C	-3.06409400	2.30338500	-0.97629700
C	-3.21004500	3.68903800	-1.06815900
C	-3.98795400	1.58346300	-0.21290100
C	-4.25623800	4.33953900	-0.41666900
H	-2.49807700	4.26097900	-1.65807300
C	-5.03449400	2.22733000	0.44014500
H	-3.88046500	0.50288100	-0.13671700
C	-5.17124700	3.61087700	0.33931600
H	-4.35792200	5.41714400	-0.50196000
H	-5.74412200	1.64916300	1.02433700
H	-5.98734300	4.11710700	0.84489100

Si-TS2a

0 1

C	-0.36129500	-0.48332500	-0.57203300
C	-0.37721400	-2.67936200	-0.26391500
C	1.85896400	-1.77191400	-0.72559000
H	2.21113400	-0.94964900	-1.35457700
N	-1.61523500	-2.34769300	-0.12058400
N	-1.60813300	-0.97292700	-0.30525500
N	0.42719600	-1.60362500	-0.54327300
C	0.27228800	-4.02245100	-0.28705900
H	-0.47813400	-4.80559900	-0.38858800
H	0.85238600	-4.19186300	0.63055700
C	2.18211400	-3.14014500	-1.43551700
O	1.09308400	-4.05085800	-1.44211800
C	3.46948900	-2.93496000	0.61068800
C	2.59593700	-1.85021800	0.59529500
C	2.44777800	-1.02313100	1.70442200
C	3.21567900	-1.28700800	2.83652900
C	4.10616700	-2.36293500	2.85150700
C	4.23644500	-3.19606700	1.74235000
C	3.41458600	-3.69814100	-0.68849300
H	1.73850200	-0.19907600	1.69627500
H	4.69324500	-2.55997700	3.74275400
H	4.91567000	-4.04291300	1.76545600
H	3.30889300	-4.77835400	-0.55090300
H	4.32218300	-3.53231100	-1.27839900
C	-2.77049000	-0.23948900	0.01566000
C	-2.78750200	0.65838000	1.08651400
C	-3.94819500	-0.42733000	-0.70977300
C	-3.93648200	1.35661400	1.42734500
C	-5.11664400	0.24898100	-0.38170600
C	-5.09000400	1.13632600	0.68542300
H	-3.93029400	2.05136700	2.25776700
H	-6.02031700	0.09381600	-0.95773700
H	2.39519800	-2.96803500	-2.49103700
H	3.11714300	-0.65662600	3.71394700
Cl	-1.36258100	0.88266500	2.05102600

Cl	-6.54222300	1.99601000	1.10766000
Cl	-3.95692400	-1.48247500	-2.08520300
C	-0.06447800	0.84680300	-0.96297500
O	-1.19299900	1.72602500	-1.05269000
H	-0.54512800	1.05274100	-2.01678300
C	1.22146200	1.53060700	-0.55355800
C	1.65763400	2.57501200	-1.58903300
H	2.04511100	0.83463700	-0.36232000
H	1.01231000	2.04589500	0.39642700
H	1.91791600	2.06241800	-2.52298700
H	0.79219400	3.21278600	-1.79392000
C	2.82369100	3.39891500	-1.10714200
C	4.13648600	3.04183600	-1.42446400
C	2.61499500	4.51141500	-0.28644700
C	5.21498900	3.77825700	-0.94008900
H	4.31289200	2.17957100	-2.06355000
C	3.68897800	5.25053700	0.20108800
H	1.59712700	4.79899900	-0.03367000
C	4.99392500	4.88579200	-0.12521500
H	6.22830400	3.48929700	-1.20182600
H	3.50705300	6.11461800	0.83284600
H	5.83268000	5.46325200	0.25043100

Re-TS2b

0 1

C	0.83450700	-0.63484900	-0.22059300
C	2.27283400	-1.21873900	-1.80902800
C	3.27490200	-0.87278600	0.46697400
H	3.36109000	0.09338700	0.96225400
N	1.12858200	-1.44677400	-2.35588400
N	0.20723900	-1.12309300	-1.35438500
N	2.17746000	-0.76938700	-0.51319900
C	3.61819600	-1.35219500	-2.46123000
H	3.63797800	-0.75262700	-3.37337200
H	3.80062100	-2.39658000	-2.74139600
C	4.56258000	-1.31718000	-0.28293600
O	4.62663200	-0.84341600	-1.61558400
C	3.82863700	-3.11426600	1.11327200

C	3.04400800	-2.00748900	1.44075200
C	2.16627300	-2.03192800	2.51989100
C	2.08772500	-3.20085200	3.27657600
C	2.87231000	-4.31209500	2.95698200
C	3.75031600	-4.27614000	1.87449700
C	4.66538400	-2.85094600	-0.11213200
H	1.57354400	-1.14080800	2.72717900
H	2.80097900	-5.21277400	3.55927700
H	4.35999500	-5.14100000	1.62918200
H	4.25062600	-3.38360600	-0.97526700
H	5.70414700	-3.17408300	-0.00799300
C	-1.08012300	-1.67796000	-1.43683800
C	-1.50068400	-2.69923700	-0.57067500
C	-1.98524500	-1.23742200	-2.41100400
C	-2.78829100	-3.21592200	-0.62604000
C	-3.27045300	-1.75570500	-2.50284800
C	-3.65854100	-2.73187400	-1.59515100
H	-3.09586900	-3.99577100	0.05970700
H	-3.95403400	-1.39493900	-3.26122700
H	5.40873200	-0.84708500	0.22280900
H	1.41192200	-3.24919000	4.12503900
Cl	-0.38864200	-3.36320000	0.58214000
Cl	-5.27140200	-3.37640500	-1.68451600
Cl	-1.50375700	-0.00949200	-3.53550600
C	0.35404100	0.23552200	0.81767500
O	1.19166200	0.66687800	1.73318400
H	0.30549800	1.10697100	-0.17383800
C	-1.12774600	0.13615900	1.20775700
C	-1.52882800	1.38424000	2.00189000
H	-1.29475800	-0.75472000	1.83120600
H	-1.77740500	0.03426400	0.32878700
H	-0.89454200	1.42778700	2.89070300
H	-1.29048500	2.27389500	1.40644900
C	-2.98971700	1.37496800	2.36833500
C	-3.93275900	2.05020000	1.58912400
C	-3.44264100	0.64390400	3.47129700
C	-5.28981100	2.00024500	1.90024800
H	-3.59675900	2.62692300	0.72950000

C	-4.79718000	0.58868400	3.78667400
H	-2.71936500	0.11521000	4.08790700
C	-5.72688800	1.26779700	3.00103400
H	-6.00579500	2.53560700	1.28400200
H	-5.12739000	0.01777700	4.64927500
H	-6.78324700	1.22844900	3.24718000
C	3.19683000	4.79302200	1.15401000
C	2.65565500	3.36331900	1.11858700
C	2.36979200	2.82496800	-0.29333600
C	2.27370700	5.85322600	0.55115700
C	1.02224500	3.26155200	-0.81122100
C	1.90248800	5.56691800	-0.90601200
H	4.15034900	4.81909000	0.60788400
H	3.38777200	2.69701400	1.58539000
H	3.15975300	3.12910400	-0.99116500
H	1.34787200	5.93537800	1.13500300
H	1.54673900	6.47727300	-1.39485900
C	-1.22916900	2.75159100	-1.37195300
H	-1.93861100	2.00177100	-1.00189700
C	-0.50696500	5.11667100	-1.31770500
C	-1.57460200	4.14168600	-0.85016000
H	-1.59797000	4.12948800	0.24548000
H	-2.55585100	4.46617100	-1.20594900
H	-0.59977700	6.06835500	-0.78449800
N	0.83032000	4.58178700	-1.04989700
N	0.10811100	2.34859900	-0.96173800
H	2.78498000	5.23910700	-1.46617900
H	2.77046600	6.82839400	0.59957700
H	3.42628700	5.06475100	2.18983300
H	1.74206200	3.25520600	1.71331700
H	2.35227600	1.73615100	-0.26004300
H	-1.29935000	2.73760300	-2.46726500
H	-0.61289700	5.32458300	-2.39029600

Si-TS2b

0 1

C	-0.76362100	-0.66194000	0.00329900
C	-1.39807600	-1.74678500	1.84164700

C	-3.11369400	-0.24360300	0.98528300
H	-3.15942300	0.73038800	0.49988700
N	-0.34438900	-2.38444500	1.47506500
N	0.03874100	-1.74477300	0.30241400
N	-1.72114500	-0.69368100	1.00766600
C	-2.29307800	-1.98657500	3.01454000
H	-1.72601300	-2.40077100	3.84872700
H	-3.09601400	-2.68970700	2.75010700
C	-3.66844400	-0.13462300	2.45196000
O	-2.80988400	-0.73169300	3.41273000
C	-5.11801100	-1.55499200	1.11197700
C	-4.02848600	-1.23641200	0.30608800
C	-3.85952200	-1.80599500	-0.95132800
C	-4.81069400	-2.71947400	-1.39824900
C	-5.90703800	-3.04602100	-0.59534700
C	-6.07027800	-2.46648400	0.66193900
C	-5.06945200	-0.79425200	2.41461000
H	-2.99922300	-1.54677100	-1.56349200
H	-6.63906700	-3.76186700	-0.95545400
H	-6.92350200	-2.72771900	1.28095400
H	-5.20835300	-1.43033800	3.29479500
H	-5.84959200	-0.02675400	2.44731100
C	1.15000500	-2.21103600	-0.41567500
C	1.01768900	-2.67498600	-1.73253700
C	2.41705600	-2.27030900	0.17153400
C	2.10866500	-3.12116500	-2.45949200
C	3.52626000	-2.73113000	-0.52983500
C	3.35608100	-3.13552900	-1.84496800
H	1.98598100	-3.46359300	-3.47943400
H	4.50048800	-2.75828200	-0.05713700
H	-3.72362600	0.91096600	2.75631200
H	-4.69974000	-3.18146500	-2.37381100
Cl	-0.55357700	-2.75963700	-2.45929200
Cl	4.73875100	-3.69394500	-2.74591600
Cl	2.65058200	-1.72492500	1.80438600
C	-0.35118200	0.38923900	-0.88193900
O	0.52902800	0.13639600	-1.81880300
H	0.27322300	0.75796200	0.20463000

C	-1.32128600	1.56423500	-1.09296700
C	-0.56395900	2.72467800	-1.74732400
H	-1.73109300	1.91502700	-0.13663200
H	-2.16762300	1.27635000	-1.73399500
H	0.25106900	3.02843200	-1.07834500
H	-0.10043500	2.34229400	-2.65995900
C	-1.46642200	3.89613900	-2.03430100
C	-1.61093700	4.93714500	-1.11303900
C	-2.22020400	3.94259900	-3.21136300
C	-2.48124800	5.99667700	-1.35848600
H	-1.02923500	4.91484400	-0.19411400
C	-3.09274100	4.99794300	-3.46187600
H	-2.11502300	3.14083000	-3.93845200
C	-3.22594300	6.03030700	-2.53516400
H	-2.57631800	6.79787400	-0.63177300
H	-3.66668900	5.01751300	-4.38333400
H	-3.90313900	6.85575600	-2.73045700
C	5.44608500	1.77702700	-0.15218900
C	4.18763100	0.96046500	-0.44481700
C	2.86861300	1.75418300	-0.39088100
C	5.49788800	2.37593500	1.25246200
C	2.32296400	1.90045500	1.00905600
C	4.30236400	3.27841400	1.56344600
H	5.51130900	2.59530800	-0.88267600
H	4.27311800	0.52691400	-1.44645600
H	3.01566800	2.74738800	-0.83596000
H	5.53850300	1.58034900	2.00783600
H	4.53341900	3.92608300	2.41310000
C	0.63503200	1.44521100	2.62458300
H	-0.04123000	0.59728900	2.78044300
C	2.71990700	2.57177800	3.34272900
C	1.75112000	1.44541600	3.66110800
H	2.27846700	0.48717100	3.62036100
H	1.35336700	1.57140100	4.67096600
H	3.63846400	2.46474500	3.92996200
N	3.08665400	2.55016400	1.92641500
N	1.17212800	1.36006400	1.27339900
H	4.09912500	3.94091500	0.71417200

H	6.41526600	2.96567000	1.35782100
H	6.33014400	1.14937700	-0.30923100
H	4.12278500	0.11552900	0.25186600
H	2.10356700	1.23385400	-0.97922600
H	0.03040100	2.35833100	2.72630500
H	2.27779200	3.54518000	3.59533700

Re-M2

0 1

C	1.06888800	-0.14517900	-0.46437600
C	2.46225500	-1.87213900	-0.24255600
C	3.51720500	0.21476000	-1.11991900
H	3.40538800	0.60904800	-2.13067400
N	1.45365100	-2.23358400	0.46157800
N	0.57768900	-1.11828500	0.43646300
N	2.34249600	-0.62246500	-0.81506600
C	3.67130500	-2.71309000	-0.53854700
H	3.36157600	-3.59939500	-1.09722200
H	4.13648000	-3.04859100	0.39559300
C	4.78652800	-0.67125600	-0.97093300
O	4.57638700	-2.01106600	-1.36333400
C	4.76626300	0.91093400	0.80300400
C	3.76578400	1.30338300	-0.09109000
C	3.16586100	2.55541400	0.02318700
C	3.56872000	3.39889800	1.05827500
C	4.56066300	3.00262700	1.95583400
C	5.17155700	1.75658800	1.82951400
C	5.28499800	-0.46368600	0.47564000
H	2.41279100	2.86850600	-0.69129400
H	4.86618900	3.67386900	2.75243400
H	5.95574200	1.45281400	2.51687800
H	4.85927600	-1.20370300	1.16288700
H	6.37222800	-0.54684500	0.54533800
C	-0.79249600	-1.46291400	0.48795800
C	-1.52813500	-1.25908400	1.66104100
C	-1.45938200	-2.04229100	-0.59934700
C	-2.87297500	-1.59793200	1.75526100
C	-2.80380300	-2.38902400	-0.54024600

C	-3.49119000	-2.15957000	0.64545900
H	-3.42250500	-1.41990500	2.67122800
H	-3.29764500	-2.83109800	-1.39695700
H	5.53697400	-0.28176800	-1.66251200
H	3.11066300	4.37740600	1.16225600
Cl	-0.75503500	-0.54102200	3.03476400
Cl	-5.18098400	-2.56003800	0.73159200
Cl	-0.59209800	-2.34888400	-2.07113100
C	0.46841000	0.95962400	-0.94303200
O	1.10329400	1.65583200	-1.97577100
H	0.95324100	1.17715900	-2.80134000
C	-0.80449100	1.57679600	-0.46172000
C	-1.93861400	1.49229600	-1.50204500
H	-0.61250800	2.63698500	-0.24387900
H	-1.12955800	1.12381500	0.47973200
H	-1.59850500	1.97681100	-2.42424000
H	-2.12481000	0.43754600	-1.73704600
C	-3.20718300	2.13886000	-1.00909600
C	-3.42498700	3.51047400	-1.16372900
C	-4.16769800	1.38190300	-0.33397200
C	-4.57656100	4.10991000	-0.65972000
H	-2.68525800	4.11054000	-1.68860100
C	-5.32089300	1.97541500	0.17178200
H	-4.00574100	0.31348600	-0.21186800
C	-5.52849700	3.34347700	0.00953500
H	-4.73320400	5.17594400	-0.79306500
H	-6.05836300	1.36873200	0.68864600
H	-6.42794700	3.80872500	0.39993800

Si-M2

0 1

C	-0.07865200	0.00197000	0.61139400
C	0.37366700	-1.58937800	2.10641400
C	-1.53074200	-2.12493200	0.61360500
H	-2.56005900	-1.77715200	0.72746200
N	1.47689400	-0.93907000	2.04368900
N	1.25409800	0.05322600	1.08307400
N	-0.61679800	-1.14044400	1.24350800

C	0.08661800	-2.71743500	3.05376600
H	-0.05077200	-2.32028600	4.06274100
H	0.93671500	-3.40974000	3.07179300
C	-1.31986300	-3.49185500	1.32065800
O	-1.11984500	-3.36691200	2.70955600
C	-0.37187900	-3.61954000	-0.85022300
C	-1.15174700	-2.45807800	-0.81455900
C	-1.47387700	-1.78763900	-1.98968000
C	-0.97462400	-2.26984100	-3.19948700
C	-0.17486700	-3.41288900	-3.23122000
C	0.12234000	-4.10234400	-2.05603800
C	-0.19777700	-4.19997800	0.52877600
H	-2.10773300	-0.90870200	-1.97797400
H	0.20600900	-3.77693100	-4.18021800
H	0.72480700	-5.00537200	-2.08285400
H	0.79544700	-3.95484000	0.92283400
H	-0.30249200	-5.28701400	0.55900300
C	2.37365600	0.62629900	0.46491800
C	2.71774700	0.37170600	-0.87126200
C	3.21468200	1.48298300	1.19183900
C	3.81804500	0.97140200	-1.47163000
C	4.33878800	2.06962800	0.62630000
C	4.61797900	1.81184300	-0.70982000
H	4.05443000	0.76489100	-2.50829100
H	4.96835900	2.72708800	1.21302900
H	-2.24580600	-4.06084600	1.20704200
H	-1.21318100	-1.75245700	-4.12293800
Cl	1.77843100	-0.74690900	-1.80170900
Cl	6.00748600	2.55815700	-1.44573200
Cl	2.82796200	1.86284200	2.84029100
C	-0.69972000	0.95650300	-0.10347500
O	0.05684800	2.00400400	-0.61901900
H	0.40779000	2.52846600	0.11458500
C	-2.16743100	1.06925400	-0.35872900
C	-2.77542500	2.27980800	0.37964500
H	-2.69367300	0.16401900	-0.04327500
H	-2.35628900	1.19492100	-1.43401600
H	-2.61044300	2.15322700	1.45524900

H	-2.23883500	3.18137100	0.06677500
C	-4.24848400	2.42174600	0.09291800
C	-5.19119700	1.74265600	0.86978500
C	-4.69853900	3.18462400	-0.98770300
C	-6.55019800	1.82753600	0.57962900
H	-4.85345800	1.14594800	1.71418600
C	-6.05682000	3.27271800	-1.28238900
H	-3.97463500	3.71763100	-1.59958200
C	-6.98731400	2.59436000	-0.49844500
H	-7.26883000	1.29788600	1.19743200
H	-6.38839100	3.87433900	-2.12305100
H	-8.04648900	2.66454100	-0.72450200

M3_{SET}

1 2

C	1.11501200	-0.39531600	-0.58817500
C	2.51522200	-2.01668600	-0.11267900
C	3.60587400	0.07626000	-1.02600800
H	3.60726200	0.25260500	-2.10303100
N	1.37601200	-2.41922700	0.36471700
N	0.50898100	-1.40482600	0.08172400
N	2.42116800	-0.77370500	-0.69169100
C	3.81017700	-2.77255100	-0.08776800
H	3.66018300	-3.74850000	-0.55324300
H	4.12601800	-2.93341300	0.94924100
C	4.86578100	-0.71192000	-0.57150600
O	4.77783000	-2.09035200	-0.84790900
C	4.52443800	1.09184200	0.92401300
C	3.68268200	1.32295200	-0.16919100
C	3.09937500	2.57254500	-0.36889400
C	3.34011500	3.57738100	0.56644400
C	4.16002200	3.34020100	1.67001000
C	4.76702000	2.09907000	1.85037500
C	5.09153800	-0.30250800	0.89875800
H	2.48785100	2.77600000	-1.24065800
H	4.34090500	4.13572300	2.38529200
H	5.42748000	1.92357300	2.69370300
H	4.54651600	-0.94770700	1.59737700

H	6.14756100	-0.34670200	1.17163300
C	-0.88507100	-1.60939900	0.26566000
C	-1.46846500	-1.41780700	1.52080800
C	-1.67195800	-2.06045000	-0.79762000
C	-2.82235200	-1.65296200	1.71520500
C	-3.02944300	-2.29558000	-0.62545100
C	-3.58349300	-2.08868900	0.63468100
H	-3.27193100	-1.49609900	2.68791300
H	-3.63812100	-2.63567900	-1.45435900
H	5.69829000	-0.34450300	-1.17472500
H	2.89576900	4.55685600	0.42571300
Cl	-0.49623900	-0.85939700	2.83406600
Cl	-5.27860500	-2.35508000	0.85875700
Cl	-0.95085100	-2.32259300	-2.34804400
C	0.49749100	0.74705600	-1.14683500
O	1.01935700	1.31017600	-2.24393100
H	1.52786300	0.68731500	-2.78332100
C	-0.66741700	1.46582200	-0.56613400
C	-1.88794900	1.48939100	-1.51245700
H	-0.34451500	2.49940800	-0.37840200
H	-0.93654000	1.04059000	0.40388600
H	-1.58781600	1.95296800	-2.45695300
H	-2.19436100	0.46099600	-1.73319700
C	-3.03339600	2.24364900	-0.88629500
C	-3.10508300	3.63572900	-0.97610500
C	-4.01483200	1.56207500	-0.16472400
C	-4.14088000	4.33166400	-0.35881400
H	-2.34767700	4.17551800	-1.53956100
C	-5.05301900	2.25377300	0.45341400
H	-3.96668200	0.47794000	-0.09802800
C	-5.11685100	3.64185600	0.35803400
H	-4.18957400	5.41268800	-0.44153900
H	-5.81334400	1.70840900	1.00353900
H	-5.92618200	4.18353400	0.83646000

M3_{HAT}

0 2

C	1.06140100	-0.20079900	-0.40709500
---	------------	-------------	-------------

C	2.40892900	-1.94334900	-0.17816700
C	3.51780400	0.13050300	-1.06882900
H	3.30896300	0.48951500	-2.07592500
N	1.30421900	-2.34686200	0.36044500
N	0.46182300	-1.24360800	0.28045500
N	2.34779400	-0.65573400	-0.63388600
C	3.64126700	-2.77340300	-0.38080100
H	3.35324300	-3.73253500	-0.81520700
H	4.13233700	-2.97053900	0.57927300
C	4.77238500	-0.78879400	-0.99539200
O	4.50114700	-2.14120000	-1.30119800
C	4.95741000	0.86510100	0.70325100
C	3.88154000	1.24621400	-0.10356900
C	3.32091100	2.51620200	0.01702200
C	3.83790400	3.38720600	0.97496200
C	4.90346100	3.00207900	1.78938200
C	5.47528400	1.73896400	1.65320400
C	5.41913700	-0.53025700	0.38221200
H	2.50490800	2.81495300	-0.63089700
H	5.29734700	3.69555400	2.52575900
H	6.31682500	1.44323200	2.27265000
H	5.06016900	-1.23305800	1.14207800
H	6.50630500	-0.62940500	0.34028200
C	-0.92432300	-1.50614000	0.36966500
C	-1.59068800	-1.39249600	1.59351400
C	-1.65092800	-1.93974100	-0.74448300
C	-2.94551300	-1.67599500	1.71042500
C	-3.00801800	-2.22602700	-0.65816000
C	-3.63416900	-2.08829900	0.57556500
H	-3.44931900	-1.57165900	2.66326400
H	-3.55946900	-2.55084500	-1.53206900
H	5.45797500	-0.45099600	-1.77558600
H	3.41127700	4.37941300	1.08207900
Cl	-0.71436700	-0.86235700	2.98816500
Cl	-5.33577800	-2.41459800	0.69589500
Cl	-0.84457800	-2.13413400	-2.26478300
C	0.51412700	1.00522700	-0.91711000
O	1.12991700	1.63501500	-1.81560000

C	-0.78113400	1.56454300	-0.36678200
C	-1.87087900	1.64865500	-1.44857900
H	-0.55818100	2.58038700	-0.01651900
H	-1.14799000	1.00746200	0.49985900
H	-1.46728200	2.21769700	-2.29160400
H	-2.09463100	0.63942600	-1.81537100
C	-3.12816200	2.29042800	-0.91962000
C	-3.33026400	3.66922600	-1.01589400
C	-4.09287800	1.51749500	-0.26850400
C	-4.47116900	4.26069300	-0.47838900
H	-2.58668800	4.28153300	-1.52041100
C	-5.23468200	2.10272900	0.27076800
H	-3.94333300	0.44298100	-0.19100400
C	-5.42691700	3.47889000	0.16668000
H	-4.61575400	5.33309500	-0.56641700
H	-5.97529500	1.48377700	0.76827800
H	-6.31749100	3.93829900	0.58340700

TS3

0 1

C	-2.73391300	-0.72672100	0.12004700
C	-4.23117100	-2.00039000	1.13400300
C	-5.03423600	0.30225700	0.63319700
H	-4.58180600	1.23404300	0.97934200
N	-3.23750300	-2.80379100	0.92333200
N	-2.30063400	-2.02065800	0.28782600
N	-4.00350100	-0.74083600	0.65085500
C	-5.49910100	-2.30551100	1.86843800
H	-5.32885500	-2.16240700	2.94600900
H	-5.79129300	-3.34082100	1.69070900
C	-6.21569800	-0.08920100	1.55399600
O	-6.52747600	-1.46685900	1.40248900
C	-7.06734200	0.73912800	-0.50585100
C	-5.70749300	0.50001500	-0.70953200
C	-5.15867600	0.48751300	-1.98457300
C	-6.00504200	0.71206500	-3.07065000
C	-7.36413800	0.95724700	-2.87343300
C	-7.90589000	0.97493800	-1.58769000

C	-7.39714000	0.68891800	0.96888100
H	-4.09895600	0.30724200	-2.13591300
H	-8.00812500	1.13077700	-3.72971900
H	-8.96586500	1.15654600	-1.43718000
H	-8.33755300	0.18169400	1.19637700
H	-7.43707000	1.69538900	1.39992400
C	-1.23251200	-2.66386100	-0.37637000
C	-1.32646700	-2.96947100	-1.73803100
C	-0.06853400	-3.01197300	0.31321500
C	-0.26647800	-3.55623500	-2.41716400
C	1.00018700	-3.61149900	-0.33891500
C	0.88710700	-3.86319300	-1.70287500
H	-0.34362000	-3.77578600	-3.47511900
H	1.90194600	-3.87426400	0.20110600
H	-6.00674200	0.13375600	2.60874200
H	-5.60130900	0.69851100	-4.07775900
Cl	-2.79129600	-2.61041600	-2.58917200
Cl	2.22688300	-4.58144600	-2.53553000
Cl	0.05094000	-2.63653300	1.99671700
C	-2.03841800	0.40564600	-0.35888100
O	-2.69814700	1.53113300	-0.39447300
H	-2.38640000	2.28178900	0.52789600
C	-0.64877400	0.32848000	-0.91400700
C	-0.56693300	0.42564100	-2.45287800
H	-0.11510100	-0.55536400	-0.56015100
H	-0.08854300	1.17809600	-0.52696400
H	-0.85676900	-0.52518900	-2.91426300
H	-1.27899600	1.18483500	-2.79479700
C	0.83537800	0.81584400	-2.85448700
C	1.91903700	-0.00191300	-2.51293000
C	1.09008200	2.02943500	-3.49537200
C	3.22267100	0.38115300	-2.80833000
H	1.74102400	-0.94729900	-2.00318000
C	2.39526500	2.41597000	-3.79981900
H	0.25823900	2.67676700	-3.76218800
C	3.46368700	1.59151900	-3.45874400
H	4.05143100	-0.26119300	-2.52463900
H	2.57414500	3.36074000	-4.30410400

H	4.47890800	1.88887200	-3.70307700
C	5.45110600	1.00045300	0.06524400
C	4.21514100	1.53329500	0.27970900
C	3.17609000	0.85850700	0.99758600
C	3.47360600	-0.45168300	1.49150800
C	4.67685800	-1.06774700	1.31019500
C	5.73950600	-0.36397500	0.55660000
H	4.02043600	2.53915100	-0.06730200
H	2.68374300	-0.98572700	2.00642900
C	1.90959500	1.46519800	1.23440700
C	1.01006900	0.97824700	2.22863500
C	1.50173800	2.64133800	0.52911600
C	-0.24708700	1.50088900	2.42058600
H	1.35840700	0.19905600	2.89367000
C	0.26041500	3.21188400	0.67494300
H	2.18741200	3.06491000	-0.19172200
C	-0.69289600	2.54206400	1.52280700
O	6.83799600	-0.90412000	0.34697300
O	-1.96318600	2.85721500	1.44715000
C	4.96830900	-2.46840200	1.84892100
C	5.24344500	-3.43031100	0.67832900
C	6.18566800	-2.43115000	2.79346600
C	3.78858400	-3.02639400	2.65094700
H	4.37653500	-3.47574000	0.00865400
H	6.10928100	-3.10465800	0.10187800
H	5.43102700	-4.43929600	1.06202100
H	5.99281800	-1.75739800	3.63499400
H	6.36603800	-3.43366600	3.19685100
H	7.07917100	-2.09443900	2.26991300
H	4.04476500	-4.02175400	3.02590600
H	3.54417000	-2.39397400	3.51152000
H	2.88652500	-3.12215200	2.03960100
C	6.56086600	1.77764100	-0.64537400
C	7.75830900	1.95746500	0.30681700
C	7.01764500	1.02610100	-1.90987900
C	6.09233600	3.17329800	-1.07442600
H	7.45707700	2.52065800	1.19631500
H	8.15784000	0.99245800	0.61882600

H	8.55063900	2.52037500	-0.19906200
H	6.18237400	0.90211600	-2.60700000
H	7.79772900	1.60303600	-2.41909400
H	7.41289300	0.04242500	-1.65931600
H	6.91150400	3.68386400	-1.58954000
H	5.24163400	3.12152800	-1.76240400
H	5.80484000	3.78723700	-0.21438600
C	-0.12579900	4.49047100	-0.08028500
C	-0.62070400	5.53965100	0.93163600
C	1.08218300	5.08299700	-0.81983700
C	-1.21993100	4.22729100	-1.13110900
H	-1.49133800	5.17630200	1.48000700
H	0.17018900	5.78648900	1.64731800
H	-0.90006200	6.45732600	0.40300700
H	1.42434000	4.42774800	-1.62886600
H	0.79002100	6.03748000	-1.26740800
H	1.92207600	5.27235300	-0.14345400
H	-1.32548600	5.11224000	-1.76817900
H	-0.94784900	3.37821800	-1.76678800
H	-2.18593800	4.01626400	-0.67525400
C	-1.12046500	1.08880100	3.61537100
C	-1.52952700	2.35832500	4.38741000
C	-2.38058700	0.33484600	3.16548900
C	-0.35628900	0.18346200	4.58930600
H	-0.64201700	2.90752000	4.71785800
H	-2.13949700	3.01811900	3.76892700
H	-2.10621100	2.07842800	5.27520400
H	-2.10639200	-0.61355000	2.68914100
H	-3.00775800	0.10776400	4.03555300
H	-2.96022000	0.93671000	2.46344400
H	-1.00002500	-0.04335300	5.44427500
H	-0.07349600	-0.76866700	4.12922200
H	0.54926800	0.66846600	4.96651300

TS3_{HTC}

0 1

C	-1.77235600	-1.01232000	0.08888600
C	-3.33057900	-1.97929600	1.30956900

C	-4.22930800	-0.22694600	-0.16563500
H	-3.87142100	0.76108100	-0.44266500
N	-2.25057800	-2.63449900	1.60241400
N	-1.28242400	-2.04185000	0.83682200
N	-3.09907000	-0.97534600	0.41244600
C	-4.71413300	-2.13547000	1.84947800
H	-4.68581500	-2.65675200	2.80615300
H	-5.33343200	-2.70897700	1.14478400
C	-5.40249900	-0.08310400	0.87260100
O	-5.21981100	-0.83612800	2.06273600
C	-6.20539400	-1.13274100	-1.16795400
C	-4.83119900	-0.97797400	-1.33269100
C	-4.17334900	-1.48407900	-2.45099700
C	-4.92260600	-2.15938700	-3.41083300
C	-6.30175800	-2.31756000	-3.25171500
C	-6.95227500	-1.80416800	-2.13267300
C	-6.68423900	-0.49266600	0.10883100
H	-3.10221800	-1.35174000	-2.57440900
H	-6.87062100	-2.84760200	-4.00882100
H	-8.02388700	-1.93071200	-2.01055000
H	-7.28917200	-1.16374200	0.72707400
H	-7.29754300	0.38887000	-0.10186100
C	0.03266100	-2.57065500	0.93595900
C	0.37279000	-3.76168700	0.29152600
C	0.96679500	-1.97545500	1.78741100
C	1.63816400	-4.31627500	0.43628400
C	2.23647700	-2.50799900	1.94761400
C	2.55712800	-3.67255000	1.25644200
H	1.89971800	-5.22722000	-0.08743400
H	2.95147000	-2.03959500	2.61315800
H	-5.43977800	0.95401300	1.20766300
H	-4.43280500	-2.56456800	-4.29007000
Cl	-0.79504500	-4.55985300	-0.70779400
Cl	4.13591100	-4.35393300	1.45452000
Cl	0.50454500	-0.56111700	2.66566800
C	-1.12776400	-0.17359500	-0.89023600
O	-1.90827600	0.60608600	-1.54612300
H	-1.87247000	1.81584700	-1.09275400

C	0.33248400	-0.28153700	-1.19265100
C	0.65103100	-1.46769300	-2.12252500
H	0.91382900	-0.34747300	-0.26448800
H	0.64022400	0.65430300	-1.66621800
H	-0.03027500	-2.30151800	-1.91953600
H	0.43010600	-1.16127300	-3.15207300
C	2.07453600	-1.97006700	-2.02614200
C	3.09847100	-1.22919200	-1.43446200
C	2.37653900	-3.23671500	-2.54096600
C	4.39757800	-1.73692200	-1.36507100
H	2.90396300	-0.23802500	-1.03119100
C	3.66515800	-3.75254300	-2.46001300
H	1.58400700	-3.82615200	-2.99865900
C	4.68238500	-3.00074100	-1.87091100
H	5.17736600	-1.12172300	-0.92440000
H	3.87713000	-4.74054600	-2.85783000
H	5.68935700	-3.40070500	-1.80717800
C	3.83623100	2.29832800	-1.37277600
C	2.52375100	2.59929500	-1.12826500
C	1.87677600	2.38146300	0.12528100
C	2.69011200	1.85403500	1.16971000
C	4.01450600	1.53275700	1.01420200
C	4.65104600	1.70389600	-0.29879500
H	1.94693700	3.03963200	-1.93172400
H	2.24061100	1.68958100	2.13956100
C	0.47171600	2.65228500	0.30310500
C	-0.15682200	2.50822200	1.61093400
C	-0.35850100	3.06372300	-0.73019200
C	-1.48928700	2.57832300	1.84623600
H	0.50231400	2.36994100	2.45820900
C	-1.78461100	3.03240300	-0.65644700
H	0.07168900	3.25496100	-1.70425200
C	-2.39977500	2.78584300	0.69502300
O	5.83847700	1.36245300	-0.49470300
O	-3.62608100	2.71889100	0.82261200
C	4.86109600	1.00877000	2.17749500
C	5.43300900	-0.38325200	1.84723500
C	6.02123800	1.98452300	2.45004300

C	4.04640900	0.88606000	3.47060600
H	4.63956200	-1.05603600	1.50138300
H	6.18294200	-0.31511800	1.05931800
H	5.89253900	-0.82187000	2.74070900
H	5.63396000	2.96179100	2.75693000
H	6.65109500	1.59880700	3.25998000
H	6.63364800	2.10985200	1.55677400
H	4.69551200	0.52187200	4.27266900
H	3.63373300	1.84989100	3.78739500
H	3.21497300	0.18069900	3.36442900
C	4.48595700	2.56187900	-2.73394200
C	5.68281500	3.51613100	-2.56175300
C	4.96258800	1.23795600	-3.35901500
C	3.51047500	3.21436500	-3.72108800
H	5.35125700	4.47067600	-2.13896100
H	6.43278800	3.07974500	-1.90211200
H	6.13925500	3.71739800	-3.53757400
H	4.11582200	0.56057800	-3.51431400
H	5.42626000	1.43611000	-4.33246400
H	5.68840200	0.74225900	-2.71408100
H	4.02495000	3.38757500	-4.67120200
H	2.64650600	2.57188500	-3.92391600
H	3.14602100	4.18098200	-3.35718200
C	-2.63613000	3.82111200	-1.69023500
C	-3.04600900	5.16483400	-1.06842400
C	-1.82123600	4.09497000	-2.96055700
C	-3.89680600	3.04384400	-2.11268400
H	-3.68674000	5.01294300	-0.19650300
H	-2.16180600	5.73289800	-0.76109500
H	-3.59921600	5.76122500	-1.80185800
H	-1.44646800	3.16491100	-3.40305700
H	-2.46382600	4.58268200	-3.69936500
H	-0.97307900	4.75890800	-2.76969400
H	-4.44241900	3.62461400	-2.86396100
H	-3.63365300	2.08001900	-2.56248400
H	-4.55888000	2.86882300	-1.26467100
C	-2.08338300	2.45308200	3.25112100
C	-2.97585000	3.66926500	3.56395000

C	-2.90870200	1.15800600	3.34164200
C	-0.99374800	2.40175800	4.32874100
H	-2.39601700	4.59586000	3.49802900
H	-3.81928400	3.73332800	2.87732700
H	-3.36228200	3.58397900	4.58492800
H	-2.27304300	0.28191400	3.16181100
H	-3.34274000	1.05874000	4.34243500
H	-3.72039000	1.15700100	2.61533800
H	-1.46909500	2.34357000	5.31211300
H	-0.34770700	1.52241600	4.23117000
H	-0.36343400	3.29673000	4.31095200

TS3_{HTC}^{C2'}

0 1

C	-1.76839100	1.25122600	-0.10151600
C	-3.34724900	2.40779200	-1.06968700
C	-4.20386800	0.38125400	0.09119500
H	-3.85876500	-0.65689800	0.03829900
N	-2.26180500	3.09158500	-1.28902500
N	-1.28529700	2.37253100	-0.67494400
N	-3.09814600	1.27117000	-0.35258200
C	-4.73623300	2.66585500	-1.55030500
H	-4.71205500	3.32221600	-2.41974900
H	-5.32815100	3.14341400	-0.75675000
C	-5.45858400	0.52972400	-0.85396600
O	-5.26988600	1.42226700	-1.93915100
C	-6.06146000	1.09889200	1.42749100
C	-4.70207400	0.79213900	1.46023500
C	-3.97544100	0.88463500	2.64633300
C	-4.63237500	1.29603700	3.80237000
C	-5.99522300	1.60162200	3.77337300
C	-6.71746600	1.50159600	2.58825700
C	-6.64643100	0.92707700	0.05219400
H	-2.92047200	0.63402200	2.67682400
H	-6.49450000	1.91786300	4.68359700
H	-7.77700000	1.73820100	2.56607900
H	-7.12274800	1.84043300	-0.32063200
H	-7.41087800	0.14537600	0.03890300

C	0.05333000	2.85964700	-0.74678900
C	0.45215200	3.94254900	0.03944000
C	0.95474700	2.31619500	-1.66592300
C	1.74467700	4.44355200	-0.04568000
C	2.25132400	2.79775300	-1.76247000
C	2.63133600	3.85402600	-0.93909900
H	2.05307400	5.26870000	0.58404100
H	2.94664100	2.36797800	-2.47382300
H	-5.62582200	-0.44154200	-1.31973900
H	-4.08256600	1.37256100	4.73451800
Cl	-0.66234500	4.65626600	1.15230200
Cl	4.24676000	4.46229800	-1.05145800
Cl	0.44081100	1.01386900	-2.67862900
C	-1.06826500	0.18364800	0.64688700
O	-1.79661300	-0.73271000	1.04812900
H	-2.10350200	-1.81039000	-0.03642300
C	0.39278000	0.24654600	0.95440200
C	0.66698300	1.25775800	2.08577800
H	0.97706800	0.48719700	0.06059300
H	0.68624900	-0.76050300	1.25814700
H	-0.01399100	2.11446200	2.00947400
H	0.41962400	0.77543600	3.03878700
C	2.08912900	1.76943900	2.11396900
C	3.13874500	1.06696600	1.52019900
C	2.36857100	2.98051300	2.75616700
C	4.44288400	1.56133500	1.56826200
H	2.95597700	0.11548800	1.02481600
C	3.66433800	3.48502000	2.79099100
H	1.55726000	3.53660200	3.22212600
C	4.70694100	2.77472200	2.19584200
H	5.24087200	0.97797400	1.11816200
H	3.86122500	4.43212000	3.28412800
H	5.71880000	3.16604800	2.22365800
C	3.76180100	-2.58232700	1.11652200
C	2.46502800	-2.88848400	0.81964200
C	1.82016600	-2.52648700	-0.40689600
C	2.62598600	-1.82453100	-1.36142600
C	3.93850400	-1.50832800	-1.16042800

C	4.57248700	-1.84122700	0.12926100
H	1.87494500	-3.40476800	1.56629900
H	2.17546900	-1.55002800	-2.30582800
C	0.44850500	-2.80075700	-0.63587700
C	-0.23196500	-2.30892700	-1.80751100
C	-0.34895000	-3.58175600	0.26785100
C	-1.58721700	-2.33207400	-1.94469000
H	0.36877100	-1.96239200	-2.63723600
C	-1.71404300	-3.61731100	0.20837400
H	0.15712900	-4.15763000	1.03044300
C	-2.44264000	-2.70249100	-0.76124700
O	5.74522600	-1.49916100	0.37693300
O	-3.75389600	-2.67869000	-0.84965500
C	4.78141900	-0.81933000	-2.23820000
C	5.32033100	0.52847000	-1.72343600
C	5.96156300	-1.72718200	-2.63073700
C	3.96752100	-0.54123700	-3.50730000
H	4.50878900	1.13098400	-1.29809800
H	6.06836200	0.37416900	-0.94658600
H	5.77412200	1.09111300	-2.54780600
H	5.59476300	-2.66475500	-3.06127200
H	6.58163000	-1.22688500	-3.38327000
H	6.57941000	-1.95502500	-1.76170900
H	4.61126000	-0.06214700	-4.25113700
H	3.57238600	-1.46144300	-3.95019600
H	3.12351600	0.12921600	-3.31025200
C	4.39995500	-2.96990800	2.45315900
C	5.63021000	-3.86259000	2.20469800
C	4.81825300	-1.70492000	3.22424200
C	3.43080100	-3.75631600	3.34407900
H	5.33813000	-4.77394000	1.67203900
H	6.38135400	-3.33622700	1.61634000
H	6.07315300	-4.15761300	3.16264900
H	3.94133200	-1.08758200	3.44933300
H	5.28992200	-1.98824400	4.17237600
H	5.52152600	-1.10829500	2.64294100
H	3.93852700	-4.02311900	4.27600200
H	2.54597400	-3.16592600	3.60547500

H	3.09959700	-4.68415700	2.86552700
C	-2.54791700	-4.39776400	1.21446100
C	-3.47387100	-5.35471900	0.44094100
C	-1.68512800	-5.22732700	2.17177500
C	-3.38688100	-3.41235600	2.05160300
H	-4.10178000	-4.78910400	-0.24789400
H	-2.88391500	-6.08476800	-0.12349600
H	-4.10655100	-5.90343200	1.14733900
H	-1.04180300	-4.59620400	2.79345200
H	-2.34115400	-5.79471400	2.83886700
H	-1.05556100	-5.94322400	1.63331200
H	-4.00459900	-3.97693700	2.75885700
H	-2.73445100	-2.74182500	2.62048300
H	-4.03245500	-2.81833500	1.40306600
C	-2.25705300	-1.95532700	-3.26324200
C	-3.15722600	-3.12975800	-3.69642100
C	-3.10549900	-0.69003400	-3.07599800
C	-1.25186000	-1.70654600	-4.39328600
H	-2.55201300	-4.02513000	-3.87403600
H	-3.89555400	-3.34193900	-2.92358600
H	-3.66516000	-2.87265600	-4.63238800
H	-2.46933800	0.17104000	-2.83242600
H	-3.64697300	-0.45475000	-3.99857000
H	-3.82486500	-0.85745900	-2.27670400
H	-1.80220800	-1.49468800	-5.31481500
H	-0.60449300	-0.84568500	-4.19915500
H	-0.61720900	-2.58008500	-4.57237500

TS3_{HTC}^{C4'}

0 1

C	-0.81508700	-1.48978400	-0.07184000
C	-2.23102900	-2.90002700	0.86045300
C	-3.34196700	-1.14130000	-0.45654300
H	-3.14581200	-0.07118300	-0.54888800
N	-1.06898000	-3.34772800	1.21422400
N	-0.18151700	-2.48334700	0.62588500
N	-2.13898100	-1.76531600	0.10154900
C	-3.59210400	-3.38586600	1.22929600

H	-3.53475100	-4.03974100	2.09911500
H	-4.04318900	-3.93662600	0.39143500
C	-4.59014100	-1.36559300	0.48394200
O	-4.33866300	-2.24037700	1.57481500
C	-5.05695700	-2.19541200	-1.75514300
C	-3.72790000	-1.77709900	-1.77388000
C	-2.92769900	-1.95795100	-2.89936300
C	-3.48417900	-2.57472800	-4.01681400
C	-4.81693000	-2.99378700	-4.00545700
C	-5.61148200	-2.80509000	-2.87774600
C	-5.71732100	-1.88778600	-0.43784300
H	-1.89614500	-1.62026900	-2.90691400
H	-5.23658500	-3.47087300	-4.88532200
H	-6.64681200	-3.13270600	-2.87101600
H	-6.19527000	-2.76346000	0.01435800
H	-6.49315500	-1.12500700	-0.55646100
C	1.16388400	-2.57621900	1.06681100
C	1.99050200	-3.62040700	0.64277500
C	1.62843600	-1.70690700	2.05979500
C	3.28405600	-3.74874000	1.13449200
C	2.91318500	-1.82062200	2.57085100
C	3.73058600	-2.83609400	2.08284500
H	3.92672900	-4.54545300	0.78109500
H	3.26618400	-1.14183000	3.33819500
H	-4.85105900	-0.41168300	0.94771700
H	-2.87960300	-2.72799700	-4.90474400
Cl	1.40000700	-4.78543500	-0.48898300
Cl	5.35458000	-2.95647900	2.67299500
Cl	0.55943300	-0.49354800	2.67432800
C	-0.26257100	-0.45441200	-0.91512800
O	-1.08876500	0.26240500	-1.56844000
H	-1.55472500	1.44430200	-1.00577800
C	1.21580500	-0.33875600	-1.14565800
C	1.75900400	-1.43490000	-2.08274300
H	1.77036000	-0.31707100	-0.20053100
H	1.37614700	0.62935400	-1.61981800
H	1.47405600	-2.42702900	-1.71463600
H	1.27526300	-1.32309300	-3.05943300

C	3.25975600	-1.35111600	-2.25064000
C	4.09900400	-1.20852900	-1.14239600
C	3.84063400	-1.40342400	-3.51989700
C	5.47920800	-1.11491900	-1.29435300
H	3.67323500	-1.16208600	-0.14358200
C	5.22122900	-1.31183400	-3.67891300
H	3.20166000	-1.50389000	-4.39371100
C	6.04565300	-1.16484800	-2.56605000
H	6.10926700	-1.00002400	-0.41712800
H	5.65193700	-1.34909400	-4.67463700
H	7.12090800	-1.08558300	-2.68891700
C	2.21274600	3.03301200	-1.47618600
C	0.91629400	2.98184000	-1.07792300
C	0.49796300	2.64971100	0.26056000
C	1.54632200	2.47374300	1.23439600
C	2.86984900	2.51552800	0.92731100
C	3.27899500	2.75996300	-0.47934700
H	0.14994500	3.15824000	-1.81918000
H	1.26133500	2.29153400	2.26172400
C	-0.86389700	2.51027500	0.57781400
C	-1.33349800	2.20494100	1.89337600
C	-1.88740100	2.52797600	-0.47898200
C	-2.64447200	1.96387700	2.19037400
H	-0.61061200	2.18802400	2.69778900
C	-3.28520000	2.42503200	-0.17239100
H	-1.65826900	3.18055700	-1.31730700
C	-3.70106600	2.02670800	1.13391300
O	4.46991100	2.75492500	-0.80758700
O	-4.90450600	1.78906100	1.43188500
C	3.96527800	2.34890900	1.98294900
C	4.84963300	1.13524000	1.64134800
C	4.83237800	3.62111200	2.03860100
C	3.37689500	2.12632800	3.38082900
H	4.23441400	0.23257200	1.55024600
H	5.37725400	1.28636400	0.69999000
H	5.58087200	0.96894700	2.44064900
H	4.22136500	4.48858800	2.30813100
H	5.60878700	3.50230300	2.80219300

H	5.31185100	3.81086600	1.07856500
H	4.19263400	1.99862900	4.09848900
H	2.77350400	2.97912700	3.70916400
H	2.74920000	1.22946300	3.42088600
C	2.61251500	3.33144100	-2.92142100
C	3.51567300	4.57774700	-2.97460500
C	3.35161100	2.11636000	-3.51444900
C	1.38762600	3.60038900	-3.80386000
H	2.99592300	5.44461700	-2.55305600
H	4.44076700	4.41786300	-2.42145800
H	3.76289800	4.80512500	-4.01709200
H	2.68278800	1.24993200	-3.56580700
H	3.67627600	2.34677600	-4.53561500
H	4.22485600	1.84467100	-2.92034100
H	1.72152700	3.80579400	-4.82530000
H	0.71684200	2.73466300	-3.84115400
H	0.81638300	4.46864700	-3.45818700
C	-4.33155500	2.74201500	-1.24389600
C	-5.21047900	3.90453900	-0.74300500
C	-3.69549100	3.16238200	-2.57563600
C	-5.22839800	1.52302000	-1.53439100
H	-5.70306400	3.63159600	0.19119300
H	-4.60136900	4.79859400	-0.57428700
H	-5.97351600	4.14632400	-1.49164900
H	-3.03137200	2.38472700	-2.97080500
H	-4.48703300	3.33102600	-3.31210800
H	-3.12744500	4.09475100	-2.48808700
H	-6.02322800	1.80753700	-2.23334700
H	-4.65150300	0.72046700	-2.00798700
H	-5.68462000	1.15877400	-0.61272400
C	-3.07331800	1.64793400	3.62458700
C	-4.09081900	2.69910700	4.11055900
C	-3.70096400	0.24176300	3.66557200
C	-1.89782100	1.66365000	4.60919800
H	-3.63083000	3.69291100	4.13040700
H	-4.96447000	2.72226800	3.46131200
H	-4.40544400	2.45251700	5.13050000
H	-3.00267100	-0.50511400	3.27033600

H	-3.93395200	-0.02490700	4.70243900
H	-4.61666900	0.20681500	3.07670500
H	-2.27721100	1.45775100	5.61427700
H	-1.15341700	0.89398000	4.37819400
H	-1.39701000	2.63684800	4.63625500

TS3_{HTC}^{C5'}

0 1

C	0.46077900	-1.47598800	-0.28514000
C	0.11714700	-3.48705500	0.54439000
C	-1.92467900	-2.45972300	-0.36260900
H	-2.30508900	-1.44007500	-0.38883500
N	1.39396200	-3.31589900	0.66626800
N	1.61110600	-2.05730900	0.14928300
N	-0.50013900	-2.40058100	-0.01382100
C	-0.73937600	-4.64017000	0.94701200
H	-0.22881000	-5.24694600	1.69437000
H	-0.97284000	-5.26150900	0.07131700
C	-2.72335000	-3.32205400	0.68352900
O	-1.90355600	-4.10312700	1.53935700
C	-3.11070600	-4.15920800	-1.55730700
C	-2.13831700	-3.17075200	-1.68126600
C	-1.49397900	-2.92901100	-2.89078400
C	-1.83299600	-3.71835500	-3.98713800
C	-2.80284500	-4.71764800	-3.86885400
C	-3.45217500	-4.94191700	-2.65712300
C	-3.67516400	-4.19841300	-0.16057600
H	-0.75604900	-2.13677800	-2.97570600
H	-3.05461100	-5.32427300	-4.73270100
H	-4.20722000	-5.71716000	-2.56939200
H	-3.72457100	-5.20484400	0.26530500
H	-4.69059000	-3.78794400	-0.14064800
C	2.94367100	-1.78218700	-0.26868900
C	3.35552300	-2.16153900	-1.55035100
C	3.88601600	-1.26304600	0.62147900
C	4.66414700	-1.96800900	-1.97119900
C	5.20317600	-1.06421100	0.22291000
C	5.56982900	-1.41416500	-1.07179200

H	4.96873500	-2.24973400	-2.97147500
H	5.92401300	-0.64560500	0.91457000
H	-3.26996700	-2.66735400	1.36851200
H	-1.34441300	-3.55364000	-4.94174300
Cl	2.21047100	-2.87940800	-2.63482100
Cl	7.20349100	-1.14321200	-1.58484100
Cl	3.39728000	-0.84431200	2.21291900
C	0.26790000	-0.21057700	-0.95207900
O	-0.83784800	-0.05864000	-1.57906800
H	-1.63364100	0.66305800	-0.77520700
C	1.35882000	0.81571300	-1.08905100
C	2.06282000	0.88393100	-2.45866900
H	2.08711300	0.73892900	-0.27267100
H	0.86861300	1.78437400	-0.96536200
H	2.65889600	-0.01241400	-2.64888700
H	1.29916900	0.94811900	-3.24039900
C	2.94243600	2.10993200	-2.46400900
C	4.17076900	2.08792300	-1.79723000
C	2.50185300	3.31212100	-3.02077300
C	4.94430700	3.23971900	-1.68896900
H	4.51625000	1.15678700	-1.35158400
C	3.27459000	4.46720700	-2.91795600
H	1.54535700	3.34241900	-3.53710500
C	4.49653300	4.43421700	-2.25065900
H	5.89533500	3.20448500	-1.16661300
H	2.91966900	5.39409400	-3.35759000
H	5.09710000	5.33437200	-2.16911800
C	1.06811300	2.02825800	2.33266100
C	0.10465000	2.08434300	1.36764700
C	-0.91508500	1.10357600	1.18481700
C	-0.94141600	0.04178300	2.14438400
C	-0.06801600	-0.05428200	3.19344300
C	1.03097700	0.92381700	3.30936200
H	0.11006600	2.93740300	0.70366700
H	-1.71867300	-0.71109800	2.05721100
C	-2.02558100	1.33325900	0.23599100
C	-3.33615200	0.73412300	0.53466100
C	-2.10358300	2.62634600	-0.46593700

C	-4.51860700	1.22572400	0.11027100
H	-3.33719400	-0.17849500	1.11906100
C	-3.24322700	3.19035200	-0.91469600
H	-1.16121200	3.10263700	-0.70739100
C	-4.53955000	2.51634300	-0.63519600
O	1.89759600	0.81784800	4.19929800
O	-5.60371300	3.00761200	-1.01165300
C	-0.23289900	-1.10846000	4.29312500
C	0.97926200	-2.05382800	4.33800200
C	-0.38888400	-0.40178000	5.65405800
C	-1.48543500	-1.96399000	4.07766600
H	1.11868700	-2.54957200	3.36992200
H	1.88885700	-1.50523300	4.58407700
H	0.81753500	-2.82740000	5.09741300
H	-1.27142600	0.24671800	5.64645300
H	-0.52579200	-1.15065000	6.44211100
H	0.48882800	0.20016000	5.88799300
H	-1.58778200	-2.66555600	4.91148700
H	-2.39409500	-1.35167100	4.04496000
H	-1.42605000	-2.55644900	3.15956100
C	2.13087600	3.12534000	2.45939700
C	1.96180200	3.84063600	3.81237500
C	3.54969100	2.53451700	2.37183700
C	2.01198100	4.17217400	1.34352000
H	0.97138700	4.30264000	3.88094000
H	2.07901700	3.13409700	4.63508500
H	2.71436800	4.63055200	3.91370200
H	3.70201000	2.03758200	1.40537500
H	4.28427900	3.34418200	2.45089900
H	3.72339200	1.81535100	3.17141300
H	2.79812600	4.92214000	1.47305400
H	2.14458900	3.72405800	0.35000400
H	1.04998900	4.69544700	1.36742700
C	-3.25174100	4.50319800	-1.70238300
C	-4.06163400	5.56695000	-0.93810400
C	-1.83344400	5.05169200	-1.90054900
C	-3.86560700	4.27671500	-3.09653800
H	-5.09748400	5.25506100	-0.80629400

H	-3.61857100	5.74823000	0.04668900
H	-4.04611100	6.50958900	-1.49582000
H	-1.20546900	4.36232300	-2.47530300
H	-1.88881900	5.99238400	-2.45607100
H	-1.33898400	5.25839200	-0.94497400
H	-3.84734200	5.21469100	-3.66190000
H	-3.28471800	3.53395700	-3.65351300
H	-4.89755600	3.93376500	-3.02421900
C	-5.84909300	0.52157500	0.38989500
C	-6.75264100	1.41767400	1.25623200
C	-6.55244500	0.19058100	-0.94029300
C	-5.64071100	-0.80017500	1.13711100
H	-6.27256600	1.62893400	2.21730400
H	-6.96732000	2.36073400	0.75393900
H	-7.69852800	0.90234100	1.45507700
H	-5.91836000	-0.45571300	-1.55699200
H	-7.48588800	-0.34513900	-0.73640500
H	-6.78311400	1.09566000	-1.50075600
H	-6.61116300	-1.27490400	1.30758600
H	-5.03160900	-1.49402000	0.54567600
H	-5.16318400	-0.65582200	2.11243200

M3

0 1

C	3.25970700	-0.76023500	-0.26388100
C	5.15816500	-1.81449100	-0.42033000
C	5.38110500	0.68917500	-0.10930200
H	5.18698800	1.30280200	-0.98775700
N	4.24816300	-2.74809900	-0.45316300
N	3.07506300	-2.08082400	-0.33932700
N	4.59022100	-0.57579600	-0.28743500
C	6.63920600	-2.00273200	-0.55066600
H	6.83503700	-2.66414300	-1.39641100
H	7.03553800	-2.47692200	0.35452900
C	6.86959200	0.27343200	0.04313100
O	7.25067400	-0.76783200	-0.82774200
C	6.06241400	0.96263300	2.16034400
C	5.10014200	1.34998000	1.22198000

C	4.10677700	2.26660700	1.55582000
C	4.05861400	2.75499600	2.86000800
C	4.99982000	2.34585900	3.80550500
C	6.01607800	1.45769100	3.45841400
C	7.07713900	0.03123900	1.55277000
H	3.39659800	2.62002600	0.81987300
H	4.95179900	2.73943400	4.81544900
H	6.76601700	1.16414300	4.18623100
H	6.86593900	-1.00447900	1.84185200
H	8.10283400	0.24934700	1.85650700
C	1.87359500	-2.85524500	-0.32887800
C	1.59215000	-3.65814700	0.77990900
C	1.05107900	-2.91714100	-1.45607600
C	0.49481100	-4.50746800	0.76998000
C	-0.05592400	-3.75341000	-1.47728400
C	-0.31377000	-4.54625500	-0.36177700
H	0.27495900	-5.12571900	1.63195000
H	-0.69541900	-3.79290900	-2.35088300
H	7.46052300	1.13932200	-0.26138400
H	3.29005800	3.47119500	3.13286800
Cl	2.59785600	-3.59004300	2.18295000
Cl	-1.66674300	-5.61760400	-0.38008700
Cl	1.40670900	-1.93164700	-2.83004500
C	2.23556800	0.36716400	-0.38553400
O	2.64932100	1.35129600	-0.95518800
H	1.99306200	3.19606900	-1.92237600
C	0.87174400	0.20109900	0.19698800
C	0.92450200	-0.08412400	1.71620800
H	0.34757100	-0.62027300	-0.30656700
H	0.31787100	1.12150800	-0.01572200
H	1.52919200	-0.97628400	1.91979600
H	1.41218700	0.75739800	2.22195500
C	-0.48224300	-0.28201700	2.22453500
C	-0.99414400	-1.56023800	2.44690800
C	-1.32434900	0.82028100	2.37077500
C	-2.33734600	-1.73460500	2.77219500
H	-0.33855500	-2.42342900	2.36259800
C	-2.66953900	0.64827500	2.67937000

H	-0.92527400	1.81761100	2.20037200
C	-3.18558900	-0.63345100	2.86066700
H	-2.72690600	-2.73375900	2.93953900
H	-3.32699800	1.50971300	2.74365600
H	-4.24475100	-0.77121600	3.05658500
C	-5.53093900	0.98441900	0.66502600
C	-4.45302600	1.68538400	0.15031500
C	-3.44737900	1.08677000	-0.62425900
C	-3.59638700	-0.27578600	-0.92039700
C	-4.65480500	-1.03944700	-0.45398100
C	-5.65584200	-0.44145200	0.41330700
H	-4.37723800	2.75328600	0.33860900
H	-2.81808400	-0.74917500	-1.51421100
C	-2.25721900	1.83813400	-1.05800400
C	-1.58403400	1.54855700	-2.25431000
C	-1.74728400	2.88108700	-0.27441000
C	-0.42715900	2.22256900	-2.65255100
H	-2.01642300	0.79674100	-2.90344700
C	-0.58304000	3.57768900	-0.60239400
H	-2.26923500	3.11664200	0.64501100
C	0.09297500	3.19751500	-1.77699600
O	-6.60147900	-1.13236800	0.92073800
O	1.28733200	3.83454200	-2.09750500
C	-4.78807600	-2.52170400	-0.82043200
C	-4.70101900	-3.39246600	0.44468600
C	-6.13963400	-2.76393800	-1.51585000
C	-3.68516300	-2.98408300	-1.77848200
H	-3.70341200	-3.30867000	0.89013800
H	-5.44677000	-3.05896800	1.16792200
H	-4.87459100	-4.44806000	0.19736100
H	-6.19345300	-2.19200100	-2.44901800
H	-6.25768500	-3.82721900	-1.76027400
H	-6.95099900	-2.44959400	-0.85903900
H	-3.83175800	-4.04206000	-2.02315100
H	-3.69160600	-2.41236800	-2.71324400
H	-2.69581700	-2.88023200	-1.31737600
C	-6.60014300	1.67997900	1.51558400
C	-7.98338200	1.50454400	0.86351900

C	-6.61922000	1.06819300	2.92811900
C	-6.34611600	3.18416500	1.66797500
H	-8.00452000	1.99747100	-0.11495300
H	-8.19595300	0.44338000	0.73126600
H	-8.76198800	1.95844500	1.48958200
H	-5.66556700	1.25507800	3.43762300
H	-7.41536100	1.52196700	3.53206000
H	-6.78282400	-0.00783900	2.86021300
H	-7.13996400	3.62631500	2.28009000
H	-5.38978400	3.38836500	2.16368500
H	-6.34384300	3.69654800	0.69982800
C	-0.05614200	4.70097600	0.30429100
C	0.06085600	6.01375100	-0.49105900
C	-0.99450600	4.97164900	1.48898300
C	1.31509300	4.31306000	0.88230800
H	0.75084400	5.91140000	-1.32828900
H	-0.91958900	6.30861100	-0.87824100
H	0.42029600	6.81429600	0.16526900
H	-1.07773000	4.10931700	2.15884500
H	-0.59607900	5.80618000	2.07400700
H	-1.99966600	5.24496900	1.15431400
H	1.66136200	5.07992000	1.58506600
H	1.24390600	3.36203600	1.42754000
H	2.06083400	4.21347700	0.09205500
C	0.17840600	1.99653000	-4.05180200
C	0.05794600	3.30537100	-4.85398900
C	1.65703900	1.56951900	-4.00587400
C	-0.57768900	0.90592700	-4.82385100
H	-0.99286600	3.59180600	-4.95933800
H	0.59397700	4.11600700	-4.35737500
H	0.47806800	3.16888900	-5.85701600
H	1.80433100	0.73818800	-3.31129100
H	1.97289000	1.23841000	-5.00104700
H	2.31695000	2.38803700	-3.71488500
H	-0.12624400	0.79117500	-5.81381100
H	-0.52637100	-0.06274100	-4.31527600
H	-1.63070000	1.16377600	-4.96622800

M03

1 1

C	-0.61626400	-0.29786800	0.19610300
C	-1.56206200	-1.07128100	1.99460300
C	-2.88731900	0.74946300	0.81968900
H	-2.51771100	1.74815000	1.06101900
N	-0.44461900	-1.73097300	1.89372900
N	0.13153900	-1.23350400	0.77055400
N	-1.71420000	-0.17997200	0.95316200
C	-2.59687000	-1.21944600	3.06931600
H	-2.09953600	-1.26274200	4.03935000
H	-3.14258700	-2.15891800	2.91976600
C	-3.96584500	0.24917000	1.81503300
O	-3.44872700	-0.10119700	3.07617500
C	-4.66421200	-0.28656000	-0.37148400
C	-3.60933800	0.62399600	-0.49915300
C	-3.40663500	1.32920700	-1.68036600
C	-4.24673900	1.07062900	-2.76069600
C	-5.27806300	0.13710000	-2.64741400
C	-5.50286000	-0.53962300	-1.44974700
C	-4.74414400	-0.82965300	1.03254600
H	-2.62120800	2.07308100	-1.77044300
H	-5.92638400	-0.04891200	-3.49737600
H	-6.32721700	-1.23925900	-1.35640800
H	-4.26247700	-1.81277000	1.09451800
H	-5.76557300	-0.93948700	1.40065200
C	1.37591900	-1.74537200	0.29841400
C	1.39794700	-2.71856400	-0.70315400
C	2.57028400	-1.29719400	0.86650200
C	2.60844100	-3.23234200	-1.14893500
C	3.78698700	-1.80357900	0.43602900
C	3.78494300	-2.76700500	-0.56968400
H	2.63063000	-3.98469600	-1.92790800
H	4.71418500	-1.45380700	0.87270800
H	-4.62886600	1.09748400	1.99793700
H	-4.10463400	1.60668000	-3.69257100
Cl	-0.08358800	-3.28998600	-1.37903700
Cl	5.29549100	-3.40605800	-1.11549700

Cl	2.52113300	-0.08611900	2.10037600
C	-0.22675800	0.40104700	-1.11357800
O	-0.78396200	0.03275500	-2.11243100
C	0.83819200	1.45550800	-1.02075900
C	0.53889400	2.53487000	0.03907900
H	0.93890100	1.89321300	-2.01656200
H	1.79084900	0.96521100	-0.77466000
H	-0.44786900	2.97217600	-0.14860800
H	0.52011300	2.08480800	1.03896600
C	1.57774600	3.63089100	-0.01985100
C	1.46370700	4.63315300	-0.98642300
C	2.67380100	3.64271900	0.84347300
C	2.42739900	5.63072100	-1.09009700
H	0.60825300	4.63316100	-1.65776100
C	3.64020700	4.64167700	0.74251100
H	2.76954800	2.87082800	1.60244600
C	3.51951500	5.63623000	-0.22439500
H	2.32370300	6.40576500	-1.84236300
H	4.48606900	4.64351500	1.42229300
H	4.27141700	6.41459900	-0.30175500

TS3N

0 1

C	-1.01834700	-0.17974600	-0.08939700
C	-2.87516200	-0.03453000	1.12947100
C	-3.22931000	-0.63601500	-1.27246500
H	-3.11724700	0.04318700	-2.11886300
N	-1.94346000	-0.04978900	2.01925700
N	-0.76102900	-0.11044200	1.28930500
N	-2.40663700	-0.11893400	-0.16073500
C	-4.34125600	0.14959900	1.39043500
H	-4.49199600	1.08882600	1.92537900
H	-4.72593400	-0.66336300	2.01684900
C	-4.69422600	-0.75290500	-0.76627400
O	-5.03761600	0.25502100	0.16712400
C	-3.80678500	-2.94946100	-1.05134100
C	-2.88866800	-2.06902200	-1.62819100
C	-1.84007100	-2.54256300	-2.41303000

C	-1.70757400	-3.91979400	-2.58541100
C	-2.61210400	-4.80302800	-1.99316200
C	-3.67427800	-4.32288200	-1.22914400
C	-4.86528100	-2.21001900	-0.27601200
H	-1.15930400	-1.84083600	-2.88362900
H	-2.49530400	-5.87229200	-2.14043200
H	-4.39073900	-5.00911800	-0.78714700
H	-4.68076600	-2.30646700	0.79941200
H	-5.87591400	-2.58144700	-0.46206700
C	0.36797500	-0.64909100	1.93948500
C	0.51150100	-2.02981800	2.11247400
C	1.39251500	0.18657400	2.38982100
C	1.63352900	-2.57301000	2.72341000
C	2.52817100	-0.32621100	3.00453200
C	2.62678300	-1.70352000	3.16207400
H	1.73388600	-3.64443200	2.84693900
H	3.31940600	0.33251200	3.33997300
H	-5.35082200	-0.58643700	-1.62308000
H	-0.89649100	-4.30875100	-3.19334000
C	-0.16719300	-0.09572300	-1.18351700
O	-0.65140400	0.25364100	-2.35092400
H	-0.80231800	1.71207100	-1.85829400
C	1.30895000	-0.35757900	-1.04513300
C	1.86939500	-1.11649600	-2.25677600
H	1.53915000	-0.93151100	-0.14508400
H	1.84603600	0.60168400	-0.94800500
H	1.35761100	-2.08473400	-2.32579200
H	1.63260400	-0.56325600	-3.16962200
C	3.35668400	-1.32080800	-2.12019900
C	3.85847600	-2.29027900	-1.24533200
C	4.26295700	-0.51201700	-2.80802400
C	5.22886900	-2.44816700	-1.06360100
H	3.16234000	-2.92572100	-0.70125800
C	5.63662400	-0.66604700	-2.63094600
H	3.88434800	0.24214400	-3.49357300
C	6.12354800	-1.63484000	-1.75733900
H	5.60025200	-3.20596900	-0.38051200
H	6.32623700	-0.03029000	-3.17783800

H	7.19298100	-1.75721200	-1.61819000
C	3.26345300	4.15335700	-1.61765100
C	2.44954300	4.60206200	-0.60973500
C	1.13080900	4.08989500	-0.46149700
C	0.71018000	3.06392900	-1.36316000
C	1.56397000	2.60749900	-2.39457300
C	2.81561000	3.16000000	-2.52399800
C	-1.43068700	3.13412500	-0.37223400
C	-0.93850200	4.12863600	0.53601000
C	-1.84905700	4.66044200	1.49204400
H	-1.46364400	5.39480400	2.19054300
C	-3.16263800	4.27024800	1.49881400
C	-3.64825200	3.34281900	0.54259300
C	-2.79763600	2.77865000	-0.37844200
H	4.25900300	4.56850300	-1.73309400
H	2.76717100	5.37104500	0.08594300
H	1.19000600	1.84388100	-3.07041700
H	3.46623500	2.83773100	-3.32950600
H	-3.84914000	4.69412300	2.22410300
H	-4.70164800	3.08264900	0.52059200
H	-3.16393500	2.09222200	-1.13246600
N	0.33469800	4.55855200	0.51737600
N	-0.53692700	2.53911000	-1.20547900
Cl	-0.71679800	-3.08585000	1.49086200
Cl	4.04610900	-2.36490300	3.91829200
Cl	1.26118800	1.89205300	2.11363000

M3N

0 1

C	-1.05442800	-0.27021300	0.05370300
C	-2.68793900	-0.52046700	1.49888900
C	-3.43241000	0.38360000	-0.68143100
H	-2.96740800	1.05176800	-1.40642800
N	-1.65249900	-1.00320900	2.11041900
N	-0.63508300	-0.85277700	1.20045400
N	-2.38089400	-0.06813600	0.24245600
C	-4.07932600	-0.28806900	1.98826100
H	-4.09946300	-0.27818700	3.07754600

H	-4.75871600	-1.06865600	1.61935300
C	-4.59410500	1.09162100	0.11703900
O	-4.44878100	0.99734600	1.52606300
C	-5.47529500	-0.76571400	-1.17729500
C	-4.09642700	-0.79158000	-1.36354000
C	-3.47739900	-1.79664000	-2.10156100
C	-4.27342600	-2.80253300	-2.64178900
C	-5.65819800	-2.79011900	-2.45063400
C	-6.26886400	-1.77166800	-1.72334900
C	-5.90458600	0.44044800	-0.38366900
H	-2.40309100	-1.77973200	-2.25996900
H	-6.26481100	-3.58197100	-2.87815500
H	-7.34543900	-1.76255800	-1.58298600
H	-6.54742700	0.19420100	0.46743700
H	-6.46094000	1.14321500	-1.01114400
C	0.55874100	-1.59895800	1.38923600
C	0.76378100	-2.78355900	0.67399500
C	1.52638400	-1.17513700	2.30313800
C	1.94016200	-3.50479700	0.81209800
C	2.71164500	-1.88534300	2.45644000
C	2.90636200	-3.03042400	1.69557200
H	2.09677700	-4.41683500	0.24869500
H	3.47037900	-1.53636400	3.14575100
H	-4.57453100	2.16380700	-0.08054900
H	-3.81686700	-3.59887800	-3.22018200
C	-0.29664700	0.05497900	-1.17078400
O	-0.93540400	0.22934600	-2.21296400
H	-1.48281900	2.45049400	-0.49986200
C	1.20217700	0.09803200	-1.14228900
C	1.84298000	-0.90022500	-2.12298800
H	1.61191600	-0.01164100	-0.13600300
H	1.47132900	1.10827500	-1.48163200
H	1.60826200	-1.93121600	-1.83780000
H	1.40187400	-0.72698400	-3.11012500
C	3.33848000	-0.70663700	-2.16216500
C	4.20234300	-1.65233200	-1.60854200
C	3.87872700	0.46238600	-2.70806800
C	5.58002300	-1.44144400	-1.60165000

H	3.79138400	-2.56450300	-1.18151800
C	5.25286300	0.67715800	-2.70156700
H	3.21344100	1.21210700	-3.13268800
C	6.10834000	-0.27525400	-2.14789000
H	6.23829000	-2.18787900	-1.16769300
H	5.65694700	1.59136800	-3.12558700
H	7.18041600	-0.10658800	-2.14111800
C	2.28435900	3.91312100	-2.91494500
C	2.58840300	3.87621300	-1.56314400
C	1.63488800	3.48206200	-0.59352100
C	0.36650700	3.06235500	-1.10163800
C	0.05874600	3.11989700	-2.45973200
C	1.01286800	3.55419400	-3.37660900
C	-0.34874300	2.76037000	1.18261600
C	0.92613400	3.24862800	1.58825000
C	1.09432100	3.46632200	2.97672800
H	2.05864200	3.84387700	3.30227800
C	0.08029200	3.21186700	3.88699600
C	-1.16565500	2.74252200	3.45483300
C	-1.37357700	2.52985200	2.09409400
H	3.04289700	4.23709500	-3.62224600
H	3.56719100	4.17275400	-1.19972000
H	-0.92389200	2.79482600	-2.79102500
H	0.77073700	3.60314000	-4.43217300
H	0.25331000	3.39133600	4.94419100
H	-1.96822700	2.56314300	4.16183600
H	-2.34718400	2.19638800	1.73924600
N	1.94008300	3.52186700	0.72624900
N	-0.51636500	2.46137100	-0.18730100
Cl	-0.46913600	-3.36949000	-0.39587800
Cl	4.40008600	-3.90031600	1.84269000
Cl	1.26192100	0.27332200	3.18866000

E-TS4a

0 1

C	3.56829300	0.69715800	0.27338200
C	5.59950400	0.93794900	1.03526000
C	4.69640500	-1.34667700	1.33518200

H	3.69160700	-1.71343800	1.53948100
N	5.30262000	2.09824300	0.52585200
N	4.03823800	1.93051900	0.05224000
N	4.56269700	0.05566900	0.90073100
C	6.78900700	0.48150100	1.81526300
H	7.35480500	1.33866700	2.17839100
H	7.44048900	-0.14818000	1.19468900
C	5.61445100	-1.43593200	2.61160000
O	6.26962300	-0.21624400	2.92909100
C	6.47739500	-2.86326100	0.84565100
C	5.40660400	-2.17170800	0.28494800
C	5.09592200	-2.28529800	-1.06863100
C	5.88321600	-3.11766100	-1.85967100
C	6.95697600	-3.81738100	-1.30278700
C	7.26112400	-3.69594800	0.05051300
C	6.60590500	-2.58552800	2.32087900
H	4.25938100	-1.74070200	-1.49730900
H	7.56171000	-4.46101800	-1.93314700
H	8.09810700	-4.23824900	0.47959000
H	7.61671600	-2.29087700	2.61955400
H	6.34136300	-3.46958500	2.90878000
C	3.39855200	2.99687100	-0.64020400
C	3.30499700	2.96787100	-2.03296900
C	2.81860300	4.04416400	0.07656000
C	2.62427000	3.96830100	-2.71253000
C	2.13457200	5.05441500	-0.58711600
C	2.04347500	4.99611100	-1.97461100
H	2.54052200	3.93993500	-3.79199600
H	1.67591500	5.86438800	-0.03284400
H	4.99937300	-1.64417000	3.48693300
H	5.65884600	-3.22415000	-2.91586900
Cl	3.98704300	1.64258000	-2.90932800
Cl	1.16999900	6.23371900	-2.80965000
Cl	2.89605300	4.04621100	1.80160800
C	2.25399600	0.04865400	-0.15019500
O	2.31138100	-1.17735600	-0.23851900
H	2.22107900	-3.17442100	-0.66994700
C	1.10102300	0.87709600	-0.32167200

C	-0.04870700	0.23316000	-1.09116700
H	1.32036500	1.89575900	-0.63689600
H	0.58599700	1.07241600	0.85127600
H	0.30737300	-0.11754200	-2.06889100
H	-0.39401700	-0.66041500	-0.56087200
C	-1.18970000	1.20157800	-1.29199300
C	-1.01677200	2.34978300	-2.07393000
C	-2.43167900	0.97635600	-0.69879900
C	-2.06042700	3.25307400	-2.25522100
H	-0.05469000	2.53150400	-2.55201800
C	-3.48447800	1.87193500	-0.88316100
H	-2.59012200	0.07856700	-0.10580900
C	-3.30004600	3.01602200	-1.65761900
H	-1.91111700	4.13726300	-2.86785000
H	-4.44902200	1.65593700	-0.43006100
H	-4.11962700	3.71271600	-1.80648200
C	-5.63418900	-1.08641700	-1.45813300
C	-4.37575200	-1.65976000	-1.50853600
C	-3.68849200	-2.14937900	-0.38381400
C	-4.35838200	-2.02262000	0.84653600
C	-5.62742300	-1.47497000	0.97937200
C	-6.33825100	-0.98490100	-0.19105700
H	-3.88971600	-1.71687400	-2.47480700
H	-3.86682600	-2.37479900	1.74815700
C	-2.30975300	-2.68583300	-0.48662800
C	-1.60535400	-3.13582200	0.64144600
C	-1.62470500	-2.75227500	-1.71151700
C	-0.28212300	-3.57874600	0.59309000
H	-2.10948900	-3.13151500	1.59804000
C	-0.30325000	-3.18794300	-1.82829800
H	-2.13703900	-2.43080800	-2.60655300
C	0.36529600	-3.57164900	-0.65356500
O	-7.51158900	-0.49608800	-0.10927600
O	1.68995000	-3.98376300	-0.73013800
C	-6.33405400	-1.41454700	2.34031700
C	-6.69860500	0.04046900	2.68669100
C	-7.62383400	-2.25539700	2.28702600
C	-5.47537100	-1.96838500	3.48364900

H	-5.79241000	0.65201900	2.76988200
H	-7.33236600	0.45596100	1.90340000
H	-7.22550700	0.08445800	3.64814900
H	-7.38269500	-3.30710900	2.09682100
H	-8.15670300	-2.19592400	3.24434800
H	-8.26951900	-1.88852900	1.48875700
H	-6.03712400	-1.90482600	4.42187800
H	-5.21125400	-3.01904900	3.32217400
H	-4.54614400	-1.40140500	3.61483600
C	-6.32102700	-0.57078100	-2.72888900
C	-7.61126100	-1.37204300	-2.97595100
C	-6.67010300	0.92110100	-2.57742300
C	-5.43528400	-0.70546200	-3.97275300
H	-7.37655200	-2.42953100	-3.14100100
H	-8.26701900	-1.28534400	-2.10945100
H	-8.13108200	-0.99561200	-3.86598500
H	-5.75409800	1.51916900	-2.51519300
H	-7.23990900	1.26619600	-3.44949700
H	-7.26224800	1.07326500	-1.67477400
H	-5.96664600	-0.30073400	-4.84121700
H	-4.49859400	-0.14703000	-3.85954100
H	-5.18824400	-1.75044300	-4.18966100
C	0.37889500	-3.30003900	-3.20493900
C	0.60464100	-4.79021200	-3.51713500
C	-0.49867800	-2.70908100	-4.31781000
C	1.73798600	-2.56913900	-3.26551100
H	1.23910400	-5.24950200	-2.75600200
H	-0.35032900	-5.32378000	-3.54815600
H	1.09136200	-4.90114400	-4.49311500
H	-0.69755500	-1.64401900	-4.15346300
H	0.01878800	-2.81289400	-5.27621800
H	-1.45757500	-3.22823800	-4.40291400
H	2.04400200	-2.45997400	-4.31168400
H	1.67902000	-1.57040100	-2.82181800
H	2.52085900	-3.12827700	-2.75081300
C	0.42392900	-4.10151600	1.85627100
C	0.75594900	-5.59287500	1.67183600
C	1.72098800	-3.32067800	2.14226300

C	-0.46183100	-3.97240700	3.10304400
H	-0.16160800	-6.17142300	1.52574900
H	1.40560200	-5.74202700	0.80812100
H	1.26311300	-5.97705900	2.56448500
H	1.53213300	-2.24149000	2.11447200
H	2.10017500	-3.58160100	3.13713900
H	2.49498900	-3.55896100	1.41097800
H	0.07780100	-4.36977500	3.96814700
H	-0.71331100	-2.92725300	3.31626300
H	-1.39342300	-4.53698000	3.00417100
C	-2.03335600	5.27065000	2.64930000
C	-0.70342300	4.59081200	2.32274900
C	-0.81594500	3.44516400	1.30182500
C	-3.08906700	4.34760500	3.25680700
C	-1.23437000	2.13529600	1.92083600
C	-3.43612000	3.15280400	2.36593700
H	-2.43932600	5.70096000	1.72392100
H	-0.01978900	5.34381500	1.91601700
H	-1.51494900	3.70810400	0.49700800
H	-2.75725500	3.97086500	4.23213300
H	-4.39908500	2.73158700	2.66315000
C	-0.71834700	-0.13250800	2.47466400
H	0.19033000	-0.60314000	2.86649700
C	-2.94389000	0.79587600	3.03257500
C	-1.77321500	-0.01372000	3.56504500
H	-1.34783300	0.48739600	4.44098800
H	-2.12132500	-1.00343100	3.87654400
H	-3.64169100	1.03737200	3.84056100
N	-2.46971000	2.05520400	2.45494400
N	-0.35605700	1.17071900	1.93349900
H	-3.54592700	3.46847600	1.32148300
H	-4.00419400	4.92354000	3.42965000
H	-1.85016800	6.10855000	3.32996700
H	-0.23352500	4.20968100	3.23839200
H	0.15447400	3.27017000	0.83305400
H	-1.09022800	-0.78052000	1.66673500
H	-3.49684600	0.22822100	2.26855900

Z-TS4a

0 1

C	1.61812600	1.85045400	-0.71571600
C	1.84107700	3.91616700	-1.38325900
C	3.28330500	3.29202700	0.59834000
H	2.71202100	3.23663700	1.52575300
N	0.90394300	3.42122300	-2.13592400
N	0.77931100	2.13163900	-1.71691900
N	2.31188100	2.98029600	-0.49605200
C	2.35385900	5.32255300	-1.40005500
H	1.51608100	6.00092700	-1.56644800
H	3.07038700	5.45184400	-2.21984600
C	3.86588100	4.70153700	0.30800100
O	2.91466600	5.63450700	-0.14777600
C	5.56321700	3.11586300	-0.07953800
C	4.53142500	2.43898800	0.58652300
C	4.76765500	1.22553600	1.22505900
C	6.05234800	0.68521800	1.17058100
C	7.07663000	1.35081300	0.49862100
C	6.83945000	2.57213300	-0.13373600
C	5.08920400	4.44915400	-0.59611800
H	3.97660400	0.71471800	1.76394600
H	8.07478000	0.92384200	0.48152500
H	7.64451100	3.10084000	-0.63442500
H	4.80942400	4.37581900	-1.65396300
H	5.83265300	5.24309400	-0.50541100
C	-0.36719300	1.40407000	-2.16429100
C	-0.44618600	0.92237500	-3.47116400
C	-1.47331500	1.28599500	-1.31869600
C	-1.59231000	0.28139700	-3.91548500
C	-2.63122700	0.64922700	-1.74218100
C	-2.66936800	0.15644300	-3.04132100
H	-1.64373500	-0.11259200	-4.92293500
H	-3.48081600	0.53504900	-1.06976900
H	4.21557100	5.08867100	1.26740300
H	6.25428100	-0.25912100	1.66506200
Cl	0.90485700	1.09438600	-4.54342700
Cl	-4.10506300	-0.64125700	-3.58089700

Cl	-1.38729700	1.89305800	0.29454400
C	1.70771900	0.63247300	0.21111300
O	1.68565600	0.96231600	1.39837200
H	1.40718000	0.19960900	3.22481000
C	1.96622600	-0.67671400	-0.29923800
C	1.56304300	-1.16381100	-1.67798800
H	1.75399300	-1.39449400	0.49318800
H	3.26603400	-0.80118600	-0.37254500
H	1.63180500	-0.34537300	-2.40600100
H	2.32638300	-1.88129500	-2.00819500
C	0.21603400	-1.85568100	-1.77891800
C	-0.74475300	-1.79386600	-0.76936600
C	-0.07098100	-2.59633300	-2.93344900
C	-1.96868800	-2.45341100	-0.91140300
H	-0.56014000	-1.21961700	0.13837400
C	-1.28415900	-3.25894600	-3.07532900
H	0.67211400	-2.65062000	-3.72683500
C	-2.23790600	-3.19073400	-2.05871000
H	-2.72430800	-2.35302100	-0.13702600
H	-1.48908500	-3.82766100	-3.97715600
H	-3.18975200	-3.70181700	-2.16644300
C	-5.86263000	-1.49270500	0.23619000
C	-4.81305900	-1.46939000	1.13949400
C	-4.17795800	-0.28950300	1.56565900
C	-4.68892600	0.91332200	1.04867500
C	-5.74058200	0.97444900	0.14510900
C	-6.38891200	-0.24737500	-0.30286700
H	-4.46446900	-2.41269400	1.54944100
H	-4.20018600	1.83810600	1.33576900
C	-2.95951900	-0.30607500	2.40031100
C	-2.49073600	0.84908100	3.04343300
C	-2.17333500	-1.45807000	2.53569400
C	-1.21964200	0.93739500	3.61141400
H	-3.13558700	1.71810500	3.05826800
C	-0.91418400	-1.45236400	3.13902600
H	-2.54451300	-2.38817000	2.12547900
C	-0.40637900	-0.21274700	3.57164000
O	-7.36112700	-0.22855700	-1.12403900

O	0.91617200	-0.13428300	3.99480900
C	-6.23059800	2.31698000	-0.41157100
C	-6.11163600	2.32722200	-1.94651800
C	-7.70105400	2.53482100	-0.01255300
C	-5.41738200	3.50370900	0.11799600
H	-5.05995900	2.23685800	-2.24728700
H	-6.67410600	1.49435000	-2.36877000
H	-6.49575000	3.27190800	-2.35158600
H	-7.79090900	2.60737500	1.07716400
H	-8.08248400	3.46729800	-0.44737700
H	-8.30561800	1.69764400	-0.36374400
H	-5.80826200	4.43248000	-0.31180900
H	-5.47722400	3.58753500	1.20859200
H	-4.35949300	3.42390900	-0.16072000
C	-6.49897900	-2.81616800	-0.20449200
C	-7.98182300	-2.84592500	0.20557900
C	-6.38670800	-2.96330800	-1.73256600
C	-5.81454200	-4.03654300	0.42317100
H	-8.07491700	-2.79598200	1.29614600
H	-8.50125200	-1.99423700	-0.23392500
H	-8.45397800	-3.77605400	-0.13484500
H	-5.33161400	-2.97744900	-2.03039100
H	-6.84999800	-3.90231600	-2.06070900
H	-6.87602100	-2.12246900	-2.22481800
H	-6.29608400	-4.94974500	0.05716500
H	-4.75178600	-4.08886400	0.15561600
H	-5.89150800	-4.03353000	1.51581100
C	-0.14563600	-2.76666200	3.36889200
C	0.17822100	-2.89659100	4.86883000
C	-0.98180200	-3.99150900	2.97060600
C	1.15206200	-2.82996000	2.54876000
H	0.82378600	-2.08475500	5.20570400
H	-0.74471500	-2.87715400	5.45680700
H	0.68266900	-3.85067200	5.05945500
H	-1.20414800	-4.00077600	1.89809800
H	-0.41655600	-4.90007000	3.20127800
H	-1.92641000	-4.03228800	3.52125200
H	1.72043100	-3.72964400	2.81516700

H	0.91547400	-2.89345600	1.48060500
H	1.78603600	-1.95825100	2.72853400
C	-0.75016800	2.23527400	4.29541600
C	-0.41280500	1.93914700	5.76779200
C	0.48208700	2.84399400	3.60044700
C	-1.84555100	3.31080500	4.27974700
H	-1.29844900	1.56699400	6.29258600
H	0.37913000	1.19310900	5.84464500
H	-0.08167600	2.85680400	6.26743400
H	0.29540200	2.99542300	2.53141100
H	0.70708600	3.81750600	4.05110700
H	1.36499400	2.21262300	3.70482900
H	-1.48318700	4.19721800	4.80945100
H	-2.10583000	3.61388900	3.25954400
H	-2.75643200	2.97030800	4.78087300
C	5.99360900	-5.01092400	1.29251000
C	5.24913000	-3.71327400	1.60595200
C	4.24427800	-3.27387100	0.52510700
C	6.87063700	-4.95590000	0.04270900
C	4.88661600	-2.52467800	-0.61773900
C	6.08896900	-4.59588200	-1.22127800
H	5.25567400	-5.81468800	1.16800600
H	4.69551100	-3.84454100	2.54071200
H	3.69280400	-4.14309200	0.14555100
H	7.68107500	-4.22762300	0.17127900
H	6.65543600	-4.88225400	-2.11010700
C	5.12687800	-0.50612600	-1.86958900
H	5.08600200	0.55143600	-1.58295800
C	6.58162200	-2.44689800	-2.38568700
C	6.56161000	-0.95031400	-2.11935900
H	7.15879500	-0.72825100	-1.22971500
H	7.00006200	-0.41618200	-2.96543600
H	7.60810100	-2.82576500	-2.36011700
N	5.81631400	-3.16241900	-1.36109100
N	4.53573800	-1.28313300	-0.79132000
H	5.14808400	-5.15637400	-1.25881000
H	7.33856400	-5.93420900	-0.10785300
H	6.60969100	-5.28528800	2.15459200

H	5.96669500	-2.90100500	1.77835500
H	3.51247100	-2.59751100	0.96799700
H	4.52864200	-0.62473800	-2.78515600
H	6.16710700	-2.67349500	-3.37645500

E-TS4b

1 1

C	1.77882100	0.16189000	0.13632700
C	3.28539700	0.25423300	1.71376800
C	3.70895000	-1.53267900	0.05733800
H	3.05102500	-2.16191900	-0.54017800
N	2.48244300	1.24488400	1.97219800
N	1.55326000	1.17563000	0.98030300
N	2.88772000	-0.43135900	0.59678200
C	4.43643200	-0.30268800	2.48626800
H	4.41158700	0.05933000	3.51332100
H	5.39124300	-0.01925600	2.02369800
C	4.38163100	-2.33257600	1.23672400
O	4.23844400	-1.70229300	2.50055100
C	6.07426600	-1.51569100	-0.29829500
C	4.86802600	-0.98053200	-0.74258800
C	4.81720900	-0.06063100	-1.78575800
C	6.01440900	0.32635200	-2.38112300
C	7.22983100	-0.20447200	-1.94027000
C	7.26908200	-1.12994000	-0.90054500
C	5.86156200	-2.49774700	0.82433600
H	3.86569700	0.33292900	-2.12991400
H	8.15410400	0.10942300	-2.41444700
H	8.21551800	-1.53870400	-0.56033300
H	6.51037600	-2.32000700	1.68746900
H	6.04738200	-3.52200000	0.48658700
C	0.53522900	2.16653300	0.89476700
C	0.62518500	3.17693000	-0.06436800
C	-0.57706300	2.09944900	1.73551400
C	-0.39596400	4.10681400	-0.20384100
C	-1.60871300	3.02038800	1.60932000
C	-1.50301600	4.00770100	0.63379400
H	-0.32976700	4.88613500	-0.95318500

H	-2.47697500	2.96559000	2.25467700
H	3.88396200	-3.29401400	1.35990800
H	6.00405800	1.04255700	-3.19587800
Cl	1.99251400	3.24050300	-1.11879500
Cl	-2.79477200	5.14485500	0.45129600
Cl	-0.69168900	0.82954500	2.90039900
C	1.03314800	-0.25601000	-1.13047700
O	1.71680800	-0.88277300	-1.93563500
C	-0.37196400	0.00283600	-1.19888100
C	-0.99951300	-0.13945200	-2.58300600
H	-0.71088100	0.88215400	-0.65503700
H	-0.92241800	-0.98278100	-0.50838300
H	-0.54402800	0.57898900	-3.27687400
H	-0.77961700	-1.13584700	-2.98004300
C	-2.49429600	0.07899800	-2.53192300
C	-3.01220000	1.34168400	-2.22261600
C	-3.38754100	-0.96816800	-2.76452900
C	-4.38602100	1.55171800	-2.14556400
H	-2.32743100	2.16957800	-2.04571300
C	-4.76470500	-0.76429000	-2.69174700
H	-2.99923200	-1.95584500	-3.00403000
C	-5.26853000	0.49685500	-2.37990200
H	-4.76962700	2.53923100	-1.90819900
H	-5.44320400	-1.59080500	-2.88250000
H	-6.34021900	0.65950500	-2.32603300
C	-5.33755100	-1.19990800	2.32267500
C	-3.88894500	-0.72983100	2.17589800
C	-3.39375800	-0.63155300	0.72131800
C	-5.61855600	-2.59726400	1.77228900
C	-2.93012800	-1.95801700	0.17427900
C	-5.26712200	-2.73353900	0.29041600
H	-5.98904100	-0.48452600	1.80262300
H	-3.80017100	0.26218400	2.63024900
H	-4.17439800	-0.21639200	0.07162000
H	-5.06133100	-3.35550800	2.33667300
H	-5.77881900	-3.59474000	-0.14568400
C	-1.18176500	-3.34754500	-0.65579700
H	-0.11043100	-3.42676400	-0.44769800

C	-3.43502300	-4.30914900	-0.31240200
C	-1.95051800	-4.51724100	-0.05658100
H	-1.76300000	-4.55713400	1.02117900
H	-1.63015400	-5.46594500	-0.49255700
H	-4.02912500	-5.00144900	0.29226300
N	-3.83811100	-2.94537500	0.04442500
N	-1.66206300	-2.08913300	-0.10191400
H	-5.60643100	-1.85275800	-0.26712500
H	-6.68260500	-2.82198400	1.89879900
H	-5.61770000	-1.16465900	3.38032600
H	-3.21585200	-1.38895700	2.73900800
H	-2.54042700	0.04801000	0.66184900
H	-1.29900000	-3.34632600	-1.74985400
H	-3.67843100	-4.49339400	-1.36665300

Z-TS4b

1 1

C	-1.69136500	-1.21510400	-0.53627800
C	-2.76587600	-2.76410400	0.56992900
C	-0.95882900	-3.63940000	-0.96495300
H	-1.25990400	-3.62845100	-2.01181400
N	-3.35793300	-1.65318100	0.89530600
N	-2.67656800	-0.69907800	0.20440000
N	-1.73495600	-2.54052500	-0.30744100
C	-3.13708300	-4.14073300	1.02745000
H	-4.22435300	-4.21835900	1.06462100
H	-2.74479200	-4.31580000	2.03627900
C	-1.30709800	-4.95887700	-0.22679700
O	-2.67147200	-5.09010200	0.10059000
C	0.90223900	-4.35679600	0.34077500
C	0.53162800	-3.54587900	-0.74128600
C	1.48647600	-2.86304300	-1.48793900
C	2.82441800	-2.97632200	-1.11188100
C	3.19491100	-3.76481300	-0.02372700
C	2.23611700	-4.46601600	0.70979100
C	-0.29621100	-5.05059800	0.93443400
H	1.20024700	-2.26132100	-2.34392000
H	4.24316000	-3.84818300	0.24650000

H	2.53012400	-5.09821100	1.54179200
H	-0.64442600	-4.51703000	1.82721500
H	-0.10383900	-6.08520200	1.22445200
C	-3.17880600	0.63341400	0.23771900
C	-3.04983800	1.39533500	1.40096100
C	-3.83541300	1.16821300	-0.87207900
C	-3.54289700	2.68961800	1.45490800
C	-4.32921900	2.46642900	-0.83796100
C	-4.17334800	3.20853400	0.32738600
H	-3.42946800	3.28297900	2.35383600
H	-4.83035100	2.88388000	-1.70268500
H	-1.10107000	-5.76447200	-0.93480200
H	3.58393000	-2.45017600	-1.68003900
Cl	-2.20737700	0.74650000	2.76554300
Cl	-4.78100900	4.82802800	0.38085100
Cl	-4.02792200	0.22215400	-2.30637500
C	-0.83207900	-0.59269300	-1.65395100
O	-0.86822700	-1.28450100	-2.66778900
C	0.00700300	0.54689200	-1.41986600
C	-0.37930200	1.68574600	-0.47114900
H	0.38051900	0.89915500	-2.38503900
H	1.09456300	0.06714800	-0.79869100
H	-1.29489500	2.18762600	-0.80873500
H	-0.57454000	1.28475200	0.53026400
C	0.70331800	2.73780700	-0.35816200
C	1.02745100	3.53992800	-1.45685100
C	1.37903400	2.94864900	0.84495200
C	2.01077800	4.52082300	-1.35730600
H	0.50066400	3.39826900	-2.39768300
C	2.36694500	3.92517900	0.94992300
H	1.12638000	2.34013800	1.71142000
C	2.68790300	4.71407000	-0.15361800
H	2.24817000	5.13633000	-2.21910500
H	2.88173500	4.07197700	1.89518500
H	3.45326500	5.47936200	-0.07326500
C	6.18497500	1.33043300	-1.26152600
C	4.94416700	0.63108100	-1.81714100
C	3.60928300	1.18959400	-1.28942700

C	6.35419400	1.22149800	0.25305800
C	3.21735800	0.61418800	0.04682900
C	5.16003900	1.77401000	1.03100200
H	6.13498500	2.39391000	-1.53153600
H	4.94476600	0.73513100	-2.90612800
H	3.65087500	2.28381900	-1.21901200
H	6.51438200	0.17776400	0.55104700
H	5.44687300	1.97899000	2.06491000
C	1.71844800	-0.73858200	1.33774600
H	1.21443000	-1.67996400	1.08706800
C	3.70168200	0.29011400	2.41551600
C	2.90553000	-0.99505100	2.25596900
H	3.54385700	-1.76283600	1.80835200
H	2.57386200	-1.35491200	3.23263000
H	4.64274500	0.09537300	2.93709000
N	4.02325800	0.85097800	1.10304400
N	2.14065200	-0.11669000	0.09314100
H	4.83196200	2.72932700	0.60312200
H	7.24691900	1.78090000	0.55138200
H	7.07467600	0.92532000	-1.75423200
H	4.99461700	-0.44436600	-1.60549700
H	2.80338100	0.94464700	-1.98358100
H	0.98112600	-0.09593600	1.84489800
H	3.13989900	1.02984700	3.00314800

IM3

0 1

C	2.45448400	-0.14627300	-0.48207300
C	1.48324100	-1.34370400	-2.01347200
C	0.19872800	0.66574200	-1.34948500
H	0.12858300	1.19164500	-0.39703200
N	2.61651200	-1.94925000	-1.80170500
N	3.21594900	-1.18400800	-0.84196200
N	1.35975800	-0.22564500	-1.23366200
C	0.29277000	-1.71350700	-2.84000100
H	0.33817000	-2.76643600	-3.11672500
H	0.25458700	-1.09907600	-3.74980100
C	-1.10106500	-0.17063700	-1.63341200

O	-0.83484900	-1.52014300	-2.01301900
C	-0.81841500	1.54459900	-3.32674000
C	0.33553800	1.58072200	-2.54621700
C	1.41467400	2.39476400	-2.87762200
C	1.32535400	3.17406600	-4.02820300
C	0.17407000	3.14055400	-4.81907400
C	-0.90567500	2.33092000	-4.47255100
C	-1.84499800	0.61217300	-2.73647100
H	2.29641600	2.42630500	-2.24457500
H	0.12080000	3.75367100	-5.71305000
H	-1.79972500	2.31092400	-5.08829400
H	-2.28047100	-0.07933200	-3.46410400
H	-2.66951600	1.17594900	-2.28600500
C	4.60259400	-1.35820100	-0.55789000
C	5.53711800	-0.53114000	-1.19042300
C	5.04374000	-2.37546800	0.28903700
C	6.89583400	-0.70853700	-0.97809100
C	6.40011300	-2.56243700	0.51886400
C	7.30543600	-1.72669700	-0.12488000
H	7.61609500	-0.06524000	-1.46703500
H	6.73899700	-3.34889400	1.18174300
H	-1.69245300	-0.25724900	-0.72267300
H	2.15417600	3.81487500	-4.31031200
Cl	5.00196900	0.70189500	-2.28011800
Cl	9.00072400	-1.96309200	0.13934600
Cl	3.89269400	-3.39666400	1.06965000
C	2.85935900	0.95901800	0.47737400
O	2.80158600	2.08692000	0.04674700
H	-9.13392300	-1.57875800	-0.82886000
C	3.32492200	0.55980600	1.84393700
C	4.22901900	1.62051200	2.47651400
H	3.81307500	-0.42059400	1.81157600
H	2.38165600	0.43815700	2.39825300
H	3.75175600	2.59773900	2.35995200
H	4.29352800	1.41486600	3.54822100
C	5.61851900	1.63973800	1.88167300
C	5.93217400	2.45427000	0.78886600
C	6.62390400	0.83369300	2.42609700

C	7.22442100	2.47443300	0.26597400
H	5.16001300	3.08513600	0.35706900
C	7.91824700	0.86182000	1.91532000
H	6.39182000	0.19830000	3.27781800
C	8.22327900	1.68562000	0.83304100
H	7.45284300	3.11795900	-0.57839300
H	8.69053600	0.24497300	2.36437200
H	9.23337500	1.71151900	0.43532300
C	-1.72201700	1.57320200	1.49121600
C	-3.05845400	1.34250300	1.17554300
C	-3.61594800	0.06061500	1.11497100
C	-2.79201800	-1.01129100	1.47836400
C	-1.44265700	-0.85758500	1.77780000
C	-0.83420800	0.44709300	1.66633000
H	-3.70685800	2.18503000	0.95417800
H	-3.24569000	-1.99556600	1.53805000
C	-5.02761900	-0.15838400	0.72599800
C	-5.39695200	-1.28403800	-0.01259200
C	-6.03555000	0.74233900	1.08139600
C	-6.71652500	-1.53994300	-0.39106000
H	-4.61150300	-1.96736000	-0.31349000
C	-7.37155100	0.55925100	0.72793500
H	-5.75587500	1.60248200	1.67775100
C	-7.69413800	-0.59853300	-0.01031600
O	0.45304400	0.60379000	1.70376800
O	-9.01740000	-0.75967500	-0.34118800
C	-0.60274700	-2.06091500	2.22430400
C	0.49864600	-2.36961600	1.19772900
C	0.04553900	-1.75793500	3.58626500
C	-1.44630400	-3.33238000	2.38495900
H	0.07057200	-2.45945100	0.19196200
H	1.23606600	-1.56560700	1.20811600
H	0.99609200	-3.31378900	1.44757600
H	-0.72307400	-1.64685800	4.35824400
H	0.71031200	-2.57852700	3.88273100
H	0.62251000	-0.83318400	3.53066600
H	-0.81043200	-4.14042300	2.76165400
H	-2.26428800	-3.18823100	3.09783100

H	-1.87395100	-3.66184600	1.43190000
C	-1.20876300	3.00858900	1.70131600
C	-0.53719000	3.09719700	3.08425800
C	-0.19406300	3.43760700	0.62943500
C	-2.35038100	4.03438100	1.67973500
H	-1.26425000	2.88185000	3.87459600
H	0.28143300	2.37872000	3.15203100
H	-0.14330700	4.10735700	3.24853200
H	-0.62278800	3.34540800	-0.37669800
H	0.08514400	4.48798400	0.77612900
H	0.71030400	2.83272600	0.69213700
H	-1.94803800	5.02303800	1.92393900
H	-2.82068900	4.10576100	0.69309400
H	-3.12636500	3.79427600	2.41390400
C	-8.44991600	1.57371100	1.14336100
C	-9.50160500	0.90152800	2.04517500
C	-7.85070800	2.73970400	1.94138700
C	-9.12560500	2.17610600	-0.10226800
H	-10.02084000	0.09458600	1.52892400
H	-9.02568600	0.49295400	2.94253000
H	-10.24186800	1.64408000	2.36345300
H	-7.10517600	3.29209600	1.36056100
H	-8.65163200	3.43668700	2.20616000
H	-7.38350600	2.39902400	2.87055600
H	-9.87358200	2.91479700	0.20714300
H	-8.38409900	2.68621300	-0.72589200
H	-9.61999300	1.41257700	-0.70244500
C	-7.07376500	-2.79878000	-1.20363600
C	-8.03731600	-3.70618100	-0.40693700
C	-7.65983300	-2.41572500	-2.58034900
C	-5.83378900	-3.65621700	-1.49716800
H	-7.54522700	-4.04847900	0.50800100
H	-8.97055400	-3.22748600	-0.09725900
H	-8.30085400	-4.58509300	-1.00388300
H	-6.91324700	-1.85749700	-3.15269500
H	-7.91520100	-3.32056200	-3.14097300
H	-8.55522100	-1.78995700	-2.54084700
H	-6.13790500	-4.53981100	-2.06608400

H	-5.09635700	-3.11040800	-2.09276400
H	-5.35257400	-3.99803400	-0.57632500

E-TS4

0 1

C	3.53460800	0.65872500	-0.36743700
C	4.47839000	1.75249500	-1.99647000
C	3.08521300	3.16301800	-0.50528000
H	2.18921900	2.95309900	0.08646000
N	4.89774000	0.52850300	-2.14044300
N	4.30003300	-0.13959700	-1.11199300
N	3.64701200	1.86910600	-0.91306200
C	4.61801600	2.96428100	-2.85985800
H	4.96268500	2.68378700	-3.85446200
H	5.32272900	3.68029400	-2.41715400
C	2.74586100	4.01698800	-1.78414500
O	3.31194500	3.49369900	-2.97872900
C	4.21515200	5.26111800	-0.31246600
C	4.11120100	3.98740700	0.24098200
C	4.88496000	3.59741800	1.32980900
C	5.78664200	4.51772900	1.85846600
C	5.90004300	5.79694800	1.30781200
C	5.11414500	6.17957500	0.22310300
C	3.25955400	5.43740800	-1.46418100
H	4.77172700	2.60556000	1.75649000
H	6.60950900	6.50107800	1.73037800
H	5.20634400	7.17419600	-0.20220500
H	3.71996000	5.87775900	-2.35340300
H	2.42212400	6.08213700	-1.17754000
C	4.57677200	-1.51228300	-0.85569600
C	5.38849100	-1.87068300	0.22306900
C	3.99375500	-2.50342000	-1.64748000
C	5.62200700	-3.20669000	0.51508400
C	4.21696100	-3.84511800	-1.36958500
C	5.02990600	-4.17368900	-0.28936900
H	6.24062500	-3.48362000	1.35900900
H	3.75756300	-4.61415400	-1.97828900
H	1.67169800	3.99884000	-1.96705100

H	6.40329500	4.24038300	2.70678700
Cl	6.11243100	-0.64366400	1.20542800
Cl	5.31935400	-5.84426200	0.06533200
Cl	2.93693000	-2.05340400	-2.93692200
C	2.76805300	0.30637800	0.89824200
O	2.93372300	1.07375900	1.83632900
H	-10.18218100	-0.50419900	-0.11089500
C	1.84317200	-0.79303000	0.76700500
C	1.37364900	-1.42552600	2.07098700
H	2.19354800	-1.53812700	0.04895100
H	0.90628400	-0.25996600	0.14052400
H	1.18455400	-0.63508900	2.80406100
H	0.42573200	-1.94300100	1.89349700
C	2.40933200	-2.39575600	2.59210700
C	3.50237000	-1.93834900	3.33542800
C	2.33069900	-3.75621600	2.28173400
C	4.48401800	-2.82463700	3.77316400
H	3.57633100	-0.87922700	3.56959000
C	3.30801300	-4.64611700	2.72199900
H	1.48840300	-4.11898900	1.69661800
C	4.38701800	-4.18272500	3.47225800
H	5.32317100	-2.45498700	4.35529000
H	3.22555700	-5.70179100	2.48232800
H	5.14692700	-4.87596900	3.82023800
C	-2.02126300	1.31541500	0.11738300
C	-3.39794700	1.20446800	0.28693100
C	-4.13939700	0.14271000	-0.23601300
C	-3.45257900	-0.81526100	-0.98460400
C	-2.07658100	-0.76542500	-1.19743400
C	-1.31492300	0.29301900	-0.60006600
H	-3.93801600	1.98186400	0.81715700
H	-4.02763000	-1.63850700	-1.39538000
C	-5.60328400	0.05405500	-0.02223400
C	-6.45418300	-0.42663500	-1.01795200
C	-6.17896100	0.45446200	1.18665400
C	-7.83695800	-0.52132400	-0.84672400
H	-6.01308900	-0.71305700	-1.96527600
C	-7.55102600	0.39739900	1.42563300

H	-5.51484200	0.80149000	1.96921800
C	-8.36835200	-0.09714000	0.38859900
O	-0.00414200	0.35320100	-0.74185000
O	-9.71587700	-0.14355600	0.64744100
C	-1.39468700	-1.82924900	-2.07331700
C	-0.64313000	-1.14929600	-3.23206100
C	-0.40757800	-2.66390900	-1.24156000
C	-2.40187400	-2.80643200	-2.69541400
H	-1.34708600	-0.60999600	-3.87540200
H	0.09251300	-0.44401500	-2.84515400
H	-0.13514900	-1.90506900	-3.84432100
H	-0.92079100	-3.14590400	-0.40177600
H	0.04575500	-3.44704100	-1.86216100
H	0.38575100	-2.02918400	-0.85377500
H	-1.86502100	-3.50814100	-3.34214200
H	-2.92821500	-3.39257600	-1.93490600
H	-3.14685600	-2.28783000	-3.30770600
C	-1.27444200	2.54394900	0.65959300
C	-0.25748700	2.12268600	1.73060700
C	-0.54942300	3.25496500	-0.49742100
C	-2.21576800	3.56834800	1.30631700
H	-0.76480500	1.64404500	2.57532300
H	0.46318800	1.41870500	1.32070000
H	0.28562100	2.99665800	2.11278600
H	-1.27382500	3.63624700	-1.22490300
H	0.02442700	4.11088600	-0.11400300
H	0.11712600	2.55302300	-1.00331800
H	-1.62792500	4.42481200	1.65277500
H	-2.96457200	3.93891700	0.59899700
H	-2.73732500	3.15025100	2.17341800
C	-8.14335300	0.84383500	2.77245000
C	-8.86668800	-0.33045700	3.45807800
C	-7.05101500	1.32687900	3.73683300
C	-9.11645400	2.01897600	2.56520500
H	-9.69724700	-0.69906700	2.85665500
H	-8.16805400	-1.15504000	3.63341800
H	-9.25720500	-0.00478400	4.42867900
H	-6.50593100	2.18737400	3.33596400

H	-7.51843400	1.63587500	4.67677400
H	-6.33027800	0.53594900	3.96647300
H	-9.50738300	2.34796700	3.53451200
H	-8.59586000	2.86538800	2.10545500
H	-9.95703800	1.74106500	1.92978900
C	-8.73592300	-1.05922700	-1.97529000
C	-9.46182300	-2.34672100	-1.52625000
C	-9.73307600	0.02212600	-2.44700500
C	-7.91878100	-1.44831900	-3.21619800
H	-8.72440300	-3.12467600	-1.30830600
H	-10.07647900	-2.23998400	-0.62813200
H	-10.11244000	-2.70661000	-2.32968100
H	-9.18203700	0.87452900	-2.85476000
H	-10.37350400	-0.38181500	-3.23759200
H	-10.38629800	0.41802300	-1.66486900
H	-8.59716000	-1.83547400	-3.98222700
H	-7.39127700	-0.58837400	-3.63854800
H	-7.18711000	-2.22913200	-2.98940000

Z-TS4

0 1

C	3.34154000	1.02678500	-0.26686100
C	4.39691900	1.01427600	-2.17779900
C	5.61785800	-0.16378300	-0.29840700
H	6.04741400	0.53209100	0.42145400
N	3.34326900	1.74451200	-2.38744300
N	2.68947600	1.74221300	-1.18940700
N	4.43958500	0.55680300	-0.88528300
C	5.49125400	0.72117200	-3.15550800
H	5.64762500	1.59825200	-3.78477800
H	5.20376900	-0.11878800	-3.79905700
C	6.58177700	-0.52025700	-1.46309400
O	6.68783600	0.47708500	-2.45608900
C	5.61659800	-2.52113300	-0.66310800
C	5.30117000	-1.52730000	0.27150100
C	4.83206400	-1.86050800	1.53835300
C	4.63951600	-3.20680400	1.84205200
C	4.93739600	-4.19630400	0.90773000

C	5.43775000	-3.86124500	-0.35038700
C	6.15398800	-1.92255400	-1.93554600
H	4.61969300	-1.09429200	2.27580600
H	4.78031400	-5.23985200	1.16186200
H	5.68482000	-4.63460600	-1.07160600
H	5.36684200	-1.87481000	-2.69780900
H	6.99122100	-2.47743700	-2.36393500
C	1.61325300	2.66933400	-1.04205400
C	0.41068800	2.47847700	-1.72894100
C	1.80386600	3.84658000	-0.31538900
C	-0.59731600	3.42786800	-1.66777000
C	0.80113100	4.80406400	-0.23478200
C	-0.38612200	4.57914700	-0.91618000
H	-1.53341300	3.26443100	-2.18724900
H	0.95053100	5.70377700	0.34897200
H	7.57718400	-0.58933500	-1.01874900
H	4.24810300	-3.48284200	2.81491700
Cl	0.14821700	1.03939500	-2.65020300
Cl	-1.64675500	5.76328700	-0.82125200
Cl	3.30668000	4.13980200	0.48896800
C	3.13094000	0.84786900	1.24570900
O	4.14880700	1.13314900	1.87085100
C	1.93626700	0.23387300	1.76436800
C	0.56116300	0.62234100	1.23478400
H	1.98887000	0.30326400	2.85462900
H	1.98475000	-1.05571600	1.59038400
H	0.54384800	0.58314100	0.13732600
H	-0.15220900	-0.15168900	1.52979700
C	0.00758400	1.94410300	1.73186100
C	0.73625200	2.82120800	2.53721500
C	-1.31297600	2.28210500	1.40256700
C	0.17141700	4.01718100	2.98340600
H	1.75878700	2.57992700	2.81507400
C	-1.87971200	3.47095600	1.84804700
H	-1.89619900	1.59468400	0.79006400
C	-1.13440600	4.34884700	2.63720200
H	0.75833300	4.68766100	3.60412800
H	-2.90156600	3.71937800	1.57490900

H	-1.57392900	5.27917100	2.98308300
C	0.08345000	-2.49614700	-0.19340300
C	-1.23049900	-2.20773500	-0.55551200
C	-2.23562400	-1.99308300	0.39213800
C	-1.91922600	-2.21528800	1.73816900
C	-0.62338000	-2.49268800	2.16249800
C	0.42758900	-2.47661800	1.19313800
H	-1.48848500	-2.10661000	-1.60560100
H	-2.72715500	-2.16868400	2.46159100
C	-3.59699300	-1.56928000	-0.01013800
C	-4.31003600	-0.65041700	0.76485000
C	-4.20026200	-2.04850200	-1.17240100
C	-5.58581300	-0.20517400	0.42307000
H	-3.82713100	-0.26265300	1.65464600
C	-5.47213500	-1.64145100	-1.58180900
H	-3.65720100	-2.77933600	-1.75966200
C	-6.15284200	-0.71753600	-0.76216200
O	1.69286700	-2.39701700	1.57226700
O	-7.40810600	-0.26163400	-1.07870700
C	-0.31125600	-2.78204200	3.63719400
C	0.44730500	-4.11739900	3.73668000
C	0.54697900	-1.66841200	4.26163800
C	-1.59007700	-2.90682400	4.47537800
H	-0.17691000	-4.93952800	3.37044700
H	1.36226300	-4.07748300	3.14273200
H	0.70792200	-4.32717900	4.78086500
H	0.07723700	-0.68744500	4.11769600
H	0.65256400	-1.83759300	5.34001200
H	1.53797300	-1.65488100	3.80857100
H	-1.32341400	-3.19077300	5.49840000
H	-2.13827100	-1.96014800	4.52690100
H	-2.26296100	-3.67260100	4.07621500
C	1.14215400	-2.85266500	-1.24650200
C	2.25683500	-1.80000000	-1.31949400
C	1.76673600	-4.20684100	-0.86529400
C	0.53460000	-2.99020400	-2.64777400
H	1.84477400	-0.82856000	-1.61630000
H	2.74764500	-1.71650500	-0.35039400

H	3.00548000	-2.09486900	-2.06860800
H	1.00209600	-4.99110200	-0.86174800
H	2.54293200	-4.48376400	-1.58967700
H	2.22263800	-4.14250900	0.12480600
H	1.31042200	-3.31888800	-3.34712300
H	-0.27336700	-3.72877300	-2.66757800
H	0.13699000	-2.03843600	-3.01716600
C	-6.10046900	-2.19678100	-2.87338800
C	-6.37461400	-1.05867300	-3.88103600
C	-5.15699700	-3.17440900	-3.58945300
C	-7.38235500	-2.99891000	-2.55797800
H	-7.01677400	-0.25822200	-3.50471800
H	-5.42911200	-0.59144300	-4.17172700
H	-6.84580700	-1.46547000	-4.78135800
H	-4.92951700	-4.04670200	-2.97031200
H	-5.63965400	-3.52983000	-4.50473800
H	-4.21631000	-2.69258900	-3.87158000
H	-7.81779800	-3.38302300	-3.48581300
H	-7.13355900	-3.85031500	-1.91810900
H	-8.16389400	-2.43692900	-2.03895400
C	-6.33229900	0.81316200	1.29954100
C	-6.62313600	2.09704200	0.50065900
C	-7.64671500	0.20531700	1.82379400
C	-5.50080000	1.21866800	2.52453700
H	-5.68765300	2.54231700	0.14472900
H	-7.26419600	1.90070800	-0.35883100
H	-7.12176600	2.82792400	1.14695500
H	-7.43969000	-0.69607200	2.40979000
H	-8.14993200	0.92607700	2.47777600
H	-8.32338900	-0.05630700	1.01043700
H	-6.07183600	1.93794400	3.11936600
H	-5.27333900	0.36071000	3.16499800
H	-4.55633500	1.69461000	2.24029300
H	-7.72608700	-0.70149100	-1.87125800

E-M4

0 1

C	0.97785800	-0.22474000	-0.32970200
---	------------	-------------	-------------

C	2.14656200	-2.04613000	-0.66030700
C	3.36145100	0.13365000	-1.10571500
H	3.06231900	0.64529100	-2.02062000
N	0.97626300	-2.47782100	-0.29267700
N	0.26052200	-1.33000900	-0.08714500
N	2.19037300	-0.67569600	-0.68943400
C	3.34271100	-2.86236900	-1.04139700
H	3.02282900	-3.71016600	-1.64857700
H	3.83183900	-3.25234100	-0.14033900
C	4.56278600	-0.83474600	-1.26802600
O	4.21779500	-2.08611000	-1.82767400
C	4.92731300	0.49929600	0.65734700
C	3.84242000	1.06620900	-0.01726300
C	3.37316100	2.33680400	0.30463900
C	4.00792400	3.02926500	1.33548200
C	5.08719300	2.46463100	2.01724500
C	5.55878200	1.19680200	1.68051300
C	5.25707700	-0.86515600	0.10967300
H	2.54056400	2.75856400	-0.25040900
H	5.57177800	3.02273600	2.81232100
H	6.40824300	0.76540500	2.20150000
H	4.83948300	-1.64435500	0.75817400
H	6.32858200	-1.05561800	0.01949200
C	-1.13586900	-1.38562100	0.17338300
C	-1.61079500	-1.67491400	1.45137500
C	-2.04626600	-1.11815900	-0.85208400
C	-2.97303400	-1.67809300	1.72082000
C	-3.41102300	-1.10644700	-0.60367900
C	-3.85203400	-1.38285600	0.68530000
H	-3.33525500	-1.89369800	2.71838700
H	-4.11115800	-0.87557800	-1.39633600
H	5.23979500	-0.37693600	-1.99249700
H	3.66387300	4.02241200	1.60536100
Cl	-0.48603300	-1.98495400	2.73053100
Cl	-5.55748500	-1.36997200	1.00895100
Cl	-1.46757200	-0.80056200	-2.44941300
C	0.49449600	1.19394300	-0.41863300
O	0.91091200	1.81280000	-1.45464500

C	-0.32212100	1.57440800	0.60500200
C	-1.09399400	2.86046100	0.54618200
H	-0.54936700	0.87390200	1.40220500
H	-1.18180500	3.32724000	1.53319800
H	-0.56703500	3.55531400	-0.11626600
C	-2.47469600	2.57577200	-0.01381600
C	-3.59599100	2.46611000	0.80942500
C	-2.61897500	2.32924000	-1.38435000
C	-4.84146700	2.13205200	0.27746700
H	-3.49339900	2.64632700	1.87699800
C	-3.86078300	2.00282500	-1.91943500
H	-1.73340800	2.37783500	-2.01461900
C	-4.97904700	1.90319600	-1.08897300
H	-5.70449000	2.05101500	0.93161600
H	-3.95757700	1.81840300	-2.98580100
H	-5.94887000	1.64609700	-1.50447400

Z-M4

0 1

C	0.13303600	-1.02708900	-0.49310900
C	0.61492900	-2.68410400	0.85987300
C	2.47334100	-1.98370600	-0.70497000
H	2.33125300	-2.36928000	-1.71400400
N	-0.62802300	-2.40793200	1.11968200
N	-0.91211500	-1.37062400	0.27185300
N	1.11640100	-1.86222900	-0.11606800
C	1.46440100	-3.73384600	1.50825000
H	0.88497500	-4.65174500	1.61762200
H	1.76494500	-3.39649300	2.50821700
C	3.29089600	-2.90191400	0.23565000
O	2.57665500	-4.02981500	0.69608600
C	4.06044500	-0.68644700	0.50727200
C	3.26181400	-0.69696900	-0.64159400
C	3.31416400	0.33641000	-1.57219800
C	4.17987400	1.40065200	-1.32210000
C	4.96680900	1.42525800	-0.16891400
C	4.91437500	0.38172600	0.75529800
C	3.87135900	-1.95237700	1.30609600

H	2.68445500	0.29455900	-2.45551700
H	5.63756800	2.26135000	0.00507700
H	5.54323700	0.39414500	1.64030000
H	3.16205400	-1.78605300	2.12626900
H	4.79461300	-2.33981500	1.74152700
C	-2.23442100	-0.85225800	0.21953300
C	-2.76627700	-0.16579600	1.31434900
C	-3.03469500	-1.06072500	-0.90793300
C	-4.06433800	0.32664800	1.28665700
C	-4.33075600	-0.56486400	-0.95813300
C	-4.82581600	0.12367400	0.14258200
H	-4.46534800	0.86120500	2.13874600
H	-4.94234100	-0.72751000	-1.83686600
H	4.11417300	-3.30675100	-0.35715400
H	4.23864900	2.22199200	-2.02877000
Cl	-1.80120200	0.10023400	2.72715600
Cl	-6.44799700	0.73845200	0.08980300
Cl	-2.42864300	-1.96406700	-2.24824700
C	0.21982400	-0.13140600	-1.71356100
O	0.69820900	-0.77656100	-2.70356300
C	-0.18451000	1.16427700	-1.58640100
C	-0.60724800	1.86524600	-0.32552200
H	-0.11510600	1.77057400	-2.48673500
H	-1.65692500	2.19274300	-0.37138400
H	-0.53092300	1.18640500	0.53084300
C	0.26574900	3.06910200	-0.02774300
C	-0.22586600	4.37000400	-0.12791300
C	1.60333800	2.88256100	0.33387200
C	0.59795600	5.46597500	0.12904400
H	-1.26403700	4.52714000	-0.41031200
C	2.42771300	3.97133500	0.59422700
H	1.99858200	1.87012600	0.39772300
C	1.92678900	5.26995800	0.49211500
H	0.19905900	6.47229500	0.04413800
H	3.46458800	3.80411600	0.87177100
H	2.56977600	6.12104200	0.69358500

TS5RR

0 1

C	-0.14059700	-0.54613500	-0.39152600
C	-1.04101900	-1.82784300	-1.93595500
C	-2.60072900	-1.26293200	-0.14164600
H	-2.46742700	-1.19603700	0.94084900
N	0.17273700	-1.64520300	-2.34596200
N	0.71981100	-0.83996300	-1.38477100
N	-1.27407100	-1.19075200	-0.74855400
C	-2.16430500	-2.57563700	-2.56806700
H	-1.77788100	-3.26187500	-3.32123900
H	-2.85318800	-1.86500800	-3.04817900
C	-3.32443500	-2.62403000	-0.46477600
O	-2.80094700	-3.33816700	-1.57063000
C	-4.76683800	-0.75402700	-1.00941000
C	-3.52818400	-0.19948700	-0.69206800
C	-3.25602900	1.14782000	-0.90960700
C	-4.26178200	1.94313500	-1.45665200
C	-5.50724500	1.39592200	-1.77073600
C	-5.76968300	0.04503400	-1.54925000
C	-4.80035700	-2.22596800	-0.68723500
H	-2.28557400	1.57795600	-0.66990300
H	-6.27742500	2.02918900	-2.19968000
H	-6.73583900	-0.37968200	-1.80510300
H	-5.23485900	-2.83799400	-1.48218100
H	-5.38136700	-2.40996100	0.22344300
C	2.05997200	-0.41016000	-1.60293700
C	2.31230000	0.79404700	-2.26322800
C	3.12402500	-1.24778300	-1.28208300
C	3.60801300	1.19264000	-2.54760500
C	4.43462000	-0.86843600	-1.55698500
C	4.65437500	0.35156800	-2.17900200
H	3.79741300	2.13560700	-3.04476600
H	5.25918800	-1.52107800	-1.29807600
H	-3.19722300	-3.31003400	0.37088900
H	-4.06758300	2.99524800	-1.63531200
Cl	0.98512900	1.80371300	-2.72324400
Cl	6.28684300	0.83813100	-2.52613800
Cl	2.82234500	-2.78647500	-0.55447800

C	0.17347200	0.54564500	0.61662100
O	1.24120100	1.14639900	0.37583100
C	-0.68356100	0.83251900	1.69448500
C	-0.59389400	2.22940300	2.27381200
H	-1.66376300	0.36669000	1.73206800
H	-1.02605400	2.25037500	3.28121300
H	0.46258500	2.50118200	2.35519700
C	-1.31084700	3.23501100	1.39844100
C	-2.61129000	3.64825900	1.69305800
C	-0.69700100	3.71987000	0.23607100
C	-3.28813400	4.53086000	0.85346900
H	-3.09778700	3.27493800	2.59120300
C	-1.37426500	4.59533700	-0.60803300
H	0.30939200	3.38555600	-0.00180500
C	-2.67080200	5.00911600	-0.29935600
H	-4.29850100	4.84330200	1.09983100
H	-0.88566500	4.96436200	-1.50527600
H	-3.19514700	5.69902100	-0.95373000
C	-1.46288900	-2.02064800	3.52335200
C	-0.66939300	-3.17539800	1.61147000
C	-1.62524500	-3.34840600	2.80713600
H	-1.45329000	-2.07235700	4.61250600
H	-2.22232000	-1.28789700	3.21052600
H	-2.64523400	-3.55327700	2.48087400
H	-1.28552300	-4.19009500	3.41741800
N	0.21012000	-2.17844500	1.84315800
N	-0.14274200	-1.57998900	3.03311300
O	-0.73119500	-3.83758800	0.57292400
C	0.31597700	-0.37183500	3.33214900
C	1.70538100	0.07670500	3.17204800
C	2.11406200	1.17029000	3.95015500
C	2.63078500	-0.52662600	2.30933400
C	3.41248700	1.65671400	3.86617300
H	1.40603800	1.63764200	4.63026100
C	3.93293800	-0.04406200	2.24021700
H	2.31513900	-1.36830100	1.70625200
C	4.32765300	1.04794600	3.00914400
H	3.71182200	2.50435200	4.47393400

H	4.64168800	-0.52088300	1.56919500
H	5.34365800	1.42402200	2.94258100
H	-0.21736600	0.08851600	4.16287800

TS5RS

0 1

C	-0.60379800	-0.52330900	0.32418300
C	-0.35063200	-1.51212400	2.26494000
C	1.74813400	-1.19533400	1.05370400
H	1.99234300	-1.17302100	-0.00774500
N	-1.62849300	-1.31363700	2.17920000
N	-1.77711500	-0.70142700	0.96128800
N	0.30775300	-1.03815600	1.16532800
C	0.47229800	-2.21783000	3.29025100
H	-0.16916400	-2.80388700	3.94775500
H	1.03636200	-1.48927400	3.88834900
C	2.20477300	-2.56926200	1.63285100
O	1.32132500	-3.11738600	2.60605900
C	3.57209200	-0.78525900	2.52330400
C	2.51073900	-0.16991600	1.86061100
C	2.27060500	1.19472400	1.97401500
C	3.13198000	1.95199300	2.76716100
C	4.20207900	1.34572100	3.42774600
C	4.43009400	-0.02600500	3.31163700
C	3.59587600	-2.26750400	2.22985000
H	1.43462600	1.66673100	1.46119900
H	4.85992200	1.94839400	4.04577000
H	5.25795300	-0.49354600	3.83626900
H	3.77609400	-2.88984800	3.11008900
H	4.37444100	-2.49755500	1.49316900
C	-3.06282600	-0.18949700	0.62909600
C	-3.30668300	1.18491100	0.67728100
C	-4.11972200	-1.05571500	0.34634900
C	-4.56623800	1.69921400	0.40816900
C	-5.39232600	-0.56133500	0.08257600
C	-5.59375100	0.81166100	0.11202600
H	-4.74108000	2.76724000	0.43882100
H	-6.20535600	-1.24086200	-0.14107300

H	2.23252600	-3.31100700	0.83204000
H	2.96384100	3.01923700	2.87045200
Cl	-2.02274700	2.27756200	1.07287600
Cl	-7.17895800	1.44221900	-0.21942000
Cl	-3.85330400	-2.75985600	0.30787300
C	-0.49461300	0.18543300	-0.99048700
O	-1.55369700	0.21945300	-1.65344900
C	0.73839700	0.75485100	-1.39877000
C	0.65813000	2.06280500	-2.17044700
H	1.56330000	0.70665300	-0.69211800
H	1.38772500	2.09031900	-2.98684300
H	-0.33592900	2.13412900	-2.62137900
C	0.92344300	3.24503700	-1.26253000
C	2.20020300	3.43165900	-0.72025400
C	-0.08542700	4.14650100	-0.92149400
C	2.45730000	4.48424900	0.15308500
H	2.99651800	2.73638700	-0.98298100
C	0.16622500	5.20092800	-0.04428800
H	-1.07908000	4.01434200	-1.34094100
C	1.43733500	5.37073600	0.49820800
H	3.45386900	4.61313500	0.56479100
H	-0.63248400	5.89000400	0.21307400
H	1.63491400	6.19109700	1.18087400
C	-0.63903600	-2.00365500	-3.51115200
C	-0.53071400	-2.95772100	-1.31750900
C	-1.50473200	-2.70409600	-2.47517900
H	-1.06244500	-1.07492900	-3.89293300
H	-0.37582100	-2.66064100	-4.34568500
H	-1.94893000	-3.63686300	-2.82394200
H	-2.29227000	-2.04318300	-2.10154000
N	0.65498200	-2.34030900	-1.53980600
N	0.59972100	-1.70864400	-2.74765600
O	-0.80261400	-3.56184700	-0.27913800
C	1.35794500	-0.62512000	-2.93285700
C	2.81499600	-0.60316300	-2.63325300
C	3.57378300	0.46293800	-3.13898700
C	3.47966500	-1.61426400	-1.92296400
C	4.93953800	0.55228000	-2.89179900

H	3.09633000	1.22062100	-3.75286500
C	4.84938200	-1.52691400	-1.68952100
H	2.91532100	-2.46938400	-1.56822500
C	5.58343700	-0.43917100	-2.15556700
H	5.50222500	1.39052000	-3.29016500
H	5.34776700	-2.32453400	-1.14688500
H	6.64940200	-0.37397400	-1.96418100
H	1.07649100	-0.06223800	-3.82192100

TS5SR

0 1

C	0.46454200	-0.25790900	-0.33218600
C	1.55191700	-0.55951900	-2.19690600
C	2.99115200	-0.55021900	-0.18812900
H	2.90764000	-0.07039600	0.78443900
N	0.30310800	-0.51766100	-2.55974800
N	-0.36850200	-0.33959700	-1.38025500
N	1.68484400	-0.43545500	-0.83951800
C	2.82393300	-0.54818700	-2.98358600
H	2.62792000	-0.26050300	-4.01623700
H	3.30226100	-1.53644900	-2.96484500
C	4.07856600	0.15643400	-1.06204500
O	3.62851800	0.45042900	-2.38600200
C	4.71968200	-2.14023700	-0.61003800
C	3.42897200	-1.99208100	-0.10781100
C	2.71387300	-3.06545000	0.41032500
C	3.31177400	-4.32341600	0.39453300
C	4.60077000	-4.48645600	-0.12003800
C	5.31567200	-3.39826300	-0.61825100
C	5.28217600	-0.81033200	-1.04996300
H	1.72422700	-2.90901800	0.83180700
H	5.05279800	-5.47332200	-0.12755000
H	6.32014800	-3.53163400	-1.00879700
H	5.76412500	-0.83742400	-2.03197400
H	6.01957300	-0.45251500	-0.32444200
C	-1.77474800	-0.56288200	-1.32683900
C	-2.25941300	-1.78419000	-0.84634600
C	-2.67553100	0.39653000	-1.78964600

C	-3.62097800	-2.04423600	-0.81286400
C	-4.04311200	0.15443300	-1.76357900
C	-4.49323100	-1.06576200	-1.27507700
H	-3.99011700	-2.98739000	-0.43105400
H	-4.73778300	0.90612300	-2.11722300
H	4.31584300	1.12002500	-0.61268100
H	2.77752900	-5.18172100	0.78891200
Cl	-1.15417300	-3.00171300	-0.30608100
Cl	-6.19822900	-1.38136000	-1.23905900
Cl	-2.08190100	1.91488300	-2.34941700
C	0.10577000	-0.04512300	1.11345700
O	0.71992100	-0.72995700	1.94500200
C	-0.84831500	0.98600900	1.35005300
C	-1.65534600	0.87452900	2.63140700
H	-1.43639100	1.27786000	0.48218800
H	-0.98877800	0.59498300	3.45288500
H	-2.09770900	1.84592900	2.88093300
C	-2.75764800	-0.15440900	2.49937400
C	-2.48387000	-1.51330500	2.69114400
C	-4.05829600	0.22798900	2.16141200
C	-3.49564400	-2.46297600	2.57324100
H	-1.46824400	-1.81508500	2.93470900
C	-5.07351300	-0.71947900	2.04772700
H	-4.27973100	1.28104400	2.00371900
C	-4.79591000	-2.06817800	2.25874200
H	-3.26955200	-3.51311700	2.73332000
H	-6.08174400	-0.40502100	1.79553700
H	-5.58694500	-2.80712700	2.17288900
C	1.65045700	2.16061700	3.52881100
C	3.53522200	1.72862600	2.15048200
C	3.16724400	2.07205000	3.60539400
H	1.19554500	2.94964500	4.13193600
H	1.18819000	1.19761500	3.77148000
H	3.53109300	1.30329400	4.28664400
H	3.62802800	3.02721100	3.87597700
N	2.51031800	1.97924000	1.32397900
N	1.45625500	2.45144000	2.09540400
O	4.63285700	1.26108300	1.80516000

C	0.24931300	2.66350700	1.55181100
H	-0.43793800	3.08687600	2.28384400
C	0.12946900	3.30459400	0.20496700
C	-0.88334500	4.25835700	0.04688000
C	0.95552200	3.01418300	-0.89081400
C	-1.05491300	4.92927100	-1.16016100
H	-1.53596800	4.48790900	0.88573800
C	0.77972000	3.68589800	-2.09719500
H	1.75531600	2.29351400	-0.77898700
C	-0.21864200	4.64788300	-2.23830000
H	-1.83791100	5.67474100	-1.25612900
H	1.43413700	3.45269800	-2.93168500
H	-0.34468600	5.17245100	-3.18010600

TS5SS

0 1

C	0.98003900	-0.35009700	-0.67166100
C	2.39875800	-1.38317400	-1.98581500
C	3.42686500	0.44727300	-0.68519800
H	3.05464100	1.41012000	-0.33863700
N	1.28279500	-2.02708700	-2.15035000
N	0.41052200	-1.38066200	-1.32276400
N	2.25955800	-0.35302900	-1.09557100
C	3.71399300	-1.52143100	-2.67807600
H	3.59708200	-2.08675000	-3.60213600
H	4.44174600	-2.02940000	-2.03062300
C	4.43348500	0.60575800	-1.88636300
O	4.11561300	-0.20702000	-3.00683900
C	5.55379100	-0.38553300	0.02773600
C	4.21228100	-0.27936700	0.38389000
C	3.72847600	-0.80391300	1.57926200
C	4.62474300	-1.45673100	2.42074700
C	5.97271200	-1.57143700	2.06994200
C	6.44782900	-1.03443700	0.87582100
C	5.82550900	0.27923700	-1.29754800
H	2.68234500	-0.68925400	1.84845500
H	6.65796300	-2.08379400	2.73763800
H	7.49641900	-1.12415800	0.60878900

H	6.38572900	-0.35222100	-1.99422300
H	6.40273100	1.19901100	-1.16123800
C	-0.89506400	-1.91072500	-1.14912400
C	-1.21214400	-2.61916200	0.01249900
C	-1.86382900	-1.72648100	-2.13653800
C	-2.49630000	-3.10940800	0.20658200
C	-3.15196400	-2.21380800	-1.96186000
C	-3.44822700	-2.89393100	-0.78434700
H	-2.74356400	-3.64148900	1.11688000
H	-3.90590000	-2.06025600	-2.72430900
H	4.38412700	1.62392600	-2.27273400
H	4.27482200	-1.87494100	3.35871200
Cl	-0.01290800	-2.85718600	1.22708000
Cl	-5.05695500	-3.49257500	-0.54417900
Cl	-1.46441800	-0.84378100	-3.56946500
C	0.43143600	0.57886700	0.36981900
O	1.28871100	1.16250100	1.05854800
C	-0.97297000	0.85091300	0.41822500
C	-1.46237800	1.28305300	1.79483800
H	-1.61244800	0.10983500	-0.05616000
H	-0.80189400	2.06717300	2.17127100
H	-2.46503500	1.70987000	1.70724900
C	-1.49378300	0.09752000	2.73080400
C	-2.57117400	-0.79337100	2.69468600
C	-0.44232100	-0.15651200	3.61610500
C	-2.60701900	-1.90499400	3.53286400
H	-3.39382400	-0.60271900	2.00667600
C	-0.47433400	-1.26940600	4.45463500
H	0.40058600	0.52864000	3.64290900
C	-1.55679100	-2.14584100	4.41699100
H	-3.46122600	-2.57609600	3.50571100
H	0.34474000	-1.44819400	5.14481300
H	-1.58468000	-3.00819100	5.07554100
C	0.94106200	3.42657400	-1.05179000
C	0.66074300	4.70859400	0.93770500
C	1.75353600	4.08436100	0.04398300
H	1.26793600	2.41972200	-1.33980600
H	0.89628900	4.03845400	-1.96113700

H	2.45964500	4.83632600	-0.30682700
H	2.27734800	3.34082500	0.65696800
N	-0.54524900	4.19748700	0.64664800
N	-0.39627800	3.35373900	-0.44473500
O	0.90990100	5.53425200	1.82494000
C	-1.23985400	2.33380800	-0.73656400
H	-0.95559600	1.87755000	-1.68647900
C	-2.73056200	2.51469500	-0.66802200
C	-3.52352900	1.55473500	-1.30805000
C	-3.35660500	3.58109000	-0.01548700
C	-4.90996300	1.64292600	-1.29242300
H	-3.04438500	0.73244600	-1.83346900
C	-4.74800200	3.67162000	-0.00936600
H	-2.74298900	4.31916900	0.48650600
C	-5.52915300	2.70686900	-0.63810400
H	-5.50460200	0.88724400	-1.79649500
H	-5.22260100	4.50500000	0.49900100
H	-6.61161800	2.78257400	-0.62181600

M5RR

0 1

C	0.02405400	-0.67326700	-0.50137100
C	1.04132700	-2.55024300	-0.99423000
C	2.50405300	-0.60974300	-1.14911500
H	2.34443000	0.45850500	-1.31777900
N	-0.19097700	-2.89604900	-0.78757300
N	-0.81353100	-1.72147800	-0.46565300
N	1.21435700	-1.20616200	-0.81376700
C	2.19602500	-3.32200100	-1.53751300
H	1.85579700	-4.29251000	-1.89768800
H	2.96467400	-3.46746900	-0.76839500
C	3.09659800	-1.25391200	-2.44620500
O	2.68117000	-2.59946800	-2.65506700
C	4.77407700	-1.18819500	-0.72501100
C	3.56413300	-0.88137600	-0.10185700
C	3.43549100	-0.87589700	1.28107800
C	4.56474100	-1.16880600	2.04649200
C	5.78385500	-1.45765600	1.43257700

C	5.89793700	-1.47171600	0.04204200
C	4.61858400	-1.16759700	-2.22616800
H	2.48130100	-0.67314600	1.76066800
H	6.65036000	-1.68943700	2.04362100
H	6.84364600	-1.71625200	-0.43218700
H	5.12328600	-1.99292500	-2.73376300
H	5.00541700	-0.23100000	-2.64467800
C	-2.21509500	-1.79903300	-0.17962400
C	-2.64321900	-2.46868100	0.96638100
C	-3.17694200	-1.35846400	-1.09564100
C	-3.99542400	-2.61558100	1.25687400
C	-4.53001800	-1.48991600	-0.82238400
C	-4.92127800	-2.10536000	0.36090300
H	-4.30786400	-3.12645200	2.15885500
H	-5.26357100	-1.12569600	-1.53057800
H	2.75414400	-0.71239900	-3.32787400
H	4.48425500	-1.17831600	3.12847100
Cl	-1.49723100	-3.17538400	2.05712800
Cl	-6.61614100	-2.26956200	0.70795000
Cl	-2.69797100	-0.69495100	-2.60910800
C	-0.45335400	0.80991200	-0.39023800
O	-1.69268200	0.86226100	-0.05687900
C	0.49870100	1.80135300	0.40281400
C	0.06831600	2.00985600	1.85654000
H	1.53125000	1.43006600	0.38824800
H	0.36978100	3.01149800	2.17755400
H	-1.02504900	1.96856400	1.87688700
C	0.66380300	1.00015600	2.80017400
C	1.82148200	1.30638100	3.52234400
C	0.09018000	-0.26486800	2.95371100
C	2.39620000	0.37383800	4.38107000
H	2.27167900	2.28962200	3.41035100
C	0.66480600	-1.20202300	3.81125200
H	-0.81891100	-0.49343400	2.39998100
C	1.81908500	-0.88654800	4.52551200
H	3.29165300	0.63080100	4.93905500
H	0.20632900	-2.17687000	3.93738200
H	2.25962100	-1.61604900	5.19784600

C	0.70348900	3.12819500	-2.93918000
C	0.19608700	0.81048200	-3.01354800
C	0.39171300	2.01357000	-3.93491500
H	0.42365300	4.12828900	-3.27298400
H	1.77994700	3.11915500	-2.69663900
H	1.17549800	1.82867100	-4.66947400
H	-0.55234700	2.19323400	-4.46012600
N	-0.07771900	1.31943900	-1.79874600
N	-0.09313100	2.74114700	-1.76626300
O	0.27470500	-0.37964200	-3.32200200
C	0.46503600	3.11946000	-0.45145000
H	1.50527900	3.45918100	-0.57274700
C	-0.33960000	4.26684400	0.11872500
C	0.29016600	5.43813400	0.53302300
C	-1.73054700	4.15879800	0.22696200
C	-0.45427000	6.49738300	1.05377700
H	1.37062800	5.52665300	0.44420800
C	-2.47165700	5.21298600	0.74699100
H	-2.20062000	3.22871000	-0.08502300
C	-1.83634600	6.38602500	1.16017700
H	0.04661800	7.40745600	1.36911200
H	-3.55027400	5.12285700	0.83323500
H	-2.41944800	7.20850400	1.56275500

M5RS

0 1

C	0.38567100	1.04954900	-0.06407100
C	0.17795100	2.42352100	1.63819400
C	-1.96042200	1.60986200	0.78197100
H	-2.33659500	1.24106200	-0.17924100
N	1.45943900	2.28312900	1.49164800
N	1.57056600	1.41905500	0.43320800
N	-0.50641600	1.68420500	0.71264400
C	-0.63634100	3.29210400	2.54215500
H	-0.02121400	4.09543700	2.94684700
H	-1.04908800	2.70188800	3.37036200
C	-2.56665700	3.01302900	1.09984700
O	-1.65067100	3.88711500	1.75116000

C	-3.48219000	1.35808300	2.59846800
C	-2.41144000	0.74940200	1.94606800
C	-1.88353600	-0.46015200	2.38498000
C	-2.48190300	-1.08485900	3.47860800
C	-3.57669700	-0.49823800	4.11596600
C	-4.07881100	0.73039800	3.68689000
C	-3.79934500	2.69479200	1.97262800
H	-1.01084500	-0.90434700	1.91012500
H	-4.03008500	-0.99462700	4.96778400
H	-4.91100400	1.19669200	4.20536900
H	-3.96158300	3.49108200	2.70360800
H	-4.69532500	2.63185400	1.34501800
C	2.85003700	0.84412400	0.18155400
C	3.29339800	-0.15568200	1.04508100
C	3.69503100	1.32062000	-0.81972100
C	4.54477700	-0.73725300	0.88037400
C	4.94739600	0.75039200	-1.00312700
C	5.34729700	-0.27734100	-0.15477200
H	4.87923800	-1.52102900	1.54839700
H	5.59972900	1.10834400	-1.78975800
H	-2.83642900	3.53400700	0.17961000
H	-2.08501500	-2.02801400	3.84030600
Cl	2.27802300	-0.67138300	2.34960500
Cl	6.91379500	-0.99440300	-0.38466200
Cl	3.19269800	2.63276100	-1.80902700
C	0.17403900	0.24087000	-1.40259600
O	1.28470200	0.06660000	-2.00778500
C	-0.75742700	-1.03781100	-1.20294800
C	0.02163300	-2.33384200	-1.39111100
H	-1.26349400	-1.01059900	-0.22923100
H	-0.67962600	-3.09827800	-1.75202300
H	0.75380500	-2.14532100	-2.18089600
C	0.71538700	-2.88222600	-0.16973900
C	-0.02758100	-3.29732600	0.94211200
C	2.09754300	-3.07961700	-0.15968400
C	0.59304200	-3.90517600	2.02991500
H	-1.10931700	-3.16711300	0.93764400
C	2.71995200	-3.70815500	0.91788800

H	2.68366600	-2.74602000	-1.01237600
C	1.97047100	-4.12312000	2.01505100
H	-0.00018500	-4.22908200	2.88001600
H	3.79346800	-3.87387800	0.89757300
H	2.45485300	-4.61239400	2.85414400
C	-2.66661800	1.14162300	-3.48972100
C	-0.80082900	2.37728300	-2.65165500
C	-2.13169900	2.57044600	-3.38977700
H	-2.23685000	0.63956400	-4.37029300
H	-3.75405300	1.06042400	-3.51900500
H	-2.77762200	3.20677100	-2.77475500
H	-1.97742800	3.05897400	-4.35173900
N	-0.86353500	1.14732600	-2.09852500
N	-2.14610800	0.53111300	-2.25547500
O	0.10434300	3.19055600	-2.53592300
C	-1.83652300	-0.89535800	-2.29427400
H	-1.37707900	-1.15887700	-3.26438200
C	-3.06394900	-1.73956300	-2.05911800
C	-3.40074800	-2.77253600	-2.93340000
C	-3.86501600	-1.51532400	-0.93401300
C	-4.51593500	-3.57364500	-2.68837300
H	-2.78493700	-2.95080200	-3.81145600
C	-4.97815300	-2.31047100	-0.68906400
H	-3.61190500	-0.71137400	-0.24707700
C	-5.30631500	-3.34399800	-1.56681900
H	-4.76537700	-4.37525200	-3.37624800
H	-5.58967500	-2.12572700	0.18862700
H	-6.17435000	-3.96635000	-1.37420800

M5SR

0 1

C	0.74883200	0.36601700	0.19663300
C	1.99324300	0.86341700	1.93616300
C	3.05452600	-0.73053200	0.38089000
H	2.66559200	-1.58144000	-0.17720200
N	0.96184500	1.63876000	2.05288400
N	0.20206000	1.32285900	0.95980800
N	1.89937400	0.06696100	0.82135400

C	3.17693000	0.68183100	2.82761200
H	2.93955400	1.00269100	3.84164600
H	4.03028200	1.26632300	2.45575300
C	3.90349600	-1.22265000	1.61038800
O	3.45779700	-0.70304700	2.85340100
C	5.28166300	0.09786000	0.09984200
C	3.98820500	0.15241000	-0.41157600
C	3.64674700	0.97601700	-1.48155300
C	4.65824800	1.74224800	-2.05608000
C	5.96476500	1.68439800	-1.56249800
C	6.28716300	0.86621500	-0.48156800
C	5.36747700	-0.83653500	1.28090100
H	2.62500900	1.02571200	-1.86019800
H	6.73762700	2.29218400	-2.02253800
H	7.30086500	0.83760900	-0.09327600
H	5.84033400	-0.38058900	2.15696300
H	5.94688300	-1.73214400	1.03644000
C	-0.94470900	2.11497600	0.67521000
C	-0.81414800	3.24748000	-0.13407300
C	-2.17465200	1.83089200	1.26740100
C	-1.91878600	4.03676200	-0.42148100
C	-3.29233500	2.61172700	0.99436800
C	-3.14576500	3.69517400	0.13730800
H	-1.82002500	4.90592100	-1.05970200
H	-4.24820300	2.38039800	1.44848600
H	3.79233100	-2.30199400	1.72100300
H	4.42749700	2.39103500	-2.89438900
Cl	0.73916900	3.71913100	-0.71426300
Cl	-4.53271600	4.67571800	-0.22036600
Cl	-2.31377400	0.49616300	2.35907900
C	0.12248000	-0.07103100	-1.20691100
O	0.02594100	0.96060600	-1.96064900
C	-1.17232100	-0.90063800	-0.87502900
C	-2.09503800	-0.89554400	-2.09711500
H	-1.71132800	-0.44721400	-0.04016000
H	-2.18414600	0.14428900	-2.42595400
H	-1.63153400	-1.45665900	-2.91758100
C	-3.43770400	-1.47924900	-1.73908100

C	-4.31175900	-0.74884800	-0.92459300
C	-3.81170500	-2.76780200	-2.12639400
C	-5.51929500	-1.29206100	-0.50197100
H	-4.03253300	0.25857100	-0.61994700
C	-5.02233900	-3.31831100	-1.70472200
H	-3.14890500	-3.34547600	-2.76692200
C	-5.87764700	-2.58399800	-0.88895300
H	-6.18365400	-0.70855700	0.12808400
H	-5.29550600	-4.32189200	-2.01565500
H	-6.81930800	-3.01085800	-0.55900100
C	0.90762400	-3.47833100	-2.00589100
C	1.68385200	-1.39109300	-2.85288800
C	1.98170100	-2.89113600	-2.91017200
H	1.18358900	-4.41316000	-1.51551300
H	-0.01671000	-3.63796400	-2.58230400
H	1.95391800	-3.25338200	-3.93740500
H	2.98912100	-3.05173100	-2.50900000
N	0.99583200	-1.19920700	-1.69341600
N	0.70605400	-2.42045800	-0.99400700
O	2.06485400	-0.55124300	-3.64908500
C	-0.68279000	-2.31053300	-0.47869000
H	-1.31077400	-3.05739100	-0.98418500
C	-0.78457400	-2.56948200	1.01299700
C	-2.05694400	-2.77260700	1.55927300
C	0.31941100	-2.56230500	1.86378700
C	-2.22030100	-2.93795500	2.93013500
H	-2.92517800	-2.78141600	0.90091100
C	0.15738800	-2.71454100	3.24058200
H	1.31076900	-2.45331100	1.43908500
C	-1.11267300	-2.89741000	3.77852700
H	-3.21356700	-3.09284700	3.34026600
H	1.02960800	-2.68897100	3.88673000
H	-1.24162800	-3.01686500	4.84955100

M5SS

0 1

C	-0.79765900	0.76778400	0.02408700
C	-2.28240300	2.17287200	0.81720300

C	-3.17538800	0.69765800	-0.93451500
H	-2.70169900	0.17450600	-1.76557900
N	-1.19144800	2.48341200	1.44691500
N	-0.27667800	1.59427300	0.94629900
N	-2.08033000	1.14027200	-0.06147500
C	-3.60632700	2.86090500	0.76461300
H	-3.54644900	3.82737800	1.26464100
H	-4.38848800	2.25212200	1.23593000
C	-4.01977700	1.92644000	-1.41216500
O	-3.85923900	3.09287900	-0.60829700
C	-5.46592900	0.24892200	-0.43867200
C	-4.15983800	-0.16458700	-0.18358700
C	-3.88197400	-1.23837400	0.65295800
C	-4.95549300	-1.89698000	1.25165900
C	-6.26782200	-1.48817700	1.00531500
C	-6.53423700	-0.41543200	0.15476300
C	-5.47902000	1.41999000	-1.39050600
H	-2.85628700	-1.55694400	0.82835900
H	-7.09035100	-2.01034200	1.48401500
H	-7.55637700	-0.09978800	-0.03286100
H	-6.15234600	2.22715300	-1.08849200
H	-5.77976500	1.09812900	-2.39353000
C	1.09882100	1.79223900	1.23968700
C	1.71444300	1.12413900	2.29904800
C	1.83998700	2.70434700	0.47947700
C	3.07573100	1.26437800	2.53511800
C	3.20214800	2.86354000	0.70299300
C	3.80181900	2.12228600	1.71486900
H	3.55353400	0.72581300	3.34412200
H	3.77944700	3.55262900	0.09927400
H	-3.69408300	2.23378900	-2.40609400
H	-4.76398400	-2.73620700	1.91216700
Cl	0.76842100	0.11227600	3.33485600
Cl	5.50938500	2.28602500	1.97853700
Cl	1.06188700	3.66835100	-0.71886900
C	-0.14047400	-0.31729700	-0.89799700
O	-1.03660300	-1.00582700	-1.50996100
C	1.02618500	-1.14627600	-0.22064400

C	0.75191800	-2.64637900	-0.36523700
H	1.08182800	-0.92853000	0.84983300
H	0.54216500	-2.88384700	-1.41046300
H	1.66161200	-3.18402600	-0.07529000
C	-0.38460300	-3.15744000	0.48967500
C	-0.31664700	-3.07676900	1.88365900
C	-1.49370300	-3.78207400	-0.08596700
C	-1.32936500	-3.60251300	2.68346600
H	0.54916600	-2.61383000	2.35087000
C	-2.49853800	-4.32751900	0.70774100
H	-1.56839200	-3.82211300	-1.16815800
C	-2.42052300	-4.23961700	2.09702900
H	-1.25629000	-3.53027600	3.76455700
H	-3.35261000	-4.80903000	0.24086800
H	-3.20323000	-4.66534000	2.71799500
C	1.69757100	-0.68462100	-3.37726100
C	0.07175000	0.97712500	-2.98614100
C	0.87840800	0.36950200	-4.12851000
H	2.63153300	-0.95622600	-3.87194200
H	1.08147700	-1.58160000	-3.21513700
H	0.21075300	-0.02514700	-4.89459700
H	1.52831600	1.13189400	-4.57004400
N	0.72566700	0.68441800	-1.79626800
N	1.97374100	0.06160300	-2.13170800
O	-0.99809000	1.54968100	-3.04563900
C	2.33885700	-0.61674600	-0.88085900
H	2.67379700	0.20522900	-0.23808700
C	3.52280600	-1.54927500	-1.00219200
C	4.66603100	-1.26301000	-0.25024000
C	3.53846400	-2.68604100	-1.82128200
C	5.79256200	-2.07917200	-0.30624500
H	4.67262300	-0.38198400	0.38739100
C	4.66456300	-3.50142000	-1.88501300
H	2.66419800	-2.94749700	-2.40730500
C	5.79540800	-3.20225400	-1.12783000
H	6.66686200	-1.83275800	0.28770600
H	4.65560900	-4.37732400	-2.52575700
H	6.67091700	-3.84155400	-1.17747100

TS6RR

0 1

C	0.42074000	-0.72724900	-0.55651600
C	1.98056500	-2.14689800	-1.29655500
C	2.74332600	0.15921900	-1.00605400
H	2.23558700	1.12619200	-1.08926200
N	0.92430300	-2.88778400	-1.18124500
N	-0.01807700	-1.99304300	-0.71479600
N	1.71530400	-0.85813900	-0.92229300
C	3.33051400	-2.42490000	-1.86661300
H	3.32879300	-3.36275200	-2.42124700
H	4.08806900	-2.47577900	-1.07247000
C	3.67321200	-0.06945400	-2.25112700
O	3.60213300	-1.38216800	-2.78841100
C	5.01101800	0.18691400	-0.24601400
C	3.68541800	0.12395300	0.17685800
C	3.34878300	0.03010700	1.52295800
C	4.38287800	0.00705900	2.45723900
C	5.71525900	0.07570800	2.04353100
C	6.04005100	0.16585000	0.69084800
C	5.09470500	0.27401500	-1.74997000
H	2.30876300	-0.03919200	1.83998400
H	6.50803100	0.04971200	2.78464700
H	7.07806900	0.20737000	0.37425300
H	5.82123500	-0.41686500	-2.18691600
H	5.37497400	1.28510300	-2.06535300
C	-1.30535800	-2.50184500	-0.39540200
C	-1.49273100	-3.21645700	0.78964300
C	-2.38556300	-2.37219800	-1.27291600
C	-2.73531500	-3.72452000	1.14578600
C	-3.64035600	-2.86607400	-0.93761500
C	-3.79797500	-3.52409100	0.27498800
H	-2.86404600	-4.26680400	2.07403700
H	-4.47276100	-2.74695200	-1.61969100
H	3.36008700	0.57410900	-3.07465900
H	4.14641600	-0.07074800	3.51324600
Cl	-0.14030500	-3.51409200	1.83349800

Cl	-5.36636300	-4.14209000	0.70451500
Cl	-2.16229300	-1.63278000	-2.81235300
C	-1.01292300	0.96673600	-0.54560200
O	-2.08007900	0.40290000	-0.41483400
C	-0.41907600	1.96759800	0.45952200
C	-1.00810000	1.87621300	1.86950300
H	0.66470000	1.81164200	0.48648600
H	-1.17007000	2.88635700	2.25724800
H	-1.99270600	1.40348000	1.79538800
C	-0.12430900	1.12980900	2.83704200
C	0.86326000	1.81921900	3.54897800
C	-0.26163600	-0.24451500	3.04071300
C	1.68603400	1.15742500	4.45473900
H	0.97751000	2.88997300	3.39588500
C	0.55731700	-0.91037700	3.95172000
H	-1.02504000	-0.78691900	2.48662100
C	1.52971600	-0.21192200	4.66324100
H	2.44408700	1.70951000	5.00215200
H	0.42873900	-1.97507500	4.11450800
H	2.16006000	-0.73166100	5.37828900
C	0.59576200	3.43083000	-2.43002500
C	0.18312200	1.14670100	-2.90887700
C	0.66016600	2.43530000	-3.57970400
H	0.47786300	4.47151500	-2.73542700
H	1.49426100	3.34271800	-1.79380800
H	1.64965500	2.29619400	-4.01451800
H	-0.04517400	2.69987900	-4.37402100
N	-0.56830400	1.53898300	-1.83628700
N	-0.60917800	2.98176800	-1.72469700
O	0.44522200	0.01153000	-3.26615500
C	-0.68085800	3.31125800	-0.28235100
H	0.12608400	4.01192200	-0.03791500
C	-2.00380000	3.96809800	0.05011900
C	-2.04290400	5.05280700	0.92659300
C	-3.19907700	3.48820400	-0.49252300
C	-3.25533900	5.64996600	1.26589800
H	-1.11451800	5.43781200	1.34315100
C	-4.41025600	4.08278000	-0.15407200

H	-3.17308400	2.64855900	-1.18015000
C	-4.44249500	5.16393700	0.72606800
H	-3.26993000	6.49697100	1.94436200
H	-5.33351700	3.70236900	-0.57961400
H	-5.38898900	5.62789000	0.98468300

TS6RS

0 1

C	-0.35910100	-1.10149100	-0.07607600
C	-0.12710100	-2.87651100	1.24567200
C	1.98297900	-1.84451400	0.53217400
H	2.31151100	-1.32016200	-0.37283900
N	-1.40981000	-2.69268500	1.19524200
N	-1.52343900	-1.59365900	0.36981200
N	0.53213700	-1.94772900	0.48264000
C	0.71077500	-3.91948500	1.91154000
H	0.12058400	-4.80920800	2.12979600
H	1.13239800	-3.53014400	2.84884500
C	2.64399500	-3.26177100	0.64009100
O	1.72345500	-4.28630600	0.99115100
C	3.45434800	-1.82457500	2.42220900
C	2.42811900	-1.12857300	1.78923300
C	1.91520600	0.05319000	2.31488600
C	2.48008800	0.55914700	3.48329300
C	3.52756100	-0.11969900	4.11119800
C	4.01651000	-1.31743100	3.59121000
C	3.77980900	-3.09745500	1.67931900
H	1.07587600	0.56065400	1.84246900
H	3.95503000	0.28227400	5.02410500
H	4.81478400	-1.85142700	4.09792200
H	3.82227400	-3.97776700	2.32758500
H	4.74721700	-3.01959400	1.17208000
C	-2.78998800	-0.97271800	0.21943900
C	-3.17380300	0.01054500	1.12999000
C	-3.66436300	-1.33769400	-0.80400200
C	-4.39758800	0.65773000	1.01361100
C	-4.89297100	-0.70501300	-0.94146400
C	-5.23481500	0.28898600	-0.03149500

H	-4.68378600	1.42513700	1.72191900
H	-5.56506000	-0.98206600	-1.74391000
H	3.03124400	-3.57505900	-0.33038200
H	2.09651900	1.47960200	3.91169100
Cl	-2.11542600	0.41403800	2.43957600
Cl	-6.76802900	1.09355000	-0.20083800
Cl	-3.21352400	-2.58389400	-1.90528700
C	-0.23618700	0.07130700	-1.69040400
O	-1.38078000	0.14096500	-2.13799900
C	0.58525100	1.31404500	-1.22638300
C	-0.23362300	2.60138300	-1.22736100
H	1.01478200	1.12122900	-0.23888400
H	0.41416900	3.42073800	-1.56683900
H	-1.03769400	2.49248200	-1.96026200
C	-0.80423000	2.98861500	0.11687500
C	0.04825800	3.20712500	1.20601500
C	-2.17091300	3.21443900	0.28421100
C	-0.45205600	3.64984700	2.42674300
H	1.11974400	3.04983800	1.08449200
C	-2.67392500	3.67551600	1.50067300
H	-2.84430300	3.03638800	-0.55066600
C	-1.81697500	3.89495800	2.57484800
H	0.22524000	3.82227500	3.25800100
H	-3.73850400	3.86481600	1.60650600
H	-2.20742900	4.25295500	3.52217300
C	2.73288300	-0.55954200	-3.54879100
C	0.79658500	-1.88190200	-3.08274600
C	2.20411500	-1.98777900	-3.67785800
H	2.39698600	0.04611500	-4.40444900
H	3.81625300	-0.48173200	-3.45134100
H	2.78215700	-2.69299600	-3.07077500
H	2.16488900	-2.36151000	-4.70067300
N	0.79041600	-0.72110500	-2.37346800
N	2.08260700	-0.09771300	-2.31178100
O	-0.11282100	-2.68316300	-3.18259900
C	1.75518900	1.32818500	-2.22794300
H	1.38131500	1.68745800	-3.20409600
C	2.93168000	2.16167400	-1.79463900

C	3.27647500	3.31168300	-2.50403900
C	3.66807700	1.81639900	-0.65584800
C	4.33818500	4.11160500	-2.08439000
H	2.71003000	3.58096000	-3.39172700
C	4.72875500	2.61236300	-0.23711700
H	3.40692300	0.91880500	-0.10021400
C	5.06598800	3.76296700	-0.95093700
H	4.59659100	5.00377300	-2.64548700
H	5.29308400	2.33551800	0.64786100
H	5.89443800	4.38277800	-0.62353500

TS6SR

0 1

C	0.68522300	0.02632000	-0.45980200
C	1.81472700	-0.16943600	-2.36208300
C	3.22196500	0.19772500	-0.37994200
H	3.08848000	0.80463100	0.51805600
N	0.58612100	-0.38998200	-2.70762500
N	-0.09093800	-0.27305600	-1.51359700
N	1.91194300	0.09354100	-1.01859400
C	3.06566800	-0.08485600	-3.17315800
H	2.83206300	0.10880800	-4.21982200
H	3.63748900	-1.02063000	-3.09940600
C	4.26989100	0.86374800	-1.34411700
O	3.79731800	1.01994900	-2.67456300
C	5.07455200	-1.30493200	-0.59474000
C	3.77830900	-1.18010600	-0.10131000
C	3.12027600	-2.24010600	0.51666000
C	3.81169100	-3.44071700	0.66155700
C	5.11886700	-3.57179300	0.18587500
C	5.75876200	-2.50866700	-0.44919700
C	5.53160100	-0.03041500	-1.25933300
H	2.09674700	-2.14310800	0.87740000
H	5.63869500	-4.51738900	0.30388700
H	6.76783200	-2.62209300	-0.83419400
H	5.94153700	-0.19004300	-2.26180100
H	6.30946200	0.46673400	-0.67074500
C	-1.47623300	-0.58614200	-1.50492500

C	-1.88491700	-1.91459400	-1.36227500
C	-2.43627900	0.40119700	-1.73512300
C	-3.23159700	-2.25249800	-1.41590200
C	-3.78659500	0.08465700	-1.79764500
C	-4.16010500	-1.24447300	-1.64324100
H	-3.54383700	-3.28326800	-1.30339300
H	-4.52554300	0.85654000	-1.97294400
H	4.47914100	1.88320100	-1.01712700
H	3.32708100	-4.28171300	1.14609400
Cl	-0.70664300	-3.16364600	-1.18828900
Cl	-5.84178200	-1.66136300	-1.76948400
Cl	-1.93657600	2.04519200	-1.95328600
C	0.09195900	-0.26177200	1.35021300
O	-0.27339100	-1.44281500	1.42021600
C	-0.84630000	0.95789400	1.53730800
C	-1.80420000	0.68240300	2.70967000
H	-1.43486300	1.14470800	0.63697400
H	-1.24579900	0.21249900	3.52810900
H	-2.16746300	1.64673700	3.08445800
C	-3.00011200	-0.15962100	2.33125900
C	-3.05759800	-1.52667000	2.60908400
C	-4.09255900	0.44423200	1.70152400
C	-4.19068500	-2.26829100	2.28319500
H	-2.19654900	-2.00590100	3.06303600
C	-5.22718600	-0.29316300	1.37507600
H	-4.05357200	1.50856700	1.47369300
C	-5.28110800	-1.65371400	1.67115200
H	-4.22174000	-3.32969800	2.50972100
H	-6.06796300	0.19151800	0.88691000
H	-6.16462400	-2.23094200	1.41678000
C	2.21074200	1.96967000	3.15408400
C	2.08043700	-0.40867400	3.01538300
C	2.99668200	0.71077300	3.50784700
H	2.82674600	2.84654500	2.94996800
H	1.50938900	2.20795800	3.96751300
H	3.21281700	0.60091900	4.56996700
H	3.93878200	0.64123600	2.95140700
N	1.29139300	0.17093700	2.06429200

N	1.46989500	1.58047800	1.93613000
O	2.09402800	-1.57480300	3.35939900
C	0.10721200	2.15341100	1.81948400
H	-0.17723800	2.59397400	2.78751400
C	0.02383700	3.23929900	0.76863200
C	-1.07441900	4.10381800	0.79706000
C	0.95987900	3.37017900	-0.25695000
C	-1.24991500	5.06372800	-0.19343800
H	-1.80342000	4.01571100	1.60029500
C	0.78705300	4.33320200	-1.25020600
H	1.82486600	2.71550100	-0.27174400
C	-0.32003400	5.17725100	-1.22681400
H	-2.11054500	5.72429600	-0.15984900
H	1.52127200	4.42086400	-2.04519100
H	-0.45371800	5.92545400	-2.00140400

TS6SS

0 1

C	0.97557300	0.14642300	-0.80222400
C	2.48704000	-0.54637900	-2.27879800
C	3.40904900	0.85329700	-0.49266200
H	3.04047300	1.63595900	0.17513900
N	1.39981700	-1.14251000	-2.65617500
N	0.48225200	-0.70194300	-1.72397200
N	2.27053400	0.23025600	-1.16766500
C	3.83937000	-0.46522500	-2.90930700
H	3.78953400	-0.76053200	-3.95724000
H	4.55667400	-1.11093500	-2.38584500
C	4.40966100	1.43291700	-1.55206100
O	4.21615000	0.89961000	-2.85908800
C	5.58337400	-0.03871000	-0.03625800
C	4.22886500	-0.17537400	0.25945300
C	3.77071700	-1.15789400	1.13116600
C	4.70565000	-2.01747000	1.70488100
C	6.06555600	-1.88711100	1.41350000
C	6.51499300	-0.89508500	0.54385000
C	5.81181200	1.10061800	-0.99810400
H	2.71226900	-1.22549200	1.36516300

H	6.77965300	-2.56746900	1.86694600
H	7.57252200	-0.79777400	0.31642100
H	6.49218500	0.85559600	-1.81894200
H	6.22591700	1.97030100	-0.47636300
C	-0.81566400	-1.27116700	-1.72032900
C	-1.12024800	-2.30820100	-0.83157000
C	-1.80877600	-0.80726000	-2.58331700
C	-2.40177100	-2.83976600	-0.76610800
C	-3.09512400	-1.33138700	-2.54483400
C	-3.37233200	-2.33618100	-1.62504000
H	-2.63295400	-3.62119700	-0.05219500
H	-3.86188900	-0.95634200	-3.21184700
H	4.25890200	2.50625300	-1.67372400
H	4.37430800	-2.79421600	2.38674300
Cl	0.09863400	-2.90510000	0.23690300
Cl	-4.98286000	-2.97793100	-1.54117600
Cl	-1.44205000	0.46355600	-3.70125600
C	0.47948800	0.98808500	0.92975300
O	1.31646000	0.55651400	1.72425000
C	-1.04288900	0.71381600	1.01284900
C	-1.46443400	0.59850800	2.49140200
H	-1.27913900	-0.24316700	0.54866300
H	-0.85223100	1.25277600	3.12007400
H	-2.50798800	0.90566500	2.59666000
C	-1.34786900	-0.83728900	2.95680500
C	-2.38323500	-1.73258600	2.66848700
C	-0.21350400	-1.31286300	3.61668500
C	-2.29070100	-3.07385600	3.03117200
H	-3.27144200	-1.36960600	2.15340100
C	-0.11848200	-2.65437000	3.98142200
H	0.60375700	-0.62803200	3.81636500
C	-1.15468400	-3.53897600	3.69046300
H	-3.10837500	-3.75315400	2.80721800
H	0.77022200	-3.00958500	4.49459600
H	-1.07892300	-4.58318200	3.97716100
C	-0.94379900	3.94434900	1.37150800
C	1.32911200	3.34995800	1.20763700
C	0.44488200	4.56524500	1.46396500

H	-1.74228400	4.64648700	1.12924900
H	-1.17457800	3.43524300	2.32090200
H	0.68610600	5.01511300	2.42659700
H	0.60564900	5.30076100	0.66914800
N	0.55704000	2.42759400	0.52447300
N	-0.74079600	3.00261200	0.25517700
O	2.49206800	3.20814800	1.52887700
C	-1.62436400	1.82727700	0.11675700
H	-1.43185200	1.47932100	-0.90780500
C	-3.10593100	2.12400000	0.18082600
C	-3.87580500	1.84442700	-0.95336000
C	-3.76120500	2.64359100	1.30565900
C	-5.25156800	2.05475000	-0.96794600
H	-3.38383300	1.46504600	-1.84469200
C	-5.13599000	2.86412100	1.29221100
H	-3.20759700	2.88664200	2.20476500
C	-5.88791600	2.56598000	0.15892000
H	-5.82212600	1.82424200	-1.86195100
H	-5.61903600	3.26965200	2.17531300
H	-6.95969200	2.73519100	0.15416100

A-TS5

0 1

C	1.14885000	-0.08531400	-0.31623800
C	2.37156700	-1.75447000	-1.18528300
C	3.48816500	0.49241800	-1.05148300
H	3.19496300	1.18486900	-1.84403400
N	1.22739700	-2.31164600	-0.92981700
N	0.50547000	-1.26453300	-0.39823900
N	2.36141700	-0.42765200	-0.82808400
C	3.59321900	-2.40185000	-1.76091000
H	3.31109600	-3.05505800	-2.58797000
H	4.08446500	-3.01489300	-0.99435100
C	4.73952300	-0.34455700	-1.41384600
O	4.46839000	-1.42411700	-2.28313100
C	5.00860400	0.50173600	0.78644800
C	3.92121400	1.17354700	0.22168800
C	3.38234800	2.30957600	0.81222100

C	3.94681600	2.76780100	2.00146900
C	5.02967100	2.09897500	2.57486700
C	5.57213800	0.96463800	1.97070000
C	5.39928900	-0.68673700	-0.05858000
H	2.55369900	2.83043200	0.34351900
H	5.46051400	2.47152600	3.49893000
H	6.42200500	0.45650700	2.41653100
H	4.98516300	-1.60820200	0.36840200
H	6.47850100	-0.82540100	-0.15330600
C	-0.84515000	-1.45898800	-0.02026500
C	-1.16408200	-2.03278100	1.21082200
C	-1.88415800	-1.02673500	-0.84902800
C	-2.48399900	-2.17229900	1.62064000
C	-3.21144700	-1.13024000	-0.45386200
C	-3.48807000	-1.71079200	0.77833800
H	-2.71849400	-2.62303800	2.57691200
H	-4.00656100	-0.75839200	-1.08955200
H	5.41271500	0.30903500	-1.97381500
H	3.54636000	3.65466400	2.48154900
Cl	0.10895400	-2.55851500	2.26269600
Cl	-5.14322700	-1.87698600	1.28387300
Cl	-1.51363500	-0.34883800	-2.39824500
C	0.09494500	2.09358800	-0.37659400
O	0.72340300	2.61270700	-1.23052600
C	-0.81198600	1.88791000	0.56828300
C	-1.93382500	2.89036700	0.75367400
H	-0.79362600	0.97215800	1.13578200
H	-2.06610600	3.09399100	1.82179000
H	-1.66092300	3.84069700	0.28282800
C	-3.24276200	2.40062600	0.16571000
C	-4.29127000	1.96784800	0.97767800
C	-3.40651600	2.35705400	-1.22224800
C	-5.48601700	1.51467000	0.41790600
H	-4.17400000	1.98999200	2.05843200
C	-4.59556900	1.90702700	-1.78627100
H	-2.58735100	2.67819700	-1.86181900
C	-5.64282800	1.48508500	-0.96514300
H	-6.29303800	1.18440000	1.06428700

H	-4.70779200	1.88565300	-2.86609600
H	-6.57352800	1.13613000	-1.40145900

A-M5

0 1

C	3.06885800	0.15512500	-0.13459500
O	4.02672500	0.65413300	0.31147200
C	1.99451600	-0.41377200	-0.63156800
C	0.94634100	-1.07758200	0.23374500
H	1.88147000	-0.37386000	-1.70891800
H	0.87486100	-2.13852500	-0.02926000
H	1.26787900	-1.04324600	1.28065200
C	-0.42828000	-0.44566400	0.11110100
C	-1.56870300	-1.24980200	0.07032300
C	-0.58247400	0.94157200	0.06817200
C	-2.83859600	-0.68171300	-0.00523800
H	-1.46034600	-2.33122100	0.09639000
C	-1.84931900	1.51303900	-0.00659900
H	0.30149100	1.57302800	0.08554100
C	-2.98254500	0.70246100	-0.04374300
H	-3.71474600	-1.32172400	-0.03877000
H	-1.95273300	2.59322300	-0.03949000
H	-3.97045300	1.14727600	-0.10751000

A-TS6RR

0 1

C	-0.64499700	1.26315400	0.20572300
O	-1.14821700	1.98554800	1.06211900
C	-0.82597100	-0.08637300	-0.10251000
C	-1.66955000	-0.91183900	0.83691800
H	-0.80895900	-0.39751300	-1.13725300
H	-1.26444900	-1.92747100	0.92214800
H	-1.61579600	-0.46004900	1.83382800
C	-3.12246000	-0.99959800	0.41023800
C	-3.71987600	-2.22245800	0.10512700
C	-3.88606800	0.16877900	0.29530200
C	-5.05237200	-2.28605100	-0.30316600
H	-3.13597200	-3.13626300	0.18669500

C	-5.21541100	0.10826400	-0.10737300
H	-3.41636800	1.12110400	0.53031800
C	-5.80434700	-1.12054700	-0.40997100
H	-5.50055500	-3.24717400	-0.53734400
H	-5.79693400	1.02211800	-0.18611300
H	-6.84186100	-1.16608100	-0.72614800
C	2.65793700	1.93110900	0.36917400
C	0.81991800	3.26386700	-0.36404200
C	2.30426500	3.36197900	-0.02664000
H	2.46138300	1.76293200	1.43327600
H	3.67063500	1.61633400	0.11930400
H	2.85536900	3.68358000	-0.91458000
H	2.45337300	4.09103000	0.76846300
N	0.50920700	1.90117100	-0.58118300
N	1.68969300	1.18698000	-0.45040000
O	0.02745400	4.16138700	-0.44840100
C	1.62410400	-0.08613700	-0.78855600
H	1.03184500	-0.29688000	-1.66636000
C	2.58768300	-1.09212100	-0.35829000
C	2.93941700	-2.09553900	-1.27262700
C	3.13129300	-1.11572000	0.93444800
C	3.85075300	-3.08048900	-0.91526500
H	2.50094200	-2.09154700	-2.26624900
C	4.03633700	-2.10728500	1.28912300
H	2.81511200	-0.38623700	1.67182700
C	4.40321100	-3.08438700	0.36425900
H	4.12595600	-3.84754300	-1.63098900
H	4.44708800	-2.12660200	2.29269100
H	5.10980800	-3.85791600	0.64658300

A-TS6RS

0 1

C	0.14458000	-1.39500000	-0.12236600
O	-0.23465700	-2.56213200	-0.14270300
C	-0.40286100	-0.21684000	-0.62522300
C	-1.62744900	-0.32716900	-1.50124800
H	-0.26463700	0.70443800	-0.08557700
H	-1.59056000	-1.28032300	-2.04056700

H	-1.62705600	0.46990600	-2.25407700
C	-2.92451700	-0.25610600	-0.71500600
C	-3.21116700	-1.23997700	0.24001600
C	-3.84038400	0.77907700	-0.90488800
C	-4.38959900	-1.19080400	0.97569200
H	-2.49240100	-2.04101600	0.39267100
C	-5.02215600	0.83277400	-0.16473900
H	-3.62894800	1.55114000	-1.64102900
C	-5.30097400	-0.15282300	0.77669800
H	-4.59925100	-1.96356200	1.70940000
H	-5.72406700	1.64557300	-0.32606900
H	-6.22033700	-0.11456400	1.35264700
C	3.13292400	-1.67038800	-1.25232300
C	2.23293000	-2.41617000	0.82634500
C	3.39130000	-2.67217300	-0.13175500
H	4.02936500	-1.24568500	-1.70157500
H	2.47675300	-2.08514900	-2.02709300
H	3.36879600	-3.71340100	-0.45187000
H	4.33800800	-2.47846700	0.37925300
N	1.58441200	-1.20168900	0.43980800
N	2.40317800	-0.62488600	-0.51558600
O	1.88071500	-3.09446800	1.74829100
C	2.07085300	0.55350000	-1.01016400
H	2.43852200	0.71583800	-2.02221300
C	1.76550200	1.76165800	-0.24901600
C	1.64261800	2.95322600	-0.97676300
C	1.66472200	1.79187900	1.15128500
C	1.41536000	4.15651600	-0.32136400
H	1.72750300	2.93016300	-2.05951900
C	1.45246300	3.00146700	1.79875800
H	1.74511400	0.87061800	1.71756200
C	1.32172200	4.18328000	1.06837200
H	1.31894800	5.07301100	-0.89352700
H	1.38051400	3.02226400	2.88092700
H	1.14693900	5.12248000	1.58252700

A-TS6SR

0 1

C	-0.14460300	-1.39492800	-0.12231900
O	0.23472800	-2.56203400	-0.14243200
C	0.40279800	-0.21680900	-0.62537200
C	1.62741500	-0.32734200	-1.50133000
H	0.26462900	0.70452100	-0.08578600
H	1.59046300	-1.28058900	-2.04048300
H	1.62711600	0.46958500	-2.25429400
C	2.92444300	-0.25620600	-0.71503300
C	3.84027200	0.77901800	-0.90487600
C	3.21107500	-1.24003900	0.24003000
C	5.02202200	0.83275300	-0.16469400
H	3.62884400	1.55105500	-1.64104600
C	4.38948300	-1.19082800	0.97574200
H	2.49228600	-2.04104700	0.39272900
C	5.30084400	-0.15283700	0.77674900
H	5.72392200	1.64556000	-0.32602800
H	4.59912900	-1.96356500	1.70947400
H	6.22020100	-0.11456500	1.35270800
C	-3.13273100	-1.67041200	-1.25241700
C	-2.23294300	-2.41616900	0.82633300
C	-3.39124000	-2.67217000	-0.13185700
H	-4.02912300	-1.24577800	-1.70183200
H	-2.47638100	-2.08513800	-2.02705900
H	-3.36880500	-3.71341700	-0.45191100
H	-4.33796900	-2.47834000	0.37907000
N	-1.58442100	-1.20164800	0.43984400
N	-2.40319800	-0.62485600	-0.51555900
O	-1.88076600	-3.09446300	1.74828500
C	-2.07080600	0.55352300	-1.01014500
H	-2.43833200	0.71584200	-2.02225500
C	-1.76549400	1.76170200	-0.24902300
C	-1.64236800	2.95323000	-0.97679200
C	-1.66489900	1.79195000	1.15129000
C	-1.41505600	4.15651000	-0.32139700
H	-1.72708500	2.93014000	-2.05956000
C	-1.45258200	3.00153200	1.79875900
H	-1.74546200	0.87070900	1.71757500
C	-1.32160400	4.18330500	1.06835300

H	-1.31843400	5.07297500	-0.89357300
H	-1.38076700	3.02235300	2.88093600
H	-1.14676300	5.12249900	1.58250100

A-TS6SS

0 1

C	-0.64499700	-1.26315400	0.20572300
O	-1.14821700	-1.98554800	1.06211900
C	-0.82597100	0.08637300	-0.10251000
C	-1.66955000	0.91183900	0.83691800
H	-0.80895900	0.39751300	-1.13725300
H	-1.26444900	1.92747100	0.92214800
H	-1.61579600	0.46004900	1.83382800
C	-3.12246000	0.99959800	0.41023800
C	-3.71987600	2.22245800	0.10512700
C	-3.88606800	-0.16877900	0.29530200
C	-5.05237200	2.28605100	-0.30316600
H	-3.13597200	3.13626300	0.18669500
C	-5.21541100	-0.10826400	-0.10737300
H	-3.41636800	-1.12110400	0.53031800
C	-5.80434700	1.12054700	-0.40997100
H	-5.50055500	3.24717400	-0.53734400
H	-5.79693400	-1.02211800	-0.18611300
H	-6.84186100	1.16608100	-0.72614800
C	2.65793700	-1.93110900	0.36917400
C	0.81991800	-3.26386700	-0.36404200
C	2.30426500	-3.36197900	-0.02664000
H	2.46138300	-1.76293200	1.43327600
H	3.67063500	-1.61633400	0.11930400
H	2.85536900	-3.68358000	-0.91458000
H	2.45337300	-4.09103000	0.76846300
N	0.50920700	-1.90117100	-0.58118300
N	1.68969300	-1.18698000	-0.45040000
O	0.02745400	-4.16138700	-0.44840100
C	1.62410400	0.08613700	-0.78855600
H	1.03184500	0.29688000	-1.66636000
C	2.58768300	1.09212100	-0.35829000
C	2.93941700	2.09553900	-1.27262700

C	3.13129300	1.11572000	0.93444800
C	3.85075300	3.08048900	-0.91526500
H	2.50094200	2.09154700	-2.26624900
C	4.03633700	2.10728500	1.28912300
H	2.81511200	0.38623700	1.67182700
C	4.40321100	3.08438700	0.36425900
H	4.12595600	3.84754300	-1.63098900
H	4.44708800	2.12660200	2.29269100
H	5.10980800	3.85791600	0.64658300

PRR

0 1

O	5.01604600	-0.95713000	-0.25872300
O	2.48726400	-2.72405400	0.21816600
N	2.76612700	-0.45095400	-0.09697600
N	1.93856700	0.71582000	-0.14341500
C	4.11914200	-0.15239200	-0.21327700
C	4.18200200	1.36948400	-0.26537700
H	4.27222500	1.66877100	-1.31471600
H	5.04834100	1.73841200	0.28232400
C	2.83294300	1.78782700	0.32411800
H	2.88436000	1.79783300	1.42384300
H	2.47124600	2.75280800	-0.03119800
C	0.80569500	0.37189500	0.72959900
H	1.11875400	0.46252800	1.78525900
C	0.61248000	-1.13759300	0.44018700
C	2.04871400	-1.59965500	0.19623700
C	-0.38836900	1.26057100	0.48772500
C	-1.41451700	1.28983900	1.43561400
H	-1.32398500	0.69763500	2.34338300
C	-2.55321300	2.05516500	1.21707900
H	-3.34961100	2.06121800	1.95447200
C	-2.67203500	2.81316500	0.05183200
H	-3.56040500	3.41297100	-0.11880800
C	-1.64626300	2.79980400	-0.88726800
H	-1.72987400	3.39134600	-1.79373900
C	-0.50838900	2.02295500	-0.67346200
H	0.28861600	1.99615300	-1.40987900

C	-0.24412200	-1.47865400	-0.79579000
H	0.02751400	-0.80699100	-1.61804600
H	0.02466900	-2.49546000	-1.10614600
C	-1.73476100	-1.41407900	-0.54131700
C	-2.55902100	-0.58609800	-1.30433300
C	-2.31715600	-2.20182900	0.45610000
C	-3.92974100	-0.52850500	-1.06568400
H	-2.11840600	0.03577200	-2.07828900
C	-3.68644800	-2.14776800	0.69818900
H	-1.69527400	-2.87027300	1.04707600
C	-4.49776500	-1.30555700	-0.06001600
H	-4.55196200	0.13089200	-1.66304000
H	-4.12108900	-2.76699000	1.47679600
H	-5.56529000	-1.25977700	0.13026900
H	0.22576900	-1.66287400	1.31670300

PRS

0 1

O	-5.04245700	-0.74097100	0.06197000
O	-2.62300600	-2.45729400	-0.89972200
N	-2.80211400	-0.25267500	-0.22648900
N	-1.92389200	0.86032600	-0.02311500
C	-4.10720500	0.01280000	0.17073400
C	-4.06150000	1.42265700	0.74758500
H	-4.40262400	2.11689500	-0.02732400
H	-4.71964100	1.50697900	1.61152000
C	-2.57547900	1.61557000	1.05984100
H	-2.33393300	1.17548500	2.03988800
H	-2.24542100	2.65402900	1.03619100
C	-0.62572900	0.23772300	0.29380300
H	-0.61375300	-0.10256900	1.34617300
C	-0.64502300	-1.01475500	-0.61061600
H	-0.37718800	-0.71271100	-1.63286000
C	-2.12481100	-1.39167400	-0.62760800
C	0.50666800	1.20716100	0.05728900
C	1.50871300	1.37469500	1.01153900
H	1.46058900	0.81783600	1.94324100
C	2.58291000	2.22572500	0.76368800

H	3.36375100	2.33808800	1.50910600
C	2.65388100	2.92755400	-0.43642100
H	3.48965900	3.59217500	-0.63081100
C	1.64502600	2.77712800	-1.38722600
H	1.69142900	3.32846600	-2.32105500
C	0.57662600	1.92120600	-1.14170700
H	-0.21627300	1.80633500	-1.87517700
C	0.21840200	-2.19327400	-0.15834800
H	0.09350100	-2.99777600	-0.89093000
H	-0.17159200	-2.57254100	0.79257100
C	1.67546000	-1.82855800	0.00225600
C	2.30154300	-1.94080100	1.24361500
H	1.73975000	-2.32644200	2.09099100
C	3.63117000	-1.55556800	1.41013500
H	4.10157800	-1.64984800	2.38403800
C	4.34929500	-1.04828600	0.33249900
C	3.73465700	-0.93875600	-0.91517900
H	4.28831400	-0.54462400	-1.76169400
C	2.41137800	-1.33077100	-1.07785700
H	1.93956300	-1.23554700	-2.05306700
H	5.38214000	-0.74033400	0.46031400

PSR

0 1

O	5.04245700	-0.74097100	0.06197000
O	2.62300600	-2.45729400	-0.89972200
N	2.80211400	-0.25267500	-0.22648900
N	1.92389200	0.86032600	-0.02311500
C	4.10720500	0.01280000	0.17073400
C	4.06150000	1.42265700	0.74758500
H	4.40262400	2.11689500	-0.02732400
H	4.71964100	1.50697900	1.61152000
C	2.57547900	1.61557000	1.05984100
H	2.33393300	1.17548500	2.03988800
H	2.24542100	2.65402900	1.03619100
C	0.62572900	0.23772300	0.29380300
H	0.61375300	-0.10256900	1.34617300
C	0.64502300	-1.01475500	-0.61061600

H	0.37718800	-0.71271100	-1.63286000
C	2.12481100	-1.39167400	-0.62760800
C	-0.50666800	1.20716100	0.05728900
C	-1.50871300	1.37469500	1.01153900
H	-1.46058900	0.81783600	1.94324100
C	-2.58291000	2.22572500	0.76368800
H	-3.36375100	2.33808800	1.50910600
C	-2.65388100	2.92755400	-0.43642100
H	-3.48965900	3.59217500	-0.63081100
C	-1.64502600	2.77712800	-1.38722600
H	-1.69142900	3.32846600	-2.32105500
C	-0.57662600	1.92120600	-1.14170700
H	0.21627300	1.80633500	-1.87517700
C	-0.21840200	-2.19327400	-0.15834800
H	-0.09350100	-2.99777600	-0.89093000
H	0.17159200	-2.57254100	0.79257100
C	-1.67546000	-1.82855800	0.00225600
C	-2.30154300	-1.94080100	1.24361500
H	-1.73975000	-2.32644200	2.09099100
C	-3.63117000	-1.55556800	1.41013500
H	-4.10157800	-1.64984800	2.38403800
C	-4.34929500	-1.04828600	0.33249900
C	-3.73465700	-0.93875600	-0.91517900
H	-4.28831400	-0.54462400	-1.76169400
C	-2.41137800	-1.33077100	-1.07785700
H	-1.93956300	-1.23554700	-2.05306700
H	-5.38214000	-0.74033400	0.46031400

PSS

0 1

O	-5.01604600	-0.95713000	-0.25872300
O	-2.48726400	-2.72405400	0.21816600
N	-2.76612700	-0.45095400	-0.09697600
N	-1.93856700	0.71582000	-0.14341500
C	-4.11914200	-0.15239200	-0.21327700
C	-4.18200200	1.36948400	-0.26537700
H	-4.27222500	1.66877100	-1.31471600
H	-5.04834100	1.73841200	0.28232400

C	-2.83294300	1.78782700	0.32411800
H	-2.88436000	1.79783300	1.42384300
H	-2.47124600	2.75280800	-0.03119800
C	-0.80569500	0.37189500	0.72959900
H	-1.11875400	0.46252800	1.78525900
C	-0.61248000	-1.13759300	0.44018700
C	-2.04871400	-1.59965500	0.19623700
C	0.38836900	1.26057100	0.48772500
C	1.41451700	1.28983900	1.43561400
H	1.32398500	0.69763500	2.34338300
C	2.55321300	2.05516500	1.21707900
H	3.34961100	2.06121800	1.95447200
C	2.67203500	2.81316500	0.05183200
H	3.56040500	3.41297100	-0.11880800
C	1.64626300	2.79980400	-0.88726800
H	1.72987400	3.39134600	-1.79373900
C	0.50838900	2.02295500	-0.67346200
H	-0.28861600	1.99615300	-1.40987900
C	0.24412200	-1.47865400	-0.79579000
H	-0.02751400	-0.80699100	-1.61804600
H	-0.02466900	-2.49546000	-1.10614600
C	1.73476100	-1.41407900	-0.54131700
C	2.55902100	-0.58609800	-1.30433300
C	2.31715600	-2.20182900	0.45610000
C	3.92974100	-0.52850500	-1.06568400
H	2.11840600	0.03577200	-2.07828900
C	3.68644800	-2.14776800	0.69818900
H	1.69527400	-2.87027300	1.04707600
C	4.49776500	-1.30555700	-0.06001600
H	4.55196200	0.13089200	-1.66304000
H	4.12108900	-2.76699000	1.47679600
H	5.56529000	-1.25977700	0.13026900
H	-0.22576900	-1.66287400	1.31670300

Re-TS1 ($\Phi = -87^\circ$)

0 1

C	-0.92383600	0.05828700	0.58974800
C	-2.55525400	-1.40242100	0.99917000

C	-3.27321500	0.94887900	0.95091600
H	-2.78939400	1.88993800	1.22469900
N	-1.51490000	-2.15078100	0.80448700
N	-0.52772300	-1.22532400	0.54665300
N	-2.23456200	-0.07173300	0.88668100
C	-3.95061800	-1.72737700	1.41998900
H	-4.00077200	-2.72527300	1.85492400
H	-4.63852500	-1.67134000	0.56520500
C	-4.37083600	0.56060800	2.00864600
O	-4.28932000	-0.79393200	2.43186700
C	-5.40364500	1.02041200	-0.13833400
C	-4.02872700	1.05241800	-0.35638600
C	-3.48673700	1.15009500	-1.63538700
C	-4.37068900	1.23276500	-2.71005500
C	-5.75235800	1.21390700	-2.50232400
C	-6.27971700	1.10494300	-1.21699900
C	-5.72117700	0.88661500	1.32965500
H	-2.40721200	1.13734200	-1.79766900
H	-6.42332200	1.27473300	-3.35343800
H	-7.35401500	1.07655000	-1.06082000
H	-6.44694500	0.09672100	1.54614600
H	-6.12980100	1.82047700	1.72971000
C	0.78371000	-1.63965400	0.20995500
C	1.08576200	-2.02513600	-1.09802700
C	1.80975100	-1.57757200	1.15477100
C	2.39591900	-2.30017900	-1.47199600
C	3.12686500	-1.84134700	0.80363100
C	3.39769000	-2.18873200	-0.51483100
H	2.62702500	-2.58423400	-2.49116900
H	3.91941700	-1.76385000	1.53730600
H	-4.23008500	1.13441300	2.92521900
H	-3.98067200	1.30702800	-3.71998300
Cl	-0.17624200	-2.17516800	-2.26478500
Cl	5.04407900	-2.49078600	-0.98025100
Cl	1.44722600	-1.11357600	2.78289200
C	-0.13153100	1.45741300	-0.52876800
O	-0.20840400	1.00717400	-1.69659100
H	-0.86044600	2.23230400	-0.19505100

C	1.24574400	1.64515900	0.10089100
C	2.05323800	2.69831200	-0.67231300
H	1.78953700	0.70027400	0.02413300
H	1.16429700	1.90975600	1.16137800
H	1.97506600	2.45990800	-1.73825200
H	1.62366000	3.69552800	-0.52507400
C	3.50077700	2.67958500	-0.24543000
C	4.32939000	1.62780900	-0.65447100
C	4.03198400	3.65534000	0.59870200
C	5.65218000	1.55293400	-0.23176000
H	3.92611100	0.86235700	-1.31564000
C	5.35788100	3.58602400	1.02471900
H	3.40047000	4.47803100	0.92479900
C	6.17145800	2.53489400	0.61177600
H	6.27921600	0.73051200	-0.56278100
H	5.75455100	4.35509800	1.68044800
H	7.20378700	2.48075600	0.94247200

Re-TS1 ($\Phi = 174^\circ$)

0 1

C	0.11899600	-0.54447100	0.29938200
C	0.25081300	-1.98474100	1.99026400
C	-2.01252300	-1.78397100	0.91109000
H	-2.61523800	-0.94820600	1.27265400
N	1.45705100	-1.52370800	1.86878900
N	1.34499800	-0.63575400	0.82497600
N	-0.58679300	-1.42207100	1.05396900
C	-0.22372900	-3.01715800	2.96776600
H	0.10727200	-2.75170100	3.97309900
H	0.21125300	-3.99144300	2.71074400
C	-2.24373800	-3.08198200	1.72270700
O	-1.63376200	-3.06683200	2.99288900
C	-2.22488500	-3.63165500	-0.57625400
C	-2.34137900	-2.23993800	-0.49126400
C	-2.74303000	-1.48546600	-1.58718600
C	-2.99336900	-2.14039100	-2.79257300
C	-2.85501400	-3.52537100	-2.88676500
C	-2.47957100	-4.28267900	-1.77712800

C	-1.84137900	-4.21987700	0.75874400
H	-2.87095700	-0.40984100	-1.51094900
H	-3.05560700	-4.02058200	-3.83138300
H	-2.39631000	-5.36283100	-1.84930500
H	-0.76283500	-4.41647400	0.79359000
H	-2.35517000	-5.15511300	0.99021400
C	2.53399600	-0.02538300	0.34122100
C	3.18039500	-0.55082800	-0.77566600
C	3.08761600	1.07575900	0.98753400
C	4.36255800	0.00149400	-1.24626400
C	4.27104400	1.64806400	0.54092400
C	4.89088900	1.09628500	-0.57342300
H	4.85430900	-0.40973200	-2.11885600
H	4.69198000	2.50832200	1.04605300
H	-3.31662600	-3.15077700	1.91709700
H	-3.30416800	-1.56885400	-3.66064600
Cl	2.48793200	-1.90330500	-1.60892500
Cl	6.37528900	1.79952600	-1.14411700
Cl	2.26623700	1.76789600	2.34686200
C	-0.17905600	0.83629800	-1.04883500
O	0.91179700	1.40420200	-1.28645000
H	-0.61014400	0.13874800	-1.80043800
C	-1.27125100	1.62563200	-0.31840100
C	-1.83720200	2.69106300	-1.26836500
H	-0.82626200	2.10965400	0.55854300
H	-2.08403700	0.97598700	0.03106100
H	-1.01994500	3.35568800	-1.56388400
H	-2.19798000	2.19896100	-2.18149900
C	-2.96050500	3.47216900	-0.63497400
C	-2.70227200	4.63689300	0.09264400
C	-4.27913300	3.01541500	-0.71515100
C	-3.73406600	5.32926900	0.72186600
H	-1.68087800	5.00302400	0.16284200
C	-5.31452000	3.70322600	-0.08771100
H	-4.49532000	2.11221000	-1.28201400
C	-5.04434100	4.86423500	0.63365600
H	-3.51457600	6.23470700	1.27927800
H	-6.33295100	3.33506300	-0.16565600

H	-5.84974200	5.40363200	1.12185500
---	-------------	------------	------------

Re-TS1 ($\Phi = 82^\circ$)

0 1

C	0.40834500	0.58068600	-0.25664600
C	0.69041400	2.71980100	-0.77616300
C	-1.70234400	1.94363600	-0.88565200
H	-1.96660600	1.41753100	-1.80460700
N	1.87844700	2.30822600	-0.46874900
N	1.67783200	0.99638600	-0.14361200
N	-0.24826300	1.71114300	-0.63231500
C	0.35825900	4.09678700	-1.26483200
H	1.05154900	4.36630700	-2.06345000
H	0.47315800	4.82380000	-0.45146400
C	-1.89180900	3.48132100	-0.99542900
O	-0.94047100	4.12168900	-1.80766600
C	-2.73913500	2.80154100	1.08550500
C	-2.61700500	1.65290200	0.29218800
C	-3.41122800	0.53937800	0.55285300
C	-4.23486300	0.54516100	1.67822600
C	-4.29045300	1.66060700	2.51277600
C	-3.56037100	2.80820100	2.20588700
C	-1.99011000	3.95447800	0.47252500
H	-3.42116000	-0.31873000	-0.10796300
H	-4.93638300	1.65043100	3.38482300
H	-3.65254200	3.70231900	2.81496000
H	-1.00110300	4.07098300	0.93048400
H	-2.51347000	4.90849200	0.56341700
C	2.79657100	0.17496500	0.14710000
C	3.00805200	-0.31002100	1.43847000
C	3.70452600	-0.16003600	-0.86096300
C	4.09651000	-1.12089800	1.73359000
C	4.80497400	-0.96178500	-0.58590800
C	4.98077400	-1.43319800	0.70916300
H	4.24757200	-1.49512400	2.73828000
H	5.50503600	-1.21633100	-1.37175800
H	-2.85642400	3.64427400	-1.48144100
H	-4.84726100	-0.32569100	1.89004900

Cl	1.89688400	0.09453200	2.70794100
Cl	6.35087500	-2.44242600	1.05899400
Cl	3.48973500	0.43675300	-2.46582100
C	0.28803600	-1.18842600	-0.59566900
O	0.88868100	-1.34692000	-1.70317000
H	0.79245100	-1.53668200	0.34152600
C	-1.19436000	-1.50816700	-0.50153300
C	-1.46273300	-2.99972300	-0.71331700
H	-1.73123400	-0.94353500	-1.27475000
H	-1.56525100	-1.20010400	0.48141900
H	-1.07608400	-3.29345100	-1.69318700
H	-0.91276800	-3.57518700	0.04236900
C	-2.94112400	-3.28653700	-0.61061300
C	-3.71414800	-3.52778100	-1.74788700
C	-3.58217300	-3.24176200	0.63326100
C	-5.09066300	-3.72563900	-1.64885600
H	-3.23024800	-3.56304000	-2.72070100
C	-4.95610900	-3.43688900	0.73736100
H	-2.99328600	-3.05131500	1.52831000
C	-5.71619800	-3.67989800	-0.40637500
H	-5.67314500	-3.91738500	-2.54480700
H	-5.43430900	-3.40415600	1.71193400
H	-6.78749600	-3.83467000	-0.32734800

Si -TS1 ($\Phi = -82^\circ$)

0 1

C	0.39490200	-0.35381100	0.70929900
C	0.36028200	-2.55807800	1.03609400
C	-1.85319200	-1.50000800	0.97845700
H	-2.23856400	-0.52537800	1.28682900
N	1.61597500	-2.29439400	0.85567800
N	1.60670700	-0.93194300	0.64978700
N	-0.39932800	-1.41480900	0.96757700
C	-0.35186200	-3.82636400	1.37631100
H	0.33915400	-4.55492700	1.79957400
H	-0.82339900	-4.25605100	0.48158100
C	-2.34466100	-2.62265900	1.96063800
O	-1.30678200	-3.50262400	2.37177400

C	-3.29584500	-2.96494300	-0.24505000
C	-2.37732700	-1.92647300	-0.37621700
C	-2.00684100	-1.42374200	-1.62130600
C	-2.61109100	-1.97397000	-2.75081700
C	-3.54970300	-3.00169600	-2.62889100
C	-3.89570500	-3.50826000	-1.37753700
C	-3.47791200	-3.35170500	1.20153900
H	-1.25443800	-0.63900600	-1.71676100
H	-4.00471500	-3.41985500	-3.52124400
H	-4.61131400	-4.32025800	-1.28895200
H	-3.40881200	-4.43000900	1.37382200
H	-4.45362800	-3.02448100	1.57594300
C	2.80000500	-0.26489200	0.27987000
C	3.31733400	-0.42094500	-1.00937900
C	3.45852600	0.57749400	1.17641300
C	4.47491800	0.24150400	-1.39638200
C	4.61358700	1.25618500	0.80955800
C	5.10338700	1.07335300	-0.47755900
H	4.87080800	0.11609800	-2.39641800
H	5.11494000	1.90990000	1.51218000
H	-2.70244400	-2.18015600	2.89077400
H	-2.34248100	-1.60575000	-3.73553400
Cl	2.52030400	-1.45724100	-2.13877400
Cl	6.54675000	1.91504200	-0.95510800
Cl	2.82671800	0.79510300	2.77568000
C	0.19081900	1.31136300	-0.32994800
O	0.42607900	0.97439200	-1.51194400
H	0.97770500	1.84488700	0.25074900
C	-1.20553600	1.78052200	0.06514800
C	-1.48319900	3.13449600	-0.60544600
H	-1.28737300	1.86986900	1.15515400
H	-1.95161900	1.05842800	-0.28684700
H	-0.72480900	3.85936000	-0.28562400
H	-1.37255800	3.00517800	-1.68679000
C	-2.86005700	3.65237200	-0.27336200
C	-3.05680700	4.55110800	0.77761000
C	-3.97664500	3.19912000	-0.98232000
C	-4.33557900	4.99133400	1.11144700

H	-2.19600000	4.91092700	1.33626900
C	-5.25663400	3.63546900	-0.65257300
H	-3.83574500	2.49769500	-1.80165700
C	-5.43998300	4.53434400	0.39669400
H	-4.46877100	5.69527300	1.92716500
H	-6.11208000	3.27762800	-1.21739500
H	-6.43691500	4.87844400	0.65294000

Si -TS1 ($\Phi = 149^\circ$)

0 1

C	-0.00712300	-0.84932200	0.58369500
C	-0.67195900	-2.84737900	-0.13907600
C	-2.43693200	-1.49265400	0.90415700
H	-2.44518100	-0.74001200	1.69801500
N	0.57473900	-2.78927000	-0.48966200
N	0.95689800	-1.54502200	-0.03376900
N	-1.05079000	-1.70215400	0.51574900
C	-1.68576800	-3.94175100	-0.21881800
H	-1.20346000	-4.90494800	-0.38289900
H	-2.40183800	-3.75376700	-1.03027700
C	-3.08181500	-2.83714000	1.40021200
O	-2.32199800	-3.98596100	1.04782600
C	-4.44701100	-1.85460600	-0.34347200
C	-3.28892900	-1.08431000	-0.27942900
C	-3.01001300	-0.10776300	-1.22984300
C	-3.93207400	0.10083100	-2.25346200
C	-5.10257100	-0.65957700	-2.31682600
C	-5.36753000	-1.64296800	-1.36576300
C	-4.49820900	-2.85541800	0.78292400
H	-2.08840100	0.46800000	-1.18196000
H	-5.80956700	-0.48774900	-3.12207200
H	-6.27206600	-2.24062100	-1.42682000
H	-4.75028200	-3.86798600	0.45438900
H	-5.24091300	-2.56153600	1.53224500
C	2.28215200	-1.09749700	-0.26751800
C	2.56647900	-0.27692700	-1.35611000
C	3.31506800	-1.46780000	0.59257000
C	3.85796700	0.17317800	-1.59810900

C	4.61384000	-1.03330700	0.37548100
C	4.86241200	-0.21545500	-0.72134600
H	4.07181300	0.81002800	-2.44733600
H	5.41023600	-1.31695100	1.05190800
H	-3.11390900	-2.86208600	2.48978400
H	-3.73903800	0.85540100	-3.00861700
Cl	1.28784700	0.19200400	-2.43206100
Cl	6.48614000	0.33863000	-1.00487500
Cl	2.96312500	-2.46050600	1.96238300
C	0.46942300	0.68091700	1.71340500
O	1.71400900	0.72381700	1.81425000
H	-0.13705700	0.28040700	2.56298300
C	-0.26467200	1.80942100	0.98819700
C	-0.06033800	3.11744800	1.76477400
H	-1.33613600	1.58387100	0.89864700
H	0.14945700	1.91401600	-0.02162300
H	-0.44659800	2.99611600	2.78435800
H	1.01722700	3.29023000	1.84723300
C	-0.73399200	4.29182700	1.10133500
C	-1.98578800	4.74192300	1.52730300
C	-0.13045100	4.93198400	0.01421600
C	-2.61844700	5.80725000	0.88998000
H	-2.46579700	4.25451300	2.37247500
C	-0.75813100	5.99594200	-0.62681300
H	0.84526000	4.59259700	-0.32581600
C	-2.00595400	6.43785600	-0.18989700
H	-3.58830200	6.14717400	1.24005100
H	-0.27118300	6.48496500	-1.46493700
H	-2.49500500	7.27022700	-0.68575700

Si -TS1 ($\Phi = 31^\circ$)

0 1

C	-0.96905000	0.27440100	0.02687600
C	-2.33426800	-0.23205100	1.70269000
C	-3.34504300	1.11686600	-0.10813800
H	-2.91512900	1.90360400	-0.73753800
N	-1.22574700	-0.82668600	2.02157500
N	-0.39859600	-0.50231200	0.96742800

N	-2.20940400	0.44488000	0.51817500
C	-3.63299300	-0.08755300	2.42590500
H	-3.51271900	-0.31213500	3.48552600
H	-4.39001000	-0.76064700	1.99894800
C	-4.31478200	1.69938100	0.98348100
O	-4.00782800	1.27218500	2.30526200
C	-5.53052500	0.21648600	-0.51018000
C	-4.19105200	0.12935300	-0.87785300
C	-3.75767700	-0.78312100	-1.83395200
C	-4.69934300	-1.61600500	-2.43267500
C	-6.04707200	-1.52959700	-2.07365800
C	-6.47170300	-0.61546700	-1.11171300
C	-5.73739500	1.27433800	0.54416100
H	-2.70480400	-0.84766500	-2.09993200
H	-6.77026500	-2.18684000	-2.54586800
H	-7.51924400	-0.55863300	-0.83101100
H	-6.30367800	0.91665100	1.41001300
H	-6.28061600	2.13274100	0.13615700
C	0.92332800	-1.01510000	0.91657600
C	1.23303900	-2.07160000	0.05827500
C	1.95403800	-0.40986700	1.63917300
C	2.54315000	-2.50199900	-0.10765400
C	3.27317300	-0.81398700	1.48399900
C	3.54696800	-1.85524600	0.60450700
H	2.77315700	-3.31671100	-0.78290700
H	4.06853600	-0.31555100	2.02405600
H	-4.21358200	2.78366700	1.02711000
H	-4.38549600	-2.33657300	-3.18079900
Cl	-0.02870900	-2.83255900	-0.85322600
Cl	5.19127700	-2.37108200	0.39630800
Cl	1.59527700	0.91160800	2.69663700
C	-0.35777300	1.45726900	-1.33693600
O	-0.92048900	2.56998800	-1.14516900
H	-0.67652800	0.82741100	-2.19967200
C	1.14299000	1.33046700	-1.08030500
C	2.00951400	2.25208300	-1.94312500
H	1.46404400	0.29472200	-1.24366900
H	1.33757300	1.58740800	-0.03305000

H	1.84378900	2.05104000	-3.00759600
H	1.72702500	3.29121300	-1.74974500
C	3.44875300	1.98916100	-1.56980200
C	4.21833600	1.07136200	-2.28856100
C	3.98612500	2.54056600	-0.40216600
C	5.49035800	0.70790800	-1.85257400
H	3.80818500	0.62909400	-3.19335900
C	5.25736600	2.18114900	0.03779100
H	3.39295400	3.24850300	0.17279900
C	6.01248900	1.25856600	-0.68443600
H	6.07187700	-0.01131200	-2.42135400
H	5.65804100	2.61877300	0.94724900
H	7.00057400	0.97065400	-0.33981700

Re-M1 ($\Phi = -104^\circ$)

0 1

C	0.80765300	-0.22765400	0.48757500
C	2.41393700	0.86784600	1.51922500
C	3.09060100	-1.33545000	0.62710300
H	2.58498600	-2.30091400	0.56724500
N	1.41777000	1.69660400	1.51533100
N	0.42754900	0.99945800	0.86964200
N	2.07606200	-0.32075700	0.92076800
C	3.78751100	0.97195700	2.09569800
H	3.81802400	1.72352100	2.88417700
H	4.50950700	1.24286800	1.31229100
C	4.19640700	-1.35578200	1.74694400
O	4.08120300	-0.28545400	2.67313900
C	5.20565500	-0.99384800	-0.43629400
C	3.82937800	-0.98343900	-0.64415000
C	3.26394900	-0.65626000	-1.87515200
C	4.13412300	-0.34944900	-2.91976600
C	5.51879400	-0.37054400	-2.72951000
C	6.06568800	-0.68940600	-1.48848700
C	5.54593800	-1.35153800	0.98845400
H	2.17794500	-0.60918700	-2.00837000
H	6.17650900	-0.12523700	-3.55754100
H	7.14168000	-0.69056500	-1.34215400

H	6.23451700	-0.64180900	1.45804800
H	6.01507500	-2.33872900	1.04742200
C	-0.77417000	1.65790600	0.50261500
C	-0.80764500	2.43725900	-0.65705800
C	-1.91762500	1.55345800	1.29319400
C	-1.98397800	3.06048900	-1.05102100
C	-3.10626300	2.16423500	0.91441600
C	-3.11848700	2.90159100	-0.26370700
H	-2.01085000	3.65832200	-1.95327500
H	-3.99527800	2.06732600	1.52508800
H	4.08340400	-2.24952000	2.36060600
H	3.73105800	-0.08577500	-3.89232900
Cl	0.62819800	2.68002700	-1.58093800
Cl	-4.59755100	3.66548000	-0.76127400
Cl	-1.86500200	0.63269200	2.75829200
C	0.08808500	-1.13853900	-0.53778900
O	0.03882300	-0.43407500	-1.66300900
H	0.74192000	-2.05342700	-0.55987900
C	-1.27596200	-1.62032000	0.00106500
C	-1.91850000	-2.55138400	-1.03017000
H	-1.93048700	-0.75159200	0.13086600
H	-1.17871200	-2.12148600	0.97361000
H	-1.86227000	-2.03782200	-1.99544300
H	-1.32697700	-3.47120200	-1.11393000
C	-3.34771300	-2.88775600	-0.68755500
C	-4.35368100	-1.92818300	-0.85124700
C	-3.69955400	-4.13591800	-0.17034200
C	-5.67285800	-2.20956200	-0.51110400
H	-4.09287500	-0.95169400	-1.25471200
C	-5.01990900	-4.42375100	0.17158500
H	-2.92946500	-4.89190400	-0.03786300
C	-6.01127600	-3.46119300	0.00200000
H	-6.43986400	-1.45383300	-0.65067800
H	-5.27364600	-5.40209800	0.56856500
H	-7.04061700	-3.68412100	0.26453600

Re-M1 ($\Phi = -164^\circ$)

0 1

C	-0.42284600	-0.20941800	0.01131300
C	-1.66693200	-1.07026200	1.60475400
C	-2.77744400	0.70906600	0.30529600
H	-2.42312300	1.61590700	-0.19027700
N	-0.57537500	-1.77027700	1.63524300
N	0.18349400	-1.22443700	0.62890900
N	-1.60823000	-0.10436700	0.63346200
C	-2.87963200	-1.06812300	2.47692600
H	-2.66971500	-1.55702500	3.42764900
H	-3.71515100	-1.58193000	1.98271900
C	-3.57907200	1.05822600	1.61351000
O	-3.17162500	0.29313100	2.73888000
C	-5.04223500	0.00546600	-0.01118500
C	-3.75891700	-0.06615600	-0.54560600
C	-3.48988700	-0.78363300	-1.70700000
C	-4.54651600	-1.43133400	-2.34202200
C	-5.83943600	-1.35747700	-1.81703100
C	-6.09695500	-0.64194800	-0.64974700
C	-5.06447000	0.83260400	1.24920200
H	-2.48048600	-0.84699100	-2.10664200
H	-6.65173600	-1.86971800	-2.32238400
H	-7.10179200	-0.59543800	-0.24107000
H	-5.58192900	0.34423000	2.08028700
H	-5.56091200	1.79309200	1.07758900
C	1.45086700	-1.80517600	0.33986200
C	1.54841400	-2.83045100	-0.60054600
C	2.57426700	-1.44564500	1.07689100
C	2.75643000	-3.46773800	-0.83339100
C	3.79727500	-2.07006500	0.86385200
C	3.86727300	-3.07188500	-0.09417400
H	2.83211700	-4.25186500	-1.57624300
H	4.67027100	-1.77883500	1.43423900
H	-3.38385800	2.08964700	1.90701500
H	-4.36355100	-1.99794600	-3.24875500
Cl	0.14638400	-3.29298900	-1.50008200
Cl	5.38963300	-3.86259900	-0.37614800
Cl	2.45365200	-0.18952700	2.26428900
C	0.20672000	0.60285300	-1.13979700

O	1.22857100	-0.04489000	-1.65479400
H	-0.67779500	0.79645900	-1.81825900
C	0.55651400	1.99151900	-0.51723800
C	1.19895300	2.86960800	-1.59154300
H	1.27773700	1.82593600	0.29306100
H	-0.32112000	2.49571000	-0.08578800
H	2.00798700	2.28134100	-2.03495800
H	0.46532900	3.06677400	-2.38307800
C	1.71645500	4.16908000	-1.02999100
C	2.93693000	4.20608400	-0.34709000
C	0.97786600	5.35025600	-1.13316200
C	3.40674300	5.38906900	0.21516200
H	3.52175300	3.29293000	-0.26180900
C	1.44359900	6.53810400	-0.57283300
H	0.02878200	5.33776400	-1.66394900
C	2.66032100	6.56123400	0.10370300
H	4.35843400	5.39849800	0.73786200
H	0.85694500	7.44702200	-0.66702600
H	3.02692500	7.48590600	0.53812200

Re-M1 ($\Phi = 84^\circ$)

0 1

C	0.42585500	0.55471400	-0.27667300
C	0.65547800	2.70491300	-0.70604100
C	-1.72922600	1.89865200	-0.87320400
H	-1.97976100	1.37837400	-1.79877800
N	1.84418800	2.31637400	-0.37600400
N	1.67831800	0.99382000	-0.08997300
N	-0.26837400	1.67325600	-0.61426800
C	0.31890700	4.07964300	-1.19917200
H	1.03056500	4.35299000	-1.98021800
H	0.40575500	4.80944400	-0.38522400
C	-1.92113600	3.43828200	-0.97754800
O	-0.96435400	4.08617000	-1.77540100
C	-2.79408200	2.75483400	1.08797500
C	-2.66390400	1.60692200	0.29404600
C	-3.48258300	0.50544200	0.53709200
C	-4.32753100	0.51915100	1.64605100

C	-4.38491700	1.63129900	2.48452200
C	-3.63616400	2.76990400	2.19266200
C	-2.03512300	3.90714300	0.48999700
H	-3.49636400	-0.35260300	-0.12284400
H	-5.04695700	1.62639900	3.34440800
H	-3.73004100	3.66575400	2.79886700
H	-1.05275100	4.02070500	0.96221100
H	-2.55844500	4.86153500	0.57692900
C	2.80908900	0.17976400	0.16900800
C	3.03028400	-0.34224900	1.44412300
C	3.71541700	-0.10999700	-0.85435700
C	4.12815200	-1.14992500	1.70924800
C	4.82493200	-0.90893500	-0.60804000
C	5.01057500	-1.41977000	0.67077900
H	4.28744800	-1.55502200	2.70065800
H	5.52583500	-1.12987800	-1.40321300
H	-2.88203300	3.59723000	-1.47200700
H	-4.95475800	-0.34472300	1.84200800
Cl	1.91761100	0.01164700	2.72638700
Cl	6.39324000	-2.42462400	0.98250000
Cl	3.49049700	0.54279800	-2.43443400
C	0.24394100	-1.00108600	-0.56078500
O	0.78914500	-1.14161100	-1.74775400
H	0.78266900	-1.46996800	0.30690900
C	-1.21580400	-1.41359300	-0.42937600
C	-1.40227400	-2.90274300	-0.71665100
H	-1.80029100	-0.85317100	-1.16920100
H	-1.59206400	-1.17556300	0.57216300
H	-0.99653100	-3.11143700	-1.71009700
H	-0.82106000	-3.48705100	0.00828500
C	-2.86369500	-3.27071300	-0.63393300
C	-3.62720400	-3.47987100	-1.78417400
C	-3.50492500	-3.32585100	0.60936600
C	-4.99419200	-3.74096100	-1.69816400
H	-3.14346300	-3.43536600	-2.75669800
C	-4.86915800	-3.58452900	0.70083700
H	-2.92362600	-3.16151100	1.51446100
C	-5.61973500	-3.79275000	-0.45595000

H	-5.56935800	-3.90430200	-2.60448700
H	-5.34720000	-3.62926000	1.67495100
H	-6.68360500	-3.99629500	-0.38763700

Si -M1 ($\Phi = -93^\circ$)

0 1

C	0.32870300	-0.30963400	0.62856700
C	0.28879500	-2.43092500	1.21598900
C	-1.94691900	-1.44132200	0.91916600
H	-2.36944300	-0.46308300	1.14768000
N	1.54941900	-2.16721500	1.07766200
N	1.55435000	-0.84632800	0.71566700
N	-0.48793200	-1.32148200	0.97214500
C	-0.41023200	-3.67547800	1.65316000
H	0.27574700	-4.32868600	2.19180200
H	-0.81350000	-4.21414300	0.78429400
C	-2.46683400	-2.50457300	1.95508600
O	-1.43086200	-3.27353700	2.54646700
C	-3.25120700	-3.04536000	-0.28203500
C	-2.38172400	-1.96828900	-0.42957100
C	-1.97320200	-1.50640600	-1.67913400
C	-2.49312000	-2.14692300	-2.80283300
C	-3.38397700	-3.21537500	-2.66952000
C	-3.76586600	-3.67662500	-1.41100700
C	-3.48489800	-3.36903300	1.17224200
H	-1.25021100	-0.68938900	-1.76666600
H	-3.77398700	-3.70118000	-3.55850600
H	-4.44363700	-4.51953700	-1.31423500
H	-3.33074800	-4.42697300	1.40739700
H	-4.50620700	-3.11736600	1.47520700
C	2.75309000	-0.22066700	0.28956200
C	3.24421400	-0.47291200	-0.99394700
C	3.44493500	0.64844300	1.13152500
C	4.41176800	0.13683400	-1.43298000
C	4.61209500	1.27238000	0.71090600
C	5.07449300	1.00350400	-0.57137000
H	4.79232700	-0.05876600	-2.42769100
H	5.14430100	1.94809600	1.36843300

H	-2.93593800	-1.99792800	2.79851500
H	-2.19627800	-1.81658900	-3.79295000
Cl	2.42015800	-1.57661700	-2.03232000
Cl	6.53500000	1.77310400	-1.11337800
Cl	2.84121600	0.95865500	2.72625700
C	0.10249000	1.05054300	-0.08731500
O	0.34006500	0.79741000	-1.37000500
H	0.84659300	1.72087000	0.42363800
C	-1.27685100	1.66229700	0.22298800
C	-1.35668200	3.05455900	-0.41105800
H	-1.46418300	1.72833500	1.30480800
H	-2.05884200	1.04208300	-0.23276800
H	-0.59552300	3.70122800	0.04238300
H	-1.10245800	2.94162200	-1.46933300
C	-2.72115800	3.67446400	-0.24939300
C	-3.00380200	4.52104000	0.82568800
C	-3.74963900	3.37275200	-1.14722900
C	-4.27802000	5.05640200	0.99957700
H	-2.21249900	4.76459900	1.53090400
C	-5.02525700	3.90424200	-0.97803000
H	-3.54117900	2.71571600	-1.98860800
C	-5.29351200	4.74926000	0.09735300
H	-4.47730900	5.71666800	1.83823800
H	-5.80992000	3.66348200	-1.68888800
H	-6.28603300	5.16852900	0.22850900

Si -M1 ($\Phi = 168^\circ$)

0 1

C	-0.24687600	-0.73088400	-0.66947100
C	0.07592500	-2.68430800	0.28886600
C	2.05269500	-1.82396800	-0.87990100
H	2.21914400	-1.14317500	-1.71968300
N	-1.14177000	-2.36788400	0.60456500
N	-1.32069600	-1.14636600	0.00520100
N	0.65417100	-1.71120200	-0.48421700
C	0.87039000	-3.93393400	0.49097700
H	0.21545800	-4.76033900	0.76522100
H	1.62757100	-3.79564900	1.27280000

C	2.38079800	-3.30195700	-1.28865000
O	1.44834900	-4.24181900	-0.76725300
C	3.98393100	-2.52426100	0.34215600
C	2.98489700	-1.55426200	0.28435400
C	2.90136800	-0.53908700	1.23052300
C	3.86557100	-0.48895800	2.23469200
C	4.88346200	-1.44287200	2.28542500
C	4.94752300	-2.46964300	1.34442900
C	3.81106100	-3.53998700	-0.76034300
H	2.09756400	0.19106500	1.20121600
H	5.62505000	-1.39254900	3.07612600
H	5.72769600	-3.22252100	1.40252500
H	3.91908900	-4.57428500	-0.42294900
H	4.53997100	-3.37591300	-1.56139400
C	-2.57732000	-0.49432700	0.16450600
C	-2.79134300	0.35716600	1.24357200
C	-3.64107100	-0.81105600	-0.67695400
C	-4.04095600	0.91551000	1.47661500
C	-4.89921500	-0.26807200	-0.46759100
C	-5.07847200	0.59027500	0.61200400
H	-4.19746300	1.58845900	2.31043200
H	-5.71897000	-0.50562100	-1.13395700
H	2.31471400	-3.42438200	-2.37025900
H	3.81966300	0.29305500	2.98501600
Cl	-1.46728300	0.74755300	2.29270200
Cl	-6.65164300	1.27711800	0.88758900
Cl	-3.36930000	-1.86317200	-2.02265400
C	-0.22489100	0.56719000	-1.51430200
O	-1.43298300	1.08305500	-1.56999700
H	0.21749100	0.19213200	-2.48622600
C	0.86347500	1.49785400	-0.90472300
C	0.89973800	2.81134200	-1.68708600
H	1.86071800	1.03355000	-0.90943300
H	0.59369900	1.71175000	0.13833900
H	1.17576100	2.60192900	-2.72820600
H	-0.11984600	3.20660100	-1.69445700
C	1.86765900	3.79789300	-1.08541800
C	3.16842900	3.92466000	-1.57930300

C	1.49821200	4.57275400	0.01934100
C	4.07697900	4.80165100	-0.99093600
H	3.46867100	3.32991600	-2.43877900
C	2.40203100	5.44964200	0.61227800
H	0.48843300	4.48434000	0.41375700
C	3.69631900	5.56751200	0.10820900
H	5.08150500	4.88970800	-1.39360200
H	2.09588400	6.04548400	1.46683200
H	4.40123100	6.25401800	0.56639500

Si -M1 ($\Phi = 34^\circ$)

0 1

C	0.87431100	0.15362700	-0.29987800
C	2.38507200	-1.24432200	-1.07782200
C	3.24582800	1.02116400	-0.62093300
H	2.73679200	1.99518100	-0.62815700
N	1.31213700	-1.96772200	-0.98045100
N	0.38315000	-1.08224900	-0.48699300
N	2.15649700	0.04268700	-0.67775300
C	3.73203400	-1.53489000	-1.65564300
H	3.69712200	-2.43288800	-2.27166600
H	4.47568100	-1.67057900	-0.85904400
C	4.22295200	0.80900900	-1.82820300
O	4.04217900	-0.43804800	-2.49421300
C	5.45495400	0.74988000	0.25818000
C	4.10549800	0.79289200	0.60086600
C	3.68845800	0.63600900	1.91829900
C	4.65424500	0.43492800	2.90238100
C	6.00918600	0.39429200	2.56525700
C	6.41883200	0.55192700	1.24254700
C	5.63998900	0.94566100	-1.22608200
H	2.63178600	0.66255500	2.17434800
H	6.75028700	0.23436600	3.34171900
H	7.47281500	0.51317400	0.98374900
H	6.31462700	0.21547900	-1.68289500
H	6.04484200	1.94085000	-1.43790100
C	-0.91326600	-1.57198800	-0.18068700
C	-1.24730000	-1.89607000	1.13526300

C	-1.85695600	-1.75659100	-1.19174600
C	-2.50795300	-2.38228100	1.45171200
C	-3.12291900	-2.24628000	-0.89984800
C	-3.42768300	-2.55066300	0.42198400
H	-2.76398600	-2.62404200	2.47579500
H	-3.85486200	-2.38113500	-1.68619800
H	4.03445800	1.55311000	-2.60203100
H	4.35231100	0.30757600	3.93671700
Cl	-0.08465700	-1.65214400	2.39394700
Cl	-5.00732400	-3.16228100	0.79867400
Cl	-1.45501900	-1.34449900	-2.82064900
C	0.25828000	1.52296500	0.15534000
O	0.82321200	2.49532000	-0.54181700
H	0.47428200	1.50833600	1.26347800
C	-1.28562800	1.47133000	0.03806400
C	-1.85331100	2.85127900	0.37787900
H	-1.72712100	0.72472400	0.71047300
H	-1.56443300	1.20980100	-0.99239900
H	-1.55797300	3.11289300	1.40213200
H	-1.38108000	3.57537600	-0.29004400
C	-3.35474800	2.88769700	0.25147100
C	-4.17454500	2.54966500	1.33218600
C	-3.96095500	3.21292000	-0.96530400
C	-5.56119500	2.53890700	1.20446200
H	-3.71576900	2.29689300	2.28556900
C	-5.34698600	3.20373800	-1.09936900
H	-3.33525300	3.47960300	-1.81368400
C	-6.15257000	2.86658700	-0.01360400
H	-6.18033600	2.27793800	2.05742000
H	-5.79939300	3.46440000	-2.05147300
H	-7.23314900	2.86256200	-0.11542900

R2_{DCE}

0 1

C	2.33722300	-1.54456300	-0.07405300
C	2.79929700	0.79570100	0.01207800
C	3.48314100	-0.57489200	0.11049500
H	2.22545900	-2.28641300	0.71538300

H	2.33850800	-2.03861000	-1.04634700
H	4.25072800	-0.65972000	-0.65862100
H	3.96097000	-0.66155700	1.08834200
N	1.44107300	0.67379100	-0.05001100
N	1.13809300	-0.63477900	-0.03576400
O	3.40037300	1.85939900	0.00936200
C	-0.06054300	-1.13203500	-0.01920500
H	-0.09214100	-2.21688200	-0.01691200
C	-1.32881800	-0.42066700	-0.00757000
C	-2.48184200	-1.22662800	0.02504500
C	-1.47487200	0.97746200	-0.02670900
C	-3.74633600	-0.65719000	0.03851200
H	-2.37539400	-2.30783900	0.04034800
C	-2.74816500	1.53797800	-0.01299300
H	-0.59350300	1.60262400	-0.05196100
C	-3.88292000	0.73075100	0.01950300
H	-4.62495500	-1.29293500	0.06307900
H	-2.85289900	2.61790100	-0.02837800
H	-4.87090100	1.17965600	0.02997800

M4_{NHCl}

0 1

C	0.98007300	-0.22344000	-0.34000600
C	2.14766400	-2.05035700	-0.64306900
C	3.36953500	0.12124300	-1.10727300
H	3.07884200	0.62303600	-2.03017700
N	0.97485700	-2.47517100	-0.27506900
N	0.25986700	-1.32418900	-0.08718800
N	2.19327400	-0.68022200	-0.68947600
C	3.34405400	-2.87326300	-1.00860600
H	3.02534400	-3.72847300	-1.60572000
H	3.82928300	-3.25137900	-0.10073800
C	4.56958500	-0.85142200	-1.25472700
O	4.22244600	-2.10746100	-1.80217100
C	4.92919400	0.50117100	0.65841900
C	3.84782900	1.06338600	-0.02598100
C	3.38033100	2.33827400	0.28160100
C	4.01204200	3.04034500	1.30786300

C	5.08735500	2.48004100	1.99978700
C	5.55767800	1.20791400	1.67737100
C	5.25999400	-0.86859700	0.12497600
H	2.55083200	2.75646900	-0.28060300
H	5.56992800	3.04498800	2.79121800
H	6.40415000	0.78000400	2.20594000
H	4.84180000	-1.64114700	0.78060300
H	6.33177600	-1.05881100	0.03913700
C	-1.13646600	-1.37736800	0.17528200
C	-1.60901600	-1.65421500	1.45716800
C	-2.04902600	-1.12483600	-0.85182500
C	-2.97087600	-1.65944500	1.72837300
C	-3.41366300	-1.11706400	-0.60256200
C	-3.85202200	-1.38055500	0.69004200
H	-3.33117700	-1.86527700	2.72871800
H	-4.11598200	-0.90148300	-1.39762200
H	5.24943700	-0.40252300	-1.98197500
H	3.66947300	4.03714400	1.56611500
Cl	-0.48128500	-1.94739400	2.73758600
Cl	-5.55740300	-1.37178400	1.01458500
Cl	-1.47377000	-0.82134500	-2.45368300
C	0.49686300	1.19470700	-0.43993500
O	0.91111900	1.80829600	-1.48114700
C	-0.31806200	1.58285600	0.58195300
C	-1.09235200	2.86734600	0.51754400
H	-0.54394900	0.88779200	1.38427800
H	-1.17193900	3.34336500	1.50085100
H	-0.57259200	3.55724000	-0.15566900
C	-2.47809800	2.57560400	-0.02645200
C	-3.59089200	2.47219600	0.80923800
C	-2.63625700	2.31569000	-1.39298400
C	-4.84098000	2.13011800	0.29302900
H	-3.47790100	2.66260300	1.87395600
C	-3.88260300	1.98155200	-1.91266100
H	-1.75793100	2.35995800	-2.03338100
C	-4.99195600	1.88730400	-1.06970900
H	-5.69694500	2.05290400	0.95678600
H	-3.98988900	1.78561600	-2.97592700

H	-5.96486400	1.62214600	-1.47256100
---	-------------	------------	-------------

TS5SR_{NHCl}

0 1

C	0.46388600	-0.25961800	-0.33341000
C	1.54902000	-0.54454800	-2.20222400
C	2.99011900	-0.55392300	-0.19265900
H	2.90797600	-0.07134100	0.77881800
N	0.29935000	-0.50085500	-2.56199500
N	-0.37066600	-0.33402500	-1.38028800
N	1.68393300	-0.43242000	-0.84381900
C	2.81883500	-0.52312900	-2.99199200
H	2.62104100	-0.22130200	-4.02010500
H	3.29808800	-1.51097500	-2.98831600
C	4.08180800	0.14716900	-1.06709900
O	3.62480200	0.46770200	-2.38131200
C	4.70523100	-2.15737600	-0.62379200
C	3.42013800	-1.99813000	-0.11086600
C	2.70229900	-3.06555400	0.41675900
C	3.29223200	-4.32724500	0.40203500
C	4.57650700	-4.50063200	-0.12159300
C	5.29366700	-3.41924300	-0.63103100
C	5.27328500	-0.83574900	-1.08027900
H	1.71559000	-2.90272800	0.84251600
H	5.02219500	-5.49033900	-0.12842300
H	6.29352700	-3.56042100	-1.03046000
H	5.72855000	-0.87392400	-2.07463900
H	6.03731800	-0.48671400	-0.37843800
C	-1.77735200	-0.55661500	-1.32684800
C	-2.26296400	-1.77844200	-0.84858000
C	-2.67707900	0.40456700	-1.78811600
C	-3.62480400	-2.03719500	-0.81614800
C	-4.04484900	0.16407000	-1.76282400
C	-4.49593400	-1.05686800	-1.27683800
H	-3.99493100	-2.98115500	-0.43711200
H	-4.73867300	0.91727900	-2.11491400
H	4.33601000	1.10058200	-0.60523700
H	2.75516900	-5.18049900	0.80340300

C	0.10821100	-0.04780900	1.11322100
O	0.72906500	-0.72797900	1.94452000
C	-0.84638700	0.98102000	1.35117800
C	-1.65258700	0.87375900	2.63325300
H	-1.43323300	1.27690100	0.48401800
H	-0.98746600	0.59105500	3.45475900
H	-2.09013300	1.84714700	2.88262200
C	-2.75946300	-0.15021400	2.49993300
C	-2.49150600	-1.51052200	2.68993100
C	-4.05820300	0.23818300	2.16126100
C	-3.50654300	-2.45635800	2.56876000
H	-1.47741200	-1.81700900	2.93421600
C	-5.07687200	-0.70540200	2.04450900
H	-4.27517200	1.29223000	2.00440500
C	-4.80483900	-2.05571400	2.25315700
H	-3.28475700	-3.50781700	2.72599500
H	-6.08334300	-0.38648900	1.79092500
H	-5.59808800	-2.79177100	2.16354100
C	1.64736400	2.14560500	3.53797900
C	3.54121400	1.71773100	2.16976600
C	3.16304800	2.04662500	3.62489700
H	1.19397900	2.93499000	4.14141200
H	1.17659500	1.18526200	3.77372800
H	3.51555300	1.26824700	4.30143700
H	3.62784500	2.99529300	3.91115900
N	2.52581000	1.97858700	1.33761000
N	1.46368000	2.44321400	2.10425200
O	4.64299800	1.25278200	1.82777400
C	0.26034500	2.65847100	1.55430900
H	-0.43085300	3.08041000	2.28311300
C	0.14661500	3.29835400	0.20658400
C	-0.86012200	4.25836300	0.04670700
C	0.97163400	3.00139800	-0.88840600
C	-1.02625900	4.92869700	-1.16164400
H	-1.51255200	4.49230600	0.88434100
C	0.80061600	3.67165600	-2.09630200
H	1.76649500	2.27549600	-0.77591500
C	-0.19152900	4.64008400	-2.23913900

H	-1.80474800	5.67856800	-1.25936300
H	1.45287900	3.43200500	-2.93072800
H	-0.31445200	5.16328300	-3.18207100
Cl	-2.08111800	1.92307400	-2.34547100
Cl	-6.20144900	-1.37100500	-1.24147900
Cl	-1.15892500	-2.99812400	-0.30949500

M4_{NHC2}

0 1

C	0.73398900	-0.40147300	-0.28513700
C	2.04165000	-2.14030700	-0.50272300
C	3.08505700	0.08578200	-1.10233300
H	2.74650700	0.50582000	-2.04967300
N	0.90159300	-2.63140700	-0.10848600
N	0.09777000	-1.53428800	0.02069100
N	1.98258500	-0.77797200	-0.62027600
C	3.29680800	-2.88820900	-0.82999900
H	3.04280100	-3.79668100	-1.37775200
H	3.81390100	-3.17869400	0.09248200
C	4.35889500	-0.79300100	-1.20359400
O	4.11420600	-2.10430600	-1.67117500
C	4.61911800	0.70004300	0.62209400
C	3.49558900	1.12949700	-0.09021300
C	2.92746200	2.38044600	0.13356000
C	3.49926400	3.19688400	1.10799500
C	4.61437000	2.76943300	1.83146000
C	5.18669900	1.52046600	1.59074200
C	5.05473100	-0.67076500	0.16949900
H	2.06748700	2.69124300	-0.45238900
H	5.04838300	3.42222300	2.58243100
H	6.06419100	1.19949400	2.14391100
H	4.70083600	-1.43258800	0.87387200
H	6.13788600	-0.78193900	0.08606400
C	-1.30155100	-1.65946100	0.32854100
C	-1.67159500	-1.91386200	1.65060000
C	-2.21780000	-1.43752000	-0.70019100
C	-3.03377800	-1.91806900	1.93991500
C	-3.56914000	-1.44983900	-0.35734000

C	-3.99197500	-1.66886800	0.95292600
H	-3.35332400	-2.09699900	2.96391700
H	-4.30656700	-1.25191100	-1.13011300
H	4.99735900	-0.33491100	-1.96232000
H	3.07780400	4.17818600	1.30093800
C	0.15799300	0.97505800	-0.45486700
O	0.49197400	1.52802600	-1.56358000
C	-0.63709500	1.40546500	0.56199700
C	-1.44997700	2.66248500	0.43164900
H	-0.83812700	0.74865000	1.40246700
H	-1.55150600	3.17622300	1.39392300
H	-0.94416800	3.34010500	-0.26461500
C	-2.82274400	2.31443700	-0.11107200
C	-3.93257900	2.18573600	0.72485900
C	-2.97197000	2.03195600	-1.47442500
C	-5.16995500	1.79412100	0.21331100
H	-3.82677100	2.39362100	1.78716600
C	-4.20494000	1.64419800	-1.98869300
H	-2.09685000	2.10724200	-2.11638100
C	-5.31114100	1.52488600	-1.14530400
H	-6.02437100	1.70187400	0.87786500
H	-4.30575100	1.43252900	-3.04959900
H	-6.27430600	1.22236200	-1.54539300
C	-0.62830800	-2.12839600	2.71499000
H	-0.02564400	-3.01619900	2.50342200
H	0.05792400	-1.27595400	2.76693800
H	-1.09667300	-2.25115900	3.69245500
C	-5.45555800	-1.62654100	1.30693200
H	-5.80652800	-2.60304800	1.65415100
H	-5.63498000	-0.90724000	2.11148500
H	-6.05774800	-1.32773900	0.44631600
C	-1.76569300	-1.17715700	-2.11258600
H	-1.21823900	-0.23142300	-2.19134700
H	-1.10307700	-1.97616500	-2.46215600
H	-2.62849300	-1.12557000	-2.77908900

TS5SR_{NHC2}

0 1

C	0.26361500	-0.31180500	-0.42600500
C	1.51182400	-0.46677000	-2.20328300
C	2.78794300	-0.50416000	-0.09193500
H	2.61619000	-0.07038400	0.89076900
N	0.29044100	-0.48555600	-2.65792800
N	-0.48029400	-0.40750100	-1.53237500
N	1.53390500	-0.39551500	-0.83971000
C	2.83473400	-0.35632900	-2.89225600
H	2.69987200	-0.00810800	-3.91613100
H	3.35317900	-1.32435000	-2.90436600
C	3.92234000	0.26505500	-0.84683900
O	3.55764400	0.62958600	-2.17840900
C	4.58026100	-2.03978100	-0.45946600
C	3.25530000	-1.93883100	-0.04213700
C	2.52922900	-3.05131900	0.36861300
C	3.15422500	-4.29580200	0.33602000
C	4.48047300	-4.40931400	-0.08999800
C	5.20392200	-3.28442400	-0.48368000
C	5.14161900	-0.68248300	-0.80637500
H	1.50620700	-2.93816400	0.71867200
H	4.95371000	-5.38590400	-0.11283500
H	6.23555900	-3.37948800	-0.80926300
H	5.67863800	-0.65925600	-1.75946700
H	5.83320100	-0.34670500	-0.02686200
C	-1.89406100	-0.68067200	-1.59404000
C	-2.34250600	-1.89920800	-1.07431800
C	-2.73970500	0.26459100	-2.17879200
C	-3.71305900	-2.14430600	-1.13049100
C	-4.10108000	-0.02826100	-2.20134300
C	-4.60391500	-1.22078000	-1.67579900
H	-4.09382500	-3.07595000	-0.72186400
H	-4.78597400	0.69786300	-2.63229900
H	4.11152200	1.20405600	-0.32824600
H	2.61062500	-5.18223500	0.64620200
C	-0.19983600	-0.14843000	0.99826100
O	0.38372000	-0.83861200	1.85245000
C	-1.19895600	0.84098100	1.20193200
C	-2.04742800	0.70299800	2.45391100

H	-1.76177600	1.11814400	0.31240100
H	-1.40426700	0.44193900	3.29920700
H	-2.52685600	1.66072100	2.68772300
C	-3.11253700	-0.35824800	2.28403500
C	-2.81925000	-1.70275200	2.53799000
C	-4.39623600	-0.02182200	1.84866800
C	-3.79232300	-2.68506300	2.37127200
H	-1.81841200	-1.96796800	2.87050800
C	-5.37379600	-1.00137200	1.68758200
H	-4.63350200	1.01975100	1.64432300
C	-5.07584600	-2.33598800	1.95270700
H	-3.55113400	-3.72366900	2.57815900
H	-6.36988300	-0.72141700	1.35712400
H	-5.83772300	-3.10010200	1.83088200
C	1.09557400	2.10009100	3.54145500
C	3.10953300	1.76810100	2.33374500
C	2.60116700	2.07694500	3.75327400
H	0.55011400	2.85328200	4.11411000
H	0.66126800	1.11103700	3.72264600
H	2.93552200	1.31648100	4.45874200
H	2.99327800	3.04761100	4.07285300
N	2.15425300	1.98754200	1.42255600
N	1.01550400	2.40807300	2.10092500
O	4.25500800	1.35318600	2.08313600
C	-0.14797500	2.57717600	1.46138400
H	-0.91134400	2.96785500	2.13291800
C	-0.18997000	3.19997800	0.10328300
C	-1.25427000	4.07471800	-0.15400100
C	0.75334600	2.97491800	-0.91114800
C	-1.36314000	4.73349600	-1.37480800
H	-1.99883900	4.24941000	0.61870300
C	0.63753900	3.63356700	-2.13344600
H	1.59108100	2.31564500	-0.72433200
C	-0.41189500	4.51865700	-2.37006200
H	-2.18938200	5.41593700	-1.54637900
H	1.38122400	3.45071100	-2.90332400
H	-0.49207800	5.03200300	-3.32285600
C	-1.39859500	-2.91380900	-0.48210500

H	-0.51621500	-3.05827000	-1.11499900
H	-1.05693000	-2.60777700	0.51258000
H	-1.90246800	-3.87585700	-0.37583500
C	-2.19062800	1.54954200	-2.72998000
H	-1.58356100	1.36715200	-3.62222900
H	-2.99848600	2.23439800	-2.99267500
H	-1.54346800	2.04141700	-1.99867900
C	-6.08094500	-1.51057500	-1.71286700
H	-6.66044000	-0.62083100	-1.45310200
H	-6.39021300	-1.82427100	-2.71504500
H	-6.34018900	-2.30834600	-1.01317400

M4_{NHC3}

0 1

C	-0.70958400	-0.71331900	-0.05424400
C	-1.51754900	-2.64048000	0.60195500
C	-3.20552000	-0.77829900	0.33401800
H	-3.16343800	-0.05720900	1.15344700
N	-0.23705500	-2.84433200	0.50828200
N	0.25147800	-1.63546300	0.09096800
N	-1.84783000	-1.35531200	0.25230400
C	-2.58407100	-3.57931200	1.08092100
H	-2.18455700	-4.21429400	1.87225000
H	-2.92928800	-4.21285700	0.25229500
C	-4.16830700	-1.93035100	0.64221100
O	-3.64382100	-2.81627800	1.61385200
C	1.65255200	-1.40082500	0.03907100
C	2.40769700	-1.83020600	-1.05066900
C	2.27787900	-0.70260900	1.07535200
C	3.76606400	-1.55221400	-1.12909200
C	3.63162700	-0.40674200	1.01465800
C	4.35333300	-0.83293200	-0.09444500
H	4.34607700	-1.87928800	-1.98301100
H	4.10824400	0.15103700	1.81052300
H	-5.09767700	-1.51850000	1.03797400
Cl	1.63052200	-2.67762200	-2.34443900
Cl	6.04727400	-0.46432500	-0.18237600
Cl	1.35674600	-0.20509100	2.44984300

C	-0.55126500	0.76963800	-0.26469000
O	-1.26156200	1.47641100	0.52708700
C	0.34157600	1.10629600	-1.23858200
C	0.81280500	2.52157200	-1.40972100
H	0.85307400	0.32494800	-1.79155300
H	0.99182800	2.76309500	-2.46289200
H	0.03866800	3.19762800	-1.03177200
C	2.08882900	2.71663700	-0.61301000
C	3.34467000	2.72927300	-1.22119100
C	2.01596800	2.80493100	0.78235900
C	4.50624700	2.84167600	-0.45616200
H	3.41460000	2.65185100	-2.30369900
C	3.17122600	2.92619600	1.54754000
H	1.03680100	2.75452300	1.25409200
C	4.42343400	2.94485200	0.92980500
H	5.47631800	2.84771100	-0.94445200
H	3.09745500	2.99791600	2.62916300
H	5.32695400	3.03398400	1.52544400
H	-4.39413800	-2.48286100	-0.28257000
C	-3.59587600	-0.05645100	-0.96176800
H	-2.74354900	0.52684800	-1.31637100
H	-3.84144100	-0.79750700	-1.73028500
C	-4.76176300	0.86937000	-0.70579200
C	-6.06520600	0.53018500	-1.07002900
C	-4.52519500	2.08421100	-0.05328200
C	-7.12303100	1.39397200	-0.78829500
H	-6.25306400	-0.41162400	-1.58009800
C	-5.58113700	2.94531100	0.22800800
H	-3.50067900	2.33091500	0.22215000
C	-6.88256100	2.60160900	-0.13873100
H	-8.13342400	1.12288800	-1.07785400
H	-5.39055400	3.88848100	0.73059600
H	-7.70556500	3.27470200	0.07956800

TS5SR_{NHC3}

0 1

C	0.21726400	-0.02740600	-0.74079400
C	0.92164400	0.60908900	-2.70109900

C	2.71304600	-0.15882900	-1.13099400
H	2.80561700	0.07512500	-0.06995800
N	-0.37577300	0.67234800	-2.79065600
N	-0.80576200	0.25643900	-1.56079700
N	1.31875100	0.14528400	-1.47631100
C	2.00479900	1.10645000	-3.60663000
H	1.60774000	1.85791900	-4.28885100
H	2.44645700	0.28419200	-4.18650200
C	3.64792100	0.77047600	-1.95546700
O	2.95644300	1.71555900	-2.75965300
C	-2.16452600	-0.13155300	-1.37534400
C	-2.49432300	-1.49159200	-1.35485400
C	-3.17788900	0.81986200	-1.25596800
C	-3.81059700	-1.89980600	-1.20212900
C	-4.50150800	0.42992100	-1.09865700
C	-4.79565800	-0.92763300	-1.07265200
H	-4.05870900	-2.95311900	-1.18269600
H	-5.28118400	1.17406000	-0.99442600
H	4.25685900	1.33916500	-1.25097100
C	0.15384200	-0.42692300	0.70623500
O	0.97635600	-1.26716700	1.10281200
C	-0.77956000	0.30689600	1.49558000
C	-1.29706000	-0.39391400	2.73987900
H	-1.54789200	0.83914200	0.93927100
H	-0.46266700	-0.89507200	3.24022200
H	-1.70893000	0.34129700	3.44016700
C	-2.36839900	-1.40465700	2.39104200
C	-2.01861000	-2.68021400	1.93416600
C	-3.72247800	-1.07516800	2.49180300
C	-3.00218000	-3.61103700	1.60917400
H	-0.96604000	-2.93486400	1.83657100
C	-4.70871600	-2.00538200	2.16986900
H	-4.00565300	-0.08454600	2.83969100
C	-4.35107800	-3.27903300	1.73318300
H	-2.71412900	-4.59916200	1.26261800
H	-5.75652100	-1.73658000	2.26320300
H	-5.11878900	-4.00635900	1.48654200
C	2.07935100	0.80244100	3.49547100

C	3.67540900	1.27104300	1.79166100
C	3.58295300	0.92035200	3.28875600
H	1.70314900	1.21763900	4.43326200
H	1.74718500	-0.23625100	3.39501200
H	4.12920100	0.00006800	3.49977600
H	4.02664000	1.72981500	3.87670000
N	2.48272000	1.64421000	1.30971900
N	1.57403600	1.59579800	2.35915200
O	4.72448300	1.19776500	1.13115000
C	0.27202100	1.85923500	2.16199100
H	-0.26351900	1.88236400	3.11100200
C	-0.13472000	2.97221500	1.24431100
C	-1.18034900	3.79781600	1.67503400
C	0.45984700	3.23452400	0.00143300
C	-1.60471400	4.87774400	0.90625700
H	-1.65736000	3.59993400	2.63178100
C	0.03310700	4.31592000	-0.76439400
H	1.28334200	2.61998200	-0.33867000
C	-0.99393700	5.14466600	-0.31710700
H	-2.40846900	5.51222300	1.26598800
H	0.51283900	4.50991800	-1.71908200
H	-1.31533000	5.99081600	-0.91607300
Cl	-2.77016700	2.49499200	-1.24976700
Cl	-6.44401700	-1.43008600	-0.87464100
Cl	-1.25926300	-2.68931100	-1.54486600
H	4.29683700	0.15282100	-2.59257900
C	2.96981400	-1.65305300	-1.37467200
H	2.16826400	-2.20985100	-0.87911700
H	2.93205300	-1.86975500	-2.44907200
C	4.30339900	-2.05851200	-0.79508000
C	5.37847500	-2.41876700	-1.60754400
C	4.47010200	-2.05671900	0.59381800
C	6.60207700	-2.77862400	-1.04396500
H	5.25564200	-2.42373700	-2.68789900
C	5.68803100	-2.41786500	1.15785700
H	3.62921100	-1.77224900	1.22410200
C	6.75812500	-2.77926200	0.33901600
H	7.43117800	-3.05878000	-1.68594600

H	5.80628300	-2.41528700	2.23695600
H	7.70968700	-3.05997300	0.77929300

TS5RR_{L3} (M06-2X/SMD)

0 1

C	-0.13935700	-0.54989200	-0.36006100
C	-0.99424500	-2.05342000	-1.72133800
C	-2.56994600	-1.31248800	-0.00170000
H	-2.43531500	-1.09115900	1.05913600
N	0.21274900	-1.88272700	-2.15567300
N	0.73038600	-0.93823500	-1.31293000
N	-1.24913100	-1.27525900	-0.62553800
C	-2.08153900	-2.94132600	-2.22416800
H	-1.66079500	-3.71135900	-2.87166900
H	-2.81046700	-2.35095900	-2.79798000
C	-3.23787400	-2.73349600	-0.12939200
O	-2.67030400	-3.57815100	-1.11441800
C	-4.75778500	-1.01291300	-0.91263600
C	-3.54320500	-0.36962900	-0.67847200
C	-3.33207900	0.94938200	-1.06910700
C	-4.37320300	1.62341500	-1.70659700
C	-5.59562200	0.98809200	-1.93576000
C	-5.79762500	-0.33247900	-1.53946500
C	-4.72687800	-2.43380700	-0.41284100
H	-2.37900100	1.44550900	-0.89361100
H	-6.39458600	1.52673100	-2.43604000
H	-6.74558200	-0.82787000	-1.72870600
H	-5.12347300	-3.15608300	-1.13200900
H	-5.31183900	-2.53360200	0.50830800
C	2.08111400	-0.55428100	-1.54942500
C	2.37754200	0.55873400	-2.33871900
C	3.11871500	-1.37485700	-1.11257800
C	3.68922000	0.90124400	-2.62355300
C	4.44461100	-1.05656200	-1.39189800
C	4.70509700	0.08712400	-2.13184900
H	3.91591900	1.77694700	-3.21967600
H	5.24690700	-1.69635300	-1.04363600
H	-3.09590500	-3.28365200	0.79947500

H	-4.22643500	2.64980900	-2.02603100
Cl	1.08714300	1.51545400	-2.98498200
Cl	6.35743400	0.50639000	-2.48203100
Cl	2.75717500	-2.81973300	-0.23279200
C	0.13826200	0.67152700	0.50032200
O	1.16919000	1.28811000	0.15865800
C	-0.70364800	1.04400500	1.56427800
C	-0.66438200	2.49955000	1.98322100
H	-1.65465300	0.53619000	1.69211300
H	-1.05434000	2.60958600	3.00185800
H	0.37824200	2.83070100	1.98302900
C	-1.47250300	3.36812400	1.04350500
C	-2.80432000	3.68370600	1.32416400
C	-0.91330500	3.81874700	-0.15877700
C	-3.56325000	4.43791900	0.43158300
H	-3.24889700	3.33592000	2.25411900
C	-1.67135300	4.56761200	-1.05535600
H	0.11984300	3.56520200	-0.38207300
C	-2.99802300	4.88432600	-0.76084200
H	-4.59608300	4.67726500	0.66787000
H	-1.22341000	4.91517400	-1.98209900
H	-3.58629000	5.47636900	-1.45576100
C	-1.34831800	-1.56737300	3.74320100
C	-0.54413000	-2.95203700	1.99741000
C	-1.46210900	-2.99138700	3.23419600
H	-1.31826600	-1.45586400	4.82752900
H	-2.14341700	-0.92364200	3.33754800
H	-2.47783600	-3.28842700	2.97085600
H	-1.06362500	-3.71725700	3.94957300
N	0.29181600	-1.89270700	2.05623700
N	-0.05739400	-1.15300400	3.16438500
O	-0.59583600	-3.76384100	1.07101600
C	0.36458600	0.09770500	3.29515900
C	1.74080300	0.55958200	3.05937500
C	2.12996600	1.74578900	3.69888900
C	2.67386200	-0.11985000	2.26419200
C	3.41825800	2.24487100	3.54938700
H	1.41460200	2.27280700	4.32570700

C	3.96647700	0.37615400	2.13042300
H	2.37158100	-1.03343700	1.76784500
C	4.34270000	1.55766600	2.76482600
H	3.70293900	3.16306100	4.05350100
H	4.68242100	-0.16294600	1.51631900
H	5.35138500	1.94243600	2.65005400
H	-0.16587600	0.64070700	4.07613000

TS5RS_{L3} (M06-2X/SMD)

0 1

C	0.58483000	-0.53604100	-0.32941100
C	0.32735400	-1.61024900	-2.22481000
C	-1.77574300	-1.20571400	-1.03172600
H	-2.01550800	-1.13743100	0.02909400
N	1.60545200	-1.41060500	-2.14737600
N	1.75798400	-0.74277400	-0.96029700
N	-0.32975500	-1.08132200	-1.14849500
C	-0.49134500	-2.39398400	-3.19615500
H	0.15492200	-3.02759600	-3.80395700
H	-1.06080100	-1.72430200	-3.85432700
C	-2.25797900	-2.59400300	-1.56717200
O	-1.33079900	-3.23698800	-2.43188400
C	-3.55891100	-0.80682100	-2.56324900
C	-2.51637100	-0.18980000	-1.87305900
C	-2.27214100	1.17465400	-1.99424600
C	-3.10692100	1.92697200	-2.81946800
C	-4.16002000	1.31768200	-3.50494300
C	-4.39262400	-0.05200800	-3.38321300
C	-3.59678900	-2.28761500	-2.27474600
H	-1.44988900	1.64918800	-1.46308300
H	-4.79973400	1.91666100	-4.14584500
H	-5.20603100	-0.52412200	-3.92685100
H	-3.69666700	-2.90342400	-3.17337500
H	-4.43595500	-2.53061400	-1.61379700
C	3.04739600	-0.22370300	-0.65144500
C	3.29931800	1.14713600	-0.74700700
C	4.10276700	-1.08188400	-0.33763200
C	4.55908200	1.66760700	-0.49120500

C	5.37611900	-0.58377800	-0.08541300
C	5.58055600	0.78652600	-0.15982600
H	4.73870000	2.73384700	-0.55827200
H	6.18675000	-1.25793100	0.16413700
H	-2.37479000	-3.28508900	-0.73078900
H	-2.93209400	2.99276500	-2.92920800
Cl	2.02455800	2.23313300	-1.19416000
Cl	7.16824500	1.42362100	0.15733600
Cl	3.83484800	-2.78465100	-0.24705400
C	0.49112000	0.20644500	0.96829200
O	1.55739600	0.23749600	1.62141000
C	-0.72571100	0.80880800	1.38000100
C	-0.59573100	2.11675600	2.14902700
H	-1.55589900	0.77831600	0.67902500
H	-1.28722400	2.15790100	2.99751500
H	0.41665600	2.16839600	2.56056100
C	-0.87011900	3.31110300	1.25981800
C	-2.15809200	3.52225400	0.75306800
C	0.14119100	4.20560400	0.90561400
C	-2.42585200	4.59653400	-0.09049400
H	-2.95600100	2.83111100	1.02165400
C	-0.12122300	5.28090500	0.05683800
H	1.14360500	4.05496200	1.29760000
C	-1.40474800	5.47846900	-0.44510500
H	-3.43178000	4.74559600	-0.47215400
H	0.67949000	5.96466100	-0.20962500
H	-1.61161500	6.31649000	-1.10366700
C	0.60943600	-1.89677600	3.58672100
C	0.54552300	-2.92855800	1.42752600
C	1.49328500	-2.63925000	2.59759500
H	1.02893500	-0.95807500	3.94907900
H	0.32238800	-2.52297800	4.43719800
H	1.92235800	-3.56186800	2.99049400
H	2.29371600	-1.99712700	2.21834100
N	-0.63849200	-2.29054000	1.59580900
N	-0.60865600	-1.62205300	2.78476500
O	0.83363600	-3.57942300	0.42280200
C	-1.37571800	-0.53807700	2.92415900

C	-2.82978900	-0.54839100	2.60164600
C	-3.60165800	0.55780900	2.98867500
C	-3.47876700	-1.63306000	1.99468400
C	-4.96736100	0.60478400	2.73031400
H	-3.13121300	1.38392300	3.51294600
C	-4.84939500	-1.58739600	1.75047300
H	-2.90345300	-2.50998200	1.72088200
C	-5.59799900	-0.46705300	2.10176100
H	-5.54120000	1.47501200	3.03380000
H	-5.33497400	-2.44145800	1.28742400
H	-6.66437700	-0.43503300	1.90219100
H	-1.11777500	0.04949900	3.80415400

TS5SR_{L3} (M06-2X/SMD)

0 1

C	0.47137000	-0.25742100	-0.35127600
C	1.53876800	-0.56541100	-2.22893000
C	3.00068000	-0.54147500	-0.23033900
H	2.92767300	-0.02505700	0.72491300
N	0.28570400	-0.52551400	-2.57531200
N	-0.37319200	-0.34520600	-1.39006300
N	1.68732400	-0.43488900	-0.87339500
C	2.79767600	-0.55416900	-3.03511000
H	2.58272800	-0.26015800	-4.06294800
H	3.27278800	-1.54418600	-3.03498900
C	4.08900000	0.12756000	-1.13643100
O	3.61600200	0.43834300	-2.44639500
C	4.70316300	-2.16842700	-0.63109000
C	3.42908400	-1.98335400	-0.09890800
C	2.72289200	-3.02714100	0.48988700
C	3.31139900	-4.28942900	0.51662300
C	4.58349100	-4.48858600	-0.02677400
C	5.28955600	-3.43119800	-0.59788100
C	5.26654500	-0.87236000	-1.15879300
H	1.74623500	-2.84499900	0.93125200
H	5.02899100	-5.47840900	0.00170400
H	6.28165500	-3.58972800	-1.01103100
H	5.67820900	-0.95471600	-2.16984400

H	6.06645700	-0.50956900	-0.50554600
C	-1.77894600	-0.56921300	-1.33124600
C	-2.26196100	-1.79307600	-0.85615300
C	-2.68216300	0.38924400	-1.79121000
C	-3.62303200	-2.05555400	-0.81900200
C	-4.04963800	0.14715100	-1.76308400
C	-4.49582800	-1.07449800	-1.27476900
H	-3.99019300	-3.00354600	-0.44587600
H	-4.74560600	0.89874600	-2.11647500
H	4.36840700	1.08361100	-0.69426900
H	2.78336500	-5.12266700	0.96966900
Cl	-1.15146800	-3.01591300	-0.33399100
Cl	-6.20276300	-1.39288500	-1.23665600
Cl	-2.09009500	1.90737200	-2.35799200
C	0.12631900	-0.03949000	1.09816100
O	0.75939300	-0.71085700	1.92689100
C	-0.83590800	0.98087700	1.34767600
C	-1.62900200	0.85880800	2.63743700
H	-1.43346900	1.27422500	0.48695400
H	-0.95068700	0.58186200	3.45037300
H	-2.07353000	1.82737100	2.89311700
C	-2.72865200	-0.17401300	2.51609400
C	-2.45049000	-1.53297400	2.70284800
C	-4.03410900	0.20554600	2.19133900
C	-3.46096400	-2.48518600	2.59139000
H	-1.43291200	-1.83402600	2.93978100
C	-5.04794800	-0.74452900	2.08339300
H	-4.25987000	1.25874200	2.03888000
C	-4.76490500	-2.09321700	2.28825000
H	-3.23043600	-3.53525600	2.74801100
H	-6.05983400	-0.43120800	1.84367100
H	-5.55480000	-2.83452300	2.20788000
C	1.68611700	2.15417100	3.52550400
C	3.55670900	1.76365700	2.11511100
C	3.20493200	2.08867800	3.57717800
H	1.23046300	2.93590100	4.13768400
H	1.24117800	1.18492800	3.77444000
H	3.59051200	1.32019700	4.24727200

H	3.65513700	3.04942400	3.84734200
N	2.51587200	2.00424800	1.30530900
N	1.46390200	2.44710600	2.09675900
O	4.65680700	1.31897500	1.74895800
C	0.24872600	2.66035200	1.57253200
H	-0.43240900	3.06528000	2.32030000
C	0.10802300	3.32753300	0.24020900
C	-0.91258600	4.27817200	0.11305200
C	0.91721000	3.05757700	-0.87257800
C	-1.10699100	4.96559600	-1.08126100
H	-1.55194800	4.49098700	0.96683600
C	0.72080300	3.74834200	-2.06521600
H	1.71869800	2.33493700	-0.78635200
C	-0.28547100	4.70591900	-2.17640700
H	-1.89585700	5.70818300	-1.15417900
H	1.36361300	3.53103300	-2.91340400
H	-0.42912000	5.24421000	-3.10836700

TS5SSL₃ (M06-2X/SMD)

0 1

C	0.98003900	-0.35009700	-0.67166100
C	2.39875800	-1.38317400	-1.98581500
C	3.42686500	0.44727300	-0.68519800
H	3.05464100	1.41012000	-0.33863700
N	1.28279500	-2.02708700	-2.15035000
N	0.41052200	-1.38066200	-1.32276400
N	2.25955800	-0.35302900	-1.09557100
C	3.71399300	-1.52143100	-2.67807600
H	3.59708200	-2.08675000	-3.60213600
H	4.44174600	-2.02940000	-2.03062300
C	4.43348500	0.60575800	-1.88636300
O	4.11561300	-0.20702000	-3.00683900
C	5.55379100	-0.38553300	0.02773600
C	4.21228100	-0.27936700	0.38389000
C	3.72847600	-0.80391300	1.57926200
C	4.62474300	-1.45673100	2.42074700
C	5.97271200	-1.57143700	2.06994200
C	6.44782900	-1.03443700	0.87582100

C	5.82550900	0.27923700	-1.29754800
H	2.68234500	-0.68925400	1.84845500
H	6.65796300	-2.08379400	2.73763800
H	7.49641900	-1.12415800	0.60878900
H	6.38572900	-0.35222100	-1.99422300
H	6.40273100	1.19901100	-1.16123800
C	-0.89506400	-1.91072500	-1.14912400
C	-1.21214400	-2.61916200	0.01249900
C	-1.86382900	-1.72648100	-2.13653800
C	-2.49630000	-3.10940800	0.20658200
C	-3.15196400	-2.21380800	-1.96186000
C	-3.44822700	-2.89393100	-0.78434700
H	-2.74356400	-3.64148900	1.11688000
H	-3.90590000	-2.06025600	-2.72430900
H	4.38412700	1.62392600	-2.27273400
H	4.27482200	-1.87494100	3.35871200
Cl	-0.01290800	-2.85718600	1.22708000
Cl	-5.05695500	-3.49257500	-0.54417900
Cl	-1.46441800	-0.84378100	-3.56946500
C	0.43143600	0.57886700	0.36981900
O	1.28871100	1.16250100	1.05854800
C	-0.97297000	0.85091300	0.41822500
C	-1.46237800	1.28305300	1.79483800
H	-1.61244800	0.10983500	-0.05616000
H	-0.80189400	2.06717300	2.17127100
H	-2.46503500	1.70987000	1.70724900
C	-1.49378300	0.09752000	2.73080400
C	-2.57117400	-0.79337100	2.69468600
C	-0.44232100	-0.15651200	3.61610500
C	-2.60701900	-1.90499400	3.53286400
H	-3.39382400	-0.60271900	2.00667600
C	-0.47433400	-1.26940600	4.45463500
H	0.40058600	0.52864000	3.64290900
C	-1.55679100	-2.14584100	4.41699100
H	-3.46122600	-2.57609600	3.50571100
H	0.34474000	-1.44819400	5.14481300
H	-1.58468000	-3.00819100	5.07554100
C	0.94106200	3.42657400	-1.05179000

C	0.66074300	4.70859400	0.93770500
C	1.75353600	4.08436100	0.04398300
H	1.26793600	2.41972200	-1.33980600
H	0.89628900	4.03845400	-1.96113700
H	2.45964500	4.83632600	-0.30682700
H	2.27734800	3.34082500	0.65696800
N	-0.54524900	4.19748700	0.64664800
N	-0.39627800	3.35373900	-0.44473500
O	0.90990100	5.53425200	1.82494000
C	-1.23985400	2.33380800	-0.73656400
H	-0.95559600	1.87755000	-1.68647900
C	-2.73056200	2.51469500	-0.66802200
C	-3.52352900	1.55473500	-1.30805000
C	-3.35660500	3.58109000	-0.01548700
C	-4.90996300	1.64292600	-1.29242300
H	-3.04438500	0.73244600	-1.83346900
C	-4.74800200	3.67162000	-0.00936600
H	-2.74298900	4.31916900	0.48650600
C	-5.52915300	2.70686900	-0.63810400
H	-5.50460200	0.88724400	-1.79649500
H	-5.22260100	4.50500000	0.49900100
H	-6.61161800	2.78257400	-0.62181600

TS5RR_{L6} (ωB97X-D)

0 1

C	-0.11839200	-0.52946100	-0.41764800
C	-1.01671400	-1.81294500	-1.96196300
C	-2.56888300	-1.26386100	-0.16317400
H	-2.43991400	-1.17648200	0.91580900
N	0.19204500	-1.61762600	-2.38051000
N	0.73845300	-0.80941200	-1.41799800
N	-1.24796000	-1.18341300	-0.77195400
C	-2.13321300	-2.57349500	-2.58709800
H	-1.74397100	-3.26232300	-3.33600800
H	-2.82535600	-1.87237300	-3.07545100
C	-3.26747100	-2.63967500	-0.46200400
O	-2.76457300	-3.33778100	-1.58854700
C	-4.75788500	-0.80955800	-0.99124200

C	-3.52166500	-0.22823700	-0.71888900
C	-3.27914300	1.11698800	-0.96927400
C	-4.30945100	1.88311900	-1.50967500
C	-5.55204600	1.30926400	-1.78082800
C	-5.78651500	-0.03993500	-1.52227200
C	-4.75698000	-2.27175200	-0.63004300
H	-2.31602800	1.57123000	-0.75557000
H	-6.34359700	1.92019000	-2.20316000
H	-6.75216300	-0.48484400	-1.74162000
H	-5.21916500	-2.91241700	-1.38492000
H	-5.29133100	-2.43698100	0.31238600
C	2.07624900	-0.37500300	-1.62994300
C	2.33179000	0.82785500	-2.29182000
C	3.14390600	-1.20324300	-1.29312300
C	3.62913800	1.24276700	-2.54048000
C	4.45535300	-0.80702300	-1.53383500
C	4.67670100	0.41896600	-2.14193000
H	3.81824600	2.18751900	-3.03320900
H	5.27947300	-1.45237900	-1.25799700
H	-3.09746100	-3.32602900	0.36525000
H	-4.13848000	2.93480400	-1.70997800
Cl	1.00977700	1.82391800	-2.80708800
Cl	6.31417300	0.93405400	-2.43775000
Cl	2.85032700	-2.75860900	-0.59049600
C	0.17725600	0.56366700	0.58973100
O	1.23000900	1.18793800	0.34479300
C	-0.67582300	0.82663100	1.67703200
C	-0.63156900	2.22161300	2.26602000
H	-1.64604200	0.34343900	1.71232000
H	-1.04302800	2.21058300	3.28157200
H	0.41261800	2.53778800	2.33568000
C	-1.41229100	3.20717000	1.42299800
C	-2.72916600	3.54119400	1.74354600
C	-0.84243500	3.75821100	0.26917800
C	-3.46376900	4.40754400	0.93786800
H	-3.18528100	3.11668800	2.63449400
C	-1.57604400	4.61947300	-0.54091500
H	0.17720300	3.49002000	0.00965400

C	-2.88861700	4.95126300	-0.20718700
H	-4.48761300	4.65413900	1.20195800
H	-1.11915600	5.03984400	-1.43187800
H	-3.45908200	5.62743100	-0.83653600
C	-1.42427900	-2.04515000	3.49849400
C	-0.57046400	-3.24541600	1.63925800
C	-1.54542200	-3.39680300	2.82194400
H	-1.42932400	-2.06769000	4.58892200
H	-2.20130100	-1.34371100	3.15964900
H	-2.55489100	-3.63060900	2.48285000
H	-1.20597700	-4.21263900	3.46677200
N	0.27137300	-2.21004100	1.84104300
N	-0.11176200	-1.58766900	3.01273300
O	-0.58840800	-3.95892900	0.63343100
C	0.32631500	-0.36793500	3.30098700
C	1.71443200	0.09407300	3.16554500
C	2.10116500	1.19644500	3.94125700
C	2.65591200	-0.49968000	2.31617900
C	3.39251300	1.70074600	3.86324200
H	1.38234800	1.65926100	4.61205000
C	3.95030000	0.00129900	2.25034400
H	2.35291500	-1.34789900	1.71693000
C	4.32210600	1.10370200	3.01403500
H	3.67533900	2.55605500	4.46838400
H	4.66825600	-0.46610700	1.58328900
H	5.33106300	1.49855900	2.94887000
H	-0.22167500	0.08614500	4.12364800

TS5RS_{L6} (ωB97X-D)

0 1

C	0.26005700	-0.62629300	-0.46475000
C	-0.43745700	-1.18584000	-2.46674600
C	-2.24510200	-0.61761700	-0.92537400
H	-2.34353500	-0.70520300	0.15425400
N	0.85347600	-1.30065600	-2.54060700
N	1.27485600	-0.94445700	-1.28478600
N	-0.83520200	-0.76435600	-1.22863800
C	-1.52029800	-1.55212300	-3.42573300

H	-1.11708600	-2.15393000	-4.23910000
H	-1.98069700	-0.64727800	-3.84386200
C	-3.06927400	-1.76730100	-1.57641000
O	-2.44788700	-2.35152200	-2.71941100
C	-4.11584700	0.37126000	-1.99816700
C	-2.85722300	0.64937000	-1.47033500
C	-2.34265100	1.93982500	-1.46623800
C	-3.13021300	2.97088400	-1.97369600
C	-4.40407600	2.70406000	-2.47602100
C	-4.90284000	1.40222500	-2.49711600
C	-4.41980500	-1.10413700	-1.91842700
H	-1.34446400	2.14669100	-1.09005500
H	-5.00706300	3.51666400	-2.86842900
H	-5.88583400	1.19770700	-2.91019700
H	-4.82524300	-1.51822500	-2.84512000
H	-5.14284400	-1.30233000	-1.12016600
C	2.65814500	-0.73023400	-1.04940300
C	3.20009000	0.53363500	-1.27938900
C	3.48376700	-1.76443700	-0.61152500
C	4.54512800	0.78429600	-1.04696900
C	4.83239200	-1.53695900	-0.37911100
C	5.33972400	-0.26058700	-0.59424100
H	4.95717800	1.77063200	-1.21464100
H	5.47090300	-2.33806200	-0.03007400
H	-3.16513800	-2.58586200	-0.86249000
H	-2.74677000	3.98591300	-1.98291800
Cl	2.18215900	1.81216200	-1.85844000
Cl	7.02743400	0.03892500	-0.28766300
Cl	2.81360700	-3.33219000	-0.33737600
C	0.48149000	-0.16869700	0.94399300
O	1.49375000	-0.64410300	1.50613000
C	-0.38521900	0.80104000	1.49384900
C	0.25393700	1.73910500	2.50563000
H	-1.09443800	1.26125500	0.81387400
H	-0.51799000	2.29840200	3.04546200
H	0.79609800	1.14467300	3.24629500
C	1.20711000	2.71427700	1.84871600
C	0.72345100	3.87302400	1.23470900

C	2.58056200	2.46066200	1.81283700
C	1.59005700	4.76301200	0.60744300
H	-0.34447300	4.08031000	1.25488600
C	3.45095500	3.35266000	1.19130100
H	2.96101600	1.55045900	2.26555200
C	2.95956000	4.50721000	0.58825300
H	1.19736600	5.66142400	0.14081500
H	4.51697400	3.14436700	1.18009500
H	3.63824900	5.20381500	0.10611400
C	-0.27506400	-2.15068300	3.60854800
C	-0.58827700	-3.26228000	1.51078100
C	0.35389600	-3.20650200	2.71719100
H	0.41943100	-1.37028500	3.92004500
H	-0.76507400	-2.57672900	4.48893000
H	0.45252600	-4.18503200	3.18821300
H	1.32807100	-2.87817400	2.34380400
N	-1.49914800	-2.25871800	1.56053700
N	-1.31642300	-1.56866800	2.72996100
O	-0.49423300	-4.07124800	0.58768400
C	-1.72134400	-0.30490600	2.81414300
C	-3.05595100	0.11926300	2.29557500
C	-3.35335200	1.47873200	2.14775300
C	-4.05199800	-0.81822900	2.00095300
C	-4.58895100	1.89072300	1.66440400
H	-2.60544900	2.22529100	2.39341100
C	-5.29300100	-0.40343300	1.52746400
H	-3.83860900	-1.87415800	2.11324700
C	-5.56180300	0.94925700	1.34057500
H	-4.78699200	2.94899500	1.53083100
H	-6.05143300	-1.14614500	1.29983900
H	-6.52227900	1.26827400	0.94951100
H	-1.40617900	0.18269900	3.73372300

TS5SR_{L6} (ω B97X-D)

0 1

C	0.43080900	-0.28700000	-0.36907200
C	1.49366700	-0.63640000	-2.24078800
C	2.95560300	-0.56922100	-0.25286700

H	2.88525700	-0.02523300	0.68788200
N	0.24065400	-0.60869800	-2.58849600
N	-0.41596600	-0.39833100	-1.40270400
N	1.64487300	-0.47557500	-0.89178500
C	2.74880100	-0.65250800	-3.04977800
H	2.53784100	-0.38684600	-4.08493600
H	3.21547800	-1.64581100	-3.02312000
C	4.03992900	0.08737400	-1.16926200
O	3.57694500	0.34895700	-2.49437300
C	4.66913900	-2.18749600	-0.61413300
C	3.38980500	-2.00483200	-0.09673100
C	2.68319400	-3.04784600	0.48991500
C	3.27625700	-4.30699700	0.52953800
C	4.55361900	-4.50357600	0.00004900
C	5.26091500	-3.44579300	-0.56774900
C	5.23353900	-0.89061400	-1.13496800
H	1.70332000	-2.86712700	0.92106700
H	5.00380100	-5.49054600	0.03757600
H	6.25696400	-3.60302100	-0.97042100
H	5.69428200	-0.97573600	-2.12333400
H	5.99143000	-0.50500900	-0.44602200
C	-1.82429600	-0.58814800	-1.33666900
C	-2.33738000	-1.79543900	-0.85103600
C	-2.70658600	0.38898800	-1.79874200
C	-3.70435600	-2.01728200	-0.79857400
C	-4.07851700	0.18159200	-1.75864300
C	-4.55657400	-1.02114800	-1.25646300
H	-4.09325800	-2.94689700	-0.40607100
H	-4.75691600	0.94659000	-2.11336800
H	4.29827500	1.06156800	-0.75785200
H	2.74643200	-5.14013300	0.97988000
Cl	-1.26308700	-3.05281200	-0.33121900
Cl	-6.27197200	-1.29212000	-1.20725100
Cl	-2.09111200	1.88535900	-2.40465300
C	0.10142600	-0.05143800	1.07943700
O	0.70482500	-0.76023900	1.90215900
C	-0.80264000	1.01376000	1.33894000
C	-1.59937700	0.93859800	2.63092100

H	-1.39113800	1.33540000	0.48340800
H	-0.93113400	0.66998500	3.45351200
H	-2.01826300	1.92450300	2.86113100
C	-2.72687700	-0.06753200	2.54255500
C	-2.48839200	-1.42467300	2.78112200
C	-4.02087900	0.33509100	2.20448300
C	-3.52171800	-2.35265200	2.69608300
H	-1.48101000	-1.74666700	3.02739300
C	-5.05849100	-0.58989100	2.12638200
H	-4.21956700	1.38681300	2.01374100
C	-4.81253500	-1.93752900	2.37444900
H	-3.31979700	-3.40221400	2.88699100
H	-6.06013200	-0.25797500	1.87157400
H	-5.62059600	-2.65996800	2.31544400
C	1.75116900	2.12097500	3.51436000
C	3.64376400	1.71220000	2.13215000
C	3.26645300	2.00876300	3.59385500
H	1.31168900	2.91312800	4.12497000
H	1.27187500	1.16704100	3.75591200
H	3.61175800	1.21126600	4.25206000
H	3.74023000	2.94477500	3.90615000
N	2.61888600	1.97703200	1.30840300
N	1.55663900	2.42108000	2.08514100
O	4.74625200	1.26957700	1.77319500
C	0.35291400	2.66414800	1.54758000
H	-0.31974700	3.09095000	2.28910100
C	0.23491600	3.32276600	0.21129300
C	-0.76497800	4.29050900	0.06204700
C	1.05198300	3.02799700	-0.88752800
C	-0.93356400	4.96485100	-1.14269700
H	-1.41280000	4.52713800	0.90220800
C	0.87950700	3.70141900	-2.09189900
H	1.84238700	2.29867800	-0.77590100
C	-0.10807300	4.67413600	-2.22581700
H	-1.70778900	5.72012200	-1.23249000
H	1.52783100	3.46189100	-2.92894900
H	-0.23463700	5.20022400	-3.16667100

TS5SS_{L6} (ωB97X-D)

0 1

C	0.99769000	-0.31264600	-0.68865200
C	2.44095800	-1.31512700	-2.00065600
C	3.43800800	0.49239900	-0.65400100
H	3.05593100	1.44391400	-0.29106900
N	1.33494400	-1.96860200	-2.18776600
N	0.44489100	-1.33973900	-1.36017600
N	2.28233200	-0.30089300	-1.09791000
C	3.76315100	-1.43667900	-2.67925600
H	3.65685500	-1.97541000	-3.61984400
H	4.47915900	-1.96975400	-2.03985400
C	4.45854300	0.68483100	-1.83547200
O	4.17537600	-0.11826900	-2.97228200
C	5.56413600	-0.31985900	0.07743300
C	4.21555800	-0.24615000	0.41139100
C	3.72317900	-0.80615800	1.58574300
C	4.61429200	-1.46682600	2.42536900
C	5.96866600	-1.55189600	2.09441800
C	6.45396600	-0.97577400	0.92316900
C	5.84637000	0.38532000	-1.22296600
H	2.67320700	-0.71275400	1.84220400
H	6.65075900	-2.07286800	2.75853400
H	7.50815700	-1.04306700	0.67297300
H	6.44569100	-0.20810700	-1.91947000
H	6.38808300	1.32024900	-1.04835300
C	-0.85220200	-1.89185400	-1.20466000
C	-1.14745700	-2.67426700	-0.08613700
C	-1.83691100	-1.66521500	-2.16696300
C	-2.42849000	-3.17020400	0.10710700
C	-3.12126500	-2.15996800	-1.99471700
C	-3.40026800	-2.89547300	-0.84749100
H	-2.65975100	-3.74945400	0.99130900
H	-3.88647900	-1.96890400	-2.73610200
H	4.39490000	1.70520100	-2.21251100
H	4.25440600	-1.91500400	3.34549300
Cl	0.08413300	-3.01168200	1.07758500
Cl	-5.01199800	-3.49324200	-0.60294800

Cl	-1.46053700	-0.72968800	-3.57719300
C	0.43352900	0.59342200	0.36375400
O	1.28483600	1.16943400	1.07129200
C	-0.97180900	0.82773100	0.42624500
C	-1.48062400	1.21369300	1.80924300
H	-1.59394100	0.08849200	-0.07027100
H	-0.84932500	2.00962800	2.20806100
H	-2.49187700	1.61657700	1.72410400
C	-1.49461100	0.01252800	2.72606000
C	-2.56652200	-0.88420900	2.69140600
C	-0.43333600	-0.24638400	3.59751700
C	-2.58157600	-2.01081600	3.50870300
H	-3.39818400	-0.69152000	2.01698400
C	-0.44544800	-1.37229800	4.41705300
H	0.40424800	0.44394600	3.62552400
C	-1.51942100	-2.25823900	4.37562200
H	-3.42740200	-2.69183300	3.47650800
H	0.38296700	-1.55473400	5.09505600
H	-1.53160000	-3.13279600	5.01866100
C	0.83843400	3.48473300	-1.06646400
C	0.58407800	4.73850800	0.94569100
C	1.66311300	4.15875500	0.00944400
H	1.18775600	2.48975200	-1.36381200
H	0.75698800	4.09317000	-1.97499900
H	2.33389300	4.93543500	-0.35800500
H	2.23615300	3.42863600	0.59273200
N	-0.62086600	4.21044300	0.67467800
N	-0.48087500	3.38169100	-0.42964100
O	0.83574900	5.54925400	1.84593700
C	-1.31368300	2.35740600	-0.71884800
H	-1.04191800	1.91498100	-1.67616800
C	-2.80175400	2.49626300	-0.60240500
C	-3.58995800	1.58396700	-1.31316700
C	-3.43545600	3.47328800	0.17128500
C	-4.97657400	1.63197200	-1.24854000
H	-3.10995800	0.83194700	-1.93186100
C	-4.82616900	3.52522600	0.22705000
H	-2.82080000	4.17289600	0.72440700

C	-5.60151400	2.60680300	-0.47393400
H	-5.56837700	0.91525300	-1.80927100
H	-5.30452600	4.28970900	0.83116600
H	-6.68458300	2.65035300	-0.41879100

TS5RR_{L7} (CAM-B3LYP)

0 1

C	-0.11998200	-0.52897800	-0.42627200
C	-1.00658900	-1.88280600	-1.91641600
C	-2.57652000	-1.27375100	-0.15026900
H	-2.45175200	-1.11258100	0.91922700
N	0.20190400	-1.70160700	-2.33411700
N	0.74367400	-0.84728100	-1.40942900
N	-1.25039400	-1.19512400	-0.76012800
C	-2.10067900	-2.70262400	-2.50025700
H	-1.68844500	-3.42221000	-3.20701900
H	-2.81028700	-2.05491600	-3.03236200
C	-3.22714300	-2.68719900	-0.35847600
O	-2.71396200	-3.42688100	-1.45798800
C	-4.79164700	-0.94995400	-0.97057100
C	-3.57367200	-0.30979900	-0.75834600
C	-3.39782000	1.03132200	-1.07340400
C	-4.47047700	1.73058000	-1.61788600
C	-5.69185900	1.09498100	-1.83457900
C	-5.86149400	-0.24778800	-1.51062000
C	-4.72944900	-2.38756200	-0.52732600
H	-2.45185100	1.53439000	-0.90175600
H	-6.51858100	1.65251700	-2.26268600
H	-6.81323600	-0.73986500	-1.68467900
H	-5.17283400	-3.08956200	-1.23736100
H	-5.24985400	-2.52094000	0.42769700
C	2.08583300	-0.43188900	-1.65329800
C	2.34540300	0.71407000	-2.40510400
C	3.14939900	-1.25085600	-1.28486700
C	3.64056100	1.07903000	-2.72658500
C	4.45740400	-0.90262400	-1.59697800
C	4.68384000	0.26421900	-2.30707300
H	3.83083100	1.97906500	-3.29578700

H	5.27724900	-1.54199100	-1.29766900
H	-3.01891700	-3.32085300	0.50104500
H	-4.35044900	2.77900900	-1.86707000
Cl	1.03220900	1.70387500	-2.95294300
Cl	6.31848700	0.71349500	-2.70383900
Cl	2.85181800	-2.73531100	-0.44539700
C	0.19440600	0.58353100	0.55349300
O	1.27502400	1.15602800	0.30267700
C	-0.67072100	0.93296800	1.61003700
C	-0.60869200	2.36406500	2.10958800
H	-1.65399100	0.47800900	1.64446700
H	-1.02075100	2.42216200	3.12244300
H	0.44021900	2.66142800	2.16704200
C	-1.36146500	3.33496200	1.22344400
C	-2.63342600	3.78801700	1.57197800
C	-0.80060700	3.78168900	0.02235700
C	-3.33441700	4.66152300	0.74583000
H	-3.08026600	3.45529100	2.50512300
C	-1.49915500	4.65174100	-0.80618300
H	0.18876500	3.43310000	-0.25586600
C	-2.76967100	5.09628200	-0.44753400
H	-4.32197100	5.00509400	1.03789700
H	-1.04635100	4.99228500	-1.73245200
H	-3.31073500	5.78293200	-1.09090300
C	-1.45723200	-1.89357300	3.60419800
C	-0.52904400	-3.17321800	1.83954600
C	-1.48687800	-3.29984800	3.03662300
H	-1.48194100	-1.82917900	4.69234600
H	-2.26929900	-1.27215400	3.20049400
H	-2.47667300	-3.63476800	2.72689400
H	-1.08618100	-4.03437200	3.74142300
N	0.25675600	-2.08543000	1.97180200
N	-0.16179700	-1.40718700	3.10222000
O	-0.51739700	-3.94773600	0.87853300
C	0.24153300	-0.16045400	3.32685300
C	1.64168300	0.29035600	3.27453400
C	1.98248500	1.40972200	4.04525800
C	2.64684600	-0.36129000	2.55172100

C	3.28956300	1.87207900	4.09118400
H	1.21484900	1.91395400	4.62465600
C	3.95584200	0.09856600	2.61046900
H	2.38651000	-1.22918200	1.96159200
C	4.28269600	1.21500100	3.37198800
H	3.53436700	2.73891400	4.69616700
H	4.72692800	-0.41864800	2.04834000
H	5.30740500	1.57053100	3.40839000
H	-0.34892700	0.32971700	4.09686200

TS5RS_{L7} (CAM-B3LYP)

0 1

C	0.34936000	-0.56568300	-0.42210000
C	-0.14793100	-1.37382500	-2.40117900
C	-2.11519700	-0.80393700	-1.07026900
H	-2.29994600	-0.76600000	0.00141900
N	1.14545900	-1.40352500	-2.36498400
N	1.44773900	-0.89042500	-1.12869100
N	-0.67186600	-0.85605100	-1.24900100
C	-1.10874000	-1.91667300	-3.40092700
H	-0.58950700	-2.56880400	-4.10242200
H	-1.58539600	-1.10243100	-3.95991700
C	-2.78103100	-2.09245100	-1.63605200
O	-2.04719600	-2.70875800	-2.69655800
C	-3.96460100	-0.14407200	-2.40868700
C	-2.78673000	0.32109200	-1.82786700
C	-2.38696000	1.64328300	-1.96885300
C	-3.19506400	2.50763800	-2.70246800
C	-4.37874700	2.05013300	-3.27749400
C	-4.77108800	0.72181300	-3.13461800
C	-4.16210600	-1.61023800	-2.11392400
H	-1.46071000	2.00205200	-1.53013100
H	-4.99684000	2.73424500	-3.84963500
H	-5.68833800	0.36768600	-3.59456100
H	-4.49401600	-2.19550200	-2.97435900
H	-4.90113600	-1.74608600	-1.31652200
C	2.81840800	-0.65958500	-0.82329000
C	3.39717500	0.57239000	-1.12021700

C	3.62012400	-1.68525200	-0.32540000
C	4.74269300	0.80539000	-0.87900900
C	4.96837600	-1.47412700	-0.08285700
C	5.50861700	-0.22585500	-0.35703400
H	5.18074200	1.76852500	-1.10396600
H	5.58284800	-2.27214000	0.31200600
H	-2.83266400	-2.85197000	-0.85566900
H	-2.89793300	3.54310800	-2.83028200
Cl	2.43400600	1.83507700	-1.81598700
Cl	7.19929100	0.04940200	-0.04966500
Cl	2.92613100	-3.23303600	-0.00444300
C	0.42570700	0.04074200	0.94409500
O	1.45992400	-0.25032900	1.58463600
C	-0.59016400	0.91857900	1.40309700
C	-0.11676800	2.05574600	2.29816400
H	-1.35923200	1.19328600	0.68726500
H	-0.96900500	2.48401500	2.83284700
H	0.56391500	1.64902700	3.04901100
C	0.58060600	3.16723000	1.54344100
C	-0.15032400	4.05724300	0.75234200
C	1.96326300	3.32995100	1.62224900
C	0.48310100	5.08109000	0.05829500
H	-1.23034100	3.95034100	0.68748600
C	2.60061700	4.35799000	0.93425800
H	2.54324500	2.64134100	2.22890000
C	1.86352800	5.23664100	0.14941500
H	-0.10248400	5.76636100	-0.54688300
H	3.67738600	4.47220100	1.01352900
H	2.35909000	6.04025900	-0.38576800
C	-0.09567400	-1.95912400	3.70137700
C	-0.33170000	-3.16641700	1.64675100
C	0.59058900	-3.01842800	2.85968500
H	0.55525200	-1.13564000	3.99271700
H	-0.57202600	-2.37627200	4.59388800
H	0.72492400	-3.97280200	3.36970500
H	1.55794800	-2.67142800	2.49040600
N	-1.27887600	-2.19702500	1.63829400
N	-1.15488500	-1.46602000	2.79108700

O	-0.19180900	-4.01224300	0.76296100
C	-1.67030200	-0.23677600	2.84884800
C	-3.08130600	0.05546400	2.47046300
C	-3.60717800	1.31549200	2.78097900
C	-3.93648300	-0.89878800	1.90848500
C	-4.93008400	1.62855800	2.50195000
H	-2.97923200	2.05640300	3.26398400
C	-5.26444800	-0.58560200	1.63977100
H	-3.54860100	-1.88591200	1.68964800
C	-5.76581600	0.67929200	1.92329600
H	-5.31183900	2.61374700	2.74917600
H	-5.91389700	-1.34359200	1.21272200
H	-6.80149600	0.92008300	1.70773000
H	-1.34366800	0.29980400	3.73576700

TS5SR_{L7} (CAM-B3LYP)

0 1

C	0.47551700	-0.30362400	-0.43082900
C	1.52671900	-0.80026300	-2.27937100
C	3.02207200	-0.50003400	-0.34158100
H	2.95086800	0.13146200	0.54144700
N	0.27226300	-0.82300600	-2.61110200
N	-0.37948500	-0.52025400	-1.44245700
N	1.68975900	-0.51170200	-0.95355900
C	2.76399500	-0.89850900	-3.10583400
H	2.52645900	-0.75212100	-4.15914300
H	3.23701000	-1.88058500	-2.98202000
C	4.06432300	0.10342100	-1.33832400
O	3.59914900	0.16318600	-2.69029800
C	4.81982400	-2.05447300	-0.54272500
C	3.52693800	-1.89538900	-0.05206700
C	2.87922600	-2.92059800	0.62573700
C	3.54305400	-4.13243800	0.78620700
C	4.83393300	-4.30306700	0.28720300
C	5.48266600	-3.26426700	-0.37321500
C	5.31381600	-0.78421400	-1.18360300
H	1.88629300	-2.76298000	1.03245300
H	5.33939900	-5.25439200	0.41908700

H	6.49078000	-3.39930400	-0.75281800
H	5.80241800	-0.93422400	-2.15009500
H	6.02804200	-0.27942200	-0.52559700
C	-1.78927000	-0.71503000	-1.38355500
C	-2.29915600	-1.92325800	-0.90173600
C	-2.66934600	0.24487300	-1.88161500
C	-3.66396300	-2.15540900	-0.86859200
C	-4.03855900	0.02502800	-1.86312500
C	-4.51593400	-1.17128300	-1.34884300
H	-4.05074500	-3.08561300	-0.47599100
H	-4.71609000	0.77787500	-2.24332900
H	4.26507200	1.13399500	-1.05431800
H	3.05524600	-4.94901600	1.30835500
Cl	-1.21922500	-3.16678800	-0.36314900
Cl	-6.23029900	-1.44844500	-1.31016900
Cl	-2.05747300	1.73329000	-2.50943400
C	0.17488400	-0.02047600	1.02088700
O	0.85624400	-0.66580000	1.83202400
C	-0.79945700	0.97695300	1.32768100
C	-1.52438400	0.80981800	2.65974700
H	-1.45540100	1.23507800	0.50129300
H	-0.78281000	0.61876600	3.43956200
H	-2.02332000	1.74987700	2.91605100
C	-2.55703800	-0.29579900	2.66375800
C	-2.19478700	-1.61481200	2.94699200
C	-3.89681200	-0.01788200	2.38806700
C	-3.14814300	-2.62679500	2.95552100
H	-1.15484000	-1.84120000	3.15894200
C	-4.85345600	-1.02721000	2.39709500
H	-4.19557300	1.00510400	2.17480900
C	-4.48146600	-2.33684100	2.68212300
H	-2.84934400	-3.64501800	3.18437700
H	-5.89152800	-0.78946400	2.18704300
H	-5.22715000	-3.12532400	2.69860700
C	1.87282500	2.29692300	3.33854300
C	3.60449700	2.09183800	1.72576400
C	3.38563400	2.39153400	3.21641000
H	1.41773400	3.03145900	4.00640500

H	1.56240000	1.29229600	3.64265500
H	3.92595200	1.67705600	3.83739500
H	3.75991900	3.39518200	3.44200700
N	2.45826200	2.19866300	1.04076800
N	1.46273600	2.55903100	1.94851200
O	4.70308300	1.77041000	1.24162100
C	0.17970600	2.69589300	1.56643000
H	-0.42377900	2.99959000	2.41813400
C	-0.17148700	3.48215000	0.34172900
C	-1.36453000	4.21320700	0.37861100
C	0.62145800	3.55481900	-0.80681800
C	-1.75564000	5.00217600	-0.69424900
H	-1.98869900	4.17358600	1.26724000
C	0.23018800	4.35186000	-1.87768500
H	1.55222500	3.00447700	-0.83291500
C	-0.95538900	5.07641500	-1.82977400
H	-2.68094600	5.56663900	-0.63922900
H	0.86379100	4.40745900	-2.75737400
H	-1.25175100	5.69887400	-2.66795300

TS5SS_{L7} (CAM-B3LYP)

0 1

C	0.90749800	-0.48175500	-0.64893300
C	2.28101200	-1.68703900	-1.86423800
C	3.37394100	0.26231400	-0.82004000
H	3.01603800	1.25752500	-0.56988800
N	1.15218600	-2.31757200	-1.94045400
N	0.30217700	-1.56659700	-1.17229000
N	2.18355700	-0.56687300	-1.08677600
C	3.56324400	-1.92674700	-2.58237900
H	3.40088900	-2.58912300	-3.43180700
H	4.31054900	-2.37758500	-1.91804000
C	4.31908100	0.28508600	-2.07730200
O	3.97115800	-0.66584700	-3.07701600
C	5.55038900	-0.43256400	-0.11467400
C	4.22505300	-0.31361900	0.28926000
C	3.82405900	-0.67078300	1.57131300
C	4.77829000	-1.17700900	2.44582600

C	6.10754300	-1.30963500	2.04373100
C	6.50344600	-0.93332800	0.76517800
C	5.74282800	0.06262300	-1.52237500
H	2.79383600	-0.54003600	1.88273600
H	6.84104000	-1.70614800	2.73812200
H	7.54023100	-1.03094400	0.45907900
H	6.28793800	-0.63618600	-2.16314400
H	6.30221200	1.00326800	-1.53201000
C	-1.01098800	-2.06842900	-0.96159400
C	-1.31328300	-2.78281100	0.19871600
C	-1.98420200	-1.92982700	-1.95167900
C	-2.58420500	-3.29927700	0.39831200
C	-3.25695300	-2.44699900	-1.77257100
C	-3.54058400	-3.11940000	-0.59105300
H	-2.81657300	-3.83743400	1.30744700
H	-4.00915900	-2.32873200	-2.54114500
H	4.23030300	1.24449600	-2.58611600
H	4.48852600	-1.46468900	3.45080000
Cl	-0.09534500	-3.03874000	1.39769800
Cl	-5.13411200	-3.76463900	-0.35103400
Cl	-1.60395900	-1.09924500	-3.42470700
C	0.40916300	0.57405400	0.28066800
O	1.29853600	1.23281000	0.85689900
C	-0.98185500	0.89970700	0.35878800
C	-1.44309500	1.41214700	1.72130000
H	-1.65680400	0.16869500	-0.07886900
H	-0.80435600	2.24722800	2.00989600
H	-2.45554600	1.80728000	1.62076500
C	-1.43027500	0.34179400	2.78850500
C	-2.52861600	-0.50185700	2.96579200
C	-0.32442500	0.17704800	3.62555500
C	-2.52460700	-1.48553200	3.94881500
H	-3.40324300	-0.37557800	2.33283600
C	-0.31640700	-0.80579300	4.60952900
H	0.53131600	0.83308900	3.50176300
C	-1.41635800	-1.64108700	4.77488800
H	-3.39349800	-2.12394300	4.07773900
H	0.54868200	-0.91237600	5.25692300

H	-1.41365300	-2.40258700	5.54829000
C	0.99310300	3.54599800	-1.23527000
C	0.76544800	4.86557000	0.72892800
C	1.83378500	4.28417600	-0.21523400
H	1.38857200	2.58081600	-1.56060500
H	0.81340900	4.15639500	-2.13018900
H	2.46273700	5.06886200	-0.63522500
H	2.45687200	3.59751200	0.36766100
N	-0.41828000	4.26417700	0.53713100
N	-0.26915900	3.36436500	-0.50828800
O	1.00685700	5.74455500	1.56641900
C	-1.15679700	2.38165100	-0.81175600
H	-0.86793000	1.91574000	-1.75178000
C	-2.63726000	2.65179400	-0.81541700
C	-3.43957200	1.83791300	-1.62119000
C	-3.24215400	3.68097400	-0.08953100
C	-4.81122300	2.03701400	-1.69864400
H	-2.98135000	1.04806600	-2.20842800
C	-4.61639600	3.88158500	-0.17442300
H	-2.61658600	4.31704500	0.52336200
C	-5.40688600	3.06224400	-0.97121900
H	-5.41367100	1.39666400	-2.33511100
H	-5.07039400	4.68836500	0.39224000
H	-6.47852300	3.22305700	-1.02974700

References

- (1) (a) Zhao, Y.; Truhlar, D. G. *J. Chem. Theory Comput.* **2008**, *4*, 1849-1868. (b) Zhao, Y.; Truhlar, D. G. *Acc. Chem. Res.* **2008**, *41*, 157-167. (c) Zhang, P.; Wolf, C. *Angew. Chem., Int. Ed.* **2013**, *52*, 7869-7873.
- (2) (a) Mennucci, B.; Tomasi, J. *J. Chem. Phys.* **1997**, *106*, 5151-5158. (b) Barone, V.; Cossi, M. *J. Phys. Chem. A* **1998**, *102*, 1995-2001.
- (3) (a) Parr, R. G.; Pearson, R. G. *J. Am. Chem. Soc.* **1983**, *105*, 7512-7516. (b) Domingo, L. R.; Picher, M. T.; Sáez, J. A. *J. Org. Chem.* **2009**, *74*, 2726-2735.
- (4) (a) Kohn, W.; Sham, L. J. *Phys. Rev.* **1965**, *140*, A1133. (b) Sham, L. J.; Kohn, W. *Phys. Rev.* **1966**, *145*, 561.
- (5) (a) Domingo, L. R.; Chamorro, E.; Pérez, P. *Eur. J. Org. Chem.* **2009**, *2009*, 3036-3044. (b) Domingo, L. R.; Chamorro, E.; Perez, P. *J. Phys. Chem. A* **2008**, *112*, 4046-4053. (c) Domingo, L. R.; Pérez, P.; Sáez, J. A. *RSC Adv.* **2013**, *3*, 1486-1494. (d) Domingo, L. R.; Perez, P. *Org. Biomol. Chem.* **2011**, *9*, 7168-7175.
- (6) Yuan, S.; Luo, Y.; Peng, J.; Miao, M.; Xu, J.; Ren, H. *Org. Lett.* **2017**, *19*, 6100-6103.
- (7) Shi, Q. Q.; Zhang, W.; Wang, Y.; Qu, L. B.; Wei, D. H. *Org. Biomol. Chem.* **2018**, *16*, 2301-2311.