

Supporting Information

**Cobalt-Catalyzed Radical-Mediated Carbon-Carbon Scission via a Radical-type Migratory Insertion**

Jian-Biao Liu,\* Xiao-Jun Liu, João C. A. Oliveira, De-Zhan Chen, and Lutz Ackermann\*

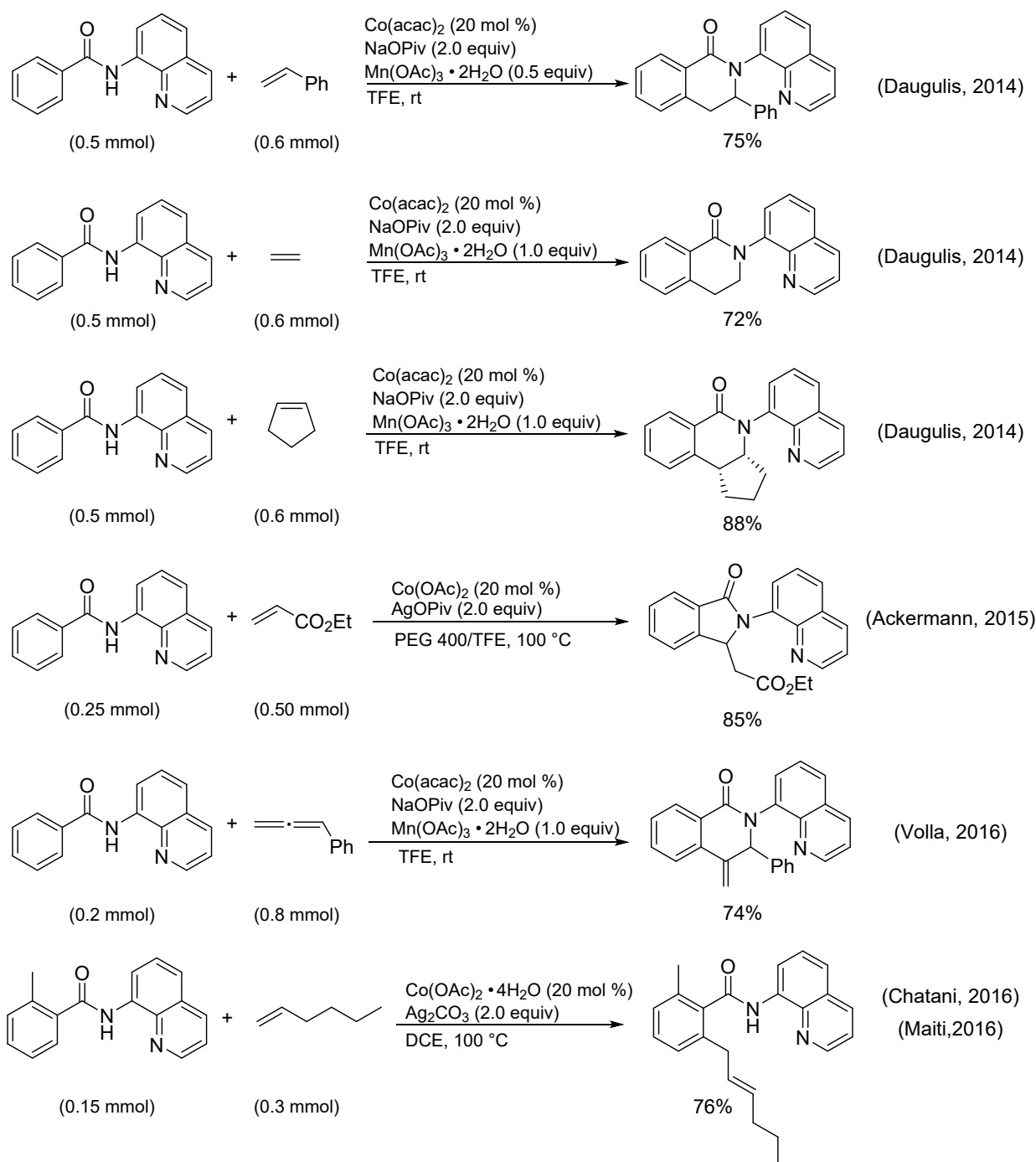
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# 1. Supplementary results for radical-type migratory insertion of alkenes into Co–C bonds

## 1.1 Selected reactions

The detailed reaction conditions for cobalt-catalyzed aminoquinoline-directed coupling of  $sp^2$  C–H bonds with various alkenes are summarized in Scheme S1.



**Scheme S1.** Selected examples of cobalt-catalyzed aminoquinoline-directed coupling of  $sp^2$  C–H bonds with alkenes.

## 1.2 Computational methods and theoretical backgrounds

- Computational details

In this section, all the geometries of the intermediates and transition states for different alkene coupling partners were optimized by Gaussian 09<sup>[1]</sup> in 2,2,2-TriFluoroEthanol (TFE) solvent at the B3LYP<sup>[2]</sup>-D3(BJ)<sup>[3]</sup>/6-31G(d,p)/ECP10MDF(Co) level of theory with the corresponding Stuttgart/Dresden (SDD) effective core potential (ECP) on the transition metals. Frequency calculations were performed at the same theoretical level to verify the nature of the stationary points and to obtain the thermal Gibbs free energy corrections ( $\Delta G_{\text{corr}}$ ) at 298.15 K. Single point calculations at B3LYP-D3(BJ)/def2-TZVP<sup>[4]</sup> were carried out in the gas phase to obtain more accurate electronic energies. The solvent corrections ( $\Delta G_{\text{solv}}$ ) were obtained from the single-point energy difference between gas phase and solution calculations at B3LYP-D3(BJ)/def2-TZVP level. The continuum solvation model SMD<sup>[5]</sup> was utilized to consider the bulk solvent effects. The correction caused by the different standard states in the gas phase and in solution was added to the free energies of all species. Numerical integrations were performed with the ultrafine grid during the calculations.

The 3D diagrams of molecules and the spin density isosurface maps were prepared by CYLview<sup>[6]</sup> and GaussView5.0 respectively. The condensed local softness, atomic charges and spin densities were calculated by Multiwfn 3.8.<sup>[7]</sup>

- Electron spin density

In open-shell systems, the electron spin density is defined as the difference between the densities of electrons with spin  $\alpha$  and those with spin  $\beta$

$$\rho_s(\mathbf{r}) = \rho_\alpha(\mathbf{r}) - \rho_\beta(\mathbf{r}).$$

Information about spin density delocalization can be obtained from the analysis of the corresponding distributions in the spin density map or the computed atomic spin population. The Mulliken spin population analyses were used to calculate the atomic spin population.

- Nucleus-independent chemical shift (NICS)

To investigate the changes of aromaticity during the migratory insertion of ethylene into Co–C bonds, the nucleus-independent chemical shift (NICS)<sup>[8]</sup> values at the ring center NICS(0) were calculated at the B3LYP/def2-SVP level. The negative NICS values denote aromaticity.

- Spin Contamination

The deviation in the expectation value  $\langle \hat{S}^2 \rangle$  from the ideal values is usually used as a quantitative measure of spin contamination in an unrestricted Hartree-Fock wave function. Similarly, the  $\langle \hat{S}^2 \rangle$  values calculated for Kohn–Sham orbitals can be used as qualitative measures of spin contamination.<sup>[9]</sup> It should be noted that the single determinant of Kohn-Sham orbitals is spin-contaminated and this is allowed since this determinant is not the correct wave function for the system.<sup>[10]</sup> For current cobalt systems, the amount of spin contamination in the Kohn–Sham determinant is small in most cases. The  $\langle \hat{S}^2 \rangle$  values for the intermediate having significant diradical character are somewhat larger than the values expected for the triplet (2.0).

### 1.3 Influence of different methods on the free energy profiles, geometries and spin populations

To investigate the influences of different DFT methods on the calculated results, we optimized the **INT1**, **TS** and **INT2** in 2,2,2-TriFluoroEthanol (TFE) solvent by PBE0-D3(BJ),<sup>[11]</sup> M06<sup>[12]</sup> and  $\omega$ B97XD<sup>[13]</sup> functionals in conjunction with 6-31G(d,p)/ECP10MDF(Co) basis set (denoted as BS1) respectively.<sup>[14]</sup> Single point calculations at XC/def2-TZVPP were carried out in the gas phase to obtain more accurate electronic energies. The solvent corrections ( $\Delta G_{\text{solv}}$ ) were obtained from the single-point energy difference between gas phase and solution calculations at XC/def2-TZVPP level. The continuum solvation model SMD was utilized to consider the bulk solvent effects. The overall free energies at each functional can be summarized as

$$G_{\text{XC}} = \Delta G_{\text{corr, XC/BS1}} + \Delta G_{\text{solv, XC/BS2}} + E_{\text{XC/BS2}},$$

where XC represents B3LYP-D3(BJ), PBE0-D3(BJ), M06 or  $\omega$ B97XD, BS1 represents 6-31G(d,p)/ECP10MDF(Co) and BS2 represents def2-TZVPP.

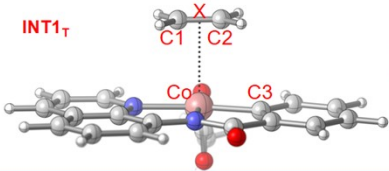
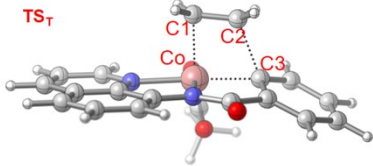
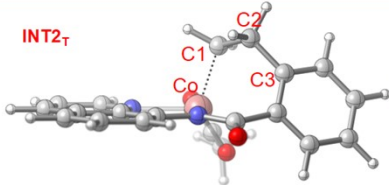
The atomic spin populations calculated by different methods, using the wavefunction obtained from the B3LYP-D3(BJ)/6-31G(d,p)/SDD(Co) level, are listed in Table S1. The Mulliken, Lowdin, Becke and Hirshfeld methods provide similar spin population changes during the insertion process.

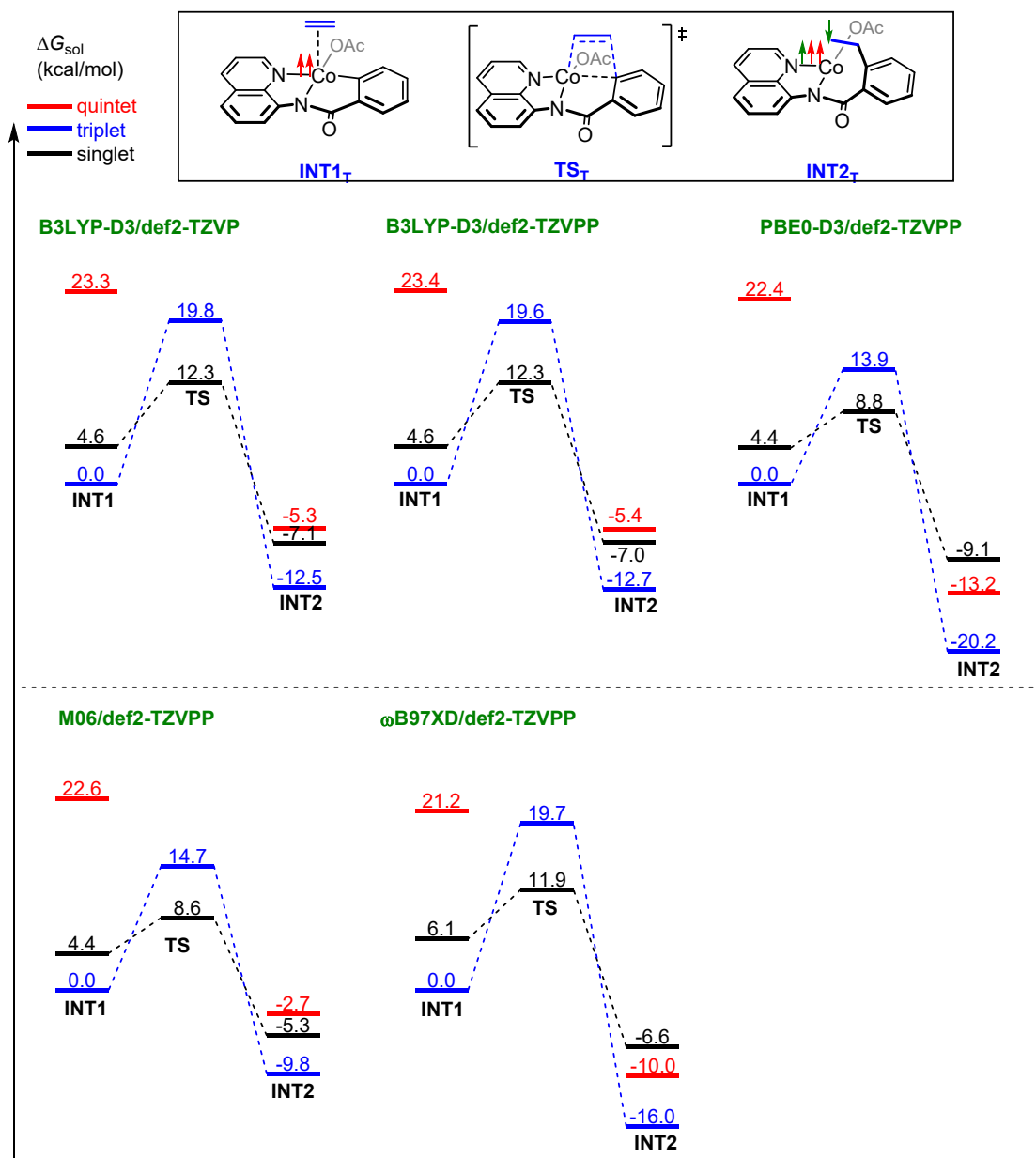
As shown in Figure S1, the B3LYP-D3(BJ), PBE0-D3(BJ), M06 and  $\omega$ B97XD functionals provide similar energy ordering of the spin states of **INT1** and **TS**. For the resulting insertion intermediate **INT2**, although deviations in the energy ordering of the singlet and quintet states were observed in these methods, the calculated results of these methods all reveal that the triplet is the most stable spin state.

The optimized structures and the calculated spin populations obtained by B3LYP-D3(BJ), PBE0-D3(BJ) and M06 methods are depicted in Figure S2. The three methods provide similar geometry changes and spin population changes during the migratory insertion of ethylene into Co–C bond.

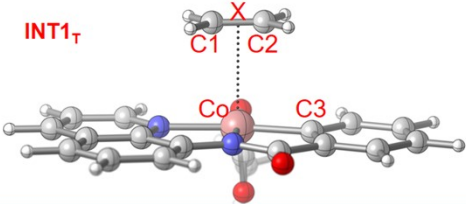
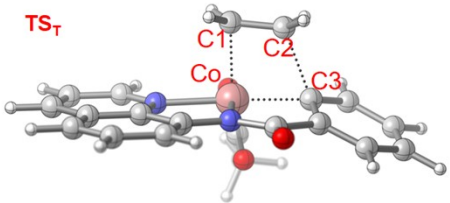
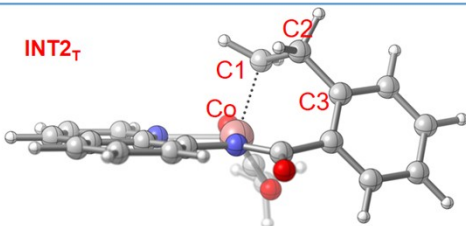
The electronic energies and bond distances obtained by the PBE0-D3 and M06 methods along the minimum energy paths of the triplet and singlet states are given in Figure S3. The results of the two methods again demonstrate that the bond-making/breaking processes in the radical-type insertion is asynchronous, while the corresponding processes occur synchronously in the typical mechanism. The calculated NICS(0) along the minimum energy paths of the triplet and singlet states also demonstrate the substantial differences between the two insertion mechanisms (Figure S4).

**Table S1.** The atomic spin populations calculated by different methods, using the wavefunction obtained from the B3LYP-D3(BJ)/6-31G(d,p)/SDD(Co) level.

	Mulliken method	Lowdin method	Becke method	Hirshfeld method
<p><b>INT1<sub>T</sub></b></p> 	<p>Spin populations: Co: 2.07; C3: -0.19</p>	<p>Spin populations: Co: 2.01; C3: -0.15</p>	<p>Spin populations: Co: 2.00; C3: -0.13</p>	<p>Spin populations: Co: 1.98; C3: -0.13</p>
<p><b>TS<sub>T</sub></b></p> 	<p>Spin populations: Co: 2.19; C3: -0.24 C2: 0.11; C1: -0.30</p>	<p>Spin populations: Co: 2.13; C3: -0.19 C2: 0.08; C1: -0.24</p>	<p>Spin populations: Co: 2.10; C3: -0.16 C2: 0.06; C1: -0.20</p>	<p>Spin populations: Co: 2.10; C3: -0.15 C2: 0.04; C1: -0.18</p>
<p><b>INT2<sub>T</sub></b></p> 	<p>Spin populations: Co: 2.42; C1: -0.55</p>	<p>Spin populations: Co: 2.36; C1: -0.47</p>	<p>Spin populations: Co: 2.31; C1: -0.38</p>	<p>Spin populations: Co: 2.32; C1: -0.37</p>

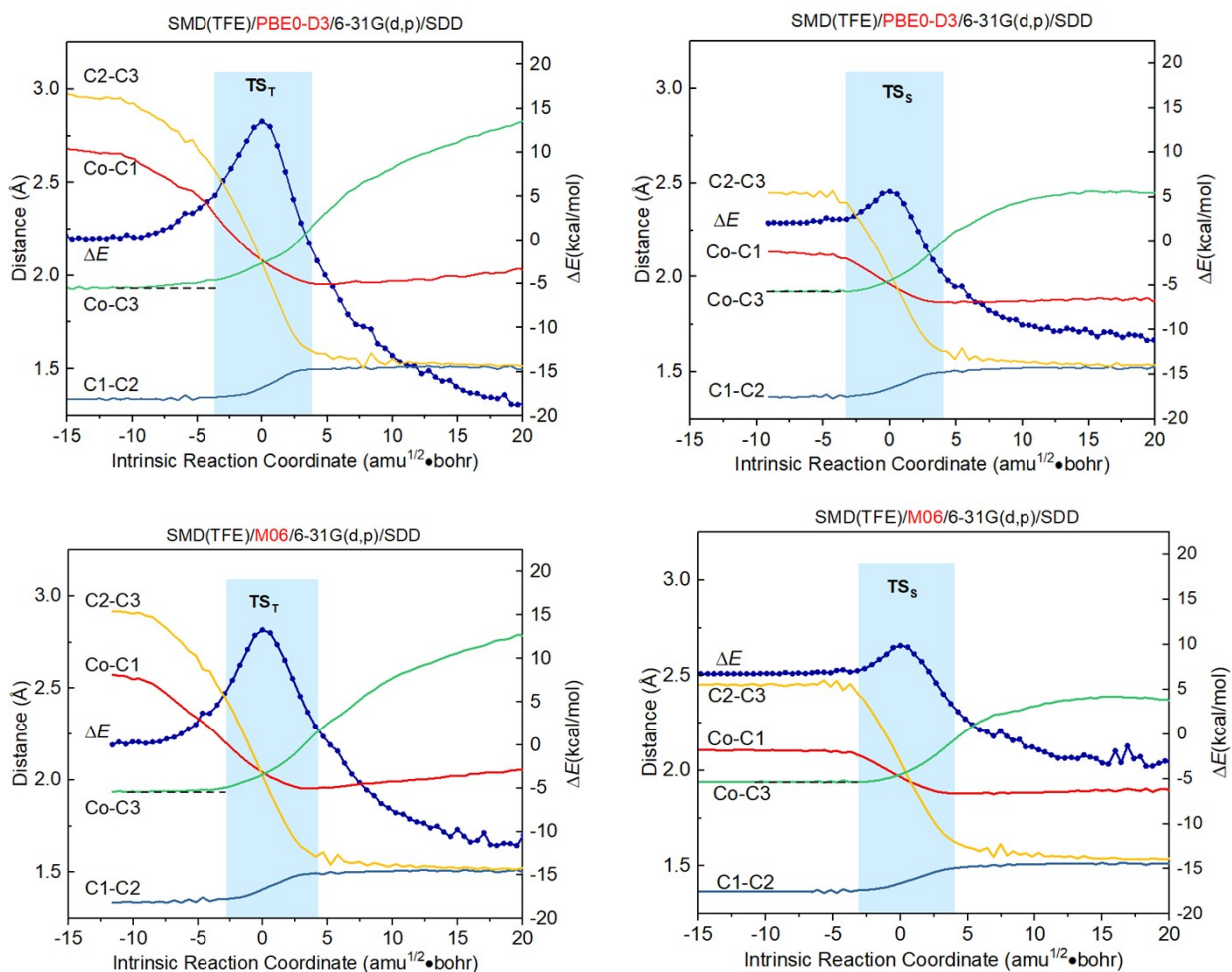


**Figure S1.** Free energy profiles for the migratory insertion of ethylene into Co–C bonds calculated at different levels. All energies are with respect to the  $\text{INT1}_T$ .

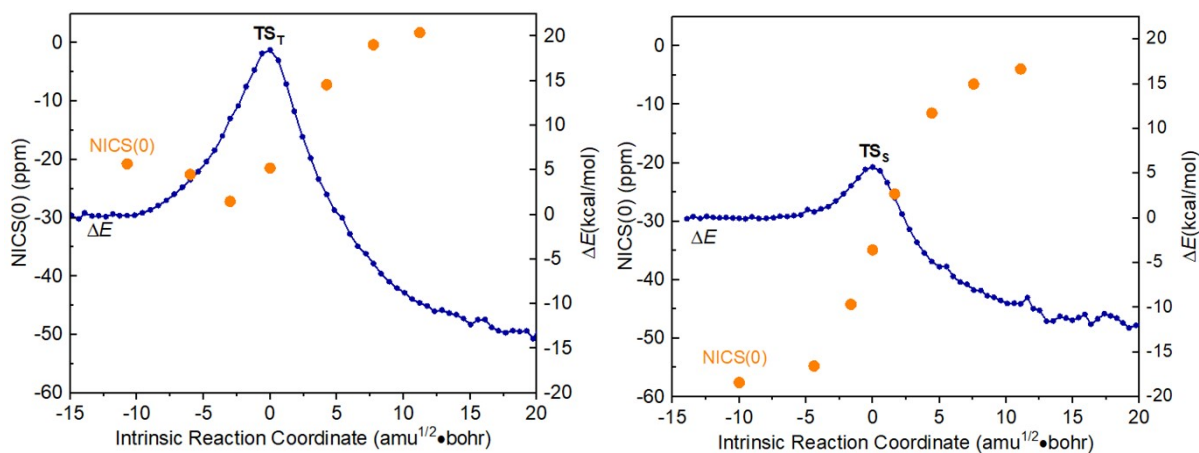
	SMD(TFE)/ <b>B3LYP-D3(BJ)</b> / 6-31G(d,p)/SDD	SMD(TFE)/ <b>PBE0-D3(BJ)</b> / 6-31G(d,p)/SDD	SMD(TFE)/ <b>M06</b> / 6-31G(d,p)/SDD
<b>INT1<sub>T</sub></b> 	<b>Bond lengths:</b> Co-X : 2.75Å (2.16Å) C1-C2 : 1.34Å (1.36Å) Co-C3 : 1.94Å (1.93Å)	<b>Bond lengths:</b> Co-X : 2.67Å (2.05Å) C1-C2 : 1.34Å (1.37Å) Co-C3 : 1.93Å (1.92Å)	<b>Bond lengths:</b> Co-X : 2.56Å (2.02Å) C1-C2 : 1.34Å (1.37Å) Co-C3 : 1.94Å (1.94Å)
	<b>Spin populations:</b> Co: 2.07; C3: -0.19	<b>Spin populations:</b> Co: 2.18; C3: -0.26	<b>Spin populations:</b> Co: 2.02; C3: -0.18
<b>TS<sub>T</sub></b> 	<b>Bond lengths:</b> Co-C1: 2.06Å (1.97Å) C1-C2 : 1.41Å (1.42Å) C2-C3 : 2.02Å (2.02Å) Co-C3 : 2.10Å (2.02Å)	<b>Bond lengths:</b> Co-C1: 2.08Å (1.96Å) C1-C2 : 1.40Å (1.41Å) C2-C3 : 2.07Å (2.02Å) Co-C3 : 2.07Å (1.98Å)	<b>Bond lengths:</b> Co-C1: 2.04Å (1.96Å) C1-C2 : 1.41Å (1.41Å) C2-C3 : 2.02Å (2.04Å) Co-C3 : 2.03Å (1.98Å)
	<b>Spin populations:</b> Co: 2.19; C3: -0.24 C2: 0.11; C1: -0.30	<b>Spin populations:</b> Co: 2.30; C3: -0.31 C2: 0.14; C1: -0.32	<b>Spin populations:</b> Co: 2.08; C3: -0.20 C2: 0.10; C1: -0.24
<b>INT2<sub>T</sub></b> 	<b>Bond lengths:</b> Co-C1: 2.08Å (1.91Å) C1-C2 : 1.51Å (1.53Å) C2-C3 : 1.52Å (1.53Å)	<b>Bond lengths:</b> Co-C1: 2.09Å (1.90Å) C1-C2 : 1.50Å (1.52Å) C2-C3 : 1.51Å (1.52Å)	<b>Bond lengths:</b> Co-C1: 2.11Å (1.91Å) C1-C2 : 1.50Å (1.51Å) C2-C3 : 1.51Å (1.53Å)
	<b>Spin populations:</b> Co: 2.42; C1: -0.55	<b>Spin populations:</b> Co: 2.54; C1: -0.63	<b>Spin populations:</b> Co: 2.54; C1: -0.65

**Figure S2.** The optimized structures and spin populations obtained by B3LYP-D3(BJ), PBE0-D3(BJ) and M06 methods respectively. The values for the singlets are given in parentheses.





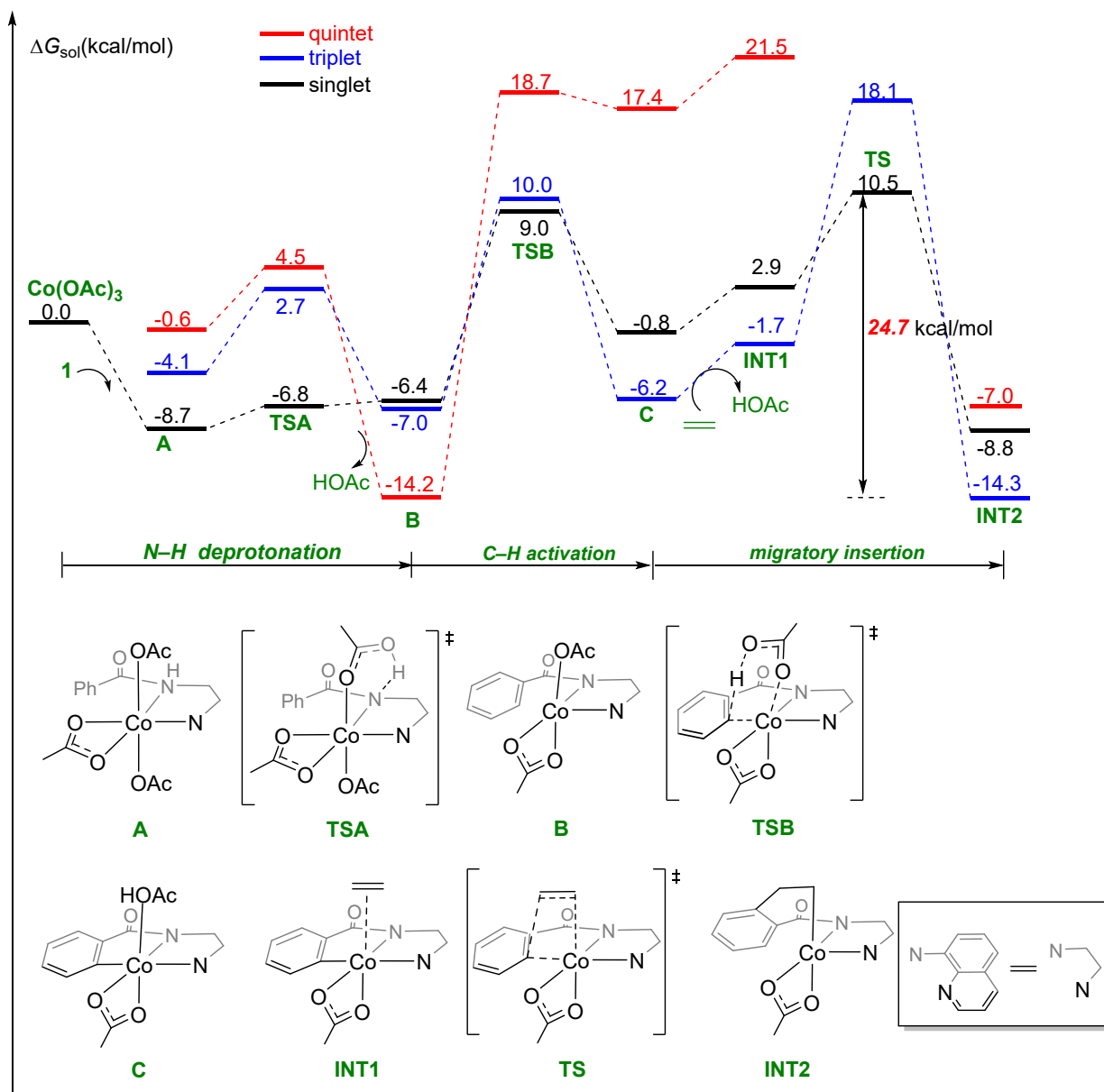
**Figure S3.** Electronic energies and bond distances obtained by the PBE0-D3 and M06 methods along minimum energy paths of the triplet and singlet states.



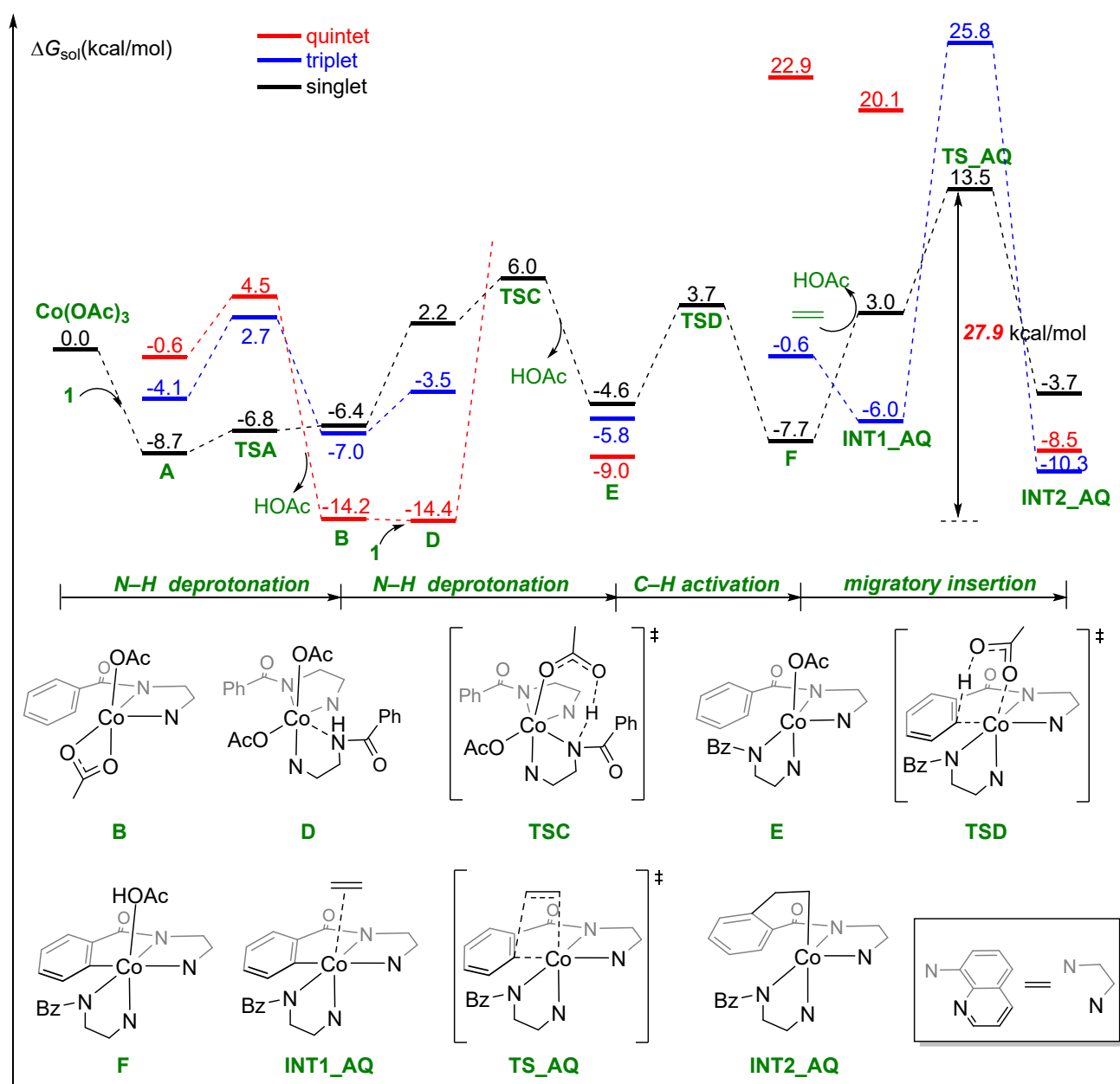
**Figure S4.** The calculated NICS(0) along the minimum energy paths of the triplet and singlet states.

#### 1.4 Potential involvement of an additional amide ligand

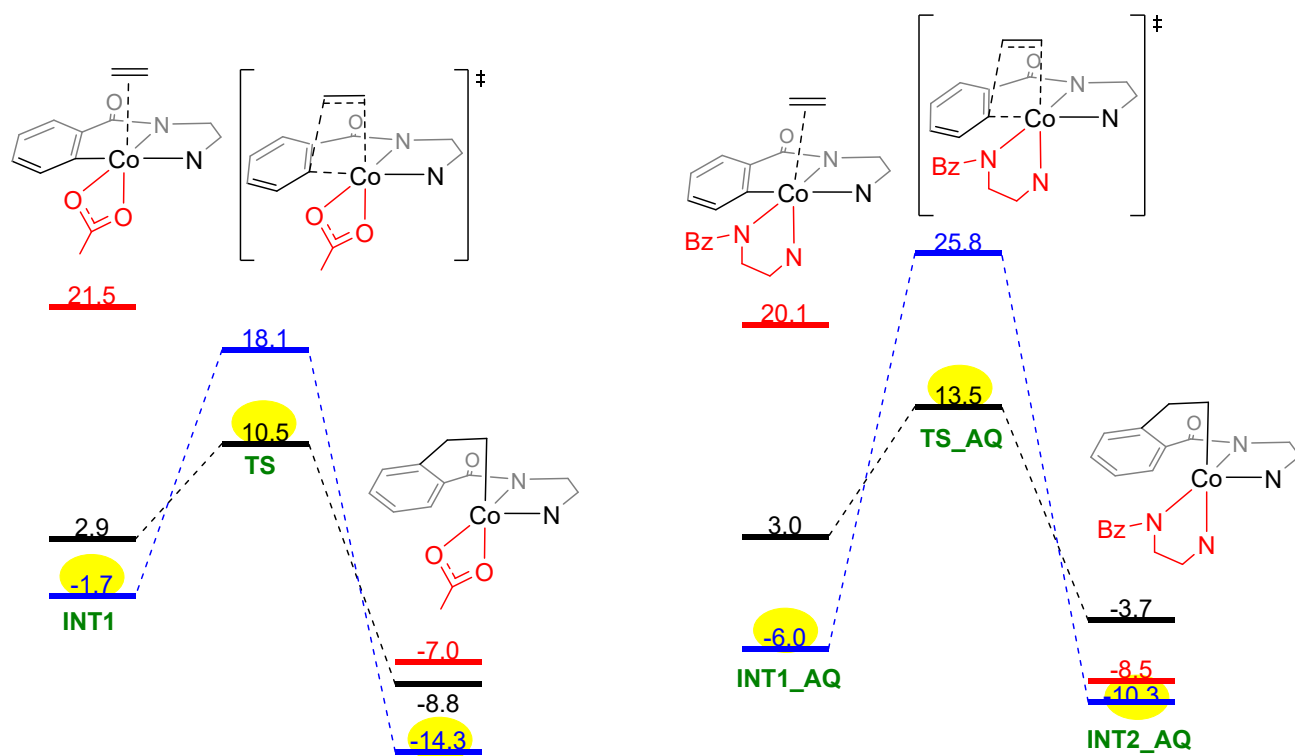
Previously, both experimental and computational studies demonstrated that an additional amide unit can coordinate with the metal center as a bis-chelating ligand.<sup>[15]</sup> The free energy profiles in the presence of one and two amide unit are given in Figures S5 and S6 respectively. In TFE solvent, the activation barrier for the C(sp<sup>2</sup>)-H activation in the presence of an additional amide is 5.3 kcal/mol lower than that with the coordination of OAc<sup>-</sup> (**TSD<sub>S</sub>** vs. **TSB<sub>S</sub>**). For the alkene-coordinated complexes, although **INT1\_AQ** is 4.3 kcal/mol more stable than **INT1**, the following migratory insertion of ethylene into Co-C bonds from **INT1** is both kinetically and thermodynamically more favorable (Figure S7). Furthermore, similar energy ordering of the intermediate and transition state and spin population changes were observed during the migratory insertion in the presence of an additional amide ligand (Figure S8).



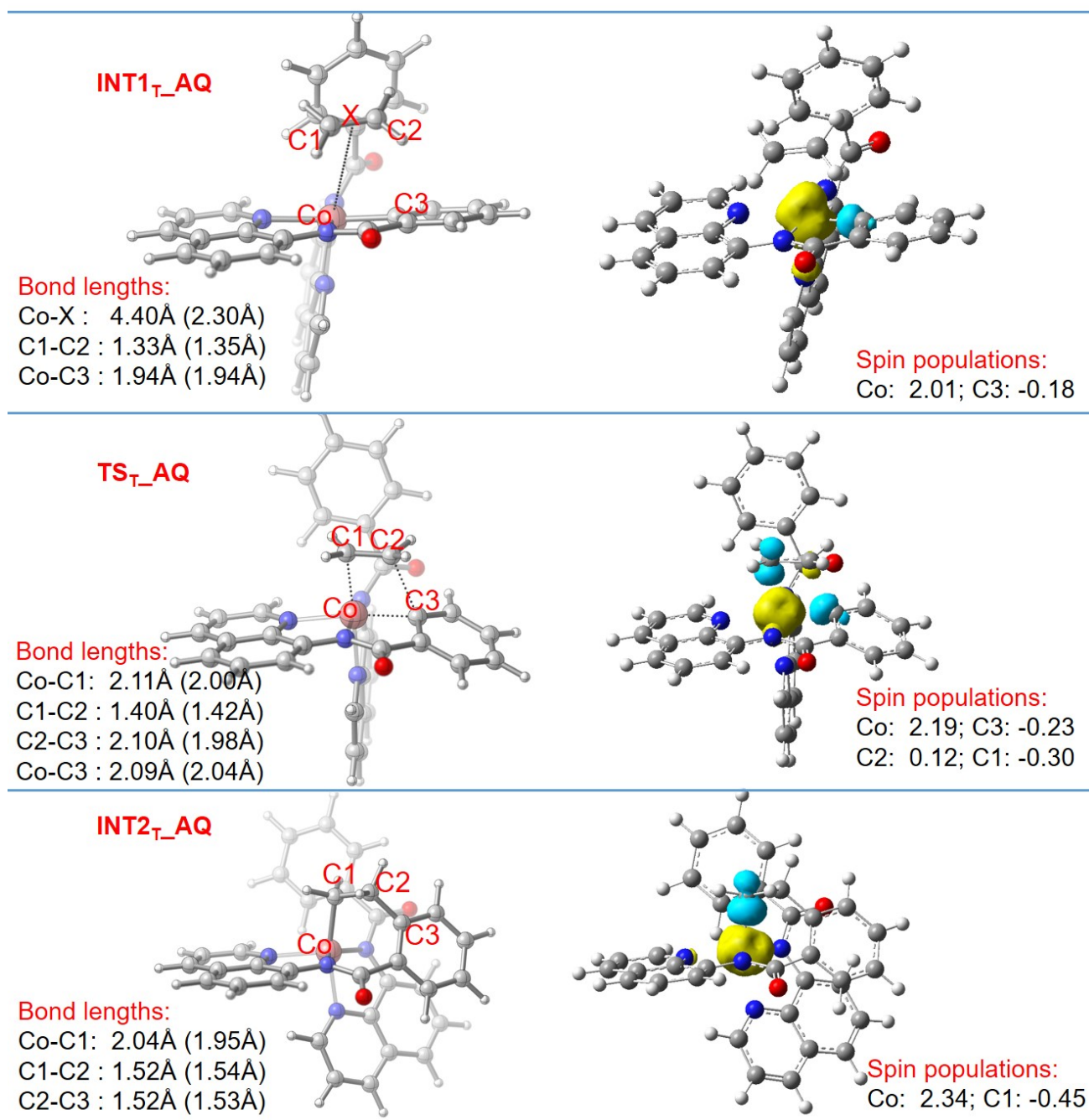
**Figure S5.** Free energy profiles for the N–H deprotonation, C–H activation and migratory insertion with the coordination of  $\text{OAc}^-$  at the SMD(TFE)/B3LYP-D3(BJ)/def2-TZVP//SMD(TFE)/B3LYP-D3(BJ)/6-31G(d,p)/SDD level. All energies are with respect to the  $\text{Co(OAc)}_3$ .



**Figure S6.** Free energy profiles for the N–H deprotonation, C–H activation and migratory insertion with an additional amide as a bis-chelating ligand at the SMD(TFE)/B3LYP-D3(BJ)/def2-TZVP//SMD(TFE)/B3LYP-D3(BJ)/6-31G(d,p)/SDD level. All energies are with respect to the  $\text{Co(OAc)}_3$ .



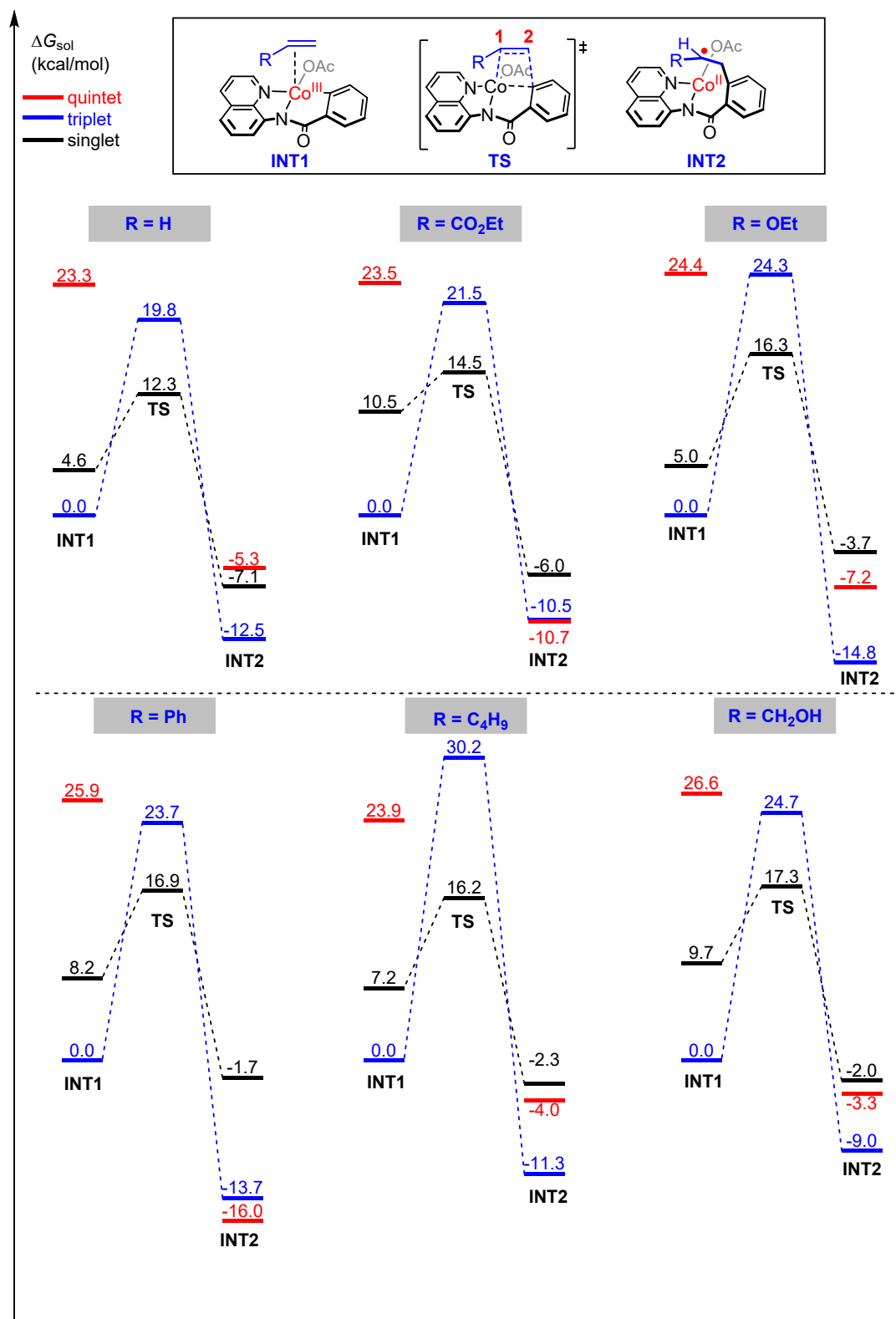
**Figure S7.** Free energy profiles for the migratory insertion of ethylene into Co–C bonds with  $\text{OAc}^-$  or an additional amide as the coordinating ligand. All energies are with respect to the  $\text{Co}(\text{OAc})_3$ .



**Figure S8.** The optimized structures and the calculated spin populations in the presence of an additional amide as a bis-chelating ligand. The values for the singlets are given in parentheses.

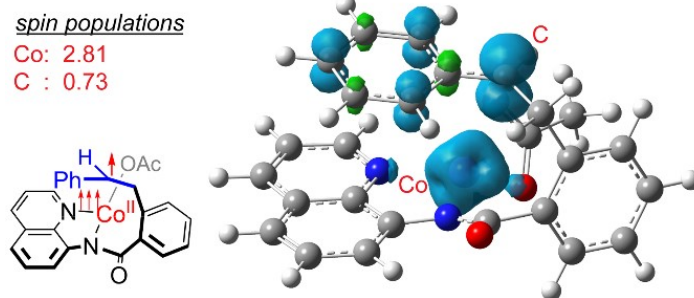
## 1.5 Free energy profiles for various alkenes as well as cyclopentene and allene

The calculated free energy profiles for migratory insertion step of various monosubstituted alkenes are given in Figure S9. Compared to the results of ethylene, both **INT1** and **TS** exhibit same energy orderings for all the monosubstituted alkenes. The main difference for the alkenes lies in the relative stability of the resulting insertion intermediates. In the case of CO<sub>2</sub>Et, the triplet and quintet states of **INT2** are quite close in energy. Interestingly, the quintet insertion product becomes more stable for styrene. The calculated spin density indicates that the **INT2<sub>Q</sub>** of styrene is actually from quartet Co(II) ferromagnetically coupled with the carbon-centered radical (Figure S10). The calculated free energy profiles for migratory insertion step of cyclopentene and allene are given in Figure S11.

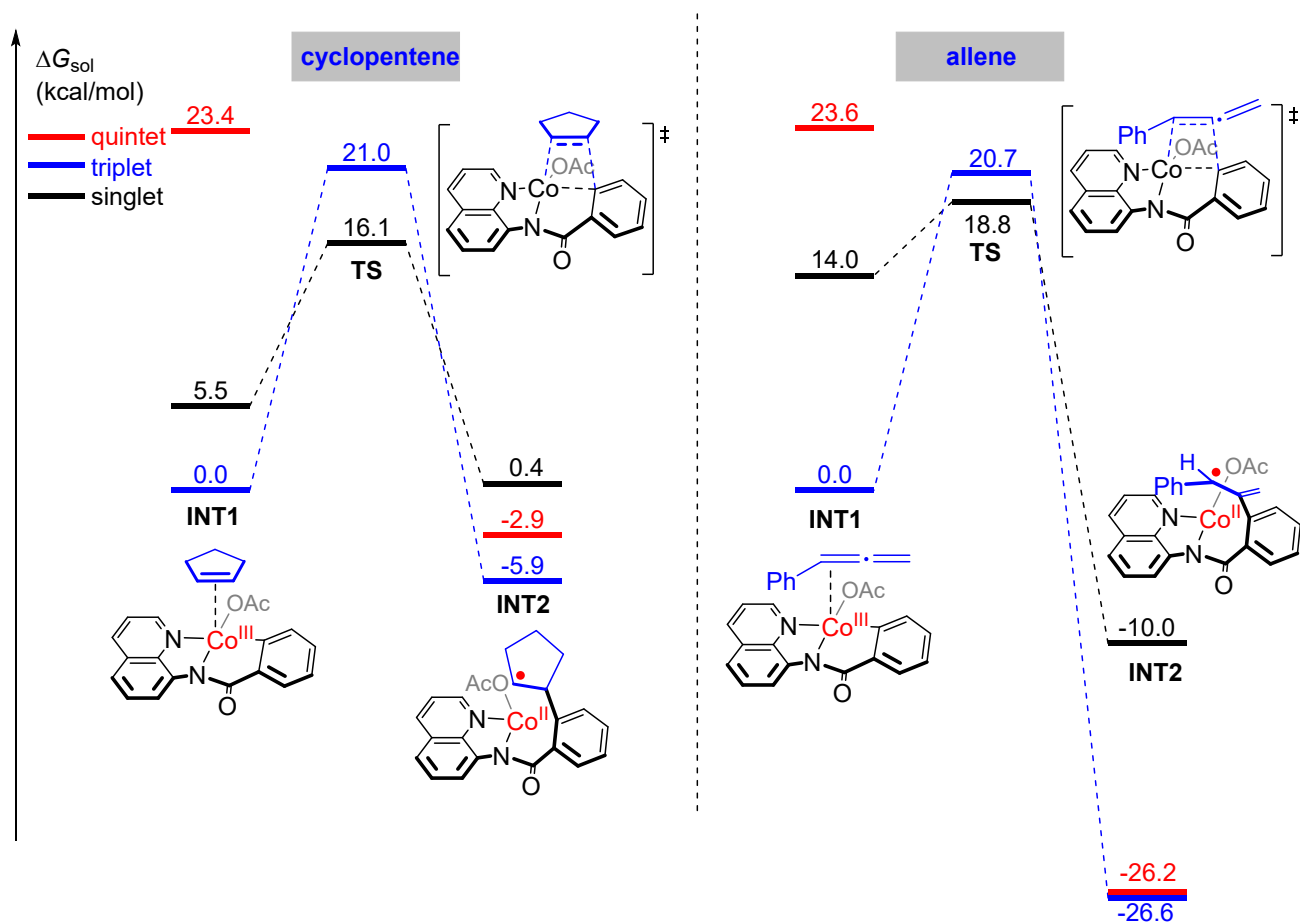


**Figure S9.** Free energy profiles for various monosubstituted alkenes at SMD(TFE)/B3LYP-D3(BJ)/def2-TZVP//SMD(TFE)/B3LYP-D3(BJ)/6-31G(d,p)/SDD level. All energies are with respect to the triplet of the corresponding INT1.





**Figure S10.** The spin density (isovalue=0.01) of INT2<sub>Q</sub> for styrene.



**Figure S11.** Free energy profiles for cyclopentene and allene at SMD(TFE)/B3LYP-D3(BJ)/def2-TZVP// SMD(TFE)/B3LYP-D3(BJ)/6-31G(d,p)/SDD level.

As shown in Figure S12, the activation free energy of the migratory insertion of different types of alkenes  $\Delta G^\ddagger(\text{TS}_S - \text{INT1}_T)$  can be separated into the energy difference between the singlet and triplet of INT1 and the activation free energy of the singlet surface using the following equation :

$$\Delta G^\ddagger(\text{TS}_S - \text{INT1}_T) = \Delta G^\circ(\text{INT1}_S - \text{INT1}_T) + \Delta G^\ddagger(\text{TS}_S - \text{INT1}_S).$$

Herein, we also investigated the possible factors influencing the two terms. As indicated in Figures S13 and S14, a linear correlation can be detected for several alkenes. The correlation of  $\Delta G^\ddagger(\text{TS}_S - \text{INT1}_S)$  with the HOMO energies of alkenes can be explained by the orbital interactions picture. For the alkenes with lower HOMO energies, the energy gap between  $\sigma_{\text{M-C}}$  and  $\pi_{\text{alkene}}$  (HOMO) becomes smaller, resulting in stronger orbital interactions.

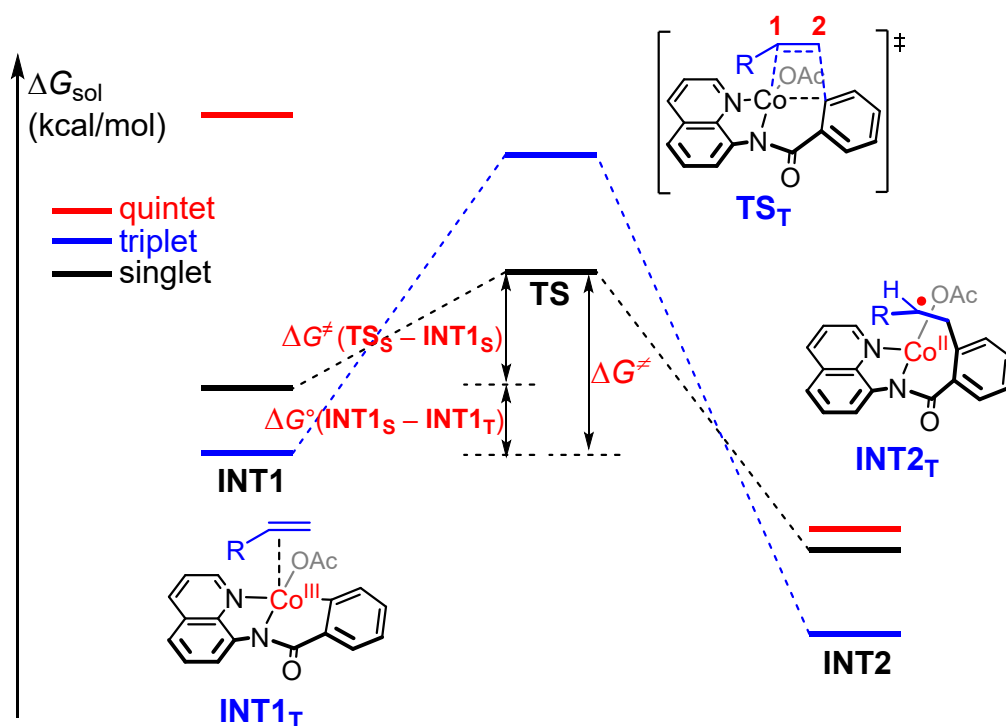
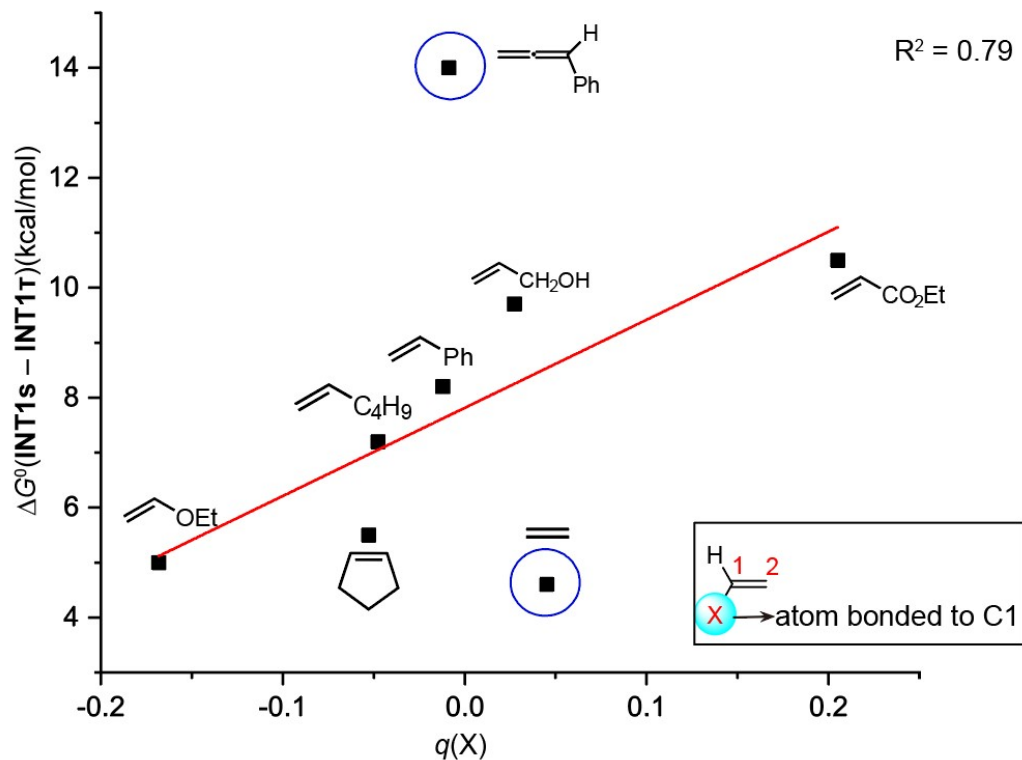
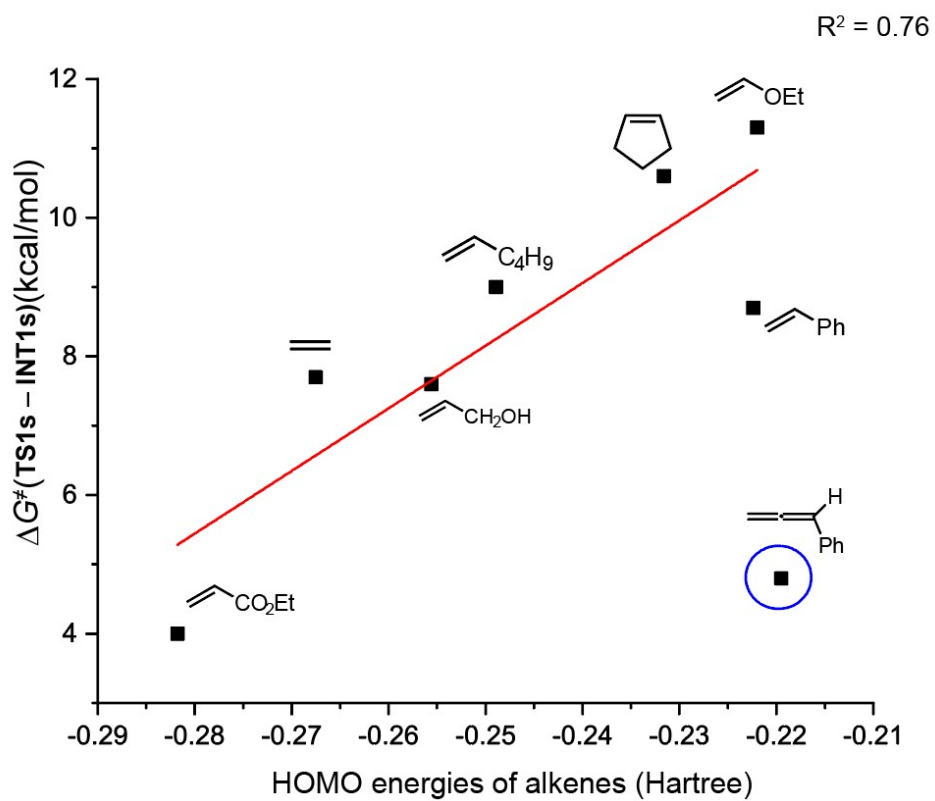


Figure S12. Free energy profiles for the migratory insertion.



**Figure S13.** Correlation of  $\Delta G^\circ(\text{INT1}_s - \text{INT1}_T)$  with the Hirshfeld charges of the atom bonded to C1 of the different alkenes. It should be noted that the values for ethylene and allene were not included during the linear fitting.



**Figure S14.** Correlation of  $\Delta G^\ddagger(\text{TS}_1\text{s} - \text{INT}_1\text{s})$  with the highest occupied molecular orbital (HOMO) energies of alkenes. It should be noted that the value for allene was not included during the linear fitting.

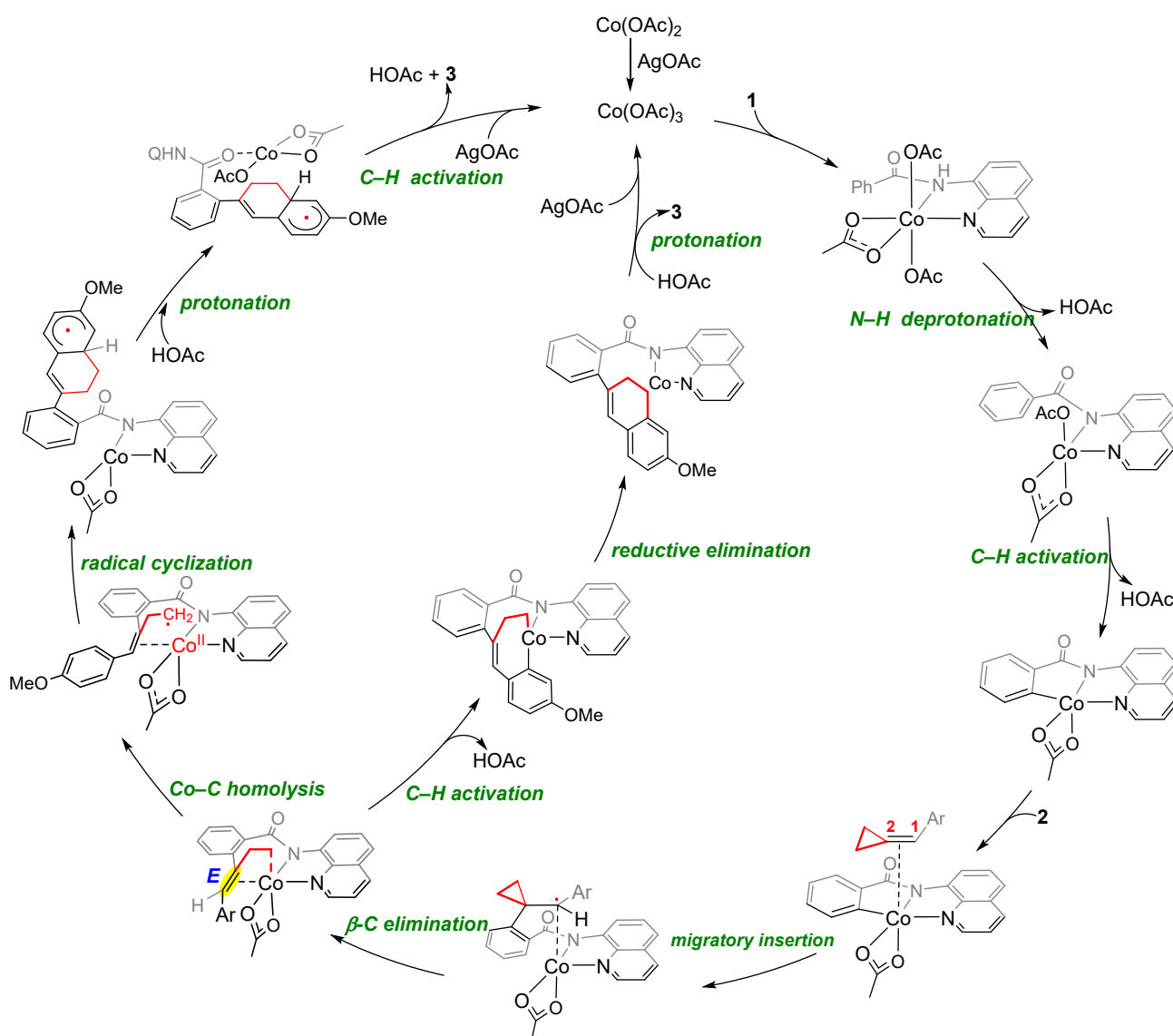
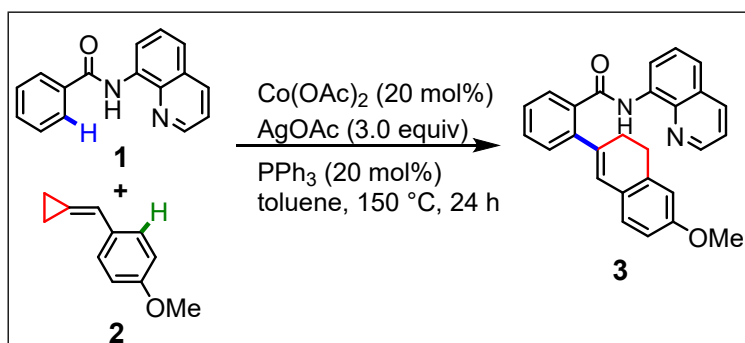
## 2. Supplementary results for Co-catalyzed coupling reaction between benzamides and ACPs

### 2.1 Computational details

In this section, all the geometries of the intermediates and transition states were optimized by Gaussian 09<sup>[1]</sup> in toluene at the B3LYP<sup>[2]</sup>-D3(BJ)<sup>[3]</sup>/6-31G(d,p)/ECP10MDF(Co) level of theory with the corresponding Stuttgart/Dresden (SDD) effective core potential (ECP) on the transition metals. Frequency calculations were performed at the same theoretical level to verify the nature of the stationary points and to obtain the thermal Gibbs free energy corrections ( $\Delta G_{\text{corr}}$ ) at 423.15 K. Single point calculations at B3LYP-D3(BJ)/def2-TZVP were carried out to obtain more accurate electronic energies. The continuum solvation model SMD was utilized to consider the bulk solvent effects. Numerical integrations were performed with the ultrafine grid during the calculations. During the calculations of the “broken symmetry” (BS) states, the Gaussian 09 procedure (Guess = Fragment = N) was employed. The minimum energy crossing points (MECPs) were searched via sobMECP, which is a modified version of Harvey’s MECP program by Tian Lu.<sup>[16]</sup>

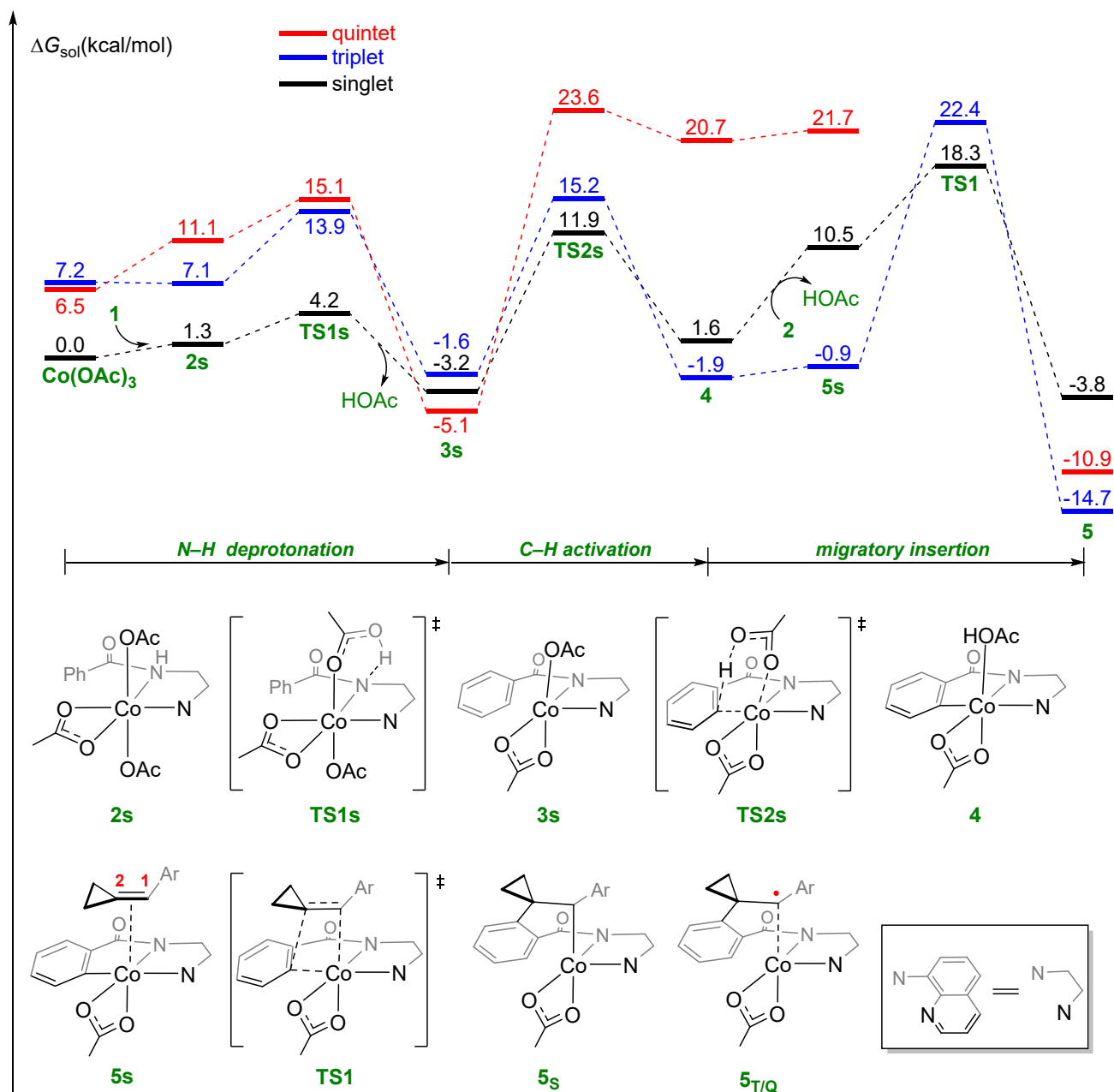
### 2.2 Results for the 1,2-insertion-*E*

The notation “1,2-insertion-*E*” means that the alkene moiety in the intermediate generated by 1,2-insertion and  $\beta$ -C elimination is *E*-alkene (see Scheme S2 for details).

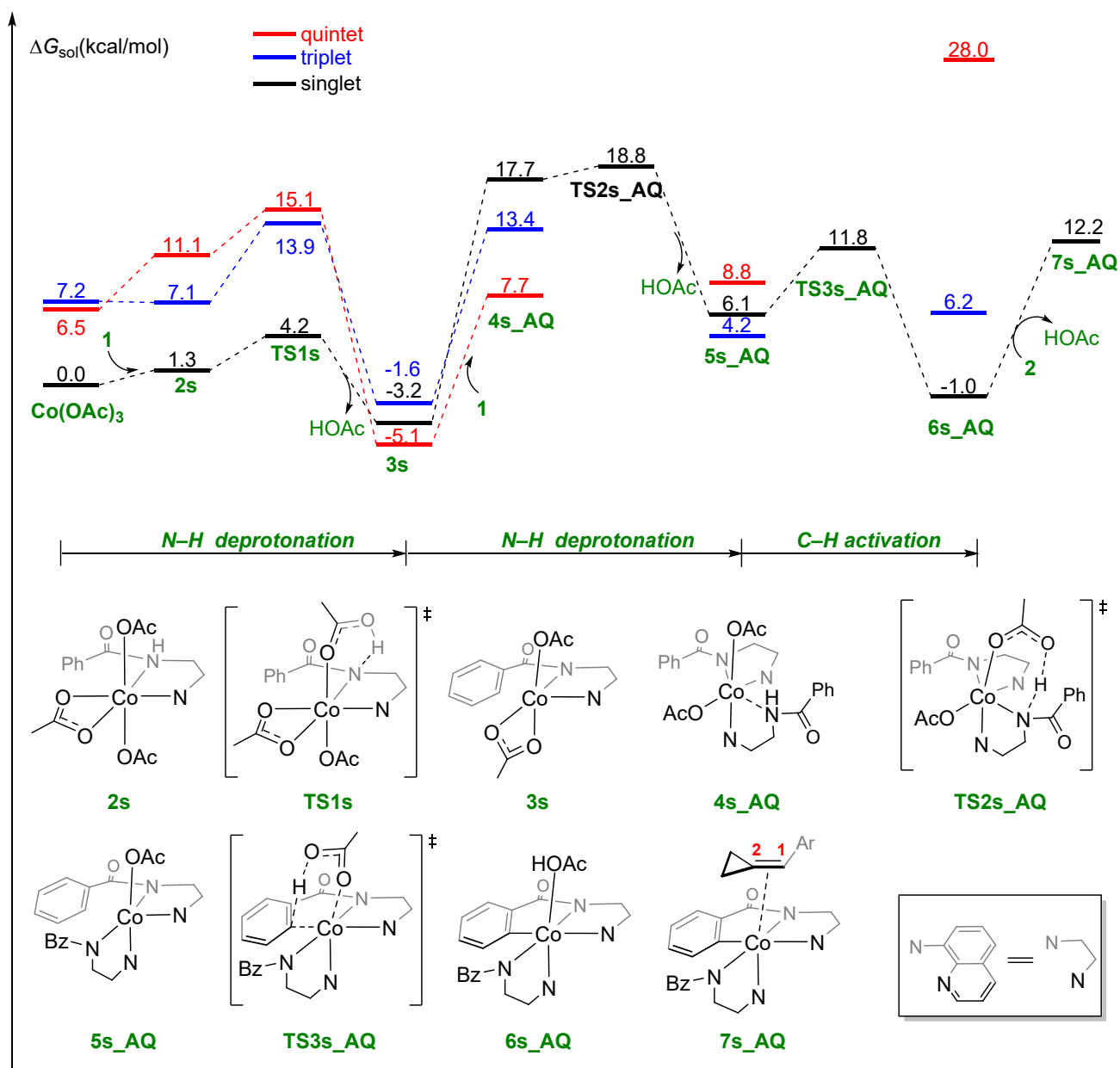


**Scheme S2.** Overall catalytic cycle for Co-catalyzed coupling reaction between benzamides and ACPs.

## 2.2.1 Free energy profiles for the 1,2-insertion-*E*

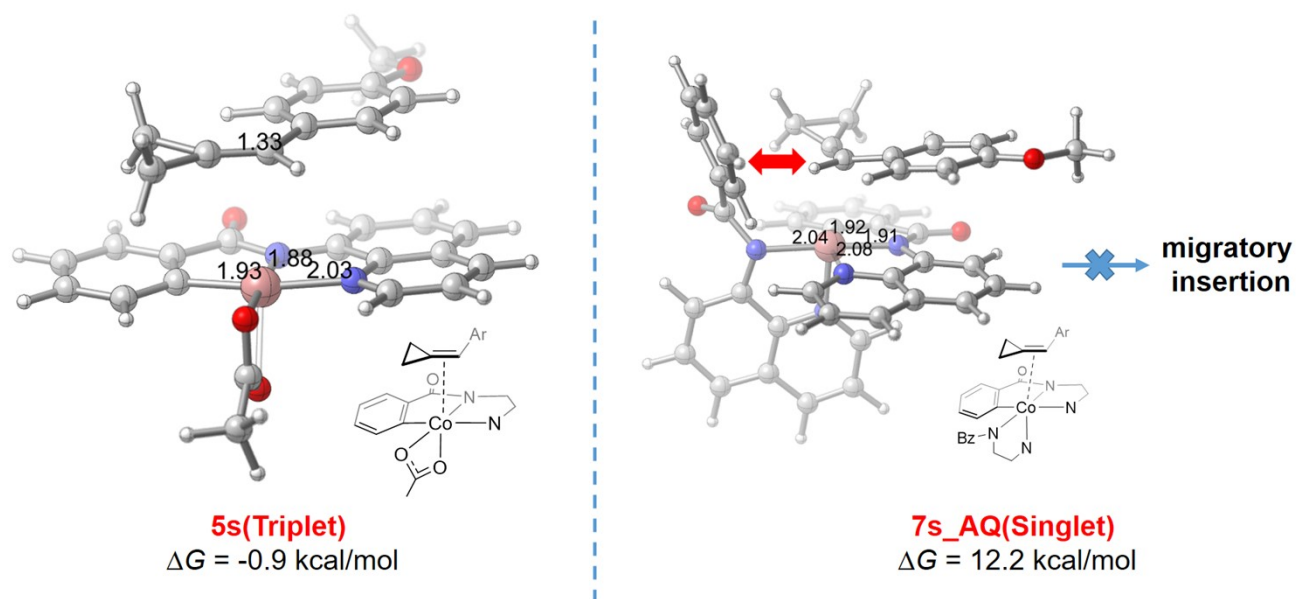


**Figure S15.** Free energy profiles for N-H deprotonation, first C-H activation and migratory insertion steps with the coordination of OAc<sup>-</sup> at SMD(toluene)/B3LYP-D3(BJ)/def2-TZVP//SMD(toluene)/B3LYP-D3(BJ)/6-31G(d,p)/SDD level.



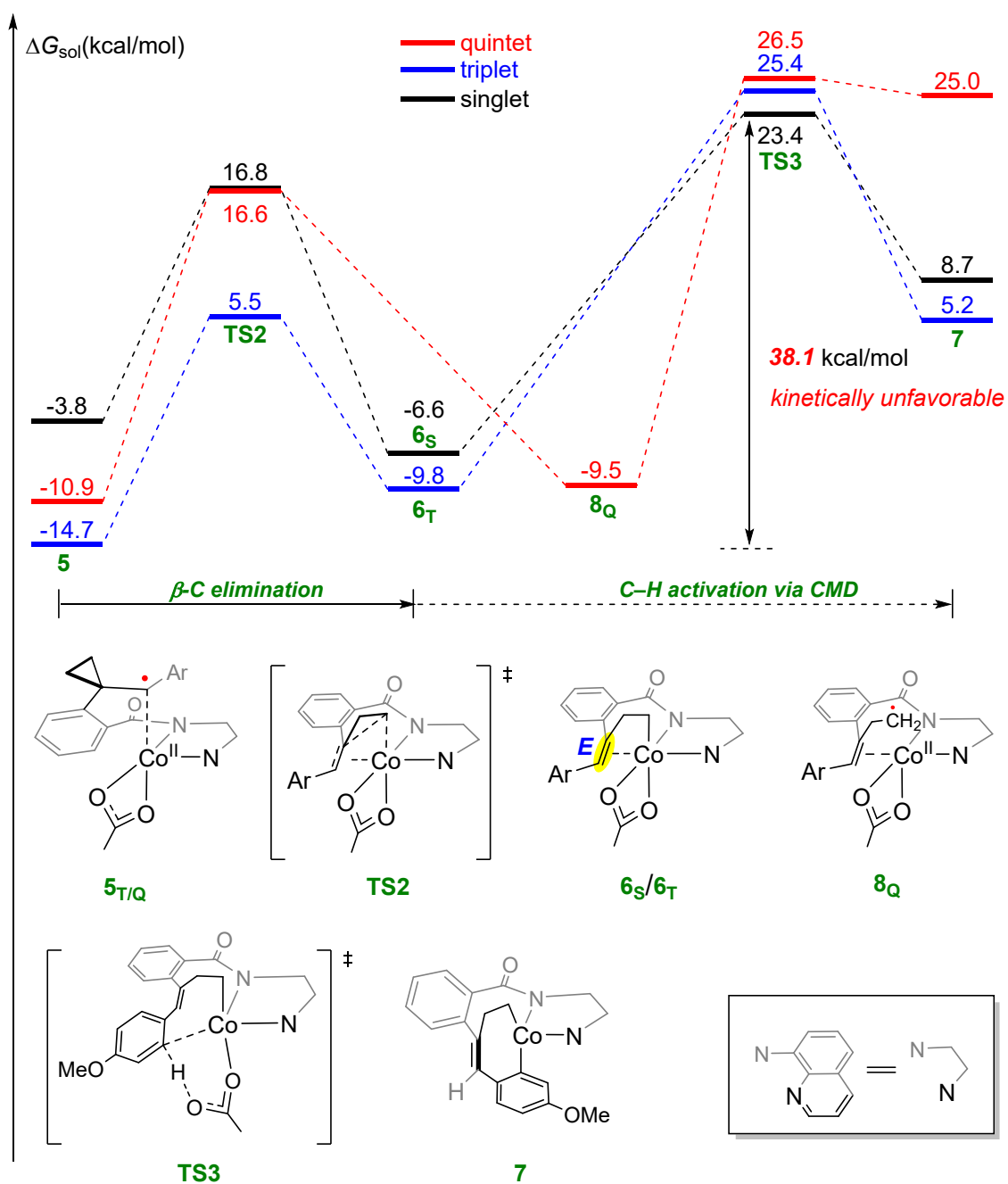
**Figure S16.** Free energy profiles for the N–H deprotonation and C–H activation with an additional amide as a bis-chelating ligand at SMD(toluene)/B3LYP-D3(BJ)/def2-TZVP//SMD(toluene)/B3LYP-D3(BJ)/6-31G(d,p)/SDD level.



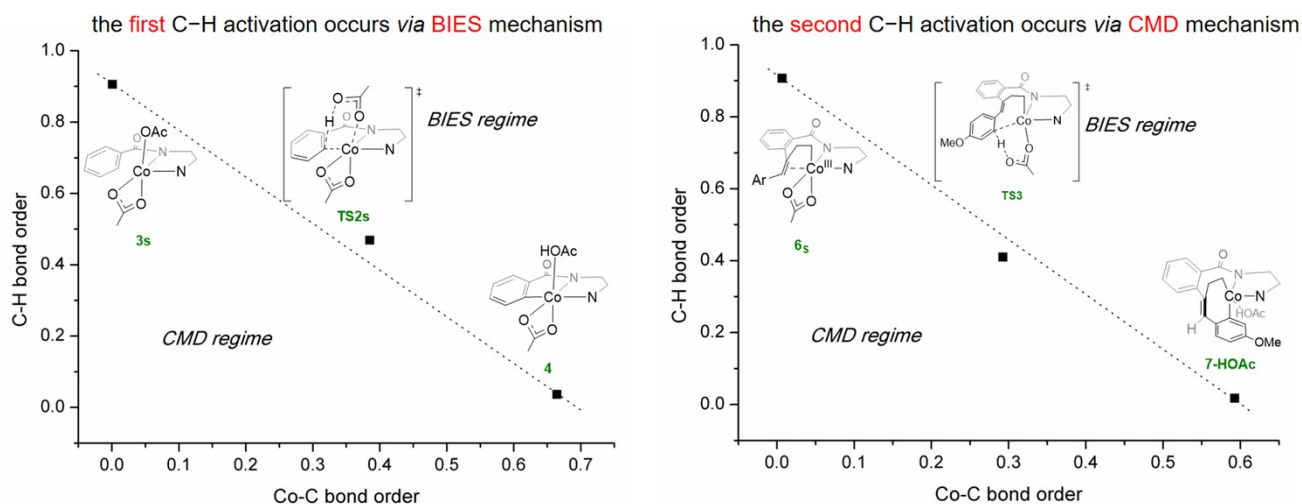


**Figure S17.** Optimized structures of the alkene-coordinated complexes with selected bond distances in Å.

In toluene solvent, as shown in Figures S15 and S16, the activation barrier for the C(sp<sup>2</sup>)-H activation in the presence of an additional amide is almost the same with that in the presence of OAc<sup>-</sup> (**TS3s\_AQ** vs. **TS2s**). However, the transition state of the second N-H deprotonation **TS2s\_AQ** is relatively high in energy. For the alkene-coordinated complexes, the **7s\_AQ(Singlet)** is 13.1 kcal/mol less stable than the counterpart **5s(Triplet)**. More importantly, our calculations indicate that migratory insertion of ACP cannot take place from such bis-ligated intermediate due to the significant steric repulsion between ACP and the additional amide unit (Figure S17).

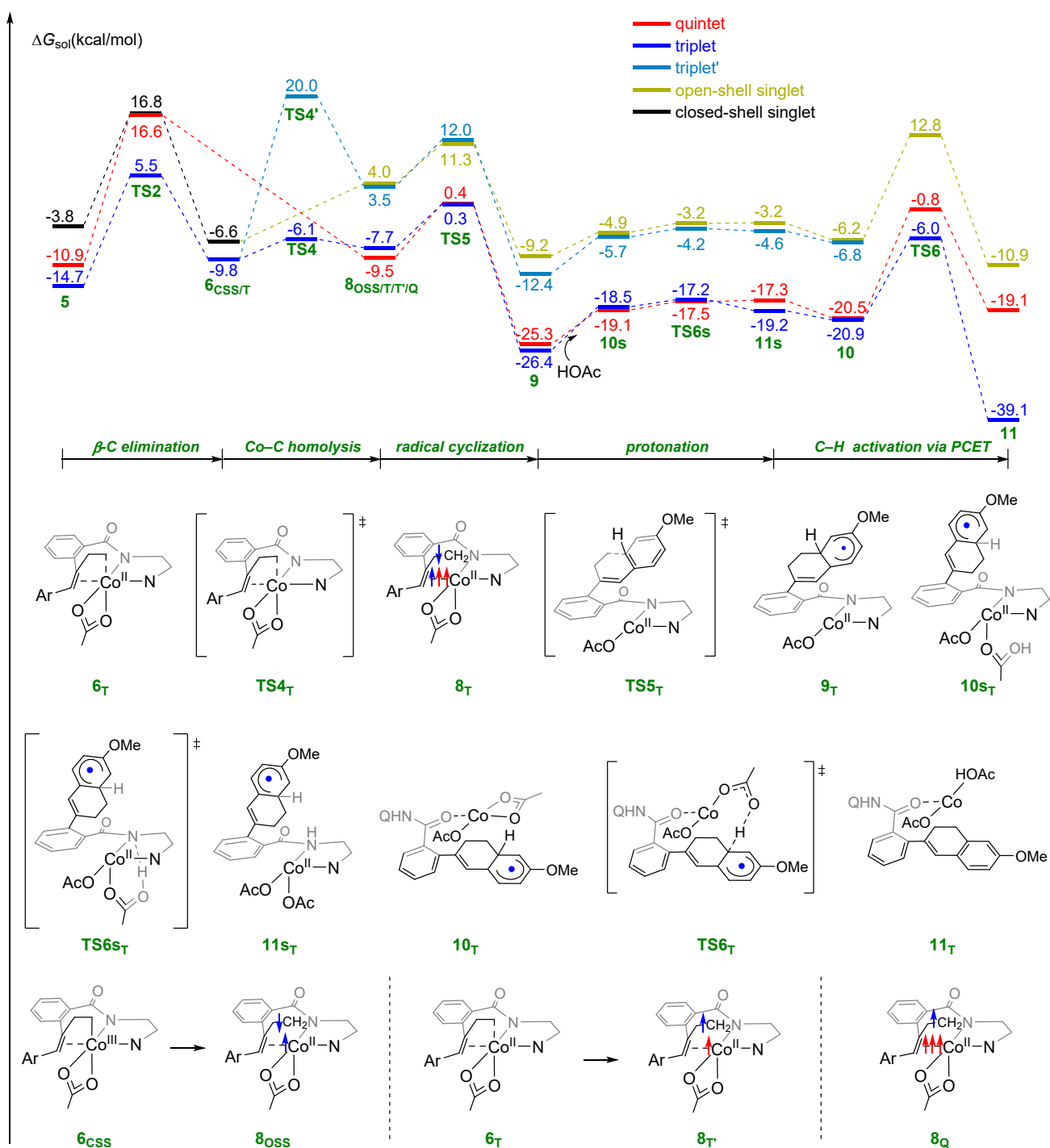


**Figure S18.** Free energy profiles for  $\beta\text{-C}$  elimination and the second C–H activation via CMD mechanism.

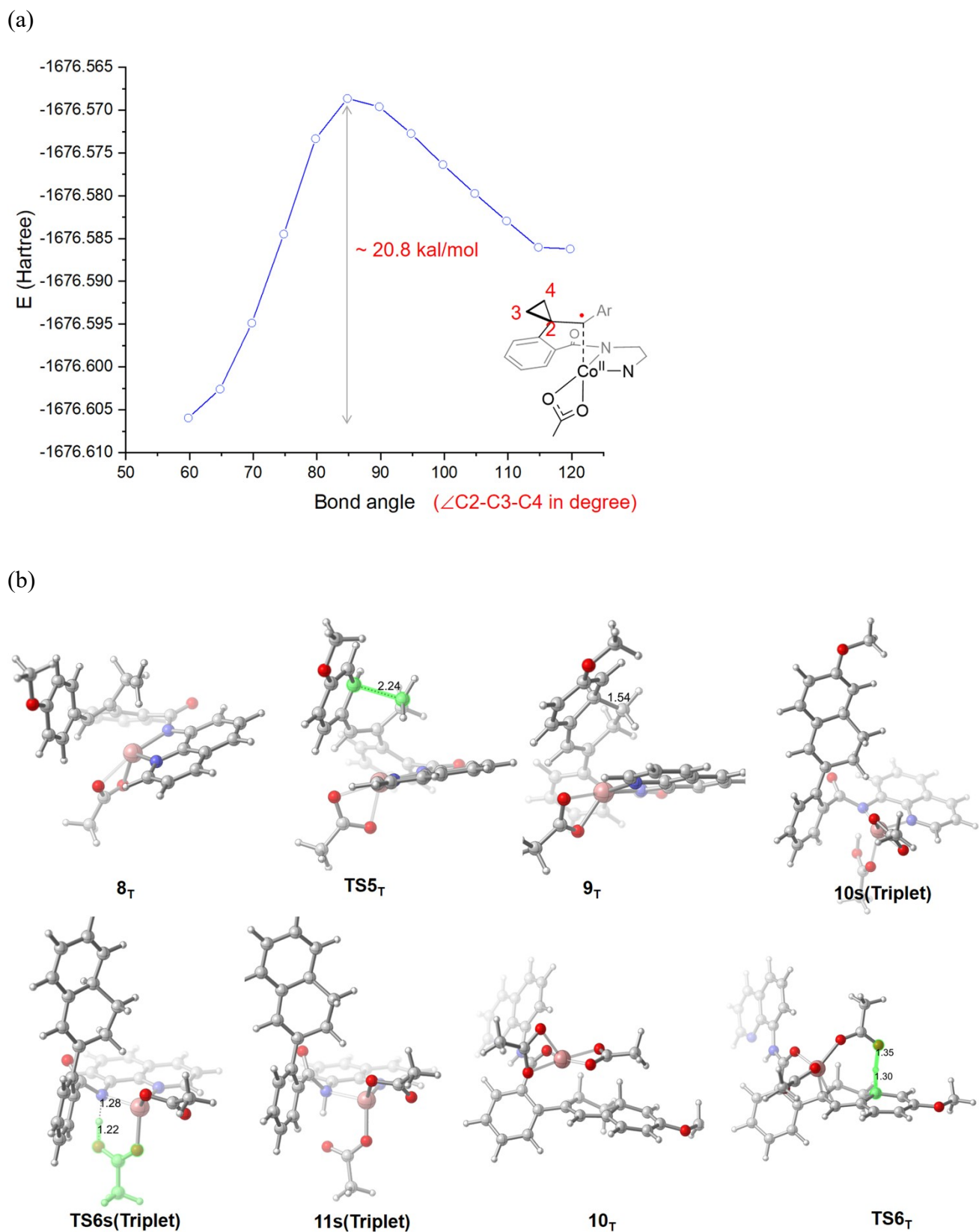


**Figure S19.** More O’Ferrall–Jencks plot for the first and the second C–H activation of the singlet PES.

A detailed Wiberg bond order analysis for both the first and second C–H activation was conducted. As seen from the More O’Ferrall–Jencks plot (Figure S19),<sup>[17]</sup> it became evident that the first C–H cleavage occurs *via* BIES mechanism, while the second C–H cleavage occurs *via* CMD mechanism. It should be noted that the CMD-type transition state **TS3** is kinetically unfavorable (see Figure S18).

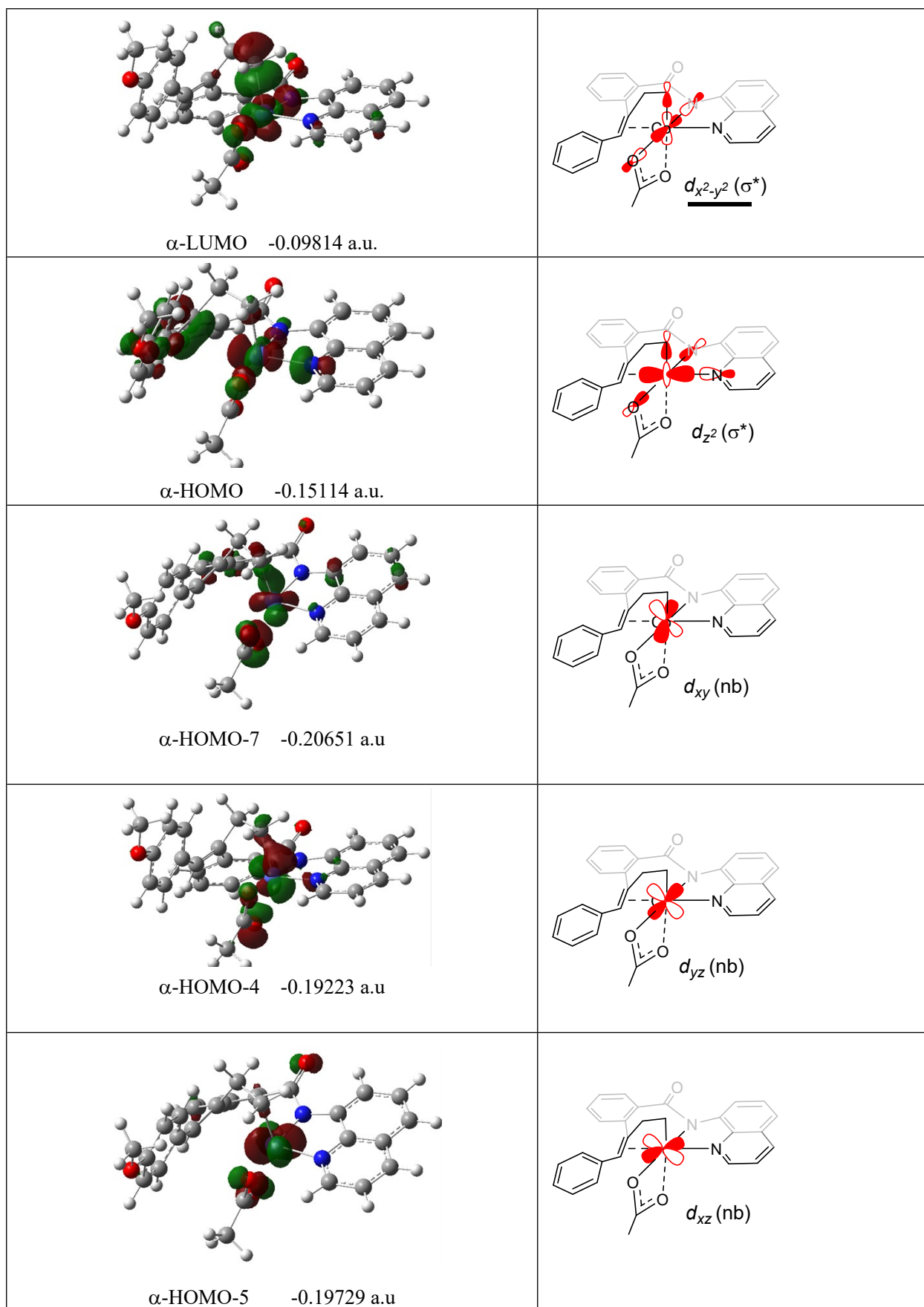


**Figure S20.** Free energy profiles for the favored C–H activation via PCET mechanism.

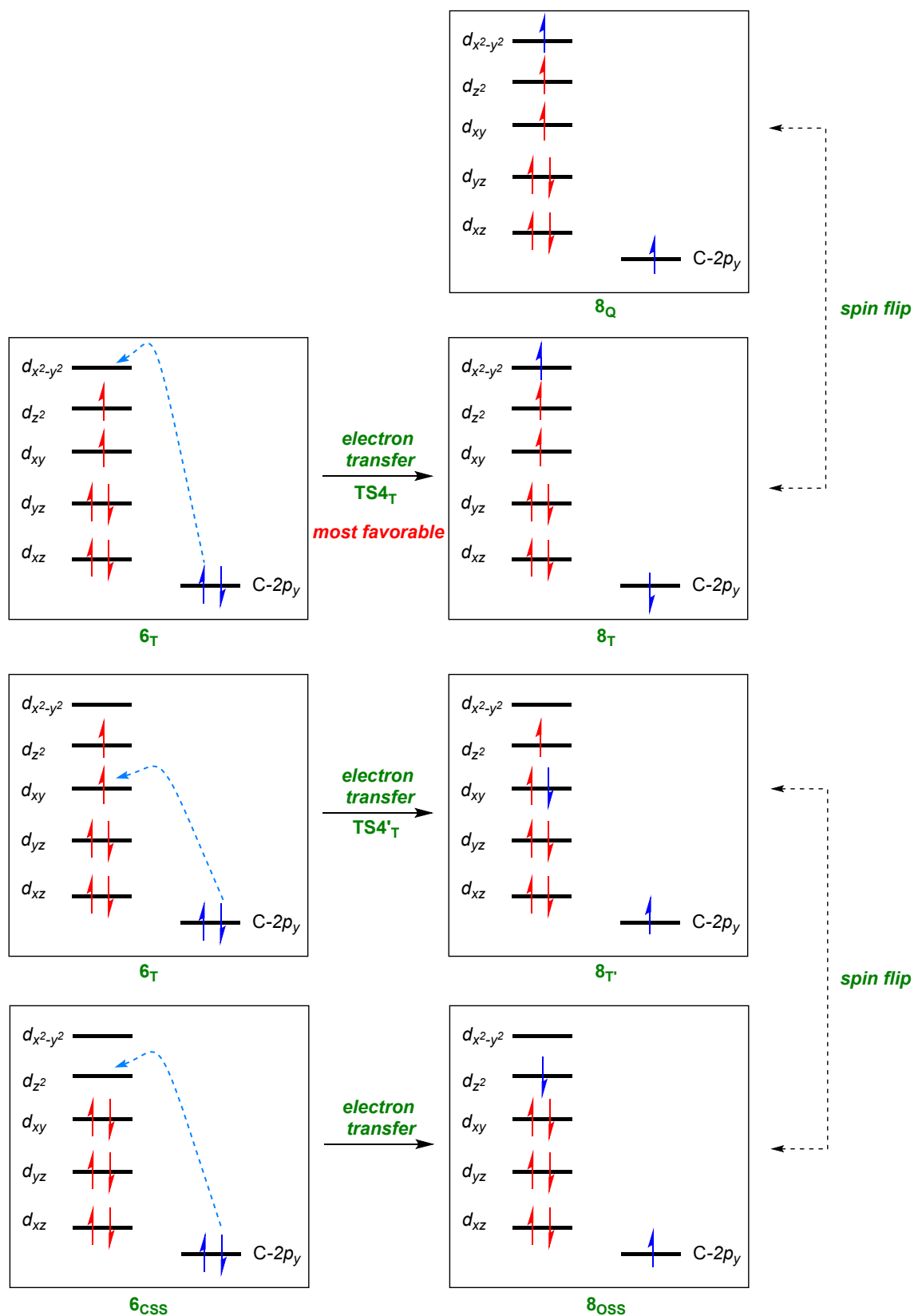


**Figure S21.** (a) The relaxed potential energy surface scan results at the B3LYP-D3(BJ)/6-31G\*/SDD(Co) level of theory for the direct carbon-carbon bond homolysis from  $5_T$ . (b) Optimized structures of the key transition states and intermediates with selected bond distances in Å.

We have also considered the direct occurrence of carbon-carbon bond homolysis in the three-membered ring from intermediate **5<sub>T</sub>**. However, we cannot locate the corresponding transition state, although the relaxed potential energy surface scans indicate there exists an energy maximum. The relaxed potential energy surface scan results with the bond angles as the scanning variable are given in Figure S21a.



**Figure S22.** Molecular orbital iso-contour surfaces of  $6_T$  (isovalue = 0.05) calculated at the SMD(toluene)/BLYP-D3(BJ)/6-31G(d,p)/SDD(Co) level.



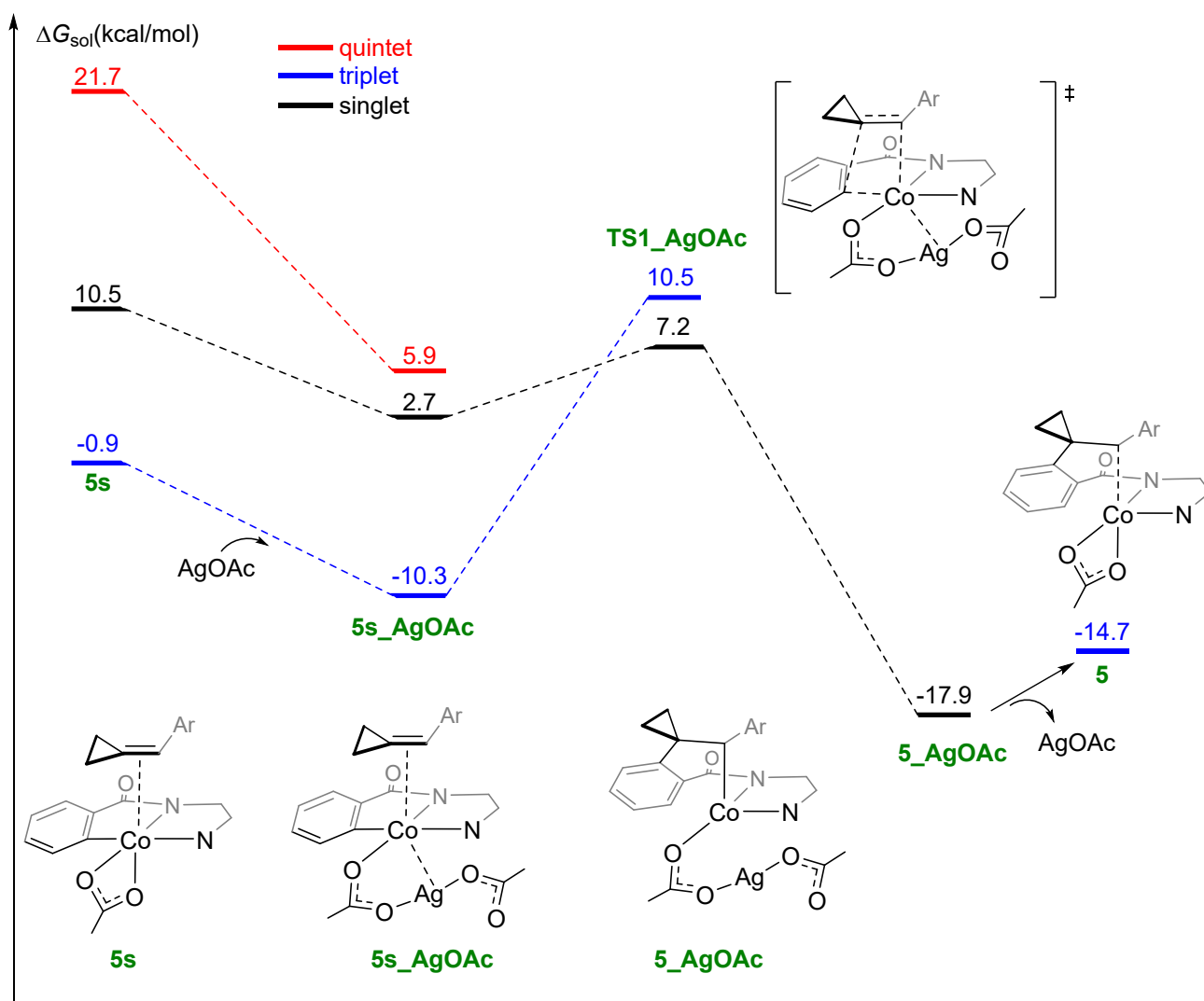
**Figure S23.** Schematic illustration of the electronic structure changes for the Co-C homolysis.



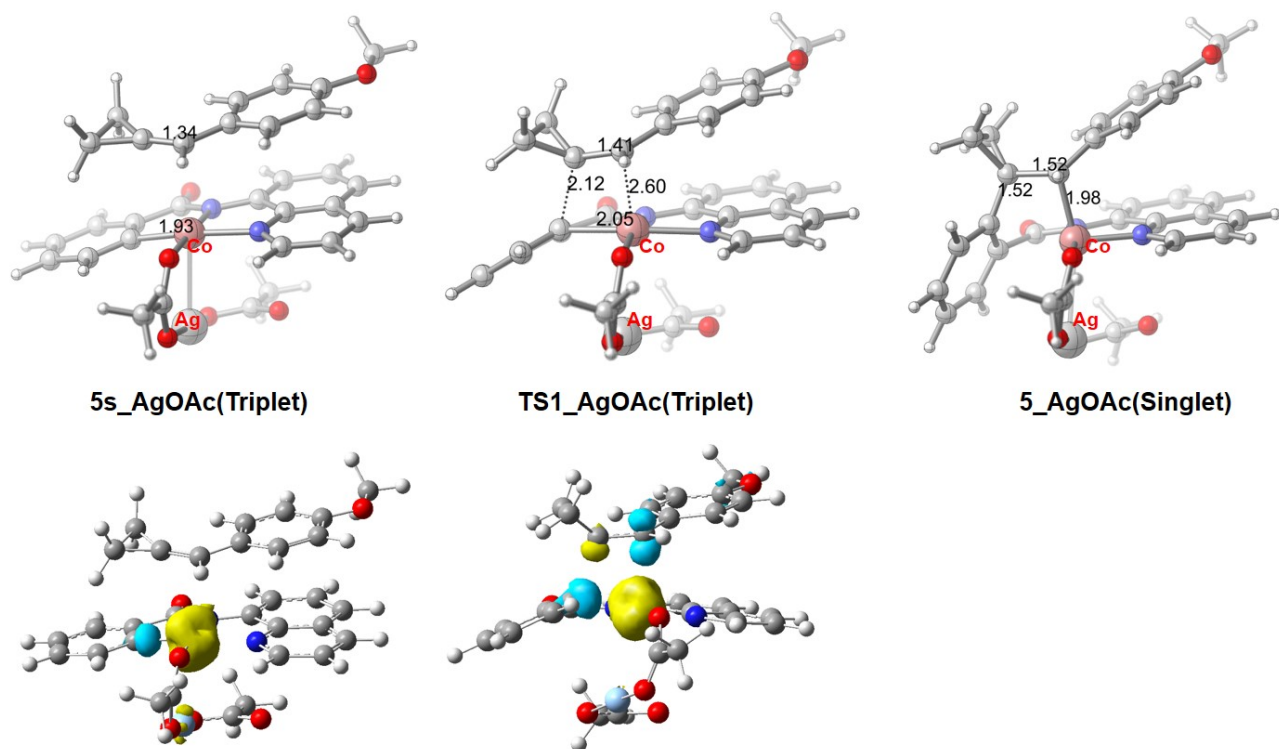
## 2.2.2 The potential roles of AgOAc

We first investigated the potential involvement of silver acetate during the migratory insertion. From complex **5s**, coordination of the AgOAc generates the stable intermediate **5s\_AgOAc**, which is exergonic by 9.4 kcal/mol for the triplet surface (Figure S24). The migratory insertion requires an energy barrier of 17.5 kcal/mol (**TS1\_AgOAc<sub>S</sub>** relative to **5s\_AgOAc<sub>T</sub>**), which is 1.7 kcal/mol lower than that from **5s** (19.2 kcal/mol, **TS1<sub>S</sub>** relative to **5s<sub>T</sub>** in Figure S15). The corresponding optimized structures and spin density contours are shown in Figure S25. The spin density changes are similar with the results without AgOAc. Attempts to locate the triplet and quintet for the intermediate **5\_AgOAc** were unsuccessful. Dissociation of one AgOAc from **5\_AgOAc** is endergonic by 3.2 kcal/mol.

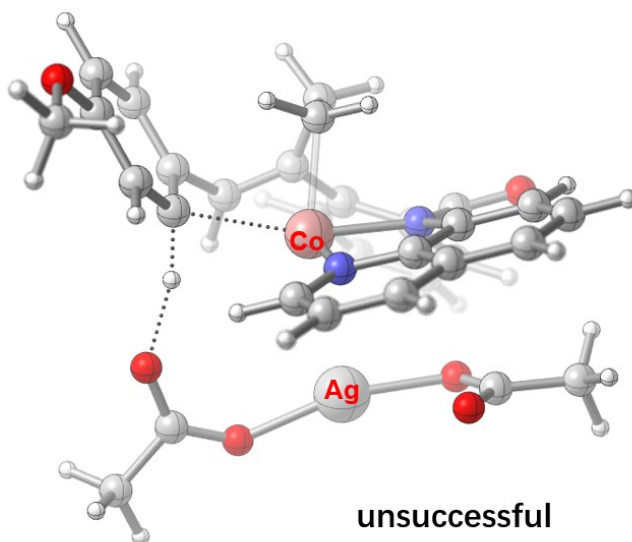
It is noteworthy that attempts to locate the transition states of bimetallic activation modes for the subsequent C–H activation *via* CMD did not meet with success (Figure S26). Free energy profiles for the C(sp<sup>2</sup>)–H activation from Co(IV) intermediate are given in Figure S27.



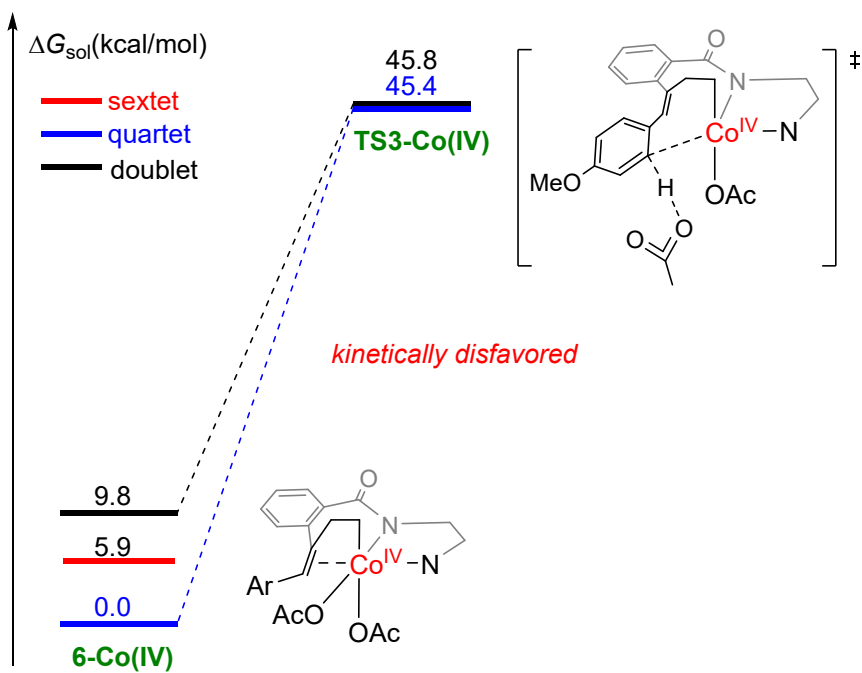
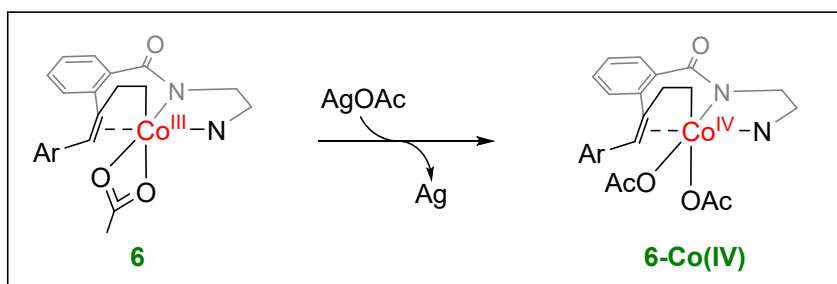
**Figure S24.** Free energy profiles for the migratory insertion from AgOAc-coordinated complex.



**Figure S25.** The corresponding optimized structures and spin density contours (isovalue=0.01; Yellow:  $\alpha$  spin density. Cyan:  $\beta$  spin density).



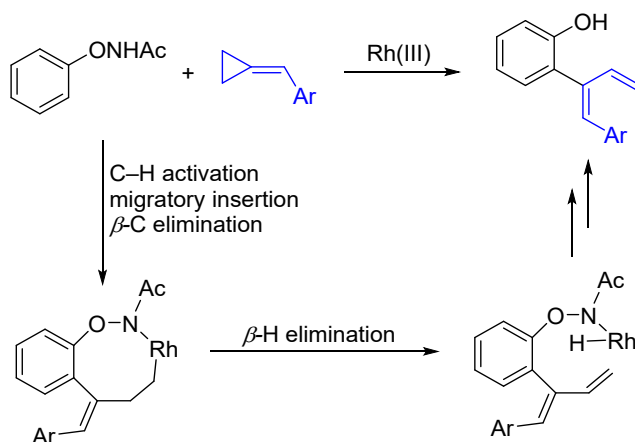
**Figure S26.** Attempts to locate the transition states of bimetallic activation modes for C-H activation did not meet with success



**Figure S27.** Free energy profiles for the  $\text{C}(\text{sp}^2)\text{-H}$  activation from  $\text{Co}(\text{IV})$  intermediate.

### 2.2.3 The competing pathway involving $\beta$ -H elimination

For the Rh(III)-catalyzed coupling of *N*-phenoxyacetamides and alkylidenecyclopropanes (ACPs), the reaction proceeds via sequential C–H activation, migratory insertion and  $\beta$ -C elimination to generate the Rh(III) homoallyl intermediate, from which  $\beta$ -H elimination may occur to produce the diene species (Scheme S3).<sup>[18]</sup> Herein, we also considered the  $\beta$ -H elimination from intermediate **6**. As shown in Figure S9, the  $\beta$ -H elimination from **6** is disfavored due to the relatively high energy barrier (34.8 kcal/mol for the triplet).



Scheme S3. Rh(III)-catalyzed ring scission via  $\beta$ -C/ $\beta$ -H elimination.

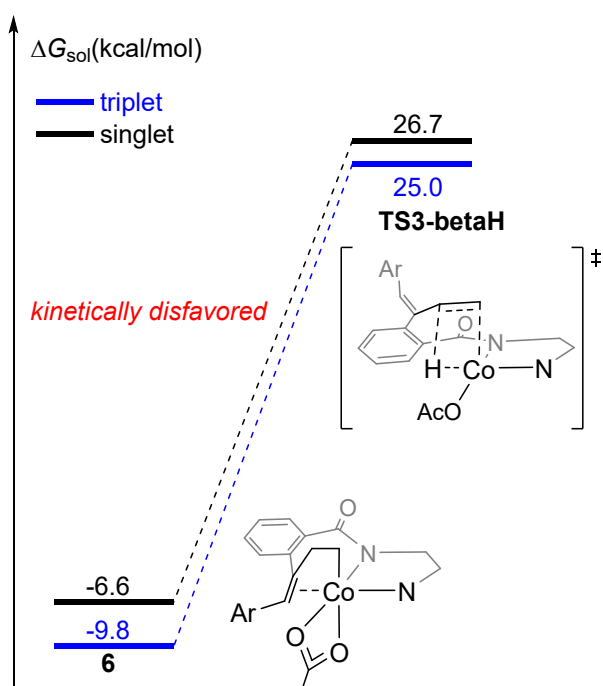
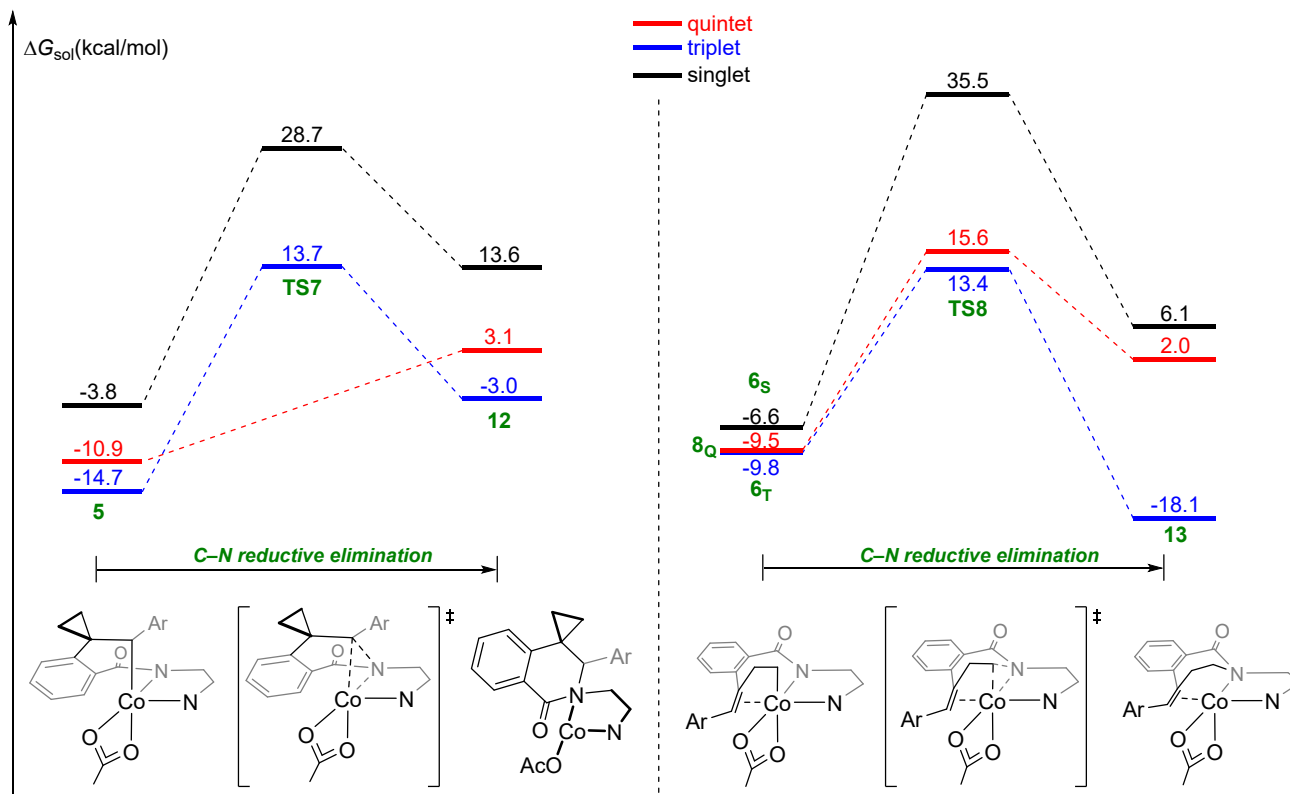


Figure S28. Free energy profiles for the  $\beta$ -H elimination from **6**.

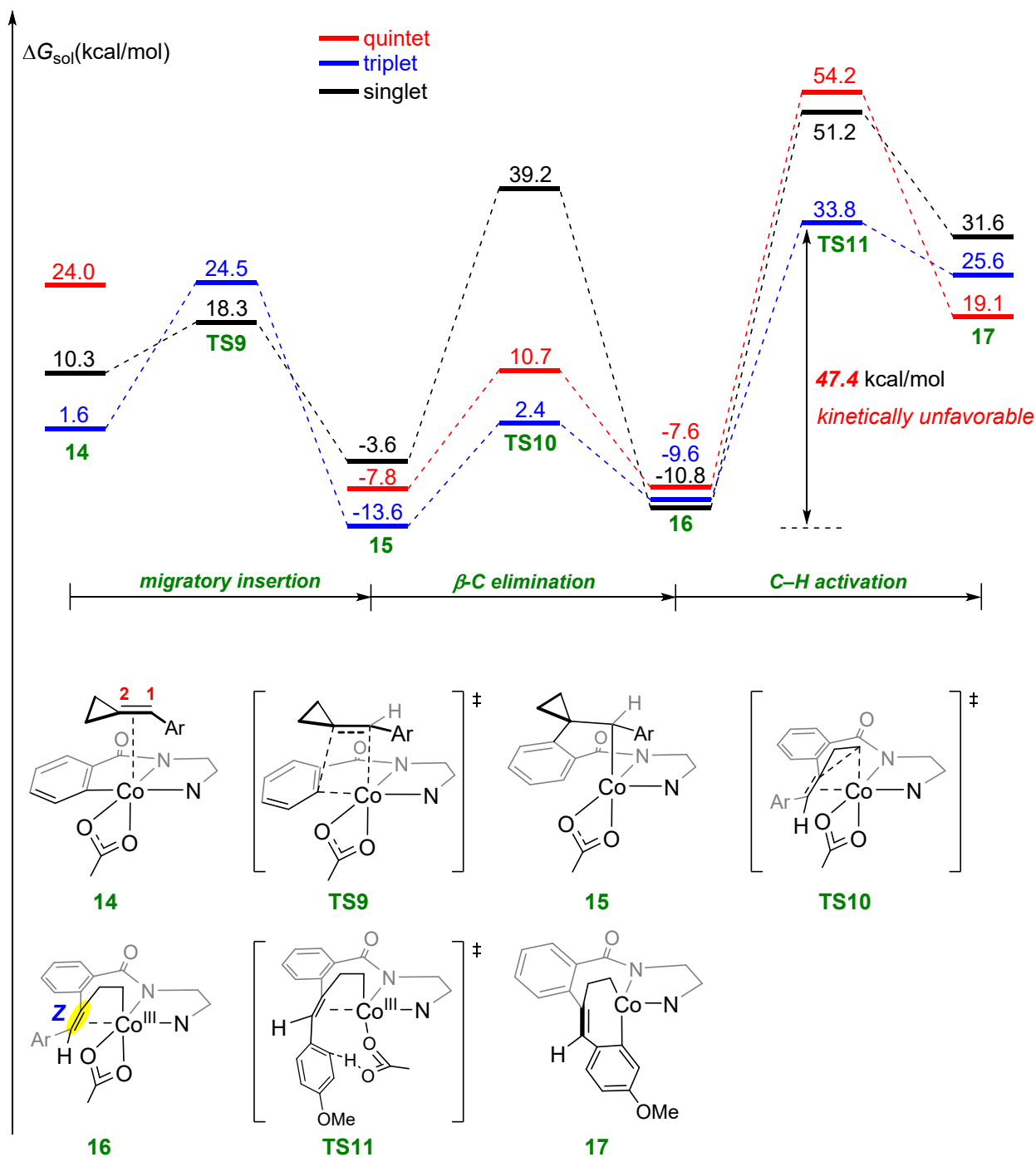
### 2.3 The side reaction pathways in 1,2-insertion-*E*



**Figure S29.** Free energy profiles for the C–N reductive elimination from intermediate **5** or **6**.

Compared to the results shown in Figure S20, the competing C–N reductive elimination from intermediate **5** or **6** in Figure S29 is kinetically unfavorable due to the relatively high energy barrier, in agreement with the experimental results that the corresponding products were not observed.

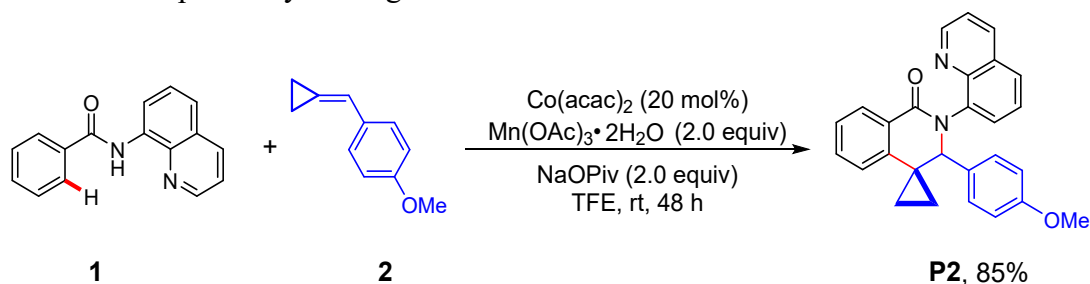
## 2.4 Results for the 1,2-insertion-Z



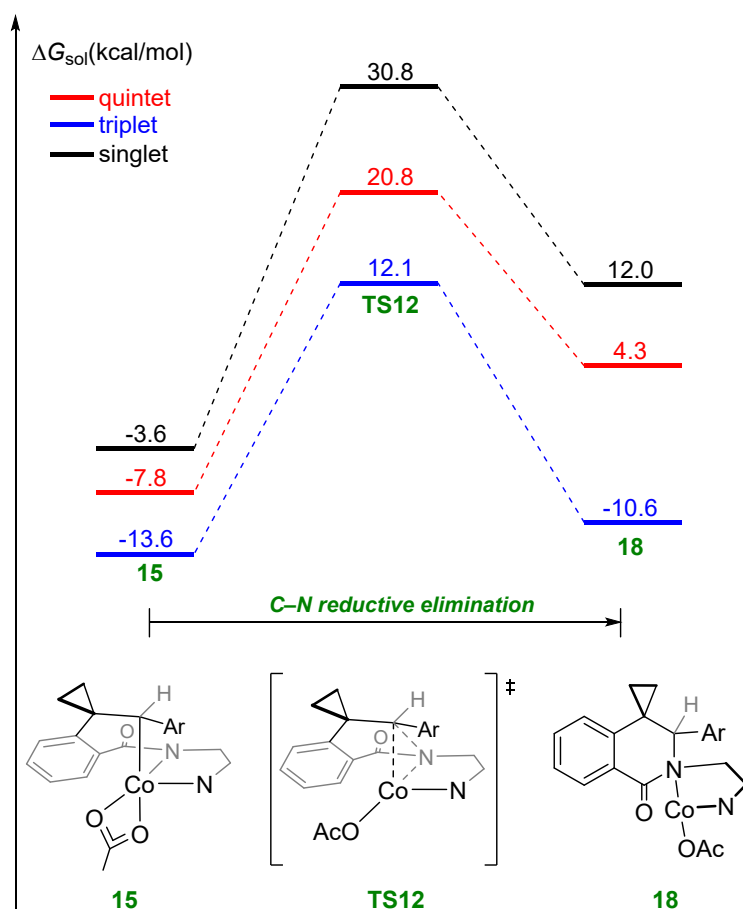
**Figure S30.** Free energy profiles for the 1,2-insertion-Z pathway.

In this case, the radical cyclization pathway is forbidden since the methylene connected with cobalt is *trans* to the aryl group. Therefore, we only considered the C-H activation via CMD in this 1,2-insertion-Z pathway. As shown in Figure S30, the second C-H activation via CMD in this pathway is kinetically unfavorable.

In 2019, Volla and coworkers reported the cobalt-catalyzed C–H activation and annulation of benzamides and alkylidenecyclopropanes under different reaction conditions (see Scheme S4).<sup>[19]</sup> The reductive elimination from the (cyclopropylmethyl)cobalt(III) occurs to afford the spiro-dihydroisoquinoline derivatives, in which the cyclopropyl ring was conserved. Herein, we also considered the possibility of reductive elimination from intermediate **15**. As shown in Figure S31, the energy barrier for the reductive elimination is 25.7 kcal/mol (**TS12<sub>T</sub>** relative to **15<sub>T</sub>**), which is 5.3 kcal/mol less favorable than the apparent activation energy of the PCET pathway (**TS6<sub>T</sub>** relative to **9<sub>T</sub>** in Figure S20). Taken together, the results in Figures S29 and S31 demonstrated that the reductive elimination from seven-membered cobaltacycle intermediate was kinetically unfavorable under the reaction conditions reported by Kwong and coworkers.



**Scheme S4.** Cobalt-catalyzed regioselective spirodihydroisoquinoline synthesis with conservation of the cyclopropyl ring.



**Figure S31.** Free energy profiles for the C–N reductive elimination from intermediate **15**.

## 2.5. Results for the 2,1-insertion-*Re*

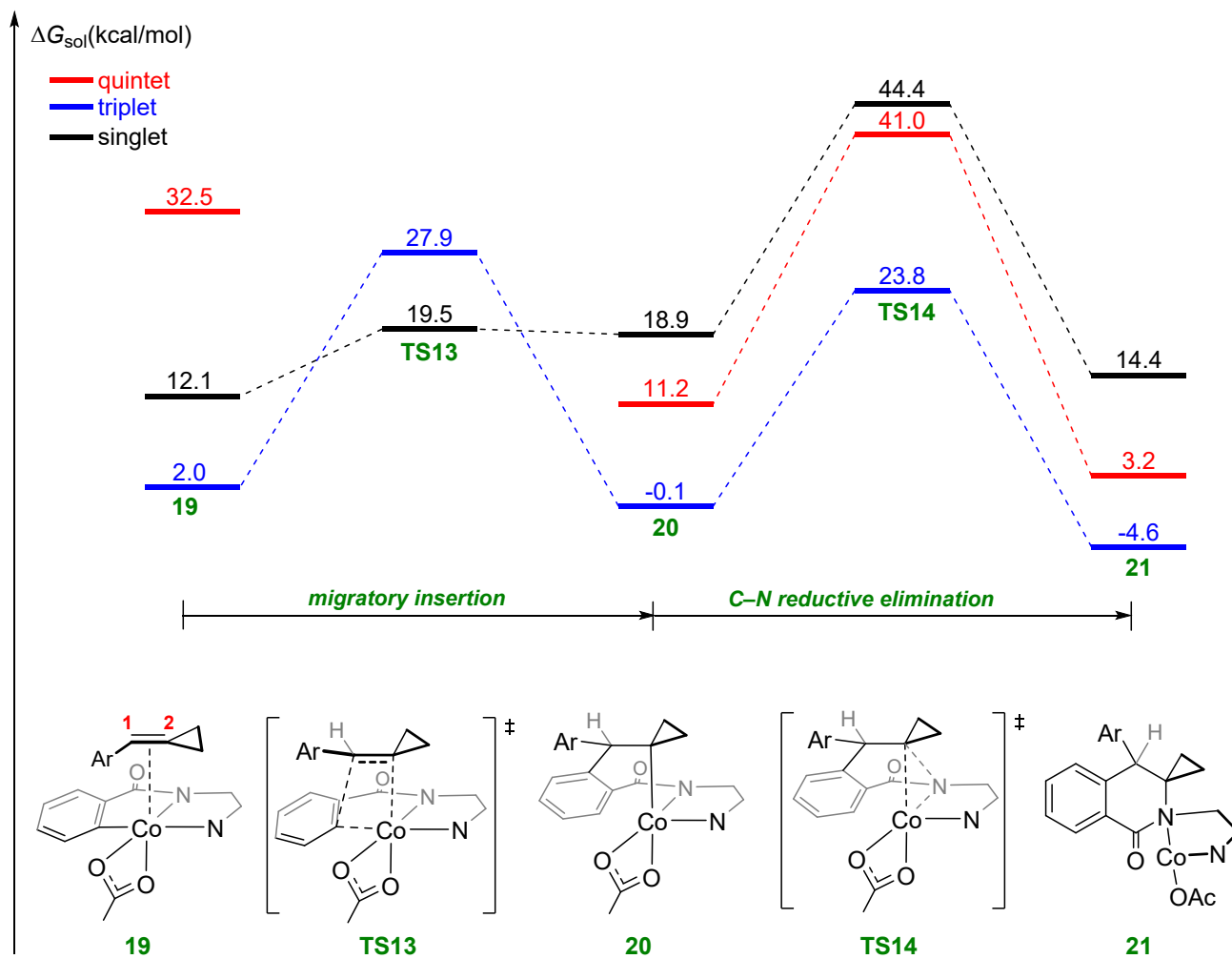


Figure S32. Free energy profiles for the 2,1-insertion-*Re* reaction pathway.





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### 3. Calculated energies and imaginary frequencies.

**Table S2.** Calculated energies and imaginary frequencies in Section 1.

Stationary point	Corrected thermal correction to Gibbs free energy at B3LYP-D3(BJ)/6-31G(d,p)/ECP10MDF(Co) (in a.u.)	Single-point energy including solvation energy at B3LYP-D3(BJ)/def2-TZVP (in a.u.)	Imaginary frequencies (in cm <sup>-1</sup> )	$\langle \hat{S}^2 \rangle$
<b>ethylene (R=H)</b>				
INT1 <sub>S</sub>	0.277841	-2490.999442		
INT1 <sub>T</sub>	0.271616	-2491.000544		2.0924
INT1 <sub>Q</sub>	0.266355	-2490.958187		6.0345
TS <sub>S</sub>	0.280376	-2490.989751	313.69 <i>i</i>	
TS <sub>T</sub>	0.272796	-2490.970172	410.57 <i>i</i>	2.2405
INT2 <sub>S</sub>	0.279856	-2491.020077		
INT2 <sub>T</sub>	0.273675	-2491.022598		2.4502
INT2 <sub>Q</sub>	0.271122	-2491.008447		6.0099
<b>R=CO<sub>2</sub>Et</b>				
INT1 <sub>S</sub>	0.343233	-2758.327085		
INT1 <sub>T</sub>	0.337987	-2758.338526		2.0915
INT1 <sub>Q</sub>	0.333268	-2758.296357		6.0318
TS <sub>S</sub>	0.345013	-2758.322401	244.66 <i>i</i>	
TS <sub>T</sub>	0.336601	-2758.302815	437.63 <i>i</i>	
INT2 <sub>S</sub>	0.34557	-2758.355663		
INT2 <sub>T</sub>	0.340059	-2758.357302		2.4694
INT2 <sub>Q</sub>	0.338117	-2758.355691		6.0126
<b>R=OEt</b>				
INT1 <sub>S</sub>	0.337296	-2644.923574		
INT1 <sub>T</sub>	0.328126	-2644.922319		2.0903
INT1 <sub>Q</sub>	0.325122	-2644.880479		6.0332

TS <sub>S</sub>	0.336001	-2644.904269	315.70 <i>i</i>	
TS <sub>T</sub>	0.332042	-2644.887505	236.33 <i>i</i>	2.4862
INT2 <sub>S</sub>	0.338086	-2644.938162		
INT2 <sub>T</sub>	0.330332	-2644.948058		2.5218
INT2 <sub>Q</sub>	0.329657	-2644.935317		6.0091
<b>R=Ph</b>				
INT1 <sub>S</sub>	0.355486	-2722.178849		
INT1 <sub>T</sub>	0.349037	-2722.185477		2.0928
INT1 <sub>Q</sub>	0.346269	-2722.141503		6.0354
TS <sub>S</sub>	0.356866	-2722.166422	310.61 <i>i</i>	
TS <sub>T</sub>	0.350225	-2722.148883	424.30 <i>i</i>	2.6136
INT2 <sub>S</sub>	0.35837	-2722.19750		
INT2 <sub>T</sub>	0.350253	-2722.208492		2.8148
INT2 <sub>Q</sub>	0.346322	-2722.208213		6.0366
<b>R=C<sub>4</sub>H<sub>9</sub></b>				
INT1 <sub>S</sub>	0.384293	-2648.341644		
INT1 <sub>T</sub>	0.376651	-2648.34551		2.0952
INT1 <sub>Q</sub>	0.371653	-2648.302502		6.0345
TS <sub>S</sub>	0.386224	-2648.32919	305.87 <i>i</i>	
TS <sub>T</sub>	0.381772	-2648.302438	346.85 <i>i</i>	2.1565
INT2 <sub>S</sub>	0.386595	-2648.359081		
INT2 <sub>T</sub>	0.379941	-2648.366826		2.4792
INT2 <sub>Q</sub>	0.377326	-2648.352514		6.0100
<b>R=CH<sub>2</sub>OH</b>				
INT1 <sub>S</sub>	0.307294	-2605.588209		
INT1 <sub>T</sub>	0.299099	-2605.595546		2.0945
INT1 <sub>Q</sub>	0.296947	-2605.55108		6.0347
TS <sub>S</sub>	0.310445	-2605.579272	287.04 <i>i</i>	
TS <sub>T</sub>	0.302659	-2605.559804	382.82 <i>i</i>	2.2434

INT2 <sub>S</sub>	0.311716	-2605.611337		
INT2 <sub>T</sub>	0.304178	-2605.614964		2.4067
INT2 <sub>Q</sub>	0.300970	-2605.602678		6.0103
<b>cyclopentene</b>				
INT1 <sub>S</sub>	0.339908	-2607.797996		
INT1 <sub>T</sub>	0.334095	-2607.800988		2.0887
INT1 <sub>Q</sub>	0.328663	-2607.758248		6.0339
TS <sub>S</sub>	0.342364	-2607.783643	320.87 <i>i</i>	
TS <sub>T</sub>	0.335548	-2607.76895	273.82 <i>i</i>	2.2180
INT2 <sub>S</sub>	0.345049	-2607.81136		
INT2 <sub>T</sub>	0.337967	-2607.814234		2.4134
INT2 <sub>Q</sub>	0.331227	-2607.802795		6.0107
<b>allene</b>				
INT1 <sub>S</sub>	0.358217	-2760.257285		
INT1 <sub>T</sub>	0.350739	-2760.272161		2.0921
INT1 <sub>Q</sub>	0.345301	-2760.229053		6.0321
TS <sub>S</sub>	0.358221	-2760.249624	228.75 <i>i</i>	
TS <sub>T</sub>	0.352026	-2760.240465	246.33 <i>i</i>	2.4847
INT2 <sub>S</sub>	0.360201	-2760.297492		
INT2 <sub>T</sub>	0.351456	-2760.315243		2.9722
INT2 <sub>Q</sub>	0.351881	-2760.315095		6.0428
A <sub>S</sub>	0.338957	-2870.814344		
A <sub>T</sub>	0.335299	-2870.803437		2.0583
A <sub>Q</sub>	0.331688	-2870.794197		6.0096
TSA <sub>S</sub>	0.335542	-2870.807934	869.06 <i>i</i>	
TSA <sub>T</sub>	0.333069	-2870.790320	1157.92 <i>i</i>	2.0944
TSA <sub>Q</sub>	0.328460	-2870.782909	898.38 <i>i</i>	6.0098
B <sub>S</sub>	0.283173	-2641.589102		

<b>B<sub>T</sub></b>	0.27689	-2641.583839		2.0383
<b>B<sub>Q</sub></b>	0.272289	-2641.590722		6.0366
<b>TSB<sub>S</sub></b>	0.278689	-2641.560074	1107.44 <i>i</i>	
<b>TSB<sub>T</sub></b>	0.272451	-2641.552227	899.72 <i>i</i>	2.0704
<b>TSB<sub>Q</sub></b>	0.267889	-2641.533858	733.66 <i>i</i>	6.0315
<b>C<sub>S</sub></b>	0.284283	-2641.581301		
<b>C<sub>T</sub></b>	0.275173	-2641.580827		2.0898
<b>C<sub>Q</sub></b>	0.273259	-2641.541328		6.0326
<b>D<sub>S</sub></b>	0.514031	-3443.678054		
<b>D<sub>T</sub></b>	0.508829	-3443.681966		2.0499
<b>D<sub>Q</sub></b>	0.501683	-3443.692113		6.0355
<b>TSC<sub>S</sub></b>	0.509838	-3443.667841	1154.68 <i>i</i>	
<b>E<sub>S</sub></b>	0.456651	-3214.465621		
<b>E<sub>T</sub></b>	0.452002	-3214.462983		2.0515
<b>E<sub>Q</sub></b>	0.445935	-3214.461936		6.0352
<b>TSD<sub>S</sub></b>	0.453071	-3214.448822	1170.75 <i>i</i>	
<b>F<sub>S</sub></b>	0.457289	-3214.471213		
<b>F<sub>T</sub></b>	0.451386	-3214.453954		2.0996
<b>F<sub>Q</sub></b>	0.447804	-3214.412987		6.0158
<b>INT1_AQ<sub>S</sub></b>	0.450921	-3063.878191		
<b>INT1_AQ<sub>T</sub></b>	0.440915	-3063.882628		2.0759
<b>INT1_AQ<sub>Q</sub></b>	0.435487	-3063.835609		6.0141
<b>TS_AQ<sub>S</sub></b>	0.452592	-3063.863183	359.73 <i>i</i>	
<b>TS_AQ<sub>T</sub></b>	0.445511	-3063.836481	381.92 <i>i</i>	2.2408
<b>INT2_AQ<sub>S</sub></b>	0.453037	-3063.891046		
<b>INT2_AQ<sub>T</sub></b>	0.448159	-3063.896653		2.3108
<b>INT2_AQ<sub>Q</sub></b>	0.443034	-3063.888780		6.0124
Stationary	Corrected thermal	Single-point energy	Imaginary	

point	correction to Gibbs free energy at B3LYP-D3(BJ)/6-31G(d,p)/ECP10MDF(Co) (in a.u.)	including solvation energy at B3LYP-D3(BJ)/def2-TZVPP (in a.u.)	frequencies (in cm <sup>-1</sup> )	
<b>ethylene (R=H)</b>				
INT1 <sub>S</sub>	0.277841	-2491.008953		
INT1 <sub>T</sub>	0.271616	-2491.010029		2.0924
INT1 <sub>Q</sub>	0.266355	-2490.967490		6.0345
TS <sub>S</sub>	0.280376	-2490.999242	313.69 <i>i</i>	
TS <sub>T</sub>	0.272796	-2490.979962	410.57 <i>i</i>	2.2405
INT2 <sub>S</sub>	0.279856	-2491.029353		
INT2 <sub>T</sub>	0.273675	-2491.032303		2.4502
INT2 <sub>Q</sub>	0.271122	-2491.018175		6.0099
Stationary point	Corrected thermal correction to Gibbs free energy at PBE0-D3(BJ)/6-31G(d,p)/ECP10MDF(Co) (in a.u.)	Single-point energy including solvation energy at PBE0-D3(BJ)/def2-TZVPP (in a.u.)	Imaginary frequencies (in cm <sup>-1</sup> )	
<b>ethylene (R=H)</b>				
INT1 <sub>S</sub>	0.282696	-2489.396967		
INT1 <sub>T</sub>	0.275072	-2489.396369		2.1375
INT1 <sub>Q</sub>	0.270028	-2489.355616		6.0477
TS <sub>S</sub>	0.283743	-2489.391057	282.44 <i>i</i>	
TS <sub>T</sub>	0.275674	-2489.374840	390.79 <i>i</i>	2.3196
INT2 <sub>S</sub>	0.282979	-2489.418813		
INT2 <sub>T</sub>	0.276708	-2489.430133		2.5439
INT2 <sub>Q</sub>	0.274996	-2489.417280		6.0102
Stationary point	Corrected thermal correction to Gibbs free	Single-point energy including solvation energy	Imaginary frequencies	

	energy at M06/6-31G(d,p)/ECP10MDF(Co) (in a.u.)	at M06/def2-TZVPP (in a.u.)	(in cm <sup>-1</sup> )	
<b>ethylene (R=H)</b>				
INT1 <sub>S</sub>	0.278618	-2490.030094		
INT1 <sub>T</sub>	0.27114	-2490.029609		2.0844
INT1 <sub>Q</sub>	0.268347	-2489.990728		6.0345
TS <sub>S</sub>	0.279592	-2490.024350	246.78 <i>i</i>	
TS <sub>T</sub>	0.273263	-2490.008288	348.44 <i>i</i>	2.1690
INT2 <sub>S</sub>	0.280196	-2490.047167		
INT2 <sub>T</sub>	0.274573	-2490.048606		2.5545
INT2 <sub>Q</sub>	0.273432	-2490.036137		6.0172
Stationary point	Corrected thermal correction to Gibbs free energy at ωB97XD/6- 31G(d,p)/ECP10MDF(Co) (in a.u.)	Single-point energy including solvation energy at ωB97XD/def2-TZVPP (in a.u.)	Imaginary frequencies (in cm <sup>-1</sup> )	
<b>ethylene (R=H)</b>				
INT1 <sub>S</sub>	0.28352	-2490.506896		
INT1 <sub>T</sub>	0.274313	-2490.507394		2.1806
INT1 <sub>Q</sub>	0.265456	-2490.464761		6.0541
TS <sub>S</sub>	0.284767	-2490.498844	309.73 <i>i</i>	
TS <sub>T</sub>	0.276878	-2490.478604	422.17 <i>i</i>	2.4207
INT2 <sub>S</sub>	0.285027	-2490.528602		
INT2 <sub>T</sub>	0.277413	-2490.536060		2.6270
INT2 <sub>Q</sub>	0.275592	-2490.524600		6.0099



**Table S3.** Calculated energies and imaginary frequencies in Section 2.

Stationary point	Corrected thermal correction to Gibbs free energy at B3LYP-D3(BJ)/6-31G(d,p)/ECP10MDF(Co) (in a.u.)	Single-point energy including solvation energy at B3LYP-D3(BJ)/def2-TZVP (in a.u.)	Imaginary frequencies (in cm <sup>-1</sup> )	$\langle \hat{S}^2 \rangle$
<b>1</b>	0.175195	-802.0801197		
<b>2</b>	0.139646	-501.7921931		
<b>HOAc</b>	0.020787	-229.2025157		
<b>Co(OAc)<sub>3</sub>_S</b>	0.087574	-2068.703606		
<b>Co(OAc)<sub>3</sub>_T</b>	0.080782	-2068.685336		
<b>Co(OAc)<sub>3</sub>_Q</b>	0.076228	-2068.68193		
<b>2s_S</b>	0.296006	-2870.810189		
<b>2s_T</b>	0.290521	-2870.79542		2.0509
<b>2s_Q</b>	0.28613	-2870.784587		6.0106
<b>TS1s_S</b>	0.293956	-2870.803476	171.53 <i>i</i>	
<b>TS1s_T</b>	0.284495	-2870.778517	725.28 <i>i</i>	2.0858
<b>TS1s_Q</b>	0.282027	-2870.774204	765.18 <i>i</i>	6.0112
<b>3s_S</b>	0.246128	-2641.590524		
<b>3s_T</b>	0.24008	-2641.581796		2.0417
<b>3s_Q</b>	0.231221	-2641.578569		6.0405
<b>TS2s_S</b>	0.243208	-2641.563407	889.94 <i>i</i>	
<b>TS2s_T</b>	0.237329	-2641.552359	668.23 <i>i</i>	2.0719
<b>TS2s_Q</b>	0.230406	-2641.532014	849.68 <i>i</i>	6.0329
<b>4_S</b>	0.247189	-2641.583897		
<b>4_T</b>	0.238198	-2641.580408		2.0845
<b>4_Q</b>	0.231851	-2641.53811		6.0307
<b>5s_S</b>	0.373972	-2914.16725224		
<b>5s_T</b>	0.362724	-2914.17413704		2.0859
<b>5s_Q</b>	0.356751	-2914.13227560		6.0305

<b>MECP1</b>	0.373332	-2914.16636660		
<b>TS1_S</b>	0.374164	-2914.15504073	276.70 <i>i</i>	
<b>TS1_T</b>	0.365374	-2914.13958240	402.70 <i>i</i>	2.4341
<b>MECP2</b>	0.372843	-2914.19053650		
<b>5_S</b>	0.376128	-2914.19216765		
<b>5_T</b>	0.366269	-2914.19970917		2.6328
<b>5_Q</b>	0.363259	-2914.19069426		6.0347
<b>4s_AQ_S</b>	0.458896	-3443.6700968		
<b>4s_AQ_T</b>	0.451839	-3443.6698974		2.0489
<b>4s_AQ_Q</b>	0.443044	-3443.6702150		6.0420
<b>TS2s_AQ_S</b>	0.455781	-3443.6651601	1098.36 <i>i</i>	
<b>5s_AQ_S</b>	0.405915	-3214.4586602		
<b>5s_AQ_T</b>	0.40023	-3214.4559216		2.0566
<b>5s_AQ_Q</b>	0.396284	-3214.4446375		6.0382
<b>TS3s_AQ_S</b>	0.40706	-3214.4507183	841.45 <i>i</i>	
<b>6s_AQ_S</b>	0.409404	-3214.4734202		
<b>6s_AQ_T</b>	0.401096	-3214.4536140		2.1015
<b>6s_AQ_Q</b>	0.395863	-3214.4137107		6.0177
<b>7s_AQ_S</b>	0.535096	-3487.0488206		
<b>5s_AgOAc_S</b>	0.403865	-3289.8582187		
<b>5s_AgOAc_T</b>	0.399388	-3289.8744661		2.0754
<b>5s_AgOAc_Q</b>	0.389089	-3289.8383568		6.0407
<b>TS1_AgOAc_S</b>	0.406387	-3289.8536729	199.28 <i>i</i>	
<b>TS1_AgOAc_T</b>	0.399085	-3289.84103100	429.27 <i>i</i>	2.3940
<b>5_AgOAc_S</b>	0.408316	-3289.89554680		
<b>TS2_S</b>	0.374982	-2914.15821894	115.87 <i>i</i>	
<b>TS2_T</b>	0.366985	-2914.16830200	266.46 <i>i</i>	2.4674
<b>TS2_Q</b>	0.361781	-2914.14536129	497.41 <i>i</i>	6.0349
<b>6_S</b>	0.376337	-2914.19690278		

<b>6_T</b>	0.365623	-2914.19125863		2.3508
<b>8_Q</b>	0.359271	-2914.18437906		
<b>MECP3</b>	0.37186	-2914.19174310		
<b>TS3_S</b>	0.36921	-2914.14198480	1218.73 <i>i</i>	
<b>TS3_T</b>	0.363247	-2914.13273734	846.40 <i>i</i>	2.3626
<b>TS3_Q</b>	0.353762	-2914.12151620	701.74 <i>i</i>	6.0151
<b>MECP4</b>	0.320319	-2684.93408690		
<b>7_S</b>	0.323448	-2684.94265164		
<b>7_T</b>	0.313728	-2684.93854796		2.1626
<b>7_Q</b>	0.313441	-2684.90661796		6.0135
<b>TS3_betaH_S</b>	0.36633	-2914.13380522	559.75 <i>i</i>	
<b>TS3_betaH_T</b>	0.357612	-2914.12776138	762.39 <i>i</i>	
<b>6_Co(IV)_doublet</b>	0.415804	-3142.73785968		
<b>6_Co(IV)_quartet</b>	0.403678	-3142.75354969		
<b>6_Co(IV)_sextet</b>	0.393921	-3142.74410530		
<b>TS3_Co(IV)_doublet</b>	0.407975	-3142.68055466	885.58 <i>i</i>	
<b>TS3_Co(IV)_quartet</b>	0.399436	-3142.68115845	1032.77 <i>i</i>	
<b>TS4_T</b>	0.362628	-2914.18241890	76.35 <i>i</i>	2.9734
<b>TS4'_T'</b>	0.364012	-2914.14223252	129.60 <i>i</i>	
<b>8_OSS</b>	0.364605	-2914.16829407		
<b>8_T'</b>	0.363300	-2914.16783821		
<b>8_T</b>	0.361852	-2914.18418150		3.0121
<b>TS5_OSS</b>	0.368299	-2914.16039146	388.03 <i>i</i>	
<b>TS5_T'</b>	0.369447	-2914.16033456	388.44 <i>i</i>	
<b>TS5_T</b>	0.364151	-2914.17378310	389.21 <i>i</i>	3.0350
<b>TS5_Q</b>	0.362520	-2914.17191679	385.56 <i>i</i>	
<b>9_OSS</b>	0.376691	-2914.20133379		
<b>9_T'</b>	0.371876	-2914.20168806		
<b>9_T</b>	0.364943	-2914.21713230		3.0134

<b>9_Q</b>	0.366163	-2914.21653491		
<b>10s_OSS</b>	0.417789	-3143.41263733		1.3457
<b>10s_T'</b>	0.416486	-3143.41266133		2.3479
<b>10s_Q</b>	0.412435	-3143.42987782		6.0555
<b>10s_T</b>	0.413479	-3143.42994980		3.0550
<b>TS6s_OSS</b>	0.413075	-3143.40525988	1041.78 <i>i</i>	1.3247
<b>TS6s_T'</b>	0.411143	-3143.40489706	1040.96 <i>i</i>	2.3099
<b>TS6s_Q</b>	0.409939	-3143.42491866	1054.68 <i>i</i>	6.0551
<b>TS6s_T</b>	0.410547	-3143.42494420	1055.11 <i>i</i>	3.0548
<b>11s_OSS</b>	0.416952	-3143.40901077		1.3913
<b>11s_T'</b>	0.414297	-3143.40869768		2.2691
<b>11s_Q</b>	0.413438	-3143.42798897		6.0549
<b>11s_T</b>	0.412669	-3143.43025030		3.0544
<b>10_OSS</b>	0.417563	-3143.41452010		1.3249
<b>10_T'</b>	0.414984	-3143.41276511		2.3585
<b>10_Q</b>	0.412790	-3143.43247781		6.0510
<b>10_T</b>	0.412398	-3143.43266970		3.0390
<b>TS6_OSS</b>	0.412613	-3143.37924006	1458.22 <i>i</i>	1.3702
<b>TS6_Q</b>	0.408082	-3143.39630403	1705.77 <i>i</i>	6.0165
<b>TS6_T</b>	0.411512	-3143.40807248	1110.99 <i>i</i>	2.6817
<b>11_S</b>	0.423893	-3143.42827798		
<b>11_T</b>	0.415191	-3143.46450336		2.1039
<b>11_Q</b>	0.414051	-3143.43149050		6.0207
<b>TS7_S</b>	0.371718	-2914.13608908	247.50 <i>i</i>	
<b>TS7_T</b>	0.362930	-2914.15118340	666.67 <i>i</i>	2.5138
<b>12_S</b>	0.371514	-2914.15994742		
<b>12_T</b>	0.367119	-2914.18194580		2.2935
<b>12_Q</b>	0.365557	-2914.17064150		6.0254
<b>TS8_S</b>	0.370416	-2914.12395301	564.47 <i>i</i>	

<b>TS8_T</b>	0.364082	-2914.15277721	637.12 <i>i</i>	2.3935
<b>TS8_Q</b>	0.361029	-2914.14617970	846.84 <i>i</i>	6.0284
<b>13_S</b>	0.374332	-2914.17459961		
<b>13_T</b>	0.370597	-2914.20946695		2.0841
<b>13_Q</b>	0.368070	-2914.17496823		6.0276
<b>14_S</b>	0.370523	-2914.16414385		
<b>14_T</b>	0.361418	-2914.16898474		2.0880
<b>14_Q</b>	0.354961	-2914.12670765		6.0343
<b>TS9_S</b>	0.373296	-2914.15425201	264.09 <i>i</i>	
<b>TS9_T</b>	0.364768	-2914.13578699	400.95 <i>i</i>	2.3902
<b>15_S</b>	0.374143	-2914.18991485		
<b>15_T</b>	0.365640	-2914.19741391		2.5548
<b>15_Q</b>	0.364166	-2914.18665254		6.0327
<b>TS10_S</b>	0.372973	-2914.12062579	302.79 <i>i</i>	
<b>TS10_T</b>	0.365367	-2914.17158637	304.51 <i>i</i>	2.4866
<b>TS10_Q</b>	0.361236	-2914.15421690	571.65 <i>i</i>	6.0411
<b>16_S</b>	0.374231	-2914.20147056		
<b>16_T</b>	0.367587	-2914.19287561		2.3740
<b>16_Q</b>	0.361042	-2914.18318424		6.0129
<b>TS11_S</b>	0.370056	-2914.09855330	1274.41 <i>i</i>	
<b>TS11_T</b>	0.359380	-2914.11561940	1533.78 <i>i</i>	2.1401
<b>TS11_Q</b>	0.360739	-2914.08441370	1447.47 <i>i</i>	6.2928
<b>17_S</b>	0.323431	-2684.90612840		
<b>17_T</b>	0.317324	-2684.90956720		2.0588
<b>17_Q</b>	0.310579	-2684.91328940		6.0167
<b>TS12_S</b>	0.372387	-2914.13332051	328.62 <i>i</i>	
<b>TS12_T</b>	0.365135	-2914.15582816	503.58 <i>i</i>	2.3914
<b>TS12_Q</b>	0.365496	-2914.14241083	677.32 <i>i</i>	6.0258
<b>18_S</b>	0.373808	-2914.16478637		

<b>18_T</b>	0.367173	-2914.19417320		2.1640
<b>18_Q</b>	0.366090	-2914.16934885		6.0224
<b>19_S</b>	0.371410	-2914.16222403		
<b>19_T</b>	0.366640	-2914.17347940		2.0882
<b>19_Q</b>	0.363386	-2914.12162173		6.0346
<b>TS13_S</b>	0.373876	-2914.15287921	246.93 <i>i</i>	
<b>TS13_T</b>	0.365639	-2914.13121701	358.68 <i>i</i>	2.1973
<b>20_S</b>	0.375191	-2914.15510099		
<b>20_T</b>	0.365232	-2914.17545392		2.1893
<b>20_Q</b>	0.362785	-2914.15495612		6.0108
<b>TS14_S</b>	0.372725	-2914.11206823	437.27 <i>i</i>	
<b>TS14_T</b>	0.366974	-2914.13916026	402.10 <i>i</i>	2.1301
<b>TS14_Q</b>	0.366860	-2914.11155427	610.24 <i>i</i>	6.0309
<b>21_S</b>	0.375076	-2914.16220429		
<b>21_T</b>	0.366262	-2914.18368283		2.1409
<b>21_Q</b>	0.364072	-2914.16898838		6.0233
<b>22_S</b>	0.370300	-2914.16485728		
<b>22_T</b>	0.368092	-2914.17207433		2.0899
<b>22_Q</b>	0.359707	-2914.12594603		6.0138
<b>TS15_S</b>	0.373482	-2914.15470376	285.95 <i>i</i>	
<b>TS15_T</b>	0.364846	-2914.13298274	381.94 <i>i</i>	2.1840
<b>23_S</b>	0.373604	-2914.15355831		
<b>23_T</b>	0.365205	-2914.17839024		2.2164
<b>23_Q</b>	0.362511	-2914.15209481		6.0116
<b>TS16_S</b>	0.372365	-2914.11534295	427.66 <i>i</i>	
<b>TS16_T</b>	0.363984	-2914.13673755	449.58 <i>i</i>	2.2394
<b>TS16_Q</b>	0.365350	-2914.11713371	556.47 <i>i</i>	6.0305
<b>24_S</b>	0.375423	-2914.16929412		
<b>24_T</b>	0.366380	-2914.19031895		2.1359

24_Q	0.362991	-2914.17428920		6.0233
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#### 4. Cartesian coordinates of all optimized structures.

##### INT1\_H\_Q

C	4.40081200	-2.62115000	-1.02786500
C	3.50972100	-3.59175400	-1.51091600
C	2.15064000	-3.30618400	-1.56802400
C	1.69476000	-2.04866800	-1.13714100
C	2.56508900	-1.05093000	-0.63529100
C	3.93132600	-1.37310300	-0.60631600
H	5.46394500	-2.84681200	-0.98277400
H	3.88188900	-4.55676400	-1.84268400
H	1.44150600	-4.03685400	-1.94748300
H	4.64997700	-0.64388200	-0.23359800
C	0.25057800	-1.73916500	-1.20076800
O	-0.62593400	-2.56318400	-1.48079800
N	-0.00481500	-0.39341500	-0.87812200
C	-1.15072000	0.25835300	-1.12930500
C	-1.15537600	1.64150800	-0.68018000
C	-2.31064600	-0.23176800	-1.78134900
C	-2.30057800	2.45559900	-0.85819700
C	-3.42918700	0.58867600	-1.95118900
H	-2.32150300	-1.25331700	-2.13263300
C	0.01184300	3.36300000	0.33634500
C	-2.23736200	3.78750800	-0.38795800
C	-3.44380100	1.90249400	-1.50072700
H	-4.30623600	0.18401500	-2.44571000
C	-1.07868500	4.23996500	0.21241300
H	0.93762200	3.68382100	0.80356300
H	-3.09883700	4.43737100	-0.50690600
H	-4.32193100	2.52556500	-1.63809700
H	-0.99427200	5.25463900	0.58430300
N	-0.02532200	2.10596300	-0.09950100
Co	1.58043700	0.62490600	0.06631800
C	0.24560800	0.17950200	2.30393000
C	1.09457200	-0.85398800	2.20467000
C	3.37358900	2.44373000	-0.10213600
O	2.95967900	1.86699400	0.97382000
O	2.86157800	2.16017600	-1.21745800
C	4.48976900	3.45095000	0.01425800
H	5.39451500	2.94579500	0.36924900
H	4.69276000	3.92493700	-0.94722500
H	4.22654400	4.21125800	0.75608300
H	0.53770100	1.11199200	2.78002900

H	0.79417000	-1.79715600	1.75867800
H	2.10557400	-0.80051600	2.60015400
H	-0.77591800	0.11344000	1.94119500

##### INT1\_H\_S

C	4.43910900	-2.36254100	-0.42554600
C	3.77638600	-3.25297700	-1.27833000
C	2.44778100	-3.01590800	-1.62905900
C	1.79535200	-1.88912800	-1.11952200
C	2.45185000	-0.99447600	-0.25767700
C	3.78117100	-1.23665400	0.08710200
H	5.47576700	-2.54669200	-0.15475800
H	4.29666000	-4.12397000	-1.66595900
H	1.91174300	-3.68743500	-2.29444100
H	4.31224100	-0.56040700	0.75157900
C	0.39289400	-1.54865500	-1.47101400
O	-0.32381500	-2.24546400	-2.21603700
N	0.03061800	-0.37209700	-0.88471900
C	-1.14153200	0.33193200	-1.12445700
C	-1.14509300	1.64714200	-0.56126300
C	-2.26584600	-0.07640600	-1.83678900
C	-2.24791700	2.52723600	-0.72826600
C	-3.36378800	0.80063200	-1.99503800
H	-2.29123900	-1.06463700	-2.27220700
C	0.04262900	3.22580200	0.67692300
C	-2.14133700	3.81439400	-0.14258700
C	-3.37241600	2.07374800	-1.46432800
H	-4.22374300	0.44950100	-2.55818500
C	-1.00248500	4.16300300	0.54991200
H	0.94920800	3.46288500	1.22403600
H	-2.96415600	4.51519900	-0.24941900
H	-4.22126700	2.73630400	-1.59979100
H	-0.89444100	5.14099300	1.00504900
N	-0.03153200	2.01672300	0.14216400
Co	1.33520400	0.52963900	0.15169700
C	0.26267700	0.15974100	2.08042500
C	1.13545000	-0.87502600	1.95012300
C	3.06208000	2.01475500	-0.35426800
O	2.81161600	1.65613500	0.84723500
O	2.30646000	1.49985400	-1.25127600
C	4.17918200	2.93875700	-0.69613500
H	5.10193600	2.35108000	-0.76871300
H	3.99508800	3.42257600	-1.65686000
H	4.30658000	3.68261900	0.09331800



H 0.53570900 1.05692400 2.62679600  
H 0.81332500 -1.83266100 1.55844300  
H 2.12510400 -0.83274000 2.39187200  
H -0.77813200 0.05385100 1.79462900

H 4.36629900 3.82971600 0.52498700  
H 0.35656900 1.10257000 2.64570900  
H 0.82977500 -1.80399700 1.70401700  
H 2.05961300 -0.69460700 2.52737700  
H -0.87305400 -0.00899500 1.82340100

INT1\_H\_T

C 4.38630600 -2.41028000 -0.56519300  
C 3.65869300 -3.39529800 -1.24399400  
C 2.33119000 -3.16132300 -1.60075600  
C 1.74645700 -1.93552500 -1.27227000  
C 2.47361000 -0.94690600 -0.59448900  
C 3.79915100 -1.18075000 -0.23723500  
H 5.41958000 -2.60019100 -0.28669000  
H 4.12962800 -4.34241100 -1.48975100  
H 1.74432400 -3.91152800 -2.12391000  
H 4.37566500 -0.43138600 0.29673200  
C 0.33744200 -1.59606400 -1.58473900  
O -0.45555300 -2.35474800 -2.16119400  
N 0.05494200 -0.32955300 -1.12959800  
C -1.17392800 0.32360400 -1.23580300  
C -1.17259600 1.64326200 -0.68755400  
C -2.35348900 -0.15048100 -1.79696700  
C -2.33434000 2.45835400 -0.70679500  
C -3.50996600 0.66602200 -1.81852200  
H -2.38258400 -1.14413100 -2.21977900  
C 0.07344600 3.29253900 0.39781800  
C -2.22774100 3.74802900 -0.13008100  
C -3.51892600 1.93939200 -1.29207600  
H -4.41312200 0.26383700 -2.26779400  
C -1.03198300 4.16301300 0.41858500  
H 1.02856800 3.57924600 0.82552300  
H -3.09629300 4.40008900 -0.12597800  
H -4.41306200 2.55405300 -1.31512100  
H -0.92656900 5.14424600 0.86695300  
N 0.00242700 2.08055500 -0.13633000  
Co 1.42583300 0.64616600 -0.25975300  
C 0.13627800 0.13746500 2.19799300  
C 1.05656800 -0.83256500 2.13307400  
C 3.36099900 2.18957500 -0.41131100  
O 2.83278600 1.69896600 0.65812000  
O 2.88099200 1.85820300 -1.52877000  
C 4.53700100 3.11247200 -0.28194400  
H 5.41998200 2.51853800 -0.02002000  
H 4.72416600 3.63437800 -1.22121200

TS\_H\_S

C -4.83223300 -1.62956000 0.24222000  
C -4.47030200 -2.38142700 1.36566700  
C -3.14732700 -2.37771400 1.80827600  
C -2.18837500 -1.63029700 1.12165400  
C -2.54153500 -0.88930900 -0.02686200  
C -3.87199300 -0.89495200 -0.45747300  
H -5.86440400 -1.62324600 -0.09655900  
H -5.22002300 -2.95985500 1.89703300  
H -2.84963200 -2.93005300 2.69481600  
H -4.15905900 -0.33740900 -1.34431900  
C -0.80107400 -1.48312800 1.64477000  
O -0.32218800 -2.21512700 2.53336800  
N -0.19312000 -0.42101200 1.05965700  
C 1.02907700 0.12750100 1.42173900  
C 1.26019000 1.40420200 0.82544500  
C 2.00451600 -0.39041400 2.26653800  
C 2.44450500 2.14403000 1.07776100  
C 3.18618500 0.34702700 2.51477900  
H 1.85337000 -1.35365400 2.73279100  
C 0.41361700 3.05918800 -0.58451700  
C 2.56515500 3.40546400 0.44125200  
C 3.41678700 1.58266800 1.94575600  
H 3.92998100 -0.08309300 3.17921700  
C 1.55601900 3.85899300 -0.38029200  
H -0.39447900 3.37973100 -1.23263000  
H 3.45620500 4.00295300 0.60999200  
H 4.32719500 2.13643200 2.15149400  
H 1.62214100 4.81923100 -0.87899800  
N 0.27381500 1.87878000 0.00159500  
Co -1.18793700 0.59779800 -0.18967900  
C -0.24250400 -0.18346200 -1.73307800  
C -1.32638200 -1.09323500 -1.62863500  
C -2.88311200 2.27096600 -0.11175500  
O -2.35562500 1.81576600 -1.19233700  
O -2.45616100 1.79220800 0.98477100  
C -3.97473700 3.29055100 -0.17082100  
H -4.91080600 2.78062000 -0.42687200

H	-4.09320300	3.78330000	0.79546900
H	-3.76438200	4.02462100	-0.95250700
H	-0.27751100	0.58751200	-2.49850000
H	-2.14247200	-0.99493100	-2.33549900
H	-1.11319500	-2.10959400	-1.31683300
H	0.74940300	-0.51144300	-1.43832900

H	2.89229800	3.68587000	-1.64557400
H	1.40990700	3.80104200	-2.60358700
H	1.58485800	4.76048300	-1.09839400
H	-0.05645700	1.48645900	2.58965100
H	2.26415900	0.67125100	2.57096800
H	1.65806900	-1.06070200	2.56014600
H	-0.66941700	-0.25554500	2.50187100

TS\_H\_T

C	4.55039000	-0.44282900	-0.18688000
C	4.39409900	-1.74893000	-0.66105200
C	3.14565300	-2.36903200	-0.59726900
C	2.05008100	-1.69167200	-0.05546200
C	2.22494900	-0.39196700	0.46422700
C	3.47089200	0.23178000	0.39085400
H	5.51716800	0.04829500	-0.24982800
H	5.23993300	-2.27508300	-1.09304800
H	2.99421500	-3.36804300	-0.99598700
H	3.60532900	1.23221600	0.79140400
C	0.67474000	-2.27454800	-0.14886400
O	0.47695200	-3.49507400	-0.31293600
N	-0.25068900	-1.28628700	-0.09101000
C	-1.62516700	-1.42739800	-0.20168300
C	-2.34364700	-0.18695900	-0.09599700
C	-2.36083000	-2.59064400	-0.40363100
C	-3.76104800	-0.14617100	-0.19815000
C	-3.77108800	-2.54304800	-0.50138500
H	-1.84191800	-3.53512900	-0.48888800
C	-2.22757200	2.12776000	0.21666900
C	-4.38671300	1.12048700	-0.08729100
C	-4.46927900	-1.35896400	-0.40456300
H	-4.30928500	-3.47309900	-0.65968300
C	-3.62554900	2.25206500	0.11328300
H	-1.59197600	2.99007200	0.38797300
H	-5.46840900	1.18426100	-0.16201700
H	-5.55136800	-1.33260100	-0.48472000
H	-4.07960900	3.23253100	0.20055300
N	-1.61496700	0.95584100	0.11225300
Co	0.36043700	0.56792000	0.30492600
C	0.14503200	0.44615200	2.35265900
C	1.47754900	-0.02356800	2.30113000
C	1.23977500	2.66051600	-0.79442500
O	0.94618700	2.78126100	0.43021000
O	1.08799000	1.52358400	-1.36828100
C	1.80461000	3.80844200	-1.58458400

INT2\_H\_Q

C	5.13482500	-1.58684500	-0.03061700
C	5.03651800	-1.06997500	-1.32478000
C	3.77975200	-0.86230400	-1.88690400
C	2.61141700	-1.12984000	-1.15897900
C	2.70471400	-1.66784500	0.13969400
C	3.97662100	-1.89171900	0.68293600
H	6.10897200	-1.76375000	0.41612300
H	5.93223500	-0.83763600	-1.89313000
H	3.68901400	-0.47539600	-2.89761900
H	4.05247300	-2.31733500	1.68042000
C	1.30153400	-0.86243600	-1.85602300
O	1.11430300	-1.38822700	-2.97198800
N	0.45846200	-0.01827100	-1.20809000
C	-0.82379000	0.27957400	-1.68308300
C	-1.49528800	1.35306900	-1.00262800
C	-1.52037400	-0.35610700	-2.70846000
C	-2.81311000	1.75281900	-1.36652400
C	-2.83010500	0.04237200	-3.06192600
H	-1.04645700	-1.16249100	-3.24690000
C	-1.39492500	2.98539100	0.66852000
C	-3.39404100	2.82477400	-0.64498800
C	-3.47678900	1.07367400	-2.41926000
H	-3.32792300	-0.48708200	-3.86928700
C	-2.69105900	3.44125400	0.36735700
H	-0.80534800	3.44182800	1.45722300
H	-4.39765100	3.15015700	-0.90344300
H	-4.47985100	1.37886500	-2.69995900
H	-3.11390800	4.26347500	0.93325400
N	-0.82560300	1.98446700	0.00865100
Co	1.02169300	1.13007900	0.37516500
C	1.08992400	-0.83326100	1.86057800
C	1.47885000	-1.97954400	0.97735100
C	2.79863800	2.66053000	1.19176200
O	1.72212600	2.59710900	1.86522300
O	2.89915100	1.97770000	0.11321900

C	3.95882200	3.48917100	1.66481300	O	2.52174500	2.25056900	-0.53670600
H	4.62242100	2.84697800	2.25602500	C	3.73401300	3.40148200	1.21803600
H	4.52795400	3.87514000	0.81661700	H	4.63477900	2.84360500	1.49916900
H	3.61524700	4.30750400	2.30022400	H	3.99610000	4.13103900	0.45014700
H	1.86498400	-0.35058900	2.45516500	H	3.35728400	3.90461500	2.11197900
H	1.70373600	-2.85603900	1.60803700	H	0.64910900	-0.31854200	2.36149500
H	0.63419100	-2.26522500	0.34406000	H	1.57439300	-2.48899900	1.87879900
H	0.07493800	-0.78610600	2.25111300	H	0.74150000	-2.57804700	0.32441900
				H	-0.62314100	-0.86564500	1.21606300

INT2\_H\_S

C	4.97762500	-1.00695000	0.37102800
C	4.99904500	-0.78703000	-1.01171800
C	3.82476700	-0.89829900	-1.74822000
C	2.61598300	-1.21572100	-1.11143300
C	2.59011300	-1.48563400	0.28024900
C	3.79028800	-1.36548700	1.00203700
H	5.89135400	-0.91523100	0.95047900
H	5.92811100	-0.52268600	-1.50748200
H	3.82218700	-0.71632000	-2.81868300
H	3.78185000	-1.57273300	2.06861900
C	1.34331600	-1.14014600	-1.91751200
O	1.18274900	-1.74102300	-2.99466600
N	0.49324600	-0.27942300	-1.32409900
C	-0.75632900	0.13370800	-1.75714200
C	-1.27995400	1.17776200	-0.94047300
C	-1.51575700	-0.31197300	-2.83025400
C	-2.54715800	1.76117200	-1.18734400
C	-2.78211500	0.26995100	-3.07960200
H	-1.13439800	-1.09521500	-3.47145600
C	-0.89089300	2.56433900	0.90460700
C	-2.96071400	2.79682100	-0.31177800
C	-3.29915700	1.27767000	-2.29035000
H	-3.35772800	-0.09441500	-3.92531200
C	-2.13800300	3.19327500	0.72162600
H	-0.21705300	2.84690500	1.70486700
H	-3.92521700	3.27121000	-0.46606700
H	-4.27031000	1.71361500	-2.50087300
H	-2.42968700	3.98400200	1.40313000
N	-0.48299400	1.59464900	0.09561900
Co	1.13660300	0.64903300	0.18694900
C	0.44681800	-0.69887400	1.35548700
C	1.30275800	-1.91327800	0.98694800
C	2.71668700	2.43000500	0.69919900
O	2.03547900	1.72414800	1.53916300

INT2\_H\_T

C	5.12307000	-1.89713400	-0.08766700
C	5.07165200	-1.48011100	-1.41997200
C	3.84198400	-1.17210800	-1.99637900
C	2.66065700	-1.24164700	-1.24519000
C	2.70428500	-1.68115900	0.09358300
C	3.94619400	-2.00471300	0.65319100
H	6.07520200	-2.15000800	0.36968200
H	5.98204200	-1.40375100	-2.00685600
H	3.78298800	-0.86517200	-3.03623800
H	3.98385000	-2.35449700	1.68155700
C	1.37447400	-0.90566400	-1.95023700
O	1.15612200	-1.41431700	-3.06645300
N	0.57029100	-0.02081500	-1.30297200
C	-0.73344400	0.28558500	-1.71731200
C	-1.39089700	1.32857500	-0.97780900
C	-1.45800700	-0.33048800	-2.73413300
C	-2.72664400	1.71883300	-1.28059800
C	-2.78562100	0.05949900	-3.02557200
H	-0.99353900	-1.11313900	-3.31415800
C	-1.24936800	2.90213300	0.74100500
C	-3.29460700	2.75853100	-0.50312500
C	-3.42053900	1.06179400	-2.32787000
H	-3.30675900	-0.45367000	-3.82854700
C	-2.56189700	3.35068200	0.50271500
H	-0.63501000	3.33748200	1.52265000
H	-4.31160300	3.07712500	-0.71295400
H	-4.43828000	1.35884600	-2.56038900
H	-2.97379300	4.14838500	1.11047400
N	-0.69199900	1.93203700	0.02945100
Co	1.20479200	1.08341300	0.19388000
C	1.07457100	-0.46841000	1.56520200
C	1.44533100	-1.78516800	0.93149600
C	2.67859500	2.78232500	1.24387800

O	1.66909700	2.35037900	1.88419900	C	1.65946300	3.16808400	-0.69076600
O	2.91092400	2.30164300	0.08130100	O	1.38530000	2.86527200	0.52086300
C	3.60030100	3.80378300	1.84531600	O	1.63875100	2.26309600	-1.58454900
H	4.41710500	3.27771900	2.35339500	C	1.97476600	4.59530100	-1.04601500
H	4.03478900	4.43368600	1.06619800	H	2.68373200	5.01086900	-0.32461000
H	3.07300600	4.41397800	2.58098700	H	2.37766900	4.67007800	-2.05705100
H	1.79727600	-0.08175600	2.28387000	H	1.05305500	5.18454500	-0.98219300
H	1.62007900	-2.51134900	1.73956300	H	-1.04355200	1.20097200	3.04503200
H	0.61313200	-2.16391600	0.33295200	H	1.56001600	-0.46014600	2.99462400
H	0.03749200	-0.35953700	1.88682900	H	1.36908000	1.28122500	3.61103800
INT1_CO2Et_Q				C	-0.99074700	-0.84598300	2.26268800
C	4.80072200	-1.31959500	0.95829400	O	-0.38211600	-1.84983000	1.91199800
C	4.70347600	-2.40695600	0.07758000	O	-2.32080800	-0.71144900	2.14273500
C	3.56910900	-2.55263300	-0.71332500	C	-3.04649800	-1.85256900	1.60874900
C	2.54214200	-1.59944000	-0.62215400	C	-4.51919600	-1.51515000	1.66662300
C	2.61608700	-0.48646600	0.24836700	H	-2.80281000	-2.73012700	2.21422100
C	3.76505600	-0.38378100	1.04780400	H	-2.70584000	-2.03495000	0.58703800
H	5.68919000	-1.20785200	1.57544000	H	-5.09710400	-2.34184600	1.24203900
H	5.50729100	-3.13533100	0.02135500	H	-4.84505300	-1.36080000	2.69994700
H	3.46231500	-3.39755000	-1.38792600	H	-4.73787200	-0.61087200	1.09254300
H	3.86908500	0.44485200	1.74644700	INT1_CO2Et_S			
C	1.31077800	-1.77043500	-1.42742700	C	4.99603500	-0.51991900	0.53453900
O	1.13693300	-2.68645700	-2.23770100	C	4.95274400	-1.75943600	-0.11400000
N	0.37025200	-0.76772400	-1.14972400	C	3.73905600	-2.24572900	-0.59925400
C	-0.94449800	-0.82874400	-1.45510900	C	2.57851100	-1.48650800	-0.42468900
C	-1.71348700	0.28570800	-0.94055400	C	2.61245400	-0.24806100	0.23664000
C	-1.63237100	-1.83607100	-2.16613700	C	3.82989800	0.23549300	0.71434700
C	-3.10756300	0.37599400	-1.17491300	H	5.94360700	-0.13935100	0.90727400
C	-3.01292100	-1.73333700	-2.38652000	H	5.86312300	-2.33756800	-0.24210400
H	-1.07717200	-2.67829800	-2.55244600	H	3.67886300	-3.19957100	-1.11635100
C	-1.71282000	2.23735300	0.31028200	H	3.88298300	1.19097700	1.22914900
C	-3.79275600	1.48325900	-0.62323000	C	1.25836100	-1.90784800	-0.95950400
C	-3.74753800	-0.65627400	-1.91497700	O	1.06574900	-2.98312500	-1.55827300
H	-3.51251700	-2.51851900	-2.94464900	N	0.32570800	-0.94147400	-0.72823400
C	-3.09280000	2.41532600	0.11705300	C	-0.97514000	-0.92634000	-1.21138000
H	-1.12942100	2.94665200	0.88732000	C	-1.67439700	0.28882400	-0.93024800
H	-4.86171800	1.58325700	-0.78467500	C	-1.65307300	-1.92313200	-1.90727200
H	-4.81556300	-0.58936300	-2.09570500	C	-3.01437800	0.49439800	-1.35321000
H	-3.58707900	3.27398400	0.55668100	C	-2.98807100	-1.71535600	-2.32509100
N	-1.04605100	1.20404200	-0.19906200	H	-1.15376200	-2.85548500	-2.12532800
Co	1.06369300	0.82169600	-0.02830400	C	-1.58247800	2.37911700	0.09909300
C	-0.38206800	0.36014700	2.86486600	C	-3.61612000	1.73195600	-1.01134000
C	0.91877400	0.39695500	3.17123700	C	-3.66760400	-0.54285500	-2.06603900

H	-3.48599300	-2.51494300	-2.86584500	N	0.26557500	-0.93062700	-1.01395100
C	-2.90530000	2.66770300	-0.29166900	C	-1.08808200	-0.89757800	-1.35423300
H	-0.99563000	3.08829100	0.67364200	C	-1.73604900	0.32998700	-1.01624400
H	-4.63970300	1.92597800	-1.31802100	C	-1.84682500	-1.89049700	-1.96163100
H	-4.69247100	-0.39969300	-2.39289100	C	-3.11301800	0.54487000	-1.28244700
H	-3.34377800	3.61937400	-0.01377800	C	-3.22007800	-1.67243400	-2.23084700
N	-0.99424000	1.23494700	-0.21375700	H	-1.38590000	-2.83103400	-2.22544800
Co	0.87618200	0.61167900	0.20043700	C	-1.50965700	2.43112700	-0.02205800
C	-0.14354900	0.04366600	2.20512700	C	-3.66249000	1.78615100	-0.87666000
C	1.15949700	-0.31935000	2.35477700	C	-3.85405300	-0.49222800	-1.90660000
C	1.79698800	2.63563800	-0.47098600	H	-3.78180300	-2.47105600	-2.70595300
O	1.53593800	2.39458900	0.75651600	C	-2.86834300	2.72082000	-0.24452900
O	1.52054400	1.68196900	-1.28321300	H	-0.84875000	3.13923100	0.46700800
C	2.41102500	3.91155600	-0.92832200	H	-4.71354800	1.98588700	-1.06302100
H	3.49312500	3.85061400	-0.76303200	H	-4.90853600	-0.34128000	-2.11349800
H	2.22401400	4.06694600	-1.99205500	H	-3.26890100	3.67318300	0.08308100
H	2.02066800	4.74561100	-0.34080700	N	-0.96708400	1.28216800	-0.40276400
H	-0.48558500	1.04127400	2.45669100	Co	0.94163600	0.63844800	-0.20224500
H	1.45221600	-1.35881000	2.26519000	C	-0.10371000	0.03557300	2.76990400
H	1.89051700	0.38247300	2.73636100	C	1.18248700	-0.30646000	2.90498500
C	-1.18957800	-0.98752400	1.95799600	C	2.05652900	2.84679100	-0.43503000
O	-0.96890800	-2.17503200	1.78066400	O	1.58738900	2.29672000	0.63494200
O	-2.41126100	-0.44527300	1.97060200	O	1.98879100	2.21529400	-1.52237600
C	-3.52102600	-1.34699900	1.69349200	C	2.68504100	4.20535800	-0.32950500
C	-4.79396400	-0.54218900	1.81664600	H	3.66420500	4.10044300	0.15135000
H	-3.48203800	-2.17145400	2.41051500	H	2.81837800	4.64650100	-1.31806200
H	-3.38199100	-1.75099900	0.68735800	H	2.07256100	4.85666100	0.29922000
H	-5.65042700	-1.18626200	1.59455500	H	-0.47405500	1.02100800	3.03330600
H	-4.91210500	-0.14873100	2.83100200	H	1.52585500	-1.30044800	2.63595900
H	-4.79868800	0.29400500	1.11233800	H	1.91614400	0.39238600	3.29281900
				C	-1.08680800	-0.92716500	2.22708700
INT1_CO2Et_T				O	-0.83086300	-2.06303100	1.84752800
C	4.86111200	-0.88931100	0.51760600	O	-2.32142400	-0.40085400	2.19957000
C	4.70838800	-2.19374900	0.03290200	C	-3.38916100	-1.27511900	1.74040500
C	3.48835700	-2.60211000	-0.50585500	C	-4.68591300	-0.51137300	1.88241600
C	2.43071500	-1.69106900	-0.55490300	H	-3.37799900	-2.18127200	2.35300300
C	2.58235300	-0.38374200	-0.07131500	H	-3.18688200	-1.55758000	0.70522800
C	3.79854400	0.02366400	0.47032500	H	-5.51199100	-1.12861000	1.51598700
H	5.81409100	-0.57953300	0.93831900	H	-4.88007300	-0.26095500	2.93000300
H	5.54195500	-2.88822500	0.07900700	H	-4.66168700	0.41364700	1.30025400
H	3.34469000	-3.61127400	-0.88238100				
H	3.92948500	1.02777200	0.86230600	TS_CO2Et_S			
C	1.08829900	-2.03058600	-1.08969200	C	4.95860800	-0.44581400	0.39055100
O	0.77027200	-3.14436100	-1.52783400				

C	4.91058700	-1.63054100	-0.35252100	C	-3.41907500	-1.18486600	1.85625000
C	3.67875400	-2.16926000	-0.72473400	C	-4.65130600	-0.31537000	1.96179600
C	2.49863500	-1.52923300	-0.34065200	H	-3.38292600	-1.94432000	2.64217500
C	2.54063200	-0.35319500	0.43526100	H	-3.34879500	-1.68357700	0.88571800
C	3.77897400	0.18677900	0.79209900	H	-5.54455800	-0.93562800	1.83866400
H	5.91781100	-0.01815900	0.66833300	H	-4.70303600	0.17314700	2.93986700
H	5.83152500	-2.12385800	-0.64831500	H	-4.65496500	0.45401700	1.18474200
H	3.61765200	-3.06848500	-1.33073400				
H	3.82844300	1.08984000	1.39378600	TS_CO2Et_T			
C	1.17381600	-1.97760000	-0.85053300	C	4.93050000	-0.67957800	0.21497200
O	0.99181900	-3.07327700	-1.41465500	C	4.78856800	-1.88921800	-0.47693100
N	0.24931700	-1.00053600	-0.67331200	C	3.51726400	-2.39343200	-0.75281000
C	-1.05065600	-1.00248700	-1.15851700	C	2.38073800	-1.70123600	-0.32727400
C	-1.71409400	0.24655800	-0.96825000	C	2.53357400	-0.52248000	0.43195700
C	-1.75488100	-2.03409800	-1.76966000	C	3.80454000	0.00131700	0.68152600
C	-3.05294300	0.45489100	-1.38752200	H	5.91998600	-0.27736700	0.41096600
C	-3.09005200	-1.82482100	-2.18852800	H	5.66701900	-2.42247500	-0.81814700
H	-1.27915600	-2.99227600	-1.91979500	H	3.38669900	-3.30385800	-1.33197400
C	-1.54978600	2.40524500	-0.09791200	H	3.91564700	0.91465600	1.25872600
C	-3.61677400	1.73079600	-1.13340700	C	1.01887600	-2.10474600	-0.80222800
C	-3.73801900	-0.61930700	-2.01133000	O	0.76009600	-3.26672100	-1.16998700
H	-3.61434600	-2.64961800	-2.66209100	N	0.19272100	-1.02675800	-0.81494100
C	-2.86990600	2.69732500	-0.49514500	C	-1.14077000	-1.02318300	-1.21206700
H	-0.93814200	3.13627200	0.41915700	C	-1.80627200	0.22806700	-0.99685400
H	-4.63926200	1.93010900	-1.44004500	C	-1.87297800	-2.06834200	-1.76466700
H	-4.76292800	-0.47684500	-2.33824500	C	-3.17132300	0.40857400	-1.35584300
H	-3.27848000	3.67879200	-0.28354300	C	-3.23470700	-1.88267200	-2.11386000
N	-0.99605700	1.22570600	-0.33596900	H	-1.39624700	-3.02237000	-1.92670100
Co	0.77829900	0.59227700	0.20152100	C	-1.65916800	2.41696200	-0.17605500
C	0.02818300	0.09645100	2.02104200	C	-3.74801600	1.67895900	-1.10879500
C	1.36239600	-0.34225400	2.15559100	C	-3.88008000	-0.67985600	-1.92313300
C	1.84151300	2.57968500	-0.47741500	H	-3.77314200	-2.72334600	-2.54285700
O	1.43605900	2.36867100	0.72219500	C	-2.99426100	2.67887600	-0.52549000
O	1.63709900	1.63736300	-1.31137500	H	-1.03597600	3.16646800	0.29951900
C	2.54285600	3.84134900	-0.85132000	H	-4.78535200	1.84890000	-1.37892400
H	3.59341800	3.75335400	-0.55027300	H	-4.92093000	-0.54812500	-2.19760800
H	2.49753900	3.99961700	-1.93001700	H	-3.41525500	3.66030400	-0.32439200
H	2.10458300	4.68847700	-0.31863800	N	-1.09281400	1.24278500	-0.41235000
H	-0.25461600	1.07603000	2.39279700	Co	0.79017400	0.65218300	0.05580600
H	2.05975400	0.30217400	2.67512800	C	0.21016800	0.06432500	2.10659200
H	1.53772200	-1.40761800	2.24560700	C	1.53648300	-0.42068200	2.21019300
C	-1.05996500	-0.90500800	1.96544600	C	1.99277500	2.85947000	-0.40995500
O	-0.90773900	-2.11696200	1.89545900	O	1.47683800	2.74576900	0.73916200
O	-2.26462600	-0.31335200	2.00038400	O	1.91304000	1.88644100	-1.24561400

C	2.74475000	4.09919400	-0.80440900	H	-5.32077900	1.95304900	-0.58592000
H	3.80682500	3.95029300	-0.57219700	H	-5.38594800	-0.36878200	-1.56390700
H	2.65881200	4.27851800	-1.87813700	H	-3.96232400	3.82451000	0.37103200
H	2.38468200	4.96195400	-0.24287100	N	-1.47460700	1.65978800	-0.27776100
H	-0.02097400	1.08126800	2.40508200	Co	0.52841200	1.20544700	-0.16389200
H	2.25844900	0.22957700	2.68638500	C	0.87440100	-1.68233800	1.80392700
H	1.66578800	-1.48669000	2.36285700	C	1.95142000	-2.51350900	1.19612600
C	-0.91753400	-0.88482900	2.02235200	C	2.52665000	2.40676800	0.57538300
O	-0.80633700	-2.09860400	1.91576400	O	1.94671800	1.56859300	1.34815600
O	-2.09738700	-0.24702400	2.08937600	O	2.01101600	2.65182100	-0.56837400
C	-3.28788000	-1.07550900	1.96123400	C	3.81298800	3.05773700	0.98956300
C	-4.48336400	-0.16791200	2.12747000	H	4.63660700	2.39240500	0.70664200
H	-3.25480100	-1.85378000	2.72752700	H	3.94696900	4.01178800	0.47660600
H	-3.26420000	-1.55472700	0.97713100	H	3.84233600	3.19595100	2.07229500
H	-5.40180500	-0.75152500	2.01626800	H	1.13851800	-0.78252800	2.34874500
H	-4.48827000	0.29635600	3.11861300	H	2.61344900	-2.89468900	1.98432800
H	-4.48233400	0.62351200	1.36985700	H	1.50797600	-3.37239200	0.68541900
INT2_CO2Et_Q				C	-0.52401800	-1.99071100	1.63244600
C	4.83723400	-0.50483600	-0.32296100	O	-0.96862000	-3.00610300	1.09291400
C	4.26368600	-0.03000200	-1.50300700	O	-1.32592100	-1.02214600	2.14259400
C	2.94637700	-0.37067000	-1.81555200	C	-2.75313900	-1.27229900	2.08099800
C	2.20237000	-1.18756800	-0.95762100	C	-3.44652600	-0.05872200	2.65846500
C	2.78020400	-1.67915100	0.22883200	H	-2.96973500	-2.17839100	2.65628100
C	4.09551400	-1.32086200	0.53500000	H	-3.03810200	-1.45146700	1.04227500
H	5.85946900	-0.24128700	-0.06771700	H	-4.53057000	-0.20164600	2.61042300
H	4.83284800	0.60723800	-2.17307500	H	-3.16465800	0.09242400	3.70535500
H	2.48476500	0.00802100	-2.72314400	H	-3.19519600	0.84300700	2.09401900
H	4.54065800	-1.68199700	1.45811500	INT2_CO2Et_S			
C	0.76851400	-1.51576000	-1.29499000	C	-4.77183900	-0.33438000	0.75412300
O	0.47916300	-2.65128000	-1.71575400	C	-4.84255200	0.67141100	-0.21739100
N	-0.07481100	-0.48140400	-1.06167800	C	-3.76597500	1.53223900	-0.40261900
C	-1.45858900	-0.54694000	-1.24149800	C	-2.60631100	1.39231400	0.37241000
C	-2.18455600	0.62058100	-0.81742500	C	-2.54046100	0.40892600	1.39143000
C	-2.19441900	-1.60817300	-1.76140400	C	-3.64028600	-0.45125100	1.55559200
C	-3.60157700	0.68923800	-0.93972900	H	-5.60706500	-1.01360000	0.89536500
C	-3.60199800	-1.53487200	-1.87157700	H	-5.73095700	0.77306800	-0.83315900
H	-1.67599200	-2.50145800	-2.07402400	H	-3.79687700	2.30321000	-1.16651900
C	-2.10230500	2.75684200	0.12809500	H	-3.60250900	-1.20470000	2.33750200
C	-4.24070100	1.87504300	-0.50179900	C	-1.39593900	2.20167100	-0.01147000
C	-4.30535800	-0.41936000	-1.47567700	O	-1.42293700	3.43552700	-0.15661000
H	-4.13169000	-2.39015500	-2.28081300	N	-0.35456800	1.37689200	-0.25055700
C	-3.49717700	2.90813200	0.02638900	C	0.91617700	1.72396300	-0.68663800
H	-1.48260900	3.54216600	0.55002800	C	1.70490000	0.57846900	-0.99035800

C	1.48792100	2.97883400	-0.84065800	C	-4.05556000	-0.15580900	1.57348600
C	3.04733400	0.68163500	-1.43119800	H	-6.05449600	-0.66438800	0.95632100
C	2.82913800	3.08658200	-1.28153600	H	-5.92126200	0.64235200	-1.16022200
H	0.90859800	3.86529200	-0.62206200	H	-3.83794500	1.89060600	-1.70353300
C	1.75589200	-1.76259500	-1.07133100	H	-4.12251900	-0.70444700	2.50909800
C	3.73230700	-0.53041500	-1.69738400	C	-1.56398700	2.01422100	-0.33075500
C	3.60242400	1.98074000	-1.57165700	O	-1.66990900	3.20841900	-0.66608800
H	3.25499900	4.07938900	-1.39149000	N	-0.41383600	1.29172000	-0.33408000
C	3.08798100	-1.73815500	-1.52643600	C	0.85100300	1.84493700	-0.53555400
H	1.22230500	-2.69011000	-0.90281100	C	1.88622600	0.89420500	-0.81237600
H	4.76387700	-0.49558700	-2.03422200	C	1.20984400	3.18630300	-0.45275100
H	4.62795600	2.08474800	-1.91046700	C	3.23368900	1.30101100	-1.01625100
H	3.58960500	-2.67802600	-1.72497300	C	2.55170400	3.58614000	-0.64957000
N	1.09638400	-0.63903100	-0.82012400	H	0.45383800	3.92948200	-0.24565300
Co	-0.66007700	-0.48578000	-0.16668600	C	2.42980400	-1.35026100	-1.12478800
C	-0.23168300	-0.57200900	1.73861300	C	4.18235100	0.28366800	-1.29007000
C	-1.33902200	0.29977900	2.32777600	C	3.55213600	2.68011400	-0.92877600
C	-1.75096100	-2.17088600	-1.53039000	H	2.78861000	4.64354900	-0.57704500
O	-1.18495000	-2.36173400	-0.38641400	C	3.78384500	-1.03479300	-1.35138800
O	-1.70493800	-1.00464900	-2.02546500	H	2.07773500	-2.37707100	-1.14794500
C	-2.45864900	-3.30343600	-2.20549800	H	5.22120400	0.55852000	-1.44810100
H	-3.43596400	-3.43732800	-1.72770000	H	4.57808600	2.99986700	-1.08128300
H	-2.60856000	-3.08649700	-3.26421000	H	4.48990800	-1.83059200	-1.55915000
H	-1.89245700	-4.22965400	-2.07978500	N	1.52452100	-0.41888300	-0.86309500
H	-0.35838700	-1.63792600	1.93583200	Co	-0.47246600	-0.68709800	-0.31452200
H	-1.67977300	-0.11806200	3.28119100	C	-0.65364600	-0.53645600	1.80637200
H	-0.93945600	1.29676800	2.52563000	C	-1.69019800	0.47942700	2.21626200
C	1.14413000	-0.12834700	2.05995900	C	-1.11748500	-2.57883100	-1.73183900
O	1.48301800	1.02000600	2.32429700	O	-0.93330800	-2.61568000	-0.45330200
O	2.03085900	-1.14319800	1.99974000	O	-0.97433900	-1.47169900	-2.32439400
C	3.42838300	-0.78975300	2.16933500	C	-1.46769200	-3.84189800	-2.45778400
C	4.22948600	-2.06958700	2.08259000	H	-2.28086900	-4.35606700	-1.93796100
H	3.55062300	-0.29654300	3.13791800	H	-1.75260500	-3.62960600	-3.48903800
H	3.70270800	-0.07993000	1.38359000	H	-0.59619400	-4.50586200	-2.45104600
H	5.29287300	-1.84253800	2.20812200	H	-0.95419800	-1.58005500	1.90080600
H	3.93215200	-2.77054300	2.86891300	H	-2.04987500	0.21223100	3.21910300
H	4.09287900	-2.55251400	1.11066400	H	-1.21868100	1.46194500	2.29175600
INT2_CO2Et_T				C	0.74908000	-0.27619300	2.18544000
C	-5.14597800	-0.12602100	0.70280900	O	1.20334400	0.81789600	2.49870400
C	-5.07245000	0.60708400	-0.48396400	O	1.50115100	-1.39235200	2.11112000
C	-3.90519800	1.30257600	-0.79313600	C	2.92699100	-1.22364900	2.33593800
C	-2.79601700	1.24403300	0.05970300	C	3.57195500	-2.58028400	2.16638200
C	-2.87104300	0.52289100	1.26847500	H	3.07412000	-0.82208000	3.34256500
				H	3.30540100	-0.49512000	1.61341100



H	4.65123500	-2.49053100	2.32435900	H	-0.89810400	0.94953300	2.62479700
H	3.17529800	-3.29596700	2.89322700	H	1.27414400	-1.20138600	2.14121200
H	3.40325300	-2.97214300	1.15914100	H	1.50679900	0.54112900	2.76356700
INT1_OEt_Q				O	-1.32914600	-0.95977600	1.93161300
C	5.26595900	-0.83855400	-0.09443200	C	-2.76616900	-0.81872500	2.10638700
C	4.98374900	-2.18174400	-0.38206300	C	-3.28630000	0.57938500	2.37267300
C	3.66532500	-2.57840700	-0.58004500	H	-3.03896700	-1.49063200	2.92719100
C	2.63930000	-1.62431500	-0.48204100	H	-3.19009600	-1.21823600	1.18254100
C	2.88937200	-0.26503800	-0.18274100	H	-4.37980900	0.52690200	2.37068000
C	4.23207100	0.10088700	-0.00695300	H	-2.97551200	0.96238800	3.34894200
H	6.29722800	-0.52991600	0.06223300	H	-2.98504500	1.28886000	1.59927700
H	5.79075200	-2.90509500	-0.45611400	INT1_OEt_S			
H	3.42236400	-3.61038200	-0.81860000	C	5.07261300	-0.59428000	0.48929000
H	4.48575300	1.13592800	0.22060300	C	4.95602000	-1.87024600	-0.07419400
C	1.23473700	-2.03832100	-0.70319600	C	3.71366700	-2.31471400	-0.52729600
O	0.88273800	-3.21067500	-0.87553300	C	2.60222100	-1.47522400	-0.40803400
N	0.36062300	-0.94006200	-0.68848200	C	2.70578500	-0.19150200	0.15918000
C	-0.93617800	-0.97743200	-1.05058100	C	3.95403600	0.24248500	0.60764100
C	-1.60940000	0.30590100	-0.95859300	H	6.04172600	-0.24828400	0.84092300
C	-1.68669700	-2.08540900	-1.50991500	H	5.82993700	-2.50979900	-0.15852400
C	-2.97153300	0.44003300	-1.32642900	H	3.59514600	-3.29939200	-0.97220400
C	-3.03650200	-1.93860600	-1.84999900	H	4.06897400	1.22894700	1.05013300
H	-1.20491900	-3.04902700	-1.58343400	C	1.24819300	-1.86858400	-0.87914000
C	-1.44823500	2.55432800	-0.42658700	O	0.99164600	-2.96761000	-1.41167900
C	-3.55265900	1.72554600	-1.23169200	N	0.36222700	-0.85640900	-0.66108500
C	-3.68013100	-0.71199400	-1.76803600	C	-0.96052300	-0.82001600	-1.06950000
H	-3.58815600	-2.80947000	-2.18925500	C	-1.60640000	0.43578800	-0.82195800
C	-2.78731200	2.78469000	-0.78398400	C	-1.70694300	-1.82758200	-1.67649300
H	-0.82543300	3.35894900	-0.04980200	C	-2.95489000	0.66883400	-1.20787600
H	-4.59316700	1.86301100	-1.50942200	C	-3.05316100	-1.59565500	-2.04043600
H	-4.72563800	-0.61335200	-2.04231400	H	-1.24808400	-2.78638600	-1.86895700
H	-3.20007300	3.78315800	-0.69671000	C	-1.38994200	2.58807900	0.04627200
N	-0.87720800	1.35512800	-0.51622200	C	-3.48990900	1.95509800	-0.94195900
Co	1.14751200	0.81980200	0.08395500	C	-3.67762400	-0.38406800	-1.82457300
C	-0.47696500	-0.00907200	2.33624100	H	-3.60400500	-2.40524300	-2.51076200
C	0.85840500	-0.22254800	2.35051700	C	-2.71055100	2.91084900	-0.32701200
C	1.95403800	3.23615800	-0.27050700	H	-0.75336400	3.30934600	0.54847900
O	1.61436900	2.70796600	0.85217800	H	-4.51539600	2.17168100	-1.22668100
O	1.84091000	2.58816200	-1.34524000	H	-4.70915000	-0.21979800	-2.11928500
C	2.51775700	4.63585200	-0.26161400	H	-3.09532700	3.90169200	-0.11326800
H	3.54119300	4.60128400	0.12921900	N	-0.86315700	1.39557000	-0.19067500
H	2.53830000	5.05613200	-1.26853900	Co	1.02286000	0.72061100	0.14685600
H	1.93189300	5.27662600	0.40305800	C	-0.46234800	0.02129500	2.23308300

C 0.91448600 -0.01199200 2.16709300  
 C 1.95377000 2.71803400 -0.66190800  
 O 1.75921400 2.51457300 0.58584500  
 O 1.61243800 1.76760200 -1.44546800  
 C 2.57015100 3.97988900 -1.16718600  
 H 3.64874200 3.94120800 -0.97615100  
 H 2.40162900 4.08854300 -2.23959800  
 H 2.16126700 4.83705000 -0.62636100  
 H -0.99525500 0.94620400 2.42931400  
 H 1.39919800 -0.98108900 2.18499800  
 H 1.44435000 0.81985200 2.61929300  
 O -1.16576600 -1.06964200 2.05721200  
 C -2.63241900 -1.06636700 2.01915100  
 C -3.30385000 0.21118100 2.46721200  
 H -2.90467200 -1.90370700 2.66487300  
 H -2.89436500 -1.32236500 0.99097300  
 H -4.38391400 0.03711100 2.43091600  
 H -3.03883200 0.47236000 3.49647200  
 H -3.08451500 1.05563300 1.81086700

INT1\_OEt\_T

C 5.05235100 -0.62609100 0.38072700  
 C 4.93187400 -1.93543700 -0.10079000  
 C 3.69771900 -2.40181500 -0.55258900  
 C 2.59348900 -1.54620900 -0.51617500  
 C 2.71092400 -0.23521700 -0.03122300  
 C 3.94384200 0.23078400 0.41836100  
 H 6.01697800 -0.26846400 0.73153400  
 H 5.80091100 -2.58632600 -0.12141900  
 H 3.57833400 -3.41406500 -0.92964700  
 H 4.05320100 1.24173700 0.80019600  
 C 1.23796400 -1.94743700 -0.96576100  
 O 0.94772000 -3.07396100 -1.39701600  
 N 0.37288100 -0.88939400 -0.82557800  
 C -0.98420300 -0.89137100 -1.14260500  
 C -1.62677200 0.36811600 -0.92612200  
 C -1.75391400 -1.94218500 -1.62736900  
 C -3.00274700 0.56196900 -1.21795600  
 C -3.12917200 -1.74996700 -1.90359100  
 H -1.29694800 -2.90685400 -1.79302000  
 C -1.38119100 2.57219200 -0.19871200  
 C -3.53795800 1.85228800 -0.98177600  
 C -3.75358600 -0.53563500 -1.71453500  
 H -3.69943600 -2.59432500 -2.27935500

C -2.73143700 2.85310600 -0.48074600  
 H -0.71888700 3.32704100 0.21205600  
 H -4.58597600 2.03863600 -1.19725100  
 H -4.80738400 -0.40143100 -1.93634000  
 H -3.11777000 3.84783700 -0.29041200  
 N -0.85253500 1.37505100 -0.41475000  
 Co 1.03771100 0.72446700 -0.08399800  
 C -0.44833800 -0.00781200 2.31325200  
 C 0.89968400 -0.10237000 2.33437000  
 C 2.08142500 2.91290000 -0.67464200  
 O 1.70683200 2.49992600 0.48917700  
 O 1.94307800 2.15105500 -1.66722000  
 C 2.68780300 4.28191600 -0.79176000  
 H 3.69095100 4.26025300 -0.35136600  
 H 2.76250400 4.58306200 -1.83746600  
 H 2.09300700 5.00678200 -0.22963700  
 H -0.95106500 0.94195100 2.46282500  
 H 1.39514900 -1.06262500 2.25283200  
 H 1.48328200 0.76295300 2.62519800  
 O -1.21212300 -1.08845800 2.10857700  
 C -2.66427100 -1.00133300 2.04404700  
 C -3.28347600 0.31334000 2.47086700  
 H -3.01211900 -1.81363300 2.68819700  
 H -2.93884000 -1.24477700 1.01513600  
 H -4.37033200 0.19785400 2.40869200  
 H -3.03008700 0.56854500 3.50469600  
 H -3.00311000 1.14299300 1.81789800

TS\_OEt\_S

C 4.94577500 -0.47233900 0.30191900  
 C 4.91112700 -1.60914800 -0.51344700  
 C 3.68369600 -2.14542800 -0.90234400  
 C 2.49634700 -1.55264000 -0.46763000  
 C 2.52526000 -0.42333100 0.37738400  
 C 3.76064100 0.11093100 0.75613800  
 H 5.90009200 -0.04423500 0.59573500  
 H 5.83677600 -2.06594600 -0.85027800  
 H 3.62961800 -3.00694200 -1.56168900  
 H 3.80196600 0.97393900 1.41449900  
 C 1.17399600 -1.99387500 -0.99158400  
 O 1.00300000 -3.06730600 -1.60369900  
 N 0.24357100 -1.03596200 -0.76309400  
 C -1.04498500 -1.00876900 -1.27268700  
 C -1.68655800 0.25360000 -1.08861500

C	-1.74822900	-2.01353400	-1.92785300	H	5.53736200	-2.23154400	-1.00844200
C	-2.99728300	0.50419100	-1.57206700	H	3.28715900	-3.31878000	-1.02116500
C	-3.05949000	-1.76636300	-2.39826000	H	3.79679100	1.30372500	0.71660600
H	-1.28684400	-2.97887000	-2.07969900	C	0.93531300	-2.24033900	-0.37537500
C	-1.49150200	2.41167700	-0.22582500	O	0.77516500	-3.47093500	-0.51248300
C	-3.53197700	1.79785800	-1.34700300	N	-0.00325000	-1.26969900	-0.47196900
C	-3.68240800	-0.54585900	-2.23700300	C	-1.35294900	-1.45438200	-0.71699800
H	-3.58367900	-2.57136300	-2.90524200	C	-2.12764400	-0.23829800	-0.69985900
C	-2.78223500	2.74436700	-0.68293300	C	-2.02119600	-2.64273100	-0.99295600
H	-0.87989100	3.12665900	0.31319800	C	-3.52323500	-0.25361600	-0.97263300
H	-4.53258000	2.02826600	-1.70073400	C	-3.40996100	-2.64903200	-1.25203700
H	-4.68627700	-0.37166100	-2.61073200	H	-1.46355100	-3.56845600	-1.01106400
H	-3.16683800	3.74046900	-0.49583700	C	-2.13605600	2.07295800	-0.39399500
N	-0.96626100	1.21128300	-0.42639900	C	-4.20241500	0.99038200	-0.94774500
Co	0.77822700	0.53893600	0.15041300	C	-4.15925700	-1.49016000	-1.25021600
C	-0.03109000	-0.03419800	1.88805300	H	-3.89252200	-3.59801900	-1.46472200
C	1.32257700	-0.44987100	1.99830100	C	-3.51333300	2.15110500	-0.66419600
C	1.88767800	2.60136900	-0.38380900	H	-1.55743300	2.96351500	-0.14217600
O	1.41950100	2.27882300	0.77149300	H	-5.26771900	1.01567200	-1.14732800
O	1.74665100	1.76689000	-1.32710200	H	-5.22364800	-1.50527200	-1.45866000
C	2.60067300	3.90429900	-0.56550800	H	-4.01013700	3.11428900	-0.63770600
H	3.62863600	3.79009300	-0.20187400	N	-1.46838100	0.92577200	-0.41314400
H	2.63020300	4.18144400	-1.62056100	Co	0.52514100	0.59765200	-0.01538800
H	2.11759000	4.68770900	0.02336200	C	0.23031700	0.30764900	2.07012900
H	-0.33740800	0.90717100	2.34032400	C	1.67406300	0.11654200	1.90824000
H	1.97884100	0.19373200	2.57108800	C	1.33070200	2.80544500	-0.88599800
H	1.49269800	-1.51534800	2.10781300	O	0.94235300	2.76393900	0.32161900
O	-1.01173400	-0.99889300	1.81833400	O	1.31582700	1.73616900	-1.59005200
C	-2.15402900	-0.77673900	2.67517200	C	1.85333300	4.08244700	-1.48323100
C	-3.13127100	0.24616100	2.12523300	H	2.94139100	4.11053900	-1.35075700
H	-1.79940500	-0.49146600	3.67318900	H	1.64085300	4.12289000	-2.55789700
H	-2.62702200	-1.75905100	2.75182300	H	1.42264200	4.94979500	-0.97888900
H	-3.98506300	0.32836800	2.80670800	H	-0.20269300	1.28560300	2.24263000
H	-2.67596700	1.23616400	2.03704100	H	2.23792800	1.01506100	2.14551800
H	-3.50311700	-0.05950700	1.14431400	H	2.01796400	-0.78372400	2.40851300
				O	-0.49903100	-0.79597100	2.42224400
TS_OEt_T				C	-1.71279400	-0.57848000	3.18546700
C	4.79491000	-0.37842100	-0.18447300	H	-2.37831100	-1.41031400	2.90803900
C	4.67086700	-1.69750000	-0.63472000	H	-1.44943800	-0.68280600	4.24883100
C	3.42006900	-2.31360400	-0.62646800	C	-2.39984600	0.76178200	2.92439000
C	2.29157700	-1.63862000	-0.16017100	H	-3.30847200	0.77771100	3.53541700
C	2.42776900	-0.32547800	0.36071900	H	-1.76711300	1.62369700	3.22555800
C	3.68431800	0.29607100	0.32752900	H	-2.68880000	0.86994300	1.86538100
H	5.76054100	0.11741700	-0.21345400				

INT2\_OEt\_Q

C	4.74943600	0.02516000	-1.05754400
C	4.79097600	0.72801800	0.14884600
C	3.66130000	1.41885500	0.58197400
C	2.47672000	1.38946000	-0.16395300
C	2.43649200	0.70885100	-1.39677400
C	3.58509300	0.03217900	-1.82595400
H	5.62596900	-0.51234400	-1.40754700
H	5.69828700	0.74053800	0.74548800
H	3.68083000	1.97313400	1.51600500
H	3.56453000	-0.48484400	-2.78203600
C	1.27609800	2.10974700	0.39548300
O	1.36101000	3.33055600	0.63782400
N	0.20984700	1.30531800	0.62242100
C	-1.03839200	1.78216100	1.02905500
C	-1.96200200	0.77464000	1.47631400
C	-1.49013400	3.09883900	1.00507500
C	-3.28303600	1.11456600	1.88636400
C	-2.80629600	3.42760000	1.40328600
H	-0.82062900	3.88087100	0.67807700
C	-2.34131300	-1.48984400	1.90874800
C	-4.12318700	0.06032900	2.32304500
C	-3.69489600	2.47075300	1.84038600
H	-3.11258000	4.46894400	1.36086600
C	-3.65544300	-1.23587700	2.34221500
H	-1.93889400	-2.49795100	1.89259600
H	-5.13567000	0.29139200	2.64151000
H	-4.70189400	2.73074300	2.15100700
H	-4.27767100	-2.05907800	2.67455600
N	-1.53246400	-0.52423700	1.49348800
Co	0.30927400	-0.72254500	0.57009300
C	0.35654000	-0.53471600	-2.06591600
C	1.19443300	0.69544800	-2.26430500
C	1.67996900	-2.70675800	1.15655700
O	0.55035300	-2.88137400	0.59251400
O	2.06780000	-1.51762800	1.41394000
C	2.55967900	-3.88031100	1.48380300
H	3.07413900	-4.19619700	0.56884900
H	3.30830500	-3.61032200	2.23040100
H	1.95571500	-4.71993900	1.83598700
H	0.82109600	-1.51943200	-2.16351600
H	1.50001700	0.75691900	-3.32149700
H	0.57333300	1.57461400	-2.06843900
O	-0.90244800	-0.41605400	-2.57954800

C	-1.64187400	-1.63603000	-2.79898700
C	-2.28533500	-2.15556100	-1.52659000
H	-0.96934700	-2.38143800	-3.24045300
H	-2.39896600	-1.37094100	-3.54148300
H	-2.91082500	-3.02320500	-1.76285300
H	-1.52963900	-2.46683000	-0.80240200
H	-2.91849300	-1.38813200	-1.07098200

INT2\_OEt\_S

C	4.60177200	-0.44444500	-0.65824000
C	4.73295100	0.61661900	0.24589700
C	3.69970000	1.53635500	0.39205300
C	2.52170700	1.40214600	-0.35516100
C	2.39771600	0.36340000	-1.31282400
C	3.45555000	-0.55521300	-1.43877100
H	5.40292000	-1.16895600	-0.76751600
H	5.63563900	0.71599000	0.84092700
H	3.77782200	2.35061400	1.10588100
H	3.37240000	-1.35050900	-2.17426900
C	1.34431600	2.27241600	0.00344000
O	1.41739300	3.50910700	0.11753100
N	0.28546100	1.47998200	0.25922500
C	-0.96475400	1.84832200	0.72837300
C	-1.73581700	0.71819100	1.12960800
C	-1.52559500	3.11158200	0.85670600
C	-3.04586900	0.85163800	1.65338800
C	-2.83684600	3.24650300	1.37306300
H	-0.95755600	3.98525500	0.56691200
C	-1.77648700	-1.60994900	1.35785500
C	-3.71217200	-0.34091100	2.03430700
C	-3.58959000	2.15828400	1.76620800
H	-3.25464600	4.24488200	1.46228200
C	-3.07800600	-1.55747900	1.89436200
H	-1.25033200	-2.54678100	1.21998800
H	-4.71828700	-0.28235500	2.43868800
H	-4.59056900	2.28269700	2.16636800
H	-3.56329600	-2.48297400	2.18199900
N	-1.13645700	-0.50792200	0.98619800
Co	0.58163000	-0.38862100	0.21882100
C	0.04449300	-0.51538100	-1.62282500
C	1.19322300	0.27108300	-2.24823400
C	1.72229100	-2.17204600	1.50356200
O	1.05624400	-2.26435500	0.39956700
O	1.80388800	-1.05922100	2.08714300

C	2.40517600	-3.40300600	2.02859600	H	-4.29669100	-2.12024200	2.15637100
H	3.29164300	-3.59990500	1.41488400	N	-1.52719000	-0.52861100	1.11527800
H	2.71532200	-3.26025300	3.06486500	Co	0.40163200	-0.66312100	0.32998600
H	1.74268700	-4.26870500	1.94543500	C	0.20157800	-0.50225500	-1.78064600
H	0.11377500	-1.59172400	-1.80391200	C	1.14755900	0.56606200	-2.28640500
H	1.50865000	-0.19789700	-3.18700200	C	1.55112500	-2.51888000	1.61166700
H	0.83123500	1.27604700	-2.47995500	O	1.30602700	-2.44058300	0.34383000
O	-1.16315500	0.01813400	-2.05984200	O	1.20899900	-1.58029500	2.37509600
C	-2.37408500	-0.75174700	-1.93045500	C	2.24722500	-3.75203800	2.11987000
C	-2.24218600	-2.23954700	-2.20805100	H	3.22096900	-3.84719400	1.62845800
H	-3.05407100	-0.29347800	-2.65433500	H	2.38335200	-3.70673500	3.20108400
H	-2.79903100	-0.58850100	-0.93567700	H	1.65926900	-4.63712600	1.85651400
H	-3.24719400	-2.67400000	-2.22854700	H	0.52452600	-1.53499900	-1.94017400
H	-1.77100100	-2.42467700	-3.17909500	H	1.36940400	0.35050600	-3.34028100
H	-1.67279100	-2.76064500	-1.43342600	H	0.62287500	1.52484100	-2.25484300
INT2_OEt_T				O	-1.07786600	-0.22667100	-2.14623700
C	4.78868800	0.03734100	-1.27433200	C	-2.12820100	-1.22639600	-2.05575800
C	4.87614400	0.79055000	-0.10117500	C	-1.67486200	-2.66738900	-1.94741700
C	3.75328000	1.47031100	0.36712300	H	-2.72060300	-1.07341500	-2.96202700
C	2.53118800	1.37975600	-0.31056400	H	-2.74641700	-0.94792800	-1.19796800
C	2.44236400	0.64061300	-1.50821200	H	-2.57054600	-3.29660100	-1.93233300
C	3.58299400	-0.02320500	-1.97416900	H	-1.06443400	-2.96883200	-2.80443200
H	5.65993900	-0.49026300	-1.65118100	H	-1.11501400	-2.86038100	-1.02843100
H	5.81443600	0.85215200	0.44198800	INT1_Ph_Q			
H	3.80899000	2.06932200	1.27126300	C	4.86331700	-1.67855300	-0.22128900
H	3.52280300	-0.58386100	-2.90326300	C	4.34040500	-2.90267800	-0.66576200
C	1.34517100	2.10838000	0.26965300	C	2.97527100	-3.02057900	-0.90055800
O	1.45692100	3.31496100	0.56617100	C	2.14295800	-1.90959700	-0.68346100
N	0.25739700	1.32396800	0.45979600	C	2.63730700	-0.66354100	-0.22761800
C	-0.97239700	1.79417500	0.92012700	C	4.02255500	-0.58028800	-0.01504800
C	-1.92329300	0.77015000	1.25552700	H	5.93131800	-1.58910000	-0.03531300
C	-1.37825200	3.11875600	1.05815900	H	5.00035300	-3.74964500	-0.82962500
C	-3.22755600	1.09697100	1.72374600	H	2.54777700	-3.95431000	-1.25561800
C	-2.67858800	3.43570600	1.51418400	H	4.45982500	0.35412800	0.33520400
H	-0.68406300	3.91128800	0.82075800	C	0.69099200	-2.02369400	-0.93663000
C	-2.35224600	-1.51471700	1.43576300	O	0.11271600	-3.07846900	-1.21807600
C	-4.09206500	0.02062600	2.04673100	N	0.04461200	-0.78583800	-0.78677800
C	-3.59388700	2.46128700	1.84659400	C	-1.19388400	-0.50107300	-1.21356600
H	-2.95049100	4.48341000	1.60550900	C	-1.64742300	0.83302300	-0.85891700
C	-3.65726400	-1.27975300	1.91119300	C	-2.07423500	-1.32917400	-1.95344700
H	-1.97539700	-2.52485200	1.30624800	C	-2.95074400	1.26751400	-1.20246700
H	-5.09442100	0.23807100	2.40430400	C	-3.34986300	-0.87536500	-2.29941200
H	-4.58729700	2.71518600	2.20285200	H	-1.75101800	-2.32241500	-2.22890500

C	-1.17203500	2.82852200	0.21161400	H	2.95651500	-3.44926500	-1.57108300
C	-3.34372800	2.55629000	-0.77721900	H	4.08144200	0.59166300	1.11804300
C	-3.79719500	0.38732600	-1.93325800	C	0.83935300	-1.73274500	-1.19516500
H	-4.00662200	-1.53334500	-2.85893900	O	0.41434200	-2.69779000	-1.86046300
C	-2.45409700	3.33357900	-0.06019300	N	0.12246100	-0.63298000	-0.83206700
H	-0.44323700	3.41373900	0.76298500	C	-1.17951200	-0.34046200	-1.20540100
H	-4.33980000	2.91727000	-1.01447200	C	-1.65193300	0.91361400	-0.70251200
H	-4.79604600	0.71926200	-2.19820700	C	-2.05079500	-1.10531000	-1.97512100
H	-2.72333400	4.32411200	0.28823500	C	-2.96346400	1.38274600	-0.98371300
N	-0.77886200	1.61882100	-0.18267300	C	-3.35605100	-0.63611700	-2.24830500
Co	1.15898600	0.70490200	0.19049800	H	-1.72561800	-2.06329200	-2.35277400
C	-0.26735000	-0.04168500	2.49357000	C	-1.16503100	2.78347000	0.60036500
C	1.02867600	-0.40980800	2.57103800	C	-3.33737200	2.62841700	-0.42109800
C	2.26934900	3.02717900	-0.06478900	C	-3.81816700	0.57459400	-1.77614400
O	1.93262100	2.42339300	1.02299900	H	-4.01023200	-1.26161800	-2.84890800
O	2.05884000	2.50034900	-1.18760800	C	-2.44389300	3.32563800	0.36376900
C	2.91282000	4.38675800	0.05754300	H	-0.43912600	3.29903700	1.22081800
H	3.79507500	4.31926000	0.70191400	H	-4.33332500	3.01816700	-0.61059700
H	3.19863000	4.77735400	-0.92020800	H	-4.82405500	0.91894900	-1.99408900
H	2.21069300	5.07754300	0.53649900	H	-2.70648800	4.27855500	0.80924900
H	-0.52764800	0.98225100	2.75637100	N	-0.78844700	1.62209900	0.08565300
H	1.36507600	-1.41682400	2.34889800	Co	0.98041200	0.65550500	0.25167300
H	1.77781400	0.28289400	2.94073300	C	-0.28524100	-0.17439500	2.23514000
C	-1.39794000	-0.88223300	2.07769300	C	1.04491400	-0.47704600	2.27370500
C	-2.65947800	-0.28550700	1.91959900	C	2.18096100	2.60080900	-0.19548900
C	-1.26027700	-2.24985400	1.77903100	O	1.95194100	2.21867300	1.00182300
C	-3.74952600	-1.02528100	1.46157600	O	1.71248400	1.83956300	-1.11436500
H	-2.77490100	0.77276500	2.13765000	C	2.96737300	3.82641600	-0.50940400
C	-2.34543500	-2.98627100	1.31566300	H	4.03294300	3.58671200	-0.41485000
H	-0.29668000	-2.73577000	1.89047300	H	2.76883800	4.15924800	-1.52940100
C	-3.59475000	-2.37709900	1.15280800	H	2.72998800	4.61622900	0.20703000
H	-4.71334800	-0.54215800	1.33216200	H	-0.59529900	0.80619800	2.58597400
H	-2.21650300	-4.03667100	1.07212100	H	1.40602200	-1.47909600	2.08190600
H	-4.43785700	-2.95322000	0.78321500	H	1.74603000	0.21231600	2.73007100
INT1_Ph_S				C	-1.37310500	-1.07508400	1.84768700
C	4.81630300	-1.23518300	0.23960700	C	-2.68545100	-0.57416900	1.83811000
C	4.51424200	-2.37958600	-0.50749100	C	-1.14800700	-2.40062100	1.43351800
C	3.21691800	-2.57364200	-0.98221100	C	-3.74838300	-1.37054600	1.41645500
C	2.23574300	-1.61912400	-0.69971200	H	-2.86091100	0.45356300	2.14350700
C	2.52609900	-0.47335000	0.06178000	C	-2.20770800	-3.19151100	1.00473600
C	3.82718700	-0.28456800	0.52729800	H	-0.14221000	-2.80597200	1.42555800
H	5.82900300	-1.08290900	0.60488300	C	-3.51020000	-2.67894300	0.99280600
H	5.28883300	-3.11111300	-0.71848500	H	-4.75583200	-0.96646400	1.40415400
				H	-2.02076600	-4.20833600	0.67315500

H -4.33381700 -3.29841100 0.65035200

INT1\_Ph\_T

C 4.58563400 -1.64826100 0.16137700

C 4.13454600 -2.83810100 -0.42242900

C 2.83204300 -2.92661800 -0.91364900

C 1.99425200 -1.81323800 -0.81599300

C 2.44304400 -0.62150400 -0.22927900

C 3.74205600 -0.53346800 0.26437200

H 5.60120700 -1.58748500 0.54362700

H 4.80060600 -3.69314200 -0.48969000

H 2.45712800 -3.84161900 -1.36427200

H 4.10233900 0.37594700 0.73571000

C 0.58585500 -1.80951600 -1.28327500

O 0.01391300 -2.78549300 -1.78964200

N 0.02365600 -0.57716600 -1.04922300

C -1.30753500 -0.23343200 -1.28995500

C -1.68825900 1.02498000 -0.73250800

C -2.26556400 -0.95720600 -1.98703800

C -3.01356200 1.51967300 -0.84832000

C -3.58249800 -0.45438500 -2.11668800

H -2.00556100 -1.91272400 -2.41760300

C -1.01102100 2.87647800 0.51722600

C -3.29775100 2.75515200 -0.21769100

C -3.96647900 0.74707100 -1.56249500

H -4.30690800 -1.04963000 -2.66445400

C -2.30505400 3.42677800 0.46692100

H -0.19983500 3.37752500 1.03523600

H -4.30339000 3.16109300 -0.27663700

H -4.98298600 1.11454200 -1.65935800

H -2.50043000 4.37077000 0.96265100

N -0.71707200 1.72177200 -0.06608100

Co 1.04692700 0.71552800 -0.12559100

C -0.23316000 -0.26934200 2.64473000

C 1.05266000 -0.61862700 2.81149700

C 2.54281100 2.67741600 -0.16254800

O 2.06300000 2.08232900 0.87580800

O 2.25916900 2.21786000 -1.30290100

C 3.43140800 3.87051500 0.02827500

H 4.39547200 3.52996700 0.42222400

H 3.59306200 4.38803100 -0.91805100

H 2.99286500 4.55042200 0.76347000

H -0.54395100 0.72586600 2.95962400

H 1.43836000 -1.59346900 2.53030400

H 1.76264000 0.07529700 3.25045500

C -1.30125800 -1.09221000 2.06024100

C -2.60410900 -0.56985400 2.00421500

C -1.06958900 -2.37069400 1.52112500

C -3.64891000 -1.30378300 1.44279800

H -2.79117700 0.42491000 2.40020000

C -2.10825600 -3.09753500 0.94793200

H -0.06894500 -2.79029000 1.53131200

C -3.40410500 -2.57052500 0.91156400

H -4.64808700 -0.88021700 1.40675700

H -1.90601400 -4.07431000 0.51849700

H -4.21138400 -3.13913300 0.45952800

TS\_Ph\_S

C 4.82102600 -1.03642400 0.15346600

C 4.59126200 -2.06777000 -0.76382300

C 3.28674400 -2.37063400 -1.15461500

C 2.21587100 -1.65315300 -0.61841600

C 2.43712400 -0.63656100 0.33663100

C 3.75081500 -0.33186700 0.70905800

H 5.83702000 -0.78727500 0.44651300

H 5.42706300 -2.62172900 -1.18037400

H 3.08596500 -3.14048300 -1.89408600

H 3.94082000 0.44400400 1.44513600

C 0.83263300 -1.83007100 -1.14341000

O 0.47742200 -2.81434000 -1.82191700

N 0.07863700 -0.74928200 -0.83157700

C -1.22003300 -0.50240400 -1.24702500

C -1.68667700 0.78987900 -0.85998900

C -2.08907400 -1.33389200 -1.94364900

C -2.99491800 1.23880700 -1.17621100

C -3.39422800 -0.88643700 -2.25582300

H -1.76442100 -2.32198700 -2.23605700

C -1.18110200 2.76200000 0.27758800

C -3.35897400 2.53170800 -0.72473700

C -3.85143500 0.36370800 -1.89288500

H -4.05203800 -1.55994400 -2.79745900

C -2.45685600 3.28802500 -0.00707900

H -0.45369500 3.31975600 0.85687100

H -4.35270400 2.91125500 -0.94373000

H -4.85640000 0.68974100 -2.14104300

H -2.71130300 4.27791900 0.35427900

N -0.81290600 1.55915100 -0.14044800

Co 0.84496000 0.59972000 0.25443200

C	0.01769200	-0.09533200	1.97392800	C	-1.35181300	2.77918200	0.08320500
C	1.32216700	-0.66657700	2.00208500	C	-3.55936700	2.38651200	-0.76984100
C	2.21509100	2.51357500	-0.09751900	C	-4.02379800	0.15521100	-1.79861600
O	1.74788300	2.15595300	1.04523500	H	-4.20535500	-1.81361400	-2.60309200
O	1.91045400	1.78837000	-1.09571500	C	-2.66394200	3.23654100	-0.14533200
C	3.10446100	3.70849500	-0.21757700	H	-0.61020900	3.39483800	0.58130900
H	4.11449200	3.42068800	0.09704100	H	-4.58374500	2.70167900	-0.94164300
H	3.14289200	4.05647000	-1.25104200	H	-5.05386700	0.43535300	-1.99149000
H	2.75743500	4.50637800	0.44342100	H	-2.95449800	4.22257100	0.18724500
H	-0.10345500	0.85556800	2.48797900	N	-0.95937400	1.57892400	-0.30902800
H	2.06157600	-0.15145000	2.60347500	Co	0.85241400	0.66714100	0.07689800
H	1.41204600	-1.74620000	2.01786600	C	0.19891600	0.01578400	2.16469800
C	-1.22370900	-0.88163600	1.84955500	C	1.52002400	-0.55562300	2.09058600
C	-2.45499800	-0.22401400	2.00842800	C	2.35511700	2.78729100	-0.11605700
C	-1.23602000	-2.25130900	1.53281700	O	1.74760800	2.52875000	0.98156800
C	-3.66016600	-0.90191200	1.83156800	O	2.25603700	1.99601300	-1.12228700
H	-2.46050200	0.83559200	2.24889400	C	3.22399200	4.00363000	-0.21131100
C	-2.43919700	-2.92906900	1.35648500	H	4.20656600	3.77501800	0.25767600
H	-0.30325800	-2.78808800	1.39727800	H	3.39803600	4.27782000	-1.26495600
C	-3.65766200	-2.25733000	1.49808600	H	2.76654100	4.83668300	0.35085900
H	-4.59953500	-0.36867600	1.94549700	H	0.10815500	1.04600700	2.49746000
H	-2.42693600	-3.98477400	1.10117000	H	2.29771700	0.04206900	2.55260300
H	-4.59419000	-2.78696900	1.35044300	H	1.60678500	-1.62232300	2.26734200
TS_Ph_T				C	-1.03960400	-0.73512800	2.01417600
C	4.80377000	-1.23715900	-0.04712200	C	-2.27468500	-0.06851200	2.13704800
C	4.46717800	-2.32957800	-0.84991100	C	-1.04409900	-2.11702900	1.72650900
C	3.13021000	-2.61321200	-1.12618200	C	-3.47580700	-0.75508700	1.98232800
C	2.10928100	-1.83272100	-0.56815000	H	-2.28117900	1.00201400	2.34491100
C	2.45983800	-0.80224500	0.32912400	C	-2.24093400	-2.79874200	1.56697200
C	3.79532000	-0.47592500	0.56016900	H	-0.10677800	-2.65218100	1.60940400
H	5.84607800	-0.98997100	0.13593000	C	-3.46349800	-2.12170400	1.69578700
H	5.25434300	-2.94204600	-1.29028100	H	-4.41937500	-0.23068200	2.07344700
H	2.85865700	-3.41243400	-1.80290500	H	-2.23211500	-3.86306900	1.33574200
H	4.05819200	0.33935200	1.22952700	H	-4.40017600	-2.65944000	1.57097600
C	0.69565600	-1.98702900	-1.06279100	INT2_Ph_Q			
O	0.27813100	-3.06045200	-1.54100600	C	4.83262000	-0.80186700	-0.19620300
N	0.02341200	-0.81625100	-0.96289200	C	4.27517000	-1.15730500	-1.42587500
C	-1.31079000	-0.59328900	-1.29238500	C	2.95663200	-1.60899500	-1.47893800
C	-1.80914700	0.71401900	-0.93111100	C	2.19326400	-1.71675900	-0.31021600
C	-2.20528300	-1.47427600	-1.88940900	C	2.75364700	-1.37592400	0.93577000
C	-3.15312500	1.09362500	-1.18171400	C	4.07465000	-0.91352600	0.97051200
C	-3.54499900	-1.08965400	-2.13744700	H	5.85693000	-0.44434900	-0.14334800
H	-1.86187100	-2.46292600	-2.15842000	H	4.85975300	-1.07903300	-2.33761700



H	2.50622200	-1.87049000	-2.43256200	H	-4.05269300	0.82593100	2.36323100
H	4.51072100	-0.63906800	1.92774700				
C	0.75124400	-2.15610400	-0.40990700	INT2_Ph_S			
O	0.42679800	-3.31260400	-0.07216700	C	4.72366500	-0.48196000	0.79102500
N	-0.06222700	-1.17067100	-0.85313000	C	4.71452500	-1.10812500	-0.46171800
C	-1.44583700	-1.31968200	-0.98683600	C	3.55080200	-1.71021400	-0.92790400
C	-2.19345400	-0.09302900	-1.03360800	C	2.38262600	-1.68398000	-0.15351500
C	-2.15773900	-2.51053900	-1.07110800	C	2.39186700	-1.09924800	1.13940900
C	-3.61252500	-0.09983400	-1.14644400	C	3.58110300	-0.49384400	1.58468000
C	-3.56744200	-2.51077500	-1.19111000	H	5.62877600	-0.00409700	1.15329500
H	-1.62412900	-3.44855400	-1.02628100	H	5.61151800	-1.11536700	-1.07340700
C	-2.15106800	2.23949700	-0.91374100	H	3.52229900	-2.18122700	-1.90577400
C	-4.27492200	1.15218500	-1.14545700	H	3.60115800	-0.04624500	2.57445200
C	-4.29387100	-1.34176300	-1.22611200	C	1.09272300	-2.15151300	-0.78111400
H	-4.08024500	-3.46644800	-1.25039100	O	0.95000500	-3.27029900	-1.30477100
C	-3.55100400	2.31877500	-1.02572400	N	0.20518600	-1.13990300	-0.74143100
H	-1.54294600	3.13318200	-0.81103100	C	-1.09069600	-1.10607000	-1.23046400
H	-5.35754100	1.17604800	-1.23065200	C	-1.66041900	0.19509800	-1.12176800
H	-5.37614400	-1.34885300	-1.30885900	C	-1.86842000	-2.13120700	-1.74890800
H	-4.03479200	3.28874600	-1.01320900	C	-2.99609200	0.46344000	-1.50707600
N	-1.50304000	1.08245300	-0.92650200	C	-3.20632000	-1.86720000	-2.12854400
Co	0.52858100	0.75448500	-0.72500000	H	-1.45539800	-3.12639400	-1.84524100
C	1.20024100	-0.12159600	2.41564500	C	-1.30080500	2.40901400	-0.46166600
C	1.92689500	-1.41831300	2.21321900	C	-3.45600300	1.79515000	-1.35070400
C	2.26546000	2.51281300	-0.71371300	C	-3.77137100	-0.61272000	-2.01382500
O	1.40274100	2.51305300	0.22175100	H	-3.80162200	-2.68672900	-2.52003100
O	2.13904300	1.67219100	-1.67097800	C	-2.60932300	2.75950000	-0.84587700
C	3.44690100	3.43870900	-0.68334300	H	-0.61677000	3.13010100	-0.03051200
H	4.29877700	2.88780400	-0.26726300	H	-4.47522900	2.04294300	-1.63153000
H	3.71250100	3.75418300	-1.69481800	H	-4.79878900	-0.43075900	-2.31195400
H	3.24819100	4.30570600	-0.05129900	H	-2.93457200	3.78577000	-0.72037200
H	1.82875100	0.75759800	2.54019300	N	-0.85124500	1.16811600	-0.59465700
H	2.60959400	-1.58396800	3.05720400	Co	0.80528700	0.48649100	-0.00219600
H	1.24063600	-2.26608400	2.18577700	C	0.21560600	0.00213000	1.80097900
C	-0.19854700	0.08315100	2.41703300	C	1.17106800	-1.16435200	2.05752400
C	-0.70814800	1.40568800	2.60388700	C	2.24856100	2.37253800	-0.62455100
C	-1.15357200	-0.96008200	2.23050600	O	1.61115200	2.20046700	0.48503700
C	-2.06916400	1.66392900	2.58621400	O	2.11160600	1.51866600	-1.54460100
H	-0.00111000	2.21788100	2.74733000	C	3.15627600	3.55882700	-0.76533900
C	-2.51338800	-0.68692300	2.21637600	H	4.08989000	3.34763700	-0.23116400
H	-0.81677400	-1.97637600	2.06111400	H	3.38521400	3.74567700	-1.81574800
C	-2.98709100	0.62098100	2.38946000	H	2.70103300	4.44207300	-0.31036900
H	-2.42545600	2.68179800	2.71914700	H	0.54349200	0.90243400	2.32802300
H	-3.21742900	-1.49662100	2.04745100	H	1.51775700	-1.14331300	3.09708000

H	0.66964000	-2.12150300	1.90441600	C	0.50864400	-0.20941700	2.09200100
C	-1.24165900	-0.20455000	1.97785200	C	1.32553600	-1.47453600	2.02300100
C	-2.04453600	0.89899500	2.32562800	C	2.40576300	2.42430200	-0.80790500
C	-1.88635200	-1.42830500	1.72477000	O	2.04329800	2.22236900	0.41185300
C	-3.43190900	0.79713500	2.38259200	O	1.77596300	1.85634900	-1.74513400
H	-1.56413000	1.85267900	2.52855300	C	3.60567600	3.28835300	-1.07676000
C	-3.27557400	-1.53477000	1.78758400	H	4.50521400	2.69583900	-0.87255300
H	-1.30600500	-2.30055800	1.44569900	H	3.62695700	3.61350400	-2.11805400
C	-4.05699100	-0.42251500	2.10661600	H	3.61385600	4.15159200	-0.40676500
H	-4.02639300	1.66948600	2.63965700	H	1.05384000	0.66668600	2.44540100
H	-3.74907900	-2.48873400	1.57343400	H	1.67943800	-1.70800000	3.03743100
H	-5.13933600	-0.50484000	2.14395000	H	0.71504700	-2.32012900	1.70081300
				C	-0.91997200	-0.14933300	2.21719600
				C	-1.53089800	1.09484400	2.53219700
INT2_Ph_T				C	-1.76865100	-1.25949700	1.97057500
C	4.85327400	-0.69360200	0.77223900	C	-2.91089400	1.22673400	2.56579400
C	4.73985100	-0.96193700	-0.59417600	H	-0.89418900	1.95372100	2.72709300
C	3.52747000	-1.41917300	-1.10953700	C	-3.14955800	-1.11915700	2.01034500
C	2.41807800	-1.58100900	-0.27204800	H	-1.33922400	-2.22347500	1.72581000
C	2.52962900	-1.32746800	1.10941600	C	-3.73030500	0.12230500	2.29648700
C	3.75797100	-0.88808900	1.61511200	H	-3.35601100	2.19034300	2.79533000
H	5.79548700	-0.34225500	1.18256200	H	-3.78121600	-1.97731900	1.80177700
H	5.59117600	-0.81984400	-1.25316300	H	-4.81064400	0.22860600	2.311159200
H	3.42547100	-1.63441800	-2.16945400				
H	3.85239900	-0.69569900	2.68074100	INT1_C4H9_Q			
C	1.09872600	-1.98759200	-0.88115400	C	-4.66330500	-2.20030500	0.12020600
O	0.98382600	-3.09917300	-1.43674500	C	-4.08290000	-3.24957600	0.84863100
N	0.16193400	-1.02142800	-0.77618600	C	-2.75164600	-3.15883900	1.23972300
C	-1.16780300	-1.16674100	-1.15933200	C	-2.01329700	-2.01475600	0.89490000
C	-1.93764500	0.04495300	-1.11799800	C	-2.56431100	-0.94375800	0.15062100
C	-1.82784800	-2.34115200	-1.50977500	C	-3.91392200	-1.06696200	-0.21365700
C	-3.32577600	0.04840200	-1.43048400	H	-5.70435000	-2.27428600	-0.18627900
C	-3.21125900	-2.33382400	-1.79979900	H	-4.67274600	-4.12341000	1.10993100
H	-1.27298800	-3.26730900	-1.54974900	H	-2.28268100	-3.95260800	1.81495300
C	-1.95346300	2.33553900	-0.69245300	H	-4.39435800	-0.27315300	-0.78472700
C	-4.00513600	1.29069400	-1.36644700	C	-0.60061700	-1.89905000	1.31194600
C	-3.95787400	-1.17580600	-1.76767000	O	0.06639000	-2.81674000	1.80098800
H	-3.68957800	-3.27498600	-2.05585000	N	-0.09430200	-0.61545000	1.04870800
C	-3.32237700	2.43224700	-1.00862600	C	0.99524200	-0.08162200	1.61977900
H	-1.38776200	3.20939200	-0.38286100	C	1.33818600	1.23758000	1.11683300
H	-5.06566100	1.32542000	-1.59884200	C	1.80958000	-0.64051800	2.63525200
H	-5.01887800	-1.18028000	-1.99684400	C	2.47993700	1.92106600	1.60160600
H	-3.81754100	3.39503700	-0.95200300	C	2.92658700	0.05399500	3.10844300
N	-1.29250800	1.18844800	-0.74338900	H	1.56446400	-1.61736100	3.02703800
Co	0.65767300	0.80325300	-0.07097700				

C	0.82082800	2.95814300	-0.34082600	H	5.55545900	1.79965200	-0.92955800
C	2.76829800	3.18863500	1.04564500	H	5.35223200	2.91247400	1.27957000
C	3.27274800	1.30319300	2.60944000	H	3.26397200	2.61118200	2.63014900
H	3.53827400	-0.40046600	3.88094800	H	3.70691200	0.41863500	-1.82130300
C	1.93867100	3.70406900	0.06905900	C	1.08335400	1.09776300	1.90859300
H	0.14874300	3.33294200	-1.10602100	O	0.84428800	1.57660900	3.03502900
H	3.63817800	3.73860900	1.39145200	N	0.27095800	0.25777600	1.20692600
H	4.14823500	1.82540700	2.98211800	C	-0.89124700	-0.33593300	1.67677300
H	2.13082800	4.67049800	-0.38290500	C	-1.44157800	-1.30705800	0.78086000
N	0.52675200	1.76500700	0.17122500	C	-1.55668000	-0.10432600	2.87730200
Co	-1.16450900	0.48450900	-0.38359400	C	-2.62663600	-2.02489700	1.09643200
C	0.76480700	-0.60463000	-2.13045500	C	-2.73499600	-0.82204100	3.18712800
C	-0.43155700	-1.20812900	-2.24304000	H	-1.16663700	0.62742300	3.56947000
C	-2.55269300	2.58537600	-0.95316000	C	-1.23641100	-2.37516500	-1.28063200
O	-1.92581800	1.81111300	-1.77034300	C	-3.09102800	-2.95852700	0.13562200
O	-2.50971200	2.38059100	0.28731400	C	-3.27093700	-1.76282100	2.33268500
C	-3.33814100	3.73570800	-1.53332700	H	-3.22736200	-0.61573400	4.13318900
H	-4.13207800	3.34289500	-2.17735800	C	-2.39915200	-3.13514000	-1.04272200
H	-3.77828000	4.34904100	-0.74566300	H	-0.67034200	-2.48320100	-2.20003800
H	-2.68327900	4.34984900	-2.15955500	H	-3.99446300	-3.52534500	0.34117500
H	0.92839200	0.34040000	-2.64977700	H	-4.17639800	-2.30508500	2.58569300
H	-0.62497800	-2.16712300	-1.77023400	H	-2.73321600	-3.84173700	-1.79403500
H	-1.22045600	-0.79904700	-2.86793100	N	-0.78035100	-1.49579500	-0.40160200
C	1.94482200	-1.17408600	-1.40165000	Co	0.88175300	-0.34877500	-0.47882500
C	3.04658600	-1.64392100	-2.36751500	C	-0.72882100	0.97492400	-1.71277500
H	1.62679300	-2.00974200	-0.76772000	C	0.49205800	1.57442300	-1.65858600
H	2.37346500	-0.41066900	-0.74067200	C	2.18361700	-2.15682100	-1.16490200
C	4.28143500	-2.16952300	-1.63054900	O	1.68915200	-1.33017300	-2.00467400
H	2.64286400	-2.42866600	-3.02071700	O	1.91673300	-1.91790200	0.06555400
H	3.33721300	-0.81153800	-3.02292400	C	3.04454300	-3.30026800	-1.57787700
C	5.38027000	-2.65113800	-2.57862200	H	4.07094400	-2.93353100	-1.69630700
H	4.67545500	-1.37702900	-0.97980500	H	3.03658300	-4.08044500	-0.81474800
H	3.98119200	-2.99110200	-0.96627100	H	2.70810300	-3.69618200	-2.53854800
H	6.25181900	-3.02031200	-2.02680400	H	-0.91056200	0.23930800	-2.49411700
H	5.02134800	-3.46624400	-3.21815200	H	0.66464900	2.41017200	-0.98850800
H	5.72001900	-1.84095300	-3.23479200	H	1.23927500	1.39243600	-2.42268700
				C	-1.92134500	1.43150400	-0.92899500
				C	-2.78343100	2.38649600	-1.77849300
				H	-1.59792200	1.94282800	-0.01698900
				H	-2.53713400	0.57642400	-0.63584300
				C	-4.04370200	2.83868200	-1.03571700
				H	-2.18303000	3.26152700	-2.05880000
				H	-3.06802900	1.88770000	-2.71462700
				C	-4.90622700	3.79298800	-1.86250000
INT1_C4H9_S							
C	4.64758500	1.67606100	-0.34423800				
C	4.53562800	2.30408500	0.90184100				
C	3.37404300	2.14169800	1.65617400				
C	2.33506100	1.35363200	1.15154800				
C	2.43418600	0.72787400	-0.10271900				
C	3.60132900	0.89204600	-0.84860500				

H	-4.63284900	1.95498400	-0.75640700	H	3.39982900	4.47034600	-0.42258300
H	-3.75174700	3.32470100	-0.09525000	H	2.16768900	4.71774400	0.85463300
H	-5.80061600	4.10220000	-1.31054100	H	-0.95568800	1.03090400	2.71991400
H	-4.34936900	4.69897300	-2.12934000	H	0.15434900	-1.74180300	1.98043600
H	-5.23668900	3.32037200	-2.79505300	H	1.01555300	-0.38615800	2.90213000
				C	-2.26480600	-0.39013300	1.65497700
INT1_C4H9_T.sp				C	-3.38410900	-0.58234100	2.69264100
C	4.73891800	-1.09654700	1.40724500	H	-2.12169000	-1.31697400	1.08666700
C	4.70515300	-2.35900800	0.80266100	H	-2.58766600	0.38014400	0.94406700
C	3.63110400	-2.71446400	-0.01230200	C	-4.72835100	-0.93206700	2.04904500
C	2.60055100	-1.79318700	-0.21618200	H	-3.09275900	-1.37327400	3.39640800
C	2.63426700	-0.52797100	0.38498900	H	-3.49106900	0.33672100	3.28528100
C	3.70446000	-0.17338600	1.20214500	C	-5.84625600	-1.12284400	3.07493600
H	5.57710900	-0.82689900	2.04436500	H	-5.00543100	-0.13729000	1.34306600
H	5.51593300	-3.06131400	0.97169900	H	-4.61500800	-1.84682800	1.45165400
H	3.57870800	-3.69010400	-0.48796400	H	-6.79711400	-1.37184300	2.59094900
H	3.74257400	0.79773900	1.68637000	H	-5.60672900	-1.93242000	3.77461900
C	1.40372700	-2.08025800	-1.04302900	H	-6.00118100	-0.21148100	3.66475700
O	1.18950500	-3.15923100	-1.61422200				
N	0.57907000	-0.98041400	-1.06192500	TS_C4H9_S			
C	-0.68003200	-0.91192500	-1.66160300	C	4.64150600	1.32057400	0.01780200
C	-1.32773000	0.35182100	-1.50120400	C	4.57262500	1.59172100	1.38900900
C	-1.35624200	-1.90986100	-2.35269900	C	3.35086300	1.49344100	2.05426700
C	-2.62817600	0.59149900	-2.01762000	C	2.19997900	1.13802200	1.34727700
C	-2.65063600	-1.66579600	-2.87197800	C	2.25522800	0.89612500	-0.04268900
H	-0.89162400	-2.87549000	-2.48801800	C	3.48917500	0.98552400	-0.69616300
C	-1.20705400	2.49102700	-0.57357300	H	5.59439900	1.38194600	-0.50030700
C	-3.19561000	1.86588200	-1.77200800	H	5.46991800	1.86617400	1.93542400
C	-3.28603800	-0.45313600	-2.71776200	H	3.27832000	1.66232600	3.12475400
H	-3.14978000	-2.47072600	-3.40316800	H	3.55051500	0.80873700	-1.76619400
C	-2.49063000	2.80999500	-1.05429400	C	0.92241600	0.85194400	2.05736800
H	-0.62669200	3.20101400	0.00631400	O	0.70529200	1.18834000	3.23872700
H	-4.19067200	2.08395500	-2.14861500	N	0.10075100	0.12542200	1.26154400
H	-4.28145100	-0.28189200	-3.11464300	C	-1.07950600	-0.49088100	1.64891900
H	-2.90678900	3.78937100	-0.84792700	C	-1.58515600	-1.38590400	0.65783700
N	-0.64884300	1.30835400	-0.79457400	C	-1.79571400	-0.34767100	2.83201400
Co	1.09131100	0.55551100	-0.07263800	C	-2.78612300	-2.11612000	0.85122400
C	-0.97155800	0.02982400	2.28650300	C	-2.99047200	-1.08052800	3.02594100
C	0.12638500	-0.73216000	2.38396000	H	-1.43553500	0.32325600	3.59882600
C	2.30609200	2.71098800	0.13376100	C	-1.26534600	-2.29050700	-1.46846400
O	1.54758500	2.14599500	1.01264500	C	-3.19984900	-2.96829300	-0.20393400
O	2.50616200	2.12186700	-0.96164200	C	-3.48787100	-1.94543700	2.07288900
C	2.92737800	4.03746800	0.45990800	H	-3.52793500	-0.94825600	3.96047800
H	3.68176900	3.89260500	1.24095300	C	-2.44366500	-3.05506900	-1.35277000

H	-0.64983700	-2.32701400	-2.36047200	O	0.50452000	1.81523900	2.96510800
H	-4.11426800	-3.54389300	-0.09461400	N	0.10836400	0.19707000	1.32497500
H	-4.40646700	-2.49898600	2.23906500	C	-1.13009600	-0.27776800	1.73025600
H	-2.73777700	-3.69692600	-2.17540900	C	-1.67730400	-1.24430900	0.82512300
N	-0.85350200	-1.49090000	-0.49520300	C	-1.86336900	0.06244000	2.85851500
Co	0.69976000	-0.31132400	-0.48177500	C	-2.93685200	-1.84987700	1.08049900
C	-0.37202600	1.09255700	-1.40337500	C	-3.11377500	-0.54724600	3.11367600
C	0.86470300	1.76814600	-1.18923000	H	-1.47034800	0.79390200	3.55305700
C	2.14156100	-1.95786900	-1.44560100	C	-1.42393100	-2.41801800	-1.16530100
O	1.49455000	-1.06671400	-2.10993100	C	-3.41435500	-2.78721200	0.13667600
O	1.99313900	-1.96512400	-0.18501300	C	-3.65086400	-1.48329300	2.25464000
C	3.05498800	-2.90937000	-2.15069600	H	-3.65881000	-0.26238900	4.01245300
H	3.99111700	-2.38581100	-2.37774900	C	-2.65651700	-3.07595100	-0.97839900
H	3.27659200	-3.77040000	-1.51813200	H	-0.80892500	-2.60815000	-2.04296400
H	2.60994000	-3.23202300	-3.09514900	H	-4.36699600	-3.27466600	0.30334900
H	-0.50116800	0.63348300	-2.38389600	H	-4.61034900	-1.94709900	2.45499800
H	1.54244800	1.86115500	-2.02976100	H	-2.98876900	-3.78697100	-1.72143700
H	0.85125100	2.62490300	-0.52233000	N	-0.94327400	-1.53684200	-0.29583800
C	-1.64768200	1.60504600	-0.78131100	Co	0.76006200	-0.46932000	-0.41737400
C	-2.27044000	2.72797000	-1.62795600	C	-0.21365300	0.83782500	-1.58940500
H	-1.44882100	1.98075100	0.22736800	C	1.06917800	1.39716100	-1.46053400
H	-2.37749600	0.79354900	-0.68646900	C	2.08182700	-2.23868800	-1.34264000
C	-3.58298300	3.24992600	-1.03712000	O	1.41009900	-1.50837600	-2.13270300
H	-1.55253800	3.55480100	-1.71773700	O	2.01489100	-1.95423400	-0.09828300
H	-2.44884700	2.35964300	-2.64773100	C	2.96217000	-3.35382800	-1.83302200
C	-4.20826000	4.36962700	-1.87025500	H	3.96202000	-2.94619600	-2.01667100
H	-4.29308900	2.41665700	-0.94700800	H	3.04343200	-4.13857200	-1.07842200
H	-3.39979000	3.60899900	-0.01532600	H	2.57671700	-3.76094400	-2.77172200
H	-5.14493700	4.72435800	-1.42613400	H	-0.39438700	0.18399500	-2.43897300
H	-3.53123500	5.22850000	-1.94979500	H	1.77660400	1.22810700	-2.26173000
H	-4.43059600	4.02829300	-2.88832400	H	1.12539100	2.38049300	-1.00208200
				C	-1.43280500	1.53941800	-1.03846400
TS_C4H9_T				C	-2.02008100	2.54656200	-2.04712400
C	4.68313000	1.21930800	0.13789700	H	-1.17270900	2.07048300	-0.11799700
C	4.51751600	1.76670400	1.41845700	H	-2.21031700	0.81110700	-0.78813100
C	3.24178300	1.80046500	1.98703100	C	-3.29026300	3.21899000	-1.51386600
C	2.14308400	1.29324500	1.28437600	H	-1.26547600	3.31369600	-2.28141000
C	2.30192100	0.76100300	-0.01149300	H	-2.24409600	2.03154400	-2.99078100
C	3.58160700	0.73503500	-0.57819900	C	-3.91090500	4.21982600	-2.49131400
H	5.67121500	1.17927000	-0.30904700	H	-4.02787300	2.43602000	-1.27057100
H	5.37323800	2.15000100	1.96274200	H	-3.05896600	3.72080800	-0.56478900
H	3.08790400	2.18950800	2.98548100	H	-4.81494200	4.67067600	-2.07356600
H	3.72658300	0.35247400	-1.58245500	H	-3.21034300	5.03026900	-2.72163300
C	0.82378900	1.15829400	1.95375800	H	-4.18059500	3.73112900	-3.43240700

## INT2\_C4H9\_Q

C	-4.74226300	0.97994500	-0.84521700
C	-4.69490100	-0.34185100	-1.29454300
C	-3.48210400	-0.88056000	-1.72037100
C	-2.30735100	-0.12030400	-1.66945400
C	-2.35084200	1.22157600	-1.24025600
C	-3.58086900	1.75310000	-0.83324400
H	-5.68346100	1.41255600	-0.51822200
H	-5.59703900	-0.94593300	-1.31861200
H	-3.43250200	-1.90451300	-2.08012600
H	-3.62468000	2.78999200	-0.50940300
C	-1.01858300	-0.76640900	-2.11294600
O	-0.89975700	-1.13372500	-3.29898000
N	-0.10883100	-0.89938000	-1.11892600
C	1.20466900	-1.32841000	-1.32067000
C	1.98690100	-1.48989400	-0.12355700
C	1.83868700	-1.57277400	-2.53629900
C	3.35655300	-1.87592500	-0.18407800
C	3.19859600	-1.95628100	-2.58766000
H	1.27624800	-1.46766000	-3.45218100
C	2.05740100	-1.37326200	2.20982200
C	4.05503300	-2.00191900	1.04242400
C	3.95557600	-2.11021400	-1.44798100
H	3.64735700	-2.13230400	-3.56114600
C	3.41223200	-1.75228400	2.23556100
H	1.51261600	-1.16468900	3.12574000
H	5.10057300	-2.29592500	1.02472100
H	4.99872200	-2.40647800	-1.49450800
H	3.92561500	-1.84032800	3.18626700
N	1.37714700	-1.25291900	1.07768400
Co	-0.57437800	-0.57917900	0.82116900
C	-0.42578900	2.02043600	0.15742200
C	-1.09912400	2.07943800	-1.18265600
C	-2.20573700	-0.79028700	2.66762900
O	-1.15123400	-0.10220400	2.86017400
O	-2.37009500	-1.36812300	1.53871400
C	-3.26294200	-0.89008100	3.72988800
H	-3.93359100	-0.02832700	3.63129500
H	-3.85202600	-1.80070200	3.60690900
H	-2.81181000	-0.85712200	4.72381200
H	-1.05200800	2.22106600	1.02752100
H	-1.38469200	3.11937800	-1.41105000
H	-0.39069700	1.77788200	-1.96141100

C	1.05254800	2.18623600	0.29715300
C	1.52617700	3.65156100	0.14758200
H	1.56438200	1.57994800	-0.46259400
H	1.37931500	1.81686300	1.27783100
C	3.04290700	3.78918400	0.30645300
H	1.22228000	4.03194600	-0.83637700
H	1.01770400	4.27375000	0.89604500
C	3.52919100	5.23257000	0.16847600
H	3.33856200	3.39285000	1.28741700
H	3.54098800	3.15856700	-0.44249200
H	4.61644400	5.30138600	0.28591800
H	3.27369600	5.64411100	-0.81517400
H	3.07091000	5.87847500	0.92682500

## INT2\_C4H9\_S

C	4.42624500	1.37090300	0.12325400
C	4.52535300	0.49182900	1.20918500
C	3.39097900	0.16989600	1.94578700
C	2.14371500	0.71077100	1.59964700
C	2.03806300	1.63908900	0.53172400
C	3.20130100	1.94685900	-0.19723100
H	5.30926200	1.61876800	-0.45797100
H	5.48408700	0.05412800	1.47019300
H	3.44848500	-0.52514000	2.77799100
H	3.13204000	2.66006400	-1.01396400
C	0.91846500	0.15812300	2.28551800
O	0.80029900	0.08557400	3.52152800
N	0.06989300	-0.30859700	1.34920600
C	-1.11416700	-1.00548900	1.52796100
C	-1.61143100	-1.52527800	0.29693500
C	-1.83986300	-1.23960300	2.68732200
C	-2.82494600	-2.25224800	0.22433600
C	-3.04944100	-1.97281900	2.61839300
H	-1.47953100	-0.86226700	3.63490700
C	-1.24733700	-1.71029000	-2.00658200
C	-3.22635800	-2.70875200	-1.05664200
C	-3.54381200	-2.47009300	1.42943800
H	-3.60040700	-2.14370400	3.53847700
C	-2.44187100	-2.44095600	-2.15892300
H	-0.60838100	-1.47239000	-2.84889100
H	-4.15230300	-3.26695500	-1.15726700
H	-4.47303900	-3.02965400	1.39827900
H	-2.72634100	-2.77845100	-3.14890500
N	-0.85247700	-1.27358100	-0.81755200

Co 0.67752500 -0.24925400 -0.43434700  
 C -0.13823300 1.47618400 -0.75309800  
 C 0.71494000 2.32443500 0.19709400  
 C 2.31119500 -1.39778600 -1.87072700  
 O 1.55347100 -0.39646600 -2.17247000  
 O 2.20468900 -1.92242600 -0.72798100  
 C 3.31848500 -1.87102200 -2.87779200  
 H 4.18872500 -1.20562800 -2.83558000  
 H 3.64259500 -2.88786000 -2.65008500  
 H 2.90326900 -1.81876100 -3.88719600  
 H 0.15200400 1.64444100 -1.79749500  
 H 0.93584800 3.30320400 -0.24334400  
 H 0.16122300 2.50017700 1.12481100  
 C -1.63542300 1.64390700 -0.57375400  
 C -2.11572900 3.07826500 -0.85269000  
 H -1.92064900 1.37219400 0.44978100  
 H -2.17107000 0.96296800 -1.24549200  
 C -3.63146600 3.23198200 -0.69564600  
 H -1.61159200 3.77701400 -0.17231400  
 H -1.82155400 3.36990600 -1.87080400  
 C -4.11753200 4.65934800 -0.95149400  
 H -4.13756900 2.54097100 -1.38356900  
 H -3.92030200 2.92170700 0.31792400  
 H -5.20376100 4.74109900 -0.83285400  
 H -3.65258700 5.36591400 -0.25357000  
 H -3.86799900 4.98636500 -1.96798800

INT2\_C4H9\_T

C -4.90211600 0.94224200 -0.55230200  
 C -4.88283100 -0.34215700 -1.10175900  
 C -3.68600000 -0.86562500 -1.58645800  
 C -2.49790800 -0.12857100 -1.49867700  
 C -2.51497800 1.17664900 -0.96734200  
 C -3.72858200 1.69516200 -0.50064100  
 H -5.83114500 1.36245000 -0.17815900  
 H -5.79487800 -0.92892600 -1.15679300  
 H -3.65693600 -1.85725700 -2.02811000  
 H -3.75004600 2.70591600 -0.10156000  
 C -1.23544500 -0.76597500 -2.01590700  
 O -1.24289100 -1.28642500 -3.14921700  
 N -0.19550400 -0.75539000 -1.14357800  
 C 1.08436300 -1.21671500 -1.46368600  
 C 1.99116400 -1.30936900 -0.35349500  
 C 1.57512400 -1.55393000 -2.72210100

C 3.33664900 -1.73984200 -0.52920800  
 C 2.91482200 -1.97430700 -2.89082100  
 H 0.91987200 -1.50034000 -3.57822300  
 C 2.29905800 -1.03932800 1.94153400  
 C 4.15511900 -1.80367700 0.62657000  
 C 3.78853400 -2.07458100 -1.83092000  
 H 3.25153400 -2.22600500 -3.89243100  
 C 3.64116500 -1.45904000 1.85770400  
 H 1.85685200 -0.75391500 2.89193200  
 H 5.18710600 -2.12707400 0.52476000  
 H 4.81369200 -2.40289800 -1.97047400  
 H 4.24607100 -1.50095300 2.75643400  
 N 1.51399100 -0.96705100 0.87757500  
 Co -0.46695500 -0.33132400 0.77663200  
 C -0.42585500 1.73463900 0.33722000  
 C -1.25246200 2.00806900 -0.89916900  
 C -1.49746700 -1.42610300 2.80427900  
 O -1.33839300 -0.16668300 2.54514100  
 O -1.11621100 -2.28792000 1.97309300  
 C -2.12972300 -1.80078800 4.11610200  
 H -3.08610800 -1.28070000 4.22621100  
 H -2.28173500 -2.87893000 4.18096500  
 H -1.48050000 -1.47210300 4.93470000  
 H -0.95165500 1.98785000 1.26359200  
 H -1.53357700 3.07074500 -0.89037600  
 H -0.63829000 1.84766900 -1.79049600  
 C 1.02161700 2.15018000 0.31356100  
 C 1.18345500 3.68390100 0.22675000  
 H 1.52722600 1.68924800 -0.54350200  
 H 1.52731800 1.79950000 1.21993500  
 C 2.65352500 4.11041600 0.27183200  
 H 0.72441100 4.04958700 -0.69998100  
 H 0.63782600 4.15386000 1.05589200  
 C 2.83199900 5.62670900 0.18223200  
 H 3.10818400 3.73918300 1.20007400  
 H 3.19400000 3.62547000 -0.55213500  
 H 3.89066800 5.90677800 0.21642700  
 H 2.41317200 6.01990000 -0.75163300  
 H 2.32590500 6.13424900 1.01198800

INT1\_CH2OH\_Q

C -4.80639600 -1.73155600 0.27888600  
 C -4.38301500 -2.58973000 1.30543700  
 C -3.08315100 -2.49276500 1.78896200

C -2.21637900 -1.53597600 1.23513700  
 C -2.60857000 -0.66474400 0.19073000  
 C -3.93230700 -0.78159300 -0.25945700  
 H -5.82319800 -1.81151100 -0.09909200  
 H -5.07022800 -3.32000100 1.72277600  
 H -2.73553700 -3.13678100 2.59225200  
 H -4.29046300 -0.13497100 -1.05978500  
 C -0.83558700 -1.41315000 1.74661300  
 O -0.30830700 -2.19635900 2.54282000  
 N -0.17731500 -0.30519900 1.18596100  
 C 0.91766200 0.28499300 1.69293500  
 C 1.43507700 1.36798500 0.87495000  
 C 1.58171000 -0.00860700 2.90811200  
 C 2.59510300 2.07929700 1.26715400  
 C 2.71935600 0.71225900 3.28444500  
 H 1.20463100 -0.80481200 3.53419200  
 C 1.21066400 2.62641400 -1.05494300  
 C 3.05332800 3.10577100 0.40936000  
 C 3.23203200 1.73033100 2.49119100  
 H 3.21246500 0.46365800 4.21850400  
 C 2.36195900 3.37426100 -0.75588800  
 H 0.63803700 2.81585100 -1.95736100  
 H 3.94187600 3.66905200 0.67748400  
 H 4.12038100 2.27517400 2.79459900  
 H 2.68584400 4.15192300 -1.43813000  
 N 0.76010000 1.65646300 -0.26262800  
 Co -1.04503300 0.47472100 -0.54721800  
 C 0.69297100 -1.13853800 -1.90793300  
 C -0.54586900 -1.65523900 -1.95075500  
 C -2.20576800 2.50098100 -1.59634500  
 O -1.68289900 1.51134600 -2.23161100  
 O -2.15634000 2.54809900 -0.33795000  
 C -2.86686500 3.59346300 -2.39827800  
 H -3.64858400 3.16115700 -3.03093800  
 H -3.29844700 4.35443300 -1.74648000  
 H -2.12698400 4.05448200 -3.06108200  
 H 0.98150100 -0.35260600 -2.60477000  
 H -0.83783000 -2.46925400 -1.29363900  
 H -1.27914000 -1.32112800 -2.67877100  
 C 1.77444300 -1.64563300 -0.99894900  
 H 1.35271400 -2.33428300 -0.25292000  
 H 2.24278200 -0.81086300 -0.46248200  
 O 2.74944900 -2.30060900 -1.82008800  
 H 3.55263000 -2.40311200 -1.28977900

INT1\_CH2OH\_S

C -4.61904500 -1.67243600 -0.34722300  
 C -4.50931100 -2.29500500 0.90176800  
 C -3.34545800 -2.13751200 1.65325300  
 C -2.30024900 -1.36164600 1.14226400  
 C -2.39771000 -0.74335400 -0.11525800  
 C -3.56748200 -0.90042700 -0.85830700  
 H -5.52899400 -1.79140300 -0.93016400  
 H -5.33006800 -2.89452600 1.28454100  
 H -3.23780500 -2.60062900 2.63044600  
 H -3.67055900 -0.43193700 -1.83342200  
 C -1.05102400 -1.10264800 1.90155000  
 O -0.82025900 -1.56643600 3.03525200  
 N -0.23160700 -0.27217100 1.19530100  
 C 0.91335800 0.34535900 1.67921700  
 C 1.45976900 1.32015100 0.78524200  
 C 1.56353500 0.13466900 2.89181700  
 C 2.62650600 2.06174600 1.11304200  
 C 2.72280800 0.87724600 3.21488400  
 H 1.17586900 -0.59825500 3.58416100  
 C 1.26346100 2.37253900 -1.28581200  
 C 3.08738700 2.99776000 0.15279400  
 C 3.25538400 1.82076600 2.36138700  
 H 3.20286100 0.68810400 4.17073600  
 C 2.40965800 3.15383500 -1.03657800  
 H 0.70791800 2.46607300 -2.21314300  
 H 3.97654400 3.58329500 0.36762600  
 H 4.14642200 2.38169600 2.62456500  
 H 2.74154700 3.86164200 -1.78774500  
 N 0.81038300 1.49182100 -0.40665900  
 Co -0.84098100 0.33573600 -0.49141400  
 C 0.67683400 -0.98448600 -1.71205600  
 C -0.53510000 -1.60031100 -1.71486300  
 C -2.15347100 2.14012300 -1.15728700  
 O -1.65800100 1.32218400 -2.00495400  
 O -1.87978700 1.89015000 0.06996300  
 C -3.02146200 3.28208900 -1.55671300  
 H -4.04567500 2.90983000 -1.67712500  
 H -3.01688600 4.05416300 -0.78547600  
 H -2.68898700 3.68953300 -2.51395300  
 H 0.90447100 -0.24378000 -2.47467000  
 H -0.72144000 -2.45119900 -1.06837500  
 H -1.27399900 -1.38794700 -2.47901200



C	1.84013900	-1.49317200	-0.90289800	H	-3.47229200	4.29023500	-1.60002400
H	1.47959900	-2.07100000	-0.04251200	H	-2.60210200	3.66530100	-3.03890000
H	2.45498600	-0.66584800	-0.53553900	H	1.19262900	-0.45639800	-2.45646500
O	2.60478900	-2.31446600	-1.79477500	H	-0.79540500	-2.57756700	-1.43101600
H	3.47363600	-2.44682500	-1.38864600	H	-1.07661600	-1.33993000	-2.77999000
INT1_CH2OH_T				C	1.78106100	-1.80741700	-0.81862800
C	-4.63067500	-1.63195100	-0.15758900	H	1.29584000	-2.58577700	-0.21137900
C	-4.37995600	-2.46374100	0.94015600	H	2.09086100	-1.00043800	-0.14227400
C	-3.20325100	-2.31716800	1.67441000	O	2.92660400	-2.32433000	-1.51026400
C	-2.28851100	-1.33058800	1.29850200	H	3.62688600	-2.45338900	-0.85483200
C	-2.53789600	-0.49652100	0.19994500	TS_CH2OH_S			
C	-3.71054400	-0.64452500	-0.53590400	C	4.63625300	1.33210000	0.02095600
H	-5.54783400	-1.75450800	-0.72765800	C	4.55996200	1.61669400	1.38899800
H	-5.10247700	-3.22575900	1.21674100	C	3.33658700	1.51712000	2.05118900
H	-2.98340500	-2.95504300	2.52625400	C	2.19122900	1.14600900	1.34299800
H	-3.91398600	-0.01968500	-1.40031100	C	2.25500100	0.88947700	-0.04300300
C	-0.99969800	-1.10594800	1.99752900	C	3.48906100	0.98062200	-0.69429400
O	-0.60294300	-1.76943200	2.96592100	H	5.59075000	1.39475300	-0.49398900
N	-0.32333900	-0.06742900	1.40138300	H	5.45333200	1.90296200	1.93572200
C	0.93378100	0.41071300	1.77414400	H	3.25846600	1.69709000	3.11942400
C	1.43974600	1.43067300	0.91058900	H	3.55603300	0.79257800	-1.76195800
C	1.72144700	0.01022200	2.84625900	C	0.91219200	0.85927000	2.04892200
C	2.70914600	2.02694200	1.12852900	O	0.68819500	1.20042400	3.22686100
C	2.98616800	0.60864900	3.06292200	N	0.09339400	0.12691100	1.25297800
H	1.36631100	-0.76377800	3.51063500	C	-1.07850600	-0.50427900	1.64570000
C	1.06532100	2.71715100	-1.00098900	C	-1.58598700	-1.39449700	0.65141300
C	3.12291300	3.01933000	0.20620000	C	-1.78237000	-0.38205200	2.83859900
C	3.48297300	1.59309400	2.23675100	C	-2.77630600	-2.14037500	0.85086600
H	3.57454300	0.27047700	3.91067700	C	-2.96643500	-1.13047300	3.03851400
C	2.30671200	3.36252000	-0.85165600	H	-1.42081100	0.28378500	3.60898000
H	0.40050300	2.95226600	-1.82556100	C	-1.27987100	-2.27494500	-1.48773100
H	4.08712300	3.50021900	0.34236100	C	-3.19222600	-2.98648200	-0.20827700
H	4.45488900	2.04218100	2.41386800	C	-3.46566100	-1.99053800	2.08216700
H	2.60291500	4.11601700	-1.57230900	H	-3.49402200	-1.01430200	3.98077200
N	0.64874200	1.78939500	-0.14888300	C	-2.44848700	-3.05328200	-1.36644400
Co	-1.07053900	0.72219200	-0.15156000	H	-0.67408900	-2.29720700	-2.38677400
C	0.82264900	-1.27566200	-1.84030100	H	-4.09842700	-3.57409700	-0.09437500
C	-0.41074100	-1.75451200	-2.02843400	H	-4.37591900	-2.55620400	2.25318600
C	-2.43309800	2.44167000	-1.29056700	H	-2.74478400	-3.69028700	-2.19203400
O	-1.74461600	1.50028700	-1.84098500	N	-0.86597400	-1.48147200	-0.51034100
O	-2.45641300	2.50970600	-0.03153900	Co	0.69002800	-0.30196600	-0.49291700
C	-3.19453100	3.39681900	-2.16098100	C	-0.37516600	1.10510400	-1.41079600
H	-4.10639100	2.89852700	-2.50954800	C	0.85796700	1.78336400	-1.21655300

C	2.11643300	-1.95291800	-1.43863600	H	-2.92335100	-3.67000900	-2.12641700
O	1.48820300	-1.06120600	-2.11857900	N	-0.93521700	-1.53262200	-0.47016500
O	1.95069000	-1.93578900	-0.17846900	Co	0.71988000	-0.36826700	-0.49434500
C	3.02102600	-2.93075600	-2.11532900	C	-0.28416500	1.16573600	-1.50149600
H	3.96532200	-2.42504700	-2.34844200	C	0.94095700	1.83548600	-1.28499400
H	3.22608500	-3.78008900	-1.46180600	C	2.17479400	-2.01244200	-1.72991800
H	2.57652700	-3.26817200	-3.05486900	O	1.46440700	-1.26072300	-2.45916300
H	-0.53850500	0.65027500	-2.38716700	O	2.12807200	-1.87714200	-0.45573500
H	1.53999400	1.85528400	-2.05535300	C	3.10449800	-3.03155200	-2.32746600
H	0.86380500	2.63716600	-0.54671300	H	4.10883500	-2.59508100	-2.38061900
C	-1.62780600	1.62460500	-0.75760400	H	3.15722800	-3.92081200	-1.69504100
H	-1.40725100	2.01369800	0.24368000	H	2.78706800	-3.29969600	-3.33678400
H	-2.37879600	0.83118900	-0.66244500	H	-0.42365100	0.64072200	-2.44454400
O	-2.12725900	2.67116300	-1.60649500	H	1.65144000	1.86181700	-2.10232200
H	-2.98091100	2.95227100	-1.24598700	H	0.92683000	2.71137000	-0.64457400
TS_CH2OH_T				C	-1.54245500	1.63486200	-0.81888800
C	4.63058600	1.39575900	0.14938800	H	-1.31279200	2.01160200	0.18551300
C	4.49857700	1.71204300	1.50496700	H	-2.26768500	0.81873000	-0.72726700
C	3.25069300	1.62140500	2.12145200	O	-2.07621900	2.68021500	-1.64495900
C	2.12853800	1.22521800	1.38759100	H	-2.94902200	2.90777600	-1.29178500
C	2.25765800	0.96275900	0.00808000	INT2_CH2OH_Q			
C	3.50959600	1.03568600	-0.60378300	C	4.65684700	-0.81363100	-0.13482100
H	5.60373000	1.44524700	-0.33054600	C	4.21150900	-1.14585200	-1.41632400
H	5.36920700	2.00913000	2.08163000	C	2.89018400	-1.54740600	-1.60272400
H	3.13396100	1.81550200	3.18381800	C	1.99818200	-1.58836600	-0.52419000
H	3.61210300	0.83093700	-1.66532000	C	2.44842100	-1.28813100	0.77605500
C	0.84452300	0.91388400	2.08838300	C	3.78283700	-0.90075200	0.94911300
O	0.56528300	1.37317600	3.21277600	H	5.68610700	-0.50471400	0.02355900
N	0.11924600	0.03452200	1.35270100	H	4.89002000	-1.09657200	-2.26279200
C	-1.07107000	-0.57137600	1.72522300	H	2.53159600	-1.81205300	-2.59344900
C	-1.61675900	-1.43434300	0.71540500	H	4.13926100	-0.67581900	1.95124400
C	-1.76564100	-0.44941700	2.92370200	C	0.57004600	-1.98355300	-0.79948400
C	-2.82731300	-2.14707700	0.93047800	O	0.33347500	-3.11597000	-1.26564600
C	-2.96810700	-1.16459700	3.13334000	N	-0.32967700	-1.00642900	-0.53020600
H	-1.37589700	0.19737700	3.69718200	C	-1.71181000	-1.18839200	-0.61710400
C	-1.40120000	-2.30334500	-1.44403700	C	-2.49714600	0.00906200	-0.47980800
C	-3.29545000	-2.96888700	-0.12466400	C	-2.40049600	-2.38759400	-0.78287300
C	-3.49868100	-1.99766500	2.17236000	C	-3.92040500	-0.03290400	-0.51208100
H	-3.48020400	-1.04601100	4.08377900	C	-3.81355300	-2.42144200	-0.81386900
C	-2.58590700	-3.04995300	-1.30373100	H	-1.84087200	-3.30428200	-0.89493100
H	-0.81784000	-2.33140500	-2.35805200	C	-2.51033000	2.32754100	-0.17832300
H	-4.21704700	-3.52788200	0.00902000	C	-4.61419400	1.19409900	-0.36772700
H	-4.42107200	-2.54318100	2.34437300	C	-4.57269200	-1.28005900	-0.68507500

H	-4.30268300	-3.38228200	-0.94620000	C	3.01969000	-1.99869800	-2.60985000
C	-3.91616700	2.37066900	-0.20070000	H	1.43310100	-0.90174700	-3.61256500
H	-1.92050600	3.23022000	-0.05021400	C	1.28027700	-1.71041100	2.03701900
H	-5.70023100	1.19064400	-0.39135900	C	3.24313700	-2.71829900	1.06424300
H	-5.65722700	-1.31276900	-0.71428000	C	3.53090500	-2.48890300	-1.42530300
H	-4.42460800	3.32140100	-0.08760900	H	3.55845300	-2.17273300	-3.53652400
N	-1.83413000	1.19411100	-0.31575800	C	2.47299000	-2.44582800	2.17556800
Co	0.21718800	0.92569400	-0.23496600	H	0.65319000	-1.46780800	2.88653900
C	0.82997400	-0.06708500	2.25557200	H	4.16807400	-3.27994500	1.15455100
C	1.52207600	-1.36501100	1.97573700	H	4.46061900	-3.04798500	-1.40287800
C	1.84360200	2.72623600	-0.72551200	H	2.76738700	-2.78328800	3.16256900
O	0.98271500	2.91397800	0.19497900	N	0.87297400	-1.27597600	0.85072800
O	1.80293500	1.63883400	-1.39754200	Co	-0.67482200	-0.27967200	0.48529800
C	2.92285200	3.73605500	-0.99078800	C	0.09153300	1.46457600	0.79452900
H	3.80514800	3.45691100	-0.40256000	C	-0.69479300	2.31712100	-0.20795200
H	3.20400900	3.73089000	-2.04589200	C	-2.24759900	-1.47743300	1.89795500
H	2.60464000	4.73385500	-0.68343800	O	-1.52295100	-0.45932100	2.22441600
H	1.43498300	0.83726400	2.29385300	O	-2.12326100	-1.95628400	0.73460100
H	2.11839900	-1.65957900	2.85364100	C	-3.21992700	-2.03033000	2.89573700
H	0.77497000	-2.15375300	1.83693000	H	-4.05295000	-1.32656200	3.00268800
C	-0.54329200	-0.05751100	2.83342100	H	-3.60561700	-2.99549600	2.56456000
H	-1.22782700	-0.61366100	2.17602800	H	-2.73829900	-2.12764300	3.87253600
H	-0.91994600	0.97086600	2.92354200	H	-0.23720400	1.65974900	1.82232000
O	-0.50948000	-0.70005300	4.12707200	H	-0.88222800	3.31625300	0.20010100
H	-1.42267700	-0.92583200	4.35768900	H	-0.10233800	2.44398000	-1.11942900
				C	1.58852200	1.62580600	0.68160600
INT2_CH2OH_S				H	1.93136200	1.33875300	-0.32145000
C	-4.44400300	1.53764100	-0.22390600	H	2.10562100	0.99293600	1.41470200
C	-4.55263600	0.62879500	-1.28357300	O	1.90063000	3.01010700	0.92260800
C	-3.41200300	0.23052500	-1.97222200	H	2.84292900	3.13139200	0.73762600
C	-2.15281800	0.72667100	-1.60505600				
C	-2.03504900	1.68234000	-0.56520700	INT2_CH2OH_T			
C	-3.20228500	2.06472000	0.11846500	C	-4.48202000	2.12040000	-0.83573700
H	-5.33122600	1.84676300	0.32053900	C	-4.61807600	0.99464500	-1.65184700
H	-5.52289000	0.22919000	-1.56252900	C	-3.48213400	0.29894400	-2.05943300
H	-3.47644900	-0.48522300	-2.78614000	C	-2.20895900	0.69846100	-1.63210400
H	-3.12462300	2.80090300	0.91389500	C	-2.06350200	1.84505800	-0.82579200
C	-0.93541000	0.12540600	-2.25696400	C	-3.21310600	2.54399000	-0.43969300
O	-0.81308100	0.02089900	-3.49056400	H	-5.36049200	2.67554000	-0.51988600
N	-0.09089100	-0.33498600	-1.31102900	H	-5.60162800	0.66604900	-1.97405000
C	1.09521800	-1.02866600	-1.49996900	H	-3.56951200	-0.56802400	-2.70728900
C	1.61372800	-1.53649400	-0.27366200	H	-3.10538100	3.43654700	0.17101300
C	1.80712100	-1.26972100	-2.66710900	C	-1.02859600	-0.10293600	-2.11073700
C	2.82753600	-2.26458800	-0.21270000	O	-0.95242700	-0.39521400	-3.31990000

N	-0.15572200	-0.48717200	-1.14233600	H	5.50556200	-2.61464300	-0.43152700
C	1.04808400	-1.14717800	-1.40938300	H	3.22907200	-3.61326700	-0.20066000
C	1.73216700	-1.65292800	-0.25320900	H	3.78884700	1.32730200	-0.35808600
C	1.66023300	-1.33013000	-2.64629600	C	0.89616100	-2.27403800	0.01493800
C	2.98106100	-2.32674400	-0.36363300	O	0.67382000	-3.48138400	0.15533900
C	2.90417100	-1.99512600	-2.74945700	N	-0.10110800	-1.28327500	0.00057300
H	1.17325800	-0.96732500	-3.53858000	C	-1.41630300	-1.50808100	-0.15823800
C	1.71345600	-1.91105500	2.06414800	C	-2.22794000	-0.30315200	-0.11996500
C	3.57557100	-2.79429900	0.83533100	C	-2.07407300	-2.74513200	-0.37020000
C	3.56220000	-2.49185200	-1.64618100	C	-3.63608900	-0.37470700	-0.25208700
H	3.34161300	-2.11440500	-3.73647600	C	-3.46497200	-2.79528000	-0.50419200
C	2.94595100	-2.59233500	2.04447200	H	-1.48572500	-3.65023100	-0.41244700
H	1.18569000	-1.72642100	2.99558700	C	-2.28116000	2.00348100	0.08255700
H	4.52911900	-3.31188500	0.78384700	C	-4.36189700	0.83756000	-0.19536300
H	4.51391000	-3.00571000	-1.73746200	C	-4.24413300	-1.64779900	-0.44174500
H	3.37884900	-2.94226400	2.97480500	H	-3.94239000	-3.75760800	-0.65730100
N	1.13904900	-1.46094500	0.95876700	C	-3.68183300	2.02755500	-0.02459100
Co	-0.66442600	-0.43066900	0.76952500	H	-1.71364900	2.91947700	0.21160400
C	-0.18909000	1.58513800	0.84310600	H	-5.44330000	0.81730400	-0.28985400
C	-0.69721500	2.31637300	-0.38044500	H	-5.32326500	-1.70428600	-0.54363900
C	-2.22410500	-1.67475700	2.24939900	H	-4.20544300	2.97549500	0.02238000
O	-1.80387600	-0.45865900	2.39238900	N	-1.57791800	0.87418100	0.03476400
O	-1.81054300	-2.35082500	1.27041800	Co	0.57195200	0.70110700	0.21211600
C	-3.18199700	-2.22673100	3.26447000	C	0.91421000	2.95153800	-0.97429000
H	-4.05928800	-1.57570600	3.33019900	O	0.99960000	2.74299600	0.29184300
H	-3.48853100	-3.23922300	2.99910500	O	0.62401200	2.01023300	-1.76075300
H	-2.70126800	-2.23197300	4.24826700	C	1.17566300	4.34665000	-1.48538600
H	-0.79888000	1.76867700	1.73343800	H	2.20598100	4.63174200	-1.24768400
H	-0.75280200	3.38535200	-0.13423700	H	1.02060000	4.40685800	-2.56366300
H	0.02923900	2.21284500	-1.19229500	H	0.51425900	5.05407800	-0.97523200
C	1.29485900	1.68340500	1.10118000	C	0.76597100	2.43549000	3.51488100
H	1.85451400	1.29933300	0.23751200	C	1.87102300	1.36108200	3.31288800
H	1.57447700	1.09465400	1.98398300	C	1.12245600	0.16544300	2.77447500
O	1.59393100	3.07283700	1.31066100	C	-0.21135100	0.34201700	2.81765200
H	2.55182000	3.14473100	1.43365300	C	-0.58976700	1.68624000	3.38936800
				H	0.84183000	3.19419500	2.73363400
				H	2.36098200	1.09152900	4.25865700
				H	2.66547300	1.69425100	2.63526200
				H	1.61701100	-0.75824000	2.49639200
				H	-0.94531800	-0.41693900	2.56849700
				H	-1.07415000	1.54409400	4.36545700
				H	-1.31227200	2.22156500	2.76272300
				H	0.86292800	2.94372000	4.47762300
INT1_cyclopentene_Q							
C	4.76938500	-0.58091300	-0.40502000				
C	4.62955400	-1.97658200	-0.35861300				
C	3.36349900	-2.53534200	-0.22630300				
C	2.24584000	-1.68858700	-0.13313100				
C	2.35355800	-0.27780100	-0.16581600				
C	3.64603400	0.24778900	-0.32124100				
H	5.76131500	-0.14577600	-0.50510900				

INT1_cyclopentene_S				H	2.15444000	0.55348600	4.31437200
C	4.62578700	-0.01982200	0.02473800	H	2.85645500	1.13094400	2.80682300
C	4.63892900	-1.38119200	-0.29916500	H	1.32717200	-1.05339200	2.42825600
C	3.43663900	-2.08338000	-0.38436800	H	-1.12680000	-0.26742500	2.43177700
C	2.23469700	-1.41398700	-0.13650100	H	-0.90454400	1.57506800	4.26583600
C	2.21202500	-0.05098800	0.20743200	H	-1.06935700	2.42243300	2.73460300
C	3.41804000	0.64624600	0.27554000	H	1.18986500	2.76275200	4.38277700
H	5.56252700	0.52909700	0.08290200	INT1_cyclopentene_T			
H	5.58166600	-1.88622400	-0.48840900	C	4.60316400	-0.08198000	0.01654900
H	3.41696700	-3.13819400	-0.64563400	C	4.62977300	-1.46989300	-0.16483500
H	3.43190400	1.70439100	0.52224800	C	3.43647400	-2.18260300	-0.28222500
C	0.91055500	-2.08065000	-0.24079600	C	2.22413900	-1.49202700	-0.21274400
O	0.76046800	-3.28214300	-0.53843100	C	2.19514100	-0.10277300	-0.02565900
N	-0.08903700	-1.18829300	0.01351200	C	3.38600400	0.61064500	0.08399600
C	-1.44893200	-1.41453300	-0.14599900	H	5.53664500	0.46731000	0.10671000
C	-2.24590300	-0.23040000	-0.03445900	H	5.58154400	-1.99038500	-0.21435700
C	-2.09989900	-2.61786300	-0.40553900	H	3.43191800	-3.26014800	-0.42311900
C	-3.65702300	-0.26487500	-0.19690100	H	3.38152100	1.68703800	0.22711000
C	-3.50500200	-2.64745800	-0.55914300	C	0.90071200	-2.15615700	-0.30568900
H	-1.52317500	-3.52686200	-0.49516000	O	0.73855800	-3.37691000	-0.45263200
C	-2.25157100	2.07434500	0.31178600	N	-0.09667900	-1.21750900	-0.19298200
C	-4.35005700	0.96795000	-0.08673400	C	-1.46815500	-1.46996100	-0.21637900
C	-4.28051800	-1.51068800	-0.46272700	C	-2.27071400	-0.29027800	-0.12590000
H	-3.97872500	-3.60362100	-0.76233000	C	-2.11665200	-2.69545200	-0.31447600
C	-3.65217300	2.12982100	0.15804800	C	-3.68853300	-0.35096600	-0.14187100
H	-1.67086000	2.96998900	0.50554100	C	-3.53096200	-2.75316600	-0.32931000
H	-5.42988100	0.98114300	-0.20281300	H	-1.53579400	-3.60368700	-0.38280900
H	-5.35783500	-1.54966600	-0.58873800	C	-2.28418100	2.03613700	0.06905300
H	-4.15651300	3.08610400	0.23943000	C	-4.38851500	0.87776700	-0.04632300
N	-1.58039800	0.93638700	0.22869300	C	-4.31285000	-1.62110500	-0.24764200
Co	0.41022300	0.60149500	0.36889100	H	-4.00336800	-3.72777200	-0.40844400
C	0.87115700	2.43048600	-1.01072200	C	-3.69177000	2.06360900	0.05578400
O	0.90491400	2.53435200	0.26069900	H	-1.69928100	2.94621900	0.15079400
O	0.57723900	1.26731800	-1.46083800	H	-5.47451800	0.87064900	-0.05506300
C	1.18394500	3.57237800	-1.91563300	H	-5.39638200	-1.68078600	-0.26111300
H	2.27367300	3.66631000	-1.98962500	H	-4.20435200	3.01591200	0.12869700
H	0.77607900	3.39637000	-2.91224700	N	-1.60418400	0.90108300	-0.01494400
H	0.78883500	4.50040300	-1.49586600	Co	0.39907400	0.59819600	0.04819000
C	1.03096500	2.23412400	3.43995500	C	0.95311900	2.66959300	-1.21449700
C	1.90920200	0.96431900	3.32445800	O	0.85030600	2.51267900	0.06320600
C	1.01532800	-0.03860300	2.63805900	O	0.78011400	1.67630300	-1.96697900
C	-0.28218600	0.38077400	2.62893600	C	1.28813700	4.03487700	-1.74130500
C	-0.42714600	1.73187300	3.28826000	H	2.30479000	4.29547600	-1.42775900
H	1.27038100	2.92181000	2.62669400				

H	1.22670900	4.05577000	-2.82990700	H	3.58550700	-3.67667000	-0.48700900
H	0.60838400	4.77592400	-1.31100800	N	1.53324700	-1.04081100	-0.19711500
C	1.10808900	2.17374300	3.38994400	Co	-0.29134600	-0.36383700	-0.02023300
C	1.89238600	0.83633700	3.38314800	C	-1.13132200	-1.74003100	-1.78972300
C	0.91032200	-0.14231300	2.78863700	O	-1.13365400	-2.07604900	-0.55121300
C	-0.33292500	0.36846600	2.72831900	O	-0.64189500	-0.60607700	-2.08560800
C	-0.38700300	1.77912100	3.26489700	C	-1.72250400	-2.64928600	-2.82083600
H	1.39951300	2.76830500	2.52006000	H	-2.81472700	-2.57595200	-2.76348000
H	2.15554900	0.51151400	4.40016400	H	-1.39966000	-2.35905000	-3.82189300
H	2.82937800	0.89306400	2.81971500	H	-1.44284900	-3.68569000	-2.61517600
H	1.17512100	-1.16209800	2.53163300	C	-2.02034100	-2.03329200	2.43000800
H	-1.21891600	-0.18888200	2.44481100	C	-2.44216900	-0.56589600	2.61634400
H	-0.89470200	1.78257500	4.24002200	C	-1.33493400	0.23359600	1.95594700
H	-0.95266000	2.45853300	2.61761100	C	-0.14844100	-0.57359300	1.93794500
H	1.30905900	2.77192000	4.28240700	C	-0.47682700	-1.97288700	2.44073500
TS_cyclopentene_S				H	-2.37712400	-2.40433200	1.46644100
C	-4.22360000	1.09427500	-0.78938400	H	-2.37999400	-0.29409300	3.68044600
C	-3.88155600	2.41175400	-1.11435500	H	-3.45183500	-0.33092100	2.27910400
C	-2.58997200	2.87805500	-0.86422700	H	-1.24995600	1.28981300	2.18013500
C	-1.65236000	2.02892200	-0.27544200	H	0.80161600	-0.12608900	2.21514500
C	-1.99953400	0.70938500	0.09457100	H	-0.09745600	-2.06883400	3.46762600
C	-3.29099400	0.24942700	-0.18206100	H	-0.01027200	-2.76934500	1.85277500
H	-5.22227900	0.72493000	-1.00523000	H	-2.42246500	-2.68277700	3.21206400
H	-4.61632500	3.06589300	-1.57415200	TS_cyclopentene_T			
H	-2.29122600	3.88427100	-1.14344800	C	-4.28538600	0.87643200	-0.71870000
H	-3.57546100	-0.76650700	0.07199700	C	-4.06035100	2.24653100	-0.88459200
C	-0.22157600	2.43012300	-0.14147300	C	-2.81533400	2.79105000	-0.56700600
O	0.17178900	3.60968000	-0.24045700	C	-1.79791900	1.96708800	-0.07867700
N	0.55386200	1.33139800	0.03363200	C	-2.04634200	0.59915100	0.13582400
C	1.94072500	1.29301300	0.02285100	C	-3.28303000	0.05121000	-0.19585200
C	2.45718900	-0.03291400	-0.10310400	H	-5.24626800	0.44590800	-0.98681500
C	2.84421400	2.34632600	0.11060100	H	-4.84808600	2.88301800	-1.27636400
C	3.85219100	-0.29028100	-0.13749300	H	-2.60547100	3.84531200	-0.72513700
C	4.23472900	2.08732900	0.07952500	H	-3.47658100	-1.00695900	-0.04992000
H	2.47882600	3.35967500	0.19922700	C	-0.40056600	2.47217200	0.08515500
C	1.93767300	-2.29553500	-0.32995000	O	-0.12966700	3.68548700	0.19054400
C	4.25565400	-1.64274200	-0.27683600	N	0.46471700	1.42972300	0.03878200
C	4.74301900	0.81012300	-0.04021500	C	1.84801000	1.49282500	0.05273700
H	4.91626500	2.92987600	0.15238700	C	2.48568100	0.21169400	-0.08070200
C	3.30518000	-2.63524000	-0.37687100	C	2.66115600	2.61685400	0.16300800
H	1.16302400	-3.05064400	-0.40086300	C	3.90232300	0.09446300	-0.10855700
H	5.31472500	-1.88144200	-0.30561700	C	4.06959400	2.49181500	0.13975200
H	5.81298300	0.63026100	-0.06621600	H	2.20448200	3.59172200	0.26100100

C	2.21638700	-2.09685300	-0.32551200	O	0.08016500	-2.86757300	0.51762900
C	4.44597100	-1.20568000	-0.25858200	N	-0.62624100	-0.86489500	-0.44351000
C	4.69108700	1.26893800	0.00661900	C	-2.00322200	-1.11190800	-0.43477000
H	4.66941000	3.39319000	0.22640200	C	-2.83393100	0.03829500	-0.67035700
C	3.60943300	-2.29503500	-0.37218400	C	-2.64055300	-2.33318500	-0.23713500
H	1.52347800	-2.92729700	-0.40714600	C	-4.25366100	-0.07178000	-0.69837800
H	5.52490400	-1.32802400	-0.28494800	C	-4.05084000	-2.43470400	-0.26762800
H	5.77287300	1.18438600	-0.01616200	H	-2.04402900	-3.21450600	-0.05421300
H	3.99973800	-3.29929800	-0.49186000	C	-2.94468400	2.33792600	-1.07663100
N	1.67931300	-0.89296400	-0.18512300	C	-4.99847800	1.11094600	-0.93065900
Co	-0.28443500	-0.41178200	-0.04224000	C	-4.85427500	-1.33941900	-0.49114400
C	-0.97998800	-1.80303700	-1.99452700	H	-4.50103100	-3.41031500	-0.10853800
O	-0.91519300	-2.39150400	-0.87517900	C	-4.35047200	2.31222000	-1.11905300
O	-0.69950700	-0.55670500	-2.05974500	H	-2.39643600	3.26385500	-1.22199700
C	-1.42321100	-2.53311000	-3.23192600	H	-6.08291800	1.05393500	-0.95646100
H	-2.51572700	-2.46671500	-3.29836900	H	-5.93629200	-1.42307900	-0.51079300
H	-0.99767900	-2.07490600	-4.12702200	H	-4.89669900	3.23120400	-1.29835200
H	-1.14745600	-3.58821400	-3.17529400	N	-2.21986900	1.24736200	-0.86103300
C	-1.94609400	-2.43527100	2.24069700	Co	-0.16064600	1.06277000	-0.77479200
C	-2.46320400	-1.03642300	2.62157500	C	1.68987200	2.65028900	-0.97972900
C	-1.37565800	-0.10676400	2.13132400	O	1.14489200	2.45162300	0.15701200
C	-0.17735300	-0.82389200	2.03765300	O	1.21208400	2.05905700	-2.00911700
C	-0.41084500	-2.29415400	2.32600300	C	2.90787900	3.51777900	-1.10259800
H	-2.23199500	-2.66274200	1.21001600	H	3.78961000	2.87782300	-0.98130100
H	-2.46766100	-0.91431700	3.71497700	H	2.95427100	3.98115500	-2.09003500
H	-3.46829300	-0.80791400	2.26360000	H	2.92344000	4.27753100	-0.31902800
H	-1.36561200	0.93655800	2.42267100	C	2.41624900	0.98959900	3.94458700
H	0.77966900	-0.35115100	2.23479100	C	2.53495100	-0.53133700	3.73008100
H	-0.04857900	-2.49681200	3.34432600	C	1.65273300	-0.83591500	2.49622900
H	0.12728300	-2.96973900	1.65465300	C	0.58338900	0.22633500	2.60172600
H	-2.34210100	-3.22345300	2.88533800	C	0.95090300	1.30644500	3.56943200
INT2_cyclopentene_Q				H	3.09060800	1.52360600	3.26663800
C	4.25959000	-0.11303800	-0.26010500	H	2.10302700	-1.05304400	4.59169100
C	3.59969200	-0.56257600	-1.40282200	H	3.56603800	-0.88002300	3.62620100
C	2.31704400	-1.09764900	-1.28020100	H	1.21660100	-1.83943400	2.56705400
C	1.69986900	-1.19419100	-0.02801600	H	-0.34848600	0.19315300	2.04930400
C	2.36533400	-0.75841600	1.13829500	H	0.30447400	1.26990400	4.46356100
C	3.64523500	-0.21106700	0.99138300	H	0.82900900	2.31605800	3.15265000
H	5.25667500	0.31150600	-0.33566900	H	2.66901800	1.29105800	4.96548400
H	4.07193200	-0.49389400	-2.37813300	INT2_cyclopentene_S			
H	1.78067100	-1.43700600	-2.16215600	C	4.30948600	-0.11873500	-0.19904700
H	4.18233600	0.14669300	1.86205600	C	3.98627400	-0.98414800	-1.24906800
C	0.29234400	-1.73626700	0.03832300	C	2.79478600	-1.69888900	-1.20604700





C	1.43380700	-0.73243700	2.29886000
C	0.20682600	0.18264400	2.12943300
C	0.37684700	1.42612900	2.99899200
H	2.49851700	1.83800200	2.78515900
H	1.58092500	-0.57328800	4.44148300
H	3.15504500	-0.41806500	3.66609900
H	1.08920400	-1.75802900	2.46759400
H	-0.75937600	-0.31149900	2.20296400
H	-0.33165700	1.35000200	3.83551300
H	0.14099700	2.36332700	2.48150000
H	1.95940700	1.85366400	4.46923300

INT1\_allene\_Q

C	4.73888100	-1.49307800	-0.59120800
C	4.20870900	-2.70554300	-1.06113700
C	2.84297900	-2.81483300	-1.29044800
C	2.01023500	-1.71002200	-1.03779600
C	2.50948700	-0.47693000	-0.54449300
C	3.90048400	-0.40232100	-0.34942100
H	5.80877500	-1.40983100	-0.41406700
H	4.86533600	-3.54977200	-1.25071700
H	2.41326400	-3.73841200	-1.66776300
H	4.34064400	0.52384500	0.01931600
C	0.55729500	-1.83769400	-1.30426300
O	0.02056500	-2.87872500	-1.69715900
N	-0.13280500	-0.64470500	-1.03584500
C	-1.43326700	-0.42119600	-1.26746500
C	-1.91442100	0.85424000	-0.75722500
C	-2.36022100	-1.26455000	-1.93235800
C	-3.27693400	1.21541900	-0.89254100
C	-3.69487600	-0.87712700	-2.07730600
H	-2.01725800	-2.21419900	-2.31519200
C	-1.42563600	2.80832400	0.38461000
C	-3.68904300	2.44277700	-0.32651100
C	-4.16124600	0.32699200	-1.56759800
H	-4.38189400	-1.54289900	-2.58921600
C	-2.76161900	3.23690000	0.32065100
H	-0.66686900	3.41011900	0.87544000
H	-4.72921600	2.74409500	-0.40374500
H	-5.20479100	0.60628500	-1.67338900
H	-3.04339400	4.18127500	0.77210800
N	-1.01552700	1.65589200	-0.14094800
Co	1.01262800	0.85283100	-0.11837700
C	-0.08285900	-0.13221400	2.67094300

C	2.06556900	3.15308900	-0.21039000
O	1.94063800	2.49749700	0.88327900
O	1.61071400	2.67527600	-1.29263600
C	2.78918200	4.47534300	-0.19631500
H	3.86752600	4.28466400	-0.14806300
H	2.57433800	5.04890000	-1.09967600
H	2.51278300	5.04968200	0.69168300
H	-0.43794200	0.86882400	2.91499300
C	-1.08874200	-1.07089800	2.14417600
C	-2.42392200	-0.65259900	2.03715600
C	-0.74693000	-2.36326200	1.71091500
C	-3.39506400	-1.50495100	1.51246000
H	-2.69352300	0.35073100	2.35577000
C	-1.71555100	-3.20957400	1.18009900
H	0.28643000	-2.69089100	1.77737700
C	-3.04464900	-2.78494300	1.07891500
H	-4.42192900	-1.16242100	1.42684000
H	-1.43170400	-4.19835500	0.83220900
H	-3.79766500	-3.44395200	0.65738000
C	1.19299300	-0.40790000	2.85234700
C	2.44809100	-0.70178800	3.05415400
H	2.78944600	-1.09908300	4.00975400
H	3.19612800	-0.56570600	2.27509800

INT1\_allene\_S

C	4.77947700	-1.05761700	-0.24640400
C	4.44099200	-2.22076100	-0.94724500
C	3.11042200	-2.45791700	-1.29163900
C	2.13195100	-1.53312900	-0.91570100
C	2.45421400	-0.38505400	-0.17339600
C	3.79195100	-0.14043300	0.13937200
H	5.81922400	-0.86320200	0.00461800
H	5.21431000	-2.92757900	-1.23347800
H	2.82284600	-3.33982100	-1.85793300
H	4.07697300	0.74918400	0.69490400
C	0.70994100	-1.65714000	-1.32778600
O	0.25219100	-2.62336400	-1.96774900
N	0.01438700	-0.55379800	-0.93423300
C	-1.30655100	-0.26706700	-1.23785600
C	-1.77054100	0.96212200	-0.67093900
C	-2.20090300	-1.01656600	-1.99589400
C	-3.09961200	1.42167700	-0.87487300
C	-3.52354500	-0.55749900	-2.19146900
H	-1.88162100	-1.95587100	-2.42199400

C	-1.24835600	2.79161200	0.67462000	H	4.90410900	-3.35208400	-1.07127100
C	-3.46255000	2.64241800	-0.25352100	H	2.49707200	-3.65542400	-1.69932600
C	-3.97956400	0.62844400	-1.65471100	H	4.06897700	0.65497800	0.26145200
H	-4.19658500	-1.17077400	-2.78376600	C	0.51886900	-1.74565200	-1.43180700
C	-2.54257400	3.32478200	0.51359800	O	-0.03245500	-2.74956100	-1.90411900
H	-0.50272500	3.29443400	1.28218400	N	-0.09167200	-0.54725500	-1.14981700
H	-4.47068900	3.02476800	-0.38449600	C	-1.44842700	-0.26547300	-1.31622100
H	-4.99905300	0.96511400	-1.81340400	C	-1.85352700	0.97543600	-0.73772200
H	-2.79580900	4.25849200	1.00303000	C	-2.41002500	-1.03383200	-1.95844600
N	-0.88130500	1.65389400	0.10309100	C	-3.20329100	1.41203900	-0.78413500
Co	0.90515100	0.70069300	0.16700000	C	-3.75268800	-0.58941200	-2.01778400
C	-0.24707600	-0.22582000	2.14423900	H	-2.13337100	-1.97999000	-2.39910800
C	2.05746000	2.68373500	-0.20051400	C	-1.19621400	2.85025700	0.48716800
O	1.88260700	2.22442500	0.97859300	C	-3.50838600	2.63438200	-0.13805200
O	1.56529300	1.96696700	-1.14415400	C	-4.15820700	0.59668900	-1.44624700
C	2.80904100	3.93897400	-0.47545200	H	-4.47893200	-1.21825300	-2.52399500
H	3.87506300	3.69301700	-0.54750800	C	-2.51261600	3.34662500	0.49927900
H	2.48709400	4.37709600	-1.42186000	H	-0.38653200	3.38119000	0.97673300
H	2.67200700	4.64622500	0.34509800	H	-4.53200100	2.99714000	-0.14624200
H	-0.57488800	0.75858700	2.47117200	H	-5.19331900	0.91970300	-1.48929300
C	-1.30232500	-1.16949200	1.74812600	H	-2.72304000	4.28065700	1.00752400
C	-2.63678500	-0.73692100	1.77297900	N	-0.88064200	1.71171800	-0.11674500
C	-1.00837600	-2.47425800	1.32061500	Co	0.91328100	0.77748200	-0.25057200
C	-3.66208100	-1.59166900	1.37163900	C	-0.08840100	-0.27758300	2.58320400
H	-2.86134600	0.27588100	2.09471000	C	2.28776300	2.82017200	-0.14257000
C	-2.03145800	-3.31947200	0.90545900	O	1.88687700	2.10501900	0.85229900
H	0.02369600	-2.80884000	1.29387400	O	1.97946700	2.44938000	-1.30940800
C	-3.36050400	-2.88053100	0.92836000	C	3.12252000	4.03844900	0.11744300
H	-4.69080900	-1.24545700	1.38829700	H	4.15295000	3.71889100	0.31119200
H	-1.79484600	-4.32040400	0.55757900	H	3.11643800	4.70060300	-0.74955900
H	-4.15593700	-3.54167100	0.59752900	H	2.76138100	4.56473900	1.00407300
C	1.04846900	-0.52953100	2.28952100	H	-0.37049600	0.74323500	2.84083500
C	2.16613400	-0.96110300	2.81201900	C	-1.15773300	-1.13339700	2.04049400
H	2.14181200	-1.33841300	3.83461000	C	-2.47679200	-0.65462100	2.02780700
H	3.11642100	-0.96507600	2.29341500	C	-0.89427300	-2.40911100	1.51370400
				C	-3.51298800	-1.44059200	1.52335000
INT1_allene_T				H	-2.68400700	0.33968500	2.41422300
C	4.62270900	-1.32711000	-0.38525100	C	-1.92609900	-3.18479300	0.99421100
C	4.19276400	-2.54474900	-0.92513800	H	0.12667100	-2.77917100	1.50012500
C	2.85435500	-2.72024500	-1.27675800	C	-3.24148500	-2.70709100	1.00384400
C	1.95874600	-1.66694700	-1.08009100	H	-4.52835600	-1.05581700	1.52090900
C	2.38264000	-0.45065500	-0.52617900	H	-1.70415000	-4.16080000	0.57286400
C	3.72005700	-0.27361400	-0.17963100	H	-4.04469400	-3.31336100	0.59578300
H	5.66730800	-1.19615200	-0.11570600	C	1.15827400	-0.65284500	2.78523300

C	2.37933100	-1.05016100	3.01581300
H	2.66038700	-1.48205900	3.97609600
H	3.15883700	-0.96665800	2.26077300
TS_allene_S			
C	4.90829100	-0.51612700	0.36930400
C	3.72361100	0.10396200	0.77251800
C	2.50164100	-0.34799400	0.26617900
C	2.47823100	-1.41684600	-0.65160700
C	3.66342100	-2.04466800	-1.04072500
C	4.87902800	-1.59658100	-0.52301700
H	5.85906500	-0.16540000	0.76098900
H	3.75140700	0.91969100	1.48827600
H	3.62236400	-2.86495800	-1.75153200
H	5.80562400	-2.08053500	-0.81697600
C	1.15708500	-1.77652000	-1.23704900
O	0.97152900	-2.78093400	-1.95187100
N	0.23320000	-0.83522800	-0.91637300
C	-1.07073800	-0.76497100	-1.38040000
C	-1.72143600	0.45456000	-1.02283400
C	-1.79163400	-1.70988300	-2.10137200
C	-3.07496800	0.70597600	-1.36564600
C	-3.14054500	-1.45678500	-2.44250700
H	-1.32089600	-2.64072200	-2.38336000
C	-1.51430000	2.50850700	0.06203600
C	-3.62565200	1.94390700	-0.94845200
C	-3.78331800	-0.28818300	-2.08880200
H	-3.68153400	-2.21789300	-2.99729600
C	-2.84799400	2.84132800	-0.24896400
H	-0.88024500	3.17977800	0.63090200
H	-4.66074600	2.17149400	-1.18551100
H	-4.82016800	-0.11197500	-2.35658200
H	-3.24399100	3.79530300	0.08009000
N	-0.97727300	1.35682200	-0.31147100
Co	0.79250000	0.62321900	0.15259100
O	1.49409000	2.31572100	0.87837500
O	1.66939300	1.85779100	-1.23985900
C	1.16567900	-0.75288200	1.85034500
C	1.78239500	-1.79157800	2.38190200
H	2.66659100	-2.26578500	1.97733300
C	0.00612200	0.00314400	1.94978400
H	1.36941200	-2.18677700	3.31014000
C	-1.34608500	-0.58892300	1.90523800
C	-2.44000300	0.21583600	2.26492900

C	-1.58427600	-1.90518900	1.48021400
C	-3.74148300	-0.27059600	2.17047200
H	-2.26154300	1.23351700	2.59905800
C	-2.88675500	-2.38933000	1.38485400
H	-0.74863500	-2.53690600	1.19896200
C	-3.97075300	-1.57301900	1.71926900
H	-4.57665900	0.36902300	2.44055800
H	-3.05675500	-3.40436800	1.03802700
H	-4.98528400	-1.95056300	1.63280000
C	1.89326000	2.67336600	-0.28788500
C	2.61413100	3.96434800	-0.49474100
H	2.18723000	4.74165200	0.14342100
H	3.66282200	3.82410600	-0.20733200
H	2.57304300	4.26285400	-1.54351800
H	0.07209100	0.96062500	2.46507600

TS_allene_T			
C	4.87596300	-0.61754100	0.31690900
C	3.71101200	0.00625900	0.75660800
C	2.46383600	-0.44626400	0.29116900
C	2.39352200	-1.50863700	-0.64871700
C	3.56555400	-2.14536300	-1.05076900
C	4.80001900	-1.70742400	-0.56204300
H	5.84256500	-0.27833100	0.67734300
H	3.75416800	0.82205900	1.47125900
H	3.50492600	-2.96144200	-1.76462200
H	5.71098100	-2.20662900	-0.87845800
C	1.06604600	-1.85935100	-1.24767000
O	0.87198500	-2.93903600	-1.84218300
N	0.18855200	-0.84256100	-1.06795900
C	-1.14880900	-0.82557000	-1.42756500
C	-1.84129800	0.37929500	-1.05062300
C	-1.87761800	-1.82851600	-2.05761700
C	-3.23310000	0.52921400	-1.29766100
C	-3.26164000	-1.67033200	-2.29798900
H	-1.37520600	-2.74004300	-2.34951100
C	-1.72039400	2.48162500	-0.03974400
C	-3.84160800	1.74043000	-0.88497300
C	-3.93870500	-0.52803100	-1.92962700
H	-3.79776800	-2.48016700	-2.78418500
C	-3.08895000	2.71723800	-0.26946700
H	-1.09767500	3.21192500	0.46691800
H	-4.90436600	1.88352100	-1.05781600
H	-5.00163900	-0.41596200	-2.11871100

H	-3.53063300	3.65302000	0.05386400	C	1.81382600	3.01103900	-0.22585000
N	-1.12420200	1.35937700	-0.41445900	C	3.50781500	0.91968600	-1.05386200
Co	0.77077300	0.71409300	0.00575800	C	3.21586400	3.18540200	-0.28630200
O	1.42874000	2.66748800	0.81062600	H	1.18552600	3.82604600	0.10098100
O	1.76569200	2.06705300	-1.27638500	C	2.29736800	-1.49219900	-1.67153400
C	1.44203100	-0.75683500	1.72639200	C	4.29711000	-0.19082500	-1.44215400
C	1.97461100	-1.81174900	2.33793100	C	4.05919200	2.17440500	-0.68878500
H	2.82463200	-2.35822000	1.94810100	H	3.62719800	4.14931000	-0.00041000
C	0.26066400	0.02242100	1.96577900	C	3.69922800	-1.39513600	-1.74213600
H	1.55704900	-2.13493400	3.29083600	H	1.78502200	-2.42200600	-1.89906900
C	-1.08340600	-0.53217900	1.99962100	H	5.37668400	-0.07943700	-1.48588900
C	-2.14606300	0.28993900	2.43355400	H	5.13488400	2.31374600	-0.72792600
C	-1.37438300	-1.84250500	1.56593500	H	4.28182200	-2.26379000	-2.02675000
C	-3.45499000	-0.17497500	2.41324300	N	1.53210900	-0.46404900	-1.32998000
H	-1.92908900	1.30157800	2.76326100	Co	-0.51057900	-0.43394200	-1.08539700
C	-2.68661700	-2.30173100	1.54771100	C	-0.75754500	-0.91103700	2.07261000
H	-0.57073800	-2.48119700	1.21709900	C	-2.31596700	-2.03973400	-1.56522000
C	-3.73263300	-1.47036800	1.96101700	O	-1.36745400	-2.37295600	-0.77894700
H	-4.26295800	0.47305300	2.73909800	O	-2.25475100	-0.91630300	-2.17167600
H	-2.89803800	-3.30626800	1.19411700	C	-3.51642100	-2.92474800	-1.73626300
H	-4.75711500	-1.82869800	1.93088500	H	-4.28298600	-2.59383900	-1.02569400
C	1.87904500	2.93585600	-0.34679500	H	-3.92481000	-2.82901300	-2.74447200
C	2.57388300	4.24155500	-0.61684400	H	-3.26775100	-3.96512600	-1.51970900
H	2.19042100	5.02466800	0.04055900	H	-1.45708500	-1.68973100	1.78148600
H	3.64314700	4.11291400	-0.41074300	C	0.61845700	-1.30603800	2.08311200
H	2.46038800	4.53169400	-1.66339800	C	0.92191900	-2.68405600	1.90312700
H	0.38845600	1.01641400	2.39249900	C	1.70993500	-0.39823000	2.13223500
				C	2.23211500	-3.12528400	1.78474900
INT2_allene_Q				H	0.10147200	-3.39395200	1.84283200
C	-4.78549800	0.20399700	0.62699100	C	3.01819500	-0.84930300	2.01142400
C	-4.69654400	1.16353000	-0.38503200	H	1.52159400	0.66480000	2.20767100
C	-3.50737800	1.86818100	-0.56759700	C	3.29281200	-2.21085300	1.83801100
C	-2.39805800	1.60513100	0.24293400	H	2.43342100	-4.18323900	1.64172800
C	-2.49431800	0.66661500	1.29063000	H	3.83214600	-0.13062800	2.02917700
C	-3.69402500	-0.03529700	1.46300500	H	4.31755500	-2.55366400	1.73264600
H	-5.70887300	-0.34838900	0.77491200	C	-1.30295000	0.41395200	2.16594600
H	-5.54737700	1.35697800	-1.03140500	C	-0.80378900	1.42937200	2.92205500
H	-3.42109600	2.60542200	-1.36094400	H	0.03135600	1.28320700	3.59753500
H	-3.77347800	-0.76438200	2.26452200	H	-1.26265700	2.41239200	2.90507900
C	-1.08763900	2.29858000	-0.03668300				
O	-0.99073700	3.52740100	0.14862100	INT2_allene_S			
N	-0.12628200	1.45457500	-0.48345500	C	4.78307000	-0.52168900	0.60107600
C	1.22376400	1.79784000	-0.57135400	C	4.77430700	-0.82876300	-0.76529900
C	2.09683400	0.73882700	-1.00414200	C	3.60922800	-1.29119400	-1.36893700

C	2.43714300	-1.44288200	-0.61611200	H	-4.02287900	0.84892600	3.05904900
C	2.44708100	-1.17463000	0.77689700	H	-3.63227200	-2.82630100	0.85687500
C	3.63473100	-0.70473900	1.36576400	H	-5.07142400	-1.14694100	1.99979400
H	5.69154600	-0.15618600	1.06981500	C	1.23111300	-1.46080600	1.61912700
H	5.67509000	-0.69785400	-1.35712400	C	1.10418400	-2.64866200	2.22137400
H	3.58658100	-1.51967600	-2.43011300	H	0.23600100	-2.88925500	2.82722800
H	3.64798300	-0.50590800	2.43303700	H	1.87302100	-3.41047600	2.12428300
C	1.14989500	-1.77628000	-1.32883400				
O	1.02961600	-2.75415000	-2.08696300	INT2_allene_T			
N	0.23521000	-0.82253700	-1.06742500	C	-4.97872700	0.06406900	0.88593100
C	-1.07168300	-0.74103000	-1.52317300	C	-5.00602200	0.89062200	-0.24065400
C	-1.70954800	0.45660800	-1.08929300	C	-3.85884600	1.58740200	-0.61674900
C	-1.80566100	-1.64766400	-2.27469100	C	-2.67131000	1.44345100	0.11011200
C	-3.06815600	0.73197800	-1.37858100	C	-2.64802700	0.63256700	1.26214700
C	-3.16427100	-1.37568100	-2.56424800	C	-3.80831000	-0.05586200	1.63599800
H	-1.34264100	-2.56196600	-2.62028100	H	-5.87055500	-0.47782900	1.18675700
C	-1.46031200	2.44867500	0.11075900	H	-5.91777700	0.99209200	-0.82166500
C	-3.59934800	1.94822900	-0.88081500	H	-3.86923200	2.23623800	-1.48782000
C	-3.79519600	-0.22623700	-2.13223200	H	-3.79183500	-0.67984400	2.52513400
H	-3.72231200	-2.10446400	-3.14452100	C	-1.43891300	2.19115000	-0.33874700
C	-2.79684300	2.80254100	-0.15440500	O	-1.49220900	3.43427300	-0.41947100
H	-0.80813100	3.07687900	0.70522400	N	-0.37880300	1.39603000	-0.62551700
H	-4.63873300	2.19449800	-1.07602500	C	0.92219300	1.87657000	-0.79316500
H	-4.83818100	-0.03698800	-2.36434500	C	1.92979700	0.87149800	-1.01380400
H	-3.17760100	3.73885600	0.23674500	C	1.34845400	3.19975400	-0.70490400
N	-0.94477400	1.31370100	-0.34298400	C	3.30644000	1.22099100	-1.11527200
Co	0.76686900	0.61939900	0.02385100	C	2.71682300	3.53771500	-0.81339900
C	0.24413300	-0.33614300	1.67441000	H	0.61574600	3.97626600	-0.54505600
C	2.01799000	2.70510700	-0.18032700	C	2.42485100	-1.40013800	-1.24552300
O	1.48309700	2.21827600	0.88888500	C	4.23779000	0.16762400	-1.29194000
O	1.88060300	2.07037400	-1.26553100	C	3.68799800	2.58305700	-1.01392700
C	2.79739400	3.98238400	-0.08873600	H	2.99645000	4.58423500	-0.73142400
H	3.74237100	3.78178500	0.42860200	C	3.80367700	-1.13783800	-1.35341700
H	3.00952100	4.37850500	-1.08271800	H	2.03966400	-2.41383400	-1.28623600
H	2.24323800	4.71612800	0.50304300	H	5.29450300	0.40743700	-1.36840300
H	0.57074800	0.43949300	2.37590100	H	4.73781500	2.84770200	-1.09203400
C	-1.19893400	-0.63905400	1.83558400	H	4.49717100	-1.96168200	-1.47752100
C	-2.02508800	0.28912200	2.49404600	N	1.53065300	-0.43498900	-1.08942600
C	-1.80552900	-1.77083500	1.26110700	Co	-0.52200900	-0.60017400	-0.80739400
C	-3.40583900	0.11143200	2.55339100	C	-0.68503200	-0.74513200	1.88417400
H	-1.57262200	1.16947400	2.94309000	C	-1.53717300	-2.66624300	-1.73027900
C	-3.18607600	-1.95177300	1.32179800	O	-0.64758300	-2.78798000	-0.83232400
H	-1.19237700	-2.50069300	0.74610800	O	-1.89123300	-1.48847000	-2.09282600
C	-3.99478100	-1.00897000	1.96103300	C	-2.14145100	-3.86971500	-2.39552000

H	-2.08010400	-4.74387900	-1.74484700	C	4.16535000	-2.28665900	-0.70840100
H	-3.17868800	-3.67298700	-2.67521200	H	3.60744800	-3.77667400	-2.13938300
H	-1.57710600	-4.07902900	-3.31200200	C	4.09662600	0.60281800	1.66263000
H	-1.30257100	-1.59267800	1.59049500	H	2.32484300	1.80874100	2.04203300
C	0.71033300	-1.03680300	2.09056200	H	5.63526300	-0.74588400	1.00913100
C	1.12212500	-2.39433100	2.08319800	H	5.20803800	-2.58470500	-0.66146800
C	1.71701800	-0.04207000	2.17729900	H	4.72938300	1.18455200	2.32257400
C	2.46377600	-2.73847800	2.17818700	N	1.91297900	0.27929700	0.73383000
H	0.36618300	-3.16878200	1.99022500	Co	0.05659800	1.03831900	0.20494800
C	3.05777900	-0.39474100	2.26654700	O	-0.40100100	0.44072000	-3.02808100
H	1.44610500	1.00399600	2.11221900	O	0.82386800	1.53666100	-1.49520800
C	3.44169000	-1.74053900	2.27169400	C	0.34201500	1.37991500	-2.70197800
H	2.75387000	-3.78510600	2.16985900	O	-1.66949000	2.31191800	-0.43368800
H	3.81277800	0.38468200	2.30899300	O	-0.00512800	3.01178000	0.81639500
H	4.49216600	-2.00846300	2.33152800	C	-1.12006400	3.24791700	0.21720700
C	-1.38146400	0.49762300	2.05746000	O	-0.96283800	0.19642600	1.54111900
C	-0.98527300	1.53321100	2.84789400	O	0.09445200	0.96042700	3.37559800
H	-0.11116900	1.47117700	3.48542600	C	-0.70788900	0.19834200	2.83861700
H	-1.57510300	2.44263500	2.89937900	C	-1.48981600	-0.84865800	3.59280800
A_Q				H	-1.13610600	-1.83762300	3.28209100
C	-4.19412900	-0.85539400	-1.33177700	H	-1.35335700	-0.72882400	4.66838300
C	-5.02656400	-1.69169200	-0.58473300	H	-2.55044900	-0.78527100	3.33372400
C	-4.47169800	-2.60965500	0.31149000	C	-1.74096300	4.60785600	0.32586600
C	-3.09054300	-2.68564400	0.46089700	H	-0.98098500	5.37867200	0.17386500
C	-2.24930800	-1.84713100	-0.28649800	H	-2.55001300	4.72212900	-0.39667600
C	-2.80955100	-0.92907400	-1.18770300	H	-2.14125600	4.72809800	1.33877000
H	-4.62219000	-0.14197400	-2.02923100	C	0.76057400	2.44144100	-3.68557200
H	-6.10451000	-1.62943500	-0.70118300	H	0.27033300	3.38218500	-3.41031100
H	-5.11533800	-3.26267400	0.89290700	H	1.84051900	2.60370800	-3.62884200
H	-2.64607400	-3.38972900	1.15525800	H	0.47089400	2.16324300	-4.69970000
H	-2.18620300	-0.26851700	-1.77895500	A_S			
C	-0.78817300	-1.97226900	-0.04385900	C	4.24367400	-0.87645100	1.43513000
N	0.07077900	-1.13658100	-0.78020300	C	5.12702000	-1.31447600	0.44692300
H	-0.26873900	-0.78071200	-1.68917700	C	4.63596800	-1.91551700	-0.71677900
O	-0.32246200	-2.74793700	0.78703400	C	3.26615800	-2.07974700	-0.88656000
C	1.45912000	-1.51422100	-0.79636700	C	2.37265800	-1.63147000	0.10085300
C	2.36326100	-0.79886400	0.02498600	C	2.86839700	-1.02563600	1.26511900
C	1.91304800	-2.56508200	-1.56247500	H	4.62415800	-0.41348600	2.34024200
C	3.73004500	-1.19595700	0.08617600	H	6.19719200	-1.18824700	0.58189900
C	3.27456600	-2.94641600	-1.52545800	H	5.32146100	-2.25396900	-1.48746300
H	1.21055400	-3.10927200	-2.18564100	H	2.86923800	-2.54302300	-1.78300800
C	2.74173000	0.95547200	1.51866100	H	2.20036800	-0.67152100	2.04097500
C	4.58974500	-0.46098000	0.94007000	C	0.93291300	-1.84266200	-0.16256100

N	-0.00498400	-1.05471800	0.60525900	C	-5.05560600	-1.59729000	-0.64669600
H	0.28195500	-0.84307300	1.59674700	C	-4.51445300	-2.47205000	0.29974200
O	0.51476000	-2.62053500	-1.00348300	C	-3.13445300	-2.56722300	0.44744100
C	-1.36634700	-1.55153000	0.57667800	C	-2.28015400	-1.78895900	-0.34923500
C	-2.32239900	-0.68983200	0.00981000	C	-2.82698900	-0.91401900	-1.30015900
C	-1.74749200	-2.77825800	1.06768600	H	-4.62800200	-0.14333400	-2.18100700
C	-3.68796200	-1.07090900	-0.07318800	H	-6.13263900	-1.52174600	-0.76373200
C	-3.10596800	-3.17098300	0.99104800	H	-5.16773800	-3.07815300	0.91988600
H	-1.00856700	-3.44278700	1.50300100	H	-2.70060700	-3.24203000	1.17652000
C	-2.74716000	1.39480000	-0.94450000	H	-2.19504400	-0.29841900	-1.92927900
C	-4.58617900	-0.13460300	-0.64348300	C	-0.81992400	-1.94373000	-0.11617500
C	-4.05673000	-2.34433100	0.43028700	N	0.05158400	-1.13579700	-0.85734600
H	-3.39326100	-4.14179200	1.38082700	H	-0.28082700	-0.71851400	-1.73829600
C	-4.11711600	1.08732100	-1.07361100	O	-0.36679200	-2.72537500	0.71800500
H	-2.34867300	2.35151200	-1.25684400	C	1.43677200	-1.51046700	-0.85104900
H	-5.63830700	-0.38894400	-0.72717900	C	2.31644900	-0.77980000	-0.01917300
H	-5.09614300	-2.65112200	0.37160000	C	1.91576000	-2.56460500	-1.59634800
H	-4.77996700	1.82735800	-1.50625600	C	3.68835700	-1.15229500	0.06845700
N	-1.89060200	0.52776100	-0.43102800	C	3.28068600	-2.92981800	-1.52801400
Co	-0.05522300	0.88642900	-0.03778000	H	1.23130000	-3.12170100	-2.22791600
O	0.25540100	-0.01935300	3.03324600	C	2.65042500	1.01353400	1.44632600
O	-0.65831900	1.53083400	1.66542100	C	4.52683800	-0.38639100	0.91536400
C	-0.36421000	1.04827800	2.82913300	C	4.14887000	-2.24801800	-0.70486000
O	1.72771200	1.64073900	0.33361700	H	3.63523600	-3.76320600	-2.12521600
O	0.09970300	2.73411100	-0.56336000	C	4.00992400	0.68725700	1.60489500
C	1.31779800	2.74404800	-0.15980400	H	2.21408000	1.87074900	1.94309200
O	0.62489400	0.26949800	-1.67549100	H	5.57606300	-0.65199600	1.00114300
O	-0.75976700	1.26977300	-3.15698200	H	5.19474600	-2.53047100	-0.63765200
C	0.13893900	0.47333200	-2.87036000	H	4.62549700	1.29858800	2.25400600
C	0.80397300	-0.40436200	-3.91334900	N	1.84328000	0.29694300	0.67631900
H	0.54088700	-1.44944400	-3.71704400	Co	0.08027200	1.02696300	0.18718700
H	0.47459000	-0.12532300	-4.91555300	O	-0.36844500	0.67725300	-2.94437400
H	1.89209700	-0.32126000	-3.83925100	O	0.89921500	1.68863000	-1.37777900
C	2.18860200	3.94156100	-0.29760900	C	0.46069200	1.53258800	-2.59801900
H	1.58640400	4.85190400	-0.28478000	O	-1.53701600	1.98757100	-0.29795500
H	2.93376500	3.95732400	0.50026800	O	-0.17048500	3.11282000	0.99047300
H	2.70953400	3.87896600	-1.26019100	C	-1.26223600	3.06327700	0.36286000
C	-0.83040300	1.89594500	3.98942400	O	-0.86883600	0.28891400	1.60277600
H	-0.25674200	2.82895800	4.00208700	O	0.43755000	0.65652000	3.40283300
H	-1.88453400	2.15784700	3.86234000	C	-0.49824500	0.08304300	2.84699400
H	-0.68518000	1.36760400	4.93254700	C	-1.35554900	-0.95007200	3.54475000
A_T				H	-1.03901300	-1.94222800	3.20542200
C	-4.21067000	-0.82228900	-1.44380000	H	-1.22512700	-0.87917500	4.62583900
				H	-2.40781600	-0.82800600	3.27741200

C	-2.26231600	4.17787600	0.36773500
H	-1.81373900	5.09188100	0.75865800
H	-2.64615300	4.34089000	-0.64253100
H	-3.10494700	3.88687300	1.00476900
C	1.05861500	2.50463000	-3.58566300
H	0.59874600	3.48669000	-3.42704100
H	2.13345300	2.60967900	-3.41782300
H	0.86286500	2.17586100	-4.60717600

TSA\_Q

C	-4.14930400	-1.04263600	-1.44098300
C	-4.92648400	-1.50161500	-0.37610700
C	-4.31600800	-2.13419900	0.71124600
C	-2.93507500	-2.30662800	0.72889500
C	-2.14694900	-1.82758000	-0.32891300
C	-2.76309500	-1.19637400	-1.41743000
H	-4.62121100	-0.56099200	-2.29208300
H	-6.00439100	-1.36981300	-0.39332300
H	-4.91682700	-2.49303500	1.54157500
H	-2.44892100	-2.79929100	1.56407100
H	-2.17545000	-0.83099800	-2.25048800
C	-0.67262200	-2.03422600	-0.22344500
N	0.14418000	-1.05204000	-0.78340300
H	-0.13698500	-0.44756700	-1.93398000
O	-0.22068700	-3.00203300	0.39520500
C	1.54479600	-1.33323200	-0.79421200
C	2.41765900	-0.38675000	-0.19886200
C	2.08809300	-2.44185600	-1.41529300
C	3.82980000	-0.57192200	-0.24320800
C	3.48722400	-2.63738200	-1.45304100
H	1.42868800	-3.16750700	-1.87888500
C	2.64732800	1.62276800	0.97134000
C	4.63702400	0.42375100	0.36194100
C	4.34863200	-1.72501100	-0.88238600
H	3.88027100	-3.52021800	-1.94709100
C	4.05143700	1.51601900	0.96410100
H	2.14731000	2.46649600	1.43441700
H	5.71702800	0.31208700	0.34110700
H	5.42361000	-1.87145000	-0.91489200
H	4.64527800	2.29250900	1.43201200
N	1.87180100	0.70510700	0.41362900
Co	-0.19177100	0.82695400	0.31757400
O	-0.18923200	0.17762500	-2.91711800
O	0.21608300	1.84633600	-1.47237600

C	0.05090700	1.41204300	-2.64649000
O	-2.13141600	1.58360800	-0.01609700
O	-0.61971100	2.78680500	1.00661900
C	-1.81565700	2.67046500	0.57537300
O	-0.52667400	-0.13924000	1.87324200
O	0.82985700	0.77746000	3.41240700
C	0.19237300	-0.18149200	2.98863600
C	0.13594900	-1.52181100	3.67557500
H	0.50883300	-2.29042100	2.99122400
H	0.72995800	-1.50918100	4.59028200
H	-0.90446000	-1.76942700	3.90875300
C	-2.82478500	3.75567200	0.78424100
H	-2.33185400	4.72165200	0.90565300
H	-3.52933500	3.78346900	-0.04957700
H	-3.38548200	3.53139200	1.69928800
C	0.10218600	2.36966900	-3.79814200
H	0.66236200	3.26549600	-3.52747200
H	0.53799000	1.88809600	-4.67578500
H	-0.92679500	2.65894300	-4.04297300

TSA\_S

C	4.18100500	-1.57078900	0.83503300
C	5.01635800	-1.21888200	-0.22702600
C	4.48319900	-1.04918600	-1.50814200
C	3.12026700	-1.23240800	-1.72311500
C	2.27402600	-1.56151600	-0.65364700
C	2.81170000	-1.73411300	0.62842100
H	4.59479600	-1.71597000	1.82842300
H	6.08023800	-1.07986100	-0.05844700
H	5.12960300	-0.77570300	-2.33664600
H	2.69321500	-1.10353100	-2.71200600
H	2.17718000	-2.00439500	1.46325800
C	0.82660100	-1.71571600	-0.96180900
N	-0.08652200	-1.26457500	0.01521800
H	0.11755600	-1.51236200	1.29680500
O	0.45706500	-2.17518900	-2.03950600
C	-1.46280800	-1.58594900	-0.22238200
C	-2.37362400	-0.52646000	-0.03078800
C	-1.95376300	-2.84307500	-0.51330700
C	-3.77798600	-0.72420300	-0.11389000
C	-3.34986600	-3.05056900	-0.62193000
H	-1.27189600	-3.67364900	-0.65265700
C	-2.63014300	1.73654500	0.48830100
C	-4.60373500	0.40097500	0.13247100



C	-4.24989500	-2.02402800	-0.42521200	N	-0.23984100	-1.03072700	0.62228500
H	-3.71041300	-4.04731400	-0.85527300	H	-0.22437500	-0.51632600	1.80025300
C	-4.03335000	1.61743600	0.43967100	O	0.48220900	-3.00241700	-0.34302800
H	-2.14607600	2.67860700	0.71522000	C	-1.61031100	-1.42803900	0.45836100
H	-5.68253400	0.28961100	0.08066800	C	-2.49703200	-0.40606000	0.04507400
H	-5.31909600	-2.19449100	-0.49968400	C	-2.12516200	-2.66130500	0.80719200
H	-4.63993700	2.49295000	0.63920600	C	-3.89955600	-0.62790100	-0.01282200
N	-1.84411900	0.69890600	0.25342700	C	-3.51955100	-2.89418000	0.73673900
Co	0.05661900	0.74899600	0.28514100	H	-1.46763100	-3.45073700	1.14753000
O	0.13648500	-1.57642600	2.46483300	C	-2.72686900	1.79574800	-0.68701200
O	0.00201800	0.65288400	2.22602200	C	-4.70902700	0.45800600	-0.43085200
C	0.07940700	-0.38715000	2.94278100	C	-4.39628200	-1.90775500	0.34056500
O	1.98647000	1.23426200	0.43745500	H	-3.89547200	-3.87397700	1.01343600
O	0.35706100	2.64517400	0.53707700	C	-4.12806700	1.66393100	-0.75939100
C	1.62518300	2.44991600	0.56051400	H	-2.22874600	2.72268900	-0.95223200
O	0.23422000	0.85927900	-1.57260100	H	-5.78515200	0.32456300	-0.48828400
O	-1.19544000	2.55106300	-2.04374100	H	-5.46469900	-2.09254400	0.29328700
C	-0.41661400	1.65477700	-2.38031900	H	-4.72374600	2.51027400	-1.08115200
C	-0.10198900	1.36157700	-3.83519600	N	-1.95042500	0.79461300	-0.30302600
H	-0.28844300	0.30407500	-4.04608400	Co	0.10601300	0.78030600	-0.29193800
H	-0.70875400	1.98847300	-4.49048400	O	-0.39697600	0.09703600	2.83086500
H	0.95946000	1.55190100	-4.02491900	O	0.10714300	1.78549600	1.44952100
C	2.59229200	3.57442000	0.68146500	C	-0.23468000	1.34333300	2.58941500
H	2.18227000	4.35732300	1.32316300	O	2.42768400	2.29732400	-0.40642400
H	3.54578500	3.21362900	1.07087900	O	0.31883300	2.43105600	-1.14405300
H	2.75464400	3.99675100	-0.31711200	C	1.54314100	2.89585300	-1.02835700
C	0.13875300	-0.23100000	4.43056300	O	1.08372100	-0.10178100	-1.64630200
H	-0.25635100	0.73927300	4.73275600	O	-0.72901800	-0.86813700	-2.73803900
H	-0.40788100	-1.04229700	4.91564700	C	0.49369500	-0.79398100	-2.59063700
H	1.18926100	-0.29824200	4.73691700	C	1.45731100	-1.54994300	-3.47742300
TSA_T				H	1.53704000	-2.57006900	-3.08476000
C	3.87703400	-0.41777800	1.82406600	H	1.06174900	-1.60331100	-4.49407700
C	4.86864500	-1.05313600	1.07566400	H	2.45080600	-1.09872900	-3.47568800
C	4.51336200	-1.99750700	0.10716000	C	1.76482400	4.21708800	-1.72025300
C	3.17342000	-2.29397400	-0.11620300	H	1.05569900	4.95833900	-1.33928600
C	2.16893300	-1.64355700	0.61976300	H	2.78726300	4.55978500	-1.55575000
C	2.53216400	-0.70779800	1.59811400	H	1.57987600	4.10180500	-2.79306400
H	4.14694800	0.30422300	2.58846600	C	-0.46714900	2.32497000	3.69602400
H	5.91474300	-0.81817700	1.24818000	H	-1.45295300	2.78016100	3.54493600
H	5.28169000	-2.49729400	-0.47470200	H	-0.44828200	1.82742500	4.66613500
H	2.88738600	-3.01802200	-0.87037600	H	0.28017300	3.12034200	3.65235700
H	1.78534700	-0.22498200	2.21006900	B_Q			
C	0.76167200	-1.97760000	0.27013000	C	3.53800500	-0.26384600	-2.06022500

C	4.80533700	-0.51089000	-1.52589700			
C	4.93584500	-1.07438100	-0.25209700	B_S		
C	3.80077600	-1.38612400	0.48916600	C	3.79409700	0.06602900 -1.92525700
C	2.52668600	-1.13018800	-0.03984700	C	4.92065100	-0.24073400 -1.15859000
C	2.39836700	-0.57131000	-1.32085800	C	4.80021200	-1.07952700 -0.04603700
H	3.43804700	0.17055900	-3.05003300	C	3.55696900	-1.60399400 0.29880100
H	5.69267200	-0.26523900	-2.10190700	C	2.41864100	-1.26903400 -0.44675500
H	5.92190700	-1.26572300	0.15971300	C	2.54463800	-0.44245800 -1.56934400
H	3.88386000	-1.82000300	1.47994000	H	3.88812200	0.70034700 -2.80199900
H	1.41474800	-0.37477200	-1.73151100	H	5.89105700	0.16395100 -1.43135900
C	1.34177300	-1.46173900	0.78060800	H	5.67558700	-1.32486700 0.54826500
N	0.10684800	-1.00243600	0.28660200	H	3.45309700	-2.26296800 1.15518200
O	1.40825300	-2.02242400	1.87301600	H	1.66925600	-0.20416800 -2.16099400
C	-0.95975100	-1.79089500	0.16016500	C	1.10793500	-1.87394300 -0.06014700
C	-2.20690700	-1.12273600	-0.17245500	N	-0.01001700	-1.09219000 -0.19006300
C	-0.96428500	-3.20729300	0.27719500	O	1.08690300	-3.05963400 0.31904100
C	-3.38745100	-1.87436500	-0.37740100	C	-1.29038000	-1.65907000 -0.21600200
C	-2.13911100	-3.92909300	0.07575500	C	-2.34516100	-0.70215400 -0.19643000
H	-0.04220500	-3.72104300	0.52093900	C	-1.65175500	-2.99848400 -0.34602700
C	-3.30052700	0.87574800	-0.58504900	C	-3.71303800	-1.06886800 -0.31443700
C	-4.56426200	-1.16351800	-0.70693000	C	-3.01134300	-3.36788300 -0.46507000
C	-3.33396000	-3.29214000	-0.24675900	H	-0.89022500	-3.76276400 -0.36248000
H	-2.11708200	-5.00990600	0.16623300	C	-2.88578400	1.57102500 -0.03645300
C	-4.51762700	0.21298800	-0.81325000	C	-4.66920300	-0.02388700 -0.28957200
H	-3.22593200	1.95655900	-0.65048300	C	-4.03265000	-2.44215100 -0.45044300
H	-5.48871800	-1.70831300	-0.87156200	H	-3.24544600	-4.42331400 -0.56900200
H	-4.24005100	-3.86730800	-0.40791800	C	-4.25829400	1.28426400 -0.15418000
H	-5.40038100	0.78941600	-1.06501000	H	-2.52730600	2.58537600 0.08603300
N	-2.18004700	0.22498600	-0.27483100	H	-5.72336000	-0.26928400 -0.37770700
Co	-0.27780400	1.09443200	0.16679200	H	-5.07203500	-2.74108500 -0.53778300
O	1.53052000	1.74237600	1.13007000	H	-4.96853200	2.10252100 -0.13077300
O	-0.14846500	1.03092700	2.36787100	N	-1.97479300	0.60615400 -0.06147100
C	1.05684400	1.43092300	2.27274500	Co	-0.10262300	0.80098200 0.23693500
O	-0.10576000	1.74968900	-1.87390100	O	1.67138500	0.95013100 1.09808800
O	-0.81375400	3.16391800	-0.33919200	O	-0.14401400	0.38850000 2.11758200
C	-0.51198900	2.91580600	-1.54994400	C	1.11993600	0.61326000 2.19720700
C	-0.60104600	3.99769400	-2.59342800	O	0.18348300	1.62777700 -1.50252600
H	-0.87314300	3.57558100	-3.56344900	O	-0.19298500	2.76890500 0.28968800
H	-1.32026000	4.76343300	-2.29633200	C	0.07625100	2.78413300 -0.96246900
H	0.38415600	4.46828800	-2.69257100	C	0.28210300	4.04432100 -1.72430500
C	1.94391600	1.45701100	3.48790700	H	0.04145500	3.89306000 -2.77817300
H	2.72027400	2.21832800	3.38887800	H	-0.32497900	4.84501500 -1.29734200
H	1.35854200	1.62290700	4.39454200	H	1.33825300	4.32717900 -1.64309700
H	2.43047700	0.47725600	3.56696500	C	1.88325000	0.43913400 3.46039000

H 2.69549300 1.16735600 3.51048400  
H 1.22262400 0.53279000 4.32385000  
H 2.32140900 -0.56593100 3.45536400

B\_T

C 3.54290800 -0.51786400 -2.16860800  
C 4.77151600 -0.79951500 -1.56520400  
C 4.81384800 -1.36852300 -0.28812200  
C 3.62950500 -1.65380900 0.38426100  
C 2.39500700 -1.35354000 -0.21025700  
C 2.35485600 -0.78877600 -1.49309800  
H 3.51121900 -0.08602600 -3.16420800  
H 5.69625500 -0.57905200 -2.09043200  
H 5.76903600 -1.58716800 0.17948400  
H 3.64479300 -2.09563100 1.37507900  
H 1.39968500 -0.56883000 -1.95533000  
C 1.15678500 -1.67839900 0.53440100  
N -0.01874400 -1.00983600 0.13739400  
O 1.14285400 -2.49590500 1.45434000  
C -1.22118100 -1.70963000 0.06038800  
C -2.34704100 -0.87129500 -0.15075400  
C -1.42008200 -3.08630900 0.08225000  
C -3.64951600 -1.39034200 -0.34332700  
C -2.71911400 -3.61180600 -0.10279400  
H -0.58707800 -3.75926200 0.24040300  
C -3.07925700 1.33277500 -0.35064300  
C -4.68907500 -0.45180300 -0.54882500  
C -3.81676200 -2.80051000 -0.31182800  
H -2.84596900 -4.68954300 -0.07914300  
C -4.40184500 0.89871600 -0.55280600  
H -2.82019300 2.38466100 -0.33792600  
H -5.70472300 -0.80444800 -0.70043100  
H -4.80754600 -3.22057400 -0.44982000  
H -5.17803600 1.63932700 -0.70661000  
N -2.08731200 0.46882800 -0.15794700  
Co -0.21338800 0.84201600 0.20972400  
O 1.59138700 1.17508200 0.83961900  
O 0.12183000 1.04591300 2.46345900  
C 1.31589600 1.21791400 2.10052000  
O 0.20649200 1.89452500 -1.79978900  
O -0.50185300 2.76755500 0.08366600  
C -0.13157500 2.91463600 -1.14651100  
C -0.11632200 4.29627800 -1.72911500  
H 0.09650000 4.25927400 -2.79817100

H -1.07938600 4.78380500 -1.55224600  
H 0.65366200 4.88830800 -1.22317700  
C 2.44064900 1.44324600 3.06535900  
H 2.97950800 2.35631400 2.79537100  
H 2.06479900 1.51724400 4.08630600  
H 3.14425200 0.60773500 2.98764500

TSB\_Q

C -4.44809600 0.74219200 -1.10273400  
C -4.14077500 2.09591200 -1.29198200  
C -2.91506900 2.59197800 -0.85949000  
C -1.99395300 1.72743700 -0.24671300  
C -2.28500100 0.35780900 -0.01375400  
C -3.53391800 -0.10074100 -0.46691100  
H -5.40373200 0.35419800 -1.44602800  
H -4.85233500 2.75405000 -1.78197200  
H -2.65145400 3.63397900 -1.01586000  
H -3.80529300 -1.14212700 -0.30108800  
C -0.65505900 2.27579000 0.09366700  
O -0.44720600 3.46912800 0.32287700  
N 0.33616500 1.28254500 0.05819000  
C 1.66092200 1.50624700 0.02288400  
C 2.46172700 0.31135000 -0.20020800  
C 2.34003700 2.74533400 0.15426100  
C 3.87339000 0.38937300 -0.27066600  
C 3.73401800 2.79930900 0.09344600  
H 1.76138200 3.64244000 0.31803700  
C 2.48805500 -1.97160900 -0.59739900  
C 4.58538900 -0.80815900 -0.51274800  
C 4.49974600 1.65744600 -0.11190800  
H 4.22756700 3.75835000 0.21059300  
C 3.89017300 -1.99052400 -0.67746800  
H 1.90496400 -2.87975300 -0.71857600  
H 5.66911600 -0.78236900 -0.57117700  
H 5.58232600 1.71830300 -0.16147400  
H 4.40359500 -2.92598300 -0.86769400  
N 1.80009500 -0.85588600 -0.36700700  
Co -0.31253700 -0.68834900 -0.01958300  
C -1.09364300 -2.46300200 -1.62392600  
O -1.06728200 -2.65751300 -0.36024900  
O -0.65720000 -1.37089300 -2.10257800  
C -0.87908200 -0.90880800 2.83038500  
O -2.06847400 -0.57994900 2.44019700  
O 0.10641500 -0.92730500 2.05224500

C -1.68994500 -3.50943100 -2.52763300  
H -2.77004600 -3.33190000 -2.59361500  
H -1.26935700 -3.44003200 -3.53283800  
H -1.53477400 -4.50983300 -2.11775300  
C -0.72848700 -1.26807600 4.27959400  
H -1.40272800 -2.09644800 4.51839000  
H 0.30119500 -1.54877000 4.50211400  
H -1.02520500 -0.41390600 4.89646000  
H -2.03615600 -0.25067600 1.32889300

TSB\_S

C 4.51490500 -0.09323300 -0.61678600  
C 4.39165200 -1.36437700 -1.18983100  
C 3.18908300 -2.06867500 -1.09822600  
C 2.11137600 -1.49273700 -0.42870000  
C 2.22076900 -0.22107900 0.18052100  
C 3.43582900 0.47446900 0.06163400  
H 5.45415700 0.44644900 -0.69518400  
H 5.23455900 -1.80300600 -1.71585800  
H 3.07479700 -3.04402900 -1.56138900  
H 3.54415200 1.44887200 0.53052200  
C 0.76572900 -2.13626900 -0.43673900  
O 0.57953200 -3.33078000 -0.73225800  
N -0.20094400 -1.22562600 -0.14926300  
C -1.57131600 -1.42545400 -0.27550100  
C -2.31149200 -0.20697000 -0.32296600  
C -2.26917900 -2.62306600 -0.36853000  
C -3.72308600 -0.19319300 -0.46574200  
C -3.67785400 -2.60952100 -0.50457800  
H -1.73266900 -3.56063900 -0.33954900  
C -2.19889300 2.12572300 -0.27729600  
C -4.35314800 1.07598800 -0.51779000  
C -4.40153600 -1.43625500 -0.55518300  
H -4.19601300 -3.56150100 -0.57262700  
C -3.59678700 2.22466900 -0.42892700  
H -1.57397300 3.00730400 -0.18631400  
H -5.43218900 1.12873700 -0.62837400  
H -5.48101900 -1.44458800 -0.66613000  
H -4.05366700 3.20687300 -0.46613800  
N -1.58932300 0.95158400 -0.23263200  
Co 0.29939600 0.57576500 0.11629600  
C 1.05902000 2.28116700 -1.27813700  
O 0.89751100 2.45959000 -0.02129600  
O 0.75797500 1.11216000 -1.70743900

C 0.48926100 0.17134700 2.90686000  
O 1.67782300 -0.23191500 2.72173000  
O -0.26621800 0.54781200 1.95258700  
C 1.60578300 3.33534200 -2.17516600  
H 2.69700500 3.22945400 -2.19777300  
H 1.22451100 3.20658400 -3.18998300  
H 1.35927200 4.32663100 -1.79022100  
C -0.07628400 0.17886700 4.29667900  
H -0.87676500 0.91512000 4.38158800  
H -0.49123200 -0.81518200 4.49944900  
H 0.71250700 0.37715100 5.02442600  
H 1.84428400 -0.15927700 1.43350700

TSB\_T

C -4.47269800 0.27396000 -0.67502400  
C -4.31666700 1.57733200 -1.16558400  
C -3.11204700 2.26448200 -0.99818200  
C -2.06477300 1.63608500 -0.33099200  
C -2.21238300 0.33392600 0.20278000  
C -3.42428200 -0.34943500 -0.00167400  
H -5.41460700 -0.24670400 -0.81811700  
H -5.13785000 2.05412100 -1.69236600  
H -2.97382000 3.26247700 -1.40232700  
H -3.55004500 -1.35144900 0.39798300  
C -0.70955800 2.24754800 -0.25467100  
O -0.47609100 3.44427300 -0.45202800  
N 0.23481300 1.28016100 -0.00412700  
C 1.61964500 1.47048200 -0.08826500  
C 2.33010400 0.25525700 -0.28914100  
C 2.33749400 2.65343100 -0.00646000  
C 3.74122600 0.22384000 -0.41206500  
C 3.74955100 2.62545000 -0.12218000  
H 1.82248900 3.59140600 0.14513900  
C 2.15541100 -2.05765400 -0.56410500  
C 4.34013600 -1.04252700 -0.62637400  
C 4.44675000 1.45279400 -0.32126400  
H 4.28884500 3.56504000 -0.05195900  
C 3.55245400 -2.17247000 -0.70388500  
H 1.50284600 -2.92274400 -0.60452400  
H 5.41909500 -1.11016000 -0.72861600  
H 5.52804200 1.45066600 -0.41305700  
H 3.98560800 -3.15252800 -0.86662500  
N 1.57517600 -0.88305500 -0.36956800  
Co -0.32022900 -0.50937400 0.05441900

C -1.21085200 -2.25942700 -1.63663500  
 O -0.89954000 -2.29008500 -0.37338600  
 O -1.06492000 -1.21812900 -2.30689000  
 C -0.48547300 -0.49608300 2.95462600  
 O -1.57478800 0.13056700 2.75266600  
 O 0.24337900 -0.94325900 2.01229700  
 C -1.76545500 -3.53125000 -2.21876200  
 H -2.75581700 -3.71487100 -1.78780000  
 H -1.85202100 -3.45079400 -3.30307600  
 H -1.12619100 -4.37757700 -1.95212900  
 C -0.01824000 -0.69602300 4.37157000  
 H 0.34857300 -1.71746500 4.50047000  
 H 0.81906000 -0.01415000 4.55827100  
 H -0.81768100 -0.48469500 5.08262200  
 H -1.79454100 0.17204500 1.40355700

C\_Q

C -4.41589900 0.70441200 -1.25533600  
 C -4.28476800 2.08566200 -1.05812000  
 C -3.06434000 2.60931700 -0.64254300  
 C -1.98483100 1.74031800 -0.42099900  
 C -2.08328500 0.33815800 -0.60035000  
 C -3.32741100 -0.14780400 -1.03609300  
 H -5.37155300 0.29671400 -1.57660600  
 H -5.13059200 2.74378900 -1.23470400  
 H -2.93574900 3.67866400 -0.49952700  
 H -2.47627200 -0.41261000 1.33357600  
 H -3.46391300 -1.21813900 -1.18664500  
 C -0.67585200 2.29771800 -0.00845100  
 O -0.50025800 3.47334900 0.32871100  
 N 0.33231400 1.32362700 -0.03374600  
 C 1.65341000 1.57591500 -0.05700400  
 C 2.48232500 0.38366500 -0.07457700  
 C 2.29880500 2.83488400 -0.10402300  
 C 3.89487600 0.48539000 -0.10652200  
 C 3.69484000 2.91582000 -0.13414400  
 H 1.69809100 3.73307400 -0.10185400  
 C 2.56518200 -1.93057600 -0.10921900  
 C 4.63747800 -0.71808500 -0.12693700  
 C 4.48987500 1.77797000 -0.12994400  
 H 4.16269300 3.89460200 -0.16077100  
 C 3.97042000 -1.92733200 -0.12502200  
 H 2.00663900 -2.86175100 -0.11672300  
 H 5.72220700 -0.67544100 -0.14843000

H 5.57212100 1.85787000 -0.15265700  
 H 4.50773800 -2.86858700 -0.14272100  
 N 1.84596700 -0.81143800 -0.08419000  
 Co -0.31697300 -0.67210300 -0.07643800  
 C -1.32365700 -0.75107000 2.81016400  
 O -2.53928100 -0.60349500 2.30128100  
 O -0.29760500 -0.69168800 2.12390600  
 C -0.66460500 -2.75375200 -1.51992600  
 O -0.88109800 -2.68980100 -0.25548700  
 O -0.19542900 -1.75915500 -2.13887400  
 C -1.31314200 -0.99775100 4.28409400  
 H -0.28793500 -1.08309300 4.64246900  
 H -1.82805000 -0.17913400 4.79587400  
 H -1.86362400 -1.91983200 4.49708500  
 C -1.00893800 -4.03089200 -2.24559200  
 H -2.09911400 -4.13483100 -2.28450000  
 H -0.61497200 -4.02282500 -3.26318100  
 H -0.61572000 -4.89191600 -1.69750100

C\_S

C -4.54786300 -0.01644800 -0.52443000  
 C -4.54530400 1.35406600 -0.80663400  
 C -3.34095300 2.05710500 -0.83687700  
 C -2.14721600 1.37427800 -0.58654600  
 C -2.13387800 -0.00687200 -0.30361200  
 C -3.34867000 -0.69746400 -0.27430100  
 H -5.48942000 -0.55885200 -0.49769600  
 H -5.48173400 1.87011300 -0.99703200  
 H -3.31497200 3.12233800 -1.04937100  
 H -2.20015400 0.62999200 1.59630000  
 H -3.37090100 -1.76246500 -0.05907000  
 C -0.81814900 2.04964200 -0.57936900  
 O -0.66299400 3.26643500 -0.79823600  
 N 0.16464400 1.14836000 -0.30666300  
 C 1.52826700 1.40320000 -0.25194900  
 C 2.32905800 0.22623400 -0.09763100  
 C 2.17752300 2.63165800 -0.32862600  
 C 3.74628200 0.29725700 -0.02315400  
 C 3.58813800 2.69629100 -0.25192600  
 H 1.59666400 3.53480500 -0.44795300  
 C 2.34375300 -2.09492600 0.10696400  
 C 4.44673000 -0.92722000 0.12451300  
 C 4.36913000 1.56931800 -0.10309600  
 H 4.06134300 3.67204900 -0.31429300

C	3.75171700	-2.11501200	0.18690900
H	1.76271600	-3.01069600	0.15361800
H	5.53110900	-0.91299800	0.18568600
H	5.45101600	1.63593200	-0.04738100
H	4.26370700	-3.06424700	0.29798100
N	1.66470800	-0.96745000	-0.02865400
Co	-0.33947800	-0.66456200	-0.09526400
C	-0.85876000	-0.02907600	2.75772100
O	-1.95406600	0.66622100	2.55086300
O	-0.21789200	-0.59819300	1.85748600
C	-0.69507300	-2.42008000	-1.57807400
O	-0.81587200	-2.58352800	-0.31710500
O	-0.37727700	-1.23428800	-1.94930800
C	-0.41332800	-0.08016500	4.17975600
H	0.41492000	-0.77881900	4.29006700
H	-0.09366600	0.92387800	4.47955100
H	-1.25198700	-0.36809800	4.81923600
C	-0.94166800	-3.51434800	-2.55816200
H	-2.01690400	-3.55267100	-2.76921500
H	-0.40890300	-3.31993200	-3.49061200
H	-0.63982200	-4.47406100	-2.13338400

C\_T

C	-4.53505200	0.20245800	-0.76134200
C	-4.49158300	1.59409400	-0.90170600
C	-3.27257400	2.26853200	-0.82926600
C	-2.10352300	1.53433700	-0.61937000
C	-2.14030500	0.13665700	-0.48578400
C	-3.36044200	-0.53461800	-0.55527000
H	-5.48921900	-0.31503200	-0.81227500
H	-5.41082600	2.14968800	-1.06130700
H	-3.21644800	3.34923700	-0.92651500
H	-2.11952100	0.37459800	1.65173000
H	-3.40915500	-1.61411400	-0.44755700
C	-0.76055500	2.15661600	-0.49306900
O	-0.54801100	3.37549100	-0.56492600
N	0.18455400	1.18310800	-0.28170400
C	1.55155800	1.39792700	-0.09666400
C	2.32111800	0.19454800	-0.05349900
C	2.21903400	2.60824200	0.04367500
C	3.73003700	0.21873400	0.11641600
C	3.62378100	2.62935200	0.21879600
H	1.66222000	3.53367100	0.01544600
C	2.28352400	-2.13580600	-0.15860200

C	4.39899800	-1.03054800	0.13714500
C	4.37591200	1.47517400	0.25430000
H	4.11299700	3.59293100	0.32619500
C	3.68157600	-2.20002200	-0.00113200
H	1.68254900	-3.03379700	-0.25927400
H	5.47759700	-1.05203900	0.26304500
H	5.45264300	1.50716300	0.38675900
H	4.17053800	-3.16741600	0.01183900
N	1.63359800	-0.98169200	-0.18380500
Co	-0.36963900	-0.63231500	-0.24606400
C	-0.75253700	-0.13363700	2.86244700
O	-1.86512400	0.53711300	2.58605800
O	-0.16246000	-0.82294600	2.02693700
C	-0.90837300	-2.61417900	-1.69066600
O	-0.87845800	-2.51859500	-0.40029800
O	-0.64974200	-1.60428500	-2.39022500
C	-0.28148100	0.04080200	4.27000700
H	0.54652300	-0.63746100	4.47330700
H	0.04949300	1.07679900	4.40230900
H	-1.10560300	-0.13649200	4.96619200
C	-1.27276700	-3.94130900	-2.29300200
H	-2.33408800	-4.13560700	-2.10266000
H	-1.09429200	-3.93882300	-3.36893900
H	-0.69858300	-4.74021900	-1.81583000

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C	2.72585600	-0.01949000	3.64835200
C	3.66987400	0.98465900	3.87775900
C	4.53920300	1.38318200	2.85614200
C	4.46075900	0.78349500	1.60268500
C	3.49740800	-0.20675200	1.36394800
C	2.63592600	-0.61357500	2.39155300
H	2.05519800	-0.33101300	4.44291800
H	3.72962500	1.45849900	4.85315300
H	5.27035800	2.16476600	3.03816600
H	5.11268000	1.09365100	0.79319200
H	1.89448700	-1.37996400	2.20077300
C	3.38381000	-0.77604600	0.00375400
N	2.11020800	-1.27012300	-0.34208500
O	4.29724500	-0.75437900	-0.81784400
C	1.94625500	-2.45114600	-0.93528900
C	0.62596700	-2.70891700	-1.48537700
C	2.93473500	-3.46911000	-1.04434900
C	0.35215600	-3.93623800	-2.13540700

C	2.63740100	-4.67744100	-1.66863600	C	-2.26142900	3.91960700	-0.04869600
H	3.92085300	-3.29606100	-0.63085100	C	-0.69595200	3.56528400	-2.33934600
C	-1.48577400	-1.89179900	-1.93137600	C	-1.88328500	5.03737800	-0.82697100
C	-0.93763400	-4.10658200	-2.68860700	H	-2.89833300	4.05255400	0.81997700
C	1.37769300	-4.92159100	-2.21067800	C	0.19831900	1.02723200	-2.90038800
H	3.40448000	-5.44190100	-1.73330400	C	0.06829000	3.33524800	-3.51147700
C	-1.85327000	-3.07726400	-2.59131900	C	-1.13467900	4.86183800	-1.96725800
H	-2.17227300	-1.05584100	-1.85998600	H	-2.21529800	6.02768000	-0.53265000
H	-1.18593600	-5.03596300	-3.19180400	C	0.48662400	2.06209700	-3.81290000
H	1.16159100	-5.86650300	-2.69900600	H	0.59052500	0.02897100	-3.07016400
H	-2.84724100	-3.16464700	-3.01515700	H	0.31186500	4.17549500	-4.15514300
N	-0.28658700	-1.72136000	-1.37942100	H	-0.86745300	5.70410800	-2.59832000
Co	0.36005800	-0.01100100	-0.12944300	H	1.06412900	1.84475200	-4.70419000
O	-0.49291700	-1.07229400	1.38888800	N	-0.50695900	1.19952300	-1.79060400
O	-0.93503500	0.66501500	2.75175000				
C	-0.76771500	-0.55777300	2.53857800	D_S			
O	1.00834000	1.71385400	0.68585900	C	2.10543100	-1.85446900	-3.79652200
O	2.54844000	1.97520000	-0.92806300	C	3.08356900	-2.84075200	-3.64732100
C	1.93118600	2.38180200	0.07743600	C	4.00844700	-2.75602500	-2.60091300
C	2.22344700	3.74999300	0.66333600	C	3.94754900	-1.69517600	-1.70080800
H	2.41671200	3.66294700	1.73663500	C	2.94196500	-0.72622400	-1.82346600
H	3.07892900	4.21415500	0.16936600	C	2.03643600	-0.79959200	-2.88787000
H	1.34126700	4.38790000	0.53769200	H	1.39667100	-1.90676100	-4.61779400
C	-0.88541900	-1.54980200	3.67865900	H	3.13153500	-3.66972200	-4.34765400
H	-1.22385700	-1.05974700	4.59282500	H	4.77372600	-3.51833700	-2.48841400
H	-1.58514500	-2.34452700	3.40461400	H	4.65348300	-1.62308100	-0.88067000
H	0.08907900	-2.01818800	3.85548400	H	1.28493300	-0.02835600	-2.99130700
C	-4.37940100	-1.02092700	3.14674400	C	2.91660900	0.42323800	-0.87459800
C	-4.70573900	-2.29422300	2.67526800	N	1.70086300	1.04500500	-0.62735100
C	-4.55914700	-2.59389900	1.31782700	O	3.98297600	0.85416600	-0.41210100
C	-4.08369800	-1.62474500	0.43752000	C	1.65369700	2.43001700	-0.55671900
C	-3.71938000	-0.35707800	0.91203200	C	0.43054800	2.96456800	-0.06708800
C	-3.88424000	-0.05523300	2.27070000	C	2.63044000	3.33359300	-0.97882600
H	-4.51011600	-0.77793400	4.19679300	C	0.20761900	4.36875900	0.01584700
H	-5.08296900	-3.04747600	3.36071600	C	2.39738900	4.72228300	-0.92377600
H	-4.82157100	-3.57957400	0.94525700	H	3.57939800	2.97000300	-1.34872700
H	-3.99018300	-1.84507500	-0.61944700	C	-1.62304900	2.49558400	0.91456100
H	-3.63672700	0.93230600	2.64207300	C	-1.02090900	4.79952600	0.57337300
C	-3.21421700	0.65456700	-0.06638500	C	1.21837100	5.24956900	-0.43690000
N	-2.30862100	1.54901600	0.40930400	H	3.18262100	5.38826500	-1.26977500
H	-1.85113800	1.37234600	1.31597400	C	-1.92059400	3.86719600	1.03309600
O	-3.62041100	0.67061100	-1.24016600	H	-2.31015500	1.76653400	1.31014800
C	-1.85709200	2.64386600	-0.38217700	H	-1.22784100	5.86305700	0.64721800
C	-1.01628700	2.44236000	-1.51638500	H	1.05448400	6.32063600	-0.38155900

H	-2.85963000	4.15734100	1.49029000	H	1.95703600	-0.65615800	5.48306100
N	-0.50444900	2.05679300	0.35538100	H	0.25807900	-2.53761800	5.60150700
Co	0.10459900	0.19640700	0.07761800	H	2.95176500	1.21284200	4.14588600
O	-0.69494200	0.27781100	-1.65994800	N	0.66589600	0.17584000	1.92771100
O	-1.29235000	-1.88718200	-1.91918500				
C	-1.17804800	-0.72256100	-2.33517600	D_T			
O	0.77678900	-1.57328700	-0.13050200	C	-2.30420900	-0.55797900	3.94809800
O	2.61989600	-1.70943900	1.18442500	C	-3.16886100	-1.64176400	4.12232400
C	1.74728800	-2.20637600	0.46368100	C	-4.07953700	-1.98226500	3.11630500
C	1.70479700	-3.69859600	0.19125700	C	-4.11976100	-1.24633100	1.93440400
H	1.51114700	-3.88839800	-0.86710200	C	-3.22859100	-0.18234300	1.74272300
H	2.64243200	-4.16822700	0.49323300	C	-2.33307400	0.16933500	2.76006900
H	0.88092300	-4.13641600	0.76671900	H	-1.60455300	-0.28469200	4.73215700
C	-1.65907000	-0.34250800	-3.71990100	H	-3.13784200	-2.21856100	5.04213300
H	-1.93801200	-1.23384300	-4.28359600	H	-4.75320300	-2.82265400	3.25431000
H	-2.53352400	0.30969900	-3.62306400	H	-4.81248200	-1.50599000	1.14076800
H	-0.88677000	0.21656000	-4.25570800	H	-1.66464500	1.00807600	2.61053300
C	-4.82176900	-1.70526100	-2.09830700	C	-3.28061500	0.58684500	0.47039800
C	-5.43540200	-0.52061700	-2.51069600	N	-2.08936700	1.16174600	0.03688000
C	-5.20437700	0.66998500	-1.81527600	O	-4.35023200	0.73809000	-0.13036800
C	-4.36505000	0.67498000	-0.70420800	C	-2.11038800	2.40643900	-0.59887300
C	-3.71891500	-0.50734500	-0.31303800	C	-0.87633100	2.76548400	-1.20110700
C	-3.95265300	-1.70026500	-1.00891500	C	-3.14072700	3.34026500	-0.63095700
H	-5.01316900	-2.63277200	-2.62860100	C	-0.67026300	4.02304600	-1.82622900
H	-6.09816900	-0.52522200	-3.37091500	C	-2.94143000	4.59750100	-1.24627900
H	-5.68445800	1.59032900	-2.13287800	H	-4.09997400	3.11090800	-0.18668400
H	-4.19277200	1.59148900	-0.15027500	C	1.28623900	2.04638200	-1.71453900
H	-3.47263000	-2.61876000	-0.69178100	C	0.60354600	4.25322500	-2.40184000
C	-2.86781800	-0.47468400	0.90149900	C	-1.74404200	4.94865600	-1.83568200
N	-1.54731200	-1.01331600	0.81125400	H	-3.76800900	5.30175300	-1.25048200
H	-1.42909100	-1.65430200	0.00532400	C	1.56992000	3.27129800	-2.34854400
O	-3.24622600	0.03535900	1.94669000	H	2.01273800	1.24429000	-1.68653300
C	-1.03138800	-1.50595700	2.07603600	H	0.80293000	5.20352600	-2.88809500
C	0.05365700	-0.81078000	2.65368600	H	-1.60904700	5.91571200	-2.30874700
C	-1.60947100	-2.56276700	2.74021300	H	2.54877500	3.41592600	-2.79097100
C	0.51771700	-1.16962100	3.94852700	N	0.10657100	1.82027000	-1.15425700
C	-1.12744200	-2.95002900	4.01296100	Co	-0.42751800	0.19644300	-0.21295000
H	-2.44784000	-3.08513200	2.29043100	O	0.63723100	0.94572000	1.28617500
C	1.66270700	0.86490900	2.45794900	O	1.12806800	-0.82220900	2.60130100
C	1.58456300	-0.41247900	4.49283000	C	0.97666800	0.39983200	2.41287000
C	-0.09910500	-2.25911000	4.61515200	O	-0.89717300	-1.44373500	0.56623800
H	-1.59215300	-3.78932300	4.51927400	O	-2.49468700	-1.92359500	-0.94919700
C	2.13570500	0.61341000	3.76002000	C	-1.76475200	-2.23892200	-0.00272500
H	2.13301100	1.61449400	1.83484000	C	-1.77573300	-3.62732100	0.59630800



H	-1.67456400	-3.58027500	1.68264300	C	-3.21685000	0.44558700	1.51850000
H	-2.69492700	-4.14780800	0.32269900	C	-2.46459500	0.59266300	2.69005000
H	-0.91790000	-4.18252400	0.19961300	H	-2.30864100	0.12160500	4.78424900
C	1.21381200	1.38795000	3.53525400	H	-4.39819500	-1.22498100	4.81954100
H	1.57918300	0.87861300	4.42797200	H	-5.74874200	-1.47323500	2.74745400
H	1.94128500	2.13884300	3.21357300	H	-4.99467500	-0.38537300	0.64137500
H	0.27998800	1.91186900	3.76532000	H	-1.55144600	1.17263000	2.66090400
C	4.69408300	0.52733900	2.96934300	C	-2.82715100	1.14199600	0.25908200
C	5.02806400	1.84798400	2.66238900	N	-1.48502200	1.42614000	0.04997800
C	4.76545400	2.35636600	1.38683900	O	-3.71262300	1.52718500	-0.51952700
C	4.16909900	1.54654300	0.42309600	C	-1.14476700	2.65646100	-0.49488900
C	3.80275800	0.23027400	0.73646100	C	0.15972800	2.73768500	-1.05448900
C	4.07866200	-0.27930000	2.01263500	C	-1.91649400	3.81914600	-0.49205600
H	4.91191100	0.12395300	3.95349800	C	0.65045000	3.93650900	-1.64634800
H	5.49874000	2.47752400	3.41181400	C	-1.41149000	5.02003100	-1.02957800
H	5.03039400	3.38072000	1.14278300	H	-2.91826000	3.80144200	-0.08254400
H	3.97920200	1.92953600	-0.57326500	C	2.03968900	1.53904600	-1.71841800
H	3.82509200	-1.30525800	2.25406400	C	1.91589200	3.87436400	-2.27955600
C	3.16401500	-0.60585400	-0.32438400	C	-0.15839300	5.09703400	-1.60511000
N	2.25685000	-1.52450900	0.09978000	H	-2.04351900	5.90283700	-0.99819800
H	1.87483000	-1.45684700	1.05352000	C	2.59017300	2.67637300	-2.33821600
O	3.45705800	-0.46182800	-1.52322200	H	2.55611800	0.59398400	-1.78316400
C	1.71008600	-2.48661700	-0.79263500	H	2.32630500	4.76965800	-2.73693400
C	0.77928600	-2.13162000	-1.81056700	H	0.21028400	6.01893300	-2.04228300
C	2.14454800	-3.79331500	-0.69007400	H	3.54250000	2.58226000	-2.84691900
C	0.42614100	-3.12051500	-2.78164800	N	0.89140400	1.58042700	-1.05448400
C	1.71979300	-4.78881500	-1.59574700	Co	-0.04224900	0.11916000	-0.13119300
H	2.85227600	-4.03890800	0.09494000	O	0.54467700	0.66151700	1.64353000
C	-0.54305100	-0.55598300	-2.91915500	O	1.24097300	-1.39115100	2.24144900
C	-0.39319100	-2.73733000	-3.87186300	C	0.94154400	-0.17680100	2.51037700
C	0.89950900	-4.44980500	-2.64533000	O	-0.99688000	-1.29240500	0.71977000
H	2.07915200	-5.80589300	-1.48030800	O	-2.72659400	-1.82804300	-0.64559500
C	-0.83908400	-1.44249600	-3.96767900	C	-2.01650600	-2.01175100	0.34896700
H	-0.97816100	0.43704200	-2.91933400	C	-2.26633200	-3.17231400	1.29460200
H	-0.65347500	-3.47928200	-4.62058100	H	-2.24267800	-2.82819500	2.33154200
H	0.60355200	-5.18377000	-3.38819000	H	-3.22679600	-3.64218900	1.07709500
H	-1.45415700	-1.10258600	-4.79230200	H	-1.46548100	-3.90970000	1.16864100
N	0.21101900	-0.87806000	-1.87048500	C	1.06897500	0.27265300	3.93400800
				H	0.24264700	-0.16254700	4.50707200
TSC_S				H	2.00606600	-0.09893900	4.35472400
C	-2.89192400	-0.00286300	3.87663300	H	1.02139300	1.35943600	4.00375200
C	-4.07003400	-0.75348000	3.89763700	C	5.28869700	-0.87092700	2.47486600
C	-4.83156500	-0.89199700	2.73239300	C	5.14649600	0.45365400	2.89590900
C	-4.41383900	-0.28400700	1.55165400	C	4.24736900	1.29559300	2.24038500

C	3.47364600	0.81749200	1.18129000	H	0.07256900	-4.48887700	-2.43287400
C	3.60352600	-0.51241500	0.76706300	H	-1.16219400	-2.58268600	-1.40433100
C	4.53260200	-1.34766300	1.40651300	C	2.07339900	2.11175500	0.08790600
H	5.99061700	-1.53173300	2.97455500	C	1.33787200	3.34006000	-0.28873600
H	5.73819200	0.82832200	3.72581100	C	1.58912400	4.51735200	0.43184000
H	4.14117600	2.33026900	2.55219200	C	0.40051800	3.34639200	-1.33232000
H	2.77377800	1.48211000	0.69698400	C	0.90419800	5.68617900	0.11558300
H	4.64325400	-2.37489400	1.07298400	C	-0.28029200	4.51953400	-1.64934600
C	2.84870100	-1.14491400	-0.36914000	C	-0.03196900	5.68804000	-0.92414200
N	1.45711300	-1.33340600	-0.23203200	H	0.20468800	2.43593600	-1.88745800
H	1.26382200	-1.51255700	1.04361100	H	1.09232200	6.59412200	0.68009000
O	3.48202000	-1.58313100	-1.32833500	H	-1.00605500	4.52171700	-2.45675100
C	0.92220800	-2.26490400	-1.19156400	H	-0.56830700	6.60045500	-1.16767200
C	-0.06132800	-1.77872500	-2.08247700	O	3.00564300	2.10913400	0.88945900
C	1.33842500	-3.57475300	-1.30566800	H	4.30802600	1.09025000	-0.87120600
C	-0.55979800	-2.58755500	-3.13875800	C	-2.70976600	-1.45227000	0.77609600
C	0.81589300	-4.40522500	-2.32549000	C	-3.69094700	-2.16008200	1.46453200
H	2.08858600	-3.96059400	-0.62351500	C	-5.03969600	-2.14227600	1.04761900
C	-1.43347300	0.00970600	-2.69305600	C	-5.44389700	-1.43155700	-0.06175200
C	-1.50498000	-1.99934900	-4.01553600	C	-4.48631800	-0.68869100	-0.79632400
C	-0.09538400	-3.92312700	-3.24075300	C	-3.12402800	-0.69024800	-0.37220200
H	1.16026100	-5.43219200	-2.39215900	N	-2.17422700	0.02334100	-1.05225600
C	-1.91499700	-0.70122000	-3.80939400	C	-2.51098800	0.71866500	-2.12661300
H	-1.80834300	0.99744500	-2.45815400	C	-3.83082100	0.76298900	-2.62006100
H	-1.90041400	-2.58440100	-4.84032200	C	-4.81209400	0.06713800	-1.95115500
H	-0.47512600	-4.55306100	-4.03882100	N	-1.35538100	-1.39171200	1.11381000
H	-2.63382700	-0.22263400	-4.46405000	H	-5.76807400	-2.70822300	1.62149700
N	-0.54997900	-0.51956400	-1.86348400	H	-6.48017200	-1.42737700	-0.38510400
				H	-5.84250200	0.08610400	-2.29464000
E_Q				H	-4.05203200	1.34694000	-3.50651500
C	2.43407900	0.00035700	-0.97516100	H	-1.71450600	1.26984900	-2.61848500
C	3.83756700	0.15973100	-1.16015300	C	-0.71812300	-2.47847700	1.60933400
C	4.60320000	-0.86999200	-1.70017800	C	0.76322000	-2.30239800	1.81541400
C	4.02682100	-2.07607800	-2.08991600	C	1.61520300	-3.33801600	1.40720400
C	2.62567100	-2.28528800	-1.95005100	C	1.31889200	-1.12506800	2.33587000
C	1.83012400	-1.25632000	-1.39108500	C	2.99809800	-3.17071500	1.45283100
N	0.50204600	-1.38521100	-1.20829300	C	2.70413300	-0.96493000	2.39698600
C	-0.09391700	-2.51756100	-1.57818800	C	3.54660300	-1.97958900	1.93945800
C	0.60817600	-3.58968900	-2.15075700	H	0.67148800	-0.32030300	2.66650300
C	1.97386800	-3.47913800	-2.33099200	H	3.64975400	-3.96405500	1.09816700
N	1.59575400	0.91814300	-0.49038100	H	3.11953600	-0.03846400	2.78049600
H	5.67124000	-0.72427200	-1.82216200	H	4.62419900	-1.84632500	1.96283600
H	4.63676500	-2.86890900	-2.51076300	O	-1.22355900	-3.60685200	1.81477400
H	2.55259500	-4.29253500	-2.75740900	H	-3.41129700	-2.73556600	2.33650100

Co	-0.39113300	0.15771000	0.06961300	C	-2.41403600	4.58295400	0.97382800
C	-0.67988100	2.40446200	1.97714100	C	-2.08186900	3.32048900	1.53011000
O	-1.23054300	1.73175300	1.01821600	C	-1.27027100	2.44962500	0.76059900
O	0.36053000	2.06461300	2.57156000	N	-0.91595200	1.21282500	1.23253600
C	-1.40568100	3.68184000	2.35806100	C	-1.26278700	0.82052800	2.44948900
H	2.30992600	4.49569600	1.24175200	C	-2.04960200	1.64328800	3.27827500
H	1.18354800	-4.25440800	1.01845400	C	-2.47401700	2.87106900	2.81598700
H	-0.83148100	4.25708800	3.08635100	N	0.08878800	1.83871600	-1.05172500
H	-2.38286900	3.43026800	2.78540100	H	-2.17878800	5.89256300	-0.69516900
H	-1.58456100	4.28760900	1.46508900	H	-3.03755700	5.26505500	1.54240800
				H	-3.09657000	3.51035600	3.43456100
E_S				H	-2.31596200	1.28613400	4.26609900
C	1.41308000	-1.93217700	1.07640200	H	-0.91515100	-0.15267000	2.77176100
C	1.96337800	-3.14507100	1.48195900	C	1.05695700	2.08688900	-1.97386000
C	3.24880100	-3.19361700	2.06592900	C	2.00614300	0.94201400	-2.15499700
C	4.00458500	-2.05813900	2.27461500	C	3.37841800	1.21486500	-2.14125200
C	3.48027900	-0.80031500	1.88606400	C	1.56374100	-0.39135300	-2.16243200
C	2.19983900	-0.76376300	1.27092500	C	4.29536600	0.16602200	-2.07855100
N	1.65327700	0.40956000	0.83156400	C	2.48881300	-1.43962800	-2.09969600
C	2.28878100	1.55789600	1.03100300	C	3.85352100	-1.16194800	-2.04352700
C	3.54759500	1.60641200	1.65564500	H	0.50703500	-0.62827900	-2.30600700
C	4.14710600	0.43550500	2.06684900	H	5.35870300	0.38351900	-2.04041100
N	0.12638000	-1.70287100	0.57401500	H	2.13021700	-2.46399600	-2.08236000
H	3.64145900	-4.16179600	2.36231900	H	4.57352400	-1.97198800	-1.97773800
H	4.98856600	-2.10763800	2.72908000	O	1.23534800	3.17759100	-2.54596300
H	5.12722800	0.44646500	2.53414300	H	-0.70304000	4.38063900	-1.97825800
H	4.02969300	2.56783400	1.78900600	Co	-0.04930200	0.16754100	-0.08813300
H	1.80487600	2.46030100	0.67957800	C	-2.13726900	-0.53489200	-1.99257600
C	-0.54911500	-2.75654800	-0.01367800	O	-1.81290700	-0.00153900	-0.85513700
C	-2.03816300	-2.77404200	0.08323200	O	-1.37309200	-1.16050200	-2.74396100
C	-2.76773600	-3.47558900	-0.88702700	C	-3.59076700	-0.31208000	-2.36177700
C	-2.71436900	-2.17817700	1.15397800	H	-2.23689200	-3.94008400	-1.71079900
C	-4.15581300	-3.55138800	-0.80324000	H	3.71586700	2.24630100	-2.13453800
C	-4.10284900	-2.26396300	1.24548800	H	-3.89185900	-0.99911600	-3.15413700
C	-4.82670200	-2.94450000	0.26319900	H	-3.70757000	0.71769200	-2.71902200
H	-2.14859600	-1.66090700	1.91717000	H	-4.23376400	-0.43886400	-1.48812200
H	-4.71604600	-4.08139700	-1.56774600				
H	-4.61837500	-1.80286400	2.08284100	E_T			
H	-5.90906700	-3.00613400	0.33007500	C	-1.91581100	1.62416100	0.82508900
O	0.02998400	-3.70217400	-0.57501600	C	-2.83914500	2.65883100	0.92867200
H	1.40849700	-4.06388200	1.34759100	C	-4.12930100	2.41410300	1.45677200
C	-0.74659400	2.81847400	-0.51211700	C	-4.52086800	1.17002700	1.90450600
C	-1.08614300	4.06598900	-1.01848400	C	-3.60285300	0.09088700	1.83174100
C	-1.92619800	4.92592700	-0.26983500	C	-2.32641600	0.33813300	1.26626000

N	-1.40743400	-0.65752000	1.11540300	C	-3.07942700	0.72993000	-2.12884400
C	-1.66000200	-1.88194500	1.56633500	C	-4.34051000	0.22668400	-1.80972900
C	-2.88696100	-2.19674000	2.17269800	H	-0.97912000	0.29943400	-2.31814900
C	-3.86119200	-1.22418000	2.28462500	H	-5.46347300	-1.51372100	-1.20315800
N	-0.57176900	1.68111900	0.42474800	H	-2.95558300	1.77213300	-2.40699300
H	-4.82421900	3.24665800	1.51151500	H	-5.21039500	0.87608100	-1.83706500
H	-5.51063600	1.00180700	2.31571200	O	-0.98364900	-3.53795100	-1.80027000
H	-4.82784900	-1.45570100	2.72168000	H	1.37403700	-3.78081400	-2.35872900
H	-3.05555900	-3.20865300	2.52190700	Co	0.12408500	-0.09147000	0.07926100
H	-0.89160200	-2.63155200	1.42247600	C	1.78692600	0.98489800	-1.99760500
C	-0.08454500	2.84150500	-0.16767700	O	1.71432000	0.44205100	-0.82027800
C	1.34442700	3.17076300	0.08941200	O	0.82024900	1.35256600	-2.67986600
C	2.02023300	3.99598100	-0.81974100	C	3.20975200	1.11975100	-2.50182100
C	2.01097400	2.70220700	1.22900000	H	1.49479800	4.35254900	-1.69919700
C	3.35742000	4.32227500	-0.60649000	H	-3.46850000	-2.99181900	-1.10442400
C	3.34557300	3.03710200	1.44680100	H	3.25586800	1.84541800	-3.31551100
C	4.02294000	3.84070000	0.52526100	H	3.53978800	0.14356700	-2.87600100
H	1.47777800	2.07991700	1.93732300	H	3.88161000	1.41505400	-1.69316700
H	3.88347100	4.94634200	-1.32264400				
H	3.85734400	2.67058100	2.33174900	TSD_S			
H	5.06611700	4.09446000	0.68990300	C	-1.05883900	-1.99324000	-1.36837800
O	-0.78998700	3.59772900	-0.84647300	C	-1.30743300	-3.17185900	-2.07009200
H	-2.58095800	3.65619800	0.60248800	C	-2.55222000	-3.39353700	-2.69533700
C	1.35275700	-2.48998500	-0.65103100	C	-3.57331800	-2.46601200	-2.64302800
C	1.88029800	-3.49812200	-1.44569300	C	-3.36619500	-1.25311900	-1.94326300
C	3.06972700	-4.16282800	-1.06875900	C	-2.11032000	-1.03755800	-1.30843700
C	3.74350900	-3.84294700	0.09085500	N	-1.85429000	0.10751700	-0.60734300
C	3.24479700	-2.81172000	0.92678100	C	-2.77216000	1.06105300	-0.53236900
C	2.05383400	-2.13514200	0.54492400	C	-4.03506200	0.92574900	-1.14012200
N	1.53665700	-1.12116000	1.29822000	C	-4.33452100	-0.22446200	-1.83405400
C	2.12626100	-0.76655900	2.42699300	N	0.15309100	-1.59541500	-0.79663500
C	3.29940600	-1.39776800	2.89149500	H	-2.69964400	-4.32534300	-3.23370300
C	3.85972600	-2.40613900	2.13872600	H	-4.52757700	-2.64481800	-3.12772000
N	0.18474500	-1.75866600	-0.90261200	H	-5.30373700	-0.35595900	-2.30595900
H	3.45171900	-4.94672600	-1.71581100	H	-4.75052300	1.73441500	-1.04464300
H	4.64980500	-4.36689900	0.37782900	H	-2.51628800	1.95452300	0.02054900
H	4.77123300	-2.90125800	2.46079400	C	1.00862000	-2.57908800	-0.36224100
H	3.74549300	-1.07192000	3.82429100	C	2.47016500	-2.27280100	-0.30146200
H	1.66944900	0.04439900	2.98542100	C	3.25672300	-2.93448200	0.65203500
C	-0.91080100	-2.33692500	-1.48715400	C	3.08599100	-1.43137800	-1.23524500
C	-2.09304200	-1.43804500	-1.67616100	C	4.63542700	-2.73693600	0.68684200
C	-3.36784000	-1.95179900	-1.39689300	C	4.46817200	-1.24847600	-1.21343400
C	-1.95772900	-0.09954100	-2.06584800	C	5.24474200	-1.89579900	-0.24907100
C	-4.48274600	-1.11879000	-1.45141500	H	2.48272000	-0.93100400	-1.98166400

H	5.23551500	-3.23943500	1.43969300			
H	4.93866200	-0.60193500	-1.94848400	F_Q		
H	6.32045400	-1.74703900	-0.22734800	C	2.60869300	0.42937600 -1.26819600
O	0.64354200	-3.73301600	-0.06118600	C	3.79385800	0.99554100 -1.73460000
H	-0.53774600	-3.92875600	-2.14174100	C	4.86305600	0.18508400 -2.17425400
C	0.08711600	2.89804900	0.47604200	C	4.78814700	-1.19216100 -2.15646700
C	0.14878300	4.20523400	0.94496300	C	3.60373400	-1.81542100 -1.68781200
C	0.63900300	5.23473700	0.10709100	C	2.52381800	-0.99887700 -1.25123600
C	1.05134300	4.99615700	-1.18754100	N	1.36762300	-1.54120000 -0.78477000
C	0.99428700	3.67673800	-1.70656500	C	1.21911400	-2.85748800 -0.73137400
C	0.52847000	2.63849200	-0.85851700	C	2.23084000	-3.73889700 -1.15524400
N	0.45389600	1.34272800	-1.29197000	C	3.41858100	-3.21869000 -1.62703900
C	0.76592700	1.03405600	-2.53941700	N	1.45401800	1.11421400 -0.88738400
C	1.22115700	2.01029200	-3.44891300	H	5.76427700	0.67107100 -2.53597400
C	1.35003800	3.31723600	-3.03163800	H	5.61507400	-1.80735900 -2.49663100
N	-0.38618600	1.76436700	1.12197800	H	4.22188100	-3.87295100 -1.95321600
H	0.67951000	6.24471900	0.50426300	H	2.06463800	-4.80876800 -1.09923500
H	1.41002400	5.80058600	-1.82158600	H	0.27716100	-3.22212400 -0.33482900
H	1.71134000	4.08427700	-3.71023400	C	1.54928200	2.42767300 -0.47991500
H	1.47038000	1.71232600	-4.46090300	C	0.31246800	3.24978300 -0.61920200
H	0.65760800	-0.00604200	-2.82383900	C	0.06416100	4.26466600 0.31454900
C	-1.12037300	1.73087500	2.26114900	C	-0.58098500	3.04887300 -1.67807100
C	-1.61831800	0.34696900	2.51799600	C	-1.08889000	5.03988300 0.21366200
C	-2.75554600	0.12884600	3.29117700	C	-1.72375500	3.83920400 -1.79079700
C	-0.97548200	-0.71487100	1.83535800	C	-1.98530300	4.82746100 -0.83905600
C	-3.28773000	-1.16058000	3.37567400	H	-0.37511800	2.27689400 -2.40950500
C	-1.53470200	-2.00051600	1.92923500	H	-1.29041000	5.80951000 0.95269500
C	-2.68230800	-2.22106100	2.69327600	H	-2.41106700	3.68131900 -2.61667700
H	0.31514800	-0.78742900	2.07056100	H	-2.88244300	5.43449600 -0.91788800
H	-4.18063000	-1.33842000	3.96802500	O	2.57346700	2.93760600 0.00784600
H	-1.05583600	-2.83359300	1.42316900	H	3.89921400	2.07170400 -1.76701500
H	-3.10405600	-3.21967800	2.76323500	C	-2.31748300	-1.88196900 0.47695300
O	-1.42355000	2.71009300	2.97068600	C	-3.35560300	-2.63211900 1.03165000
H	-0.18413800	4.43027400	1.94815800	C	-4.48565800	-2.98935200 0.26232300
Co	-0.07865900	0.14747900	0.16109500	C	-4.61427600	-2.62904700 -1.06186200
C	2.20381100	-0.09290700	1.83372300	C	-3.58612900	-1.86741900 -1.67326600
O	1.76567300	0.35223200	0.73038100	C	-2.45224000	-1.48671900 -0.89960200
O	1.49997000	-0.81926500	2.60640200	N	-1.44397800	-0.74341300 -1.43973800
C	3.59178900	0.29277400	2.25296200	C	-1.49024000	-0.39188300 -2.71565300
H	-3.23116000	0.96454600	3.79575100	C	-2.56822800	-0.73448200 -3.55570500
H	2.77456600	-3.59337800	1.36649100	C	-3.61476000	-1.46006300 -3.03105000
H	3.52246400	1.23546400	2.80866400	N	-1.14834500	-1.45601700 1.08042600
H	4.01986800	-0.46649300	2.90799000	H	-5.26941000	-3.57177000 0.73901700
H	4.22397100	0.45009300	1.37884200	H	-5.48216800	-2.91759500 -1.64660300

H	-4.46712700	-1.73388200	-3.64645500	C	-2.24993900	1.41792100	-0.89506000
H	-2.55928400	-0.41894100	-4.59297100	C	-3.10947900	0.20183700	-1.03626900
H	-0.64824600	0.17885700	-3.09454500	C	-4.31627800	0.14517900	-0.32526100
C	-0.75602600	-1.82590400	2.31702800	C	-2.79330600	-0.82504900	-1.93374900
C	0.54403700	-1.19200900	2.70961700	C	-5.17638600	-0.93976400	-0.48291800
C	1.17167700	-1.53332500	3.91269100	C	-3.66478200	-1.89929400	-2.10994000
C	1.12949200	-0.25057900	1.85566800	C	-4.85348200	-1.96337100	-1.37887100
C	2.38804600	-0.93904600	4.25167000	H	-1.86992900	-0.77731300	-2.49592000
C	2.34836300	0.33967300	2.18686200	H	-6.09932000	-0.98610200	0.08759600
C	2.97519600	-0.00509100	3.39380200	H	-3.41538200	-2.68638600	-2.81558000
H	-0.07076800	1.35178100	2.26938800	H	-5.52741600	-2.80529600	-1.50788600
H	2.87972100	-1.20304900	5.18372900	O	-2.82552600	2.51658100	-0.74930600
H	2.81483200	1.07206600	1.53396800	H	-1.55302400	3.53747700	-2.44592900
H	3.92120300	0.45951800	3.66053300	C	1.85987500	-2.17760500	0.60352900
O	-1.34225300	-2.61048600	3.09879000	C	2.62226900	-3.21049300	1.14288000
H	-3.28540300	-2.94433000	2.06309700	C	3.16795600	-4.20736500	0.30159300
Co	0.04284500	-0.09394100	-0.03677100	C	2.98834100	-4.19457200	-1.06594700
C	-1.76423300	1.90784200	1.60976600	C	2.22504700	-3.15530100	-1.65749000
O	-1.63401200	1.30931000	0.54162400	C	1.65050200	-2.16535000	-0.81464500
O	-0.82279600	1.92893000	2.54614500	N	0.89364600	-1.14421900	-1.31951400
C	-3.01156800	2.63972600	1.99129000	C	0.72877000	-1.02931600	-2.62649000
H	-3.59674600	1.99084400	2.65363400	C	1.27317700	-1.96008200	-3.53548200
H	-2.77076000	3.55320700	2.53795100	C	2.00398900	-3.02319200	-3.05257100
H	-3.59791400	2.86542400	1.10131400	N	1.27821400	-1.10569300	1.26066700
H	0.70100100	-2.26327700	4.56531800	H	3.75439100	-4.99983500	0.75778500
H	0.76746900	4.42033900	1.12595700	H	3.42536600	-4.95970800	-1.69975000
				H	2.42676500	-3.76119300	-3.72818600
				H	1.10285700	-1.82644700	-4.59793400
F_S				H	0.15024200	-0.17733700	-2.96707100
C	-0.12382500	2.37448500	-1.34137000	C	1.32705300	-0.84183000	2.59113000
C	-0.52395700	3.45793500	-2.12357800	C	0.55962000	0.39707100	2.89922200
C	0.39687300	4.45489500	-2.50728000	C	0.49846300	0.92854100	4.18782600
C	1.72326800	4.41205200	-2.12780100	C	-0.11171500	1.00241900	1.81412700
C	2.17751200	3.33124100	-1.33455700	C	-0.23772100	2.09348100	4.41406400
C	1.24472200	2.32581800	-0.95147000	C	-0.83699600	2.17404100	2.05476600
N	1.62526300	1.25773200	-0.18729800	C	-0.89971400	2.71164500	3.35120100
C	2.88503100	1.13708100	0.20958600	H	-1.93256500	0.15469800	2.08995000
C	3.86549300	2.08801500	-0.13290100	H	-0.29577500	2.51708900	5.41244000
C	3.51662400	3.17845600	-0.89632700	H	-1.36784100	2.67402600	1.25066400
N	-0.89137900	1.26565400	-0.97483900	H	-1.47130600	3.61957500	3.52592300
H	0.03970400	5.27711500	-3.12076000	O	1.92877600	-1.51055800	3.45689600
H	2.42379600	5.18556300	-2.42520700	H	2.79965800	-3.23969000	2.20831800
H	4.25360500	3.92698100	-1.17166600	Co	0.19694200	0.03684900	0.17517600
H	4.88107900	1.94081400	0.21639800	C	-2.06543700	-1.56630700	1.30908900
H	3.13013600	0.27395700	0.81282800				

O	-1.18036100	-1.36332700	0.46736800	C	-1.60210700	-2.16448100	-0.88392000
O	-2.46900000	-0.66758200	2.18378300	N	-0.74486100	-1.22076800	-1.38095500
C	-2.74090100	-2.89177600	1.42047400	C	-0.57785700	-1.10221700	-2.68893300
H	-2.20108300	-3.47864700	2.17347600	C	-1.29127800	-1.89521400	-3.60885500
H	-3.77361100	-2.77377100	1.75012700	C	-2.18946500	-2.82878600	-3.13722900
H	-2.69277800	-3.41387400	0.46558300	N	-0.82293300	-1.42444700	1.21928500
H	1.02345500	0.42825900	4.99720700	H	-3.98988300	-4.77703500	0.66351400
H	-4.56376500	0.95119500	0.35775800	H	-3.84125000	-4.58793000	-1.80498000
F_T				H	-2.75964900	-3.44830500	-3.82344600
C	2.47745300	0.79149700	-1.22612000	H	-1.12574300	-1.75536900	-4.67111000
C	3.44343300	1.52069700	-1.91590400	H	0.13966600	-0.35853100	-3.01801000
C	4.73243900	0.99366000	-2.14669700	C	-0.59524500	-1.41518400	2.56182100
C	5.10011400	-0.25737200	-1.69788500	C	0.36656600	-0.33427500	2.90304200
C	4.15371400	-1.04068400	-0.99371800	C	0.80188500	-0.10109800	4.20890600
C	2.84796200	-0.51393000	-0.76849100	C	0.82152900	0.45965600	1.83360600
N	1.90658600	-1.22898800	-0.09741900	C	1.70107000	0.93656300	4.45439100
C	2.18251900	-2.43497600	0.36605000	C	1.72685600	1.49268400	2.08270800
C	3.44612700	-3.03523200	0.18499400	C	2.15665800	1.72910300	3.39661700
C	4.42392400	-2.33915500	-0.49006900	H	-0.96102800	1.72735100	2.00202200
N	1.14520900	1.18337300	-1.02808300	H	2.04565000	1.13097400	5.46574400
H	5.44750600	1.60194400	-2.69323200	H	2.09794800	2.12500500	1.28340000
H	6.09562700	-0.65270700	-1.87371200	H	2.85446900	2.53950300	3.59006300
H	5.40912000	-2.77003100	-0.64427900	O	-1.09835700	-2.18243000	3.40376900
H	3.62747300	-4.02872600	0.57994600	H	-2.61259700	-3.35210200	2.14270200
H	1.38652900	-2.94540000	0.89988500	Co	0.09287300	-0.12027900	0.11893400
C	0.85268900	2.51873000	-0.95431600	C	-2.62747300	1.43330100	1.14542100
C	-0.57615700	2.90861100	-1.16086600	O	-2.13041000	0.78500600	0.23201000
C	-1.12498500	3.92110000	-0.36337500	O	-1.90238600	1.96569400	2.13368800
C	-1.34650500	2.34038800	-2.18207100	C	-4.09711600	1.67641900	1.29539000
C	-2.44670600	4.32063500	-0.54982400	H	-4.48158400	0.99926700	2.06701400
C	-2.65993900	2.76106100	-2.38802600	H	-4.28693500	2.70111400	1.62102800
C	-3.21695800	3.74060600	-1.56322200	H	-4.60456700	1.47244500	0.35308100
H	-0.91372900	1.57600800	-2.81543700	H	0.43041300	-0.73029800	5.01318400
H	-2.87674400	5.08536600	0.09023900	H	-0.51603100	4.37154400	0.41403900
H	-3.24933700	2.32040000	-3.18684500	INT1_AQ_Q			
H	-4.24506000	4.05754800	-1.71220100	C	-2.90574100	-0.25798900	0.89781600
O	1.68445900	3.42149200	-0.72994100	C	-4.15250700	-0.04532800	1.47965200
H	3.20601900	2.50922300	-2.28489700	C	-5.25723900	-0.86041000	1.14507500
C	-1.67354600	-2.28800900	0.54035800	C	-5.15345800	-1.88777300	0.23161900
C	-2.54198800	-3.23624300	1.07081600	C	-3.90389800	-2.14151300	-0.38962200
C	-3.32040600	-4.04969400	0.21349400	C	-2.79011300	-1.32597300	-0.04853100
C	-3.24589100	-3.95021000	-1.15933800	N	-1.56749400	-1.52510000	-0.61972800
C	-2.36770400	-2.99895400	-1.74124400	C	-1.39074700	-2.49318700	-1.51049500

C	-2.43825500	-3.34833500	-1.89637800	H	-0.88068800	3.70975500	-4.57474100
C	-3.68841700	-3.16974700	-1.33977700	H	-2.48953900	2.11962700	-0.91553800
N	-1.71832400	0.42493500	1.17069000	H	-2.66517000	3.65353400	-2.84827200
H	-6.20945300	-0.66299300	1.62821200	O	2.54619400	0.45394900	-3.17730000
H	-6.00752800	-2.50839400	-0.01994800	H	3.85453800	-1.20319600	-2.49127700
H	-4.51879200	-3.81015100	-1.62258400	Co	-0.18670500	-0.13032300	-0.00570200
H	-2.24939700	-4.12838600	-2.62487500	H	1.10016400	2.19898300	-4.36704700
H	-0.39458900	-2.58942700	-1.93085900	H	-0.84477300	4.21032100	1.32096300
C	-1.73316500	1.71054800	1.64755100	C	3.58341700	2.03391900	-0.18562900
C	-0.40404900	2.24753000	2.08023500	C	2.93278300	3.02668300	-0.79046700
C	-0.11209300	3.59626100	1.83451700	H	3.65021900	1.96836300	0.89741100
C	0.52934000	1.45163500	2.75901100	H	4.06774700	1.24424900	-0.75416500
C	1.10947600	4.13294200	2.23583600	H	2.86525300	3.08150300	-1.87388300
C	1.74685500	1.99402600	3.17145900	H	2.44028900	3.81624500	-0.22882100
C	2.04150200	3.33280300	2.90489400				
H	0.28947800	0.41999900	2.98290800				
H	1.33552000	5.17515400	2.03124300	INT1_AQ_S			
H	2.46017100	1.37315000	3.70541600	C	-1.37800300	-1.43129200	1.54793200
H	2.99121300	3.75399000	3.22093800	C	-2.32683700	-2.01786300	2.38671400
O	-2.73404800	2.44727100	1.68728200	C	-1.95262200	-2.97112100	3.35484100
H	-4.27765300	0.75105800	2.20004900	C	-0.64139700	-3.37024700	3.51896800
C	2.44985300	-1.28262100	-0.87798700	C	0.35749200	-2.80387300	2.69224100
C	3.62424300	-1.65041800	-1.53588400	C	-0.02582500	-1.84251800	1.71258900
C	4.50616700	-2.59971100	-0.97021700	N	0.89682200	-1.26750400	0.88307400
C	4.25193800	-3.20739600	0.24018100	C	2.17895400	-1.59139800	0.98871000
C	3.07007700	-2.86883700	0.94751800	C	2.63484700	-2.52526900	1.93841300
C	2.18470700	-1.90223100	0.39109300	C	1.73289000	-3.13211300	2.78111000
N	1.04185900	-1.53238700	1.03701900	N	-1.59486300	-0.39507600	0.63633400
C	0.71791300	-2.10194700	2.19050200	H	-2.72752900	-3.39556200	3.98677000
C	1.53022200	-3.07282200	2.80548100	H	-0.36004400	-4.10474500	4.26644000
C	2.70446900	-3.44694100	2.18841700	H	2.05825200	-3.86029500	3.51804100
N	1.47274500	-0.39464100	-1.28916900	H	3.69434800	-2.75029500	1.98138900
H	5.40796100	-2.85442800	-1.52011900	H	2.87178200	-1.11257700	0.31217900
H	4.93226600	-3.94100800	0.66103500	C	-2.86736400	-0.26396200	0.13151200
H	3.35774100	-4.18901000	2.63851900	C	-3.35297500	1.10672600	-0.22245300
H	1.22240900	-3.50635700	3.75031300	C	-4.18324400	1.27542200	-1.33972500
H	-0.21444800	-1.78327300	2.64666700	C	-3.09221000	2.20245300	0.60977000
C	1.58941400	0.40659800	-2.37298400	C	-4.69343000	2.53281800	-1.65306000
C	0.40686200	1.30991700	-2.53578300	C	-3.62735400	3.45664000	0.31249500
C	0.30775500	2.18516200	-3.62397300	C	-4.41492900	3.62700500	-0.82761100
C	-0.59533900	1.28944700	-1.56553500	H	-2.48295800	2.06731700	1.49379800
C	-0.79938400	3.02724700	-3.73354700	H	-5.31328900	2.66066500	-2.53551200
C	-1.70549700	2.12264000	-1.66744700	H	-3.42634300	4.29831800	0.96863000
C	-1.80385300	2.99582300	-2.76145700	H	-4.82002800	4.60564400	-1.06790400
				O	-3.67061000	-1.20736200	-0.00220200



H	-3.36817300	-1.73743000	2.30022800	C	-3.92514100	1.57417600	-0.89767900
C	2.58885800	1.29934800	-0.70636500	C	-2.56979400	1.31330500	-0.54868800
C	3.83210900	1.74788600	-1.14483500	N	-1.87774800	0.28591400	-1.11764200
C	4.50180500	2.78009000	-0.44832900	C	-2.45388100	-0.49110300	-2.01872200
C	3.97336000	3.36770100	0.68228900	C	-3.78950300	-0.29896300	-2.42847500
C	2.71253400	2.93444200	1.16677000	C	-4.51882100	0.72633300	-1.86754300
C	2.02240800	1.91673700	0.45495000	N	-0.56336700	1.72902400	0.71227300
N	0.79703500	1.45999000	0.85959500	H	-4.44821100	4.22447200	1.16628200
C	0.25841300	1.92408200	1.97456400	H	-5.63526900	2.85322600	-0.53016300
C	0.87995200	2.92665600	2.74711100	H	-5.55162700	0.89805000	-2.15683800
C	2.09060900	3.43967600	2.33748400	H	-4.22094200	-0.96077700	-3.17103700
N	1.80429200	0.28417900	-1.23373700	H	-1.84771000	-1.29430500	-2.42723100
H	5.46831900	3.10749900	-0.82056500	C	0.33993400	2.61796100	1.22434900
H	4.50628800	4.15013500	1.21314400	C	1.62566300	2.02987800	1.72318200
H	2.58669800	4.22011200	2.90707900	C	2.81868600	2.73110900	1.49831600
H	0.39166400	3.27891300	3.64878500	C	1.65485500	0.84233700	2.46716700
H	-0.68690800	1.48610500	2.27056200	C	4.02681300	2.23302700	1.98013800
C	2.17950300	-0.60265700	-2.19631900	C	2.86292900	0.35858300	2.97223600
C	1.13396400	-1.64214600	-2.37678900	C	4.05107900	1.04715200	2.72237700
C	1.28346500	-2.69617100	-3.28275900	H	0.73172000	0.31046800	2.66798000
C	-0.01916800	-1.51361300	-1.57862000	H	4.94974800	2.77111200	1.78501600
C	0.27240900	-3.64969800	-3.39498400	H	2.87299000	-0.55097700	3.56494500
C	-1.02122800	-2.47824400	-1.69288800	H	4.99205400	0.66641500	3.10825700
C	-0.87233800	-3.53800000	-2.59845400	O	0.17285800	3.84935100	1.29174900
H	0.37278600	-4.47518700	-4.09373100	H	-2.10620500	3.77275000	1.75781200
H	-1.92274600	-2.41946300	-1.09189900	C	0.03332400	-2.72558400	-0.38955000
H	-1.66025400	-4.28283900	-2.68135900	C	0.20923200	-4.03579600	-0.82152000
O	3.25373000	-0.58187200	-2.83185900	C	-0.45630400	-5.09703100	-0.16254400
H	4.28295900	1.29620600	-2.01631800	C	-1.29081400	-4.88495900	0.91398500
Co	0.13117400	-0.01352700	-0.36263400	C	-1.49487600	-3.56236000	1.38643200
H	2.18633000	-2.75689200	-3.88465000	C	-0.82744900	-2.49544100	0.72882300
H	-4.40876800	0.41689500	-1.96469700	N	-0.97145700	-1.19703000	1.13319000
C	-0.55629500	1.92476300	-1.56357500	C	-1.75527700	-0.91010300	2.16187000
C	-0.90383800	0.87943000	-2.34891800	C	-2.45881200	-1.90706000	2.86673200
H	-1.24748100	2.37001500	-0.86157400	C	-2.32889500	-3.22418600	2.48179200
H	0.38860900	2.43398000	-1.71374800	N	0.59262100	-1.56131400	-0.90866600
H	-0.24809900	0.54179900	-3.14187400	H	-0.29734900	-6.10753700	-0.52750000
H	-1.89215000	0.43950400	-2.32314700	H	-1.79603900	-5.70910800	1.40739800
				H	-2.85835400	-4.01301500	3.00813600
INT1_AQ_T				H	-3.08939400	-1.62161100	3.70111400
C	-1.88009800	2.11515800	0.41787500	H	-1.83240400	0.13635600	2.43724000
C	-2.58873400	3.15142800	1.01678600	C	1.55204200	-1.50549600	-1.88531100
C	-3.93536400	3.40508000	0.67122000	C	1.87857500	-0.09182100	-2.19877400
C	-4.60268800	2.64692000	-0.26675900	C	2.81279700	0.26171700	-3.17536300

C	1.18151800	0.88285800	-1.46588100	H	0.31375000	-5.63636400	1.61506100
C	3.04774800	1.61116200	-3.43610200	H	-2.09215400	-2.46821400	3.25672500
C	1.40790800	2.23075800	-1.74474300	H	-1.78097800	-4.87745500	2.71870400
C	2.34120300	2.58842800	-2.72765300	O	3.25156800	-1.76728800	1.38817300
H	3.77122500	1.90378800	-4.19128200	H	4.42417300	0.06557100	1.47355100
H	0.87701200	3.01428200	-1.21459300	C	-2.70679500	0.36801600	-1.13615100
H	2.51551200	3.64026600	-2.93895200	C	-3.74353600	0.27676200	-2.06288900
O	2.07341900	-2.47946900	-2.45203500	C	-5.05034500	0.70791100	-1.73799700
H	0.85642200	-4.23904600	-1.66202900	C	-5.36110900	1.23438400	-0.50373900
Co	-0.01736400	0.08261100	-0.16201900	C	-4.34201800	1.34651000	0.47584900
H	3.33677300	-0.51984300	-3.71879100	C	-3.02385200	0.90976600	0.15775900
H	2.78876800	3.65857800	0.93589800	N	-2.01310100	0.99220300	1.07228000
C	3.53381500	-2.29701600	0.62905100	C	-2.24462700	1.49373300	2.27662300
C	4.27070000	-1.40881500	-0.03620900	C	-3.51742300	1.94887700	2.67222200
H	3.31757200	-2.18416600	1.68842800	C	-4.55944000	1.87213700	1.77425200
H	3.11258800	-3.16906900	0.13549800	N	-1.37286800	-0.00180500	-1.29987400
H	4.47952300	-1.52723100	-1.09614200	H	-5.82479300	0.61647600	-2.49446200
H	4.68562200	-0.52860900	0.44837700	H	-6.36736100	1.56382400	-0.26444200

INT2\_AQ\_Q

C	2.57219600	0.96210500	0.88786900
C	3.94666600	0.96485300	1.11690200
C	4.72727600	2.11921400	0.87746200
C	4.17706200	3.29036500	0.40611800
C	2.78201200	3.34322800	0.15974200
C	1.98999200	2.18448700	0.40251800
N	0.64646800	2.19079600	0.16528500
C	0.05051000	3.28226000	-0.29145400
C	0.75777300	4.47192500	-0.54933900
C	2.11744900	4.49710900	-0.32628600
N	1.66777200	-0.08334700	1.10206900
H	5.79482200	2.06597900	1.07182800
H	4.78497800	4.17006000	0.21929800
H	2.69610600	5.39579700	-0.52033600
H	0.22747100	5.34133300	-0.92149600
H	-1.01959500	3.21512600	-0.46472200
C	2.07702000	-1.34226500	1.40554800
C	0.97772400	-2.29758600	1.77992900
C	1.15939700	-3.66161900	1.51244500
C	-0.19772800	-1.87909900	2.42233000
C	0.16945700	-4.58436700	1.84293300
C	-1.18852900	-2.80452900	2.75676800
C	-1.00952600	-4.15757100	2.46195000
H	-0.33059900	-0.83294500	2.68385700

H	0.31375000	-5.63636400	1.61506100
H	-2.09215400	-2.46821400	3.25672500
H	-1.78097800	-4.87745500	2.71870400
O	3.25156800	-1.76728800	1.38817300
H	4.42417300	0.06557100	1.47355100
C	-2.70679500	0.36801600	-1.13615100
C	-3.74353600	0.27676200	-2.06288900
C	-5.05034500	0.70791100	-1.73799700
C	-5.36110900	1.23438400	-0.50373900
C	-4.34201800	1.34651000	0.47584900
C	-3.02385200	0.90976600	0.15775900
N	-2.01310100	0.99220300	1.07228000
C	-2.24462700	1.49373300	2.27662300
C	-3.51742300	1.94887700	2.67222200
C	-4.55944000	1.87213700	1.77425200
N	-1.37286800	-0.00180500	-1.29987400
H	-5.82479300	0.61647600	-2.49446200
H	-6.36736100	1.56382400	-0.26444200
H	-5.55511300	2.21106800	2.04599300
H	-3.65673300	2.34801000	3.67063100
H	-1.39836200	1.53782600	2.95627200
C	-0.90320000	-0.63319100	-2.40187800
C	0.57028200	-0.94905000	-2.31669000
C	1.50543500	0.08805300	-2.41876100
C	1.00014300	-2.27601000	-2.11183200
C	2.87035300	-0.16908900	-2.27938200
C	2.37014500	-2.51194800	-1.95840200
C	3.30044700	-1.47187600	-2.03217200
H	3.58532000	0.64567000	-2.34001500
H	2.71150700	-3.52700500	-1.77360400
H	4.35675600	-1.68192200	-1.89322000
O	-1.54148600	-0.95621200	-3.42553200
H	-3.53942800	-0.13094400	-3.04133400
Co	-0.17364100	0.28167300	0.32263600
H	1.15601800	1.10382800	-2.57989400
H	2.07796400	-3.98330400	1.03381000
C	-1.13617500	-3.24189900	-1.13542500
C	0.00737500	-3.42604000	-2.07643700
H	-0.97638000	-2.84071000	-0.14335400
H	-2.12499200	-3.60908000	-1.38874600
H	-0.38462500	-3.58519400	-3.08949700
H	0.56554300	-4.34288200	-1.82351700

INT2\_AQ\_S

C	-0.95887000	-1.82070900	1.44781200	H	-0.12182400	0.76429300	2.71279200
C	-1.70279600	-2.54330600	2.37663500	C	1.55190600	0.27626500	-2.64672500
C	-1.20749600	-3.73897500	2.93760200	C	0.24583300	-0.40269800	-2.95318900
C	0.03208000	-4.24218800	2.59605400	C	0.27751800	-1.72555100	-3.41539900
C	0.82827900	-3.53739300	1.66094900	C	-0.99011000	0.24174000	-2.70244700
C	0.32487700	-2.32792200	1.09919500	C	-0.90464200	-2.43971500	-3.58807400
N	1.04357200	-1.59894800	0.19777100	C	-2.16839100	-0.49727500	-2.89336300
C	2.23917800	-2.02210000	-0.18244400	C	-2.13097200	-1.82376800	-3.31665500
C	2.81147600	-3.21105000	0.31499600	H	-0.87322600	-3.47024400	-3.92865100
C	2.11265500	-3.96051100	1.23499200	H	-3.12314100	-0.01250800	-2.71480400
N	-1.34837100	-0.58700500	0.90277200	H	-3.05764100	-2.37509200	-3.44568100
H	-1.82364400	-4.26752800	3.65937500	O	2.48440500	0.33427000	-3.47288100
H	0.40792300	-5.16324900	3.03017300	H	4.03028300	1.71641000	-2.28806000
H	2.53137500	-4.87651100	1.64192400	Co	0.12697500	0.22653300	-0.21523300
H	3.79371100	-3.51229500	-0.03172500	H	1.23886100	-2.18994600	-3.61396600
H	2.77234000	-1.40914800	-0.90040800	H	-4.58824000	0.56931700	-1.00629300
C	-2.67790000	-0.46355500	0.57722000	C	-0.67017700	1.90992700	-0.78734000
C	-3.29849300	0.89170400	0.68211300	C	-1.05675700	1.70086500	-2.26326900
C	-4.30383900	1.26124500	-0.22060700	H	-1.52852200	2.13846500	-0.16586300
C	-2.95239700	1.76238400	1.72377600	H	0.07279600	2.70307200	-0.67691800
C	-4.91783400	2.50793000	-0.11520800	H	-0.39185300	2.28385200	-2.90934200
C	-3.58638800	2.99840400	1.84582800	H	-2.07634100	2.05730700	-2.44345600
C	-4.55978800	3.37880900	0.91831400				
H	-2.18564800	1.46689100	2.43067800				
H	-5.67911600	2.79933800	-0.83286600	INT2_AQ_T			
H	-3.31930300	3.66545200	2.66027300	C	2.25880400	-0.20425300	-1.16832900
H	-5.04396900	4.34722100	1.00482400	C	3.63915100	-0.31816800	-1.31852400
O	-3.40699500	-1.41767200	0.24177000	C	4.21835500	-1.47731700	-1.88379500
H	-2.68199600	-2.18386000	2.67279200	C	3.45814900	-2.54334000	-2.30939700
C	2.59543000	1.38469100	-0.73037500	C	2.04744100	-2.47337200	-2.18707200
C	3.79673800	1.86138600	-1.24256800	C	1.45869700	-1.30954200	-1.61485700
C	4.70747400	2.52899500	-0.39038900	N	0.10750400	-1.20171000	-1.45837800
C	4.45435100	2.72267100	0.95268500	C	-0.68565900	-2.18621700	-1.85482500
C	3.24231700	2.24232100	1.51323900	C	-0.18910900	-3.36455200	-2.44306200
C	2.32612900	1.58103400	0.65652900	C	1.17249300	-3.50798000	-2.60033300
N	1.13602500	1.08364500	1.12263100	N	1.52869200	0.89177500	-0.68887100
C	0.82197900	1.19510100	2.40619300	H	5.30036800	-1.51770800	-1.97235300
C	1.68329500	1.83638100	3.31870900	H	3.91287900	-3.43259700	-2.73445500
C	2.87913600	2.36110300	2.87898200	H	1.59082800	-4.40882600	-3.04011600
N	1.56776100	0.71518000	-1.37431000	H	-0.88072500	-4.13956300	-2.75378400
H	5.63733400	2.89373200	-0.81680200	H	-1.75064900	-2.05110900	-1.69659700
H	5.16918300	3.23040500	1.59211200	C	2.14879300	2.05125100	-0.32291600
H	3.55347700	2.86175700	3.56722900	C	1.27852200	3.27137800	-0.30749200
H	1.38384400	1.90615300	4.35814000	C	1.60543300	4.33028300	0.55046000
				C	0.15650300	3.38182100	-1.13837500

C	0.79380000	5.46155200	0.61000300	H	-0.47674000	0.13647800	3.43191700
C	-0.65086800	4.51761900	-1.08679700	H	0.73117900	1.41948300	3.50553100
C	-0.33965400	5.55473900	-0.20390900				
H	-0.06848100	2.57539700	-1.82664000	TS_AQ_S			
H	1.04131800	6.27033200	1.29126500	C	-1.26870800	-1.58402600	1.44406100
H	-1.51864800	4.59504000	-1.73527400	C	-2.18286900	-2.28103800	2.23538500
H	-0.97201600	6.43647600	-0.15606600	C	-1.75939300	-3.26961900	3.14606100
O	3.35409000	2.17548800	-0.02643700	C	-0.42708300	-3.59372300	3.30271100
H	4.27761000	0.48405400	-0.98433800	C	0.54034100	-2.90761700	2.53128100
C	-2.54419600	-1.24000900	0.93658600	C	0.10906700	-1.91062300	1.60676200
C	-3.39492400	-2.13734800	1.58102800	N	1.00095100	-1.21888700	0.83921400
C	-4.78358500	-2.13186100	1.32839900	C	2.29811500	-1.45711400	0.95882700
C	-5.35719300	-1.25345100	0.43493700	C	2.80743500	-2.42162900	1.85113300
C	-4.53360500	-0.32458200	-0.24863800	C	1.93419000	-3.14643000	2.62828900
C	-3.13118600	-0.31462200	0.00697100	N	-1.56907000	-0.51446700	0.58976600
N	-2.29664300	0.55725800	-0.63806700	H	-2.51229700	-3.78155800	3.73870300
C	-2.79473600	1.40439800	-1.52780200	H	-0.10624500	-4.35587100	4.00556400
C	-4.16789100	1.46325700	-1.83550800	H	2.29546900	-3.89932700	3.32278400
C	-5.03233800	0.60524200	-1.19476800	H	3.87925900	-2.57571900	1.90554200
N	-1.17608300	-1.10653100	1.11963100	H	2.96748200	-0.87846700	0.33557700
H	-5.40672500	-2.84822400	1.85624800	C	-2.83342900	-0.49355200	0.05462400
H	-6.42468400	-1.26016500	0.23873400	C	-3.44627400	0.83073400	-0.27832800
H	-6.09755900	0.62362500	-1.40632500	C	-4.25272000	0.93851400	-1.42003600
H	-4.51824800	2.18028400	-2.56933500	C	-3.30792600	1.93568000	0.57114200
H	-2.09235500	2.06180500	-2.02530400	C	-4.86292200	2.14950100	-1.73842800
C	-0.40285400	-2.02253900	1.74824300	C	-3.94067100	3.14107600	0.26656800
C	1.02463100	-1.59830500	1.95268600	C	-4.70644400	3.25453500	-0.89590600
C	2.03405300	-2.51589400	1.63492200	H	-2.71361200	1.84698200	1.47096700
C	1.35865900	-0.31560400	2.43577100	H	-5.46492700	2.23217200	-2.63853100
C	3.37587300	-2.16098700	1.74846700	H	-3.83461600	3.99027600	0.93524800
C	2.71154900	0.02218600	2.55121100	H	-5.18806900	4.19685100	-1.14033500
C	3.71376300	-0.88317600	2.20014500	O	-3.53179600	-1.50859400	-0.14711700
H	4.15185600	-2.86904400	1.47424300	H	-3.23954300	-2.06276100	2.15417400
H	2.97847200	1.00867400	2.92015800	C	2.43048700	1.66985200	-0.62761700
H	4.75677200	-0.59209500	2.28378000	C	3.61129500	2.28893000	-1.02501300
O	-0.76188800	-3.16350200	2.11081300	C	4.11485000	3.38762700	-0.29037200
H	-2.97833900	-2.84878600	2.27866200	C	3.48203700	3.87097100	0.83637600
Co	-0.30348500	0.31508600	-0.04191800	C	2.28166100	3.25845200	1.28041000
H	1.75127600	-3.50219300	1.28000700	C	1.75823200	2.17451000	0.52789100
H	2.48503400	4.24414700	1.18004500	N	0.60381500	1.53334600	0.89327800
C	-0.40596300	1.38572900	1.68884700	C	-0.01732700	1.88281900	2.00871800
C	0.27810500	0.66840600	2.84601400	C	0.44206800	2.94177900	2.81818700
H	0.08300600	2.30962200	1.39372600	C	1.57239700	3.63682900	2.44905000
H	-1.47732700	1.52769200	1.83309600	N	1.79214300	0.57376500	-1.18754700

H	5.03616700	3.85313000	-0.62830900	C	2.96784700	0.12727000	0.23991300
H	3.89103000	4.70478200	1.39794900	C	3.40116800	-1.25277700	-0.14698600
H	1.94026900	4.46348200	3.04969600	C	4.23069300	-1.42530100	-1.26339700
H	-0.10796600	3.19296800	3.71806900	C	3.05572400	-2.36523400	0.63187700
H	-0.89451100	1.30522500	2.26985400	C	4.66580900	-2.69819300	-1.62582400
C	2.31144900	-0.26935800	-2.11342600	C	3.51409000	-3.63667700	0.28482000
C	1.40520700	-1.43180900	-2.31439300	C	4.30771600	-3.80666400	-0.85193900
C	1.86867700	-2.62400000	-2.87107200	H	2.43385400	-2.22804000	1.50872200
C	0.08967000	-1.32958400	-1.80890800	H	5.28776400	-2.82779600	-2.50664800
C	1.03037700	-3.73892000	-2.91217400	H	3.24942600	-4.49296700	0.89823300
C	-0.74106800	-2.45475500	-1.85476600	H	4.65349200	-4.79792500	-1.13038000
C	-0.26653500	-3.65335800	-2.39350500	O	3.77480600	1.06531000	0.06280400
H	1.38595400	-4.67248300	-3.33785900	H	3.45152800	1.36149600	2.55680800
H	-1.75624600	-2.40099000	-1.47470800	C	-2.81352700	-1.15376000	-0.65881900
H	-0.91603800	-4.52422500	-2.41458600	C	-4.11241400	-1.48356000	-1.04229800
O	3.41629700	-0.15382000	-2.68472900	C	-4.88563000	-2.38177800	-0.27319600
H	4.14277000	1.92234100	-1.89135100	C	-4.40075000	-2.95972000	0.88092200
Co	0.12762000	0.11783800	-0.36840100	C	-3.08554300	-2.65236000	1.31520000
H	2.88784800	-2.67215500	-3.24355800	C	-2.29395300	-1.76020600	0.53860400
H	-4.38023500	0.07099700	-2.05974400	N	-1.01759000	-1.43886300	0.91469100
C	-0.69443200	1.46824400	-1.59793500	C	-0.50718900	-1.93342400	2.03185600
C	-0.87129700	0.30046200	-2.38864700	C	-1.23005700	-2.81228100	2.86224000
H	-1.54267300	1.89281900	-1.08263600	C	-2.50763800	-3.17670200	2.49924100
H	0.06019500	2.18279600	-1.90867000	N	-1.93324400	-0.28497800	-1.26966500
H	-0.34270600	0.24630600	-3.33369200	H	-5.89317100	-2.61319100	-0.60713100
H	-1.85411300	-0.15634000	-2.41322600	H	-5.00700000	-3.64147100	1.46905200
				H	-3.08769900	-3.85979000	3.11309100
				H	-0.76761800	-3.18951000	3.76737800
TS_AQ_T				H	0.50060300	-1.61913400	2.27899200
C	1.50678400	1.31847700	1.65468700	C	-2.20321800	0.53175600	-2.30752300
C	2.45519500	1.78732300	2.56226700	C	-1.04518700	1.44699500	-2.55889500
C	2.14958900	2.80360400	3.49003300	C	-1.21522000	2.64435400	-3.25802400
C	0.89744500	3.38008000	3.54404400	C	0.20889800	1.14894500	-1.99073800
C	-0.10428100	2.93605200	2.64750700	C	-0.15982400	3.55190100	-3.36449400
C	0.20556800	1.90679700	1.70807200	C	1.26784100	2.04871500	-2.09968700
N	-0.72893000	1.45127500	0.82380100	C	1.07236800	3.26017100	-2.77357900
C	-1.94925700	1.96517900	0.82728400	H	-0.29925000	4.48672300	-3.89907500
C	-2.33768700	2.98165100	1.72206500	H	2.23723700	1.82136200	-1.66907100
C	-1.41943900	3.46368000	2.62652700	H	1.89385900	3.96741800	-2.84675300
N	1.71326500	0.25690400	0.76688300	O	-3.26706800	0.61761800	-2.96229100
H	2.92541400	3.13067100	4.17642800	H	-4.52597900	-1.03809300	-1.93610100
H	0.66348100	4.16375700	4.25758500	Co	-0.07267700	-0.11757600	-0.35289100
H	-1.68579200	4.24729700	3.32998600	H	-2.18794300	2.86136400	-3.68992700
H	-3.35133700	3.36431100	1.68187300	H	4.51597500	-0.55547500	-1.84676100
H	-2.64956600	1.56384300	0.10548500				

C 0.50244400 -1.77652200 -1.51803900  
 C 0.89555400 -0.78294000 -2.42674700  
 H 1.22756500 -2.23541600 -0.85902700  
 H -0.41122600 -2.33142400 -1.69612600  
 H 0.34986000 -0.69249100 -3.35837500  
 H 1.93887800 -0.49385400 -2.46614100

INT1\_H\_Q(m06)

C 4.35444300 -2.74498100 -0.62741600  
 C 3.55794100 -3.58068100 -1.41374200  
 C 2.24824600 -3.21762700 -1.69995500  
 C 1.74824600 -2.01376800 -1.19604900  
 C 2.53305700 -1.17112000 -0.40422000  
 C 3.84466500 -1.54702200 -0.12153500  
 H 5.38180900 -3.03220600 -0.40683900  
 H 3.96478900 -4.51206400 -1.80189000  
 H 1.60910700 -3.85080200 -2.31414500  
 H 4.48334900 -0.91041600 0.49509200  
 C 0.36436000 -1.58135000 -1.49598500  
 O -0.42021300 -2.27567100 -2.14601600  
 N 0.08211000 -0.32850100 -0.97314100  
 C -1.10878300 0.33718300 -1.19627700  
 C -1.14707600 1.65239400 -0.63137600  
 C -2.23604500 -0.10012800 -1.88639800  
 C -2.28504700 2.48195900 -0.76791600  
 C -3.36678800 0.72993500 -2.01589000  
 H -2.24263500 -1.08860800 -2.32734000  
 C -0.01160500 3.27008700 0.57416500  
 C -2.22703000 3.76461300 -0.18161400  
 C -3.40800200 1.99345500 -1.47673600  
 H -4.22659000 0.34833100 -2.56201500  
 C -1.09289000 4.16126300 0.48617000  
 H 0.90141000 3.54930600 1.10006500  
 H -3.08737700 4.42586200 -0.26875400  
 H -4.28497600 2.62849500 -1.58375000  
 H -1.01768100 5.14176500 0.94635600  
 N -0.03932100 2.06245300 0.03471700  
 Co 1.52743100 0.54826500 0.09796700  
 C 0.35957800 0.21894900 2.31920400  
 C 1.24391900 -0.78196400 2.16691100  
 C 3.22353100 2.30082000 -0.31731200  
 O 2.83375200 1.92477500 0.84546500  
 O 2.71513800 1.75356500 -1.33139500

C 4.24172400 3.38196900 -0.42768200  
 H 5.09914600 3.15052600 0.21215100  
 H 4.56711400 3.51621000 -1.46113900  
 H 3.80241600 4.31630700 -0.05887500  
 H 0.64758800 1.16978300 2.76653700  
 H 0.94280900 -1.75397700 1.78144500  
 H 2.27515000 -0.68616100 2.50700900  
 H -0.68571800 0.10232600 2.03680600

INT1\_H\_Q(pbe0)

C 4.36715300 -2.60892800 -1.03501600  
 C 3.48231500 -3.56358800 -1.55085600  
 C 2.12419500 -3.28543900 -1.58675400  
 C 1.66682200 -2.05092500 -1.10404100  
 C 2.52882100 -1.06644200 -0.57253200  
 C 3.89439700 -1.38442200 -0.56216300  
 H 5.43250900 -2.82881500 -1.00557500  
 H 3.85925600 -4.51172200 -1.92449300  
 H 1.41533700 -4.00412500 -1.99130900  
 H 4.61332500 -0.66691200 -0.16600900  
 C 0.22468200 -1.74868600 -1.15208500  
 O -0.64939100 -2.56463500 -1.43738600  
 N -0.03147100 -0.41366400 -0.80613900  
 C -1.14530200 0.25345400 -1.11386500  
 C -1.16083900 1.62685200 -0.64487300  
 C -2.26206900 -0.20994700 -1.85151000  
 C -2.28272900 2.45227600 -0.87380300  
 C -3.35635400 0.62391800 -2.07426600  
 H -2.25854300 -1.22491900 -2.22624300  
 C -0.03355600 3.31411900 0.44786400  
 C -2.23379200 3.77244200 -0.38009400  
 C -3.38760200 1.92488900 -1.59528000  
 H -4.20319800 0.24083900 -2.63510300  
 C -1.10633500 4.20163200 0.28624400  
 H 0.87377300 3.62106100 0.96100300  
 H -3.08165500 4.43372100 -0.53466700  
 H -4.24963200 2.56088500 -1.77417100  
 H -1.03100000 5.20955000 0.67918500  
 N -0.06032600 2.06802400 -0.00591000  
 Co 1.54279000 0.59061200 0.16109800  
 C 0.31414900 0.21639800 2.35782900  
 C 1.21058100 -0.77519100 2.24010500  
 C 3.31474200 2.40594800 -0.11816700  
 O 2.94829000 1.86404800 0.98473400

O	2.75985700	2.09606500	-1.19978600	C	0.75422000	3.08851000	-0.86076400
C	4.43537000	3.40477700	-0.07360800	O	0.93882900	2.80237000	0.36286500
H	5.36050800	2.88912400	0.20548100	O	0.40874000	2.18439500	-1.67796100
H	4.57125200	3.89011500	-1.04100800	C	0.96242000	4.50477800	-1.32537900
H	4.23458500	4.15435600	0.69734300	H	2.01712100	4.76762500	-1.19845600
H	0.57928200	1.17150700	2.80609700	H	0.68196000	4.62619100	-2.37214000
H	0.93308200	-1.74566500	1.83745500	H	0.37553600	5.18381400	-0.70073200
H	2.23108800	-0.66590400	2.60045800	H	-0.85594200	1.59645400	3.09053300
H	-0.71928200	0.08686800	2.04647500	H	1.30668900	-0.60902600	3.07056100
				H	1.58748700	1.21909100	3.10253700
				H	-1.13834600	-0.23331400	3.05636300

INT1\_H\_Q(wb97xd)

C	4.80286200	-0.48427900	0.15727500
C	4.68413400	-1.86237700	-0.05725600
C	3.42925800	-2.41435500	-0.25964200
C	2.29745600	-1.58259200	-0.24356300
C	2.37721700	-0.18533700	-0.03290400
C	3.67075300	0.32738400	0.16516500
H	5.78669300	-0.04938700	0.31733300
H	5.56816000	-2.49335100	-0.06415800
H	3.31434800	-3.48168400	-0.42701300
H	3.80038200	1.39593700	0.33378400
C	0.96905700	-2.21955500	-0.44718400
O	0.81812800	-3.41037000	-0.69881600
N	-0.09232700	-1.30178900	-0.32042000
C	-1.38634300	-1.59219800	-0.31328600
C	-2.25962200	-0.43107400	-0.13132000
C	-1.99960400	-2.87011500	-0.44867100
C	-3.65723600	-0.59119600	-0.09781800
C	-3.38386000	-2.99768200	-0.42163800
H	-1.37026600	-3.73861900	-0.57982500
C	-2.43176300	1.84448700	0.19458200
C	-4.44824600	0.56160200	0.09453800
C	-4.20969700	-1.89554200	-0.25366900
H	-3.82460800	-3.98204100	-0.53605700
C	-3.83158500	1.78305800	0.24321500
H	-1.91321500	2.79098700	0.31526100
H	-5.52941100	0.46910400	0.12660600
H	-5.28855700	-2.01379100	-0.23447400
H	-4.40156600	2.69155700	0.39733900
N	-1.66985800	0.77423400	0.01060300
Co	0.52458200	0.70823100	-0.07958100
C	-0.43350600	0.59466600	3.07604800
C	0.88234200	0.39180600	3.08414800

INT1\_H\_S(m06)

C	4.43062700	-2.31802500	-0.46822000
C	3.77844600	-3.18755500	-1.34331900
C	2.44535600	-2.96574700	-1.66780900
C	1.77651600	-1.87689700	-1.10960000
C	2.42563200	-1.00599400	-0.22712300
C	3.76033500	-1.22925800	0.09416300
H	5.47595400	-2.49009700	-0.21619200
H	4.31326400	-4.03326300	-1.76993100
H	1.91217600	-3.62114200	-2.35568000
H	4.28826300	-0.56758900	0.78147900
C	0.37333100	-1.54984800	-1.44487100
O	-0.32592400	-2.22526000	-2.21347700
N	-0.00618100	-0.40179700	-0.81830800
C	-1.16820400	0.30921000	-1.07984700
C	-1.15798500	1.63506100	-0.55563800
C	-2.29257400	-0.10459300	-1.77971800
C	-2.24461100	2.51963500	-0.75201800
C	-3.37614800	0.77840400	-1.96770500
H	-2.33225800	-1.10807400	-2.18624400
C	0.03633100	3.22710500	0.64333000
C	-2.12644600	3.81790800	-0.20467800
C	-3.36938700	2.06255000	-1.47697200
H	-4.24051200	0.42040500	-2.52328200
C	-0.99255100	4.17257800	0.48377100
H	0.94272800	3.47132600	1.19646600
H	-2.94354300	4.52467800	-0.33867800
H	-4.20959900	2.73557200	-1.63379400
H	-0.87552000	5.16293700	0.91299000
N	-0.04600000	2.00911500	0.14199700
Co	1.29890000	0.51098800	0.20144300
C	0.31525100	0.20582200	2.04238200

C 1.20570200 -0.82246300 1.89609400  
C 3.03288000 1.96577500 -0.30778600  
O 2.75759400 1.61867600 0.88834400  
O 2.29395200 1.46861000 -1.21740100  
C 4.17424000 2.85716700 -0.61755100  
H 5.09076000 2.25393000 -0.60984700  
H 4.05918700 3.30675100 -1.60632300  
H 4.27204900 3.62982400 0.14986700  
H 0.58684100 1.10487300 2.59400000  
H 0.87092600 -1.80523000 1.57390300  
H 2.19665500 -0.76770400 2.34207500  
H -0.74137500 0.06518300 1.82436700

INT1\_H\_S(pbe0)

C 4.42734800 -2.31836900 -0.43944200  
C 3.77710100 -3.20097800 -1.30481000  
C 2.44574700 -2.98029200 -1.64210200  
C 1.77943600 -1.87818600 -1.10637600  
C 2.42287000 -0.99220500 -0.23162000  
C 3.75613800 -1.21807600 0.10048100  
H 5.46911500 -2.48971200 -0.17854200  
H 4.31073300 -4.05466700 -1.71316100  
H 1.91611600 -3.64553000 -2.32006000  
H 4.27992500 -0.54817900 0.77838900  
C 0.37690300 -1.54845800 -1.44840200  
O -0.33297900 -2.23749700 -2.19767300  
N 0.01357600 -0.38482400 -0.84973300  
C -1.15184000 0.31547400 -1.09663100  
C -1.14380000 1.63570400 -0.55658200  
C -2.27835700 -0.09482200 -1.79746900  
C -2.23421100 2.52099700 -0.73561400  
C -3.36591000 0.78784600 -1.96730300  
H -2.31337500 -1.09111600 -2.21697000  
C 0.06076600 3.21295900 0.64973500  
C -2.11240000 3.81379700 -0.17356800  
C -3.36194700 2.06732800 -1.46020200  
H -4.23088200 0.43507600 -2.52251800  
C -0.97043300 4.15887200 0.50907300  
H 0.97072400 3.44719000 1.19448800  
H -2.92749000 4.52292900 -0.29033800  
H -4.20524200 2.73561400 -1.60596900  
H -0.84901500 5.14302700 0.94818500  
N -0.02830900 2.00102500 0.13533500  
Co 1.30658300 0.51821800 0.17369200

C 0.28951200 0.18741800 2.01998300  
C 1.17667800 -0.84066700 1.87833800  
C 3.03089700 1.97450300 -0.32410500  
O 2.75821600 1.62186600 0.87085100  
O 2.29220300 1.46777700 -1.22991600  
C 4.15689400 2.88645400 -0.64051500  
H 5.07982000 2.29556600 -0.66374400  
H 4.01201300 3.35037100 -1.61726000  
H 4.25666800 3.64553000 0.13820500  
H 0.55620200 1.07933600 2.58009600  
H 0.84717600 -1.81222600 1.52595300  
H 2.16028100 -0.79268300 2.33525000  
H -0.75836600 0.05716100 1.76723100

INT1\_H\_S(wb97xd)

C 4.43002700 -2.35697900 -0.43627700  
C 3.77076400 -3.23816300 -1.29551400  
C 2.44517400 -2.99911300 -1.64392100  
C 1.79483200 -1.88045300 -1.12512900  
C 2.44471800 -0.99518000 -0.25710000  
C 3.77268700 -1.23982200 0.08441100  
H 5.46638600 -2.54263000 -0.16664400  
H 4.29179100 -4.10487400 -1.69090700  
H 1.91190500 -3.66605300 -2.31628500  
H 4.30266800 -0.56908300 0.75597800  
C 0.39019800 -1.53620800 -1.47506000  
O -0.31643600 -2.22553900 -2.22612800  
N 0.02981400 -0.37221500 -0.87721500  
C -1.14581100 0.32779600 -1.11876300  
C -1.14815300 1.64475500 -0.56388900  
C -2.26697000 -0.08373300 -1.81897400  
C -2.24351200 2.51882500 -0.73369900  
C -3.36585000 0.79211100 -1.98093300  
H -2.29910700 -1.07509200 -2.24803300  
C 0.03793100 3.22213600 0.66091300  
C -2.13745300 3.80952100 -0.15851400  
C -3.37087700 2.06326900 -1.46324400  
H -4.22733400 0.43622400 -2.53816800  
C -1.00302100 4.16069600 0.52875200  
H 0.94363100 3.46243100 1.20933200  
H -2.95986400 4.51004800 -0.27028200  
H -4.21905000 2.72631600 -1.60093200  
H -0.89251600 5.14074700 0.97766900



N -0.03486300 2.01488200 0.13669900  
 Co 1.33272400 0.52572000 0.15642900  
 C 0.28289100 0.18109700 2.07632000  
 C 1.15800300 -0.84639500 1.94287400  
 C 3.05181400 1.99392000 -0.34051300  
 O 2.79553800 1.63473200 0.85461200  
 O 2.30456800 1.48768900 -1.23958400  
 C 4.17319800 2.91460500 -0.66828000  
 H 5.09808000 2.32844600 -0.69403000  
 H 4.01830200 3.37445900 -1.64484600  
 H 4.27038600 3.67663300 0.10717300  
 H 0.55797700 1.08149900 2.61733700  
 H 0.83200500 -1.81117100 1.57085100  
 H 2.14995400 -0.79514200 2.37981000  
 H -0.76206500 0.06283700 1.80836300

H -0.95377200 5.11739200 0.93094400  
 N -0.04033600 2.03345500 -0.01285400  
 Co 1.36612800 0.57230500 -0.08855200  
 C 0.27294700 0.18036000 2.27595900  
 C 1.13330000 -0.83769200 2.14677100  
 C 3.24012500 2.14519000 -0.42176900  
 O 2.86280300 1.62272900 0.68650100  
 O 2.62087200 1.85174800 -1.47466400  
 C 4.41909300 3.05857500 -0.41847700  
 H 5.32118800 2.46368800 -0.23176900  
 H 4.52076600 3.57233300 -1.37652200  
 H 4.33145100 3.78549200 0.39470500  
 H 0.57754400 1.13006100 2.71498300  
 H 0.82125100 -1.80245800 1.75007400  
 H 2.16700200 -0.75554800 2.48053200  
 H -0.77276500 0.08633400 1.98580100

INT1\_H\_T(m06)

C 4.38338900 -2.40372600 -0.54282400  
 C 3.67646000 -3.35431800 -1.27923500  
 C 2.34977100 -3.11920300 -1.62256100  
 C 1.74589600 -1.92979400 -1.22100900  
 C 2.45344900 -0.98049200 -0.47830300  
 C 3.77844600 -1.21000100 -0.13621300  
 H 5.42244200 -2.59155900 -0.27710900  
 H 4.16499900 -4.27688700 -1.58438800  
 H 1.77354600 -3.84199800 -2.19929500  
 H 4.34663200 -0.48221900 0.44226100  
 C 0.34448100 -1.58917800 -1.54684200  
 O -0.41876600 -2.31801600 -2.18150300  
 N 0.03696300 -0.34657500 -1.04193900  
 C -1.17365000 0.32570000 -1.21496400  
 C -1.18124700 1.63305000 -0.64739900  
 C -2.31801000 -0.11358800 -1.85857500  
 C -2.31408900 2.47321500 -0.74039000  
 C -3.44996800 0.72642700 -1.94556600  
 H -2.34203300 -1.10278200 -2.29990800  
 C 0.02238400 3.23714300 0.52614900  
 C -2.21623700 3.75510400 -0.15354200  
 C -3.46461900 1.99015000 -1.40800900  
 H -4.33155000 0.34964900 -2.45957900  
 C -1.05508300 4.13806600 0.47348800  
 H 0.95512700 3.50329900 1.02313400  
 H -3.06997300 4.42834100 -0.20823000  
 H -4.34127400 2.62977800 -1.48465300

INT1\_H\_T(pbe0)

C 4.39068900 -2.39227000 -0.56559800  
 C 3.67664900 -3.36456800 -1.26953100  
 C 2.35160400 -3.13485800 -1.62627600  
 C 1.75605900 -1.92523300 -1.27218900  
 C 2.47148200 -0.95208200 -0.56990100  
 C 3.79419500 -1.17812600 -0.21106100  
 H 5.42483300 -2.57969000 -0.28702100  
 H 4.15783600 -4.30140100 -1.53568600  
 H 1.77288600 -3.87723200 -2.17087500  
 H 4.36253000 -0.43562800 0.34266500  
 C 0.35009700 -1.58649100 -1.58486500  
 O -0.43098500 -2.33401900 -2.18111700  
 N 0.06346200 -0.33815400 -1.10541600  
 C -1.16042200 0.31018400 -1.21304700  
 C -1.16106200 1.63160800 -0.67596000  
 C -2.33840900 -0.16868200 -1.76571500  
 C -2.32029300 2.44279200 -0.70328300  
 C -3.49329000 0.64383200 -1.79171200  
 H -2.36674700 -1.16735600 -2.18013700  
 C 0.07958600 3.28434100 0.39126500  
 C -2.21462300 3.73589300 -0.14117100  
 C -3.50311400 1.91965300 -1.27962500  
 H -4.39756400 0.23536900 -2.23420800  
 C -1.02194100 4.15558100 0.40134000  
 H 1.03471700 3.57483000 0.81920900  
 H -3.08407600 4.38786700 -0.14385500

H	-4.39841000	2.53343600	-1.30665900	H	-1.58159300	2.94248600	0.33159500
H	-0.91544300	5.14190100	0.83917400	H	-5.43055500	1.04318000	0.01331000
N	0.00834300	2.07146000	-0.12773000	H	-5.46080300	-1.48068600	-0.35710700
Co	1.42014200	0.63258800	-0.21498600	H	-4.07714600	3.11512500	0.33329800
C	0.15742200	0.21886700	2.20464300	N	-1.56987400	0.91569900	0.02221000
C	0.97344300	-0.83180200	2.06225900	Co	0.42752200	0.53471500	-0.01424400
C	3.34366400	2.16113300	-0.38907500	C	-0.38034000	0.41452000	3.02980900
O	2.82913300	1.68549900	0.68736900	C	0.91646900	0.11466200	3.09553400
O	2.85677400	1.81681700	-1.49405500	C	1.16647300	2.71784700	-0.86377800
C	4.51304900	3.08489400	-0.28445700	O	0.99729500	2.40151100	0.36777000
H	5.40080100	2.49495000	-0.03087200	O	0.96006100	1.83969900	-1.73985800
H	4.68586000	3.59925000	-1.23040900	C	1.62360400	4.10137900	-1.20742300
H	4.35324400	3.80740500	0.51959600	H	2.68442300	4.18891700	-0.95069500
H	0.49017300	1.13685900	2.68314600	H	1.49601500	4.29773200	-2.27211100
H	0.63271200	-1.75968600	1.61046400	H	1.07365000	4.83621100	-0.61531700
H	1.99745000	-0.80964800	2.42743000	H	-0.73064600	1.44332300	3.06127000
H	-0.87737400	0.18346600	1.87259000	H	1.26627100	-0.91415300	3.06226700
				H	1.67620200	0.88797900	3.17964100
				H	-1.13999300	-0.35948400	2.94905300

INT1\_H\_T(wb97xd)

C	4.59324300	-0.40029000	0.09464500
C	4.54399300	-1.78053800	-0.10696200
C	3.31840500	-2.41970400	-0.27264200
C	2.15068400	-1.66160200	-0.23685100
C	2.20336900	-0.28139300	-0.04142300
C	3.42136900	0.36211600	0.12904000
H	5.55316800	0.09072000	0.22772400
H	5.46401600	-2.35627000	-0.13090600
H	3.25753000	-3.49406900	-0.42440600
H	3.47517400	1.43414300	0.29385900
C	0.79033700	-2.24632500	-0.37304800
O	0.57197200	-3.44863500	-0.53892800
N	-0.14852000	-1.25735300	-0.27650700
C	-1.53357100	-1.44237200	-0.31721400
C	-2.28376600	-0.23736500	-0.15191900
C	-2.23132400	-2.62252700	-0.49214600
C	-3.69484100	-0.23855100	-0.16291400
C	-3.64707100	-2.62044100	-0.50510300
H	-1.69414400	-3.55141400	-0.62098800
C	-2.20180200	2.06268300	0.19022100
C	-4.34502000	1.00672000	0.01609900
C	-4.37555200	-1.46955300	-0.34621900
H	-4.15952600	-3.56712300	-0.64620000
C	-3.60482400	2.15024200	0.19204600

INT2\_H\_Q(m06)

C	5.09779300	-1.66270400	0.01673400
C	5.07053800	-1.13515500	-1.27167300
C	3.84838900	-0.87441800	-1.87717200
C	2.64727900	-1.09863800	-1.19839400
C	2.66799000	-1.66180900	0.08905800
C	3.90480000	-1.93444300	0.67772500
H	6.04795500	-1.87628600	0.50192000
H	5.99754900	-0.93216100	-1.80327500
H	3.80945800	-0.46916500	-2.88703000
H	3.92387600	-2.37445200	1.67518500
C	1.38607500	-0.73415700	-1.92510800
O	1.23693000	-1.13725700	-3.08850500
N	0.53011400	0.06252900	-1.23448500
C	-0.75836600	0.34225800	-1.68842600
C	-1.45726300	1.34978300	-0.94881200
C	-1.44754200	-0.27285300	-2.72565700
C	-2.78706200	1.71691400	-1.27569200
C	-2.77403300	0.08817800	-3.03843500
H	-0.95512500	-1.04087900	-3.30884700
C	-1.39699100	2.88512200	0.80336200
C	-3.39405600	2.72793900	-0.49833200
C	-3.44312000	1.06507400	-2.34442500
H	-3.26835100	-0.42809300	-3.85883800

C	-2.70517400	3.31510300	0.53504700	H	-3.21610400	-0.37924200	-3.89958800
H	-0.81976000	3.31764700	1.61873500	C	-2.67029400	3.36316900	0.49905500
H	-4.41374800	3.02889800	-0.73305900	H	-0.81011600	3.31634300	1.62667000
H	-4.46389900	1.34719200	-2.59336800	H	-4.35001900	3.12586800	-0.81471500
H	-3.15035400	4.09387300	1.14639200	H	-4.39583300	1.43069500	-2.67586700
N	-0.80109400	1.94356800	0.09011000	H	-3.10366400	4.16342800	1.08883000
Co	1.04547700	1.08859000	0.43646400	N	-0.80270400	1.92412900	0.12098200
C	0.98825900	-0.76114500	1.70120800	Co	1.04140300	1.07235700	0.47661000
C	1.40724800	-1.93609400	0.87305300	C	1.00106200	-0.89079300	1.79847100
C	2.83900700	2.60865000	1.14637200	C	1.41031300	-2.02920000	0.92463000
O	1.70908600	2.65116800	1.72446400	C	2.76057400	2.74108800	1.03770300
O	3.01107100	1.76505200	0.21054600	O	1.72053100	2.64668800	1.75987900
C	3.92533800	3.55183300	1.53645900	O	2.88278200	1.96908200	0.03483600
H	3.98011200	3.63421100	2.62578100	C	3.83896200	3.71943700	1.37694500
H	4.88859600	3.23838700	1.12860100	H	4.50102200	3.25933400	2.11942900
H	3.68089000	4.54598100	1.14416500	H	4.43040400	3.96743700	0.49409600
H	1.73050800	-0.36652000	2.40545100	H	3.41172800	4.62180500	1.81896900
H	1.59405100	-2.79498800	1.54112400	H	1.74885800	-0.46142700	2.46825800
H	0.58811500	-2.23756800	0.20939200	H	1.59553100	-2.91323900	1.55674300
H	-0.04327300	-0.73126400	2.06112800	H	0.59135400	-2.29589600	0.25012500
				H	-0.03664200	-0.82109900	2.12418400

INT2\_H\_Q(pbe0)

C	5.10161800	-1.74150000	0.05877600
C	5.06738400	-1.17297100	-1.21340600
C	3.84204100	-0.88913200	-1.80347100
C	2.64373700	-1.13187500	-1.12382800
C	2.67133400	-1.72503100	0.15071700
C	3.91198100	-2.02392400	0.72214100
H	6.05268300	-1.97849300	0.52789300
H	5.99038500	-0.95945900	-1.74500200
H	3.79911300	-0.46099600	-2.80134600
H	3.93755800	-2.49434800	1.70264200
C	1.37102500	-0.79268900	-1.84732700
O	1.22356900	-1.22240300	-3.00383700
N	0.51131500	-0.00259400	-1.16502400
C	-0.75661800	0.30913500	-1.64533100
C	-1.44730000	1.34199800	-0.92832200
C	-1.43078900	-0.28457800	-2.70620500
C	-2.75522800	1.75099100	-1.29992100
C	-2.73437300	0.11883400	-3.06243900
H	-0.94011300	-1.06348900	-3.27260800
C	-1.38374600	2.89326200	0.80706900
C	-3.35120500	2.78992300	-0.54859600
C	-3.39622900	1.11727900	-2.38987400

INT2\_H\_Q(wb97xd)

C	4.67553700	-0.83106900	-0.08135700
C	4.14766900	-1.20799700	-1.31478700
C	2.82105900	-1.61451600	-1.39763300
C	2.00546000	-1.62035300	-0.26274200
C	2.53549900	-1.26340900	0.98764500
C	3.87585600	-0.87185200	1.05648000
H	5.71265000	-0.51882700	-0.00297500
H	4.76789000	-1.19116600	-2.20571900
H	2.40072700	-1.91797400	-2.35255400
H	4.29660100	-0.60244000	2.02232400
C	0.56756500	-2.04821700	-0.43691900
O	0.33860100	-3.20754600	-0.81893100
N	-0.33619600	-1.07603900	-0.18453700
C	-1.71789500	-1.29266200	-0.22105700
C	-2.52969900	-0.11253500	-0.08261500
C	-2.38070700	-2.50329300	-0.34692500
C	-3.94341200	-0.18873000	-0.08748700
C	-3.79309000	-2.57232000	-0.34273900
H	-1.80749300	-3.41212400	-0.45516300

C	-2.59437300	2.20194200	0.17736900	H	-1.15490700	-1.08086200	-3.49742900
C	-4.66691100	1.02153600	0.04389600	C	-0.82532900	2.50385100	0.91823300
C	-4.57216900	-1.45213500	-0.22110900	C	-2.88174700	2.80402800	-0.29021600
H	-4.26017200	-3.54758700	-0.44315500	C	-3.25061800	1.33390300	-2.28909400
C	-3.99954900	2.21356800	0.17344100	H	-3.34545900	-0.00597300	-3.94627900
H	-2.02668200	3.12166200	0.28139100	C	-2.05610400	3.16189400	0.74843800
H	-5.75277900	0.98944800	0.04013600	H	-0.14850600	2.75867600	1.73071500
H	-5.65614700	-1.50962400	-0.22419000	H	-3.83869600	3.30084700	-0.43903000
H	-4.52786400	3.15423600	0.27455200	H	-4.21167300	1.80100700	-2.49260200
N	-1.89412800	1.08901100	0.05455900	H	-2.33339800	3.94493200	1.44725100
Co	0.18086700	0.86875000	0.11084100	N	-0.43393500	1.54496800	0.09534700
C	1.12637800	0.06382400	2.58238400	Co	1.15956900	0.54463100	0.17619900
C	1.69475500	-1.27731700	2.25136100	C	0.38787200	-0.76093900	1.33333200
C	1.53034500	2.80879100	-0.55940700	C	1.29106100	-1.92582400	0.98909200
O	0.72575200	2.91475800	0.41712700	C	2.72065500	2.31931800	0.70573500
O	1.60736200	1.69733700	-1.17253500	O	2.05020300	1.61155500	1.54081200
C	2.40258900	3.96017600	-0.96034000	O	2.54143200	2.13881700	-0.52684600
H	3.29642100	3.94927400	-0.32724600	C	3.71894000	3.29726000	1.22556200
H	2.71382800	3.86651300	-2.00159000	H	4.65443800	2.76070900	1.42687900
H	1.88344700	4.90662500	-0.79919800	H	3.91967300	4.07683200	0.48682600
H	1.76501700	0.94374200	2.52819900	H	3.37622700	3.73863100	2.16548900
H	2.33333400	-1.61310200	3.08481200	H	0.53796900	-0.35296500	2.34110900
H	0.88851300	-2.01279100	2.17227900	H	1.60918900	-2.47720400	1.88395800
H	0.20876500	0.13870300	3.15977000	H	0.77391500	-2.63489000	0.33239000
				H	-0.67445700	-0.92983000	1.13004400

INT2\_H\_S(m06)

C	4.89854600	-0.82181900	0.38858400
C	4.94197600	-0.69206900	-1.00212500
C	3.79398000	-0.89216000	-1.75230500
C	2.58802300	-1.21718700	-1.12328300
C	2.53975100	-1.40941500	0.27926000
C	3.71930300	-1.19602000	1.01285600
H	5.79589800	-0.65362000	0.97952500
H	5.87278400	-0.42037300	-1.49461300
H	3.80424600	-0.76821200	-2.83366300
H	3.69436700	-1.34512000	2.09225000
C	1.33386300	-1.17024900	-1.94626600
O	1.20140800	-1.73339600	-3.03896500
N	0.47281700	-0.34258800	-1.32969400
C	-0.75395300	0.11728500	-1.76748700
C	-1.24339800	1.16344700	-0.94170000
C	-1.51687300	-0.29102900	-2.84685600
C	-2.49045200	1.77798900	-1.18052200
C	-2.76130800	0.32906500	-3.09196500

INT2\_H\_S(pbe0)

C	4.96118600	-0.99303300	0.36330700
C	4.98389300	-0.78418000	-1.01787800
C	3.81305300	-0.89959300	-1.75342500
C	2.60660600	-1.21068300	-1.11586800
C	2.57878500	-1.47040700	0.27470700
C	3.77623500	-1.34582400	0.99520700
H	5.87495900	-0.89751900	0.94291400
H	5.91403000	-0.52409600	-1.51486400
H	3.81133600	-0.72568400	-2.82597100
H	3.76736900	-1.54755900	2.06356500
C	1.33730200	-1.14120500	-1.91900300
O	1.17773400	-1.73499400	-2.99348600
N	0.48988200	-0.28865800	-1.31832700
C	-0.75260600	0.12595100	-1.75135000
C	-1.26843500	1.17066300	-0.93671600
C	-1.51390900	-0.31542000	-2.82061800
C	-2.52964500	1.75761200	-1.17931400

C -2.77436400 0.27245200 -3.06692800  
 H -1.13822000 -1.10163800 -3.46345300  
 C -0.86579100 2.54711200 0.90000000  
 C -2.93519500 2.79157900 -0.30311900  
 C -3.28459300 1.27984600 -2.27834500  
 H -3.35337000 -0.08841300 -3.91241700  
 C -2.10838700 3.18062600 0.72529700  
 H -0.18649600 2.82547000 1.69859300  
 H -3.89864100 3.27099400 -0.45298900  
 H -4.25454200 1.72057700 -2.48734300  
 H -2.39339700 3.97109100 1.41065100  
 N -0.46616100 1.58085300 0.09047000  
 Co 1.14144700 0.63853700 0.17312900  
 C 0.44519400 -0.68863200 1.33563900  
 C 1.29640500 -1.89965900 0.97608600  
 C 2.71142700 2.42236900 0.69672100  
 O 2.02398300 1.71422600 1.52189200  
 O 2.53975400 2.24996400 -0.53818500  
 C 3.71123700 3.39169100 1.23519300  
 H 4.61396400 2.83651000 1.51448500  
 H 3.97432800 4.13413600 0.48041600  
 H 3.32486500 3.87765900 2.13413600  
 H 0.64529300 -0.30199200 2.34065500  
 H 1.56758800 -2.47305600 1.86997100  
 H 0.73894700 -2.56755200 0.31247500  
 H -0.62575500 -0.85222000 1.19303500

INT2\_H\_S(wb97xd)

C 4.43675500 -0.26364700 0.07555100  
 C 4.11753800 -0.97619900 -1.08227900  
 C 2.90180800 -1.63875000 -1.17111000  
 C 1.99090000 -1.58728600 -0.11080000  
 C 2.31954400 -0.90743000 1.08213100  
 C 3.55304100 -0.24290900 1.14610400  
 H 5.38447400 0.26096000 0.14745000  
 H 4.81442500 -1.00699800 -1.91392500  
 H 2.63413200 -2.18466200 -2.07096700  
 H 3.81891000 0.28220500 2.05962900  
 C 0.61650200 -2.17420400 -0.32055400  
 O 0.43113600 -3.33984900 -0.69444400  
 N -0.30672400 -1.22253900 -0.10929400  
 C -1.68358100 -1.32433000 -0.23245500  
 C -2.32320400 -0.06619100 -0.04235900

C -2.46835400 -2.42652500 -0.50788600  
 C -3.72103400 0.08055900 -0.12480800  
 C -3.87440400 -2.28191500 -0.59068400  
 H -2.00918400 -3.39371500 -0.66456700  
 C -2.01147200 2.19959300 0.40697700  
 C -4.24630900 1.38105500 0.07544600  
 C -4.49881100 -1.07207000 -0.40761700  
 H -4.46938500 -3.16320800 -0.80989100  
 C -3.39791700 2.42868700 0.33719900  
 H -1.31061900 3.00050900 0.61411200  
 H -5.31936900 1.53738300 0.01822500  
 H -5.57766400 -0.97941800 -0.47928100  
 H -3.77122100 3.43375700 0.49297400  
 N -1.50062900 0.99646300 0.21923500  
 Co 0.31295900 0.50975800 0.27876900  
 C 0.28425200 0.14463700 2.14589200  
 C 1.38160600 -0.91083000 2.28922000  
 C 1.32572300 2.35501500 -0.88754300  
 O 1.08661100 2.28923600 0.37236300  
 O 0.95466800 1.39565900 -1.61586000  
 C 2.06402100 3.53460700 -1.43653700  
 H 3.13278900 3.38790000 -1.24720800  
 H 1.90479100 3.62083700 -2.51196300  
 H 1.75189300 4.44856600 -0.92720300  
 H 0.54162800 1.09491800 2.62492900  
 H 1.98077900 -0.73410300 3.18840200  
 H 0.93542600 -1.90509700 2.38281600  
 H -0.68995800 -0.20275900 2.49703700

INT2\_H\_T(m06)

C 5.07710400 -1.86933300 0.16573900  
 C 5.08455400 -1.39442600 -1.14314000  
 C 3.88149700 -1.09966300 -1.77227800  
 C 2.66736600 -1.24396900 -1.09606600  
 C 2.65247000 -1.74891300 0.21650500  
 C 3.86850700 -2.05424200 0.82985500  
 H 6.01256800 -2.11126600 0.66561100  
 H 6.02424200 -1.26045400 -1.67421900  
 H 3.86876000 -0.74198100 -2.80048600  
 H 3.85946000 -2.45783900 1.84219000  
 C 1.41603000 -0.88855000 -1.84753600  
 O 1.27297800 -1.31507100 -3.00311300  
 N 0.56573700 -0.06708000 -1.18400900  
 C -0.68912100 0.29997900 -1.66996500

C -1.36980000 1.29089500 -0.89053400  
 C -1.35456900 -0.20150300 -2.78022800  
 C -2.66210100 1.75235300 -1.24457300  
 C -2.64464200 0.25546800 -3.12214100  
 H -0.87265700 -0.94936400 -3.39724400  
 C -1.28854800 2.71477100 0.94704100  
 C -3.24556800 2.74445000 -0.42404200  
 C -3.29789100 1.21224700 -2.38553000  
 H -3.12333300 -0.16807400 -4.00268100  
 C -2.56469300 3.23042000 0.66543300  
 H -0.71087000 3.07170300 1.80019900  
 H -4.23801200 3.11576700 -0.67430700  
 H -4.28987100 1.56543300 -2.65938100  
 H -2.98947900 3.99614600 1.30731300  
 N -0.72496000 1.78141800 0.20257200  
 Co 1.17232500 0.97104700 0.39365000  
 C 0.84884200 -0.71974000 1.61453400  
 C 1.35681400 -1.96653300 0.95913100  
 C 2.68724300 2.89225500 0.79758600  
 O 2.44371200 1.90215000 1.58619200  
 O 2.11816200 2.94514600 -0.31721200  
 C 3.64593800 3.93827800 1.25992100  
 H 4.61782900 3.47550500 1.46261600  
 H 3.76131900 4.72616400 0.51294800  
 H 3.28996300 4.36856200 2.20215300  
 H 1.46135700 -0.32851600 2.43412500  
 H 1.52455100 -2.72227000 1.74408800  
 H 0.59226500 -2.37468300 0.28816000  
 H -0.22818700 -0.65878600 1.79007100

INT2\_H\_T(pbe0)

C 5.07567600 -1.90678000 0.14156100  
 C 5.08849000 -1.40398900 -1.15834300  
 C 3.88827800 -1.08393600 -1.78213300  
 C 2.67343100 -1.22860000 -1.10589500  
 C 2.65228200 -1.75369300 0.19882900  
 C 3.86530100 -2.08976600 0.80453700  
 H 6.00739500 -2.17005500 0.63468800  
 H 6.02856800 -1.26933100 -1.68580700  
 H 3.87897800 -0.70787300 -2.80163100  
 H 3.85421200 -2.51038200 1.80736200  
 C 1.41848200 -0.86552000 -1.84655900  
 O 1.26884700 -1.28680000 -3.00511700  
 N 0.56846300 -0.05629000 -1.17366700

C -0.68693300 0.29636200 -1.65611600  
 C -1.36629800 1.30023600 -0.89253400  
 C -1.35689000 -0.23152400 -2.75313600  
 C -2.66789800 1.74405400 -1.24264500  
 C -2.65230500 0.21153700 -3.09377900  
 H -0.87340200 -0.98611600 -3.35717100  
 C -1.27722500 2.74972200 0.92000100  
 C -3.25319800 2.74277200 -0.42966800  
 C -3.30837100 1.17766700 -2.36927000  
 H -3.13417200 -0.23089000 -3.96150100  
 C -2.56332500 3.24652000 0.64725100  
 H -0.69618000 3.12301200 1.75957700  
 H -4.24996100 3.10251700 -0.67106200  
 H -4.30359400 1.51515900 -2.64309900  
 H -2.98804800 4.01364700 1.28558500  
 N -0.71087900 1.81487100 0.17955800  
 Co 1.18837600 0.99119700 0.39643700  
 C 0.85419200 -0.69765500 1.58644900  
 C 1.34841600 -1.95496800 0.93302000  
 C 2.69788800 2.89411800 0.84410600  
 O 2.41622700 1.93303700 1.65174300  
 O 2.15578400 2.91892100 -0.28927900  
 C 3.65105600 3.95263800 1.29736200  
 H 4.57953300 3.48669700 1.64016700  
 H 3.86095200 4.66036800 0.49484800  
 H 3.21605800 4.48275400 2.15091000  
 H 1.46482700 -0.32720800 2.41404100  
 H 1.49914200 -2.71189500 1.71697900  
 H 0.58612600 -2.34460500 0.25243300  
 H -0.22100700 -0.63202900 1.75991500

INT2\_H\_T(wb97xd)

C 4.86960100 -0.65246600 0.26401300  
 C 4.49546700 -1.04349600 -1.01977700  
 C 3.18658600 -1.44560000 -1.26071800  
 C 2.23663000 -1.43059700 -0.23618300  
 C 2.61208200 -1.05290600 1.06493900  
 C 3.93497500 -0.66879900 1.29553900  
 H 5.89155500 -0.34561100 0.46554800  
 H 5.22096500 -1.04230300 -1.82745300  
 H 2.88622300 -1.76890800 -2.25326000  
 H 4.23463800 -0.38588700 2.30140200  
 C 0.83971100 -1.89157300 -0.57126500

O	0.70793700	-2.96606000	-1.17990400	C	0.71935800	-2.19737600	-0.20515600
N	-0.15177300	-1.05279700	-0.19408100	O	0.50317800	-3.37039200	-0.54207400
C	-1.50699300	-1.38131100	-0.30134000	N	-0.21509500	-1.25953700	0.08916600
C	-2.41576700	-0.31703000	0.02136300	C	-1.58378100	-1.39460800	-0.08345900
C	-2.06144500	-2.60599800	-0.63818600	C	-2.27412100	-0.15125700	-0.02829600
C	-3.81764900	-0.50624100	-0.01095800	C	-2.32474400	-2.54535500	-0.30386300
C	-3.46341000	-2.79070800	-0.66384900	C	-3.67515100	-0.06987100	-0.19517200
H	-1.41519500	-3.43316200	-0.89085600	C	-3.72364300	-2.46189600	-0.46920600
C	-2.65944400	1.90718600	0.65410700	H	-1.82578800	-3.50642600	-0.35212700
C	-4.63480100	0.60361700	0.31686300	C	-2.08073000	2.14861500	0.25228800
C	-4.33592300	-1.77728400	-0.36361600	C	-4.25811800	1.21633700	-0.12904700
H	-3.84636400	-3.77008200	-0.93513300	C	-4.39812700	-1.26463000	-0.42005700
C	-4.06251900	1.80639100	0.64661800	H	-4.27698900	-3.38267400	-0.64164900
H	-2.16489700	2.84108400	0.90635600	C	-3.46735800	2.31737100	0.09114600
H	-5.71461800	0.48651800	0.30127000	H	-1.42636100	2.99871500	0.43898300
H	-5.41080700	-1.92643400	-0.39039100	H	-5.33476400	1.31719200	-0.25418600
H	-4.66323800	2.67227200	0.89936400	H	-5.47675300	-1.21522500	-0.55261200
N	-1.87657100	0.88779800	0.35822700	H	-3.88904200	3.31617900	0.14771400
Co	0.21289900	0.86409200	0.27253100	N	-1.50865300	0.95969500	0.18886500
C	0.78491000	0.21593800	2.23423800	Co	0.38329700	0.49974600	0.42221500
C	1.60540000	-1.04397500	2.19739800	C	0.01215300	0.38246300	2.34820100
C	0.90877000	2.92412700	-0.93009000	C	1.36007600	-0.02018500	2.25005500
O	1.15541700	2.63276200	0.29787200	C	1.12175800	2.33506600	-0.86299700
O	0.22659000	2.12957900	-1.62349200	O	1.00451100	2.34622600	0.41168200
C	1.44746200	4.20962500	-1.48376800	O	0.80361600	1.26774400	-1.46372600
H	2.53817900	4.20756700	-1.40062800	C	1.65644300	3.52216700	-1.57733200
H	1.15640400	4.33871500	-2.52632100	H	2.74801200	3.52622000	-1.46578800
H	1.07228900	5.04538600	-0.88617000	H	1.41252400	3.47908900	-2.64114200
H	1.33565700	1.13364600	2.45173400	H	1.27061400	4.44296500	-1.13081300
H	2.14574700	-1.11888500	3.15178400	H	-0.22328000	1.40520400	2.64517200
H	0.94727500	-1.91392800	2.13263800	H	2.12883800	0.69771800	2.52940600
H	-0.19131700	0.14796400	2.71462100	H	1.60227900	-1.05830900	2.46824400
TS_H_S(m06)				H	-0.75902600	-0.36096000	2.54483900
C	4.53148400	-0.31714400	-0.17845100	TS_H_S(pbe0)			
C	4.41713300	-1.61122600	-0.68678900	C	-4.81893900	-1.62371700	0.22808300
C	3.18396800	-2.25259600	-0.66672600	C	-4.46401900	-2.39086800	1.33943300
C	2.07514100	-1.60316100	-0.13010700	C	-3.14887800	-2.38194000	1.79385000
C	2.18972500	-0.30802200	0.40435200	C	-2.19461000	-1.61409200	1.13017200
C	3.42816600	0.33166200	0.37253200	C	-2.53897300	-0.85844500	-0.00592500
H	5.49337300	0.19152500	-0.20242000	C	-3.86279700	-0.86760000	-0.44797800
H	5.28773100	-2.11158100	-1.10440900	H	-5.84810100	-1.62063500	-0.12148000
H	3.05852000	-3.25141300	-1.08225400	H	-5.21452000	-2.98550900	1.85228200
H	3.54157700	1.33270700	0.78833600	H	-2.85156900	-2.94782200	2.67310400

H	-4.14931800	-0.29571700	-1.32703200	H	-5.21371900	-2.99802600	1.85761400
C	-0.81394100	-1.46712300	1.65346100	H	-2.85807400	-2.94106700	2.68353600
O	-0.33871500	-2.18380700	2.54848300	H	-4.15701100	-0.32149900	-1.33265700
N	-0.20511000	-0.41977300	1.05186400	C	-0.81675200	-1.45662200	1.66346000
C	1.01019700	0.12780500	1.41427100	O	-0.34792000	-2.17426100	2.56042400
C	1.24197300	1.39725800	0.81170600	N	-0.20847600	-0.41097900	1.06242400
C	1.98045900	-0.38107700	2.26532300	C	1.01533700	0.13620100	1.42420200
C	2.41962100	2.13938500	1.06308100	C	1.25295200	1.40515700	0.81694100
C	3.15636900	0.35945400	2.51269200	C	1.98174100	-0.37504200	2.27102900
H	1.82923100	-1.34218300	2.73868900	C	2.43089300	2.13890200	1.06691300
C	0.39784400	3.02989100	-0.60921000	C	3.16509600	0.36040300	2.51841300
C	2.53893000	3.39332200	0.41863200	H	1.83027700	-1.33415900	2.74667100
C	3.38726100	1.58869700	1.93742000	C	0.42177100	3.04037100	-0.60934900
H	3.89835000	-0.06442900	3.18388700	C	2.56074900	3.39327700	0.42068200
C	1.53351400	3.83483300	-0.40842200	C	3.39925100	1.58490800	1.94308100
H	-0.40917700	3.34232400	-1.26446700	H	3.90452700	-0.06712600	3.18892100
H	3.42773600	3.99569200	0.58588200	C	1.56245700	3.84063000	-0.40790100
H	4.29616800	2.14587400	2.14340400	H	-0.38072500	3.35819400	-1.26698600
H	1.59736300	4.79132600	-0.91548400	H	3.45291900	3.98918800	0.58928700
N	0.26064200	1.85836400	-0.01575000	H	4.31020300	2.13865400	2.14672600
Co	-1.19190600	0.58194900	-0.19350400	H	1.63309100	4.79510300	-0.91596500
C	-0.21843000	-0.17091000	-1.72054400	N	0.27414000	1.87153900	-0.01669700
C	-1.31540200	-1.05203600	-1.60207900	Co	-1.20124600	0.58871400	-0.19580800
C	-2.84956300	2.24444000	-0.10526400	C	-0.23052600	-0.17475200	-1.74232800
O	-2.34667600	1.78904800	-1.19060000	C	-1.31199000	-1.06827900	-1.62710000
O	-2.40678000	1.75812600	0.97733000	C	-2.86629300	2.25607700	-0.10315100
C	-3.92744700	3.26864400	-0.13729500	O	-2.36591500	1.80520300	-1.19052600
H	-4.87423400	2.76386100	-0.36113900	O	-2.42161700	1.76874300	0.97743300
H	-4.01335100	3.76710600	0.82926700	C	-3.95032300	3.28067100	-0.13117300
H	-3.73566900	3.99525500	-0.93013400	H	-4.89271700	2.77413100	-0.36564700
H	-0.24461000	0.60897700	-2.47826900	H	-4.04211600	3.76974300	0.83915800
H	-2.13519100	-0.94130800	-2.30515400	H	-3.75405100	4.01505800	-0.91505400
H	-1.12136000	-2.07102000	-1.28173800	H	-0.26758700	0.60476300	-2.49892400
H	0.76801900	-0.50499300	-1.41128500	H	-2.13827000	-0.96412300	-2.32198600
				H	-1.11238100	-2.08133800	-1.29548600
				H	0.75965600	-0.49787900	-1.43608600

TS\_H\_S(wb97xd)

C	-4.82356800	-1.64622200	0.22514200
C	-4.46656100	-2.40259700	1.34219000
C	-3.15288300	-2.38166300	1.80019900
C	-2.20198300	-1.61298900	1.13370500
C	-2.54734700	-0.86955500	-0.00706800
C	-3.86953500	-0.88900800	-0.45175900
H	-5.85107900	-1.65181500	-0.12693400

TS\_H\_T(m06)

C	4.51981000	-0.37988700	-0.19833100
C	4.38806100	-1.68860100	-0.65720500
C	3.15118200	-2.32150800	-0.59149400
C	2.04953100	-1.65725800	-0.05878600
C	2.19774700	-0.35146900	0.44850900
C	3.43251800	0.28659500	0.36507100



H	5.48087400	0.12632400	-0.26201000	C	3.44855100	0.31307100	0.36688900
H	5.24510600	-2.20744100	-1.07997300	H	5.50058800	0.15278100	-0.24980600
H	3.01100200	-3.32811800	-0.98301200	H	5.27895700	-2.19478800	-1.03053000
H	3.55753700	1.29613700	0.75501800	H	3.05360100	-3.32828800	-0.92455400
C	0.68897000	-2.26061600	-0.15595500	H	3.56079300	1.32743900	0.74073600
O	0.50364200	-3.46783800	-0.35710000	C	0.71378800	-2.25176900	-0.12315200
N	-0.25128600	-1.28915700	-0.05281700	O	0.53440800	-3.46656800	-0.30494300
C	-1.62157200	-1.43231200	-0.18904200	N	-0.22135500	-1.28122400	-0.03776100
C	-2.32853400	-0.19530500	-0.06291100	C	-1.58459800	-1.43926600	-0.18414100
C	-2.35492300	-2.58071700	-0.43952700	C	-2.32087100	-0.21421100	-0.07302300
C	-3.73522800	-0.13645100	-0.19816000	C	-2.29693500	-2.60387800	-0.43434500
C	-3.75902100	-2.51693900	-0.56819200	C	-3.73019500	-0.18808600	-0.22043500
H	-1.84069900	-3.53017600	-0.54196700	C	-3.70046800	-2.57058800	-0.57735400
C	-2.19010300	2.10010400	0.30511200	H	-1.76266000	-3.54079300	-0.52500100
C	-4.34760100	1.13102400	-0.07211900	C	-2.23964000	2.08568800	0.28261700
C	-4.44653100	-1.33285900	-0.45512300	C	-4.37247400	1.06650200	-0.10630500
H	-4.30259900	-3.43817100	-0.76684000	C	-4.41544700	-1.40040500	-0.47719400
C	-3.58162100	2.24436000	0.17375600	H	-4.22154100	-3.50323100	-0.77578000
H	-1.55005400	2.95725300	0.51124500	C	-3.63218300	2.19872200	0.14001000
H	-5.42874700	1.20785900	-0.17412500	H	-1.61873300	2.95335100	0.48456400
H	-5.52845500	-1.29198800	-0.56209000	H	-5.45226900	1.12067100	-0.21690500
H	-4.02629700	3.22967600	0.27374300	H	-5.49491500	-1.38469600	-0.59435700
N	-1.59027900	0.92874000	0.18780200	H	-4.09871900	3.17347600	0.23067900
Co	0.36474900	0.51508200	0.36761100	N	-1.61363400	0.92673200	0.17605000
C	0.12239800	0.49683100	2.39489600	Co	0.36626700	0.56983200	0.34832300
C	1.44831200	0.03707300	2.28652500	C	0.14493000	0.52111300	2.41833300
C	1.20785200	2.53714500	-0.82905800	C	1.46862600	0.07455700	2.32919400
O	1.08347000	2.62359800	0.42472900	C	1.12965000	2.60817300	-0.86179900
O	0.88150800	1.45412700	-1.41400200	O	0.89968400	2.73412500	0.37394100
C	1.78497700	3.66238000	-1.62339200	O	0.97824300	1.46730200	-1.41209800
H	2.87452900	3.53462900	-1.65157400	C	1.62162100	3.76152400	-1.67802200
H	1.41573000	3.64853100	-2.65198600	H	2.71756000	3.73652400	-1.68013200
H	1.56845300	4.62410500	-1.15128900	H	1.27959800	3.67818400	-2.71157700
H	-0.08074000	1.54588300	2.60901200	H	1.29950800	4.70907700	-1.24253200
H	2.24070200	0.74216800	2.52728000	H	-0.07266800	1.56849100	2.61109100
H	1.64732500	-0.99800300	2.55735100	H	2.26035000	0.78336100	2.54792500
H	-0.68974700	-0.20404800	2.58375300	H	1.67607900	-0.96245200	2.57348800
				H	-0.66227300	-0.18958200	2.57418500
TS_H_T(pbe0)							
C	4.54292800	-0.35631000	-0.18180700				
C	4.41808900	-1.67450800	-0.62071700	TS_H_T(wb97xd)			
C	3.18465200	-2.31548200	-0.55155200	C	4.55728300	-0.46757600	-0.15750500
C	2.07435000	-1.64705000	-0.03699800	C	4.39898900	-1.76637800	-0.63959300
C	2.22054300	-0.33619500	0.44688300	C	3.14861500	-2.37682200	-0.59945200

C	2.05206500	-1.69471400	-0.07472400
C	2.23361100	-0.40560900	0.44211000
C	3.47595700	0.21453700	0.40061100
H	5.52881300	0.01552900	-0.20151200
H	5.24796500	-2.29695600	-1.05906900
H	3.00036500	-3.37568300	-1.00022900
H	3.60713300	1.21519600	0.80205700
C	0.67039800	-2.26791000	-0.16868500
O	0.47477500	-3.48323900	-0.32946400
N	-0.24338600	-1.27865000	-0.10484700
C	-1.61971700	-1.42806800	-0.20537500
C	-2.34602200	-0.19253100	-0.10477600
C	-2.34566200	-2.59200800	-0.38902900
C	-3.75601100	-0.16472900	-0.19740700
C	-3.75706500	-2.55704900	-0.47547900
H	-1.82438500	-3.53601000	-0.46974500
C	-2.24660200	2.11539000	0.18637700
C	-4.39354800	1.09590700	-0.09399200
C	-4.45931900	-1.38254800	-0.38574400
H	-4.28843500	-3.49317400	-0.61874000
C	-3.64474700	2.23104200	0.09113000
H	-1.61863500	2.98623800	0.34693900
H	-5.47632600	1.14884400	-0.16245800
H	-5.54238700	-1.36392600	-0.45583900
H	-4.10493900	3.20865200	0.17316100
N	-1.62490900	0.95484200	0.09026300
Co	0.38716700	0.58114400	0.29011200
C	0.10800600	0.47192400	2.39645900
C	1.41785400	-0.00294300	2.33683300
C	1.23927500	2.67342100	-0.78958400
O	0.91738300	2.76849100	0.42663000
O	1.13645100	1.54462900	-1.37460300
C	1.77863500	3.84855100	-1.55138600
H	2.86871300	3.75527700	-1.60209000
H	1.39413700	3.84618300	-2.57358000
H	1.52715300	4.78518700	-1.05231400
H	-0.09076000	1.52069400	2.59707300
H	2.22130900	0.68198300	2.58422300
H	1.59458400	-1.05097300	2.55165300
H	-0.72059200	-0.22165500	2.50428300

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C	-5.11503300	1.15067000	-0.00037100
C	-3.94722700	1.79153600	0.41550100
C	-2.73539300	1.10311100	0.42362900
C	-2.68323700	-0.23742600	0.01534600
C	-3.86281500	-0.87857600	-0.38411000
C	-5.07056200	-0.18721700	-0.39841600
H	-6.05723500	1.69020100	-0.00792200
H	-3.97971700	2.82654600	0.74120400
H	-1.84435800	1.61168600	0.77934200
H	-3.80860000	-1.92019800	-0.67978600
H	-5.97771700	-0.69082900	-0.71795300
C	-1.42262400	-1.05072500	0.00560700
O	-1.44868800	-2.28027200	0.00458400
N	-0.26407900	-0.31822700	-0.01417900
H	-0.31609700	0.69064400	-0.10931900
C	1.05363500	-0.76985500	0.01547900
C	2.04474000	0.26828000	-0.03247700
C	1.45422000	-2.09301200	0.09103600
C	3.42787500	-0.07709000	-0.00283600
C	2.83095000	-2.41346500	0.12120700
H	0.70456400	-2.86976400	0.12299700
C	2.50655200	2.52096800	-0.15162900
C	4.35605900	0.99276400	-0.05440900
C	3.80467800	-1.44210000	0.07546500
H	3.11454100	-3.45978100	0.18068200
C	3.90101600	2.28878900	-0.12870500
H	2.12601600	3.53869100	-0.20992500
H	5.41977700	0.77299700	-0.03457400
H	4.85868500	-1.70132400	0.09773800
H	4.58790700	3.12724400	-0.16935000
N	1.60797100	1.55551100	-0.10524700

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C	-3.82720300	-2.83382100	3.61966700
C	-2.78849300	-3.65269300	3.76559800
C	-2.15485400	-4.94341600	3.47406800
C	-1.46207700	-3.88185800	4.34461600
H	-1.75791000	-5.12257200	2.47572300
H	-2.53222300	-5.83903000	3.96583800
H	-1.37780700	-4.07787800	5.41254700
H	-0.60370100	-3.36119700	3.92258600
H	-3.78359500	-1.86155100	4.10999800
C	-5.05097400	-3.10018400	2.85562400

C	-6.06075300	-2.12076500	2.80230200
C	-5.27621300	-4.29930900	2.16153000
C	-7.23539900	-2.32512100	2.09362600
H	-5.91531200	-1.18175800	3.32974100
C	-6.45003700	-4.52027600	1.44529000
H	-4.51967700	-5.07588800	2.18085500
C	-7.44056000	-3.52964000	1.40737400
H	-8.00984600	-1.56613100	2.05647700
H	-6.58374000	-5.45996800	0.92356800
O	-8.62256500	-3.64234300	0.73900000
C	-8.87421700	-4.84739700	0.02840900
H	-9.85912300	-4.72875500	-0.42619100
H	-8.13192000	-5.01423000	-0.76212400
H	-8.89032700	-5.71665600	0.69766700

HOAc

C	-0.09030500	0.12322700	-0.00019400
O	-0.64170300	1.20280700	-0.00008300
O	-0.77830300	-1.04285900	0.00004900
H	-1.72166500	-0.80310600	0.00009300
C	1.39467700	-0.11156900	0.00002900
H	1.68022400	-0.69305600	0.88193000
H	1.68046900	-0.69298900	-0.88183500
H	1.91745200	0.84414600	0.00013900

CoOAc3\_Q

Co	-0.10976800	-0.03788900	0.02928600
C	-2.49528400	-0.06882000	0.01033400
O	-1.81646100	-0.51152200	-0.98070500
O	-1.84044600	0.38345400	1.01436200
C	1.20769100	2.00143800	0.07211300
O	1.37974700	1.18946600	1.01895800
O	0.33036500	1.67685200	-0.82728300
C	1.37962400	-1.95902500	-0.07178100
O	1.48922900	-1.12842500	-1.00712300
O	0.47740600	-1.71060100	0.83394300
C	-3.98903100	-0.04519300	-0.01719300
H	-4.38974900	-0.13789600	0.99360400
H	-4.30924500	0.91973800	-0.42734500
H	-4.37115300	-0.83744600	-0.66272100
C	1.96117800	3.28432600	-0.06027600
H	2.58081400	3.24044500	-0.96203200
H	1.25753400	4.11264800	-0.18330600
H	2.59147900	3.45037200	0.81365800

C	2.21925300	-3.18782200	0.05157300
H	2.78160100	-3.14403900	0.98965900
H	1.57162800	-4.06865800	0.09649900
H	2.90548500	-3.26915000	-0.79165700

CoOAc3\_S

Co	0.00078400	0.00552500	-0.01827800
C	1.49510500	-1.71917700	-0.03812600
O	0.57526600	-1.61766900	0.84530800
O	1.51022500	-0.78803300	-0.91484900
C	0.74997100	2.16167700	-0.00284900
O	-0.06855500	1.72558400	-0.88318200
O	1.12289900	1.29835900	0.86479100
C	-2.23996100	-0.42940700	-0.00149900
O	-1.67774900	0.31093200	0.87703100
O	-1.45578700	-0.89922100	-0.89641400
C	2.49774400	-2.82210500	-0.02597700
H	2.83639100	-3.03498200	-1.04166300
H	3.36121900	-2.50250500	0.56828500
H	2.07094000	-3.71483300	0.43443400
C	1.21332900	3.57806500	0.03263600
H	0.65978900	4.10830700	0.81584100
H	2.27603700	3.61523100	0.28398700
H	1.02806300	4.06372000	-0.92662400
C	-3.69465500	-0.75272600	0.03457000
H	-4.08129100	-0.85420200	-0.98154600
H	-3.82687200	-1.71072100	0.55045000
H	-4.24124100	0.01755000	0.58102800

CoOAc3\_T

Co	-0.06739700	-0.01366900	0.00105500
C	1.26941600	-1.99559100	0.05634700
O	0.44795600	-1.89304000	0.99920900
O	1.31355200	-1.03342300	-0.81593000
C	1.07324400	2.08677700	-0.07444800
O	0.24942000	1.90629100	-1.00361300
O	1.22412700	1.13325500	0.79519600
C	-2.37280700	-0.11770600	0.01602000
O	-1.71128400	0.68889100	0.76021300
O	-1.65108500	-0.86791100	-0.73098700
C	2.20667300	-3.15263200	-0.10723600
H	2.12463300	-3.55423500	-1.12103300
H	3.23500500	-2.80292100	0.02926500
H	1.98209800	-3.92781000	0.62574200

C	1.89901900	3.32782300	0.07423300
H	1.81886500	3.70643400	1.09688300
H	2.95022300	3.08179400	-0.10795200
H	1.57241500	4.08664400	-0.63719800
C	-3.85903600	-0.15394900	-0.00384300
H	-4.21400700	0.57287400	-0.74358600
H	-4.20948700	-1.14615100	-0.29372300
H	-4.25490800	0.12694100	0.97409400

2s\_Q

C	-4.24304900	-0.73284000	-1.21785600
C	-5.06990200	-1.57176200	-0.47004700
C	-4.50805700	-2.52114100	0.38824300
C	-3.12579300	-2.62439800	0.49809200
C	-2.28963900	-1.78113400	-0.24905600
C	-2.85679200	-0.83330700	-1.11219200
H	-4.67473300	0.00729500	-1.88427200
H	-6.14936600	-1.48707300	-0.55487700
H	-5.14812200	-3.17679400	0.97080400
H	-2.66900100	-3.35151000	1.15951100
H	-2.23892100	-0.16835000	-1.70298500
C	-0.82282200	-1.94567200	-0.05033200
N	0.02843300	-1.08128000	-0.78547100
H	-0.31916700	-0.72439100	-1.69890800
O	-0.34945600	-2.76064200	0.72693300
C	1.41491700	-1.46593900	-0.83999600
C	2.36651000	-0.71867500	-0.09951600
C	1.83000200	-2.55401500	-1.57576400
C	3.73348500	-1.12302000	-0.09057400
C	3.18863500	-2.94401700	-1.59006000
H	1.09534100	-3.12356000	-2.13538500
C	2.82063200	1.08335700	1.31251800
C	4.63620300	-0.35707200	0.68904400
C	4.12319300	-2.25204700	-0.85364300
H	3.48520700	-3.80611900	-2.17820100
C	4.18336600	0.73322500	1.39609400
H	2.41989800	1.94061800	1.84039200
H	5.68320100	-0.64440200	0.71836000
H	5.16504200	-2.55703400	-0.84662500
H	4.84999600	1.33269000	2.00479900
N	1.95948200	0.38801800	0.58874700
Co	0.03807500	1.04588400	0.20829000
O	-0.48010600	0.36830800	-3.04950500
O	0.64478600	1.59946200	-1.54054500

C	0.14808900	1.38881300	-2.72648300	C	-4.00768900	-2.40476000	0.49664100
O	-1.71879600	2.20677000	-0.19850400	H	-3.30162200	-4.15098100	1.50817500
O	0.02248200	2.95202800	0.91094800	C	-4.13772100	0.96292300	-1.14624000
C	-1.15454800	3.14690900	0.43586800	H	-2.37766300	2.24494600	-1.38783900
O	-0.77781300	0.22371600	1.64357500	H	-5.62985100	-0.52583500	-0.74125200
O	0.64328300	0.50673100	3.37206800	H	-5.03913900	-2.74004900	0.45181900
C	-0.33611000	-0.02555900	2.87588400	H	-4.81449400	1.66564400	-1.61779900
C	-1.18016600	-1.05957500	3.58582400	N	-1.90877100	0.48438200	-0.46106000
H	-1.03689700	-2.02268300	3.08555000	Co	-0.09526000	0.90357800	-0.03749000
H	-0.88534100	-1.13695400	4.63315100	O	0.34033200	-0.01271300	3.00406900
H	-2.24032800	-0.80359400	3.50574800	O	-0.72944800	1.48324400	1.68619000
C	-1.83947100	4.46282500	0.66586100	C	-0.32933800	1.02825400	2.82516000
H	-1.13452200	5.28461800	0.51814900	O	1.64423200	1.69220300	0.39447800
H	-2.69870700	4.57211700	0.00304200	O	0.00926100	2.75786500	-0.53247000
H	-2.18301000	4.50146100	1.70546900	C	1.21193300	2.78413300	-0.09988100
C	0.39720300	2.50167900	-3.71725900	O	0.63085600	0.34896000	-1.66474300
H	-0.18706800	3.37747300	-3.41412600	O	-0.86572400	1.20440400	-3.14069400
H	1.45134900	2.79182000	-3.70212500	C	0.12241300	0.53390800	-2.85940700
H	0.10133600	2.19754500	-4.72189400	C	0.91352000	-0.22328500	-3.91670200
2s_S				H	0.76321900	-1.29802400	-3.76968600
C	4.28646000	-0.79632500	1.31953800	H	0.57707300	0.05904200	-4.91561700
C	5.15906700	-1.34145100	0.37799400	H	1.98398400	-0.02682500	-3.80908300
C	4.65269000	-2.02632900	-0.73120800	C	2.06312900	4.00561000	-0.20830900
C	3.27954900	-2.16446600	-0.89136400	H	1.44372700	4.90430600	-0.19451200
C	2.39683900	-1.60872800	0.04875400	H	2.79443000	4.02913000	0.60196400
C	2.90729900	-0.92115000	1.15815600	H	2.60315100	3.96979900	-1.16117000
H	4.67681900	-0.26560200	2.18231700	C	-0.72701000	1.88002200	4.01266800
H	6.23232300	-1.23469300	0.50633300	H	-0.07377800	2.75917900	4.04793000
H	5.32956400	-2.45052100	-1.46650100	H	-1.75373100	2.23716500	3.90259300
H	2.86525800	-2.69470000	-1.74106600	H	-0.61561100	1.31848800	4.94119000
H	2.24950200	-0.47962900	1.89644800	2s_T			
C	0.94973800	-1.82111000	-0.19620800	C	-4.27023400	-0.62658400	-1.31285500
N	0.02119400	-1.02921100	0.59505900	C	-5.10528900	-1.47014500	-0.57965400
H	0.32508900	-0.80276700	1.58511700	C	-4.55267400	-2.44168300	0.25962800
O	0.51912200	-2.61801800	-1.00482300	C	-3.17153600	-2.56394000	0.36236800
C	-1.33051100	-1.54862500	0.60316700	C	-2.32713700	-1.71549400	-0.36990300
C	-2.31252400	-0.72692900	0.01644800	C	-2.88476800	-0.74348200	-1.21191100
C	-1.68690000	-2.76475500	1.13710700	H	-4.69544700	0.13061800	-1.96431200
C	-3.66850500	-1.14279300	-0.05384800	H	-6.18393900	-1.37201300	-0.66099200
C	-3.03704700	-3.18827900	1.08366700	H	-5.19883600	-3.10074200	0.83151800
H	-0.93266800	-3.40228000	1.58562600	H	-2.72172000	-3.31151800	1.00537600
C	-2.77392400	1.30720100	-1.02342600	H	-2.25979400	-0.06806900	-1.78305300
C	-4.58306500	-0.24742700	-0.66384200	C	-0.86223600	-1.91418500	-0.19043400

N	0.00143400	-1.02832700	-0.87397200	C	-5.10057800	-1.26310800	-0.53747100
H	-0.34426700	-0.55164200	-1.72934500	C	-4.53852500	-2.30373100	0.20784900
O	-0.39939300	-2.78415500	0.53371700	C	-3.15963400	-2.48084900	0.22152700
C	1.38141200	-1.41724700	-0.94723400	C	-2.32112400	-1.61466600	-0.49781900
C	2.32409600	-0.69325700	-0.17625600	C	-2.89127100	-0.57641600	-1.24490200
C	1.80590500	-2.47716800	-1.71716200	H	-4.70586800	0.40080900	-1.84930200
C	3.69599000	-1.07846400	-0.17798400	H	-6.17759100	-1.12306500	-0.55115800
C	3.16809600	-2.85523600	-1.73785600	H	-5.17652000	-2.97519100	0.77472600
H	1.07753200	-3.03198600	-2.29903900	H	-2.70492300	-3.28764400	0.78440100
C	2.75630000	1.07333800	1.29325800	H	-2.27339300	0.10122000	-1.81665400
C	4.58993000	-0.32332300	0.62079100	C	-0.85256000	-1.88519200	-0.42372400
C	4.09518400	-2.17858300	-0.97790400	N	0.01819000	-0.86314400	-0.85526400
H	3.47451800	-3.69494200	-2.35266300	H	-0.24327700	-0.14780100	-1.94930400
C	4.12403700	0.74250100	1.35545600	O	-0.43484400	-2.94765900	0.02748700
H	2.34679400	1.90951700	1.84578100	C	1.39148200	-1.25470400	-0.95897800
H	5.64080200	-0.59631800	0.64060200	C	2.36615300	-0.51591500	-0.23741400
H	5.13992300	-2.47323400	-0.98046600	C	1.81801400	-2.28838300	-1.77169500
H	4.78259100	1.33708700	1.97719600	C	3.75065000	-0.84132000	-0.33587900
N	1.90600400	0.38060800	0.55531100	C	3.18814000	-2.61456500	-1.87726800
Co	0.08909600	1.02155300	0.27049800	H	1.08402500	-2.86156800	-2.32644800
O	-0.47178700	0.73346700	-2.90924900	C	2.80522100	1.21891700	1.26458600
O	0.72034700	1.81134500	-1.32278900	C	4.65583400	-0.06197600	0.42729200
C	0.23078300	1.67920200	-2.52212200	C	4.14339300	-1.91206400	-1.17525400
O	-1.61629900	1.91767800	-0.02545300	H	3.48341800	-3.43538400	-2.52303200
O	-0.12980100	2.98121700	1.17884500	C	4.18961200	0.95917300	1.22509800
C	-1.28254800	2.94869300	0.66829400	H	2.39007400	2.01215800	1.87569900
O	-0.67360600	0.20325400	1.72137500	H	5.71777900	-0.28447200	0.37466700
O	0.95944000	0.03347400	3.28231600	H	5.19600300	-2.16573300	-1.25295300
C	-0.12443400	-0.29069800	2.82222100	H	4.86182800	1.56468700	1.82166500
C	-1.02376400	-1.32138700	3.47720800	N	1.94317800	0.51034400	0.55657500
H	-0.96185000	-2.24450400	2.89231000	Co	-0.06987600	0.86505600	0.45940900
H	-0.69098400	-1.51088500	4.49888900	O	-0.28012800	0.58105400	-2.85851400
H	-2.06539900	-0.99150800	3.46840200	O	0.47895300	1.98128700	-1.27553000
C	-2.28367400	4.04881400	0.86925700	C	0.16856600	1.72240700	-2.46558600
H	-1.77947200	4.97727400	1.14125700	O	-1.84191300	1.92083900	0.18779700
H	-2.88465800	4.18814500	-0.03198600	O	-0.16695400	2.74999000	1.32834300
H	-2.95727700	3.76145800	1.68419300	C	-1.35574200	2.87226400	0.88430600
C	0.60610400	2.80732100	-3.45778400	O	-0.59079600	-0.13417400	1.89002600
H	0.03532700	3.69943800	-3.17722700	O	1.07344100	-0.29328700	3.39661800
H	1.66656900	3.05172700	-3.35670500	C	0.06151900	-0.74195300	2.89104000
H	0.37345800	2.54000800	-4.48917900	C	-0.59994900	-2.03302200	3.30792600
				H	-0.50781000	-2.75062400	2.48619500
TS1s_Q				H	-0.12449800	-2.42899000	4.20616200
C	-4.27517200	-0.40693400	-1.26556600	H	-1.66720800	-1.86966900	3.48268500

C	-2.17501200	4.08758500	1.20324900	C	-0.18633200	0.00990000	2.99896600
H	-1.53130300	4.95853500	1.33927800	O	1.84581800	1.29756800	0.64873900
H	-2.91017100	4.27035700	0.41749900	O	0.26282700	2.72857400	0.29805900
H	-2.71211100	3.90709000	2.14143600	C	1.49606200	2.51946800	0.55870100
C	0.29120900	2.79659000	-3.51076000	O	0.46888500	0.73991700	-1.57304700
H	0.98698000	3.57016200	-3.18421800	O	-1.01256400	2.21795500	-2.45877400
H	0.60454400	2.36990800	-4.46566700	C	-0.09816500	1.40701500	-2.55208800
H	-0.69632300	3.25107900	-3.65204400	C	0.52203200	1.03657800	-3.89276600
TS1s_S				H	0.28010300	-0.00523000	-4.12724800
C	4.23917300	-1.34021400	0.99602300	H	0.13357600	1.68700300	-4.67802300
C	5.07355400	-1.29468300	-0.12042000	H	1.61188800	1.11515300	-3.84386500
C	4.52658300	-1.40124400	-1.40258300	C	2.47245800	3.64035700	0.70377900
C	3.15409000	-1.56001200	-1.56096300	H	1.97820700	4.52687700	1.10595200
C	2.30805200	-1.58387800	-0.44292600	H	3.30443200	3.33878100	1.34280400
C	2.86003300	-1.47325500	0.83773300	H	2.86812000	3.88596600	-0.28822700
H	4.65996100	-1.26620700	1.99446000	C	-0.30916500	0.32837800	4.45983200
H	6.14628900	-1.17974900	0.00588700	H	-0.77365000	1.30364400	4.60325100
H	5.17205500	-1.36693200	-2.27527800	H	-0.88396000	-0.45106000	4.96594400
H	2.71358400	-1.65961000	-2.54633000	H	0.69482600	0.33741600	4.89836300
H	2.22778300	-1.49692500	1.71584800	TS1s_T			
C	0.85418200	-1.80079600	-0.70113300	C	4.11292600	-1.14008500	1.15220300
N	-0.06569300	-1.20080500	0.20381000	C	4.97411600	-1.62585800	0.16936000
H	0.14551500	-1.28701100	1.58123100	C	4.45077200	-2.21476300	-0.98608700
O	0.48585800	-2.47805500	-1.64920700	C	3.07448800	-2.31276100	-1.15166300
C	-1.42530000	-1.60303300	0.01004900	C	2.20120200	-1.81376000	-0.17217500
C	-2.37102600	-0.56076200	-0.10834000	C	2.73137900	-1.22857100	0.98391800
C	-1.87825000	-2.90819900	-0.00926800	H	4.51278300	-0.68360700	2.05222100
C	-3.76180900	-0.81913200	-0.24751300	H	6.04941000	-1.54842600	0.30152900
C	-3.25891500	-3.18204600	-0.14960200	H	5.11733700	-2.59564300	-1.75406300
H	-1.17130200	-3.72485400	0.07295400	H	2.64821700	-2.76978200	-2.03729200
C	-2.69138900	1.75149100	-0.18897200	H	2.08695700	-0.84106900	1.75979200
C	-4.61507500	0.30777000	-0.35563000	C	0.74177100	-1.96681500	-0.43896000
C	-4.18878300	-2.16993300	-0.26724300	N	-0.15347900	-1.18402900	0.35224100
H	-3.58509600	-4.21716400	-0.16474300	H	0.03717700	-1.09587800	1.68262300
C	-4.08505900	1.57893500	-0.32516900	O	0.33040300	-2.73527900	-1.29429100
H	-2.22514200	2.72737300	-0.17845500	C	-1.53850200	-1.53810200	0.19019300
H	-5.68500100	0.15519600	-0.46354200	C	-2.44832100	-0.53977700	-0.24481500
H	-5.24578800	-2.39148900	-0.37585900	C	-2.02371700	-2.79795700	0.47951400
H	-4.71624400	2.45568600	-0.41052300	C	-3.83212000	-0.83461500	-0.40855700
N	-1.88380200	0.71253900	-0.08262800	C	-3.39788800	-3.09445100	0.33069100
Co	-0.00926100	0.81059500	0.21722600	H	-1.33901900	-3.57007700	0.81150400
O	0.13789000	-1.20177700	2.69737100	C	-2.73960000	1.66200500	-0.94757000
O	-0.38563600	0.91440700	2.15051000	C	-4.66237500	0.21790200	-0.87160500

C	-4.29065000	-2.14089200	-0.10836800	N	0.16072100	-1.00243400	0.22164400
H	-3.74479600	-4.09618200	0.56328500	O	1.45785500	-2.20101900	1.68508600
C	-4.12182500	1.45438900	-1.14695000	C	-0.91942500	-1.78540000	0.09706600
H	-2.26200600	2.61195600	-1.15688200	C	-2.18231100	-1.10739900	-0.14062800
H	-5.72369000	0.03206400	-1.01004100	C	-0.92655400	-3.20254500	0.14550200
H	-5.34378900	-2.37475600	-0.23006500	C	-3.37773600	-1.84844700	-0.31270300
H	-4.73561900	2.27055600	-1.51052400	C	-2.11431300	-3.91653300	-0.02798500
N	-1.95123700	0.70180800	-0.50395600	H	0.00182200	-3.72848300	0.32708000
Co	0.04674700	0.82127900	0.08605000	C	-3.29003100	0.91197300	-0.39410600
O	-0.00775800	-0.85032700	2.81200000	C	-4.56745500	-1.11717200	-0.53953700
O	-0.65195100	1.11594300	1.93867900	C	-3.32225400	-3.26970400	-0.25323800
C	-0.45862100	0.34731600	2.92087300	H	-2.08693400	-5.00034900	0.01299200
O	1.89257000	1.73577300	1.06031300	C	-4.52287100	0.26192500	-0.58212900
O	0.29478600	2.74317900	-0.05849700	H	-3.19955700	1.99330400	-0.41324700
C	1.40634800	2.79511500	0.59479000	H	-5.50359200	-1.65042400	-0.67547600
O	0.87960900	0.53488300	-1.51869400	H	-4.23622600	-3.83896100	-0.39002500
O	-0.32867900	1.91973800	-2.85031800	H	-5.41746300	0.84974500	-0.75326400
C	0.62087800	1.18175100	-2.64896100	N	-2.16180500	0.24258400	-0.18375300
C	1.65851300	0.85062200	-3.70726000	Co	-0.23340400	1.05985500	0.18413300
H	1.66809100	-0.22830400	-3.88900600	O	1.47929500	1.73275500	1.21101000
H	1.43014800	1.38146200	-4.63244100	O	-0.30573600	1.07086200	2.31680900
H	2.65457100	1.12924500	-3.34987300	C	0.88840000	1.51146700	2.31667100
C	2.07713700	4.13275800	0.74153100	O	0.01034600	1.63876300	-1.81650800
H	1.34969700	4.88676400	1.05357800	O	-0.88168000	3.06537600	-0.39092900
H	2.89306600	4.07274900	1.46281700	C	-0.46928000	2.79539100	-1.55741500
H	2.47561500	4.43914200	-0.23146800	C	-0.50615200	3.84071600	-2.64498100
C	-0.73931000	0.85717400	4.30374600	H	-0.67420200	3.37858200	-3.62039800
H	-1.47383400	1.66262200	4.27154300	H	-1.27467000	4.58795300	-2.43836200
H	-1.07660300	0.04619700	4.95142500	H	0.46554200	4.34685500	-2.67505800
H	0.19568000	1.25693700	4.71337300	C	1.62058500	1.71722600	3.61798400
3s_Q				H	2.34873500	2.52569300	3.52606800
C	3.63647200	-0.16480500	-2.07851200	H	0.91892700	1.92509200	4.42806500
C	4.88803500	-0.56298800	-1.60584200	H	2.16234400	0.79567300	3.86043100
C	4.99363800	-1.26698000	-0.40178700	3s_S			
C	3.84927700	-1.56921400	0.32701300	C	3.77228400	0.05496800	-1.93572900
C	2.58984100	-1.16538000	-0.14213000	C	4.92560700	-0.32607300	-1.24797700
C	2.48590600	-0.46401900	-1.35180500	C	4.83052600	-1.19530200	-0.15719800
H	3.55370700	0.38639500	-3.00992300	C	3.58671100	-1.67595600	0.24222700
H	5.78287700	-0.32388900	-2.17307100	C	2.42385700	-1.26837900	-0.42365500
H	5.96786000	-1.57459300	-0.03442000	C	2.52392100	-0.41102900	-1.52447400
H	3.90668200	-2.11232200	1.26385600	H	3.84404700	0.71495300	-2.79560400
H	1.52069800	-0.13314500	-1.71571600	H	5.89646300	0.04401200	-1.56520400
C	1.40142200	-1.52884300	0.66380200	H	5.72691800	-1.50168000	0.37435800



H	3.49684900	-2.36927500	1.07207200	H	3.53374400	0.17880100	-3.09449800
H	1.62720000	-0.11075600	-2.05084900	H	5.71521300	-0.56120800	-2.16245100
C	1.11537900	-1.85139000	0.01023600	H	5.78839100	-1.80791700	-0.01383700
N	-0.01129900	-1.06274600	-0.14549000	H	3.66506700	-2.31486600	1.19248200
O	1.08597700	-3.01099400	0.43427300	H	1.43809300	-0.29641200	-1.86997700
C	-1.27617500	-1.64186000	-0.19784600	C	1.19190200	-1.69292000	0.49049800
C	-2.34955100	-0.70248500	-0.20811300	N	0.00577600	-1.00028300	0.14464900
C	-1.61852000	-2.98949200	-0.32011100	O	1.18722000	-2.57096700	1.34505400
C	-3.71062900	-1.09143500	-0.35631200	C	-1.19621100	-1.70151200	0.06338900
C	-2.96695600	-3.37676000	-0.47626500	C	-2.33205200	-0.86707400	-0.12598300
H	-0.84246100	-3.73829100	-0.29001200	C	-1.39834300	-3.07777200	0.07253600
C	-2.92649400	1.55950300	-0.03953700	C	-3.63774200	-1.38719400	-0.30931400
C	-4.67964000	-0.05883400	-0.34396800	C	-2.69734200	-3.60351100	-0.11322800
C	-4.00538600	-2.46848200	-0.49753200	H	-0.56532400	-3.74810600	0.23337900
H	-3.18297900	-4.43658400	-0.57625800	C	-3.07540200	1.33949200	-0.26275700
C	-4.29243000	1.25440900	-0.18713100	C	-4.68145400	-0.44526700	-0.47527400
H	-2.57643400	2.57384300	0.10475100	C	-3.80119200	-2.79699700	-0.30114600
H	-5.72886700	-0.31717700	-0.45441800	H	-2.81969200	-4.68213400	-0.10094900
H	-5.03642700	-2.78737600	-0.60938700	C	-4.40152100	0.90607900	-0.44993700
H	-5.01769300	2.05969100	-0.16787400	H	-2.80665700	2.38861800	-0.22827100
N	-2.00267000	0.60865500	-0.05796200	H	-5.69904900	-0.79723000	-0.61714700
Co	-0.13402200	0.82598700	0.27164700	H	-4.79119900	-3.22095500	-0.43277900
O	1.62628100	0.97679600	1.10671300	H	-5.18513000	1.64543300	-0.56852800
O	-0.18482700	0.45438400	2.15882500	N	-2.08174900	0.47373600	-0.11167200
C	1.07682500	0.67099300	2.21512600	Co	-0.20240800	0.84861200	0.24191300
O	0.19427400	1.65334600	-1.46396400	O	1.57924600	1.16873100	0.94452400
O	-0.25063000	2.79757600	0.31767500	O	-0.02094400	1.11223200	2.44383400
C	0.07154000	2.80156100	-0.91912900	C	1.19988300	1.25743400	2.17569500
C	0.32619200	4.06557400	-1.67184000	O	0.19413900	1.76888700	-1.80408700
H	0.12328700	3.92376600	-2.73488200	O	-0.48033800	2.78287200	0.02196600
H	-0.28082900	4.87778200	-1.26725200	C	-0.10482900	2.83502200	-1.21247600
H	1.38242300	4.33262700	-1.55263200	C	-0.01642400	4.17980000	-1.87922500
C	1.85617700	0.52211000	3.47742600	H	0.00305200	4.06790400	-2.96425800
H	2.66777500	1.25202300	3.50594800	H	-0.85169300	4.81520100	-1.57484000
H	1.20568800	0.63256300	4.34640600	H	0.90940300	4.66940000	-1.55756500
H	2.29760000	-0.48094800	3.49154400	C	2.24272400	1.51482500	3.22493400
				H	2.74689100	2.46294100	3.01443200
3s_T				H	1.79021100	1.54698600	4.21640400
C	3.56904700	-0.36325700	-2.15441600	H	2.99735500	0.72339100	3.18358200
C	4.79392400	-0.78016100	-1.63023200				
C	4.83612600	-1.48204800	-0.42151400	TS2s_Q			
C	3.65596100	-1.76429900	0.25810900	C	-4.47379200	0.69373700	-1.02137300
C	2.42506900	-1.33290400	-0.25713100	C	-4.16906700	2.03088600	-1.30635400
C	2.38550400	-0.63564600	-1.47133900	C	-2.93808400	2.55498300	-0.92717300

C	-2.01011000	1.73684800	-0.26624100	C	4.51062700	-0.06169200	-0.61336100
C	-2.30244700	0.39030400	0.06881500	C	4.38412400	-1.32590400	-1.20240700
C	-3.55294700	-0.10296000	-0.34077000	C	3.18795700	-2.03795600	-1.10282100
H	-5.43444800	0.28403500	-1.32281300	C	2.11709400	-1.47521600	-0.41317500
H	-4.88743800	2.65387100	-1.83117400	C	2.22697100	-0.21064200	0.20949600
H	-2.67030500	3.58125100	-1.15841100	C	3.43963200	0.49078100	0.08710600
H	-3.81875800	-1.12931900	-0.09610400	H	5.44820600	0.48082600	-0.69477000
C	-0.65666500	2.29769400	-0.00686800	H	5.22264200	-1.75304600	-1.74504700
O	-0.41851400	3.49820000	0.08326100	H	3.06567400	-3.00995400	-1.56993200
N	0.31984400	1.28050500	0.04836900	H	3.54877600	1.45733700	0.57161900
C	1.65596600	1.49630500	-0.01927800	C	0.77474000	-2.13388200	-0.40434500
C	2.44868700	0.29278600	-0.18431400	O	0.58963800	-3.31825300	-0.69521200
C	2.33562200	2.73112800	0.04159800	N	-0.19438700	-1.21570200	-0.09767300
C	3.86270400	0.35959500	-0.27069500	C	-1.55488800	-1.41452800	-0.25272700
C	3.73519400	2.77777900	-0.03651600	C	-2.30231000	-0.19854500	-0.29723500
H	1.75621200	3.63403200	0.16512500	C	-2.24724800	-2.61408700	-0.38441700
C	2.45522700	-2.00926100	-0.45550000	C	-3.71434200	-0.18857500	-0.45352300
C	4.56148500	-0.85713200	-0.45319100	C	-3.65223300	-2.60200300	-0.53959600
C	4.49575000	1.63047700	-0.18765500	H	-1.69645900	-3.54358600	-0.37476100
H	4.22840600	3.74248700	0.02527100	C	-2.19506900	2.13250500	-0.22893600
C	3.85891100	-2.04133500	-0.54631800	C	-4.34502500	1.08021000	-0.49186200
H	1.86088200	-2.91578000	-0.51881400	C	-4.38480000	-1.43256200	-0.57221900
H	5.64512300	-0.84396600	-0.52272700	H	-4.16510100	-3.55451000	-0.63672200
H	5.57801200	1.68603400	-0.25161800	C	-3.59304600	2.23030400	-0.38295200
H	4.36622800	-2.98867900	-0.68871200	H	-1.56466900	3.00856900	-0.12570800
N	1.78063200	-0.88063600	-0.28310300	H	-5.42361500	1.13303000	-0.60915200
Co	-0.32709700	-0.63394400	0.02961500	H	-5.46294800	-1.44742300	-0.69512200
C	-1.03560000	-2.30523100	-1.63029700	H	-4.05469500	3.21078700	-0.40883700
O	-1.00556000	-2.56588000	-0.37856600	N	-1.58539800	0.95990200	-0.19431700
O	-0.63561300	-1.17788300	-2.04446800	Co	0.30716700	0.58914800	0.13096400
C	-0.90491100	-0.91391600	2.86250800	C	1.04880600	2.24776400	-1.31385000
O	-2.05048200	-0.41969400	2.55668300	O	0.90358900	2.47007600	-0.06381000
O	0.04339100	-1.02166700	2.04427100	O	0.74104100	1.07659500	-1.71575100
C	-1.59145600	-3.32470500	-2.59203900	C	0.48907600	0.15697000	2.91532500
H	-2.67859400	-3.19432800	-2.64472100	O	1.64273400	-0.32883500	2.74514200
H	-1.18128700	-3.17772900	-3.59298300	O	-0.22451000	0.62580600	1.97039400
H	-1.39049900	-4.33915200	-2.24063000	C	1.59509500	3.27920600	-2.24725200
C	-0.73354900	-1.40014500	4.27705700	H	2.68353700	3.15879200	-2.29431700
H	-1.22843500	-2.37313900	4.37261600	H	1.19222800	3.13665800	-3.25184700
H	0.32399700	-1.51708900	4.51633700	H	1.37303900	4.28310300	-1.88052100
H	-1.21332300	-0.71238900	4.97691600	C	-0.10868700	0.16638400	4.29747800
H	-2.04382400	-0.11584700	1.41218700	H	-0.75240900	1.03790400	4.42861700
				H	-0.72464300	-0.73285900	4.41005300
				H	0.67621300	0.14789600	5.05454700

TS2s\_S

H 1.84517800 -0.20050900 1.44671200

TS2s\_T

C -4.46884000 0.20845600 -0.60459800

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C -2.07308800 1.60096200 -0.30751000

C -2.21250800 0.32377300 0.28214400

C -3.42171900 -0.37262500 0.10543700

H -5.40686300 -0.32449100 -0.72845900

H -5.13953600 1.93557800 -1.70672200

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C -0.72023800 2.22917300 -0.26664000

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C 1.61248000 1.45887900 -0.16078200

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C 3.74333300 0.20952500 -0.44632400

C 3.72711400 2.62568700 -0.36414300

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C 2.17357200 -2.08887400 -0.37169300

C 4.34625900 -1.06628700 -0.57323100

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H 4.25654700 3.57312800 -0.39416200

C 3.56836700 -2.20492200 -0.53837200

H 1.51896200 -2.95213100 -0.32822000

H 5.42278100 -1.13519600 -0.69979500

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C -1.69881900 -3.27925100 -2.38635900

H -2.76675300 -3.36637600 -2.15662000

H -1.58233600 -3.09621900 -3.45544200

H -1.22137000 -4.22142800 -2.10583400

C -0.08596100 -0.79820300 4.43174600

H 0.12147400 -1.86490700 4.55141800

H 0.85043000 -0.25851800 4.60889600

H -0.83253700 -0.47325800 5.15693900

H -1.79217800 0.21251800 1.46510300

4\_Q

C -4.49314600 0.66673100 -1.09101100

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C -2.01383400 1.74214100 -0.47007200

C -2.15533700 0.33475500 -0.45252600

C -3.41707100 -0.17696600 -0.79509100

H -5.46545500 0.24414600 -1.33262900

H -5.16148000 2.70799100 -1.31489100

H -2.91504800 3.67216100 -0.78188000

H -2.46702500 -0.28082300 1.38562100

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C -0.66887900 2.32267100 -0.21677100

O -0.45237200 3.52771000 -0.10986100

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C 3.89097000 0.45402000 -0.07787800

C 3.71727400 2.87373700 -0.20441600

H 1.71794400 3.70731100 -0.24049100

C 2.52346900 -1.94443600 0.01060500

C 4.61282600 -0.76198500 -0.02672700

C 4.50200800 1.73616300 -0.14164400

H 4.19127400 3.84897600 -0.25385300

C 3.93073800 -1.96060500 0.01941600

H 1.94400500 -2.86213100 0.04165200

H 5.69874200 -0.73745100 -0.02753500

H 5.58538200 1.80580400 -0.14375600

H 4.45673000 -2.90778100 0.05784600

N 1.82620700 -0.81780700 -0.03516200

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C -1.32214500 -0.79106600 2.80295700

O -2.53130100 -0.51924500 2.35067900

O -0.30972100 -0.74996300 2.09758500

C -0.60986600 -2.59494500 -1.51753600

O -0.77177800 -2.61800800 -0.24253400

O -0.22966800 -1.53772300 -2.08734800

C -1.28600600 -1.16335300 4.25411500

H	-0.25459400	-1.26841000	4.58833000	O	-0.79589900	-2.60229800	-0.34613100
H	-1.80491800	-0.40580600	4.84784100	O	-0.34944200	-1.21671200	-1.95024400
H	-1.81693000	-2.11114700	4.39196600	C	-0.45792200	-0.07881900	4.17821000
C	-0.91426600	-3.84227300	-2.31160300	H	0.25010600	-0.89231000	4.32956000
H	-2.00138900	-3.95742500	-2.38700900	H	0.00426600	0.86995100	4.47126200
H	-0.49771800	-3.77450200	-3.31782900	H	-1.34599700	-0.22027600	4.79970300
H	-0.52556200	-4.72558600	-1.79786400	C	-0.92729900	-3.47415700	-2.61088000
4_S				H	-1.99127500	-3.45689900	-2.87367300
C	-4.54733200	-0.05134600	-0.48975700	H	-0.34680900	-3.29210900	-3.51716400
C	-4.55302200	1.32074500	-0.76683200	H	-0.69202700	-4.45503300	-2.19317200
C	-3.35275100	2.02789000	-0.80543400	4_T			
C	-2.15349000	1.34865600	-0.56871900	C	-4.50780600	0.18348800	-0.59931100
C	-2.13225000	-0.03374400	-0.29244200	C	-4.47101600	1.56882200	-0.79364400
C	-3.34486300	-0.72838800	-0.25306000	C	-3.25198600	2.24573700	-0.78250000
H	-5.48715000	-0.59666400	-0.45619000	C	-2.07582300	1.52117300	-0.57900700
H	-5.49350000	1.83322600	-0.94657900	C	-2.10313200	0.12862900	-0.39044000
H	-3.32281600	3.09326400	-1.01395400	C	-3.32680300	-0.54301200	-0.39965300
H	-2.04268900	0.81859300	1.52347600	H	-5.46244000	-0.33581100	-0.60395400
H	-3.35592500	-1.79442400	-0.04324300	H	-5.39552400	2.11712300	-0.94792400
C	-0.82560000	2.03794700	-0.56796300	H	-3.19350900	3.32090700	-0.92410500
O	-0.66996400	3.24005400	-0.79876300	H	-2.14225100	0.56159000	1.62347100
N	0.15680100	1.13137000	-0.25692100	H	-3.36323400	-1.61829700	-0.25282400
C	1.51458200	1.38751800	-0.23340500	C	-0.72803300	2.15578100	-0.52330000
C	2.32481900	0.21601400	-0.07749100	O	-0.51355600	3.35869800	-0.65739500
C	2.15924700	2.61808100	-0.34111800	N	0.22197300	1.17773500	-0.28190300
C	3.74422300	0.29346700	-0.02025300	C	1.59249100	1.39521200	-0.18229600
C	3.56882700	2.68660100	-0.28410000	C	2.35927200	0.19265900	-0.07506300
H	1.56365500	3.50980100	-0.47373400	C	2.27323500	2.60726000	-0.17940900
C	2.34682900	-2.10228100	0.14779700	C	3.77496600	0.21721400	0.03626000
C	4.44643700	-0.92859100	0.13412400	C	3.68369500	2.62785000	-0.06762400
C	4.35942300	1.56640200	-0.12519100	H	1.71224600	3.52616100	-0.26984200
H	4.03819000	3.66255900	-0.37013500	C	2.29751500	-2.13663000	0.00424700
C	3.75554800	-2.11786800	0.21708000	C	4.43158800	-1.03428800	0.13412800
H	1.76224800	-3.01482800	0.20678500	C	4.43210600	1.47519100	0.03966300
H	5.53166600	-0.91330500	0.18333400	H	4.18358200	3.59200600	-0.06865600
H	5.44141500	1.64142900	-0.08441700	C	3.70015900	-2.20353900	0.11829900
H	4.27287500	-3.06369800	0.33362700	H	1.67763400	-3.02723800	-0.00869800
N	1.66589200	-0.97794700	0.00684700	H	5.51430500	-1.05942900	0.21999800
Co	-0.33725700	-0.68743500	-0.08816800	H	5.51357900	1.51144600	0.12362100
C	-0.84879100	0.00332200	2.73707500	H	4.18324200	-3.17126700	0.19198200
O	-1.82166900	0.84889000	2.48699400	N	1.65918900	-0.98141300	-0.08801200
O	-0.27557300	-0.67752100	1.87464700	Co	-0.33015300	-0.62481300	-0.18877200
C	-0.67121800	-2.40242500	-1.60036000	C	-0.92605800	-0.14973300	2.88116800

O	-1.96759400	0.61664000	2.59054000	Co	-1.36626000	-0.16276400	-0.67115000
O	-0.30273500	-0.79660200	2.03985800	C	0.15117300	-2.15694000	2.74143200
C	-0.81630200	-2.52680300	-1.66833400	C	-1.17321700	-2.08436900	2.86044500
O	-0.83881700	-2.51626700	-0.37635900	C	-2.40178700	-1.28727900	2.77217100
O	-0.51996600	-1.47804100	-2.28796000	C	-2.42865400	-2.77041100	3.17747000
C	-0.56976800	-0.14179100	4.33680700	H	-2.78880100	-1.03727600	1.78644500
H	0.19593500	-0.89007600	4.53727300	H	-2.60227400	-0.54044500	3.53904700
H	-0.19213600	0.85100600	4.60373600	H	-2.64887500	-3.01367700	4.21599700
H	-1.45901200	-0.33001000	4.94421100	H	-2.84222300	-3.47629000	2.45867500
C	-1.17576000	-3.80501900	-2.37888500	C	-3.14942300	-1.39670600	-1.82668000
H	-2.26060900	-3.94762000	-2.32087000	O	-2.93624000	-1.64999500	-0.59631300
H	-0.88094700	-3.75782500	-3.42790600	O	-2.41888800	-0.54456300	-2.43091000
H	-0.70385100	-4.66048100	-1.88876000	C	-4.28073000	-2.07275700	-2.55442300
				H	-5.20574000	-1.52310200	-2.34547800
5s_Q				H	-4.11042800	-2.06542700	-3.63218600
C	-3.34446900	3.33795500	1.13449800	H	-4.40929600	-3.09527700	-2.19279300
C	-2.56275900	4.36292400	0.58577700	H	0.63169900	-3.11650600	2.93293200
C	-1.45677200	4.04453600	-0.19606600	C	1.05005800	-1.06750700	2.34663600
C	-1.14912600	2.69726600	-0.42847300	C	2.40165900	-1.34901700	2.07359300
C	-1.92594500	1.64462600	0.10551000	C	0.62096100	0.26096600	2.19508500
C	-3.02165300	1.99616100	0.90446400	C	3.27629800	-0.36106100	1.64486900
H	-4.21019500	3.59020800	1.74225300	H	2.76378100	-2.36729900	2.18680800
H	-2.81661000	5.40158700	0.77661200	C	1.48778300	1.26436600	1.76915000
H	-0.82097000	4.81675000	-0.61901900	H	-0.41057200	0.51996200	2.40294700
H	-3.64925900	1.22303800	1.34234200	C	2.82300800	0.95565800	1.47800700
C	0.06725200	2.33601100	-1.19868100	H	4.31354700	-0.58507000	1.42032600
O	0.86229100	3.15058700	-1.66767900	H	1.10826500	2.27096700	1.64748500
N	0.21702500	0.94187100	-1.27133800	O	3.74247200	1.85114400	1.02781700
C	1.39350900	0.30565100	-1.50312200	C	3.32770900	3.20361600	0.85282400
C	1.34192300	-1.11146900	-1.23093600	H	4.20620200	3.73957200	0.48885800
C	2.61714800	0.85641300	-1.92085200	H	2.52238600	3.29070300	0.11599000
C	2.49070800	-1.92660400	-1.38407700	H	3.00582700	3.64850400	1.80273000
C	3.74802600	0.03705300	-2.07055700				
H	2.66464200	1.91405000	-2.13404700	5s_S			
C	0.05614000	-2.90139300	-0.49829300	C	4.40830400	-2.42639300	-0.46825600
C	2.35725900	-3.29834800	-1.06675000	C	3.67879300	-3.38485000	-1.17873200
C	3.70354600	-1.32154000	-1.81327500	C	2.35060000	-3.12972900	-1.52303100
H	4.67926600	0.49021700	-2.39471800	C	1.76369800	-1.92460900	-1.13472000
C	1.14164600	-3.78557900	-0.62952300	C	2.47573800	-0.97113600	-0.38542400
H	-0.91658200	-3.23708300	-0.15766800	C	3.81297200	-1.21906200	-0.07673400
H	3.21685500	-3.95480800	-1.16634400	H	5.44835300	-2.61842200	-0.21624300
H	4.58853800	-1.93896600	-1.93160300	H	4.14970700	-4.31865900	-1.47184400
H	1.01077700	-4.83232900	-0.37975800	H	1.76268900	-3.84261900	-2.09417500
N	0.16074000	-1.60731100	-0.78143800	H	4.39644900	-0.48550100	0.47276700

C	0.36759400	-1.55563400	-1.50301000	H	-4.53097400	0.59074100	1.46881400
O	-0.39336100	-2.26996300	-2.16196800	H	-2.84470900	-3.17251000	0.23799000
N	0.07683000	-0.30501000	-1.00536100	O	-5.07812000	-1.59954200	0.32539900
C	-1.08383200	0.40550400	-1.24088900	C	-5.26677400	-2.81530600	-0.39148300
C	-1.12093200	1.69530200	-0.61652400	H	-6.30592300	-2.80918300	-0.72440100
C	-2.19525700	0.00805700	-1.98206800	H	-4.60590300	-2.87097600	-1.26468600
C	-2.24701300	2.55580300	-0.74961000	H	-5.09946500	-3.69097900	0.24730300
C	-3.30987400	0.86528200	-2.10412200				
H	-2.18673300	-0.96547800	-2.44885600	5s_T			
C	0.00281900	3.22352400	0.73822400	C	4.42843200	-2.17661900	-0.63480600
C	-2.18236400	3.80339700	-0.08174500	C	3.73367400	-3.21156100	-1.27108100
C	-3.35593900	2.11068200	-1.51136100	C	2.39207200	-3.04519400	-1.61578400
H	-4.16110600	0.51938200	-2.68357300	C	1.75896300	-1.83925600	-1.31109200
C	-1.06588400	4.13854200	0.65518300	C	2.44742400	-0.80552700	-0.66137000
H	0.89942500	3.44409900	1.30910200	C	3.79022800	-0.96730600	-0.32949600
H	-3.02277300	4.48791900	-0.15628000	H	5.47412700	-2.31218100	-0.37172800
H	-4.22396200	2.75371500	-1.61632400	H	4.24247500	-4.14361100	-1.49840400
H	-0.99614500	5.08849400	1.17338000	H	1.82898200	-3.82846300	-2.11501200
N	-0.03204500	2.04806600	0.12961000	H	4.33718900	-0.17546700	0.17212400
Co	1.39799400	0.55777800	0.03106600	C	0.33417300	-1.56140900	-1.63609500
C	-0.00916800	-0.06613200	2.20156400	O	-0.42594800	-2.34222500	-2.20540800
C	1.13762800	-0.78473900	2.24633400	N	0.01141800	-0.28984500	-1.19078600
C	1.67340000	-2.14038900	2.42133300	C	-1.23371900	0.31417000	-1.31575800
C	2.40583500	-0.90509300	2.97217000	C	-1.32860600	1.58043400	-0.66248600
H	2.14134600	-2.64868400	1.58503700	C	-2.35876200	-0.16754900	-1.97456100
H	1.14351900	-2.79211000	3.11389800	C	-2.53416500	2.33160400	-0.66239500
H	2.39958700	-0.71476500	4.04363600	C	-3.55508800	0.58662100	-1.98111000
H	3.32602300	-0.63043000	2.46702600	H	-2.30510800	-1.12681600	-2.46751400
C	3.14855000	2.11374600	-0.41019600	C	-0.22602600	3.16934200	0.64151200
O	2.94843900	1.74008700	0.79128000	C	-2.52541900	3.55439000	0.04956700
O	2.37699700	1.61821800	-1.30566000	C	-3.66091400	1.80451800	-1.34475900
C	4.25188600	3.05279200	-0.78501400	H	-4.41720700	0.17687800	-2.49831600
H	5.14592500	2.46329700	-1.01819600	C	-1.38188500	3.97006400	0.70233300
H	3.98141500	3.62826800	-1.67242000	H	0.69681800	3.45354300	1.13645900
H	4.48395700	3.71771000	0.04906900	H	-3.42945700	4.15600300	0.08019900
H	0.02643500	0.95738400	2.56804200	H	-4.59044900	2.36449400	-1.35069300
C	-1.31824800	-0.54818400	1.78109200	H	-1.35709500	4.90061100	1.25789200
C	-2.43109800	0.30844100	1.87997200	N	-0.20519400	2.02060300	-0.01900200
C	-1.50665000	-1.81364200	1.20359400	Co	1.31809700	0.70897700	-0.28404200
C	-3.67683400	-0.07476200	1.41287400	C	0.23385400	-0.29559700	2.53743700
H	-2.30190300	1.29774700	2.30993200	C	1.33058000	-1.05526100	2.57905800
C	-2.74571500	-2.20546000	0.71367900	C	1.95512900	-2.36760900	2.38502200
H	-0.66223600	-2.48337600	1.09526700	C	2.72178500	-1.19193900	3.01220800
C	-3.83789300	-1.32876200	0.80436200	H	2.24118900	-2.67411800	1.38201400

H	1.64708900	-3.18614300	3.03424200	C	2.42551200	2.16066700	1.10715600
H	2.93902100	-1.22757600	4.07869700	C	3.11461000	0.40546800	2.61657800
H	3.49982100	-0.73018100	2.40915600	H	1.75273400	-1.27765200	2.85433100
C	3.06897500	2.39626800	-0.33364900	C	0.43802100	3.03011100	-0.63362900
O	2.63630700	1.78626400	0.71758300	C	2.57747000	3.38623000	0.41292300
O	2.56936300	2.10805900	-1.45139100	C	3.37542100	1.61731000	2.00819900
C	4.17428000	3.40582600	-0.18690100	H	3.84327300	-0.01065500	3.30665600
H	5.12983500	2.87287800	-0.12492900	C	1.59093800	3.81922300	-0.44737900
H	4.20276100	4.07178600	-1.05045400	H	-0.35707500	3.32529100	-1.30940800
H	4.05171200	3.97853000	0.73522800	H	3.47797000	3.97440800	0.56495000
H	0.30121100	0.71746000	2.93283300	H	4.29351400	2.16079000	2.20692100
C	-1.07954800	-0.69185000	2.02029700	H	1.68618300	4.75353500	-0.98924900
C	-2.17530600	0.17711100	2.16979600	N	0.27150700	1.88012600	0.00148900
C	-1.29078200	-1.89490700	1.32954300	Co	-1.20360500	0.59559500	-0.17723300
C	-3.42243300	-0.13293500	1.64680600	C	-0.22975900	-0.21054800	-1.77316700
H	-2.03654100	1.11961600	2.69294800	C	-1.36010100	-1.05761500	-1.65581200
C	-2.53142600	-2.21429800	0.78768800	C	-1.47911200	-2.50618700	-1.95519200
H	-0.46257100	-2.57854300	1.18337300	C	-2.26372200	-1.46873600	-2.76081500
C	-3.60449200	-1.32445600	0.93359300	H	-2.06364600	-3.14245300	-1.30076900
H	-4.26107900	0.54729200	1.74704700	H	-0.60973800	-2.98246900	-2.40044100
H	-2.64187400	-3.13419000	0.22795300	H	-1.92793100	-1.21807700	-3.76369500
O	-4.84352900	-1.51921100	0.40301200	H	-3.33742900	-1.47346900	-2.63185700
C	-5.04009700	-2.66312600	-0.41724800	C	-2.84968600	2.28775900	-0.12158600
H	-6.06723800	-2.60067200	-0.78141000	O	-2.35159700	1.81833600	-1.20914600
H	-4.35271500	-2.67081300	-1.27158400	O	-2.41972400	1.81389400	0.97036500
H	-4.91802000	-3.59480700	0.14953400	C	-3.92879500	3.32848800	-0.16635300
				H	-4.89277600	2.82660800	-0.30864200
TS1_S				H	-3.96366700	3.88411200	0.77225300
C	-4.83711300	-1.62066600	0.33012700	H	-3.77254500	4.00694500	-1.00818700
C	-4.43060500	-2.47044000	1.36374200	C	1.16588200	-0.62702100	-1.57342700
C	-3.09336600	-2.48490400	1.76343900	C	2.19396400	0.22223900	-2.02559400
C	-2.16595900	-1.67463700	1.10995900	C	1.54262000	-1.80149400	-0.90532000
C	-2.55469800	-0.86339200	0.02264000	C	3.52975900	-0.06871500	-1.79802800
C	-3.90379500	-0.82498300	-0.33935500	H	1.93093500	1.14058900	-2.54310000
H	-5.88336000	-1.58114500	0.03964100	C	2.87960400	-2.10687600	-0.66569900
H	-5.15763300	-3.09997000	1.86807200	H	0.78329400	-2.47078100	-0.52163300
H	-2.75464600	-3.09240000	2.59717400	C	3.88400700	-1.23173400	-1.09928900
H	-4.22756700	-0.17986500	-1.14970800	H	4.31676900	0.59887600	-2.13283900
C	-0.77538800	-1.52289200	1.63044400	H	3.12383000	-3.01157700	-0.12316200
O	-0.25655000	-2.29227300	2.44777700	H	-0.34748300	0.62413300	-2.46291700
N	-0.22464700	-0.38714900	1.11241800	O	5.21511900	-1.42097900	-0.89019200
C	0.97485900	0.17366700	1.49454900	C	5.60954000	-2.52849200	-0.09025700
C	1.23112800	1.43001300	0.86484500	H	5.33889000	-3.48387000	-0.55700200
C	1.93164300	-0.32667500	2.37379600	H	6.69614400	-2.46867500	-0.00666000

H	5.16601900	-2.47694500	0.91180200	C	1.52275500	-0.92234600	1.81660600
				C	1.62829800	-2.36472400	2.14230400
TS1_T				C	2.49680200	-1.33168500	2.86295200
C	5.02618100	-1.20002800	-0.17117000	H	2.14162400	-3.02703500	1.45428000
C	4.74137700	-2.22123900	-1.08432800	H	0.79171700	-2.81467800	2.67085500
C	3.42179300	-2.46454300	-1.46808800	H	2.24810700	-1.06244700	3.88639500
C	2.38623700	-1.69931400	-0.92973300	H	3.55662200	-1.35337200	2.64238100
C	2.66728100	-0.72412400	0.04674400	H	0.63163900	0.89311400	2.47930700
C	3.99091200	-0.45886800	0.40324300	C	2.64590800	2.70318000	-0.03809300
H	6.05548400	-0.98806200	0.10459700	O	2.04174200	2.40873800	1.04141900
H	5.54908600	-2.80822600	-1.51114700	O	2.49537300	1.96951600	-1.06568000
H	3.17519000	-3.21607600	-2.21225100	C	3.57430200	3.89040100	-0.09682500
H	4.21240300	0.30964500	1.13740800	H	4.59385900	3.54813200	0.11527800
C	0.99365000	-1.79975000	-1.46986500	H	3.57062800	4.33205900	-1.09565100
O	0.57249100	-2.79171300	-2.07597000	H	3.29962500	4.63602400	0.65177300
N	0.33118500	-0.62990500	-1.21868000	O	-5.06721800	-0.91372700	1.17909000
C	-0.96375700	-0.34723800	-1.60253700	C	-5.55100100	-2.02767800	0.43399600
C	-1.44871300	0.92531300	-1.14053500	H	-5.35313200	-2.97469700	0.95030600
C	-1.83314300	-1.14536300	-2.34179600	H	-6.62955400	-1.88555700	0.34966000
C	-2.78250900	1.34497400	-1.40145100	H	-5.10704500	-2.05601000	-0.56745700
C	-3.15554300	-0.71958900	-2.59683900				
H	-1.47932600	-2.10289100	-2.69662000	5_Q			
C	-0.97475700	2.88665800	0.03134600	C	-5.03206900	-0.01438700	0.28885000
C	-3.17124600	2.61108900	-0.90004700	C	-4.53500700	0.51771500	1.47886300
C	-3.64046900	0.48738700	-2.13772300	C	-3.27328700	0.13073200	1.92898100
H	-3.80518000	-1.37218300	-3.17374500	C	-2.50189300	-0.78711800	1.20260800
C	-2.27196500	3.38459300	-0.19753900	C	-2.99899600	-1.32961000	-0.00045100
H	-0.23678200	3.44332500	0.60020300	C	-4.26712700	-0.92623400	-0.43783300
H	-4.18428100	2.96125000	-1.07741100	H	-6.01195100	0.28058400	-0.07535700
H	-4.65982000	0.80057800	-2.33995800	H	-5.12005200	1.23081200	2.05155700
H	-2.54702500	4.35922100	0.18992100	H	-2.86963100	0.54941700	2.84625300
N	-0.58717800	1.70242100	-0.41584900	H	-4.64953500	-1.32889200	-1.37087300
Co	1.17805900	0.70785300	-0.03463500	C	-1.12390100	-1.13301800	1.73184700
C	-3.29284400	0.35508300	2.02702000	O	-0.90891400	-2.18067800	2.34743900
C	-3.73104200	-0.81523300	1.38176100	N	-0.22958000	-0.14747900	1.43216700
C	-2.79423200	-1.78367100	0.99251000	C	1.11183800	-0.17547600	1.78834100
C	-1.44001300	-1.56324000	1.20831300	C	1.91888400	0.81241900	1.12790400
C	-0.97614300	-0.37982800	1.81534100	C	1.74165200	-1.04687200	2.67045100
C	-1.94384800	0.56450500	2.23316600	C	3.32041100	0.89472300	1.35970500
H	-4.03096800	1.09003300	2.32930200	C	3.13132800	-0.94761800	2.90921200
H	-3.10678700	-2.68980500	0.49007100	H	1.15295500	-1.81264800	3.15423600
H	-0.72912400	-2.29793800	0.85246300	C	1.99896600	2.53839600	-0.43666200
H	-1.61029700	1.48464400	2.70352700	C	4.04297100	1.86464000	0.62352900
C	0.42549700	-0.05325100	1.98334800	C	3.91788400	-0.00721200	2.27879500



H	3.58462900	-1.64279900	3.61012700	C	-4.95743100	-0.76136600	1.10083100
C	3.38891900	2.68343100	-0.27123700	C	-3.77317600	-0.95054200	1.80370900
H	1.44842900	3.16111800	-1.13505900	C	-2.58155500	-1.23676100	1.12511100
H	5.11633000	1.94724500	0.76887000	C	-2.58679400	-1.40217500	-0.28590800
H	4.98418300	0.05833600	2.47178600	C	-3.79692200	-1.18664600	-0.97386600
H	3.92211100	3.42804300	-0.85115300	H	-5.88356700	-0.68971400	-0.84892500
N	1.29533900	1.64004700	0.23727100	H	-5.87230400	-0.52357500	1.63504200
Co	-0.72666200	1.17228200	0.06127100	H	-3.74614600	-0.85127600	2.88393800
C	-1.27002600	-1.42125500	-1.77961500	H	-3.80846000	-1.30299700	-2.05268300
C	-2.15109200	-2.21982000	-0.88325600	C	-1.29019600	-1.20491300	1.91400400
C	-1.77820200	-3.60406500	-0.40428100	O	-1.08538700	-1.87103000	2.93048000
C	-2.83367000	-3.45344700	-1.46309800	N	-0.48595300	-0.26507500	1.35687700
H	-2.07898000	-3.87114400	0.60205100	C	0.73947600	0.17659700	1.80989600
H	-0.81995600	-4.00764000	-0.71011000	C	1.26020200	1.22896900	0.99896100
H	-2.57676400	-3.73086700	-2.48078800	C	1.50358300	-0.27567400	2.87862200
H	-3.86892400	-3.63036100	-1.18803900	C	2.53381500	1.80267000	1.23666400
C	-2.21580900	2.88759900	-0.74835700	C	2.77402100	0.29740900	3.11705600
O	-1.83000100	1.91537600	-1.48829600	H	1.11874100	-1.06977900	3.50400300
O	-1.72548000	2.99590300	0.41854200	C	0.87425900	2.59887800	-0.85540400
C	-3.26263700	3.84403200	-1.24485300	C	2.94539700	2.83362800	0.35574400
H	-4.24658100	3.39953800	-1.05635000	C	3.29426300	1.30438500	2.32687800
H	-3.20397000	4.79451800	-0.71226400	H	3.35698000	-0.07525500	3.95439100
H	-3.16292700	3.99863300	-2.32120400	C	2.11836300	3.23325600	-0.67291700
C	0.13986700	-1.29408800	-1.76432900	H	0.20048000	2.85840100	-1.66336200
C	0.76624800	-0.42858300	-2.71808100	H	3.91558100	3.30036200	0.49860800
C	1.00517600	-1.94145100	-0.83634900	H	4.27114000	1.73010500	2.53220000
C	2.12970000	-0.22538400	-2.73317600	H	2.41262100	4.02028900	-1.35762200
H	0.13878000	0.08757500	-3.43884000	N	0.47084300	1.62987500	-0.04598900
C	2.37836100	-1.74641900	-0.85861100	Co	-1.11566400	0.61190200	-0.18780400
H	0.58555800	-2.56027900	-0.05510600	C	-0.39721200	-0.76227200	-1.39447400
C	2.95646700	-0.88197000	-1.80032100	C	-1.35561000	-1.89131400	-1.03947100
H	2.59081200	0.44089900	-3.45524400	C	-0.89888700	-3.30369200	-0.74843400
H	2.98800000	-2.23670500	-0.11015300	C	-1.58100300	-2.99544900	-2.05380600
H	-1.80016000	-0.79915200	-2.49781600	H	-1.45500800	-3.85985100	-0.00006700
O	4.28533000	-0.60290000	-1.88082500	H	0.16107400	-3.52164500	-0.77656200
C	5.16901900	-1.32045600	-1.02713100	H	-0.96512300	-2.96872200	-2.94815300
H	5.11883400	-2.39975200	-1.21808200	H	-2.59197500	-3.35952000	-2.20838200
H	6.17239600	-0.96107400	-1.26273200	C	-2.71126900	2.37122500	-0.75957300
H	4.95467500	-1.13181200	0.03034900	O	-1.99225400	1.68061300	-1.58227800
				O	-2.56648900	2.20184900	0.47829700
				C	-3.73007500	3.32668400	-1.32000900
				H	-4.61982400	2.75653800	-1.61037400
				H	-4.01777900	4.06510800	-0.56995700
				H	-3.34317100	3.82057100	-2.21466300
5_S							
C	-4.96396800	-0.85488000	-0.29579600				

C	1.07162600	-0.95212800	-1.37303800	H	-3.98198700	3.83067100	-0.08339700
C	1.85105900	-0.31861300	-2.36256900	H	-4.12741900	-0.07152000	2.78483100
C	1.76545800	-1.62545700	-0.35459300	N	-1.18910600	0.43522200	1.23971600
C	3.23725900	-0.32916500	-2.32413600	Co	0.77351000	-0.18545700	0.87774000
H	1.34732700	0.20975000	-3.16790000	C	0.77874200	-1.61671100	-0.77991000
C	3.15834000	-1.64926000	-0.30062600	C	1.74106900	-1.11853900	-1.81352400
H	1.21433100	-2.10659500	0.44166900	C	1.33412800	-0.61634100	-3.17928600
C	3.90498100	-0.98593000	-1.28017000	C	1.93560900	-1.98760100	-3.05605700
H	3.82575300	0.17331200	-3.08506400	H	1.94507000	0.17504900	-3.60108400
H	3.64381300	-2.16091400	0.52095800	H	0.28557900	-0.55560800	-3.43721700
H	-0.70248700	-0.30583500	-2.34128200	H	1.27099000	-2.83850700	-3.16965000
O	5.26598400	-0.91860600	-1.30174300	H	2.95152400	-2.14836900	-3.40195100
C	5.97066800	-1.49459900	-0.21031900	C	1.59407100	-0.64710400	3.16082800
H	5.81336100	-2.57902000	-0.15135300	O	1.39774100	-1.50957100	2.21506600
H	7.02842500	-1.29825500	-0.39514600	O	1.36885600	0.56769600	2.94939300
H	5.67806500	-1.03624900	0.74292100	C	2.09551500	-1.15427700	4.48774300
5_T				H	3.06880200	-1.63543300	4.34804900
C	5.26316900	-0.79943400	-0.38237500	H	2.18902000	-0.33803800	5.20485400
C	5.31068300	0.55433400	-0.04410900	H	1.40936200	-1.91387000	4.87530000
C	4.20240000	1.36462700	-0.27984000	C	-0.65686900	-1.76535400	-0.91436600
C	3.03096500	0.82985700	-0.82898700	C	-1.30161200	-2.80405900	-0.19244800
C	2.98834500	-0.52803300	-1.20030700	C	-1.48700700	-0.84242800	-1.59090000
C	4.11258200	-1.32835400	-0.96565400	C	-2.67818600	-2.90480300	-0.13984200
H	6.12247900	-1.43889400	-0.20338200	H	-0.69147700	-3.52422900	0.34490500
H	6.20764700	0.97734300	0.39819700	C	-2.87083600	-0.93203400	-1.54144300
H	4.22824300	2.42074200	-0.03083300	H	-1.04444800	0.00603500	-2.09316300
H	4.08203600	-2.37547600	-1.25216200	C	-3.48022500	-1.95793400	-0.80291200
C	1.85548400	1.75997900	-1.02290100	H	-3.16483100	-3.69657000	0.42006600
O	1.98565900	2.77224500	-1.71891500	H	-3.46494700	-0.18059800	-2.04593600
N	0.74911800	1.38067200	-0.31715100	H	1.23738600	-2.39060600	-0.16093300
C	-0.43888700	2.10642400	-0.30638300	O	-4.81856300	-2.11007200	-0.65917400
C	-1.47268400	1.57171200	0.53948900	C	-5.67246600	-1.13335000	-1.24897100
C	-0.73778200	3.25366200	-1.03944500	H	-5.57221700	-1.11774600	-2.34059700
C	-2.75485800	2.18730500	0.61898900	H	-6.68969700	-1.42753700	-0.98654600
C	-2.00965800	3.86133800	-0.94684500	H	-5.46878800	-0.13311300	-0.84918900
H	0.02576600	3.67191800	-1.67782800	TS2_Q			
C	-2.11022100	-0.11935700	2.00864600	C	0.84510600	5.41434400	0.80190500
C	-3.71988600	1.57096300	1.45484700	C	0.07352100	4.30183000	1.11707900
C	-3.00782800	3.35527800	-0.14330800	C	0.32915100	3.02567100	0.58039300
H	-2.19531600	4.75600600	-1.53453500	C	1.39326800	2.89616400	-0.34208100
C	-3.40480800	0.42211700	2.14486200	C	2.15027200	4.03841200	-0.66381700
H	-1.82328900	-1.02550000	2.53262900	C	1.90308200	5.27998800	-0.09352400
H	-4.70757600	2.01624100	1.53813900				

H	0.60790400	6.37765700	1.24327500	O	-0.46242500	-1.64140800	-0.94922200
H	-0.77744800	4.43956000	1.77336800	C	-2.28583000	-3.12551100	-0.44443600
H	2.94842100	3.92081700	-1.38656600	H	-3.03760000	-2.63243200	-1.06837700
H	2.52107800	6.13287100	-0.35708200	H	-1.83290300	-3.92261700	-1.04052700
C	1.89920900	1.66656000	-1.07524000	H	-2.77058100	-3.54359300	0.43872000
O	2.30275700	1.82109900	-2.23167900	Co	0.45107800	-0.40026800	0.49201300
N	2.01369300	0.50362700	-0.35305800	O	-6.32297500	-1.07772400	-1.21590300
C	-1.37667300	1.41129000	-0.20281800	C	-7.13601500	-1.62421500	-0.18392900
C	-2.64196200	0.74041400	-0.33834300	H	-7.43755100	-0.85755600	0.54028300
C	-3.14817800	0.59829200	-1.66031100	H	-8.02478800	-2.01899000	-0.67875500
C	-3.42945500	0.18680500	0.69782300	H	-6.62452000	-2.43964900	0.34226800
C	-4.36343300	-0.00123100	-1.92191900				
H	-2.55699300	0.98160600	-2.48669600	TS2_S			
C	-4.65605700	-0.41846300	0.44637400	C	0.39175600	5.36679300	0.90076700
H	-3.06653400	0.17290400	1.71431200	C	-0.16892200	4.14855900	1.27268600
C	-5.14069600	-0.51004800	-0.86562600	C	0.22562400	2.93248100	0.69134900
H	-4.73814000	-0.09276000	-2.93595300	C	1.20441500	2.96045300	-0.33053900
H	-5.21563200	-0.83347200	1.27560600	C	1.75053500	4.20302000	-0.69674600
C	3.03245500	-0.40346300	-0.65536400	C	1.36790000	5.39327200	-0.09045500
C	2.98544700	-1.65324800	0.05496900	H	0.05453700	6.28299200	1.37607200
C	4.13254800	-0.19340500	-1.48718600	H	-0.96209900	4.15191500	2.01000400
C	4.03079600	-2.61702400	-0.05727600	H	2.49330300	4.20125900	-1.48421500
C	5.16536900	-1.14891100	-1.58965200	H	1.82170200	6.33019000	-0.39876100
H	4.18654600	0.71463400	-2.06886000	C	1.82305900	1.80319500	-1.09681400
C	1.77510000	-3.02556900	1.50112100	O	2.41133100	2.07566500	-2.15016300
C	3.88875900	-3.81488400	0.68641200	N	1.83922200	0.55718800	-0.51932700
C	5.13740300	-2.33960500	-0.89598600	C	-1.08609800	0.94244300	-0.07157900
H	6.00299700	-0.92946100	-2.24575900	C	-2.47106100	0.44005400	-0.23289500
C	2.77156300	-4.02082000	1.46556900	C	-3.02539800	0.50372900	-1.52910400
H	0.85881300	-3.15643900	2.06829400	C	-3.26938000	-0.14171200	0.76473900
H	4.67049100	-4.56714000	0.62637500	C	-4.30316900	0.04464800	-1.80907700
H	5.93533800	-3.06954900	-0.98907700	H	-2.42972200	0.92600000	-2.33344200
H	2.64103100	-4.93230600	2.03825400	C	-4.56099500	-0.59997700	0.50489100
N	1.88922600	-1.89132500	0.82843500	H	-2.87422800	-0.29825400	1.75825200
C	-0.68226600	1.95924000	0.91963700	C	-5.09029400	-0.50604900	-0.78792800
C	-0.10917800	0.91454900	2.43402100	H	-4.71420800	0.10547200	-2.81143700
C	-1.16670200	1.95732800	2.33754500	H	-5.13340000	-1.04310600	1.31064600
H	0.88771800	1.22467600	2.72853600	C	2.91255900	-0.30758600	-0.78223700
H	-0.42246000	-0.10072800	2.65456500	C	2.95661800	-1.47302500	0.05494600
H	-2.18285400	1.61329200	2.48966200	C	3.97458800	-0.13748900	-1.67225500
H	-0.98110200	2.86786600	2.89945000	C	4.05248300	-2.38236700	0.03538100
H	-0.91052400	1.64874900	-1.15466600	C	5.05758300	-1.04488900	-1.69124700
C	-1.24075700	-2.11121000	-0.06248800	H	3.96506700	0.70200100	-2.34800100
O	-1.14177300	-1.69902900	1.14058500	C	1.84616800	-2.71848600	1.68333800

C	3.98968200	-3.48648400	0.92109200	N	1.97778300	0.51980700	-0.48800100
C	5.12150800	-2.14331700	-0.86237200	C	-1.13938000	1.19536100	-0.14067400
H	5.86212500	-0.85983200	-2.39753300	C	-2.48461800	0.65267900	-0.29055500
C	2.89847800	-3.65314900	1.74576900	C	-3.00106900	0.61380600	-1.60836800
H	0.94898700	-2.83030800	2.28286800	C	-3.30376300	0.13131100	0.72859600
H	4.80989000	-4.19882800	0.93476400	C	-4.26454300	0.12693100	-1.88666500
H	5.95876600	-2.83321800	-0.89608300	H	-2.38334100	0.97996500	-2.42282300
H	2.82924000	-4.49157900	2.42992600	C	-4.57898700	-0.35932300	0.46479000
N	1.88548100	-1.67366800	0.87180000	H	-2.93567900	0.04667600	1.73980500
C	-0.56112800	1.71100200	1.07956700	C	-5.07330000	-0.36083800	-0.84682800
C	0.19835400	0.78532900	2.36569100	H	-4.64953200	0.10889500	-2.90065100
C	-1.03581400	1.63224200	2.48315500	H	-5.16783000	-0.75648500	1.28207200
H	1.14811000	1.21362800	2.66110200	C	2.93090300	-0.46203100	-0.76370800
H	0.05843600	-0.26937900	2.58320700	C	2.83461400	-1.64046400	0.05704800
H	-1.96015700	1.10103300	2.66962800	C	3.99889200	-0.40125700	-1.65876300
H	-0.93661000	2.52763100	3.08526400	C	3.81969500	-2.66902600	0.00373800
H	-0.76466500	1.40158900	-1.00295900	C	4.96554300	-1.43007700	-1.71247300
C	-1.02192200	-2.32236500	-0.31825800	H	4.08062900	0.45217200	-2.31395500
O	-0.99929900	-1.89095700	0.88805600	C	1.62103600	-2.78433500	1.68417500
O	-0.27457200	-1.75714800	-1.17900000	C	3.64983000	-3.77476900	0.87212400
C	-1.95768200	-3.42641500	-0.70948500	C	4.90106700	-2.54253400	-0.90354400
H	-2.93996800	-2.98199200	-0.90575400	H	5.78214200	-1.32862200	-2.42192200
H	-1.61151200	-3.92594300	-1.61583700	C	2.56242200	-3.83154300	1.71589000
H	-2.06579100	-4.14401800	0.10696900	H	0.72392100	-2.81042800	2.29270500
Co	0.36229700	-0.38804800	0.32849700	H	4.38600200	-4.57380700	0.85909900
O	-6.33524200	-0.92405100	-1.14864400	H	5.65028200	-3.32637700	-0.95493100
C	-7.16119100	-1.49854200	-0.14524900	H	2.41077400	-4.66761400	2.38958300
H	-7.36375600	-0.78991900	0.66779300	N	1.75697500	-1.73597800	0.88701100
H	-8.10083800	-1.75516500	-0.63766500	C	-0.48653500	1.80880200	0.99015600
H	-6.71546000	-2.40980600	0.27367600	C	0.11166200	0.66234700	2.33382900
				C	-0.93271000	1.72760800	2.41319800
TS2_T				H	1.11549200	0.91641400	2.65564900
C	0.78646200	5.35565300	0.91440400	H	-0.22836800	-0.35248200	2.52441200
C	0.12171900	4.17675700	1.23509600	H	-1.94690000	1.38977000	2.58936700
C	0.44703000	2.94166800	0.64507300	H	-0.68230200	2.58311200	3.03059400
C	1.46839200	2.91861300	-0.33592100	H	-0.73318600	1.53616700	-1.08815400
C	2.11952200	4.12396400	-0.65172700	C	-1.22346400	-2.19404900	-0.13848200
C	1.80361800	5.32788200	-0.03525200	O	-1.21416600	-1.88518900	1.08513300
H	0.49912200	6.28467900	1.39740100	O	-0.49091800	-1.56261800	-0.97685500
H	-0.69970000	4.22802700	1.93946900	C	-2.14123900	-3.27279000	-0.65665300
H	2.89095100	4.08036700	-1.41043800	H	-3.05249500	-2.79427000	-1.03246600
H	2.33988600	6.23335800	-0.30236500	H	-1.67779800	-3.81097400	-1.48662200
C	2.03283400	1.73557700	-1.10550700	H	-2.41633500	-3.96483900	0.14141600
O	2.59726300	1.96989000	-2.18145100	Co	0.35241100	-0.28241800	0.37207100

O	-6.29793100	-0.81864500	-1.20943000	H	-5.35980800	-3.90323200	-0.71471600
C	-7.14303000	-1.35229100	-0.19588200	H	-0.99187500	-5.20212800	0.96249400
H	-7.38441700	-0.59999500	0.56492800	N	-1.35191100	-1.93196300	0.32695800
H	-8.06048300	-1.65873000	-0.70070500	C	0.52473000	1.74523300	-0.68927100
H	-6.68883200	-2.22579600	0.28769900	C	-0.00531700	-0.48311000	-1.59174300
6_S				C	0.18335700	0.98458900	-1.97513300
C	-0.37132600	5.19067400	0.57538500	H	-0.77586700	-0.99149900	-2.17350200
C	0.32817200	4.07490100	0.12945000	H	0.91678000	-1.06862900	-1.57366300
C	-0.32610600	2.88357700	-0.24279500	H	0.95468200	1.15159400	-2.73888400
C	-1.73435000	2.85269000	-0.19332000	H	-0.74290200	1.38597100	-2.38763800
C	-2.42807700	3.99447800	0.23727000	H	1.69947000	2.05364000	0.99043400
C	-1.76383200	5.14803000	0.63722200	C	0.68459700	-0.56716900	2.36192300
H	0.16807500	6.09082200	0.85513200	O	-0.38180000	0.09470400	2.45802400
H	1.40809600	4.12429700	0.03602500	O	1.06010800	-0.98379900	1.20147900
H	-3.51044200	3.94975800	0.24899200	C	1.51943000	-0.91940900	3.56374500
H	-2.32888500	6.01034500	0.97784700	H	1.14691500	-1.85907400	3.98821700
C	-2.63089400	1.70908800	-0.59914100	H	2.56412200	-1.06244400	3.28146700
O	-3.71837800	2.01621600	-1.10946500	H	1.42924500	-0.14516600	4.32843400
N	-2.24406000	0.42522100	-0.32048500	Co	-0.50061700	-0.24248000	0.25412000
C	1.66451800	1.52105300	0.04270200	O	6.51150900	-1.29871500	-0.49658600
C	2.88052300	0.76079300	-0.20681300	C	6.91647400	-1.90863600	-1.71775100
C	3.78394700	0.63564300	0.87349600	H	7.03494100	-1.16757100	-2.51748400
C	3.25809200	0.17388000	-1.42669600	H	7.88197700	-2.37441400	-1.51459800
C	4.97681100	-0.05184200	0.75555400	H	6.20442000	-2.67882800	-2.03781900
H	3.52600500	1.09035000	1.82575300	6_T			
C	4.45942100	-0.51686400	-1.56509400	C	-0.27245800	5.14696100	0.89049600
H	2.62036900	0.25501800	-2.29502000	C	0.47693800	4.11093400	0.34847500
C	5.32519200	-0.64258800	-0.47043500	C	-0.11716500	2.94295100	-0.17533700
H	5.66108300	-0.14535400	1.59218400	C	-1.52974600	2.87523600	-0.18739200
H	4.71053900	-0.94973400	-2.52547000	C	-2.27464500	3.94473600	0.33650400
C	-3.15023500	-0.62531000	-0.50181600	C	-1.66472100	5.06128700	0.89467700
C	-2.64356300	-1.90321600	-0.11285800	H	0.22836600	6.02624200	1.28477900
C	-4.46589500	-0.59566900	-0.97426400	H	1.55536200	4.21069900	0.29387600
C	-3.42077400	-3.09406000	-0.18402700	H	-3.35637400	3.88022900	0.29646800
C	-5.23985700	-1.77542600	-1.03845500	H	-2.26933700	5.86478400	1.30391200
H	-4.88889100	0.34417700	-1.28563000	C	-2.40877000	1.78781600	-0.76961300
C	-0.78513900	-3.07682900	0.68979700	O	-3.28408100	2.14720600	-1.56349600
C	-2.80032000	-4.30054800	0.22027700	N	-2.25626400	0.50715200	-0.28840200
C	-4.75219800	-3.00588500	-0.65651300	C	1.94404900	1.65166300	-0.02202200
H	-6.25819200	-1.69432600	-1.40797400	C	3.09215700	0.78519400	-0.27359600
C	-1.49277200	-4.29194200	0.65287800	C	3.99252900	0.59780300	0.80000800
H	0.24649700	-3.01721000	1.01072700	C	3.40293300	0.13490200	-1.48033200
H	-3.36706600	-5.22622800	0.17908500	C	5.10999600	-0.21066800	0.69127600

H	3.79325400	1.09960300	1.74300000	8_Q			
C	4.52883500	-0.67600400	-1.61015000	C	2.64529400	-4.37004100	-0.44592400
H	2.77416900	0.26063800	-2.35079700	C	1.46586200	-3.65047800	-0.61796400
C	5.38717200	-0.86364800	-0.51978800	C	1.48365000	-2.27339300	-0.89893300
H	5.78876200	-0.35011600	1.52621800	C	2.73673000	-1.62151100	-1.00750000
H	4.72646400	-1.15315300	-2.56227200	C	3.91302200	-2.36436700	-0.86549300
C	-3.24628600	-0.46646500	-0.51219800	C	3.87621700	-3.72556000	-0.57583400
C	-2.93758300	-1.80148900	-0.06962600	H	2.60201800	-5.43349000	-0.23065100
C	-4.51558900	-0.26799400	-1.05554900	H	0.50897400	-4.16006900	-0.56626900
C	-3.88695900	-2.86127500	-0.16785800	H	4.85922800	-1.84520100	-0.97328700
C	-5.45287700	-1.32170400	-1.14364700	H	4.80153500	-4.28057900	-0.45505100
H	-4.78134500	0.71278400	-1.41505600	C	2.90304600	-0.13567800	-1.24291900
C	-1.34107500	-3.22847200	0.86251600	O	3.79105200	0.25715900	-2.00972100
C	-3.48448700	-4.13837000	0.29361900	N	2.03773000	0.63167200	-0.52193600
C	-5.16629400	-2.59715400	-0.71504400	C	-0.84260800	-1.78862600	-0.23483500
H	-6.42776200	-1.10226700	-1.56937000	C	-2.25468400	-1.38393300	-0.32716200
C	-2.21982800	-4.32666400	0.80783800	C	-2.97489200	-1.13938300	0.86065900
H	-0.32963500	-3.31806700	1.24521900	C	-2.94801600	-1.27605700	-1.54291400
H	-4.18776800	-4.96427300	0.23287000	C	-4.30731100	-0.75986400	0.82896000
H	-5.89232700	-3.40032100	-0.79228700	H	-2.45923000	-1.22511900	1.81069900
H	-1.89168900	-5.29648200	1.16467900	C	-4.29271500	-0.90874500	-1.58771900
N	-1.69526600	-2.02359500	0.44395700	H	-2.45128700	-1.51843700	-2.47328200
C	0.78409600	1.88037100	-0.69689200	C	-4.97752400	-0.63358200	-0.39803200
C	0.10307600	-0.35990100	-1.54267200	H	-4.85559300	-0.55896000	1.74369500
C	0.34449700	1.08629300	-1.92291100	H	-4.79252400	-0.84656200	-2.54642300
H	-0.66255000	-0.88408900	-2.11421400	C	1.96035600	2.01511500	-0.63410700
H	0.99203300	-0.96146900	-1.36228600	C	0.94928700	2.64035100	0.17973000
H	1.09859800	1.16436700	-2.71754700	C	2.72745000	2.84618100	-1.44877300
H	-0.56323100	1.52312200	-2.34014500	C	0.73361700	4.04815800	0.14104200
H	2.04268200	2.19628500	0.91310300	C	2.51020600	4.24176300	-1.47483600
C	0.94256900	-0.71744000	2.19757500	H	3.49529000	2.39859300	-2.06193700
O	-0.01505700	0.11035700	2.33127800	C	-0.76816200	2.35125000	1.74339200
O	1.09067700	-1.29989500	1.07555700	C	-0.29658900	4.56959700	0.96128700
C	1.86101000	-1.02924700	3.34745200	C	1.54086900	4.84782300	-0.70651300
H	1.40475300	-1.81348500	3.96264100	H	3.13425500	4.84638000	-2.12680800
H	2.82418300	-1.38913000	2.98285900	C	-1.04634300	3.73050400	1.75772800
H	1.99440600	-0.14635100	3.97644800	H	-1.31755100	1.64536700	2.35691700
Co	-0.59308700	-0.27870100	0.36097900	H	-0.48596000	5.63943800	0.95101400
O	6.50305800	-1.63847700	-0.53772500	H	1.38124200	5.92100500	-0.73738000
C	6.82670200	-2.31723700	-1.74523100	H	-1.83984600	4.11045000	2.39120300
H	7.01396900	-1.61376200	-2.56593100	N	0.18841200	1.83538900	0.98393000
H	7.73991100	-2.87810500	-1.53970200	C	0.18211700	-1.56831700	-1.11560300
H	6.03393200	-3.01569500	-2.04016300	C	-0.73123500	0.50066000	-2.32513400
				C	0.05181600	-0.76331600	-2.40302800

H	-1.09931700	0.96465200	-3.23337200	C	-0.00330700	2.51309000	-0.32113200
H	-0.83485600	1.04194900	-1.39411800	C	-1.21527100	2.37640500	0.44270600
H	-0.37487800	-1.43027400	-3.16932400	C	0.09470100	3.63191700	-1.14596500
H	1.06116300	-0.54952700	-2.78072000	C	-2.24847600	3.36035600	0.38593300
H	-0.60811800	-2.38933000	0.64164000	C	-0.93885800	4.59109500	-1.21369100
C	0.63252800	-1.10743500	3.12009300	H	0.99023400	3.77410300	-1.73071600
O	1.68686800	-1.04071400	2.39252100	C	-2.43171200	1.09953700	1.97623100
O	-0.46041900	-0.66843900	2.66721000	C	-3.39068500	3.15247600	1.19671600
C	0.73697000	-1.69388000	4.50351300	C	-2.08912900	4.48118700	-0.46424600
H	1.33329000	-1.02447300	5.13272800	H	-0.80779900	5.44126600	-1.87683900
H	-0.25049800	-1.82277700	4.94837800	C	-3.48228500	2.03531200	1.99891700
H	1.26038500	-2.65319100	4.46244900	H	-2.47287600	0.19243700	2.57221000
Co	0.79442100	-0.12210800	0.83955600	H	-4.19046600	3.88749600	1.17676600
O	-6.28142400	-0.25524100	-0.32807200	H	-2.87189800	5.23153400	-0.51205000
C	-7.00270400	-0.11508700	-1.54579900	H	-4.34464700	1.86045100	2.63227400
H	-7.06437700	-1.06531100	-2.09076800	N	-1.35224600	1.26503600	1.22643800
H	-8.00861000	0.20195100	-1.26545900	C	1.76259300	-1.06151400	-1.48467000
H	-6.55325600	0.64601400	-2.19564300	C	-0.13513300	-0.09148700	-2.95488900
				C	1.32255400	-0.30106700	-2.73644100
TS3_Q				H	-0.71139600	0.51447400	-2.26687300
C	5.32024800	-1.29375400	-0.19735000	H	-0.64010100	-0.49392700	-3.82398700
C	4.10833500	-1.61597200	-0.80412300	H	1.75608000	-0.83988200	-3.59042800
C	3.07151700	-0.67715000	-0.89424100	H	1.83622000	0.66998900	-2.72232100
C	3.26301800	0.61686300	-0.36599600	H	1.54554400	-2.51729900	-0.01380200
C	4.49644900	0.93258300	0.22007100	C	0.75818000	-1.82195900	2.82142900
C	5.51393300	-0.01200100	0.31970600	O	1.12910200	-0.76131100	2.25674300
H	6.11070500	-2.03627000	-0.13739700	O	-0.23708200	-2.53212000	2.41044600
H	3.95328700	-2.60439700	-1.22640600	C	1.50412100	-2.33284700	4.02175000
H	4.63847200	1.93928300	0.59696700	H	0.80596100	-2.72463600	4.76495700
H	6.45585300	0.25349100	0.79034600	H	2.15001700	-3.15914700	3.70418000
C	2.26400100	1.75330900	-0.43974800	H	2.12304900	-1.54451600	4.45072100
O	2.71922900	2.87929600	-0.67547900	Co	0.06385100	-0.11501000	0.65265500
N	0.93795000	1.47972600	-0.19577200	O	-4.51216300	-2.61791600	-1.34282800
C	1.06727600	-2.04238000	-0.87002800	C	-5.35786700	-2.06327100	-0.34627400
C	-0.37963700	-2.32757200	-1.03573200	H	-5.20131500	-2.53951000	0.63021600
C	-1.15183500	-1.80020400	0.02336600	H	-5.20978700	-0.98004300	-0.24527600
C	-0.98534600	-2.94514300	-2.13586500	H	-6.38073500	-2.25487700	-0.67584400
C	-2.55394500	-1.87893900	-0.07156300				
H	-0.63013500	-2.10622800	1.39638000	TS3_S			
C	-2.37101300	-3.03592800	-2.19650300	C	4.38024100	-3.44654900	-0.01242100
H	-0.38107900	-3.34131900	-2.94701300	C	3.05192400	-3.25099800	-0.37957800
C	-3.16354200	-2.49207900	-1.17207900	C	2.51356400	-1.96047200	-0.50159500
H	-3.16526900	-1.46699100	0.72461100	C	3.32724100	-0.84423600	-0.24875400
H	-2.86784600	-3.51232000	-3.03583300	C	4.66362700	-1.05836200	0.12255000

C	5.18913500	-2.33961800	0.24685800	O	0.64668100	-0.10048900	2.03917400
H	4.77682500	-4.45383500	0.07367600	O	-1.40170400	-0.54775100	2.82110800
H	2.41128900	-4.10390000	-0.58282100	C	0.30290600	-0.03100300	4.40521700
H	5.27643600	-0.18418500	0.30561600	H	-0.08227200	0.93116100	4.76097700
H	6.22574300	-2.47385100	0.54103300	H	-0.09869500	-0.80982100	5.05805100
C	2.91970900	0.60055300	-0.38985600	H	1.39220800	-0.01534600	4.45151300
O	3.84111700	1.42508400	-0.49333800	Co	-0.03223400	-0.06548000	0.08783400
N	1.59367400	0.94638200	-0.40614100	O	-5.28593200	-1.88486200	-1.03471400
C	0.19137000	-2.38691500	0.04045500	C	-5.99438400	-0.73945500	-0.58146200
C	-1.27533600	-2.40110600	-0.17298800	H	-6.01480700	-0.68343200	0.51427500
C	-1.89607800	-1.25509400	0.34061200	H	-5.56456800	0.18710300	-0.98322800
C	-1.95931300	-3.31965300	-0.97468300	H	-7.01504600	-0.84996400	-0.95182100
C	-3.25811800	-1.05215500	0.04864400				
H	-1.54517600	-0.78350200	1.61745100	TS3_T			
C	-3.30845400	-3.11676200	-1.23551300	C	4.34486400	-3.44952700	0.35768400
H	-1.44318000	-4.17586000	-1.40043400	C	3.03942200	-3.35107300	-0.11131900
C	-3.96358500	-1.98343600	-0.72150100	C	2.47321300	-2.11123300	-0.45334100
H	-3.77800100	-0.18025700	0.42659300	C	3.25551100	-0.94400600	-0.34016200
H	-3.87952500	-3.81396500	-1.83996100	C	4.57699100	-1.06500200	0.12021900
C	1.25854400	2.28229400	-0.65179900	C	5.11679700	-2.29389500	0.48296200
C	-0.05390200	2.65350800	-0.23557000	H	4.75778100	-4.42063200	0.61427900
C	2.02671300	3.27881000	-1.25973200	H	2.43706200	-4.24598000	-0.23322300
C	-0.54045000	3.98873400	-0.34308700	H	5.17659200	-0.16443400	0.18195000
C	1.52560800	4.58852300	-1.41676200	H	6.13837200	-2.35061900	0.84659900
H	3.02612100	3.04907500	-1.58961300	C	2.87003400	0.46887900	-0.73917100
C	-2.00341800	1.95083400	0.83219200	O	3.75803900	1.10916300	-1.32100200
C	-1.82214500	4.25933100	0.19327300	N	1.64072700	0.96695400	-0.38390300
C	0.28025900	4.96248300	-0.95971200	C	0.13158000	-2.67277000	-0.06621600
H	2.16295800	5.32374500	-1.89963400	C	-1.33110500	-2.50867500	-0.26960700
C	-2.53609000	3.25275200	0.80302500	C	-1.87914100	-1.30335000	0.21885200
H	-2.53780000	1.14421400	1.30853000	C	-2.10452300	-3.39954000	-1.02515400
H	-2.22095500	5.26760700	0.12987100	C	-3.22191900	-1.01253000	-0.09168600
H	-0.07975200	5.98166300	-1.05652500	H	-1.63329300	-0.85388400	1.57855200
H	-3.50700600	3.43381700	1.24990600	C	-3.42982400	-3.09769000	-1.31188300
N	-0.82327300	1.65950000	0.30057600	H	-1.66501000	-4.31574900	-1.41036600
C	1.07471600	-1.85420300	-0.84950000	C	-3.99543800	-1.89712800	-0.84900700
C	-0.39671800	-0.14967400	-1.83372000	H	-3.66408000	-0.09185300	0.27176200
C	0.61476800	-1.24500100	-2.18042000	H	-4.04753900	-3.76920600	-1.89953500
H	-0.16234600	0.80729300	-2.29986200	C	1.34498400	2.32517200	-0.58366800
H	-1.43222000	-0.42165200	-2.03410300	C	0.05149500	2.77726900	-0.12528200
H	0.20166600	-2.03357300	-2.82080300	C	2.17136600	3.30263700	-1.14752800
H	1.48841200	-0.83120000	-2.68753200	C	-0.33221300	4.15167900	-0.20533800
H	0.58290500	-2.75757500	0.98599900	C	1.77586500	4.65500900	-1.23522600
C	-0.16349900	-0.24360300	2.98789900	H	3.14071800	3.00732900	-1.51120100



C	-1.97850700	2.21914000	0.88513600	O	-2.25634600	1.54018500	-2.15895500
C	-1.60394000	4.50902100	0.30434200	N	-0.88078900	1.17626200	-0.32876600
C	0.55707200	5.09397000	-0.77491500	C	-1.18793000	-2.02234600	-0.85849200
H	2.47130000	5.36093800	-1.68045900	C	0.24089600	-2.38651300	-0.85585100
C	-2.42391200	3.55315100	0.86102400	C	1.07954900	-1.57366400	-0.05982700
H	-2.58569300	1.43354600	1.32003400	C	0.79597100	-3.38368400	-1.67520800
H	-1.91525100	5.54868800	0.25427200	C	2.46159800	-1.79884800	-0.06839000
H	0.26348400	6.13712900	-0.83766900	C	2.16463800	-3.61209200	-1.66089400
H	-3.39545500	3.80489300	1.27127900	H	0.15568000	-3.98950300	-2.31190600
N	-0.80264600	1.85308700	0.39888200	C	3.00495700	-2.82357800	-0.85448500
C	1.04754900	-2.07224900	-0.86085600	H	3.11229300	-1.16100900	0.52112400
C	-0.32646100	-0.18599900	-1.88071500	H	2.61396200	-4.38916100	-2.27080700
C	0.63539200	-1.33698600	-2.15053500	C	0.01270800	2.21201900	-0.62137600
H	-0.01667500	0.77913900	-2.27360800	C	1.16189600	2.30224100	0.24474200
H	-1.37608700	-0.38933300	-2.06709500	C	-0.10187700	3.19311600	-1.60866800
H	0.17352900	-2.07086100	-2.82185500	C	2.11756800	3.35438500	0.11451100
H	1.53811900	-0.96697400	-2.63996500	C	0.84649100	4.23159500	-1.72787200
H	0.47741100	-3.18490600	0.83046300	H	-0.93312300	3.14311100	-2.29345800
C	-0.34610700	-0.39821300	3.01572900	C	2.36007200	1.35683700	2.02001100
O	0.53477600	-0.26994800	2.13005000	C	3.21259700	3.35575700	1.01274900
O	-1.58108300	-0.64178500	2.74320400	C	1.93783500	4.33131200	-0.89437500
C	0.01592200	-0.24569800	4.46763400	H	0.70104000	4.96790300	-2.51322500
H	-0.35978900	0.72066500	4.82207200	C	3.33665200	2.36725400	1.96515200
H	-0.46425800	-1.02607000	5.06265900	H	2.42294700	0.54827500	2.74224300
H	1.09811400	-0.27478700	4.59587000	H	3.95289200	4.14716000	0.93553200
Co	-0.02104300	-0.04746700	0.16455100	H	2.66442400	5.13063000	-1.00029600
O	-5.29984800	-1.69504000	-1.18908200	H	4.16741400	2.35139300	2.66154400
C	-5.91282200	-0.48191900	-0.77480300	N	1.32197300	1.33467300	1.19555600
H	-6.93372000	-0.51251500	-1.15949000	C	-1.94083300	-1.81301700	0.25236800
H	-5.94409700	-0.39684800	0.31881500	C	-1.03357700	-1.06178500	2.44983600
H	-5.39786300	0.39385600	-1.19024500	C	-1.53308900	-2.26351600	1.65754700
				H	-1.81205200	-0.37209400	2.78273700
7_Q				H	-0.30586900	-1.28529900	3.23346400
C	-5.57115000	-0.81433600	0.64948400	H	-0.74991700	-3.02079500	1.58375200
C	-4.38018000	-1.52813800	0.71075000	H	-2.40176900	-2.72919600	2.14420600
C	-3.18874700	-1.01771900	0.16727800	H	-1.63198400	-1.76679400	-1.82103200
C	-3.20185300	0.26018700	-0.43449200	Co	-0.03722100	-0.17413600	0.86722400
C	-4.42021400	0.95775400	-0.50874600	O	4.33296100	-3.12661200	-0.92454700
C	-5.58985400	0.43977000	0.03520400	C	5.23299600	-2.35073100	-0.14695700
H	-6.47973100	-1.23568200	1.06921300	H	5.21193500	-1.29267300	-0.43762500
H	-4.36917500	-2.51491000	1.16388500	H	5.01667600	-2.43309400	0.92603600
H	-4.42868700	1.92344700	-1.00143200	H	6.22792300	-2.75525900	-0.34242800
H	-6.51219900	1.00996900	-0.02207700				
C	-2.03694300	1.01109300	-1.06467100	7_S			

C	-4.73187600	-2.80738400	0.91610500	H	0.38815800	-2.75766900	1.83506100
C	-3.34494900	-2.80928700	1.01436200	H	-1.18820700	-2.39820800	2.58478800
C	-2.56466100	-1.81582400	0.39927400	H	-0.95692600	-2.22794900	-1.62634200
C	-3.20471100	-0.77823100	-0.30908500	Co	0.14109300	-0.12454700	0.25848700
C	-4.60677100	-0.80390300	-0.41338800	O	5.20893000	-2.07929500	-0.76026500
C	-5.36694200	-1.79832200	0.18969800	C	5.91150500	-1.09101000	-0.02114600
H	-5.31057300	-3.59259400	1.39339000	H	5.67690200	-0.07840800	-0.37361300
H	-2.84568300	-3.61115600	1.55043800	H	5.69537000	-1.15795000	1.05275600
H	-5.08043300	-0.00825700	-0.97598100	H	6.97244900	-1.28870900	-0.18480400
H	-6.44896300	-1.78328600	0.09983100				
C	-2.56146100	0.44438300	-0.93168400	7_T			
O	-3.17155800	1.00824000	-1.84943000	C	-5.33450700	-1.54446700	0.92007800
N	-1.40537400	0.92102200	-0.35947700	C	-4.06277700	-2.10538100	0.92204600
C	-0.38553500	-2.16948500	-0.69986600	C	-2.98093000	-1.47059100	0.28777900
C	1.08083000	-2.23761300	-0.76623500	C	-3.18888800	-0.22277800	-0.33827900
C	1.69094700	-1.20564100	-0.02566100	C	-4.48651900	0.31749700	-0.35504900
C	1.83492900	-3.13443800	-1.53960000	C	-5.54739500	-0.32400900	0.27434000
C	3.08897700	-1.13107200	0.00214500	H	-6.15686900	-2.05944200	1.40778100
C	3.21823500	-3.05489400	-1.50084100	H	-3.90003500	-3.06921600	1.39565800
H	1.34653800	-3.89472200	-2.14442800	H	-4.64577900	1.26035700	-0.86670600
C	3.84641100	-2.06246100	-0.72229500	H	-6.53619800	0.12468000	0.26044900
H	3.59730400	-0.34449400	0.54513800	C	-2.15753000	0.65044400	-1.03605100
H	3.84279200	-3.74103600	-2.06313500	O	-2.45517700	1.06744000	-2.15862000
C	-1.05052500	2.26199600	-0.51822600	N	-1.04445100	1.04649500	-0.31379100
C	0.20231200	2.60305900	0.08420200	C	-0.93415500	-2.21819200	-0.85788500
C	-1.77337400	3.30526600	-1.09864100	C	0.52433300	-2.41588600	-0.87110600
C	0.66955200	3.94548500	0.16187500	C	1.28847900	-1.57397000	-0.03767800
C	-1.29585000	4.63385200	-1.04602500	C	1.19192300	-3.32034400	-1.71488500
H	-2.70808100	3.08569600	-1.59061600	C	2.68079300	-1.68714200	0.01314800
C	2.05098600	1.81105700	1.27004700	C	2.57449800	-3.43327900	-1.67522900
C	1.88877400	4.16979000	0.84452500	H	0.61943000	-3.95157600	-2.38982900
C	-0.10990600	4.97039000	-0.42967800	C	3.32633300	-2.62470400	-0.80592100
H	-1.89812800	5.41131800	-1.50747600	H	3.25700500	-1.02804000	0.65203800
C	2.56638400	3.11127300	1.41103200	H	3.10060800	-4.13987000	-2.30864800
H	2.55343700	0.95620100	1.70184200	C	-0.44456800	2.28074900	-0.59042800
H	2.27259000	5.18270000	0.92509400	C	0.74010500	2.59629000	0.16918500
H	0.23910800	5.99719200	-0.39067400	C	-0.90452400	3.27361100	-1.45837100
H	3.49213500	3.25800600	1.95570600	C	1.38147300	3.86763300	0.06545400
N	0.92589100	1.56562000	0.60986700	C	-0.26394300	4.52744500	-1.55584100
C	-1.09079700	-1.98037100	0.46476500	H	-1.76626800	3.06838300	-2.07424400
C	0.04173900	-0.64311900	2.10617900	C	2.31608100	1.86352600	1.73226600
C	-0.44864500	-2.05477000	1.85329100	C	2.52978500	4.08474900	0.86421200
H	-0.71262600	0.01939000	2.54155700	C	0.85488000	4.84140300	-0.81728500
H	0.98725400	-0.57373200	2.64638500	H	-0.67646100	5.25932800	-2.24458900

C	2.99728000	3.09307900	1.70026800	H	6.81395300	-0.20959000	1.05396900
H	2.65504000	1.04843600	2.36541000	H	4.48018200	-2.38362100	-1.83059900
H	3.03579700	5.04436100	0.80626000	C	-2.87624000	-0.43985400	-1.22601400
H	1.34297500	5.80688000	-0.90371800	C	-2.95233000	-1.63649900	-0.43689400
H	3.87330700	3.24096100	2.32166700	C	-3.75237400	-0.33242100	-2.30688200
N	1.23709500	1.63108000	0.99770800	C	-3.88664300	-2.67085800	-0.72552300
C	-1.64410200	-2.09767100	0.28777400	C	-4.67702900	-1.36257600	-2.58774400
C	-0.30232900	-1.25537600	2.20614400	H	-3.71493900	0.55170100	-2.92337700
C	-1.03834800	-2.45988800	1.64097400	C	-2.09596600	-2.81344400	1.39230000
H	-0.95961600	-0.51927400	2.69044500	C	-3.87738500	-3.80688700	0.12246000
H	0.54858500	-1.49955100	2.84553100	C	-4.76047700	-2.51060300	-1.82917000
H	-0.33903900	-3.28940400	1.51314400	H	-5.34187200	-1.23342900	-3.43711400
H	-1.83233500	-2.79076300	2.32173800	C	-2.99143100	-3.87923200	1.17485500
H	-1.43275800	-2.03527900	-1.80842600	H	-1.38109500	-2.81888200	2.20815200
Co	0.22045300	-0.13306600	0.69584300	H	-4.57779200	-4.61456100	-0.07023800
O	4.67572500	-2.81016400	-0.84930900	H	-5.47634300	-3.29259700	-2.06159800
C	5.48498200	-2.01419500	0.00457200	H	-2.96875000	-4.73754300	1.83692300
H	5.38562800	-0.94518800	-0.22350100	N	-2.08192000	-1.74345900	0.61287300
H	5.24410500	-2.18141100	1.06230200	C	1.48282500	1.64858300	-0.38056400
H	6.51519700	-2.32413000	-0.17989200	C	0.75214200	-0.96034500	-0.07445000
				C	0.69209700	0.38825800	-0.50344400
TS3_betaH_S				H	0.51828100	-1.73041200	-0.80265300
C	0.28520500	5.19973000	0.22726800	H	1.37612100	-1.25961300	0.76129100
C	1.07015400	4.06319900	0.10036000	H	0.16538000	0.44074500	-1.45112700
C	0.56683300	2.83552200	-0.37110400	H	-0.10153100	1.02218800	0.56891800
C	-0.82167800	2.77512000	-0.73252900	H	3.27839800	2.70441300	-0.24529300
C	-1.58537600	3.95103500	-0.60831100	C	-1.23702700	0.17271600	3.03349800
C	-1.06257900	5.14219000	-0.12333100	O	-2.05336100	0.69214500	2.21578200
H	0.72128400	6.11753300	0.60993700	O	-0.26804500	-0.51352300	2.54468500
H	2.10691300	4.11760000	0.41104400	C	-1.36400900	0.36083900	4.51614600
H	-2.62432000	3.91266700	-0.91457900	H	-1.13692600	-0.57300600	5.03653200
H	-1.70099300	6.01479100	-0.02586400	H	-0.63567400	1.11137500	4.84283200
C	-1.68574600	1.67436500	-1.40468200	H	-2.36634700	0.70650900	4.77340500
O	-2.21453400	2.00515900	-2.47156900	Co	-0.93128600	-0.16805900	0.72138200
N	-1.93509400	0.48062400	-0.76929900	O	6.74158700	-2.35690800	-0.28615000
C	2.82915100	1.71768700	-0.32415400	C	6.61675300	-3.52946000	-1.08066900
C	3.80278000	0.61943000	-0.35688500	H	5.71544800	-4.09879800	-0.82142100
C	4.96979400	0.72026500	0.42710500	H	6.59952600	-3.29239700	-2.15177700
C	3.66696600	-0.51316800	-1.17264200	H	7.49765200	-4.13586400	-0.86324600
C	5.92399500	-0.28466900	0.43789900				
H	5.11575700	1.59900200	1.04937900	TS3_betaH_T			
C	4.62108100	-1.53000000	-1.17892700	C	0.36822800	5.08086600	0.11392100
H	2.81419800	-0.59668200	-1.83578900	C	1.13242700	3.92361500	0.06318500
C	5.75353500	-1.42543700	-0.36164300	C	0.63039800	2.71108700	-0.44958300

C	-0.71858800	2.68818300	-0.90789300	H	3.28169400	2.57552600	-0.55438300
C	-1.46818200	3.87468000	-0.85782900	C	-1.27215700	0.32716700	3.31951400
C	-0.94816000	5.05765100	-0.34803000	O	-1.57954600	1.14999700	2.38535000
H	0.79223000	5.98992400	0.52942500	O	-0.75789100	-0.78832000	3.03986600
H	2.13875100	3.94221900	0.46644500	C	-1.52981200	0.73989400	4.74848200
H	-2.48550100	3.85457300	-1.23540400	H	-1.35739900	-0.09257500	5.43208500
H	-1.56486600	5.95021500	-0.30871400	H	-0.86148900	1.56720500	5.01008000
C	-1.48814800	1.56227200	-1.61246900	H	-2.55539000	1.10550200	4.85212600
O	-1.67205100	1.70064400	-2.82588700	Co	-1.08651100	-0.09793300	0.85229900
N	-1.99757700	0.55837000	-0.82949700	O	6.89145800	-2.36659400	-0.26511600
C	2.85481500	1.57922100	-0.46653800	C	6.73234700	-3.64259700	-0.87287500
C	3.85224700	0.50263900	-0.44467100	H	5.88856000	-4.19378400	-0.43948300
C	5.09330400	0.74499700	0.17856600	H	6.59129000	-3.55838100	-1.95760900
C	3.66965600	-0.74608000	-1.05763700	H	7.65620200	-4.18815600	-0.67363800
C	6.07989600	-0.22653600	0.23186300				
H	5.27401700	1.71238700	0.63930900	6_Co(IV)_doublet			
C	4.65614500	-1.73063700	-1.02235000	C	-0.44243600	5.00509000	-0.24671200
H	2.75511400	-0.95080600	-1.60148100	C	0.30725100	3.88177000	-0.57452300
C	5.86695100	-1.47891000	-0.36470600	C	-0.29071500	2.62906100	-0.83514300
H	7.02853300	-0.03923900	0.72398000	C	-1.69887800	2.55792000	-0.82709500
H	4.47746400	-2.67628200	-1.51941400	C	-2.44412800	3.70470100	-0.50845600
C	-2.90145600	-0.37881700	-1.33265000	C	-1.83364500	4.91240800	-0.19559500
C	-3.09555700	-1.55308700	-0.52460800	H	0.05741700	5.94869500	-0.04878100
C	-3.66435700	-0.27655800	-2.49613100	H	1.38473600	3.97057200	-0.65937300
C	-4.04600700	-2.55370200	-0.88532300	H	-3.52378900	3.61824100	-0.51195900
C	-4.60104300	-1.27266500	-2.84695700	H	-2.43741000	5.77704200	0.06220700
H	-3.52393000	0.58161600	-3.13564100	C	-2.55016500	1.36375100	-1.17917900
C	-2.48042300	-2.74171400	1.39769700	O	-3.58815100	1.59585200	-1.81551300
C	-4.17554100	-3.66982900	-0.02312200	N	-2.17801000	0.13084300	-0.72743700
C	-4.80437900	-2.39247700	-2.07098300	C	1.77267900	1.44403900	-0.37143900
H	-5.17385600	-1.13981600	-3.76030800	C	3.02439000	0.71457200	-0.49842500
C	-3.40290400	-3.76565600	1.11383100	C	4.00150300	0.96953000	0.49352200
H	-1.85342000	-2.75599900	2.28231900	C	3.37754200	-0.18601200	-1.52126400
H	-4.89397800	-4.44574100	-0.27260600	C	5.24242900	0.35938800	0.47786100
H	-5.52622200	-3.15349700	-2.34995700	H	3.76363300	1.66205900	1.29537600
H	-3.49076100	-4.60898600	1.78944800	C	4.62192900	-0.80771100	-1.55130800
N	-2.33418400	-1.68655200	0.60733900	H	2.68175900	-0.41859800	-2.31283600
C	1.50739600	1.50350200	-0.39908800	C	5.56503300	-0.54358900	-0.54780500
C	0.97366400	-0.86195800	0.59518400	H	5.98058300	0.56234100	1.24637900
C	0.78764400	0.18977800	-0.29939200	H	4.84758600	-1.49356600	-2.35828300
H	0.76595200	-1.88155900	0.28946100	C	-3.05814900	-0.94694500	-0.83355400
H	1.50857400	-0.71871600	1.52688000	C	-2.59155500	-2.13819100	-0.20079300
H	0.32192400	-0.09997700	-1.24022000	C	-4.31806100	-1.00924000	-1.43478300
H	-0.24154200	1.03401900	0.50018900	C	-3.36385500	-3.33306400	-0.14843200

C	-5.08319400	-2.19524400	-1.38626500	C	0.25694400	2.58671500	-0.86485800
H	-4.70606200	-0.13389500	-1.92770700	C	-1.13272900	2.41011300	-1.08630100
C	-0.83205200	-3.13422000	0.97445600	C	-2.02821400	3.47256500	-0.86407200
C	-2.79644600	-4.44404500	0.52021000	C	-1.59491900	4.70400400	-0.39770800
C	-4.63986300	-3.34035900	-0.76116800	H	0.14816700	5.87437300	0.11206500
H	-6.05917700	-2.18953500	-1.86318200	H	1.72639800	4.08171600	-0.36887700
C	-1.54242500	-4.34384600	1.08059500	H	-3.08275500	3.29750500	-1.03964500
H	0.16443800	-3.01274400	1.37511200	H	-2.30855100	5.50084100	-0.21369200
H	-3.36116800	-5.36984300	0.58126200	C	-1.83021200	1.21823200	-1.68229300
H	-5.24293600	-4.24207000	-0.72981000	O	-2.40665700	1.35008400	-2.75371100
H	-1.08397200	-5.17901700	1.59775700	N	-1.87807900	0.02768700	-0.92364200
N	-1.34799300	-2.07882800	0.35800300	C	2.48051000	1.65387700	-0.40447400
C	0.61640200	1.47692000	-1.10771600	C	3.62632400	0.73021500	-0.43608000
C	0.10704500	-0.88968100	-1.66443000	C	4.21755100	0.34781500	0.78598100
C	0.32097400	0.50547800	-2.25400600	C	4.20568400	0.24566600	-1.61647600
H	-0.63334900	-1.47912500	-2.20651700	C	5.30254900	-0.51455800	0.82332000
H	1.02198200	-1.46328300	-1.51160700	H	3.79216700	0.72965000	1.70805500
H	1.13508400	0.54296400	-2.99073700	C	5.30333000	-0.61677300	-1.59535100
H	-0.57810100	0.83198900	-2.77714600	H	3.81685400	0.57047500	-2.57654400
H	1.79311100	2.13437000	0.46616000	C	5.85248300	-1.00975800	-0.36918200
C	1.58055300	-0.57324700	2.01805700	H	5.74921700	-0.81521600	1.76570800
O	1.15757000	0.45265500	2.60468400	H	5.72625200	-0.95958400	-2.53181100
O	1.09391000	-1.08235500	0.95184500	C	-2.64775900	-1.04645100	-1.29875900
C	2.75314800	-1.31229300	2.63287600	C	-2.67975900	-2.12353600	-0.34087400
H	2.35320800	-2.11688700	3.26130600	C	-3.40867200	-1.20362200	-2.47177800
H	3.37271900	-1.75257700	1.85087100	C	-3.45804500	-3.28949500	-0.55903000
H	3.34770300	-0.64879200	3.26158200	C	-4.17279300	-2.36455300	-2.68101100
Co	-0.49990100	-0.40037800	0.10080600	H	-3.40767000	-0.41730900	-3.20838800
O	6.79888900	-1.10052200	-0.48451200	C	-1.91103400	-2.91324300	1.70342800
C	7.17703500	-2.01768300	-1.50696200	C	-3.42978800	-4.28466000	0.44627500
H	7.17565400	-1.54114500	-2.49456400	C	-4.21268500	-3.39190100	-1.75755700
H	8.19169500	-2.33587500	-1.26329600	H	-4.74681600	-2.44431900	-3.59847500
H	6.51807400	-2.89413000	-1.52401200	C	-2.66068600	-4.09667700	1.57751300
C	-1.70578100	1.43065200	2.27009000	H	-1.27200300	-2.71887700	2.55828500
O	-2.92091300	1.35653100	2.15325700	H	-4.01518800	-5.18983200	0.31468000
O	-0.98813600	0.36188500	1.94445100	H	-4.81300400	-4.27876300	-1.93450700
C	-0.96017500	2.63166500	2.77614800	H	-2.62084600	-4.84316900	2.36259300
H	-0.32965500	2.34985000	3.62253600	N	-1.93161100	-1.96661900	0.77344300
H	-0.30510200	3.01349000	1.98954000	C	1.29739500	1.54298300	-1.05203400
H	-1.67299200	3.40377800	3.06771900	C	0.54894500	-0.81333900	-0.77926100
				C	0.94787900	0.25731500	-1.77747500
6_Co(IV)_quartet				H	0.08598900	-1.69536900	-1.22617900
C	-0.22610600	4.90716300	-0.20996600	H	1.36733000	-1.08009100	-0.11242400
C	0.66706500	3.87827300	-0.46298800	H	1.82159800	-0.11628700	-2.31913900

H	0.17860400	0.41387200	-2.53629400	H	-2.95553600	-0.17795100	-2.63272500
H	2.58799600	2.45567300	0.31643400	C	-5.39937100	-0.55313000	-0.31965700
C	1.21322900	-0.03445300	2.63312600	H	-5.19320300	-1.57395200	1.55909400
O	1.39752000	1.13968300	2.32435800	H	-5.29755600	0.35245800	-2.28605100
O	0.35262300	-0.83800100	2.05547500	C	1.52207000	2.14510700	-0.75528800
C	2.01531300	-0.71231000	3.73255700	C	0.77749600	2.71667000	0.35061500
H	1.35954500	-1.28789400	4.39195100	C	1.96896000	3.03356100	-1.76335000
H	2.72373500	-1.41414000	3.27818600	C	0.50493400	4.10705600	0.41258400
H	2.56796800	0.02911500	4.31172800	C	1.69549500	4.40387100	-1.68582300
Co	-0.78649400	-0.22396500	0.67401200	H	2.53135500	2.63531700	-2.59298000
O	6.91771300	-1.84742000	-0.23122100	C	-0.36711300	2.32401900	2.33537100
C	7.52858800	-2.34736000	-1.41256300	C	-0.24109700	4.57739100	1.51833200
H	7.92949200	-1.53735700	-2.03494600	C	0.98115900	4.94755900	-0.63036400
H	8.35122000	-2.98373200	-1.08143100	H	2.05367400	5.05156400	-2.47954500
H	6.82881300	-2.94718100	-2.00832200	C	-0.67851700	3.68682100	2.47804500
C	-2.97399100	1.48309200	1.53606200	H	-0.69154600	1.57281400	3.04727000
O	-3.69856600	1.19877500	0.57177000	H	-0.46407100	5.63742200	1.59669000
O	-1.76869900	1.05742300	1.74387000	H	0.77527000	6.01250000	-0.58707300
C	-3.46865400	2.45745100	2.59555200	H	-1.25572500	4.01742400	3.33391800
H	-3.26989400	2.06321400	3.59564000	N	0.34015000	1.86561200	1.30581300
H	-2.90600800	3.39122200	2.49087700	C	-0.26586000	-1.19579100	-1.69262900
H	-4.53336200	2.65994600	2.47088100	C	-0.93868000	1.16482800	-2.40314200
				C	-0.40276000	-0.16841400	-2.80454100
6_Co(IV)_sextet				H	-1.08106100	1.93809700	-3.15086700
C	2.10964700	-4.14420500	-1.47598100	H	-1.23275800	1.37303100	-1.38332400
C	0.95056900	-3.37586100	-1.53457800	H	-1.03551200	-0.60854000	-3.59724400
C	1.00471600	-1.97363900	-1.61321200	H	0.56784800	-0.03973400	-3.30265300
C	2.27902500	-1.36631800	-1.63736400	H	-0.96836900	-2.27231800	-0.06607100
C	3.44215100	-2.14394400	-1.61594900	C	-0.66033000	-1.93099000	2.65448500
C	3.36279700	-3.52960900	-1.52245300	O	-0.37530400	-2.88979300	1.93061200
H	2.03324700	-5.22509700	-1.40676300	O	-0.40751300	-0.68375600	2.37511500
H	-0.01959900	-3.86080500	-1.53660600	C	-1.38008100	-2.13063200	3.97910200
H	4.40075300	-1.63790800	-1.62803600	H	-0.75568100	-1.75635600	4.79717900
H	4.26940400	-4.12543700	-1.48307900	H	-2.30859600	-1.54976900	3.98854200
C	2.46216600	0.11400500	-1.66009000	H	-1.60377100	-3.18561100	4.14414700
O	3.25543600	0.64238200	-2.42797400	Co	0.88191300	-0.13020200	1.02893400
N	1.67924300	0.80230100	-0.70978200	O	-6.69988800	-0.29589700	-0.02842600
C	-1.26215500	-1.55726300	-0.83120200	C	-7.47712800	0.40912000	-0.98940600
C	-2.66293300	-1.16444800	-0.72682300	H	-7.54933200	-0.14421500	-1.93364700
C	-3.34745700	-1.56806800	0.44508900	H	-8.47345700	0.50904400	-0.55573500
C	-3.41335700	-0.47749500	-1.70032400	H	-7.06711700	1.40768300	-1.18441300
C	-4.67999800	-1.26420200	0.65473800	C	3.74487900	-0.55492400	1.38448500
H	-2.80597200	-2.14438200	1.18693800	O	4.06637900	0.31828300	0.56905100
C	-4.75859500	-0.17279400	-1.50702600	O	2.53252700	-0.82849700	1.75925500

C	4.80469100	-1.43594100	2.02702800	H	-2.97066800	3.57494100	1.95820400
H	4.67620800	-1.44991100	3.11322600	N	-0.63559400	1.79193800	0.34760500
H	4.67178600	-2.46276800	1.66984600	C	0.71402800	-1.82269100	-1.41523000
H	5.80686700	-1.08836800	1.77142700	C	-0.48310600	0.23595900	-2.14843100
TS3_Co(IV)_doublet				C	0.33080100	-0.96921400	-2.64527600
C	3.88933600	-3.62613300	-0.44820500	H	-0.13094900	1.18741600	-2.54923700
C	2.56505000	-3.36157700	-0.78605000	H	-1.55737100	0.14244600	-2.29453400
C	2.13554100	-2.05690700	-1.07017400	H	-0.22546500	-1.58171800	-3.36185000
C	3.07034700	-1.00776500	-1.00792700	H	1.24579700	-0.64621900	-3.14669200
C	4.40758300	-1.28666200	-0.69366600	H	0.00972500	-2.79787300	0.35645600
C	4.81668900	-2.58376300	-0.40468800	C	-1.45921300	-1.82128700	3.09554400
H	4.19661000	-4.64372400	-0.22744800	O	-0.96470400	-2.79973700	2.52281400
H	1.84542600	-4.17147000	-0.84728900	O	-2.06686100	-0.82455100	2.52853600
H	5.11328800	-0.46489500	-0.65611700	C	-1.39153000	-1.70352200	4.61771900
H	5.85249300	-2.77987100	-0.14638900	H	-0.78473800	-0.83312100	4.88993800
C	2.76962500	0.43307800	-1.26635400	H	-2.39194100	-1.54108200	5.03210900
O	3.55742000	1.09953600	-1.92623500	H	-0.95273800	-2.60198900	5.05634400
N	1.60362800	0.99894000	-0.69221600	Co	-0.05167500	0.07392200	-0.20925300
C	-0.25228900	-2.33772600	-0.59573100	C	1.78023700	-0.14034700	2.04974600
C	-1.68554300	-2.07086200	-0.84002000	O	2.64834500	0.58582000	1.51281500
C	-2.19726600	-1.02682600	-0.05187700	O	0.62391400	-0.42258500	1.59391500
C	-2.41217200	-2.59882400	-1.91538600	C	2.09467900	-0.75577700	3.40875900
C	-3.46104500	-0.49898100	-0.38325800	H	1.73351700	-0.07989600	4.19133800
H	-1.92214400	-0.90393400	1.20648900	H	1.56754100	-1.70692200	3.50090400
C	-3.66858900	-2.08951200	-2.20705000	H	3.17071200	-0.88802000	3.53362700
H	-1.98917800	-3.38861200	-2.52997500	O	-5.43396400	-0.60273200	-1.82323400
C	-4.19691700	-1.02819700	-1.44475700	C	-6.00895800	0.48290700	-1.10859100
H	-3.87942400	0.30164000	0.21592300	H	-6.16261100	0.23435300	-0.05113200
H	-4.26362900	-2.48420400	-3.02431300	H	-5.38974500	1.38648900	-1.18062900
C	1.45592800	2.37210800	-0.61407000	H	-6.97654000	0.67357500	-1.57610200
C	0.22654900	2.78375900	-0.00237600	TS3_Co(IV)_quartet			
C	2.36836100	3.37906900	-0.96484300	C	3.77540700	-3.73231300	-0.12075700
C	-0.05461100	4.14298300	0.28380700	C	2.44928100	-3.52994900	-0.49160000
C	2.06584100	4.73209200	-0.72408500	C	1.99529700	-2.27726100	-0.93139000
H	3.30776400	3.11135800	-1.41889500	C	2.92117600	-1.21509200	-1.00456300
C	-1.72489400	2.06984100	1.05875800	C	4.26099100	-1.43630000	-0.65658800
C	-1.25275600	4.42826900	0.98026100	C	4.68844500	-2.68013500	-0.20402700
C	0.89138800	5.12411400	-0.11283500	H	4.09587000	-4.71122000	0.22245800
H	2.79380200	5.48106400	-1.01839100	H	1.74319500	-4.35289800	-0.45454100
C	-2.06830100	3.39321000	1.38618600	H	4.95883700	-0.60905300	-0.72231200
H	-2.30523000	1.22674300	1.40608800	H	5.72658900	-2.82717800	0.07640200
H	-1.50167800	5.45946500	1.21155900	C	2.62254600	0.18431900	-1.45811800
H	0.68440000	6.17111800	0.08382200	O	3.30277800	0.68546700	-2.34554900

N	1.58143400	0.88309000	-0.80671000	C	1.96100800	-0.26363900	1.95028600
C	-0.39333300	-2.55245100	-0.42670000	O	2.68334000	0.63092300	1.47325900
C	-1.82563800	-2.21610800	-0.62558100	O	0.83836700	-0.66913100	1.47214400
C	-2.25900000	-1.04198500	0.01977600	C	2.43173500	-1.01732100	3.18620200
C	-2.65016600	-2.87432700	-1.54661900	H	2.83364500	-0.32190200	3.92747700
C	-3.53053400	-0.53145100	-0.29883800	H	1.61781400	-1.60781800	3.60779000
H	-1.91929200	-0.64714700	1.24073700	H	3.24386000	-1.68801000	2.88455900
C	-3.90737300	-2.36198300	-1.84382200	O	-5.59807200	-0.76283400	-1.58918400
H	-2.30118700	-3.77241200	-2.04918100	C	-6.10137400	0.42173400	-0.98740400
C	-4.35285000	-1.18073700	-1.22490600	H	-6.18532000	0.31817100	0.10150500
H	-3.87772700	0.36383100	0.20538400	H	-5.47343200	1.29188800	-1.21955500
H	-4.56375500	-2.85442700	-2.55408600	H	-7.09588100	0.57609800	-1.40993600
C	1.53203300	2.24910800	-0.82194100				
C	0.35917600	2.82949100	-0.21025600				
C	2.52491200	3.13156200	-1.28979500	TS4_T			
C	0.21091300	4.23840100	-0.10797900	C	-1.20758500	4.97214200	-0.01959500
C	2.36111600	4.52126000	-1.19270500	C	-0.30434300	3.95104300	-0.29709000
H	3.42303100	2.72846700	-1.73010100	C	-0.73574800	2.66051200	-0.65630700
C	-1.64504600	2.46444400	0.91426000	C	-2.12764800	2.41779800	-0.74548500
C	-0.95059300	4.73028200	0.53254000	C	-3.02271300	3.46518300	-0.49576300
C	1.23253000	5.07930800	-0.62285000	C	-2.57750800	4.72908500	-0.12156400
H	3.14914600	5.16494000	-1.56972200	H	-0.84135400	5.95718900	0.25390700
C	-1.87120300	3.84503100	1.05170600	H	0.76114900	4.15475000	-0.27028200
H	-2.30653800	1.72944600	1.35625400	H	-4.08276600	3.25864200	-0.59274100
H	-1.09406700	5.80297500	0.62171500	H	-3.29334600	5.52006500	0.08040600
H	1.11908800	6.15607200	-0.54632400	C	-2.76988200	1.09001500	-1.08664500
H	-2.75839800	4.19016400	1.57014600	O	-3.75999800	1.09519800	-1.83124500
N	-0.57517400	1.98174100	0.28760700	N	-2.20546400	0.00552300	-0.48513900
C	0.56352400	-2.10610400	-1.27467300	C	1.39920400	1.55136600	-0.14177100
C	-0.52874000	-0.03541800	-2.19844700	C	2.67844600	0.84651900	-0.31101900
C	0.18241300	-1.32769300	-2.54843300	C	3.41036500	0.49992500	0.84524900
H	-0.11002500	0.87893300	-2.60891100	C	3.26454200	0.56072000	-1.55448400
H	-1.61368000	-0.05352000	-2.21095800	C	4.63991700	-0.13050200	0.76162800
H	-0.46709700	-1.95749400	-3.16553000	H	2.97401800	0.69948000	1.81696300
H	1.08491400	-1.12387300	-3.12739300	C	4.50712600	-0.06332800	-1.65443400
H	-0.10371600	-3.01700700	0.51256300	H	2.76381000	0.84449700	-2.47111300
C	-1.40983800	-0.97969700	3.31460800	C	5.20083800	-0.42175000	-0.49188600
O	-1.27414600	-2.19172900	3.15139000	H	5.19109300	-0.40635700	1.65463800
O	-1.90696700	-0.14368900	2.44125300	H	4.92302400	-0.25774500	-2.63534900
C	-0.97846200	-0.30204600	4.61152500	C	-2.68441400	-1.29005700	-0.66690500
H	-0.11463600	0.34021000	4.40675700	C	-1.96610600	-2.32331400	0.03646600
H	-1.77658300	0.34129000	4.99555600	C	-3.76538800	-1.69365800	-1.45100400
H	-0.70552500	-1.04330800	5.36518400	C	-2.34767800	-3.69319100	-0.06445300
Co	-0.14612900	0.00227200	-0.06948800	C	-4.13637000	-3.05363400	-1.54287000



H	-4.32026400	-0.93920100	-1.98703000	C	-2.44226400	1.63659100	-0.94266800
C	-0.19781800	-2.85549600	1.47450500	O	-3.36604800	1.92882700	-1.71280300
C	-1.57957600	-4.63772700	0.65963800	N	-2.17506700	0.37966100	-0.46655100
C	-3.45708600	-4.04606400	-0.87271700	C	1.80021200	1.42370200	-0.07359600
H	-4.98811800	-3.31147500	-2.16595800	C	2.97362000	0.58534800	-0.30989600
C	-0.51078400	-4.22666100	1.42631700	C	3.79599800	0.30721200	0.80513000
H	0.62503400	-2.47042100	2.06720900	C	3.38788500	0.06709000	-1.54908100
H	-1.84818600	-5.68887600	0.60031200	C	4.94240600	-0.45908500	0.69951700
H	-3.75089300	-5.08814600	-0.95017000	H	3.51391700	0.70602500	1.77452800
H	0.08837700	-4.93369200	1.98892700	C	4.54302200	-0.70278800	-1.67454600
N	-0.89730000	-1.95164300	0.80362200	H	2.81858600	0.26686700	-2.44632800
C	0.30863100	1.63650700	-0.96596900	C	5.32608300	-0.97870700	-0.54678000
C	0.30769400	-0.64438100	-2.06131400	H	5.56186700	-0.66987100	1.56494400
C	0.14762600	0.82889300	-2.25772700	H	4.82258000	-1.07715100	-2.65166200
H	-0.40272900	-1.32745000	-2.51062900	C	-3.05005900	-0.68519400	-0.72502700
H	1.20305600	-1.05804000	-1.61447300	C	-2.73540500	-1.89482000	-0.02400700
H	0.86286400	1.22024100	-2.99958800	C	-4.17363800	-0.71067500	-1.55099800
H	-0.83591700	1.03269600	-2.68164700	C	-3.53566600	-3.06641000	-0.13534900
H	1.34794100	2.14041400	0.77107600	C	-4.96542000	-1.87719100	-1.66206100
C	0.04076200	0.69239100	3.04046600	H	-4.43923300	0.17863400	-2.09901700
O	-0.99641400	1.12068300	2.42484100	C	-1.25216100	-2.95096700	1.43889900
O	0.83958300	-0.08682200	2.44619200	C	-3.12903500	-4.20011700	0.60985600
C	0.30726900	1.15902000	4.44840300	C	-4.67510600	-3.03619300	-0.97746300
H	-0.62469100	1.20754000	5.01643700	H	-5.83276500	-1.84331400	-2.31523000
H	1.02303200	0.50290200	4.94616500	C	-1.99682700	-4.14460400	1.39433300
H	0.72509700	2.17167300	4.41143600	H	-0.34452100	-2.85745300	2.02467300
Co	-0.60844800	0.07959900	0.72309400	H	-3.71958300	-5.11008300	0.55143300
O	6.41033600	-1.03942200	-0.47370600	H	-5.29411900	-3.92269100	-1.07264600
C	7.02611600	-1.34393500	-1.71952200	H	-1.66637600	-5.00110700	1.97113500
H	7.22944100	-0.43646300	-2.30129700	N	-1.61667800	-1.87344800	0.75747500
H	7.97127400	-1.83217300	-1.47651200	C	0.69369100	1.70498400	-0.81757400
H	6.41113300	-2.02800400	-2.31714500	C	0.20666300	-0.44459800	-2.02153300
				C	0.36991900	1.03696400	-2.15299800
TS4'_T'				H	-0.59189100	-0.94988800	-2.55302400
C	-0.33046200	5.04555000	0.63411000	H	1.00285200	-1.05404600	-1.60811200
C	0.41626800	3.96919200	0.16795000	H	1.16051200	1.29615600	-2.87651900
C	-0.19176600	2.80576800	-0.34271600	H	-0.54258800	1.46977700	-2.56537600
C	-1.60142800	2.76877700	-0.40538700	H	1.83432600	1.91897400	0.89327300
C	-2.34208300	3.87446800	0.03567100	C	0.58084200	0.02085800	2.62204700
C	-1.72308300	4.99889500	0.57061300	O	-0.38602800	0.81514600	2.43820300
H	0.17486500	5.92487700	1.02263900	O	0.86977400	-0.81081300	1.68933000
H	1.49929400	4.03188500	0.16530900	C	1.38073200	0.04162100	3.89583500
H	-3.42244800	3.82847700	-0.04494700	H	0.72161900	-0.17511900	4.74254300
H	-2.32085200	5.83578900	0.91860600	H	2.18988300	-0.68901000	3.86425000

H 1.78950800 1.04446600 4.05389000  
Co -0.63359600 -0.16130100 0.56089400  
O 6.46336000 -1.72104100 -0.55784900  
C 6.89525800 -2.26644100 -1.79883400  
H 7.11327600 -1.47977800 -2.53157500  
H 7.81185000 -2.81755500 -1.58228700  
H 6.15112600 -2.95555700 -2.21683200

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C 3.39411800 -3.91671900 -0.32243300  
C 2.10412000 -3.43787200 -0.54002200  
C 1.87370600 -2.09103100 -0.86769600  
C 2.98752200 -1.22188200 -0.97457900  
C 4.27920400 -1.72282300 -0.78662700  
C 4.48773700 -3.05871400 -0.45323700  
H 3.54532800 -4.96232500 -0.07129600  
H 1.25728900 -4.11474800 -0.48564000  
H 5.11408600 -1.03846900 -0.89372300  
H 5.49640400 -3.42935300 -0.29844600  
C 2.84994500 0.25357700 -1.26663000  
O 3.63455800 0.80448800 -2.04860100  
N 1.83255600 0.84334100 -0.58183800  
C -0.50003200 -1.95987400 -0.23613900  
C -1.95095200 -1.73394100 -0.28487500  
C -2.63031400 -1.52748900 0.93411400  
C -2.71154400 -1.73157400 -1.46380800  
C -3.99319800 -1.27977300 0.96737800  
H -2.05962300 -1.54118300 1.85719200  
C -4.08681400 -1.49790900 -1.44331000  
H -2.23898800 -1.94494000 -2.41408800  
C -4.73325400 -1.25425300 -0.22537100  
H -4.51192500 -1.10732000 1.90486900  
H -4.63999700 -1.51182100 -2.37431400  
C 1.44064200 2.16310800 -0.76352200  
C 0.31242800 2.54399000 0.03217900  
C 1.97891400 3.11960200 -1.62124200  
C -0.26359600 3.84092500 -0.05224500  
C 1.41014900 4.41111100 -1.69380700  
H 2.83379000 2.85618000 -2.22609400  
C -1.25763100 1.85166300 1.61577200  
C -1.39605200 4.09594900 0.76152000  
C 0.31644300 4.78241800 -0.93933600  
H 1.85789400 5.13022800 -2.37391000  
C -1.89231600 3.10939600 1.58617300

H -1.60324300 1.04807300 2.25590300  
H -1.86512400 5.07504800 0.72394100  
H -0.10806200 5.77862300 -1.01323300  
H -2.75928600 3.28199200 2.21393000  
N -0.19942500 1.58607900 0.86389700  
C 0.47362700 -1.62654200 -1.13307800  
C -0.73800700 0.20008100 -2.46895700  
C 0.22948500 -0.93139300 -2.46543300  
H -1.12185400 0.57457900 -3.41156800  
H -0.98515500 0.73479800 -1.56340800  
H -0.08532300 -1.70392600 -3.18670300  
H 1.19580200 -0.58907100 -2.86212900  
H -0.16857300 -2.47255700 0.66335500  
C 1.15457600 -0.41196100 3.20143000  
O 2.08537200 0.21795400 2.63374100  
O 0.17450900 -0.84820400 2.48394800  
C 1.13682800 -0.65739900 4.68465600  
H 0.29025000 -0.12323100 5.12881900  
H 0.99117900 -1.72363600 4.88183200  
H 2.06481200 -0.31604800 5.14447800  
Co 0.89338000 -0.06003700 0.82558100  
O -6.06251100 -1.00027800 -0.09390100  
C -6.85442000 -0.95462500 -1.27431600  
H -6.85200900 -1.91722300 -1.80069700  
H -7.87066100 -0.72908400 -0.94664900  
H -6.51349600 -0.16749700 -1.95837100

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C 2.59038300 -4.40466100 -0.43012500  
C 1.42080400 -3.67003500 -0.60551300  
C 1.45707700 -2.29379400 -0.88901300  
C 2.71859100 -1.65852500 -0.99670000  
C 3.88487000 -2.41660200 -0.85172300  
C 3.82985000 -3.77657100 -0.55946800  
H 2.53282800 -5.46705200 -0.21303500  
H 0.45727000 -4.16699900 -0.55481000  
H 4.83795300 -1.91013800 -0.95926600  
H 4.74767600 -4.34339100 -0.43636100  
C 2.90515700 -0.17581000 -1.23579400  
O 3.79927600 0.20238400 -2.00293700  
N 2.04995000 0.60607500 -0.51829600  
C -0.86505800 -1.78091900 -0.23378000  
C -2.27284900 -1.36195100 -0.33101000  
C -2.99485500 -1.11318000 0.85474900

C	-2.96082600	-1.24546800	-1.54888100	H	-6.54910900	0.70694400	-2.21052700
C	-4.32392200	-0.72235800	0.81928900				
H	-2.48251700	-1.20414800	1.80611800	8_T'			
C	-4.30213200	-0.86662000	-1.59758400	C	3.39884700	-3.91253900	-0.32113100
H	-2.46254200	-1.48840800	-2.47829800	C	2.10801800	-3.43621500	-0.53952500
C	-4.98888300	-0.58823300	-0.40968100	C	1.87535100	-2.09014400	-0.86856700
H	-4.87356000	-0.51837500	1.73253000	C	2.98759500	-1.21905600	-0.97589600
H	-4.79782100	-0.79777800	-2.55797200	C	4.28010800	-1.71743500	-0.78706900
C	1.99272500	1.99009400	-0.63677900	C	4.49093000	-3.05268500	-0.45240800
C	0.99382400	2.63453400	0.17696800	H	3.55188500	-4.95763700	-0.06899500
C	2.76957000	2.80572100	-1.45776400	H	1.26234500	-4.11450300	-0.48468400
C	0.80004600	4.04538400	0.13316400	H	5.11383200	-1.03171200	-0.89446500
C	2.57347400	4.20431900	-1.48976000	H	5.50022100	-3.42136000	-0.29699200
H	3.52892800	2.34395100	-2.07095100	C	2.84724900	0.25595400	-1.26904600
C	-0.72256700	2.37866200	1.74757300	O	3.63046300	0.80762400	-2.05183000
C	-0.21865300	4.58623900	0.95517300	N	1.82949400	0.84451600	-0.58373600
C	1.61641400	4.82880000	-0.72082100	C	-0.49832100	-1.96067300	-0.23683500
H	3.20445400	4.79615100	-2.14677800	C	-1.94932900	-1.73549300	-0.28517400
C	-0.97858300	3.76223500	1.75778100	C	-2.62851000	-1.53045700	0.93418600
H	-1.28036300	1.68329300	2.36550900	C	-2.71023600	-1.73210300	-1.46388800
H	-0.39121200	5.65887100	0.94135100	C	-3.99149200	-1.28343300	0.96806600
H	1.47361900	5.90422200	-0.75566700	H	-2.05760100	-1.54478800	1.85712400
H	-1.76336400	4.15733600	2.39285300	C	-4.08559200	-1.49898900	-1.44280600
N	0.22298000	1.84505100	0.98657400	H	-2.23793000	-1.94417000	-2.41456800
C	0.16519600	-1.57280100	-1.11083400	C	-4.73186700	-1.25700900	-0.22445900
C	-0.71058500	0.51218100	-2.31907600	H	-4.51004700	-1.11219100	1.90587500
C	0.04957700	-0.76551700	-2.39781100	H	-4.63895200	-1.51203900	-2.37371900
H	-1.03967200	1.00016500	-3.22980700	C	1.43680000	2.16431700	-0.76418200
H	-0.84102800	1.03505800	-1.38101500	C	0.30887700	2.54391900	0.03255200
H	-0.38928600	-1.42478000	-3.16434800	C	1.97416200	3.12180000	-1.62130900
H	1.06191200	-0.56994800	-2.77694100	C	-0.26820900	3.84045000	-0.05083600
H	-0.64011800	-2.38370100	0.64367800	C	1.40443700	4.41296400	-1.69270100
C	0.59726900	-1.10372900	3.12004800	H	2.82886100	2.85937400	-2.22683700
O	1.66031200	-1.06340900	2.40672100	C	-1.25927200	1.84966200	1.61713900
O	-0.48027500	-0.63952900	2.65072100	C	-1.40020700	4.09421000	0.76397000
C	0.64707400	-1.68538500	4.50882800	C	0.31071000	4.78293000	-0.93760800
H	0.49298800	-0.88308900	5.23828000	H	1.85143400	5.13290900	-2.37242300
H	-0.16721000	-2.40416600	4.63674900	C	-1.89499100	3.10690200	1.58860900
H	1.60629800	-2.16722000	4.70127600	H	-1.60376100	1.04550100	2.25716200
Co	0.79222800	-0.12421600	0.84362200	H	-1.87008900	5.07295200	0.72724500
O	-6.28979800	-0.19912700	-0.34348300	H	-0.11447800	5.77891200	-1.01058000
C	-7.00618400	-0.05182100	-1.56328900	H	-2.76158800	3.27852500	2.21715000
H	-7.07313100	-1.00074300	-2.10987300	N	-0.20144900	1.58526400	0.86432200
H	-8.01059600	0.27219700	-1.28559700	C	0.47476800	-1.62785600	-1.13451100

C	-0.73539400	0.19896300	-2.47145600	H	-4.17745500	-1.56544100	1.94831700
C	0.22966500	-0.93464600	-2.46767300	H	-4.16057600	-2.03873400	-2.32550200
H	-1.12447600	0.56945700	-3.41347700	C	0.85023500	2.29306900	-0.80904700
H	-0.97946000	0.73595500	-1.56643800	C	-0.28074400	2.42245200	0.06009100
H	-0.08833800	-1.70800600	-3.18662000	C	1.07364000	3.31167900	-1.73350300
H	1.19581900	-0.59524500	-2.86718400	C	-1.16698600	3.53129700	-0.01841600
H	-0.16620600	-2.47217800	0.66310200	C	0.19557600	4.41668300	-1.80169700
C	1.15745100	-0.41211200	3.20092300	H	1.92646900	3.24120900	-2.39201700
O	2.08675100	0.21936100	2.63239100	C	-1.51178600	1.44604900	1.78647900
O	0.17712100	-0.84911300	2.48433300	C	-2.26881600	3.53864300	0.87380800
C	1.14179600	-0.65819300	4.68404500	C	-0.90319400	4.54195500	-0.97688300
H	0.29509300	-0.12528200	5.12947600	H	0.40249800	5.19038500	-2.53566000
H	0.99770200	-1.72470100	4.88089500	C	-2.44192700	2.50437800	1.76781100
H	2.06990700	-0.31590200	5.14290700	H	-1.59761500	0.61742700	2.47914900
Co	0.89401900	-0.05952000	0.82567700	H	-2.97058200	4.36731500	0.84138900
O	-6.06122300	-1.00382400	-0.09239700	H	-1.56817500	5.39692000	-1.04777300
C	-6.85342600	-0.95738800	-1.27257800	H	-3.27823500	2.48862400	2.45761700
H	-6.85034300	-1.91933000	-1.80015100	N	-0.47802800	1.41010100	0.95853800
H	-7.86978100	-0.73308100	-0.94441900	C	0.75510600	-1.60296400	-1.06742500
H	-6.51329400	-0.16914100	-1.95574200	C	-1.14391500	-0.36121400	-2.23506100
TS5_OSS				C	0.21215700	-0.98580200	-2.35036400
C	4.16253100	-3.18016400	-0.53333800	H	-1.69866900	-0.19081600	-3.15316100
C	2.78557200	-3.00089500	-0.64072500	H	-1.31362700	0.36237900	-1.44602900
C	2.23595700	-1.74106100	-0.93589400	H	0.19637400	-1.77536600	-3.11649500
C	3.11766000	-0.64746700	-1.12277400	H	0.92980500	-0.24863700	-2.72904300
C	4.49928600	-0.84914000	-1.04731500	H	0.40075000	-2.54611400	0.78682100
C	5.02500700	-2.10244600	-0.74482900	C	1.47597100	-0.21079600	3.19273800
H	4.56154700	-4.16360000	-0.30331500	O	2.22911800	0.55930800	2.53809200
H	2.11612200	-3.84704700	-0.52160200	O	0.52868700	-0.82448200	2.56913800
H	5.15053200	0.00217100	-1.21472100	C	1.62836800	-0.41386200	4.67439100
H	6.09980500	-2.23897900	-0.67492600	H	0.78580600	0.06096000	5.18897600
C	2.63488100	0.75767000	-1.38836000	H	1.59893200	-1.48124600	4.91029000
O	3.21177400	1.45945600	-2.22824700	H	2.56072300	0.02528400	5.03097900
N	1.56576100	1.11711600	-0.62470700	Co	0.95578500	0.05691000	0.85407800
C	-0.06131100	-2.12679100	-0.10281100	O	-5.65554800	-1.51594700	-0.10050400
C	-1.51868800	-2.11699600	-0.13548700	C	-6.41219300	-1.50623700	-1.30392300
C	-2.24397000	-1.92994900	1.05122000	H	-6.37328700	-2.47708400	-1.81376400
C	-2.22522500	-2.12290000	-1.37369700	H	-7.44278300	-1.29780100	-1.01140900
C	-3.61708800	-1.72525000	1.03331900	H	-6.06635900	-0.72394900	-1.99120200
H	-1.70433800	-1.90730100	1.99299400	TS5_Q			
C	-3.63245100	-1.96659200	-1.38296000	C	4.26685900	-3.03235500	-0.68924500
H	-1.77016500	-2.60153400	-2.23361500	C	2.88443200	-2.89862300	-0.79336500
C	-4.31366100	-1.72381100	-0.19385700	C	2.28855000	-1.65072100	-1.04641900

C	3.13075900	-0.51851800	-1.18764200	H	0.50256000	-2.55130600	0.67124400
C	4.51903100	-0.67426200	-1.11872000	C	1.50087200	-0.31303500	3.30821200
C	5.09002600	-1.91767800	-0.86033700	O	2.09332500	0.61738000	2.67841000
H	4.70049600	-4.00837100	-0.49282600	O	0.69840500	-1.07989400	2.67471000
H	2.24587100	-3.77183600	-0.70425400	C	1.69888200	-0.48955700	4.78917900
H	5.14057500	0.20477500	-1.25335600	H	0.85148800	-0.03291100	5.31329900
H	6.16902300	-2.01711100	-0.79255500	H	1.71665800	-1.55124000	5.04583600
C	2.60184600	0.88101200	-1.39991200	H	2.61706500	-0.00163900	5.11918700
O	3.13520700	1.61541300	-2.23791300	Co	1.03917100	0.07076000	0.93968000
N	1.54028200	1.18567800	-0.59277200	O	-5.58663800	-1.62686400	-0.09434700
C	0.01605400	-2.13067400	-0.20595800	C	-6.36395800	-1.60744100	-1.28420800
C	-1.44101400	-2.15033000	-0.21245100	H	-6.31313900	-2.56575200	-1.81627900
C	-2.14819900	-2.00085800	0.99047100	H	-7.39361000	-1.42800000	-0.96996200
C	-2.16823700	-2.14187000	-1.43818900	H	-6.04708200	-0.80294500	-1.95979200
C	-3.52510800	-1.82122800	0.99981700				
H	-1.59322000	-1.99023400	1.92401900	TS5_T			
C	-3.57804300	-2.01140700	-1.42065600	C	4.23145600	-3.04419600	-0.69622700
H	-1.71771900	-2.59098900	-2.31640500	C	2.84987700	-2.89590500	-0.79002400
C	-4.24266900	-1.80708700	-0.21505200	C	2.26575800	-1.64305300	-1.04734000
H	-4.07264300	-1.69147500	1.92725500	C	3.11940400	-0.52149300	-1.20561800
H	-4.12080700	-2.07223600	-2.35568000	C	4.50610200	-0.69263300	-1.14806000
C	0.74891500	2.31927300	-0.76387800	C	5.06535700	-1.94042000	-0.88504400
C	-0.39329000	2.39674900	0.10885700	H	4.65594200	-4.02333700	-0.49549000
C	0.91689500	3.34032800	-1.69567400	H	2.20279600	-3.76176200	-0.69111900
C	-1.32987100	3.46478900	0.00721100	H	5.13600100	0.17861500	-1.29380300
C	-0.01279400	4.40109400	-1.78219100	H	6.14375200	-2.05151900	-0.82637400
H	1.77337400	3.30614300	-2.35236800	C	2.60551000	0.88618400	-1.40524800
C	-1.60321000	1.39968600	1.83500600	O	3.14250400	1.62098400	-2.24121300
C	-2.43924900	3.43989700	0.88902600	N	1.55843900	1.19686900	-0.58354000
C	-1.11633600	4.47798500	-0.96142500	C	-0.01712900	-2.11621900	-0.22070500
H	0.15849300	5.17506800	-2.52492000	C	-1.47497700	-2.12546300	-0.24207500
C	-2.58006300	2.41420500	1.79753700	C	-2.19585900	-1.98692900	0.95410700
H	-1.66971000	0.57429900	2.53578200	C	-2.18760000	-2.09765600	-1.47625400
H	-3.17365800	4.23874700	0.83474200	C	-3.57231800	-1.80303000	0.94842000
H	-1.82458900	5.29685900	-1.04076700	H	-1.65173800	-1.98734300	1.89355900
H	-3.42249900	2.37271000	2.47876700	C	-3.59729500	-1.96497000	-1.47423900
N	-0.55889200	1.39404700	1.02211900	H	-1.72813500	-2.53612700	-2.35524200
C	0.80445100	-1.56957700	-1.17045600	C	-4.27586600	-1.77394900	-0.27439300
C	-1.13961900	-0.33144500	-2.26250200	H	-4.13037700	-1.68219400	1.87080000
C	0.23063300	-0.91418500	-2.41895500	H	-4.12848800	-2.01331700	-2.41657600
H	-1.71288200	-0.14340000	-3.16561800	C	0.79391200	2.35246700	-0.71639600
H	-1.31583200	0.35868400	-1.44565500	C	-0.33750500	2.43801400	0.17071400
H	0.22764700	-1.66786700	-3.22045300	C	0.97924400	3.39386100	-1.62257300
H	0.92510000	-0.14183300	-2.77138900	C	-1.24507800	3.53397700	0.10733000

C	0.07846400	4.48149900	-1.67093700	H	6.10028100	-2.25197700	-0.70886500
H	1.82743600	3.35319300	-2.28969400	C	2.65110900	0.78019900	-1.34178600
C	-1.55928200	1.43019500	1.88556700	O	3.24196900	1.49855600	-2.15852600
C	-2.34554200	3.51662900	1.00009500	N	1.57172000	1.12832000	-0.58825600
C	-1.01410300	4.56665400	-0.83639400	C	-0.05553600	-2.11704300	-0.12022900
H	0.26329800	5.26984700	-2.39507200	C	-1.51390600	-2.10989300	-0.15178800
C	-2.50677100	2.47221400	1.88406300	C	-2.24034800	-1.94619700	1.03704400
H	-1.63904000	0.58854000	2.56533100	C	-2.21987500	-2.09928600	-1.39035100
H	-3.05780200	4.33669100	0.97395100	C	-3.61454600	-1.74648800	1.02224200
H	-1.70082900	5.40588500	-0.88649200	H	-1.70146800	-1.93754200	1.97940700
H	-3.34343900	2.43728200	2.57270600	C	-3.62767900	-1.94642700	-1.39761800
N	-0.52348800	1.41753400	1.06105300	H	-1.76369900	-2.56564400	-2.25650900
C	0.78288100	-1.54664700	-1.17150300	C	-4.31025400	-1.72546400	-0.20493900
C	-1.14565500	-0.27859800	-2.25852500	H	-4.17578100	-1.60486700	1.93970900
C	0.21962600	-0.87251300	-2.41568500	H	-4.15530300	-2.00471300	-2.34143000
H	-1.71073800	-0.07077900	-3.16247200	C	0.86297000	2.30856900	-0.76669900
H	-1.31982000	0.40205300	-1.43275900	C	-0.28896100	2.42036600	0.07582000
H	0.21114600	-1.62012200	-3.22279700	C	1.10739100	3.34567800	-1.66578900
H	0.92229800	-0.10472500	-2.76030100	C	-1.17659300	3.52794400	-0.00340800
H	0.45788400	-2.55670300	0.65258400	C	0.22821000	4.44941500	-1.73465500
C	1.45956500	-0.49914300	3.26945100	H	1.97612500	3.28920300	-2.30437600
O	2.16726600	0.34331400	2.62820400	C	-1.55759700	1.40783000	1.75419800
O	0.53188500	-1.12132700	2.65766300	C	-2.29978200	3.51499500	0.86186600
C	1.68486400	-0.71963100	4.74101800	C	-0.89161400	4.55697500	-0.93557400
H	1.01717900	-0.05383600	5.30026000	H	0.45156000	5.23754900	-2.44820500
H	1.44404500	-1.74853200	5.01593600	C	-2.49060500	2.46352400	1.73186700
H	2.71388100	-0.48079100	5.01480900	H	-1.65752000	0.56702700	2.42957400
Co	1.01898900	0.04284200	0.91804900	H	-3.00345300	4.34199200	0.82825700
O	-5.62090200	-1.59312600	-0.16774500	H	-1.55635800	5.41208100	-1.00671700
C	-6.38437500	-1.56293400	-1.36636700	H	-3.34296700	2.43238500	2.40117000
H	-6.32728100	-2.51651300	-1.90623700	N	-0.50415000	1.39040700	0.95029400
H	-7.41762600	-1.38620100	-1.06254500	C	0.75866400	-1.57936500	-1.07861400
H	-6.05974100	-0.75250700	-2.03108900	C	-1.14454700	-0.32596100	-2.22881200
				C	0.21553300	-0.94023600	-2.35062100
				H	-1.69883400	-0.14662300	-3.14551700
TS5_T'				H	-1.31910600	0.38666800	-1.43122700
C	4.15863600	-3.18836400	-0.59917300	H	0.20822100	-1.71430800	-3.13246000
C	2.78251500	-2.99892100	-0.70083900	H	0.93036900	-0.19089100	-2.71049400
C	2.23933100	-1.72786900	-0.95600200	H	0.40856000	-2.55634700	0.75872900
C	3.12565600	-0.63296900	-1.10784800	C	1.47812400	-0.24948100	3.17815000
C	4.50630700	-0.84367900	-1.03772500	O	2.23773400	0.50470800	2.50917500
C	5.02615400	-2.10833600	-0.77495000	O	0.50002700	-0.82702200	2.56871800
H	4.55282300	-4.18062800	-0.40078600	C	1.67281300	-0.48633300	4.64871100
H	2.10865600	-3.84487500	-0.60751800	H	0.77300000	-0.17728800	5.19004800
H	5.16139200	0.00941500	-1.17882800				

H	1.81374500	-1.55629500	4.83127100	C	-3.08858300	1.05670300	1.77402200
H	2.53571500	0.06812400	5.01879800	H	-1.83138700	-0.70406300	2.09105500
Co	0.93697200	0.05491400	0.86728200	H	-4.01195700	2.93857400	1.31183200
O	-5.65281600	-1.52260800	-0.10872000	H	-2.75950200	4.80140500	0.05692500
C	-6.40850000	-1.49016400	-1.31225500	H	-3.95686400	0.62845200	2.26194500
H	-6.36811400	-2.45060300	-1.84134500	N	-0.82391200	0.76195700	1.07513700
H	-7.43958700	-1.28887100	-1.01645300	C	1.15862600	-1.16274500	-1.39432100
H	-6.06320300	-0.69392200	-1.98363500	C	-0.97335500	-0.17246700	-2.34787700
				C	0.52548400	-0.40403800	-2.54330800
9_OSS				H	-1.41088900	0.23875700	-3.26345000
C	4.80536300	-2.11753600	-0.99655400	H	-1.12706700	0.56632400	-1.55931900
C	3.42409800	-2.20143600	-1.15329800	H	0.69276000	-1.00618100	-3.44999500
C	2.62455500	-1.04494200	-1.17745500	H	1.03431600	0.54523500	-2.71830800
C	3.25455700	0.21699600	-1.02266400	H	0.87369200	-2.68331900	0.07476500
C	4.64483000	0.28719300	-0.89992500	C	1.39673800	-0.84841700	3.11678600
C	5.42089000	-0.86925400	-0.87913300	O	1.95433000	0.22308400	2.75268600
H	5.40214200	-3.02472000	-0.98540300	O	0.66514500	-1.48275900	2.26772400
H	2.95010900	-3.16842200	-1.29089100	C	1.53763700	-1.38848300	4.51271300
H	5.10150600	1.26659800	-0.80417500	H	0.59008100	-1.25251100	5.04548000
H	6.49872000	-0.79865100	-0.76980400	H	1.74653700	-2.46126500	4.47972200
C	2.47890700	1.51137300	-0.95656400	H	2.32939800	-0.86634100	5.05118400
O	2.90431300	2.51908400	-1.53408500	Co	0.93777800	-0.11238200	0.86799500
N	1.33727700	1.41755500	-0.21934000	O	-5.16117300	-1.75261400	-0.41375800
C	0.39782700	-2.07493600	-0.68956400	C	-5.89704900	-0.79235600	-1.15671000
C	-1.01408000	-2.19794300	-0.83539200	H	-5.93030700	-1.04526700	-2.22421600
C	-1.77013100	-2.91510400	0.10062400	H	-6.91140100	-0.80531500	-0.75371700
C	-1.71298500	-1.47127800	-1.96385000	H	-5.47041800	0.21239700	-1.03975500
C	-3.14888000	-2.80713300	0.15575200				
H	-1.24891800	-3.50567000	0.84940600	9_Q			
C	-3.17667700	-1.23372600	-1.70618100	C	4.77436300	-2.12468100	-1.00315100
H	-1.63422800	-2.13642900	-2.84858600	C	3.39500200	-2.18898100	-1.17781400
C	-3.83687400	-1.89032400	-0.71588700	C	2.60748600	-1.02432400	-1.19518700
H	-3.73007900	-3.33382000	0.90461500	C	3.24432700	0.22934900	-1.01397500
H	-3.68586200	-0.54800700	-2.37316500	C	4.63501900	0.27893400	-0.87510300
C	0.36493600	2.40818600	-0.16953000	C	5.39985400	-0.88452800	-0.86020700
C	-0.82593200	2.01365000	0.52405400	H	5.36089300	-3.03858000	-0.99685000
C	0.38740600	3.67894100	-0.74091900	H	2.91087800	-3.14834100	-1.33317900
C	-1.96873800	2.85559700	0.59648800	H	5.10235700	1.25117300	-0.76059800
C	-0.74029900	4.52462200	-0.63993200	H	6.47675300	-0.82512500	-0.73545100
H	1.27564100	4.00017800	-1.26448800	C	2.50572000	1.54765200	-0.92498900
C	-1.90586000	0.29525900	1.67932400	O	2.97547000	2.53893300	-1.49665300
C	-3.11534500	2.32869300	1.24478700	N	1.36959100	1.49698700	-0.16929100
C	-1.89981900	4.14091300	0.00226900	C	0.38339500	-2.02255700	-0.67331600
H	-0.68400100	5.50936500	-1.09517100	C	-1.03839600	-2.14952200	-0.81324800

C	-1.80113600	-2.84143600	0.12916100	H	-7.02572400	-1.18171600	-1.17612500
C	-1.71422500	-1.45245200	-1.97152800	H	-5.67459900	-0.04433400	-1.44005300
C	-3.18752500	-2.78636400	0.12447900				
H	-1.28913800	-3.36827700	0.92815800	9_T			
C	-3.19983400	-1.29849700	-1.80593800	C	4.60852400	-2.43248300	-0.92880100
H	-1.54596400	-2.09456700	-2.86086700	C	3.22347800	-2.40811600	-1.06274100
C	-3.87756100	-1.96060400	-0.82908400	C	2.51667400	-1.19348600	-1.12103300
H	-3.77699200	-3.30347600	0.87342200	C	3.24555300	0.01965300	-1.02847900
H	-3.71055200	-0.68048800	-2.53513400	C	4.63991600	-0.02220400	-0.93044800
C	0.47234700	2.55538400	-0.06752800	C	5.32262600	-1.23413800	-0.87064200
C	-0.73863300	2.26618800	0.65950900	H	5.13010600	-3.38408500	-0.88905100
C	0.59497200	3.83191000	-0.61492500	H	2.67141400	-3.33820500	-1.15572100
C	-1.77850400	3.23190200	0.78399000	H	5.17613000	0.91959600	-0.88426000
C	-0.43381600	4.78920500	-0.46903600	H	6.40434100	-1.24453800	-0.77829400
H	1.49543500	4.07351500	-1.15946900	C	2.60614800	1.39112400	-0.99428000
C	-1.98214300	0.67350000	1.84193100	O	3.13383400	2.31901500	-1.61909500
C	-2.95093500	2.83703400	1.47474800	N	1.48446000	1.45654100	-0.21926300
C	-1.60198200	4.51482000	0.20745400	C	0.24358600	-2.08575400	-0.58067000
H	-0.28892400	5.76965400	-0.91384400	C	-1.17363400	-2.17536700	-0.74611600
C	-3.05993200	1.56542600	1.99541000	C	-1.96863100	-2.84157200	0.19059700
H	-2.00643500	-0.33620800	2.23679700	C	-1.81684000	-1.46522400	-1.91601400
H	-3.76280200	3.55122200	1.58199400	C	-3.35106900	-2.74775100	0.16865200
H	-2.38887700	5.25617000	0.30485000	H	-1.48133800	-3.37838000	0.99854600
H	-3.95207500	1.24209400	2.51963600	C	-3.29956400	-1.26892100	-1.76875500
N	-0.87309300	1.01832300	1.20375200	H	-1.65836500	-2.11474000	-2.80161100
C	1.14493500	-1.14028400	-1.41292200	C	-4.00683700	-1.90814000	-0.79830400
C	-1.00492900	-0.11876800	-2.29091400	H	-3.96432600	-3.24385800	0.91268400
C	0.49318300	-0.33292800	-2.51692600	H	-3.78433900	-0.64080900	-2.50702100
H	-1.45552800	0.33482900	-3.17969800	C	0.66363400	2.57727500	-0.14875600
H	-1.16007100	0.57462300	-1.45983400	C	-0.55805800	2.39601600	0.59419100
H	0.64788700	-0.88999300	-3.45395000	C	0.87426600	3.82425100	-0.73485200
H	0.99918800	0.62392600	-2.65335900	C	-1.52079100	3.44010400	0.70382900
H	0.86736600	-2.64103100	0.07892300	C	-0.07999000	4.85844500	-0.60732100
C	1.26147500	-1.51770600	2.88341300	H	1.78464700	3.98305300	-1.29338600
O	2.08325100	-0.69416800	2.33827500	C	-1.89858000	0.93352900	1.83603200
O	0.11516900	-1.67064900	2.38094200	C	-2.70856700	3.15376900	1.42138300
C	1.69649700	-2.26837300	4.11459900	C	-1.25654200	4.68995500	0.08899900
H	1.86890800	-1.55708300	4.92899100	H	0.13102900	5.81272400	-1.08156800
H	0.94029700	-2.99327100	4.41813000	C	-2.90300200	1.90895800	1.98051800
H	2.64617800	-2.77585000	3.92109500	H	-1.99105800	-0.05987900	2.26152400
Co	0.81715300	-0.10153300	0.89679600	H	-3.46311500	3.92940200	1.51970900
O	-5.22660200	-1.91408900	-0.62650500	H	-1.98485400	5.49039400	0.17332100
C	-5.98739000	-1.09480000	-1.50125800	H	-3.80737500	1.66885100	2.52808900
H	-5.90519600	-1.43184600	-2.54263200	N	-0.77782400	1.17512000	1.17134600



C 1.04318900 -1.22314800 -1.30676100  
 C -1.06438000 -0.15502100 -2.23120200  
 C 0.42747400 -0.42269900 -2.43905400  
 H -1.48886000 0.30945300 -3.12721400  
 H -1.20481500 0.54621500 -1.40327700  
 H 0.56857700 -1.01387400 -3.35716100  
 H 0.96534500 0.51186800 -2.59997400  
 H 0.69452500 -2.70293900 0.19156900  
 C 1.11055400 -1.48368600 2.91860500  
 O 2.00041500 -0.73137700 2.37358800  
 O -0.03325300 -1.56887300 2.40068000  
 C 1.47708600 -2.24008400 4.16946100  
 H 1.74290300 -1.53019300 4.95922900  
 H 0.64988900 -2.86756100 4.50336700  
 H 2.36024100 -2.85777700 3.97942100  
 Co 0.83921500 -0.06466800 0.88569300  
 O -5.35657900 -1.82597000 -0.61329500  
 C -6.08550000 -0.99564500 -1.50464500  
 H -5.99746800 -1.34323600 -2.54208700  
 H -7.12985800 -1.05472600 -1.19289600  
 H -5.74831700 0.04745600 -1.44760800

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C 4.85769400 -2.08719400 -0.87473700  
 C 3.48198100 -2.19957200 -1.06343700  
 C 2.66507200 -1.05786800 -1.13183100  
 C 3.26854500 0.21890800 -0.99384500  
 C 4.65361700 0.31639800 -0.84096300  
 C 5.44862600 -0.82601000 -0.77296800  
 H 5.46923500 -2.98322100 -0.82509500  
 H 3.02756900 -3.17797300 -1.18606800  
 H 5.09059700 1.30570800 -0.75585300  
 H 6.52184800 -0.73389800 -0.63738400  
 C 2.46823700 1.50030800 -0.96496700  
 O 2.89981900 2.51202800 -1.53172100  
 N 1.30172300 1.39396400 -0.26940400  
 C 0.43729400 -2.09816400 -0.64901900  
 C -0.97485800 -2.21831500 -0.79609800  
 C -1.73628000 -2.91463000 0.15302500  
 C -1.66821700 -1.51472700 -1.94161900  
 C -3.11389500 -2.80232800 0.19898300  
 H -1.21924000 -3.48846400 0.91729200  
 C -3.13415100 -1.27721400 -1.70236000  
 H -1.58093800 -2.19766500 -2.81190900

C -3.79969800 -1.91138000 -0.70156400  
 H -3.69929600 -3.31101100 0.95704200  
 H -3.64033400 -0.61201500 -2.39195500  
 C 0.33060500 2.38457000 -0.22426200  
 C -0.85362900 2.00739100 0.49224500  
 C 0.34918700 3.64359700 -0.82247300  
 C -1.99304600 2.85547300 0.55741400  
 C -0.77590700 4.49291900 -0.73079800  
 H 1.23367300 3.95193000 -1.35989000  
 C -1.92553100 0.32430200 1.70404000  
 C -3.13339400 2.34982600 1.23315100  
 C -1.92946800 4.12577000 -0.06851100  
 H -0.72296100 5.46623200 -1.21047100  
 C -3.10409600 1.09277200 1.79633300  
 H -1.85167600 -0.66613700 2.13789400  
 H -4.02707700 2.96468200 1.29432500  
 H -2.78807600 4.78825100 -0.02106200  
 H -3.96759700 0.68144400 2.30690800  
 N -0.85001500 0.76907300 1.07332400  
 C 1.20320300 -1.19610400 -1.36688000  
 C -0.92707400 -0.22351100 -2.34570900  
 C 0.57160100 -0.46544200 -2.53552500  
 H -1.36127500 0.17172100 -3.26979900  
 H -1.08006100 0.52886400 -1.57070400  
 H 0.73493900 -1.09524500 -3.42402700  
 H 1.08422500 0.47586600 -2.73782400  
 H 0.91020200 -2.69928100 0.12245600  
 C 1.34696100 -0.75572500 3.09679000  
 O 1.84915400 0.33200900 2.70035700  
 O 0.68989700 -1.47623300 2.25489800  
 C 1.45984300 -1.21134900 4.52502500  
 H 0.49996100 -1.04521600 5.02701200  
 H 1.67369300 -2.28259200 4.56424200  
 H 2.23503200 -0.65048100 5.04881300  
 Co 0.90239600 -0.13599700 0.81934800  
 O -5.12721200 -1.77552100 -0.41588400  
 C -5.86445500 -0.84761100 -1.19814000  
 H -5.88154200 -1.13558300 -2.25711000  
 H -6.88338200 -0.85902400 -0.80706700  
 H -5.45005000 0.16496700 -1.10860200

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C -0.19098500 -4.42880500 -0.09201000  
 C -1.20542400 -3.47607400 -0.07576200

C	-1.02453500	-2.17531700	-0.58755300	H	-1.03502000	0.32188900	0.47428600
C	0.25792200	-1.85540600	-1.10204000	H	-3.60414600	-2.70952300	-0.93686600
C	1.26913400	-2.82553600	-1.12644200	C	1.22985200	-1.04204000	2.81899600
C	1.05565500	-4.11049600	-0.62903200	O	2.46461400	-1.24674700	2.54856900
H	-0.37397100	-5.41618500	0.32168600	O	0.50183900	-0.55037400	1.90087100
H	-2.15856500	-3.72603900	0.37758800	C	0.66201300	-1.40635300	4.15862300
H	2.22295800	-2.58379000	-1.58158700	H	-0.17752600	-0.75376000	4.40617500
H	1.85256800	-4.84674200	-0.66182500	H	0.29142500	-2.43673300	4.11270000
C	0.55327300	-0.49610600	-1.68164000	H	1.43225100	-1.35270400	4.93051600
O	-0.07500300	-0.06386800	-2.64656400	Co	2.19309500	-0.55403300	0.71971900
N	1.57256400	0.15581000	-1.00963800	C	4.56625200	-1.17670400	-1.00383100
C	-3.43351800	-1.66157200	-0.70031500	O	4.03623700	-1.26110500	0.11062700
C	-4.58241100	-0.83430700	-0.58893500	O	3.94864500	-0.67844100	-2.05556300
C	-5.88109400	-1.35740600	-0.64642200	H	3.02934800	-0.38788100	-1.76355100
C	-4.38297300	0.65008800	-0.37741000	C	5.96823700	-1.63293300	-1.26391600
C	-6.99209600	-0.58663300	-0.35160400	H	5.98221800	-2.32119200	-2.11376400
H	-6.01028700	-2.41166100	-0.88158000	H	6.58329300	-0.76787000	-1.53291500
C	-5.60912700	1.36701400	0.11781800	H	6.37743500	-2.11553200	-0.37731200
H	-4.13321900	1.07697000	-1.37043200	O	-8.01193000	1.36520300	0.44997300
C	-6.83316900	0.77801200	0.08192800	C	-7.95214700	2.70759700	0.90342700
H	-7.99447600	-0.99961500	-0.37657100	H	-7.55897300	3.37854400	0.12829200
H	-5.48055200	2.39528000	0.43590800	H	-8.97737600	2.99656200	1.14304300
C	1.79687500	1.53745400	-1.17711600	H	-7.33027300	2.80154800	1.80337000
C	2.52572700	2.15892000	-0.11085600				
C	1.41098600	2.33030000	-2.25135900	10s_Q			
C	2.85484400	3.54399300	-0.15165300	C	-0.12679300	-4.53656100	-0.36964900
C	1.73328200	3.70704000	-2.28090800	C	-1.13468700	-3.58070200	-0.28333300
H	0.85489600	1.88175100	-3.06053900	C	-0.95074700	-2.25766600	-0.72901300
C	3.54653400	1.89401300	1.96538200	C	0.31938400	-1.91924000	-1.25861000
C	3.57706800	4.07025500	0.94887500	C	1.32478800	-2.88894800	-1.34844000
C	2.44142600	4.31413400	-1.26775700	C	1.11239500	-4.19513100	-0.90982200
H	1.41210500	4.29159800	-3.13803200	H	-0.30774600	-5.54377200	-0.00591300
C	3.92350800	3.25270300	2.00173000	H	-2.08151500	-3.84644000	0.17459600
H	3.78664300	1.21496900	2.77804200	H	2.27348100	-2.62769900	-1.80450000
H	3.84670100	5.12261800	0.94903400	H	1.90410300	-4.93340000	-0.99263600
H	2.68665400	5.37097700	-1.30565400	C	0.58707800	-0.54529300	-1.81945100
H	4.47306700	3.63272600	2.85574400	O	-0.05463100	-0.13257400	-2.78354300
N	2.87773000	1.37339600	0.95011100	N	1.56801300	0.14710900	-1.12810900
C	-2.14510800	-1.21650400	-0.52230500	C	-3.35171600	-1.69228900	-0.78894700
C	-3.12814200	0.87821300	0.48791400	C	-4.48228000	-0.84791900	-0.62131400
C	-1.90480700	0.24078900	-0.18035500	C	-5.79229000	-1.33545900	-0.70673700
H	-2.95775000	1.95179700	0.62713200	C	-4.24545400	0.61577400	-0.32243500
H	-3.29180500	0.44064900	1.48010800	C	-6.88504100	-0.55598400	-0.36747500
H	-1.67079600	0.79845300	-1.09486900	H	-5.94659300	-2.37106200	-1.00185100

C	-5.45524400	1.33443200	0.20923500	H	6.14560900	-2.43045100	0.34386600
H	-3.97652200	1.09348800	-1.28680700	O	-7.85773700	1.37259800	0.54101000
C	-6.69324300	0.77792500	0.14092900	C	-7.76608600	2.68594500	1.06793400
H	-7.89704400	-0.94263100	-0.41475300	H	-7.35638200	3.38902700	0.33077600
H	-5.30266600	2.34007600	0.58404200	H	-8.78426200	2.98575200	1.32373000
C	1.80477900	1.51274900	-1.39366800	H	-7.14295600	2.71521800	1.97145500
C	2.41396500	2.25567000	-0.32634400				
C	1.53974700	2.18828600	-2.57929200	10s_T			
C	2.74541100	3.63327700	-0.48553800	C	-0.11752900	-4.53935900	-0.36864800
C	1.86381000	3.55652200	-2.72711600	C	-1.12526600	-3.58360700	-0.28234800
H	1.06925500	1.65373100	-3.39025800	C	-0.94208900	-2.26083700	-0.72989700
C	3.21441600	2.24952600	1.87076300	C	0.32792500	-1.92300000	-1.26068400
C	3.34610500	4.29009200	0.61625500	C	1.33318500	-2.89306200	-1.35081800
C	2.45725300	4.27608400	-1.71543700	C	1.12118200	-4.19865400	-0.91077800
H	1.63732400	4.04033800	-3.67258000	H	-0.29799700	-5.54608100	-0.00331200
C	3.58303700	3.60567000	1.78837200	H	-2.07136900	-3.84905400	0.17719100
H	3.36005800	1.66471300	2.77299200	H	2.28166900	-2.63198600	-1.80749700
H	3.61193300	5.33928200	0.52208500	H	1.91277000	-4.93705800	-0.99350700
H	2.70707400	5.32522000	-1.83856300	C	0.59543300	-0.55033800	-1.82530800
H	4.03931400	4.08954300	2.64446900	O	-0.04026900	-0.14342200	-2.79577400
N	2.65562400	1.60751200	0.85434700	N	1.56956900	0.14684700	-1.12965500
C	-2.05529600	-1.28878300	-0.58461000	C	-3.34403600	-1.69845200	-0.78401000
C	-2.99257700	0.75812200	0.56429500	C	-4.47450200	-0.85408600	-0.61847200
C	-1.77765200	0.13038900	-0.12851400	C	-5.78454400	-1.34349500	-0.69647000
H	-2.79683700	1.81640500	0.77152400	C	-4.23849100	0.61194700	-0.33054500
H	-3.17695800	0.26396700	1.52566300	C	-6.87669800	-0.56298900	-0.35851300
H	-1.50158400	0.74927100	-0.99123100	H	-5.93879400	-2.38113000	-0.98436600
H	-0.92368500	0.12856800	0.55318600	C	-5.44704700	1.33267200	0.20117800
H	-3.54346600	-2.71794600	-1.09668600	H	-3.97444100	1.08337000	-1.29935300
C	1.26809000	-0.90816900	3.10669600	C	-6.68460100	0.77444700	0.14078800
O	2.47063700	-0.54707400	3.05005100	H	-7.88848200	-0.95090200	-0.39982900
O	0.57487800	-0.97466300	2.02162500	H	-5.29417100	2.34081600	0.56908900
C	0.60326000	-1.28543600	4.40418300	C	1.80419800	1.51253600	-1.39636700
H	-0.34748900	-0.75378100	4.50301600	C	2.40603500	2.25854100	-0.32703500
H	0.37700600	-2.35687100	4.39146300	C	1.54305000	2.18559500	-2.58423500
H	1.24991600	-1.06234200	5.25364800	C	2.73439900	3.63682700	-0.48647800
Co	2.04437800	-0.36043300	0.81899600	C	1.86405000	3.55453400	-2.73231500
C	4.47220000	-1.43457800	-0.52819600	H	1.07802000	1.64848600	-3.39668300
O	3.82432700	-1.42487500	0.52818200	C	3.19544600	2.25751000	1.87401200
O	4.04370100	-0.88583500	-1.64597500	C	3.32763300	4.29684300	0.61746200
H	3.11115300	-0.51536800	-1.50430000	C	2.45051200	4.27710600	-1.71870600
C	5.81231200	-2.09245100	-0.63633500	H	1.64085800	4.03646300	-3.67952600
H	5.73767400	-2.94596500	-1.31817100	C	3.56055400	3.61462800	1.79166000
H	6.53519100	-1.39324300	-1.06592900	H	3.33835100	1.67423500	2.77766900

H	3.59094900	5.34666200	0.52324000	H	1.85123900	-4.84156400	-0.65392500
H	2.69798000	5.32677600	-1.84204400	C	0.55142500	-0.49304300	-1.68050000
H	4.01110200	4.10091400	2.64942400	O	-0.07857300	-0.05745700	-2.64281000
N	2.64355000	1.61255600	0.85569000	N	1.57423600	0.15544700	-1.01029900
C	-2.04684300	-1.29238300	-0.58749600	C	-3.43789100	-1.65902800	-0.70429000
C	-2.98216200	0.76200900	0.54978300	C	-4.58657000	-0.83183300	-0.59169800
C	-1.76950900	0.13071500	-0.14372000	C	-5.88542500	-1.35453400	-0.65117800
H	-2.78665400	1.82193800	0.74864200	C	-4.38698300	0.65205200	-0.37660800
H	-3.16173100	0.27442700	1.51540100	C	-6.99633500	-0.58428600	-0.35503300
H	-1.49813100	0.74343400	-1.01230800	H	-6.01469300	-2.40818400	-0.88898900
H	-0.91279100	0.13566900	0.53436900	C	-5.61324900	1.36798600	0.11982700
H	-3.53618500	-2.72629500	-1.08397700	H	-4.13678300	1.08122400	-1.36852400
C	1.25682200	-0.90312200	3.10743700	C	-6.83734900	0.77930500	0.08195500
O	2.45845600	-0.53882400	3.05345400	H	-7.99879700	-0.99698200	-0.38147000
O	0.56638600	-0.97270600	2.02075400	H	-5.48461700	2.39543300	0.44052700
C	0.58966900	-1.28090500	4.40360900	C	1.80061600	1.53689700	-1.17683400
H	-0.36265000	-0.75154300	4.49960700	C	2.53021800	2.15662600	-0.11017500
H	0.36612800	-2.35291300	4.39128500	C	1.41625000	2.33100700	-2.25068600
H	1.23362900	-1.05542800	5.25449500	C	2.86178700	3.54112600	-0.15003600
Co	2.03634700	-0.35693500	0.82006500	C	1.74091800	3.70722200	-2.27939900
C	4.47053300	-1.43337800	-0.51484800	H	0.85944100	1.88398000	-3.06020300
O	3.81727800	-1.42219900	0.53814600	C	3.55002500	1.88855600	1.96619300
O	4.04835000	-0.88489000	-1.63518500	C	3.58479000	4.06535700	0.95093700
H	3.11532600	-0.51415300	-1.49834100	C	2.44992400	4.31258000	-1.26580300
C	5.81054800	-2.09259900	-0.61581200	H	1.42092100	4.29279200	-3.13627400
H	5.73804100	-2.94739300	-1.29629300	C	3.92954000	3.24650900	2.00336100
H	6.53591000	-1.39488800	-1.04365700	H	3.78855700	1.20852000	2.77847600
H	6.13927300	-2.42905800	0.36646200	H	3.85640600	5.11720900	0.95180200
O	-7.84836100	1.37023700	0.54123400	H	2.69700400	5.36901000	-1.30313200
C	-7.75630400	2.68688900	1.05982400	H	4.47965200	3.62501200	2.85769100
H	-7.35000900	3.38592200	0.31695000	N	2.88051200	1.36986900	0.95039000
H	-8.77388500	2.98713100	1.31745200	C	-2.14943000	-1.21445500	-0.52482100
H	-7.12994200	2.72230900	1.96088400	C	-3.13254000	0.87800600	0.48981200
				C	-1.90896600	0.24186900	-0.17929600
10s_T'				H	-2.96204700	1.95124100	0.63156500
C	-0.19477200	-4.42566400	-0.09139400	H	-3.29679300	0.43822600	1.48093200
C	-1.21017800	-3.47392400	-0.07906300	H	-1.67402100	0.80159900	-1.09233000
C	-1.02883100	-2.17299600	-0.59039200	H	-1.03942600	0.32104100	0.47606100
C	0.25458800	-1.85233200	-1.10206100	H	-3.60853400	-2.70647900	-0.94307700
C	1.26693100	-2.82142100	-1.12220100	C	1.23122000	-1.04298300	2.81883200
C	1.05336600	-4.10623000	-0.62424000	O	2.46586200	-1.24841900	2.54771500
H	-0.37811500	-5.41298900	0.32225700	O	0.50266000	-0.55149200	1.90125300
H	-2.16439300	-3.72449900	0.37168400	C	0.66464400	-1.40652000	4.15927300
H	2.22157900	-2.57952200	-1.57541700	H	-0.17520500	-0.75435900	4.40688900

H	0.29487000	-2.43724700	4.11461200	C	1.85054400	1.97533300	-2.53320600
H	1.43541700	-1.35159800	4.93055100	C	3.28258600	3.38536200	-0.56311700
Co	2.19478200	-0.55622600	0.71880700	C	2.26905600	3.30808700	-2.75378200
C	4.56784100	-1.17808400	-1.00678200	H	1.30635800	1.45092700	-3.30574500
O	4.03905600	-1.26343400	0.10814900	C	3.81216300	2.01495300	1.78175000
O	3.94865600	-0.68009100	-2.05774800	C	4.00890500	4.02008500	0.47577600
H	3.02953200	-0.38976500	-1.76474500	C	2.96823900	4.00785100	-1.79644300
C	5.96999700	-1.63289100	-1.26865100	H	2.03264400	3.77733400	-3.70368700
H	5.98362800	-2.32097400	-2.11865200	C	4.27435100	3.34157300	1.64341600
H	6.58388700	-0.76719000	-1.53824300	H	3.99853500	1.44461500	2.68724800
H	6.38074400	-2.11527400	-0.38264400	H	4.34947100	5.04198600	0.33496300
O	-8.01618000	1.36572900	0.45098100	H	3.28906100	5.03022100	-1.97142300
C	-7.95632300	2.70683100	0.90823900	H	4.82791300	3.80324800	2.45335200
H	-7.56263700	3.37987900	0.13518900	N	3.13391600	1.39562300	0.83251100
H	-8.98160000	2.99534600	1.14818900	C	-2.32692700	-1.12058100	-0.38890600
H	-7.33484200	2.79809800	1.80872900	C	-3.44058300	0.73277000	0.91214100
				C	-2.13083800	0.20885300	0.31091700
TS6s_OSS				H	-3.28847900	1.74231800	1.31065600
C	-0.55231800	-4.44191900	-0.14901800	H	-3.76415200	0.09719900	1.74565200
C	-1.51009700	-3.43353600	-0.10653400	H	-1.75075800	0.94588100	-0.40561600
C	-1.22726400	-2.10717100	-0.48877000	H	-1.36184800	0.10937300	1.08081000
C	0.10027700	-1.81839700	-0.90452900	H	-3.71210900	-2.44368200	-1.31032400
C	1.05377000	-2.84717700	-0.95438200	C	1.31063400	-0.63304100	2.93457200
C	0.73978800	-4.15169500	-0.58372400	O	2.50381100	-1.05338600	2.76704500
H	-0.81571900	-5.44890800	0.16099000	O	0.71124300	-0.16295200	1.90989000
H	-2.50597900	-3.65988000	0.25886700	C	0.62449600	-0.70944100	4.26470600
H	2.04393800	-2.63887700	-1.33814600	H	0.04279700	0.19901000	4.43927000
H	1.49627800	-4.92797700	-0.63972500	H	-0.07290500	-1.55455800	4.25295300
C	0.47275300	-0.45052300	-1.39059300	H	1.34921300	-0.85995600	5.06617100
O	-0.31091300	0.23930700	-2.02400600	Co	2.36465000	-0.54549600	0.84324300
N	1.78224100	-0.02340100	-1.04192500	C	4.45249200	-1.55845300	-0.89584400
C	-3.57583400	-1.47353500	-0.83680900	O	4.05488800	-1.39459200	0.29040400
C	-4.72517100	-0.64495100	-0.71729200	O	3.76804100	-1.23434200	-1.93020000
C	-6.00326000	-1.09320900	-1.07119700	H	2.72234500	-0.69356800	-1.54417300
C	-4.54633000	0.75063600	-0.16262500	C	5.80959600	-2.16499700	-1.13392200
C	-7.14070900	-0.35714400	-0.78414200	H	5.72733400	-2.98018200	-1.85799300
H	-6.10408100	-2.06891600	-1.54156200	H	6.46691200	-1.40550500	-1.57047100
C	-5.82778900	1.39879600	0.28486700	H	6.24215000	-2.52788100	-0.20157600
H	-4.13763000	1.36716200	-0.98921100	O	-8.25333900	1.42602700	0.25132000
C	-7.03751500	0.88000600	-0.05432000	C	-8.25187700	2.64281500	0.97968500
H	-8.13109200	-0.71566200	-1.04200500	H	-7.73887500	3.44226900	0.42903200
H	-5.74065800	2.33307800	0.82767000	H	-9.29908600	2.91768500	1.12039500
C	2.12125300	1.33861500	-1.33598000	H	-7.77427900	2.52440400	1.96118900
C	2.85464100	2.04356900	-0.33683700				

TS6s_Q			H	-2.80726600	1.67161600	1.02288300	
C	-0.21481000	-4.59231400	-0.48614300	H	-3.25893000	0.05596700	1.57890100
C	-1.19652600	-3.60965400	-0.40284200	H	-1.43593200	0.77182200	-0.77581300
C	-0.95303900	-2.27501500	-0.77888300	H	-0.94843100	-0.02232500	0.72118100
C	0.35170100	-1.95587900	-1.23538800	H	-3.51996700	-2.62291900	-1.35287000
C	1.33512200	-2.95026900	-1.31323500	C	1.14898400	-0.75886600	3.18149100
C	1.06010300	-4.26569300	-0.94642000	O	2.24997500	-0.15926700	3.23121200
H	-0.44388500	-5.60879300	-0.17978000	O	0.62396400	-1.03653100	2.03414900
H	-2.17198100	-3.86355400	-0.00206300	C	0.41037000	-1.19002100	4.42107700
H	2.31748100	-2.70095400	-1.69675100	H	-0.63559300	-0.87637400	4.35906000
H	1.83340400	-5.02380700	-1.02218400	H	0.41936100	-2.28362700	4.47971300
C	0.66378900	-0.57677600	-1.73527700	H	0.87634600	-0.77670300	5.31635300
O	-0.07132300	-0.00189000	-2.52500100	Co	2.08211200	-0.25953500	0.93417500
N	1.82511400	0.00192200	-1.18211000	C	4.42925700	-1.54115300	-0.21769400
C	-3.32891400	-1.63670400	-0.93507000	O	3.81060500	-1.30612500	0.85743900
C	-4.45195500	-0.78599600	-0.74729500	O	4.02333400	-1.17391900	-1.37854200
C	-5.76298500	-1.22917600	-0.96063500	H	2.92039200	-0.64687600	-1.31093000
C	-4.20666400	0.63139000	-0.27956800	C	5.70640000	-2.33479700	-0.15957000
C	-6.85985100	-0.46234000	-0.60574500	H	5.45542600	-3.39676100	-0.26633400
H	-5.91811400	-2.22391100	-1.37267100	H	6.37062800	-2.05913800	-0.98036200
C	-5.43321900	1.32047900	0.25257600	H	6.19927800	-2.19553000	0.80355400
H	-3.86930200	1.20160900	-1.16925400	O	-7.85062700	1.38487700	0.44120900
C	-6.67497900	0.80586900	0.05146000	C	-7.76787800	2.63399700	1.10749600
H	-7.87407400	-0.81634700	-0.75373000	H	-7.29998200	3.39911400	0.47404300
H	-5.28514700	2.27750600	0.73967400	H	-8.79434400	2.93091000	1.33137100
C	2.09633800	1.36192600	-1.52633800	H	-7.20214300	2.55407600	2.04503000
C	2.44851800	2.24438300	-0.46300200				
C	2.08034700	1.85399100	-2.81827000	TS6s_T			
C	2.76639700	3.60890600	-0.73263600	C	-0.21318900	-4.59217800	-0.48589400
C	2.39211700	3.20663000	-3.08507300	C	-1.19454600	-3.60931400	-0.40262300
H	1.81606500	1.19333800	-3.63296500	C	-0.95109400	-2.27476800	-0.77957500
C	2.79428100	2.54885800	1.82804800	C	0.35376700	-1.95617000	-1.23642600
C	3.10398900	4.43069200	0.37054700	C	1.33682100	-2.95104500	-1.31449700
C	2.72796300	4.07417300	-2.07049900	C	1.06161800	-4.26618800	-0.94715900
H	2.36525400	3.55650700	-4.11213200	H	-0.44233700	-5.60840000	-0.17872800
C	3.11734900	3.90751300	1.64441100	H	-2.16972600	-3.86289500	-0.00101300
H	2.79134100	2.08326300	2.80783800	H	2.31912800	-2.70202800	-1.69834700
H	3.34968200	5.47418800	0.19485500	H	1.83463400	-5.02457800	-1.02303800
H	2.96721700	5.11282000	-2.27636400	C	0.66666800	-0.57766300	-1.73769700
H	3.37240700	4.51602900	2.50442300	O	-0.06648500	-0.00397300	-2.53006500
N	2.47368000	1.75449100	0.81647100	N	1.82664300	0.00165200	-1.18245000
C	-2.04001500	-1.28628000	-0.61797700	C	-3.32765200	-1.63848400	-0.93262000
C	-3.00783200	0.64676700	0.68982500	C	-4.45066300	-0.78780300	-0.74589000
C	-1.76522500	0.07106300	0.00035400	C	-5.76191500	-1.23268200	-0.95509700

C	-4.20556300	0.63155500	-0.28410100	C	5.70185400	-2.34036100	-0.14997800
C	-6.85849200	-0.46538300	-0.60073600	H	5.44901100	-3.40204200	-0.25513700
H	-5.91714800	-2.22900200	-1.36323600	H	6.36810900	-2.06742800	-0.97001700
C	-5.43147600	1.32159200	0.24830600	H	6.19325800	-2.20037500	0.81381600
H	-3.87102000	1.19868300	-1.17682300	O	-7.84854400	1.38483300	0.44157700
C	-6.67323700	0.80536100	0.05157100	C	-7.76548400	2.63669800	1.10267100
H	-7.87277100	-0.82061400	-0.74538500	H	-7.29946300	3.39959900	0.46518000
H	-5.28310000	2.28048400	0.73162200	H	-8.79174500	2.93368200	1.32738300
C	2.09874700	1.36143800	-1.52678200	H	-7.19783000	2.56103100	2.03939600
C	2.44949500	2.24408100	-0.46313000				
C	2.08499000	1.85303700	-2.81891100	TS6s_T'			
C	2.76830000	3.60839600	-0.73271400	C	-0.47304700	-4.41437300	-0.07140600
C	2.39764900	3.20549000	-3.08563600	C	-1.44530000	-3.41926200	-0.04930200
H	1.82179200	1.19219400	-3.63379100	C	-1.18659200	-2.10137400	-0.47615400
C	2.79153700	2.54923600	1.82836900	C	0.13098400	-1.80850200	-0.91721000
C	3.10432700	4.43046700	0.37073700	C	1.09977000	-2.82346700	-0.94684700
C	2.73217400	4.07322900	-2.07079900	C	0.80939900	-4.12018700	-0.53176700
H	2.37255400	3.55505300	-4.11284600	H	-0.71761300	-5.41443400	0.27429900
C	3.11537100	3.90772100	1.64479300	H	-2.43295500	-3.64830300	0.33621700
H	2.78682200	2.08397500	2.80830800	H	2.07970500	-2.61346800	-1.35471600
H	3.35066300	5.47381800	0.19508700	H	1.57628600	-4.88709400	-0.57281700
H	2.97208700	5.11173400	-2.27660900	C	0.48829000	-0.44737500	-1.43152300
H	3.36921900	4.51643700	2.50502100	O	-0.29267800	0.21806400	-2.09285400
N	2.47233700	1.75460300	0.81655600	N	1.78650400	0.00034900	-1.06519900
C	-2.03805600	-1.28611300	-0.61974200	C	-3.54834600	-1.50722600	-0.80456500
C	-3.00432200	0.65170500	0.68214000	C	-4.70472300	-0.68714100	-0.69579900
C	-1.76308900	0.07428000	-0.00838600	C	-5.98344000	-1.16149000	-1.01155400
H	-2.80365100	1.67802000	1.01058100	C	-4.53225700	0.72980800	-0.19602400
H	-3.25255900	0.06421800	1.57420500	C	-7.12397900	-0.42693600	-0.73325000
H	-1.43684300	0.77190000	-0.78864400	H	-6.08117500	-2.15505100	-1.44364600
H	-0.94425000	-0.01483800	0.71063900	C	-5.81326800	1.38090000	0.24843600
H	-3.51916300	-2.62635000	-1.34623300	H	-4.14406600	1.31949500	-1.05159500
C	1.14297700	-0.75504100	3.18207200	C	-7.02255600	0.83761900	-0.05167600
O	2.24478700	-0.15701500	3.23203100	H	-8.11444800	-0.80489300	-0.96129200
O	0.61810100	-1.03264000	2.03467300	H	-5.72747200	2.33545200	0.75500600
C	0.40331000	-1.18470800	4.42156700	C	2.10111300	1.37506000	-1.32262300
H	-0.64293600	-0.87240600	4.35784500	C	2.80718300	2.06868500	-0.29555000
H	0.41358200	-2.27820500	4.48220300	C	1.82915300	2.03710300	-2.50570300
H	0.86788000	-0.76936100	5.31664100	C	3.20920800	3.42440100	-0.48241100
Co	2.07817500	-0.25903100	0.93466300	C	2.22115300	3.38404500	-2.68604200
C	4.42630100	-1.54437900	-0.21164500	H	1.30472900	1.52136300	-3.29738000
O	3.80453500	-1.30946200	0.86172300	C	3.73987400	2.00583000	1.83294400
O	4.02484100	-1.17512900	-1.37336700	C	3.91052800	4.04720600	0.58070900
H	2.92158200	-0.64720900	-1.30842700	C	2.89525700	4.07229800	-1.70285800

H	1.98508100	3.87349100	-3.62579300	H	0.96981400	5.55521200	-0.04761500
C	4.17667300	3.34460600	1.73376700	H	2.64533300	3.74911000	0.06479100
H	3.92683400	1.41702800	2.72650900	H	-2.02961700	2.70269300	-1.11811300
H	4.23152800	5.07906000	0.46956300	H	-1.40335500	5.00962400	-0.61629500
H	3.19676900	5.10527000	-1.84742700	C	-0.45310900	0.49135000	-1.18351700
H	4.71134800	3.79661600	2.56166600	O	0.33555800	-0.34253900	-1.58575000
N	3.08529300	1.39697600	0.86071400	N	-1.84755700	0.16444700	-1.03042500
C	-2.29609700	-1.12467600	-0.39146200	C	3.58874300	1.41876400	-0.93836500
C	-3.40886400	0.76322500	0.85985100	C	4.72959900	0.57953300	-0.80109600
C	-2.10332000	0.23148500	0.25630800	C	5.97356700	0.92075000	-1.34301500
H	-3.26146300	1.78825800	1.21855800	C	4.57715100	-0.70528800	-0.01802800
H	-3.71129400	0.15531000	1.72143300	C	7.11797700	0.19299300	-1.06003300
H	-1.74323100	0.94634200	-0.49228600	H	6.04702200	1.80942000	-1.96610000
H	-1.32180600	0.16687900	1.01737100	C	5.88240400	-1.33255800	0.38750000
H	-3.68164100	-2.49527200	-1.24038000	H	4.06078000	-1.42282900	-0.68775700
C	1.30542400	-0.66513900	2.89548100	C	7.06218300	-0.91762700	-0.14545400
O	2.48395500	-1.12091700	2.71600100	H	8.08417600	0.47075800	-1.46645800
O	0.71925600	-0.15157600	1.88508400	H	5.83062900	-2.17278800	1.07042700
C	0.62056300	-0.75215200	4.22614500	C	-2.24439000	-1.14259100	-1.49877500
H	0.04826500	0.15922600	4.41511200	C	-2.90324000	-1.99735800	-0.57652300
H	-0.08457100	-1.59071700	4.20391200	C	-2.04387100	-1.56443500	-2.79449000
H	1.34494800	-0.92224800	5.02411600	C	-3.34374000	-3.28862000	-0.99172100
Co	2.36428300	-0.56512300	0.80280800	C	-2.47792700	-2.84512900	-3.20808600
C	4.45262800	-1.53816700	-0.94788400	H	-1.54234100	-0.91071900	-3.49824400
O	4.03887900	-1.41481900	0.23880400	C	-3.72245100	-2.31872700	1.57105200
O	3.78466800	-1.17211700	-1.97801100	C	-4.00034100	-4.09236400	-0.02560300
H	2.73415400	-0.64366200	-1.58435900	C	-3.11235500	-3.69484100	-2.32958600
C	5.80676800	-2.14987900	-1.18761800	H	-2.30447200	-3.15299300	-4.23405400
H	5.72124200	-2.95480600	-1.92294000	C	-4.18867200	-3.61295200	1.25029300
H	6.47141600	-1.38988900	-1.61162900	H	-3.85723600	-1.90347700	2.56565800
H	6.23191500	-2.52949900	-0.25861300	H	-4.34954200	-5.08136200	-0.30818300
O	-8.23919300	1.38231300	0.25293000	H	-3.44560800	-4.67805800	-2.64769100
C	-8.23943000	2.62548000	0.93534900	H	-4.68810100	-4.20417700	2.00953200
H	-7.74405100	3.40907700	0.34703900	N	-3.10778900	-1.54507000	0.69536700
H	-9.28721800	2.89457400	1.08275300	C	2.38792500	1.17812900	-0.32124200
H	-7.74504400	2.54891300	1.91268500	C	3.60096100	-0.47200900	1.15360300
				C	2.24359900	-0.00006600	0.61954900
11s_OSS				H	3.47303500	-1.39798500	1.72568000
C	0.67429700	4.53192400	-0.25995000	H	4.03182900	0.27504700	1.83148500
C	1.62243300	3.51483500	-0.20991900	H	1.75720600	-0.82936200	0.09531400
C	1.29603900	2.16947400	-0.46417500	H	1.56809800	0.26128700	1.43798400
C	-0.05721400	1.87304900	-0.78710900	H	3.68994800	2.29808900	-1.57160600
C	-1.00559200	2.91005500	-0.83163900	C	-1.29955600	0.20449500	3.00186000
C	-0.65079600	4.22907500	-0.56948200	O	-2.48159500	0.67656000	2.95944900



O	-0.75965600	-0.12885000	1.89154700	H	5.64354100	-2.12236500	1.19023500
C	-0.54771400	0.06535300	4.29204500	C	-2.37447600	-1.05842300	-1.65155800
H	0.02797900	-0.86331000	4.29395000	C	-2.87196200	-2.03670800	-0.75253200
H	0.16044300	0.89732200	4.37816000	C	-2.35895500	-1.32911500	-3.00289700
H	-1.23005300	0.09532900	5.14286000	C	-3.33957500	-3.28980700	-1.24817400
Co	-2.43338000	0.42094400	0.95320200	C	-2.82818200	-2.56625500	-3.49977500
C	-4.51805900	1.76816100	-0.56871700	H	-1.97169800	-0.58270100	-3.68739400
O	-4.07514100	1.34243700	0.56011900	C	-3.33811700	-2.66110300	1.44932100
O	-3.90588300	1.69521200	-1.66206000	C	-3.81313500	-4.23165100	-0.30177000
H	-2.54784200	0.87908100	-1.39680200	C	-3.30740600	-3.53226700	-2.64392900
C	-5.88823100	2.41144100	-0.51929200	H	-2.80350000	-2.74913300	-4.56894700
H	-6.19632600	2.74415900	-1.51106500	C	-3.80839300	-3.92415700	1.04065200
H	-6.61565500	1.69521500	-0.12490100	H	-3.31772500	-2.36876600	2.49427500
H	-5.86818100	3.26294700	0.16817500	H	-4.17548800	-5.19415000	-0.65104500
O	8.28933500	-1.46116200	0.11524300	H	-3.66451400	-4.48558900	-3.02093700
C	8.33434200	-2.55857100	1.01252700	H	-4.16244400	-4.62783400	1.78492500
H	7.74864800	-3.40904400	0.63948300	N	-2.89351300	-1.75560800	0.58755600
H	9.38368200	-2.85020500	1.08829800	C	2.30305600	1.18174000	-0.53205500
H	7.96369700	-2.28083300	2.00796100	C	3.42653700	-0.41028200	1.07068300
				C	2.10101000	0.04594600	0.45004000
11s_Q				H	3.26247800	-1.30290200	1.68563200
C	0.67689800	4.57550700	-0.71355200	H	3.83479500	0.36851200	1.72642700
C	1.60163300	3.54248800	-0.59626400	H	1.64021900	-0.80300700	-0.06741100
C	1.24051000	2.19065800	-0.74732000	H	1.38900400	0.35396100	1.22000300
C	-0.12287900	1.90483800	-1.03320700	H	3.67398400	2.20974700	-1.78885200
C	-1.04781900	2.95552800	-1.13852000	C	-1.07175300	0.26315800	3.19437200
C	-0.65919900	4.28211800	-0.98038700	O	-2.19421400	-0.27822900	3.35579200
H	0.99895400	5.60442800	-0.58192200	O	-0.72122900	0.68181700	2.02062100
H	2.63115800	3.77294500	-0.34427900	C	-0.09700600	0.44376200	4.32685500
H	-2.08592400	2.75096800	-1.37090900	H	0.83186800	-0.08734300	4.09494500
H	-1.39484200	5.07501700	-1.07126900	H	0.15296400	1.50452300	4.42574000
C	-0.54869400	0.51058800	-1.34718800	H	-0.51209800	0.07076700	5.26358900
O	0.21939800	-0.34105600	-1.76776100	Co	-2.40950700	0.13887100	1.13809200
N	-1.90829200	0.18672000	-1.10921300	C	-4.44330300	1.95375500	0.09042400
C	3.53048300	1.36599100	-1.11672800	O	-3.91180700	1.35821500	1.10860200
C	4.64995500	0.51791400	-0.89120400	O	-4.06980800	1.82201000	-1.09354500
C	5.91842900	0.80991900	-1.40572400	H	-2.64045900	0.93260000	-1.18930600
C	4.45106200	-0.71741100	-0.04090500	C	-5.59921900	2.87262800	0.42298900
C	7.04129700	0.08828900	-1.03545800	H	-6.04953100	3.27534500	-0.48494100
H	6.02743900	1.65799400	-2.07825100	H	-6.34920300	2.33133900	1.00712800
C	5.73201300	-1.32881200	0.45701200	H	-5.23558000	3.69505300	1.04820300
H	3.95787500	-1.46968200	-0.68994700	O	8.14598200	-1.49794600	0.28912800
C	6.93633900	-0.96079500	-0.05461100	C	8.14283000	-2.53293400	1.25849500
H	8.02578500	0.32936100	-1.42092400	H	7.56211100	-3.40118500	0.92015200

H	9.18487300	-2.82860800	1.39527400	C	-2.30305600	-1.18174000	-0.53205500
H	7.73682900	-2.18571800	2.21768000	C	-3.42653700	0.41028200	1.07068300
				C	-2.10101000	-0.04594600	0.45004000
11s_T				H	-3.26247800	1.30290200	1.68563200
C	-0.67689800	-4.57550700	-0.71355200	H	-3.83479500	-0.36851200	1.72642700
C	-1.60163300	-3.54248800	-0.59626400	H	-1.64021900	0.80300700	-0.06741100
C	-1.24051000	-2.19065800	-0.74732000	H	-1.38900400	-0.35396100	1.22000300
C	0.12287900	-1.90483800	-1.03320700	H	-3.67398400	-2.20974700	-1.78885200
C	1.04781900	-2.95552800	-1.13852000	C	1.07175300	-0.26315800	3.19437200
C	0.65919900	-4.28211800	-0.98038700	O	2.19421400	0.27822900	3.35579200
H	-0.99895400	-5.60442800	-0.58192200	O	0.72122900	-0.68181700	2.02062100
H	-2.63115800	-3.77294500	-0.34427900	C	0.09700600	-0.44376200	4.32685500
H	2.08592400	-2.75096800	-1.37090900	H	-0.83186800	0.08734300	4.09494500
H	1.39484200	-5.07501700	-1.07126900	H	-0.15296400	-1.50452300	4.42574000
C	0.54869400	-0.51058800	-1.34718800	H	0.51209800	-0.07076700	5.26358900
O	-0.21939800	0.34105600	-1.76776100	Co	2.40950700	-0.13887100	1.13809200
N	1.90829200	-0.18672000	-1.10921300	C	4.44330300	-1.95375500	0.09042400
C	-3.53048300	-1.36599100	-1.11672800	O	3.91180700	-1.35821500	1.10860200
C	-4.64995500	-0.51791400	-0.89120400	O	4.06980800	-1.82201000	-1.09354500
C	-5.91842900	-0.80991900	-1.40572400	H	2.64045900	-0.93260000	-1.18930600
C	-4.45106200	0.71741100	-0.04090500	C	5.59921900	-2.87262800	0.42298900
C	-7.04129700	-0.08828900	-1.03545800	H	6.04953100	-3.27534500	-0.48494100
H	-6.02743900	-1.65799400	-2.07825100	H	6.34920300	-2.33133900	1.00712800
C	-5.73201300	1.32881200	0.45701200	H	5.23558000	-3.69505300	1.04820300
H	-3.95787500	1.46968200	-0.68994700	O	-8.14598200	1.49794600	0.28912800
C	-6.93633900	0.96079500	-0.05461100	C	-8.14283000	2.53293400	1.25849500
H	-8.02578500	-0.32936100	-1.42092400	H	-7.56211100	3.40118500	0.92015200
H	-5.64354100	2.12236500	1.19023500	H	-9.18487300	2.82860800	1.39527400
C	2.37447600	1.05842300	-1.65155800	H	-7.73682900	2.18571800	2.21768000
C	2.87196200	2.03670800	-0.75253200				
C	2.35895500	1.32911500	-3.00289700	11s_T'			
C	3.33957500	3.28980700	-1.24817400	C	0.66423200	4.49988600	-0.34033900
C	2.82818200	2.56625500	-3.49977500	C	1.61633000	3.48727600	-0.27283200
H	1.97169800	0.58270100	-3.68739400	C	1.29481100	2.13676600	-0.50390300
C	3.33811700	2.66110300	1.44932100	C	-0.05678200	1.82961600	-0.82272300
C	3.81313500	4.23165100	-0.30177000	C	-1.00903800	2.86197200	-0.88561700
C	3.30740600	3.53226700	-2.64392900	C	-0.65934700	4.18666200	-0.64537200
H	2.80350000	2.74913300	-4.56894700	H	0.95581200	5.52782200	-0.14577100
C	3.80839300	3.92415700	1.04065200	H	2.63854800	3.72998100	-0.00284100
H	3.31772500	2.36876600	2.49427500	H	-2.03125000	2.64656000	-1.17186400
H	4.17548800	5.19415000	-0.65104500	H	-1.41489600	4.96333400	-0.70618900
H	3.66451400	4.48558900	-3.02093700	C	-0.44904000	0.43884800	-1.19065400
H	4.16244400	4.62783400	1.78492500	O	0.34213200	-0.40286000	-1.57100400
N	2.89351300	1.75560800	0.58755600	N	-1.84341200	0.11657700	-1.03290300

C	3.58753400	1.38030400	-0.97033200	O	-4.06717600	1.35469500	0.51665800
C	4.73117700	0.54721800	-0.81747600	O	-3.89310500	1.62164000	-1.71691200
C	5.97217400	0.87840500	-1.37182500	H	-2.54641400	0.81988100	-1.42330600
C	4.58445400	-0.71883700	-0.00335200	C	-5.88047200	2.37560600	-0.60744100
C	7.11943900	0.16001500	-1.07618600	H	-6.17715200	2.68653500	-1.60971600
H	6.04122800	1.75226400	-2.01601000	H	-6.61048900	1.66389400	-0.20933700
C	5.89265600	-1.33395000	0.41126200	H	-5.87329300	3.24037200	0.06330600
H	4.06618300	-1.45297300	-0.65330800	O	8.29877700	-1.46390000	0.13267800
C	7.06949700	-0.92907300	-0.13584200	C	8.34968800	-2.53981900	1.05528400
H	8.08345300	0.43030900	-1.49270700	H	7.76442700	-3.40006700	0.70465200
H	5.84537200	-2.15822400	1.11367700	H	9.39996700	-2.82732700	1.13374000
C	-2.24337800	-1.20422200	-1.45497100	H	7.98228000	-2.23962600	2.04538700
C	-2.93861400	-2.00692100	-0.51242100				
C	-2.01922700	-1.68553500	-2.72589600				
C	-3.39192700	-3.30761400	-0.88188600	10_OSS			
C	-2.46410100	-2.97673900	-3.09286200	C	-0.47413000	2.93427800	3.64193200
H	-1.49190500	-1.07102700	-3.44572500	C	0.46259600	2.09301900	3.04630400
C	-3.81573900	-2.21864400	1.62470700	C	0.10616000	1.20245700	2.02153200
C	-4.08687000	-4.05666100	0.10111500	C	-1.24701500	1.18827200	1.60793900
C	-3.13446700	-3.77637800	-2.19430500	C	-2.18819900	2.02495600	2.22138500
H	-2.27115000	-3.33261300	-4.09965400	C	-1.80851600	2.89790800	3.23715000
C	-4.29849100	-3.51734600	1.34903500	H	-0.16185000	3.61030000	4.43218800
H	-3.96849600	-1.75977800	2.59738400	H	1.48928900	2.09766800	3.39632900
H	-4.44645500	-5.05128800	-0.14632000	H	-3.21278100	2.02853700	1.86240400
H	-3.47671400	-4.76719900	-2.47732600	H	-2.54366400	3.55057800	3.69659200
H	-4.82765700	-4.06511800	2.12064900	C	-1.66975400	0.40332000	0.42131000
N	-3.16438100	-1.49509700	0.73294700	O	-0.98169700	0.31477100	-0.62128500
C	2.39032900	1.15194600	-0.34237500	N	-2.86936800	-0.20774100	0.51095100
C	3.61347300	-0.45915700	1.16712100	C	2.40272500	0.72915700	1.22228400
C	2.25268800	-0.00189600	0.62901300	C	3.47000200	-0.12592500	0.83753600
H	3.49000800	-1.37132300	1.76188700	C	4.77317800	0.35542700	0.66539300
H	4.04653300	0.30462400	1.82467500	C	3.17202700	-1.58808300	0.60342300
H	1.76245300	-0.84432700	0.12999100	C	5.84007200	-0.49993300	0.44964300
H	1.58268900	0.28120500	1.44481600	H	4.95045200	1.42526200	0.74194300
H	3.68363700	2.24424800	-1.62520700	C	4.39412800	-2.46119000	0.57002600
C	-1.24580500	0.34777300	2.96005400	H	2.70313000	-1.64310300	-0.39741600
O	-2.40211200	0.88332700	2.89759500	C	5.63952200	-1.92604100	0.45077100
O	-0.76294000	-0.12212100	1.87496500	H	6.85153000	-0.12772100	0.33073300
C	-0.46572600	0.30099300	4.23893800	H	4.23249700	-3.53293600	0.56034700
H	0.15775300	-0.59494500	4.27068900	C	-3.57612800	-0.93046800	-0.45961700
H	0.19395700	1.17547400	4.27908000	C	-4.81177500	-1.48546000	0.01110900
H	-1.13600600	0.33484900	5.09964600	C	-3.18599000	-1.12567900	-1.77221500
Co	-2.41936700	0.45563400	0.93692500	C	-5.62733600	-2.23717400	-0.88382800
C	-4.50772100	1.73546700	-0.62682300	C	-4.01168900	-1.87335100	-2.64478400

H	-2.25592300	-0.70813800	-2.12843400	C	0.01612100	1.31683600	2.00585200
C	-6.28652400	-1.76732900	1.75545000	C	-1.32312900	1.28295200	1.55190600
C	-6.83659300	-2.76113900	-0.36167200	C	-2.27249100	2.17283100	2.07072900
C	-5.20192800	-2.42128600	-2.22458500	C	-1.91304400	3.11569000	3.02999500
H	-3.68362400	-2.01014800	-3.67031900	H	-0.29522600	3.90257100	4.21749400
C	-7.16802900	-2.52909300	0.95352300	H	1.37143600	2.30230100	3.34447800
H	-6.53095200	-1.57181000	2.79758700	H	-3.28583200	2.16015900	1.68051100
H	-7.48746900	-3.34086200	-1.01010700	H	-2.65383600	3.80847100	3.41583900
H	-5.82520900	-2.99461900	-2.90408500	C	-1.71162900	0.41660400	0.40915700
H	-8.08615900	-2.91666400	1.38165800	O	-0.97718300	0.25131200	-0.58938300
N	-5.15163000	-1.26179000	1.30966200	N	-2.92178400	-0.17376800	0.49858700
C	1.12445000	0.28282700	1.47047300	C	2.30015600	0.79249100	1.20973900
C	2.07549600	-2.05678500	1.58031400	C	3.37536600	-0.08503000	0.88380400
C	0.81439100	-1.20373000	1.38589800	C	4.66806500	0.39094100	0.65028600
H	1.84032900	-3.11174500	1.40247400	C	3.08646000	-1.56343800	0.78483300
H	2.44205600	-1.96890100	2.61007500	C	5.74146000	-0.47133500	0.49006700
H	0.37604100	-1.44373200	0.41066900	H	4.83603500	1.46460300	0.63078200
H	0.06133300	-1.45959900	2.13947600	C	4.31570100	-2.42653100	0.79449500
H	2.62044400	1.78907900	1.32665600	H	2.59524800	-1.70374500	-0.19714700
C	-0.54388000	3.31798800	-1.65326100	C	5.55450500	-1.89302200	0.60984900
O	-0.50795800	2.52192600	-2.62200000	H	6.74673300	-0.10115900	0.32284500
O	0.00572700	2.99983500	-0.53109200	H	4.16398600	-3.49680600	0.87402200
C	-1.21470000	4.66702300	-1.74793500	C	-3.59742000	-0.96845200	-0.43732600
H	-1.91686800	4.79111100	-0.91800200	C	-4.87419600	-1.44193700	0.01214200
H	-0.45924000	5.45464500	-1.65746300	C	-3.13940700	-1.30656900	-1.69775300
H	-1.73745100	4.77483600	-2.69929300	C	-5.66084100	-2.25912900	-0.85061500
Co	0.67033500	1.26891300	-1.11726400	C	-3.93707000	-2.11724300	-2.53961200
C	2.61802300	0.53054000	-2.18901000	H	-2.17642500	-0.95386400	-2.03599000
O	2.49396600	1.74194900	-1.82733700	C	-6.45172700	-1.51155700	1.68647200
O	1.63606000	-0.25791000	-1.94168700	C	-6.91300900	-2.69782100	-0.35131100
C	3.85365900	0.02110600	-2.86835300	C	-5.16634400	-2.58819100	-2.13900600
H	4.28481700	-0.79434300	-2.28023500	H	-3.55535000	-2.36643800	-3.52462100
H	3.58892400	-0.38099700	-3.85142800	C	-7.31016800	-2.32709700	0.91286500
H	4.58890600	0.81833000	-2.98145600	H	-6.74770900	-1.20747000	2.68846000
H	-3.35071800	-0.19949100	1.40793800	H	-7.54412100	-3.32295200	-0.97668500
O	6.80265000	-2.63257900	0.33862500	H	-5.76804200	-3.21066200	-2.79426900
C	6.70379100	-4.04830000	0.33148600	H	-8.26234300	-2.64676700	1.32228900
H	6.09748500	-4.40516500	-0.51126400	N	-5.27880000	-1.08144700	1.26042600
H	7.72269200	-4.42582800	0.22765000	C	1.04332300	0.35465000	1.55231700
H	6.27172000	-4.42628400	1.26711500	C	2.02210500	-1.95861400	1.82849800
				C	0.74656700	-1.13378900	1.60798100
10_Q				H	1.79269100	-3.02631800	1.74372900
C	-0.59131000	3.17044100	3.47232900	H	2.41786000	-1.78578200	2.83647000
C	0.35344500	2.27845500	2.97007000	H	0.27357300	-1.45778700	0.67315700

H	0.02337700	-1.32888100	2.40769600	C	5.78323300	-0.55946600	0.50856500
H	2.50579600	1.86077600	1.21419600	H	4.89707700	1.36820300	0.79772700
C	-0.27074200	3.34360800	-1.74841900	C	4.32725000	-2.51442200	0.59548300
O	-0.20604000	2.45645800	-2.65260400	H	2.65142500	-1.67988400	-0.38488300
O	0.19065200	3.09289500	-0.58359700	C	5.57688300	-1.98397100	0.49656700
C	-0.88310900	4.69284600	-2.02601200	H	6.79736800	-0.19026800	0.40442300
H	-1.65921800	4.90287000	-1.28389500	H	4.16111200	-3.58533100	0.57510300
H	-0.11422800	5.46540600	-1.92223100	C	-3.62388300	-0.92053100	-0.49202400
H	-1.30617400	4.73385100	-3.03050300	C	-4.88050400	-1.45117400	-0.04977300
Co	0.75633400	1.20256200	-1.23466600	C	-3.20570700	-1.12803500	-1.79384700
C	2.74244200	0.22262200	-2.26471400	C	-5.68915300	-2.18841500	-0.96274000
O	2.73081200	1.47065500	-2.06359200	C	-4.02442700	-1.86155700	-2.68488200
O	1.71392200	-0.47422900	-1.93854900	H	-2.25777800	-0.73241000	-2.12710400
C	3.93676000	-0.46950200	-2.86513300	C	-6.39977400	-1.70345500	1.66045300
H	4.30373300	-1.23004400	-2.16964100	C	-6.92028000	-2.68798000	-0.46848400
H	3.63804800	-0.98074200	-3.78578800	C	-5.23564000	-2.38366600	-2.29270300
H	4.73389400	0.24248300	-3.08042700	H	-3.67399300	-2.00847400	-3.70156900
H	-3.44751300	-0.07372500	1.36480300	C	-7.27745700	-2.44814300	0.83852000
O	6.72133300	-2.59849000	0.53314900	H	-6.66396100	-1.50298000	2.69679100
C	6.63318600	-4.01129600	0.63240700	H	-7.56722100	-3.25560800	-1.13136100
H	6.01424300	-4.43306700	-0.17026900	H	-5.85395700	-2.94562500	-2.98607900
H	7.65286900	-4.38906900	0.53746100	H	-8.21278300	-2.81709700	1.24531500
H	6.22144700	-4.32216800	1.60136200	N	-5.24545800	-1.22019300	1.24063400

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C	-0.53105000	2.85617900	3.70498700	C	1.06279100	0.23574900	1.49445300
C	0.40335400	2.02100900	3.09726200	C	2.00035100	-2.10876400	1.58355500
C	0.04631700	1.15355300	2.05304400	C	0.74550400	-1.24707200	1.38654500
C	-1.30492200	1.15566300	1.63244600	H	1.76150700	-3.16053300	1.39243400
C	-2.24356100	1.98657300	2.25749100	H	2.35661500	-2.03375300	2.61796300
C	-1.86329500	2.83651600	3.29255400	H	0.31646200	-1.47039500	0.40296800
H	-0.21863800	3.51440200	4.51005100	H	-0.01748800	-1.50892100	2.12788900
H	1.42837300	2.01173500	3.45210100	H	2.56388400	1.73854900	1.36605300
H	-3.26674900	2.00384000	1.89480300	C	-0.29562200	3.49517200	-1.56662600
H	-2.59669200	3.48467300	3.76108300	O	-0.20359700	2.66293500	-2.51906500
C	-1.72315800	0.39736600	0.42506200	O	0.12269300	3.17326600	-0.40277100
O	-1.02035900	0.33793900	-0.60754000	C	-0.87018600	4.87020900	-1.79478900
N	-2.92493500	-0.21204900	0.49471800	H	-1.51372500	5.15310600	-0.95786700
C	2.34095400	0.68066600	1.24670000	H	-0.04830200	5.59341800	-1.84078800
C	3.41053500	-0.17739500	0.86663500	H	-1.42680600	4.91022700	-2.73237800
C	4.71639000	0.29960500	0.71452300	Co	0.72067100	1.32886100	-1.14598900
C	3.10887900	-1.63643900	0.62177200	C	2.73628600	0.45079500	-2.21274100
				O	2.70764400	1.67606200	-1.90090700
				O	1.71270700	-0.28335900	-1.96557300
				C	3.94696800	-0.16968900	-2.85793100
				H	4.31889900	-0.98442100	-2.22963700

H	3.66514500	-0.60051900	-3.82391300	C	-7.18973800	-2.40259700	1.01935400
H	4.73592300	0.56931200	-3.00009000	H	-6.62756200	-1.24738100	2.77204700
H	-3.42167400	-0.20481800	1.38340700	H	-7.42914300	-3.42584600	-0.85488200
O	6.73786400	-2.69536800	0.39393900	H	-5.68539500	-3.29238600	-2.70178800
C	6.63193900	-4.11033800	0.36899700	H	-8.12754700	-2.73986800	1.44743100
H	6.03522000	-4.45405500	-0.48596300	N	-5.18388100	-1.10450100	1.32004600
H	7.65022500	-4.49192000	0.27437200	C	1.08571500	0.41918500	1.57500200
H	6.18549200	-4.49707400	1.29427800	C	2.08097200	-1.88108200	1.89732100

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C	-0.56725400	3.29170200	3.39456500
C	0.38211600	2.38216900	2.93352400
C	0.05536000	1.39377300	1.99336700
C	-1.27606000	1.35051000	1.51944100
C	-2.23067200	2.25765300	1.99755100
C	-1.88239600	3.22734000	2.93387700
H	-0.28032900	4.04505000	4.12199600
H	1.39533800	2.41464600	3.32035500
H	-3.23851500	2.23428200	1.59390300
H	-2.62682200	3.93276500	3.28858500
C	-1.65454000	0.44456800	0.40554500
O	-0.92328300	0.23677100	-0.58889400
N	-2.86270500	-0.14794500	0.50959000
C	2.33085200	0.85224800	1.19413500
C	3.40183000	-0.03108000	0.86540100
C	4.68492400	0.44146700	0.58245800
C	3.11438400	-1.51250400	0.81345400
C	5.75662500	-0.42249200	0.41079200
H	4.84906400	1.51484600	0.53277800
C	4.34647100	-2.37205300	0.81026900
H	2.59515000	-1.68236300	-0.14910600
C	5.57754400	-1.84055500	0.57358300
H	6.75546500	-0.05431700	0.20498300
H	4.20086400	-3.44015600	0.92340900
C	-3.53177300	-0.97237400	-0.40507200
C	-4.78961000	-1.47086900	0.07014000
C	-3.08674200	-1.31203200	-1.66997200
C	-5.57004500	-2.31655500	-0.77065700
C	-3.87838000	-2.15096000	-2.48949500
H	-2.13996700	-0.93722600	-2.02958600
C	-6.33952600	-1.55708200	1.76944500
C	-6.80336600	-2.77888700	-0.24654700
C	-5.08854500	-2.64820300	-2.06325300
H	-3.50742000	-2.40034400	-3.47857100

H	-6.62756200	-1.24738100	2.77204700
H	-7.42914300	-3.42584600	-0.85488200
H	-5.68539500	-3.29238600	-2.70178800
H	-8.12754700	-2.73986800	1.44743100
N	-5.18388100	-1.10450100	1.32004600
C	1.08571500	0.41918500	1.57500200
C	2.08097200	-1.88108200	1.89732100
C	0.79646000	-1.06697700	1.68903100
H	1.85411700	-2.95166900	1.85016900
H	2.50427300	-1.67733100	2.88815300
H	0.29585200	-1.42311700	0.78035600
H	0.09882500	-1.23772600	2.51665800
H	2.52983000	1.92063800	1.15619700
C	-0.49140300	3.14404800	-1.87427100
O	-0.50393600	2.26576000	-2.77007600
O	0.10882600	2.92019800	-0.75566500
C	-1.16228700	4.48414500	-2.05438400
H	-1.82283500	4.68386200	-1.20523400
H	-0.40151100	5.27170500	-2.06917800
H	-1.73021300	4.51239700	-2.98531700
Co	0.72665800	1.13355600	-1.21337000
C	2.63656300	0.25777700	-2.24546200
O	2.53619900	1.50297400	-2.01392200
O	1.64608100	-0.48251400	-1.90168000
C	3.85200000	-0.34230100	-2.88514400
H	4.25050400	-1.13202500	-2.24199800
H	3.57131700	-0.79903300	-3.83980600
H	4.61628400	0.41728700	-3.05153700
H	-3.38454000	-0.03626600	1.37658800
O	6.74381600	-2.54525500	0.48035600
C	6.66414700	-3.95473500	0.62415400
H	6.02309200	-4.40232500	-0.14657000
H	7.68199500	-4.33209700	0.50981000
H	6.28277700	-4.23785300	1.61380200

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C	0.48266000	4.35807600	-1.82590800
C	-0.41197700	3.32118900	-1.57742300
C	0.00669300	2.09460100	-1.03437900
C	1.38726100	1.95075000	-0.74755700
C	2.28613200	2.99507300	-1.01156400
C	1.84157400	4.19866700	-1.54867600
H	0.11910900	5.28977000	-2.24970600

H	-1.45852300	3.44101700	-1.83536100	H	-1.51917400	4.20095100	3.68192700
H	3.33302500	2.88446200	-0.74492300	H	-3.05837800	3.82518300	2.87892200
H	2.54394900	5.00435200	-1.73562700	H	-2.65103900	3.00231700	4.38968200
C	1.87798800	0.74703200	-0.03814200	Co	-0.68217100	0.54784000	1.31443600
O	1.20392900	0.15280900	0.83843000	C	-1.77647400	-2.31015300	1.55882300
N	3.11809400	0.32000500	-0.35650900	O	-0.89502500	-1.41080500	1.56877400
C	-2.31259900	1.32244400	-0.54917400	O	-2.72269700	-2.43501700	0.71567000
C	-3.38748100	0.43082000	-0.72450000	C	-1.71413100	-3.35185700	2.65632400
C	-4.70088800	0.74108700	-0.27442700	H	-2.30041600	-4.23529000	2.40024900
C	-3.16412100	-0.86095900	-1.35542800	H	-0.67519500	-3.62546500	2.85546200
C	-5.76040800	-0.08357500	-0.55046900	H	-2.12221400	-2.90879500	3.57184900
H	-4.86186600	1.66448600	0.27569300	H	3.61126200	0.78301100	-1.11710600
C	-4.33227500	-1.61955700	-1.76561700	H	-2.85601300	-1.59803600	-0.26278800
C	-5.58327800	-1.27474700	-1.32213900	O	-6.73597200	-1.97118800	-1.55598700
H	-6.76293200	0.15530600	-0.20977700	C	-6.62485800	-3.17141700	-2.30363400
H	-4.16842800	-2.52167100	-2.34446100	H	-7.63319900	-3.58402900	-2.37255900
C	3.87073100	-0.72582400	0.19228600	H	-6.24329600	-2.98302900	-3.31606200
C	5.17040900	-0.87906100	-0.39514700	H	-5.96997600	-3.89784000	-1.80483300
C	3.46664800	-1.57736900	1.20489800				
C	6.03568100	-1.90851900	0.07642100	TS6_Q			
C	4.34162200	-2.59244200	1.65888000	C	0.49084300	4.40197600	-2.03440000
H	2.48521500	-1.46772800	1.64178000	C	-0.44229300	3.40358000	-1.79356200
C	6.71134300	-0.15009800	-1.94164500	C	-0.06084600	2.14036000	-1.30002100
C	7.30694500	-2.01029900	-0.54266100	C	1.31230500	1.94230500	-0.98372600
C	5.59550900	-2.76436900	1.11871000	C	2.25082200	2.95717700	-1.24958000
H	4.00072600	-3.24654100	2.45530000	C	1.85125600	4.17581700	-1.78014000
C	7.64681700	-1.13553900	-1.54892000	H	0.16552200	5.35666800	-2.43751300
H	6.96060600	0.55043300	-2.73599700	H	-1.48771800	3.56877100	-2.03393800
H	7.99758800	-2.78111900	-0.21255300	H	3.29179800	2.81301600	-0.97486400
H	6.25702500	-3.54767900	1.47616000	H	2.58385300	4.95398800	-1.96800100
H	8.61151700	-1.18860700	-2.04182300	C	1.73424300	0.77769600	-0.18229500
N	5.51875600	-0.01997000	-1.39126400	O	1.01740800	0.24456300	0.71126800
C	-0.97219700	0.99554100	-0.83766300	N	2.98108600	0.30434200	-0.40968500
C	-1.91948700	-0.91277100	-2.24098800	C	-2.32098400	1.30854300	-0.62815900
C	-0.68269400	-0.35254700	-1.52416000	C	-3.36706400	0.34183500	-0.65220000
H	-1.72192900	-1.94212400	-2.56090300	C	-4.61238200	0.57705900	-0.02033400
H	-2.11178900	-0.32473200	-3.15013300	C	-3.16112500	-0.92957600	-1.33046200
H	-0.33493600	-1.08982900	-0.79570000	C	-5.65787800	-0.30788100	-0.14353700
H	0.13008600	-0.22141300	-2.24698500	H	-4.74461300	1.49230500	0.55161100
H	-2.52605700	2.29708700	-0.11953300	C	-4.32823200	-1.75563200	-1.56791500
C	-1.58217600	2.30937700	2.66355100	C	-5.52151500	-1.48381300	-0.94339700
O	-2.10702200	1.14372700	2.62511600	H	-6.61333500	-0.12344300	0.33634800
O	-0.53537900	2.52632300	1.97946700	H	-4.20095400	-2.64620000	-2.17330700
C	-2.23243000	3.40425100	3.46410700	C	3.69019200	-0.70627400	0.24644100

C	4.99139100	-0.95905900	-0.30533900	H	-5.81798900	-4.12550300	-1.41336600
C	3.25091500	-1.44319900	1.33359200				
C	5.81612500	-1.96750100	0.27310700				
C	4.08557600	-2.43848400	1.89270200				
H	2.27310700	-1.25412600	1.75001800	TS6_T			
C	6.57426800	-0.42919100	-1.89093300	C	0.45354700	4.30772200	-2.08578100
C	7.08979000	-2.16867600	-0.31628700	C	-0.44552500	3.28139500	-1.80160200
C	5.33728200	-2.70555000	1.38593800	C	-0.03225300	2.09403700	-1.18234400
H	3.71676600	-2.99917100	2.74613000	C	1.33654400	1.96780800	-0.84524200
C	7.47074300	-1.40388300	-1.39494000	C	2.23803400	2.99823900	-1.14367700
H	6.85588600	0.18613700	-2.74299100	C	1.80307100	4.16690900	-1.76370400
H	7.75069600	-2.92714200	0.09376900	H	0.09922400	5.21513500	-2.56591000
H	5.96753600	-3.47294800	1.82477300	H	-1.48934200	3.38364100	-2.07974700
H	8.43866200	-1.53492700	-1.86665000	H	3.27736100	2.90819000	-0.84166100
N	5.38058000	-0.20954200	-1.37186600	H	2.50849300	4.96343900	-1.97694300
C	-1.04618200	1.06907200	-1.16891200	C	1.81295800	0.80110500	-0.05455200
C	-2.02439300	-0.93560500	-2.35289100	O	1.13927300	0.27444800	0.85928400
C	-0.75247500	-0.30684100	-1.75767300	N	3.04631100	0.34276100	-0.36075600
H	-1.81123700	-1.96081900	-2.67556600	C	-2.30330700	1.29717700	-0.47882900
H	-2.32563800	-0.37210700	-3.24750100	C	-3.38036000	0.37382100	-0.55396400
H	-0.34161900	-0.99396300	-1.00707000	C	-4.63836500	0.65529000	0.03790300
H	0.01820000	-0.20989700	-2.52972900	C	-3.21415300	-0.88079700	-1.27508900
H	-2.54099600	2.29174300	-0.21884000	C	-5.72160600	-0.15973500	-0.17559900
C	-1.30771300	2.71086900	2.58887500	H	-4.74327700	1.54958600	0.64596200
O	-1.81201100	1.55546700	2.83852200	C	-4.42390300	-1.62302500	-1.60578900
O	-0.53193600	2.84144300	1.60425900	C	-5.62343500	-1.30689100	-1.02310600
C	-1.67019100	3.87336500	3.47504800	H	-6.68555000	0.05900200	0.27261000
H	-1.12332900	4.77120700	3.18501800	H	-4.31631600	-2.49849500	-2.23588700
H	-2.74678900	4.06017500	3.40409500	C	3.78252400	-0.69082800	0.23216300
H	-1.45231700	3.62387000	4.51780000	C	5.08002600	-0.88944500	-0.34604100
Co	-0.89978800	0.67445100	1.26749600	C	3.36203100	-1.49468300	1.27675500
C	-1.41596300	-2.38277100	1.34963100	C	5.92664500	-1.91435200	0.16755500
O	-1.21315200	-1.21648600	1.77696800	C	4.21832800	-2.50659400	1.77175500
O	-2.02597200	-2.68306700	0.27016900	H	2.38265000	-1.34877800	1.70778000
C	-0.87661700	-3.53385800	2.16440500	C	6.63562000	-0.24860300	-1.91668500
H	-1.36938400	-4.47060200	1.90195700	C	7.19724200	-2.06173600	-0.44379800
H	0.19555400	-3.62801100	1.95576100	C	5.46979000	-2.72127900	1.24131600
H	-0.99207700	-3.32316700	3.22983500	H	3.86535000	-3.12245900	2.59304400
H	3.50697700	0.68534800	-1.19339400	C	7.55378800	-1.23304700	-1.48272000
H	-2.56810900	-1.76226200	-0.36984600	H	6.89808300	0.41559600	-2.73758000
O	-6.65065500	-2.25131300	-1.01719600	H	7.87439700	-2.83038100	-0.08207300
C	-6.58108300	-3.43462600	-1.79563500	H	6.11716900	-3.50102900	1.63088700
H	-7.56241200	-3.90747900	-1.72282400	H	8.51843300	-1.32188300	-1.97056200
H	-6.36575600	-3.21345400	-2.84957800	N	5.44442400	-0.07664100	-1.37491500



C	-1.00863600	1.00042800	-0.95064900	O	1.01816300	-0.18058100	0.31238700
C	-2.07125000	-0.86862400	-2.29689200	N	3.15452400	0.20108600	-0.40204500
C	-0.77457100	-0.33458900	-1.67157400	C	-2.12362400	1.62337300	-0.40402100
H	-1.90624500	-1.87956300	-2.68434500	C	-3.28389600	0.78946300	-0.70265400
H	-2.35351500	-0.23443300	-3.14844700	C	-4.39151900	0.72363700	0.16147200
H	-0.37096500	-1.08935800	-0.98795200	C	-3.27382900	-0.02459900	-1.85669000
H	-0.02058100	-0.18992600	-2.45208800	C	-5.44490500	-0.14413100	-0.08626000
H	-2.50143600	2.28446700	-0.07135900	H	-4.40752100	1.34758600	1.05132700
C	-1.34069300	2.50911900	2.71643200	C	-4.33029700	-0.89874600	-2.10594500
O	-1.82428700	1.32658000	2.83287200	C	-5.41238100	-0.97359000	-1.21684600
O	-0.56713700	2.78561100	1.76165900	H	-6.29276400	-0.21090500	0.58710600
C	-1.72839500	3.54892000	3.74145000	H	-4.29845200	-1.52060800	-2.99307700
H	-1.24439000	4.50424700	3.53378400	C	3.80017400	-0.91757800	0.08798700
H	-2.81557600	3.67837700	3.73931300	C	5.16546800	-1.05839600	-0.35819900
H	-1.44628300	3.20194300	4.74051200	C	3.27230900	-1.87442300	0.95268600
Co	-0.88285800	0.60806100	1.17735400	C	5.94748100	-2.16693500	0.08823800
C	-1.47450200	-2.49678900	1.28572000	C	4.06503400	-2.95888600	1.37735600
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O	-2.28304700	-2.75017700	0.33787800	C	6.90338500	-0.20981600	-1.61523700
C	-0.98080500	-3.67479800	2.10315600	C	7.28063900	-2.23834000	-0.38816000
H	-1.49213900	-4.59689200	1.82464900	C	5.37289700	-3.12081400	0.96633000
H	0.09640400	-3.79194000	1.94264000	H	3.62074700	-3.68596300	2.05152700
H	-1.13233500	-3.46806400	3.16637700	C	7.76103600	-1.26486600	-1.23683100
H	3.54468000	0.76447200	-1.14162300	H	7.25904400	0.57124300	-2.28442300
H	-2.74555300	-1.70564800	-0.39083800	H	7.91060000	-3.06638900	-0.07444300
O	-6.79286100	-1.99371300	-1.17834400	H	5.96958000	-3.96285000	1.30347100
C	-6.75935600	-3.15025200	-2.00067500	H	8.77773500	-1.29701100	-1.61445200
H	-7.77083100	-3.56037700	-1.99261900	N	5.65350000	-0.10671200	-1.19539000
H	-6.47896200	-2.90258000	-3.03302300	C	-0.90797700	1.46113300	-1.04951100
H	-6.06062700	-3.90149400	-1.61036100	C	-2.10606800	0.11158300	-2.80767900
				C	-0.78374100	0.31688100	-2.05637200
				H	-2.03622800	-0.76692900	-3.45656900
				H	-2.28678700	0.97621100	-3.46313300
				H	-0.50360000	-0.61734000	-1.55547400
				H	0.02469000	0.54297400	-2.75620000
				H	-2.24105000	2.43440200	0.31053700
				C	-1.11084500	1.54069100	3.11959100
				O	-1.56624100	0.35124100	2.82854900
				O	-0.35447700	2.10118700	2.30728300
				C	-1.52910900	2.15653300	4.42419300
				H	-1.08905500	3.14668400	4.54282300
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				Co	-0.72852100	0.21346500	1.00569900
11_Q							
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C	1.55405100	1.97701500	-0.67910000				
C	2.58097900	2.96501800	-0.77279400				
C	2.28625100	4.29864600	-0.96309800				
H	0.71251900	5.77737200	-1.20673400				
H	-1.10210600	4.09239100	-1.16099300				
H	3.61621600	2.68006200	-0.61352200				
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11\_S

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C 0.07881700 1.80699900 -1.51313200  
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C	0.82860100	4.32845900	-2.12545500	H	-0.38416200	-1.08160500	-1.19140500
C	-0.12017200	3.33336200	-1.89380200	H	0.24868600	-0.14758800	-2.54574200
C	0.22234600	2.12761700	-1.26733500	H	-2.30131200	2.38031000	-0.27451800
C	1.56871100	1.94954600	-0.86787000	C	-1.53005400	2.15260700	2.97532500
C	2.52137800	2.94787700	-1.11433600	O	-1.68344900	0.87412600	2.77319600
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H	0.53075900	5.25296000	-2.61147600	C	-2.18701900	2.72593200	4.20946700
H	-1.14699000	3.47570300	-2.21465900	H	-1.98629900	3.79425100	4.29800900
H	3.54247200	2.81704400	-0.76781000	H	-3.26793300	2.55668800	4.16025800
H	2.89824300	4.90873200	-1.91579800	H	-1.81857500	2.20500200	5.09899100
C	1.94896100	0.75479100	-0.06610700	Co	-0.82864800	0.70429500	0.93787000
O	1.19092600	0.25378700	0.79309900	C	-2.43411900	-1.88867900	1.49747200
N	3.18567600	0.25546900	-0.29449600	O	-1.41821700	-1.45845700	0.94579000
C	-2.07504600	1.36080900	-0.57979000	O	-3.05151000	-1.27998900	2.49260800
C	-3.21303600	0.45823200	-0.82066800	C	-3.08557100	-3.18230000	1.09615500
C	-4.39693500	0.54257100	-0.07116700	H	-3.09034500	-3.87326600	1.94509900
C	-3.11292800	-0.53750100	-1.81128900	H	-4.12549000	-2.99107800	0.81859900
C	-5.44925100	-0.33875900	-0.27942600	H	-2.55237600	-3.62579400	0.25623000
H	-4.48045200	1.30359000	0.70024700	H	3.74172200	0.65689900	-1.04603900
C	-4.16634000	-1.43181400	-2.01910200	H	-2.58986400	-0.41148600	2.70552300
C	-5.33455800	-1.34115400	-1.25244500	O	-6.40480100	-2.18209700	-1.37369500
H	-6.36004900	-0.28056700	0.30732100	C	-6.32902300	-3.21682700	-2.34203400
H	-4.06273500	-2.19250200	-2.78456500	H	-7.26897500	-3.76759800	-2.27139900
C	3.85017000	-0.79971200	0.34051100	H	-6.22432800	-2.81663600	-3.35876600
C	5.16678300	-1.05517600	-0.16894500	H	-5.49610600	-3.90292400	-2.13987800
C	3.34842700	-1.57364100	1.37158800				
C	5.94580700	-2.10612900	0.39685200	TS7_S			
C	4.13840200	-2.61161000	1.91951700	C	-5.37143500	-0.88698700	0.38626600
H	2.35540900	-1.38393400	1.75117800	C	-4.26454700	-0.63198200	1.19257700
C	6.82411900	-0.49267600	-1.66402500	C	-2.98484100	-0.98129100	0.75887900
C	7.23838700	-2.31003900	-0.14839700	C	-2.80650200	-1.64191900	-0.46922300
C	5.40508600	-2.88173800	1.45453000	C	-3.92161100	-1.89562600	-1.26830200
H	3.72075900	-3.20332100	2.72812300	C	-5.19741800	-1.51298300	-0.84850200
C	7.67937100	-1.50775100	-1.17560600	H	-6.36398800	-0.59736300	0.71769200
H	7.15387700	0.15219900	-2.47609900	H	-4.37626000	-0.14553200	2.15579200
H	7.86548200	-3.10064200	0.25399400	H	-3.79749000	-2.39512600	-2.22368700
H	6.00047200	-3.68163100	1.88400600	H	-6.05477700	-1.71111100	-1.48516000
H	8.66317600	-1.63947400	-1.61303900	C	-1.41220600	-2.08748200	-0.82383400
N	5.61488800	-0.26848100	-1.18492600	C	-0.49252000	-0.93525100	-0.99959800
C	-0.79222500	1.05516300	-1.07815800	C	0.93424700	-0.94487400	-1.25250000
C	-1.86827800	-0.57902600	-2.66995800	C	1.46756600	0.12954900	-2.00937600
C	-0.60344300	-0.24911100	-1.86606300	C	1.85391400	-1.87184500	-0.72677700
H	-1.76959300	-1.55968900	-3.14787400	C	2.82115900	0.27084900	-2.22287100

H	0.78634100	0.88049700	-2.39792400	H	5.87343800	-1.25251200	-0.15345400
C	3.22547800	-1.73603800	-0.92133000				
H	1.51642000	-2.69286900	-0.11445700	TS7_T			
C	3.72052400	-0.65315000	-1.65669100	C	1.98164200	-4.66858800	0.01426200
H	3.21916800	1.10476300	-2.79055400	C	0.89315200	-3.85287800	-0.27900200
H	3.89458400	-2.45978500	-0.47423400	C	1.06591100	-2.53636200	-0.73611300
C	-1.81400400	-0.72137400	1.64855700	C	2.38612600	-2.03872300	-0.89318000
O	-1.85954600	-0.96537600	2.85022300	C	3.47187900	-2.88683800	-0.62507900
N	-0.69097000	-0.17514100	1.01079700	C	3.27921200	-4.18482100	-0.16819000
Co	-0.88996600	1.57268700	0.17478900	H	1.81744800	-5.68423000	0.36113700
C	-2.46498200	2.88894000	-0.91537000	H	-0.11438700	-4.24620900	-0.19096100
O	-2.76025700	1.72767900	-0.48166200	H	4.47029200	-2.48874200	-0.76496900
O	-1.26702600	3.29251300	-0.74552000	H	4.13550600	-4.81705400	0.04519000
C	-3.50060300	3.76240300	-1.56454800	C	2.74662400	-0.63068300	-1.27098900
H	-3.03121000	4.48028300	-2.24011900	O	3.82299800	-0.38962300	-1.81224300
H	-4.23006100	3.15211900	-2.10146900	N	1.79233200	0.35230700	-0.91666600
H	-4.03356700	4.31999600	-0.78561100	C	-1.23339100	-1.74478900	-0.29678000
C	-1.01430100	-3.44514600	-0.26027000	C	-2.55459100	-1.12885700	-0.43951500
C	-1.22284700	-3.29593300	-1.73651800	C	-3.58457000	-1.63089600	0.38670000
H	-1.79196300	-3.94738900	0.30605300	C	-2.88402400	-0.06667600	-1.29969700
H	-0.01686700	-3.61436300	0.11898200	C	-4.87356800	-1.13224500	0.33178700
H	-0.34312800	-3.28239900	-2.37116500	H	-3.35541700	-2.43252800	1.08254800
H	-2.10362200	-3.73900100	-2.18801500	C	-4.17609000	0.45191700	-1.36013300
C	0.56661800	-0.29960800	1.62479700	H	-2.12864700	0.39947900	-1.91663200
C	1.46637900	0.74836600	1.30145300	C	-5.18421300	-0.08417700	-0.54919900
C	1.03295000	-1.36561800	2.38149900	H	-5.65829100	-1.52906400	0.96701300
C	2.83048700	0.71028100	1.68550000	H	-4.38119000	1.27647100	-2.03154300
C	2.38446300	-1.39965400	2.79040100	C	2.20820400	1.69916500	-0.76189500
H	0.36012400	-2.16625700	2.66006600	C	1.44036300	2.47073100	0.16545300
C	1.70880500	2.80802100	0.24843600	C	3.17041600	2.35220600	-1.54965300
C	3.64445300	1.80058300	1.28316500	C	1.69287900	3.87329100	0.32484400
C	3.27610000	-0.40271400	2.44388900	C	3.41961600	3.71894700	-1.37360800
H	2.72657400	-2.24201700	3.38445100	H	3.73028500	1.78179100	-2.27420100
C	3.07916000	2.83923700	0.57378600	C	-0.29110400	2.54856700	1.76604700
H	1.23292500	3.60835500	-0.30667400	C	0.88952200	4.57720900	1.25660500
H	4.69873500	1.80866200	1.54314100	C	2.70708000	4.47713900	-0.45521500
H	4.31367900	-0.44830200	2.76088000	H	4.18692100	4.19249900	-1.97959900
H	3.67364200	3.68966600	0.25798700	C	-0.10068300	3.91229300	1.97185100
N	0.92363400	1.78726100	0.58798100	H	-1.03271200	1.97397700	2.30901300
H	-0.99742800	-0.11627100	-1.50426200	H	1.05913700	5.64022500	1.40046800
O	5.03393900	-0.40276300	-1.86725500	H	2.90433400	5.53791400	-0.33299300
C	5.98771700	-1.25774400	-1.24409900	H	-0.72243100	4.43755000	2.68889500
H	5.90756300	-2.28687100	-1.61392200	N	0.45248900	1.85137300	0.88485400
H	6.96752800	-0.85703200	-1.50774300	C	-0.13434500	-1.73055100	-1.11078800

C 0.47578800 0.38171500 -2.35526000  
 C -0.04735100 -1.02463100 -2.45736800  
 H 1.07555500 0.75203100 -3.18195900  
 H -0.18892700 1.12761500 -1.92831900  
 H -1.03710500 -1.04086900 -2.93239400  
 H 0.61562600 -1.61093800 -3.09994000  
 H -1.15251000 -2.36258500 0.59383600  
 C 0.23812500 -0.99749600 2.96037300  
 O 1.32524100 -1.05441700 2.27731200  
 O -0.80093400 -0.52016600 2.42828600  
 C 0.24716400 -1.48321200 4.38579100  
 H 0.79895500 -0.76500900 5.00221500  
 H -0.76878500 -1.57746700 4.77162200  
 H 0.76977800 -2.44106600 4.45283200  
 Co 0.53980300 -0.15043200 0.66604400  
 O -6.47149200 0.34411500 -0.53379400  
 C -6.83040300 1.42163200 -1.39196100  
 H -6.67216100 1.16647400 -2.44688900  
 H -7.89332900 1.59958600 -1.22170200  
 H -6.26908900 2.33245500 -1.15021500

12\_Q

C 5.70931500 -0.19831100 -0.35276000  
 C 4.53000700 -0.90963400 -0.23763700  
 C 3.27188000 -0.24266800 -0.23266100  
 C 3.23514100 1.18139700 -0.43935800  
 C 4.44855000 1.86231600 -0.53644700  
 C 5.67911900 1.19952800 -0.48134300  
 H 6.66080400 -0.72275300 -0.33609100  
 H 4.53528900 -1.98823700 -0.12237500  
 H 4.44791100 2.93911200 -0.68039200  
 H 6.60203700 1.76549300 -0.56056900  
 C 1.91428900 1.88947400 -0.60610000  
 C 0.74295600 0.92075100 -0.81847300  
 C -0.66491400 1.47310300 -0.86820100  
 C -1.40389500 1.29931200 -2.05102800  
 C -1.30840600 2.08910500 0.21221600  
 C -2.71931000 1.72922800 -2.15672400  
 H -0.94154000 0.79192000 -2.89105100  
 C -2.63342100 2.52291000 0.12509600  
 H -0.78948300 2.22923100 1.15130200  
 C -3.34675300 2.34646200 -1.06548900  
 H -3.28307000 1.59227600 -3.07374700  
 H -3.09188400 2.99303800 0.98642000

C 2.07883200 -0.96952400 -0.02501500  
 O 1.89957500 -2.26483000 -0.03505700  
 N 0.82978000 -0.24723800 0.11327900  
 Co -0.06651000 -2.16765500 -0.50617800  
 C -1.25695500 -2.69006800 -2.55546600  
 O -0.37848800 -1.76793300 -2.54666400  
 O -1.46600800 -3.36596400 -1.49087200  
 C -2.07261000 -2.94696900 -3.79205400  
 H -2.48994500 -3.95495400 -3.78139800  
 H -2.89879800 -2.22686400 -3.81710600  
 H -1.46565200 -2.79183500 -4.68648000  
 C 1.73443500 3.25045800 0.05349600  
 C 1.87297800 3.15976800 -1.43453700  
 H 2.57967100 3.61516200 0.62960400  
 H 0.76504400 3.52083400 0.45316200  
 H 0.97671500 3.32181900 -2.02622800  
 H 2.79175500 3.48690400 -1.90916300  
 C 0.49420500 -0.04094400 1.50389900  
 C -0.56570300 -0.83428400 2.02784300  
 C 1.13780000 0.85629800 2.34044100  
 C -1.02388400 -0.62942000 3.36396700  
 C 0.70015600 1.04259200 3.66849500  
 H 1.97401900 1.43032100 1.96601000  
 C -2.13136800 -2.52780500 1.67662500  
 C -2.11090700 -1.42453200 3.80849600  
 C -0.37303600 0.33463700 4.17167100  
 H 1.21430300 1.76560300 4.29379900  
 C -2.67152600 -2.35928100 2.96609200  
 H -2.51913600 -3.27419800 0.99072000  
 H -2.48651500 -1.28991200 4.81873800  
 H -0.71917000 0.49249500 5.18840200  
 H -3.50357300 -2.97850500 3.28135300  
 N -1.11695300 -1.79757500 1.23050200  
 H 0.92526300 0.45668600 -1.79159300  
 O -4.63770800 2.73287800 -1.25842700  
 C -5.31476600 3.35531000 -0.17488300  
 H -4.82539700 4.29064900 0.12458700  
 H -6.32063000 3.57797400 -0.53513700  
 H -5.38426400 2.68966400 0.69475700

12\_S

C -5.68583100 -0.34783900 0.12587200  
 C -4.55486200 0.28098800 0.62712100  
 C -3.28111900 -0.25680100 0.39122400

C	-3.12570400	-1.44342600	-0.35742000	C	1.96325000	-1.08512400	3.63768000
C	-4.28160000	-2.08159000	-0.82371600	H	0.63290700	-2.70009100	4.08944300
C	-5.54383500	-1.54101800	-0.58914000	C	3.43921500	2.01986100	2.16049400
H	-6.67005300	0.07576600	0.29775900	H	2.46714000	3.20080500	0.60702400
H	-4.62858900	1.18732400	1.21759600	H	4.11573000	0.66467700	3.69395600
H	-4.20268300	-3.00466600	-1.38686200	H	2.69903900	-1.37268100	4.38300100
H	-6.42210000	-2.05041500	-0.97479600	H	4.29689800	2.68147400	2.22149800
C	-1.74065600	-1.95069900	-0.61606100	N	1.32669800	1.56187900	1.09760100
C	-0.76506600	-0.77694200	-0.66032300	H	-1.19678500	-0.09206000	-1.39320200
C	0.65307200	-1.03265500	-1.12104200	O	4.52058000	-1.45392600	-2.65748900
C	1.07366600	-0.39986400	-2.30451800	C	5.49520900	-2.23145700	-1.97466800
C	1.57995400	-1.83872300	-0.45322200	H	5.19430200	-3.28419000	-1.90105000
C	2.35875300	-0.56050700	-2.79841500	H	6.40761200	-2.16186700	-2.56937600
H	0.37710400	0.24087400	-2.83616900	H	5.69072800	-1.84015800	-0.96844400
C	2.88304700	-2.00368000	-0.93017300				
H	1.31633600	-2.33225700	0.47224000	12_T			
C	3.28006200	-1.36181100	-2.10733400	C	5.74557100	-0.14380600	-0.17551900
H	2.67711100	-0.06399400	-3.70890600	C	4.57225000	0.11214700	-0.87229900
H	3.57143300	-2.62762000	-0.37382300	C	3.33587800	-0.30119400	-0.35745200
C	-2.13772900	0.36099300	1.10307400	C	3.26211600	-0.98212900	0.87811900
O	-2.27643500	1.05046600	2.09661700	C	4.45864800	-1.25890400	1.54989700
N	-0.80774700	0.04873200	0.62099500	C	5.68415600	-0.84362500	1.03308600
Co	-0.07419800	1.84303400	-0.05268400	H	6.70085100	0.18599200	-0.57112000
C	-0.64242200	3.37045100	-1.69360600	H	4.58424500	0.61872800	-1.83092700
O	-1.38621600	2.35995500	-1.44846800	H	4.43936300	-1.79171700	2.49407100
O	0.41687100	3.50231700	-0.99966500	H	6.59585300	-1.06013100	1.58225000
C	-1.02599400	4.37612100	-2.74101200	C	1.91194100	-1.35968500	1.40806000
H	-0.16656800	4.98504300	-3.02619600	C	0.87734200	-0.36610100	0.88954100
H	-1.44024600	3.86888400	-3.61603600	C	-0.52618100	-0.39890600	1.45354800
H	-1.80518700	5.03256200	-2.33713600	C	-0.97075300	0.73685600	2.15547900
C	-1.37174500	-3.33947500	-0.11380200	C	-1.42782700	-1.45790000	1.29431100
C	-1.52162500	-3.09201200	-1.58362100	C	-2.25834800	0.81765800	2.66670100
H	-2.15878300	-3.88484800	0.39828600	H	-0.29440800	1.57633300	2.28572900
H	-0.37652200	-3.50769600	0.27823600	C	-2.72636300	-1.39205100	1.80051300
H	-0.61385400	-3.04634100	-2.17545400	H	-1.14236300	-2.34604900	0.74694000
H	-2.37599200	-3.50472500	-2.10782500	C	-3.15118800	-0.24786400	2.48710100
C	0.07864800	-0.36395900	1.70035300	H	-2.59642000	1.70017400	3.19926100
C	1.22101500	0.43513300	1.88950300	H	-3.39363300	-2.23082000	1.64612700
C	-0.14715600	-1.46794000	2.49510000	C	2.14376800	-0.15908200	-1.23434000
C	2.19907600	0.07450000	2.85494000	O	2.23472000	0.02052100	-2.44062800
C	0.81039800	-1.82620800	3.47063000	N	0.87514900	-0.31973800	-0.62330200
H	-1.04448500	-2.06078900	2.36227000	Co	-0.18774800	1.75345200	-0.81495000
C	2.41881700	2.32480300	1.24308900	C	0.30994400	3.96370300	0.14022300
C	3.34245900	0.90726300	2.97204500	O	1.02651000	2.91558200	0.33466000

O	-0.71055900	3.91193300	-0.59958500	H	4.13550600	-4.81705400	0.04519000
C	0.72156600	5.25104400	0.81359000	C	2.74662400	-0.63068300	-1.27098900
H	-0.00474400	6.04284200	0.62634000	O	3.82299800	-0.38962300	-1.81224300
H	0.82403000	5.08679600	1.89071800	N	1.79233200	0.35230700	-0.91666600
H	1.70299600	5.55931800	0.43838500	C	-1.23339100	-1.74478900	-0.29678000
C	1.61213000	-2.82914800	1.66179200	C	-2.55459100	-1.12885700	-0.43951500
C	1.76195900	-1.88559400	2.81685700	C	-3.58457000	-1.63089600	0.38670000
H	2.42231100	-3.52269900	1.45787700	C	-2.88402400	-0.06667600	-1.29969700
H	0.62457100	-3.20954000	1.43089800	C	-4.87356800	-1.13224500	0.33178700
H	0.85893400	-1.59154400	3.34133400	H	-3.35541700	-2.43252800	1.08254800
H	2.64184000	-1.95441400	3.44674700	C	-4.17609000	0.45191700	-1.36013300
C	-0.02126800	-1.19608400	-1.34540400	H	-2.12864700	0.39947900	-1.91663200
C	-1.23664600	-0.67472200	-1.84711700	C	-5.18421300	-0.08417700	-0.54919900
C	0.29742000	-2.53169100	-1.52444300	H	-5.65829100	-1.52906400	0.96701300
C	-2.15682600	-1.55404300	-2.49444600	H	-4.38119000	1.27647100	-2.03154300
C	-0.60638800	-3.39887800	-2.16613900	C	2.20820400	1.69916500	-0.76189500
H	1.24569000	-2.90415100	-1.15478700	C	1.44036300	2.47073100	0.16545300
C	-2.66185300	1.15059500	-2.18913200	C	3.17041600	2.35220600	-1.54965300
C	-3.37383500	-1.00817700	-2.98265000	C	1.69287900	3.87329100	0.32484400
C	-1.81618500	-2.92247500	-2.63004100	C	3.41961600	3.71894700	-1.37360800
H	-0.34586800	-4.44505500	-2.29177600	H	3.73028500	1.78179100	-2.27420100
C	-3.61175300	0.34460900	-2.82618200	C	-0.29110400	2.54856700	1.76604700
H	-2.82859800	2.21348900	-2.05254300	C	0.88952200	4.57720900	1.25660500
H	-4.09105500	-1.65667500	-3.47561500	C	2.70708000	4.47713900	-0.45521500
H	-2.52055900	-3.58776800	-3.12094300	H	4.18692100	4.19249900	-1.97959900
H	-4.52710600	0.79961600	-3.18961000	C	-0.10068300	3.91229300	1.97185100
N	-1.49982200	0.67497000	-1.69900500	H	-1.03271200	1.97397700	2.30901300
H	1.28015200	0.61125200	1.16686700	H	1.05913700	5.64022500	1.40046800
O	-4.39304100	-0.07994000	3.01237200	H	2.90433400	5.53791400	-0.33299300
C	-5.34466400	-1.12026700	2.82539600	H	-0.72243100	4.43755000	2.68889500
H	-5.02112700	-2.05466900	3.30081300	N	0.45248900	1.85137300	0.88485400
H	-6.26374200	-0.77654700	3.30279400	C	-0.13434500	-1.73055100	-1.11078800
H	-5.53801800	-1.30308000	1.76111300	C	0.47578800	0.38171500	-2.35526000
TS8_Q				C	-0.04735100	-1.02463100	-2.45736800
C	1.98164200	-4.66858800	0.01426200	H	1.07555500	0.75203100	-3.18195900
C	0.89315200	-3.85287800	-0.27900200	H	-0.18892700	1.12761500	-1.92831900
C	1.06591100	-2.53636200	-0.73611300	H	-1.03710500	-1.04086900	-2.93239400
C	2.38612600	-2.03872300	-0.89318000	H	0.61562600	-1.61093800	-3.09994000
C	3.47187900	-2.88683800	-0.62507900	H	-1.15251000	-2.36258500	0.59383600
C	3.27921200	-4.18482100	-0.16819000	C	0.23812500	-0.99749600	2.96037300
H	1.81744800	-5.68423000	0.36113700	O	1.32524100	-1.05441700	2.27731200
H	-0.11438700	-4.24620900	-0.19096100	O	-0.80093400	-0.52016600	2.42828600
H	4.47029200	-2.48874200	-0.76496900	C	0.24716400	-1.48321200	4.38579100
				H	0.79895500	-0.76500900	5.00221500

H -0.76878500 -1.57746700 4.77162200  
H 0.76977800 -2.44106600 4.45283200  
Co 0.53980300 -0.15043200 0.66604400  
O -6.47149200 0.34411500 -0.53379400  
C -6.83040300 1.42163200 -1.39196100  
H -6.67216100 1.16647400 -2.44688900  
H -7.89332900 1.59958600 -1.22170200  
H -6.26908900 2.33245500 -1.15021500

TS8\_S

C -0.93497700 5.00164300 0.61828900  
C -0.07560200 4.00010500 0.17665000  
C -0.56802900 2.79870100 -0.35510100  
C -1.96415500 2.62725600 -0.45211800  
C -2.82089600 3.65713300 -0.03763200  
C -2.31601000 4.83292100 0.50680300  
H -0.52575600 5.91865400 1.03140200  
H 0.99754800 4.15251800 0.21963000  
H -3.88933100 3.50447800 -0.13636900  
H -2.99429000 5.61339700 0.83719200  
C -2.64405300 1.39263700 -0.95615500  
O -3.74969900 1.48679000 -1.48531400  
N -2.02600600 0.14482400 -0.70629900  
C 1.51921600 1.52151600 -0.17021000  
C 2.71327300 0.73128400 -0.46283000  
C 3.80318500 0.90672100 0.42022000  
C 2.88696200 -0.18975700 -1.51051000  
C 4.99745400 0.22787400 0.25810600  
H 3.69591800 1.59651600 1.25224500  
C 4.08176500 -0.88577300 -1.68482800  
H 2.08260500 -0.40700400 -2.19841700  
C 5.14978000 -0.67793000 -0.80308900  
H 5.82688000 0.37568300 0.94160900  
H 4.16579400 -1.59015700 -2.50323400  
C -2.85608400 -1.01375700 -0.74153600  
C -2.39647500 -2.05488300 0.10718600  
C -3.97277400 -1.24941900 -1.53168300  
C -3.08185200 -3.29613700 0.20161800  
C -4.65736800 -2.48391900 -1.43970800  
H -4.33345200 -0.48224500 -2.19730200  
C -0.78952700 -2.72184600 1.65360400  
C -2.55689200 -4.26281800 1.09539400  
C -4.23853500 -3.48806100 -0.59477400  
H -5.53714800 -2.63201900 -2.05850500

C -1.42198600 -3.96935500 1.81798000  
H 0.11688400 -2.45268900 2.18039100  
H -3.05652000 -5.22144700 1.19877000  
H -4.77745300 -4.42823400 -0.52981100  
H -0.99504200 -4.68560300 2.51125000  
N -1.25710600 -1.79402000 0.82117600  
C 0.37049200 1.76704500 -0.86346000  
C -0.59544300 -0.24613800 -1.89120400  
C 0.00307200 1.10591200 -2.18156400  
H -1.27713900 -0.63596600 -2.64374600  
H 0.11277200 -1.01106600 -1.57621600  
H 0.88177500 1.00796100 -2.82807600  
H -0.71407200 1.72750000 -2.72283400  
H 1.58825200 2.04855800 0.77588000  
C 1.11413600 0.32028900 2.66971400  
O 0.51621700 1.39553100 2.80854700  
O 0.93049200 -0.51430100 1.69308000  
C 2.16228800 -0.13205000 3.67826800  
H 1.77385200 -0.97919100 4.25556900  
H 3.06403900 -0.47588600 3.16344500  
H 2.40856900 0.67822200 4.36688400  
Co -0.47020300 -0.11471500 0.44249500  
O 6.35273900 -1.30119600 -0.88685200  
C 6.55321000 -2.23268900 -1.94354800  
H 6.45458400 -1.75488300 -2.92603600  
H 7.57225800 -2.60488200 -1.82708600  
H 5.85270300 -3.07415500 -1.87711100

TS8\_T

C 0.76649900 4.97997800 -1.38272500  
C -0.09070600 4.02236600 -0.85003300  
C 0.38875600 2.92757900 -0.10917000  
C 1.78406000 2.82625100 0.10838500  
C 2.63260600 3.82276500 -0.40097300  
C 2.13942600 4.88307400 -1.15241400  
H 0.35998000 5.81121900 -1.95103000  
H -1.16204500 4.13802100 -0.97431500  
H 3.69384200 3.73194600 -0.20119800  
H 2.81938400 5.63208500 -1.54655000  
C 2.49905200 1.71276800 0.82457500  
O 3.56775800 1.95136400 1.39229500  
N 1.97601600 0.41710400 0.69303700  
C -1.70223000 1.64335000 -0.21703400  
C -2.90249700 0.88200800 0.12179500





C -0.52425700 -1.57173000 -1.07434000  
 C 0.07660500 0.60462400 -2.20262600  
 C -0.54672900 -0.77475800 -2.36663400  
 H 0.36112300 1.03845100 -3.16970600  
 H -0.61343000 1.29588800 -1.70792100  
 H -1.56364000 -0.67696600 -2.75100900  
 H 0.02648800 -1.33068100 -3.11597400  
 H -1.47983300 -2.34354900 0.63439900  
 C 1.58205900 -1.38370200 2.60042500  
 O 2.36794100 -0.81309700 1.78360100  
 O 0.32050300 -1.32467800 2.39470300  
 C 2.11855800 -2.16833500 3.76634800  
 H 1.42482400 -2.13273700 4.60897600  
 H 2.22177000 -3.21360200 3.45336300  
 H 3.10252200 -1.79998800 4.06171700  
 Co 0.67619300 -0.34466600 0.60078200  
 O -6.82224200 0.51138600 0.13630800  
 C -7.23626400 1.62068500 -0.64688000  
 H -7.16858100 1.40660400 -1.72133700  
 H -8.27985600 1.80464500 -0.38486200  
 H -6.64706400 2.51920100 -0.42192200

13\_S

C 2.11328100 -4.15577000 -0.52118600  
 C 0.91753300 -3.46617400 -0.54707500  
 C 0.84181400 -2.15011300 -1.06626700  
 C 2.06029200 -1.53261200 -1.50388500  
 C 3.26222800 -2.27479300 -1.50076400  
 C 3.29284100 -3.56775400 -1.02049500  
 H 2.13886800 -5.17095500 -0.13561100  
 H 0.00398900 -3.93998600 -0.20400600  
 H 4.16581000 -1.78058700 -1.83887500  
 H 4.22543500 -4.12243500 -1.00610900  
 C 2.18288200 -0.09629700 -1.79928100  
 O 3.17602900 0.44662100 -2.24626600  
 N 1.00408300 0.74239300 -1.38012200  
 C -1.38180600 -1.47111900 -0.20142700  
 C -2.74633900 -0.93742300 -0.13298700  
 C -3.61472100 -1.53186000 0.81134000  
 C -3.27391500 0.11894400 -0.89525100  
 C -4.92885500 -1.12310100 0.96245200  
 H -3.23709200 -2.33868300 1.43307000  
 C -4.59407500 0.54526600 -0.75342600  
 H -2.65018900 0.65341100 -1.59708800

C -5.43599600 -0.07971800 0.17367400  
 H -5.58408200 -1.59448800 1.68762300  
 H -4.94912000 1.36893800 -1.36074000  
 C 1.40430000 2.08475800 -0.99429200  
 C 1.39927900 2.32940300 0.39743500  
 C 1.76225000 3.08151900 -1.87418600  
 C 1.76254500 3.60827400 0.90086200  
 C 2.12375400 4.35675500 -1.37986700  
 H 1.78170200 2.88980300 -2.93999900  
 C 0.99453700 1.50323900 2.53287900  
 C 1.72324700 3.79174400 2.30694900  
 C 2.12763000 4.61731900 -0.02658100  
 H 2.40787700 5.13301200 -2.08287100  
 C 1.33924700 2.74182100 3.11042500  
 H 0.68613900 0.65649900 3.13328200  
 H 1.99315200 4.75485700 2.72918700  
 H 2.40760700 5.59740600 0.34778300  
 H 1.29595000 2.84623500 4.18886300  
 N 1.02118600 1.29352000 1.22043200  
 C -0.44131800 -1.44513700 -1.22161600  
 C -0.09336400 0.74540500 -2.39528000  
 C -0.60954800 -0.68562700 -2.52829800  
 H 0.26309900 1.14400700 -3.35145000  
 H -0.85590000 1.42121500 -2.00493400  
 H -1.65581400 -0.68158700 -2.84298000  
 H -0.04498400 -1.20882900 -3.30533700  
 H -1.15028700 -2.12869700 0.62975100  
 C 1.68547700 -1.74720600 2.31612300  
 O 2.77669700 -1.37911400 1.87462500  
 O 0.51913300 -1.35392300 1.88144500  
 C 1.59692500 -2.75607400 3.45487900  
 H 0.86396700 -2.43738100 4.20230300  
 H 1.25674600 -3.71821000 3.05523500  
 H 2.57353700 -2.89375000 3.92257500  
 Co 0.56636400 -0.29941300 0.28511900  
 O -6.73679400 0.25486800 0.38796100  
 C -7.29040600 1.31074700 -0.38650900  
 H -7.26806000 1.08027400 -1.45905300  
 H -8.32820400 1.40949000 -0.06368000  
 H -6.76767300 2.25909600 -0.20950700

13\_T

C -1.89191400 4.96189400 -0.04274900  
 C -0.88244600 4.03196800 -0.28352400

C	-1.16605300	2.66784900	-0.44945700	H	0.08641100	1.83558700	-2.87238900
C	-2.52064200	2.25433100	-0.35369100	H	1.03178300	2.47068900	0.92437600
C	-3.52545900	3.19594700	-0.09921300	C	-0.40161300	-0.62803800	3.01915700
C	-3.22169300	4.54535800	0.04505000	O	-1.44896400	-0.49053900	2.30993200
H	-1.63956000	6.01181500	0.07452600	O	0.73253200	-0.27134600	2.57582700
H	0.15003700	4.35939000	-0.35375600	C	-0.50992500	-1.27399700	4.38280600
H	-4.54479600	2.83974300	0.00196800	H	0.29503200	-0.93587000	5.03878300
H	-4.01206600	5.26477200	0.23483100	H	-1.48211500	-1.06313600	4.83364100
C	-2.94733700	0.81449200	-0.37548300	H	-0.42104000	-2.36053200	4.26467500
O	-3.96136900	0.42685800	0.18275000	Co	-0.27384900	0.26230100	0.70911800
N	-2.06834700	-0.05295500	-1.05022900	O	6.50987900	0.19655900	-0.50703100
C	1.08913000	1.74522000	0.11348800	C	6.88447800	-0.98438200	-1.20093700
C	2.46945100	1.26995900	-0.11728400	H	7.97385400	-1.03212400	-1.15179300
C	3.52253000	2.01777700	0.44817800	H	6.46466200	-1.88221300	-0.72930900
C	2.82542800	0.10483000	-0.81408400	H	6.57453200	-0.95262200	-2.25337700
C	4.85022400	1.64390700	0.30279900				
H	3.28567800	2.91412600	1.01494600				
C	4.15551600	-0.28619200	-0.97130500	14_Q			
H	2.05557700	-0.54287600	-1.21200000	C	5.41613000	-0.02887900	-0.00383900
C	5.18116400	0.48694000	-0.41550300	C	5.38891900	-1.38686700	-0.35941400
H	5.64983100	2.23112600	0.74265900	C	4.18677700	-1.97681600	-0.72953400
H	4.37519700	-1.19744800	-1.51465500	C	3.01563700	-1.20214100	-0.74336300
C	-2.29942900	-1.46584800	-1.00243000	C	3.00525100	0.16858400	-0.37894500
C	-1.24287200	-2.29587900	-0.52745700	C	4.24381600	0.72789000	-0.01837100
C	-3.47319700	-2.03069900	-1.45258500	H	6.35820500	0.42929600	0.28838000
C	-1.40875000	-3.71416200	-0.56568500	H	6.30429100	-1.97152800	-0.34589200
C	-3.64141200	-3.43385200	-1.46535800	H	4.13608300	-3.02438400	-1.01001400
H	-4.27221600	-1.38435700	-1.79505700	H	4.29345500	1.77607600	0.27096500
C	0.87050100	-2.50619800	0.40873100	C	1.73966800	-1.85359900	-1.13250700
C	-0.33618800	-4.51679700	-0.10282300	O	1.62501800	-3.04932700	-1.39186100
C	-2.62675900	-4.26132500	-1.04332000	N	0.66882100	-0.93012600	-1.16032600
H	-4.57761900	-3.85245800	-1.82021400	C	-0.58697800	-1.20938200	-1.53182700
C	0.80408800	-3.91501200	0.37412200	C	-1.51031300	-0.09138500	-1.39771500
H	1.73590800	-2.00238600	0.82469400	C	-1.09758300	-2.43554300	-2.03003600
H	-0.43531500	-5.59816100	-0.12449100	C	-2.87037900	-0.22871900	-1.77197200
H	-2.74426900	-5.34073700	-1.06107000	C	-2.44428400	-2.55004300	-2.38743500
H	1.64295800	-4.49641100	0.74034100	H	-0.42004800	-3.27169500	-2.12111100
N	-0.10536800	-1.71907200	-0.02343000	C	-1.82192600	2.10475200	-0.75123600
C	-0.04405500	1.70543300	-0.71941900	C	-3.70806500	0.89872500	-1.61897300
C	-1.47478100	0.45796800	-2.32124000	C	-3.32370200	-1.48352800	-2.26669300
C	-0.09285100	1.07687500	-2.09710800	H	-2.80680400	-3.50074200	-2.76505300
H	-2.16404100	1.19195900	-2.74668000	C	-3.17955800	2.06970800	-1.11316000
H	-1.42640400	-0.37911400	-3.01902300	H	-1.37674400	2.99645300	-0.32389500
H	0.68048200	0.32082200	-2.20609100	H	-4.75551300	0.82809100	-1.89436400

H	-4.36741000	-1.59222600	-2.54475500	H	6.06158700	-2.67005800	-0.23850800
H	-3.79047700	2.95631500	-0.98673800	H	5.56791500	-0.27459100	-0.81558300
N	-1.01418900	1.05978300	-0.89309300	H	1.95128700	-3.22273400	0.91827000
Co	1.14200600	0.96130400	-0.44995900	C	3.13961100	0.96939800	-0.59932300
C	-3.18692400	-1.82264300	1.12866800	O	3.93165600	1.80939300	-1.03687100
C	-3.57331900	-0.52914400	1.50295500	N	1.81146700	1.18212300	-0.31214900
C	-2.63375500	0.33041500	2.08811700	C	1.18824000	2.41338700	-0.28455400
C	-1.32048500	-0.09655900	2.26412800	C	-0.12427300	2.38489300	0.28893700
C	-0.90634700	-1.37987400	1.87180000	C	1.68145900	3.64278600	-0.72169700
C	-1.87437200	-2.23390400	1.30879400	C	-0.90366800	3.56620600	0.43470500
H	-3.92649200	-2.47968100	0.68449200	C	0.89618800	4.80823100	-0.58769500
H	-2.90985200	1.33254700	2.39187900	H	2.67226700	3.68427800	-1.15023400
H	-0.60089800	0.58542400	2.70239100	C	-1.76874700	1.06357200	1.27572400
H	-1.58208000	-3.23436900	1.00330400	C	-2.17406800	3.42344600	1.04955700
C	0.47587800	-1.84632500	2.00280700	C	-0.36559800	4.79354900	-0.02645900
C	1.49562600	-1.15790800	2.51690100	H	1.31188700	5.74865500	-0.93860000
C	2.91594800	-1.13245100	2.86398400	C	-2.59945700	2.18504100	1.47646300
C	2.00413200	0.07677000	3.12567000	H	-2.08131400	0.06620300	1.56466100
H	3.64650800	-1.04622300	2.06385700	H	-2.80055600	4.30130800	1.18044000
H	3.25224700	-1.71072600	3.72340800	H	-0.94819500	5.70377100	0.07430200
H	1.73264500	0.30372300	4.15592200	H	-3.56635700	2.05118900	1.94813000
H	2.13396300	0.95233800	2.49171500	N	-0.58349400	1.16483800	0.69846100
H	0.67072600	-2.85323000	1.63615000	Co	0.81945400	-0.26795100	0.38137600
C	1.28526700	3.42454400	-0.40821000	C	-4.19742000	0.17744300	-1.28183000
O	1.08387400	2.74736100	0.66168000	C	-4.61155800	-1.03295900	-0.70308900
O	1.31500100	2.84953000	-1.53366200	C	-3.66613700	-2.03642200	-0.44329700
C	1.52516800	4.91188100	-0.30051600	C	-2.32811000	-1.82649900	-0.76477900
H	2.57976300	5.07995500	-0.05393200	C	-1.89802700	-0.62063300	-1.33971000
H	1.31005300	5.40994500	-1.24767800	C	-2.86109100	0.37742000	-1.58498600
H	0.92357300	5.34203900	0.50381300	H	-4.93996700	0.94488200	-1.47238400
O	-4.86833100	-0.19171700	1.24023500	H	-3.96134700	-2.97505400	0.00902700
C	-5.33350900	1.06762200	1.70731800	H	-1.60227800	-2.59667300	-0.53685400
H	-4.78940000	1.89922600	1.24470200	H	-2.54591300	1.32476900	-2.01289900
H	-6.38537800	1.12580900	1.42144600	C	-0.50278600	-0.35419700	-1.68613600
H	-5.25181100	1.14688500	2.79831300	C	0.48834000	-1.28006000	-1.78177400
				C	1.57769300	-1.65966900	-2.69382600
				C	0.65228200	-2.71262600	-2.06054900
14_S				H	2.60438400	-1.65387900	-2.34840600
C	4.03360500	-3.08083800	0.37356000	H	1.44576300	-1.40445800	-3.74308000
C	5.05999900	-2.26788900	-0.11702700	H	-0.11230200	-3.19572200	-2.66605500
C	4.79277600	-0.93748500	-0.44181600	H	1.11302400	-3.34738500	-1.31125000
C	3.49778900	-0.44078300	-0.28220400	H	-0.28290000	0.65234200	-2.03515600
C	2.45476400	-1.25445900	0.19055700	C	0.46010000	-1.17002600	2.48631800
C	2.73534200	-2.57643400	0.53282800	O	-0.10466300	-1.66273000	1.45273700
H	4.24334800	-4.11533800	0.63467600				

O	1.21426500	-0.16053600	2.28695100	C	-2.43714700	0.06005300	2.26556000
C	0.28714000	-1.76151400	3.84860000	C	-1.13033600	-0.41707200	2.35075000
H	1.02313900	-2.56391700	3.97429600	C	-0.74788400	-1.62490000	1.74602400
H	0.46237900	-1.00876100	4.61915100	C	-1.73675800	-2.34615200	1.05046700
H	-0.71117000	-2.19212100	3.95142000	H	-3.79474100	-2.43686100	0.40796400
O	-5.93665900	-1.13495500	-0.42670000	H	-2.69028400	0.99880200	2.74264800
C	-6.41074500	-2.34477800	0.15476700	H	-0.39434500	0.16270700	2.89652400
H	-5.95069300	-2.52893400	1.13341400	H	-1.46696600	-3.27949900	0.56538200
H	-7.48637700	-2.21453600	0.28341000	C	0.62042600	-2.15135300	1.80359100
H	-6.22733600	-3.20526400	-0.50005300	C	1.65710200	-1.58518300	2.41659700
14_T				C	3.08041500	-1.64333400	2.75095400
C	5.11040500	0.13765300	0.11119500	C	2.19744500	-0.46601000	3.19703100
C	5.21724400	-1.12776500	-0.47708300	H	3.80980800	-1.45864500	1.96648700
C	4.08803100	-1.74938700	-1.01143200	H	3.41062700	-2.34476000	3.51601300
C	2.86264500	-1.08519200	-0.96051500	H	1.94326900	-0.38771500	4.25341600
C	2.75213000	0.18294700	-0.37648300	H	2.34318500	0.49138000	2.69950600
C	3.87625700	0.79875800	0.16762000	H	0.78364200	-3.09311400	1.28112200
H	5.99216200	0.61208900	0.53345200	C	1.55014500	3.21506000	-0.23506700
H	6.18074200	-1.62735700	-0.51217100	O	1.22514700	2.43893100	0.74069600
H	4.13930100	-2.73412100	-1.46653400	O	1.56570100	2.74168500	-1.40157200
H	3.80467800	1.77184400	0.64252600	C	1.92809000	4.64205100	0.05199500
C	1.60130800	-1.65951300	-1.50033800	H	3.00313000	4.68347800	0.26129000
O	1.49149600	-2.77478000	-2.00405100	H	1.72547500	5.27194200	-0.81583800
N	0.57779600	-0.73870300	-1.33826600	H	1.39771600	5.01488700	0.93046800
C	-0.74214700	-0.92097800	-1.73749000	O	-4.69583400	-0.27854900	1.38722400
C	-1.60498400	0.16065200	-1.38367600	C	-5.13034000	0.88603200	2.07384000
C	-1.29389700	-2.00473200	-2.40981900	H	-4.57792000	1.77710700	1.75328200
C	-2.98920000	0.14611300	-1.69835700	H	-6.18536200	1.01017700	1.82221400
C	-2.67420200	-2.01767300	-2.72048900	H	-5.03050000	0.77296800	3.16067800
H	-0.65844600	-2.83533400	-2.68002000	TS9_S			
C	-1.76998000	2.23714500	-0.33704900	C	3.45442900	-3.43312900	0.53011900
C	-3.75197100	1.26604200	-1.29288600	C	4.60592000	-2.73182100	0.15836000
C	-3.51655600	-0.98136400	-2.37988400	C	4.50204600	-1.41657200	-0.29828800
H	-3.07321600	-2.88209200	-3.24292100	C	3.24784900	-0.81701200	-0.40002000
C	-3.14536900	2.30923100	-0.62184700	C	2.07874100	-1.53189400	-0.06570500
H	-1.25878700	3.02222200	0.20964900	C	2.19499600	-2.83757500	0.41539800
H	-4.81526900	1.29049800	-1.51066900	H	3.53617100	-4.44950200	0.90570300
H	-4.57396400	-1.01044600	-2.62175200	H	5.57984700	-3.20546500	0.23793400
H	-3.70866700	3.18022600	-0.30698200	H	5.37971500	-0.83340200	-0.55985100
N	-1.03079300	1.20161900	-0.70778500	H	1.30495500	-3.39326100	0.69359800
Co	0.94788300	0.87163200	-0.44800200	C	3.10292600	0.62590300	-0.75694100
C	-3.04108200	-1.88454300	0.95761300	O	4.01508700	1.31602100	-1.22390800
C	-3.39965800	-0.67044600	1.55822800	N	1.84502600	1.04917400	-0.42902600

C	1.41760200	2.36145900	-0.40227400	C	-6.50682500	-2.10658800	-0.00277800
C	0.15840700	2.52676500	0.25446000	H	-6.12931400	-2.30472800	1.00833100
C	2.04634500	3.49628200	-0.90898000	H	-7.58306000	-1.93188500	0.04548400
C	-0.45930300	3.79892400	0.38720900	H	-6.31256600	-2.97983500	-0.63796500
C	1.42992400	4.76048200	-0.77329600				
H	3.00582200	3.39107500	-1.39513700	TS9_T			
C	-1.58393900	1.45196700	1.37261700	C	3.17596200	-3.65343000	0.54715300
C	-1.70657300	3.83695500	1.06160900	C	4.38176900	-3.04536600	0.18398200
C	0.20936900	4.92878600	-0.14924600	C	4.38962200	-1.72351400	-0.26746800
H	1.94355300	5.62737800	-1.17921600	C	3.19365200	-1.01459800	-0.37311500
C	-2.26133000	2.67531300	1.55297900	C	1.97228500	-1.65162200	-0.06820700
H	-1.99435600	0.51022500	1.71807800	C	1.96897000	-2.96081700	0.41445400
H	-2.21465700	4.78923500	1.18431400	H	3.17227000	-4.67194000	0.92551200
H	-0.24363700	5.91062700	-0.05570200	H	5.31433300	-3.59455300	0.27268500
H	-3.21509000	2.67974000	2.06824000	H	5.31566100	-1.21202900	-0.51294000
N	-0.41833200	1.39001300	0.74966100	H	1.03132300	-3.44102400	0.67657800
Co	0.65980800	-0.20002300	0.35726800	C	3.18982600	0.45000700	-0.69387800
C	-4.07670800	0.30561700	-1.26457700	O	4.14660300	1.02977500	-1.21857800
C	-4.59086000	-0.88183200	-0.72152700	N	2.01143900	0.99787500	-0.26730700
C	-3.71479800	-1.92434600	-0.39353800	C	1.67804000	2.33696000	-0.30626000
C	-2.34513500	-1.77465700	-0.60740200	C	0.38891900	2.63565500	0.26001600
C	-1.81249500	-0.59653500	-1.15116600	C	2.42536900	3.39773300	-0.81285400
C	-2.71296200	0.43933700	-1.47089000	C	-0.10845900	3.96777500	0.30752700
H	-4.76524700	1.10632500	-1.51380200	C	1.92259400	4.71755500	-0.76273300
H	-4.08558500	-2.84914400	0.03139300	H	3.39731700	3.18827900	-1.23756500
H	-1.67977000	-2.57829800	-0.32042400	C	-1.53359600	1.79382100	1.28650500
H	-2.32520600	1.36727300	-1.88245900	C	-1.38554700	4.15904600	0.89203400
C	-0.37775100	-0.37195400	-1.37975700	C	0.68970900	5.01527100	-0.22116800
C	0.59048200	-1.39766600	-1.50802000	H	2.53667300	5.51802000	-1.16563300
C	1.35174300	-1.77099200	-2.72814700	C	-2.09316100	3.08297600	1.38397600
C	0.40785700	-2.76674600	-2.05034400	H	-2.05609600	0.91083700	1.63890300
H	2.41021600	-1.99085800	-2.65775200	H	-1.79555700	5.16372900	0.94712700
H	1.04319300	-1.29440700	-3.65494400	H	0.32004900	6.03528600	-0.18710000
H	-0.55917000	-2.97173200	-2.50190500	H	-3.07101400	3.20786400	1.83522200
H	0.87443200	-3.61796400	-1.57208800	N	-0.34333000	1.58643600	0.74608100
H	-0.15265700	0.55113300	-1.90835300	Co	0.63248500	-0.19814100	0.49007200
C	0.39850600	-1.07522800	2.53671400	C	-4.00345000	0.50988700	-1.26611000
O	-0.36151800	-1.40015000	1.55492800	C	-4.59685900	-0.67287400	-0.79082000
O	1.31531900	-0.23241600	2.30911000	C	-3.79645000	-1.79758100	-0.53864200
C	0.21929900	-1.71141900	3.88265300	C	-2.42668900	-1.73672900	-0.76415600
H	0.72318500	-2.68479900	3.87738400	C	-1.81391700	-0.56554400	-1.24832000
H	0.66699400	-1.09315600	4.66246500	C	-2.63907000	0.55871300	-1.48304200
H	-0.84050500	-1.87947600	4.08793600	H	-4.63595100	1.37124600	-1.45276300
O	-5.94082800	-0.92342000	-0.55103700	H	-4.23011700	-2.71375600	-0.15793300

H -1.81659000 -2.60007900 -0.53399600  
H -2.18621600 1.47815400 -1.84254700  
C -0.39288500 -0.45138400 -1.51344800  
C 0.52978800 -1.51336600 -1.60969300  
C 1.33820500 -1.91161000 -2.79137100  
C 0.32585600 -2.87268200 -2.16583800  
H 2.38577100 -2.15770500 -2.66079000  
H 1.09438700 -1.43221400 -3.73608000  
H -0.61768900 -3.05027400 -2.67587500  
H 0.73382800 -3.73591600 -1.65450500  
H -0.06627200 0.50818800 -1.90827800  
C 0.02425200 -1.21882200 2.66985700  
O -0.76874300 -1.37062600 1.68644500  
O 1.10254600 -0.56466300 2.51743400  
C -0.29067200 -1.85137600 4.00248800  
H 0.08059500 -2.88278700 3.99569600  
H 0.20580500 -1.31562900 4.81363300  
H -1.36974400 -1.88150800 4.16882300  
O -5.93943000 -0.62755500 -0.60534400  
C -6.59350500 -1.79970300 -0.12916700  
H -6.22700500 -2.09012500 0.86282000  
H -7.65217700 -1.54497900 -0.06064400  
H -6.46862500 -2.63921000 -0.82359500

15\_Q

C -1.79124700 4.28995600 -0.68066700  
C -0.94884800 4.24955900 -1.79336000  
C 0.22927900 3.51104900 -1.73653500  
C 0.55730700 2.76637600 -0.59724000  
C -0.29819200 2.78568900 0.52206700  
C -1.45486700 3.57497100 0.46688500  
H -2.69947300 4.88527800 -0.70123500  
H -1.19792700 4.80789700 -2.69079100  
H 0.91458200 3.50595800 -2.57825300  
H -2.09528500 3.62602800 1.34281700  
C 1.90473600 2.08093500 -0.56928600  
O 2.91880200 2.77978200 -0.68263700  
N 1.85146000 0.72574200 -0.42846000  
C 2.98777600 -0.05647900 -0.23843100  
C 2.75199000 -1.47368400 -0.14807800  
C 4.30606800 0.37688000 -0.09907800  
C 3.81695200 -2.39281900 0.08232400  
C 5.35518300 -0.54094400 0.13059900

H 4.51163200 1.43367300 -0.17797600  
C 1.18024700 -3.20452200 -0.22175200  
C 3.48188000 -3.76700200 0.15667500  
C 5.13757200 -1.89798800 0.22269200  
H 6.36395100 -0.15098600 0.23323400  
C 2.17351300 -4.17513300 0.00654100  
H 0.13625400 -3.46541200 -0.35728700  
H 4.27215100 -4.49203800 0.33084600  
H 5.95270200 -2.59344100 0.39622500  
H 1.89822500 -5.22259300 0.05720500  
N 1.46624100 -1.91207400 -0.29244200  
Co 0.15916300 -0.34195500 -0.58853100  
C -2.70614700 -2.25062800 1.64851100  
C -3.79869800 -1.66723000 0.97524600  
C -3.73614600 -0.31696100 0.59962500  
C -2.60282400 0.43485000 0.87181600  
C -1.46860700 -0.13064800 1.52661100  
C -1.57837300 -1.51061500 1.90899400  
H -2.77565400 -3.29301700 1.94174000  
H -4.56773900 0.15585400 0.09156600  
H -2.57577400 1.46749700 0.55637200  
H -0.73825200 -1.97208000 2.42037000  
C -0.26804900 0.56193900 1.85094500  
C 0.04675500 2.01478700 1.77418100  
C 1.31435500 2.43767900 2.49312800  
C -0.01113400 2.77746600 3.10484700  
H 1.89261200 3.23619700 2.04145400  
H 1.91094300 1.65195900 2.94770300  
H -0.33648200 2.22342800 3.97949800  
H -0.34200600 3.81081400 3.07078400  
H 0.46002100 -0.02644800 2.40644600  
C -1.69424500 -0.89783300 -2.10814800  
O -1.38693200 -1.77154700 -1.25075300  
O -1.01759500 0.18971900 -2.16323900  
C -2.84235400 -1.09881700 -3.06159700  
H -3.57425500 -0.29793300 -2.91773800  
H -2.48283900 -1.02760600 -4.09279000  
H -3.31679600 -2.06779700 -2.90172400  
O -4.85425200 -2.48640800 0.74126000  
C -5.97494500 -1.95423600 0.04380400  
H -5.69551300 -1.60547300 -0.95773300  
H -6.68928700 -2.77393600 -0.04757300  
H -6.44091700 -1.13064400 0.59852500

## 15\_S

C	0.89020900	-4.29466100	0.70344100
C	2.24973400	-4.09276100	0.97199400
C	2.91268100	-3.00396500	0.41889000
C	2.22860700	-2.09952600	-0.40277500
C	0.86132200	-2.31806700	-0.72579400
C	0.21507100	-3.42787400	-0.14689700
H	0.36838900	-5.14078900	1.14020300
H	2.78365800	-4.77990700	1.62141500
H	3.96034000	-2.82121100	0.63380400
H	-0.82434400	-3.61462900	-0.39551400
C	2.93309700	-0.82202900	-0.80469000
O	4.05326400	-0.78103300	-1.31646600
N	2.15450500	0.21415300	-0.40956000
C	2.43592400	1.56163300	-0.44670600
C	1.43453300	2.33252700	0.21719900
C	3.51606800	2.22764900	-1.01430500
C	1.50339900	3.74621300	0.29980900
C	3.58588800	3.63743700	-0.92960500
H	4.28972600	1.65487900	-1.50800100
C	-0.57673800	2.25366900	1.40972600
C	0.44706100	4.39726200	0.98700700
C	2.61645100	4.39292300	-0.29790800
H	4.43791600	4.13764500	-1.38072000
C	-0.57826100	3.65771200	1.53782400
H	-1.36796600	1.63054300	1.80810400
H	0.45672500	5.47983200	1.07419500
H	2.69531900	5.47393100	-0.24491000
H	-1.39558100	4.13514900	2.06604400
N	0.40000500	1.62519100	0.77193600
Co	0.55491100	-0.23060000	0.47573800
C	-3.71591000	1.61519700	-0.93637400
C	-4.58222200	0.56641400	-0.59476000
C	-4.07534800	-0.73416300	-0.48599600
C	-2.71862300	-0.96940800	-0.70628300
C	-1.83199800	0.06224500	-1.04488500
C	-2.37074900	1.35957000	-1.15927100
H	-4.12252100	2.61713900	-1.03056800
H	-4.72240600	-1.56364700	-0.22735400
H	-2.34256900	-1.97993300	-0.60394400
H	-1.71290200	2.18075700	-1.43137800
C	-0.37857900	-0.13766900	-1.23634600
C	0.14784400	-1.46292900	-1.76818800
C	0.72981600	-1.48193200	-3.16374200

C	-0.57683000	-2.17878800	-2.88677700
H	1.60890100	-2.09408900	-3.34029100
H	0.70947000	-0.54900000	-3.71924600
H	-1.49257400	-1.72391100	-3.24937400
H	-0.58141700	-3.26473800	-2.88342200
H	0.05278100	0.70386000	-1.78040500
C	-0.03435300	-1.06198500	2.64405100
O	-0.86794500	-0.81613500	1.69378100
O	1.18586100	-0.80011400	2.45890700
C	-0.53247300	-1.68709300	3.91725800
H	-0.64767100	-2.76466300	3.75460100
H	0.18081500	-1.53017800	4.72797500
H	-1.51142100	-1.28198800	4.18462700
O	-5.88738900	0.90960700	-0.39712700
C	-6.80043400	-0.12369500	-0.05717300
H	-6.52842600	-0.61118200	0.88774900
H	-7.77357500	0.35755700	0.05688500
H	-6.86628800	-0.88268000	-0.84713000

## 15\_T

C	1.34055000	4.32563200	0.59425500
C	0.14773600	4.49154800	1.29993900
C	-0.96528000	3.72636300	0.95980800
C	-0.88994000	2.76334200	-0.05321800
C	0.31582900	2.58390800	-0.76412200
C	1.41221100	3.38975800	-0.43585000
H	2.20940600	4.93025000	0.83709500
H	0.08010200	5.22371600	2.09906500
H	-1.90840700	3.86331300	1.47905500
H	2.33101900	3.28818500	-1.00505900
C	-2.14200300	1.96629000	-0.35096300
O	-3.19149600	2.54497300	-0.65018400
N	-1.95829500	0.62991100	-0.17131000
C	-2.94616300	-0.33254300	-0.29699600
C	-2.53547900	-1.67207500	0.03649200
C	-4.26520900	-0.14104400	-0.70333900
C	-3.45449800	-2.75973800	-0.03249400
C	-5.16315800	-1.22828400	-0.77651500
H	-4.58743300	0.86034100	-0.94920600
C	-0.82163800	-3.07128000	0.77255700
C	-2.97205100	-4.04065500	0.33332300
C	-4.78605500	-2.51344600	-0.45189200
H	-6.18290700	-1.03298900	-1.09604400
C	-1.66510500	-4.19904000	0.73901700



H	0.21627700	-3.15497100	1.08019400	C	-2.23312600	3.07114100	1.08466600
H	-3.64840200	-4.89002300	0.29350100	H	-3.60790800	4.57865100	0.41806600
H	-5.48803500	-3.33958000	-0.50680500	H	-2.11246400	5.32183500	-1.45002300
H	-1.27567300	-5.16796100	1.03084000	H	0.10739200	4.25754600	-1.71354500
N	-1.23993900	-1.86263900	0.42972700	H	-2.87989500	2.73837100	1.89028100
Co	-0.23944500	-0.03376500	0.49730700	C	1.27182600	2.40478800	-0.43798500
C	3.02012700	-2.63786400	-0.92594800	O	2.08646200	3.31285800	-0.65055500
C	4.17165700	-1.92106000	-0.55056500	N	1.54840100	1.06915400	-0.51283400
C	4.13006900	-0.51823100	-0.49687600	C	2.83046000	0.67132900	-0.93089100
C	2.95289300	0.15033200	-0.80038100	C	3.31988100	-0.57417700	-0.41349100
C	1.78404900	-0.54429400	-1.17954600	C	3.65221300	1.35164100	-1.82532500
C	1.85612100	-1.96121000	-1.23374200	C	4.60445900	-1.07795900	-0.77868800
H	3.07516300	-3.72031700	-0.97563300	C	4.91459200	0.84149000	-2.19795800
H	5.00513300	0.05154100	-0.21022600	H	3.32111100	2.29679400	-2.22810800
H	2.92658000	1.22916200	-0.72959200	C	2.91541900	-2.41194000	0.96760100
H	0.97278800	-2.51893000	-1.52970700	C	5.01110400	-2.30258600	-0.19507600
C	0.52166900	0.10985700	-1.46438300	C	5.40119200	-0.34244900	-1.68921400
C	0.40225500	1.55952800	-1.87236300	H	5.51317900	1.41190600	-2.90226200
C	-0.42665000	1.82641400	-3.10883800	C	4.17810500	-2.96510800	0.67971900
C	1.07147200	1.96207900	-3.17537300	H	2.20494100	-2.90973600	1.61887200
H	-1.02492200	2.73143200	-3.12275100	H	5.98611000	-2.70884300	-0.44972200
H	-0.88882900	0.97132200	-3.59382700	H	6.37903800	-0.72095100	-1.97006700
H	1.63509100	1.19744300	-3.70050500	H	4.46928200	-3.90354200	1.13816200
H	1.49110300	2.96074900	-3.24372600	N	2.51059600	-1.26523600	0.44288200
H	-0.19720500	-0.54052600	-1.96190200	Co	0.59482900	-0.43556900	0.39788300
C	0.50261200	0.49379700	2.79443100	C	-4.28245500	-1.99118300	0.35573800
O	1.24638500	0.40249800	1.74179400	C	-4.44012300	-1.44802800	-0.93102700
O	-0.71207800	0.19064900	2.72091500	C	-3.67376600	-0.33526600	-1.30337400
C	1.12730700	1.00796200	4.06507600	C	-2.76852000	0.22288300	-0.40845900
H	1.30161000	2.08408800	3.95528100	C	-2.58915000	-0.30307400	0.89220900
H	0.46960100	0.83840200	4.91869700	C	-3.37824700	-1.43164700	1.23785400
H	2.09703500	0.53129600	4.23188600	H	-4.87805300	-2.85483500	0.63304100
O	5.26513600	-2.66777200	-0.26826400	H	-3.76593600	0.09808600	-2.29158500
C	6.45447600	-1.99682700	0.13990300	H	-2.18194600	1.06740700	-0.74124600
H	6.29587800	-1.42838500	1.06387900	H	-3.25577700	-1.87135300	2.22330400
H	7.19233400	-2.77974500	0.32039300	C	-1.65842700	0.17228000	1.88466900
H	6.82495500	-1.32516100	-0.64358300	C	-0.80080000	1.29416700	1.88806400
				C	1.04317600	0.96663400	2.57747400
				C	-0.11350300	1.65838900	3.18524400
TS10_Q				H	1.82970300	1.53114600	2.09549900
C	-2.64542400	4.10326400	0.25473600	H	1.23918000	-0.06320100	2.85334800
C	-1.81040100	4.51869000	-0.78478600	H	-0.54607300	1.18361800	4.06699400
C	-0.57414000	3.91093900	-0.94563300	H	0.00169500	2.73227500	3.32702100
C	-0.14566400	2.84627200	-0.12660200	H	-1.61753500	-0.43676000	2.78323500
C	-1.00190500	2.40699000	0.90031300				

C -0.49556500 -2.65314300 0.36232900  
O -0.08361200 -2.25493300 1.49134600  
O -0.35870200 -1.89606000 -0.65984100  
C -1.10746300 -4.01870400 0.19049300  
H -1.91228500 -3.98194400 -0.54585400  
H -0.33862800 -4.70593300 -0.18188100  
H -1.48223400 -4.39785400 1.14242500  
O -5.34817900 -2.06648800 -1.73089000  
C -5.51956800 -1.57151200 -3.05380400  
H -6.27294800 -2.20972100 -3.51858200  
H -5.87753800 -0.53454100 -3.05327400  
H -4.58861700 -1.63320900 -3.63051100

TS10\_S

C -2.10910900 4.17044400 0.53454200  
C -1.26412600 4.64809000 -0.46487100  
C -0.10885000 3.94244900 -0.77788900  
C 0.23797100 2.73354900 -0.14993000  
C -0.64396000 2.23822000 0.84592900  
C -1.78273100 2.98597600 1.18661400  
H -3.00874300 4.71188800 0.81137400  
H -1.49503700 5.56968500 -0.99047900  
H 0.57433400 4.31846300 -1.52934100  
H -2.42881700 2.61205800 1.97569700  
C 1.58320400 2.18765800 -0.64102100  
O 2.37973500 2.99522800 -1.14056400  
N 1.85426500 0.85809700 -0.51878600  
C 3.10603000 0.30801100 -0.72935600  
C 3.24163100 -0.98712900 -0.13845700  
C 4.21121000 0.82888800 -1.40187300  
C 4.43687400 -1.74988900 -0.24063800  
C 5.39959100 0.07152100 -1.49886900  
H 4.14150400 1.81077000 -1.84441900  
C 2.17587200 -2.65154400 1.10849500  
C 4.43976300 -3.02502900 0.37892700  
C 5.52998300 -1.18692900 -0.94493300  
H 6.23814400 0.50427500 -2.03712000  
C 3.31891900 -3.47316000 1.04456700  
H 1.27072400 -2.97016500 1.61409800  
H 5.33200600 -3.64159500 0.31985200  
H 6.45275200 -1.75050600 -1.03772100  
H 3.29685200 -4.44688700 1.52047500  
N 2.15206700 -1.45478300 0.54264500  
Co 0.63962700 -0.29934200 0.37081400

C -3.99037700 -2.45484200 0.65377300  
C -4.79525900 -1.62667000 -0.14148500  
C -4.39420800 -0.30526300 -0.37138800  
C -3.20714200 0.17435100 0.18134900  
C -2.38945200 -0.63356200 0.98669700  
C -2.81784400 -1.96038500 1.20319500  
H -4.30365600 -3.47925800 0.82678200  
H -4.99053900 0.35905600 -0.98497300  
H -2.91089200 1.18803500 -0.04222600  
H -2.20428600 -2.61701900 1.81459600  
C -1.13248700 -0.22878800 1.63644600  
C -0.46410100 1.02788700 1.72619400  
C 1.41905300 0.63281800 2.16343700  
C 0.34890800 1.30712600 2.96024200  
H 2.23097900 1.25401800 1.80760200  
H 1.72068700 -0.32871500 2.56345800  
H 0.01409900 0.78049800 3.85326200  
H 0.49972400 2.36677800 3.15357800  
H -0.91240300 -0.85893600 2.49874500  
C -0.78451500 -0.88865100 -1.55630500  
O -0.07961300 -1.69979900 -0.85980100  
O -0.75668700 0.33620800 -1.26408100  
C -1.65351800 -1.42268600 -2.66009400  
H -2.54889000 -1.86696400 -2.21259500  
H -1.95760400 -0.61886300 -3.33253400  
H -1.12841400 -2.20389000 -3.21569100  
O -5.93219900 -2.19142600 -0.63781200  
C -6.76242600 -1.38961900 -1.46627000  
H -7.60043500 -2.02434300 -1.75997700  
H -7.14706600 -0.51369300 -0.92860600  
H -6.23257700 -1.05438800 -2.36693100

TS10\_T

C 3.54742300 3.53096000 -1.00353300  
C 3.04399000 4.12560900 0.15424600  
C 1.81002100 3.72445500 0.64744200  
C 1.04958000 2.70775600 0.03799700  
C 1.56238000 2.11282100 -1.12896000  
C 2.79978500 2.54767100 -1.63805900  
H 4.50722800 3.83223200 -1.41198700  
H 3.60627900 4.90147300 0.66497700  
H 1.38834000 4.18967900 1.52969000  
H 3.17904600 2.08543600 -2.54483900  
C -0.25320000 2.41206500 0.76030600

O	-0.71199600	3.32563600	1.46254400	H	-1.03145700	-4.54070300	-2.30053200
N	-0.81274800	1.17406500	0.63351500	O	4.50003100	-3.05813500	2.09446600
C	-1.96624800	0.92340500	1.39901800	C	4.93262200	-2.45117900	3.30765500
C	-3.00958200	0.18073300	0.76197300	H	5.50815000	-3.21315400	3.83556100
C	-2.17408500	1.31660200	2.71567200	H	5.57471000	-1.58271200	3.11658500
C	-4.23441500	-0.10774400	1.43522700	H	4.08251800	-2.14561200	3.92912000
C	-3.37472100	1.00833100	3.39051900				
H	-1.40846300	1.88593600	3.22333300				
C	-3.72219300	-0.90847200	-1.16577100	16_Q			
C	-5.22183400	-0.81644700	0.70678700	C	-2.31687700	4.04083200	0.30682300
C	-4.39909400	0.32176000	2.77418200	C	-1.54788800	4.51502000	-0.75832600
H	-3.48888600	1.33512500	4.42011400	C	-1.87590800	2.94044000	1.03112700
C	-4.97610000	-1.20421300	-0.59133900	H	-3.25339300	4.52314200	0.57045000
H	-3.46318300	-1.25138200	-2.16228500	C	-0.33447300	3.90604400	-1.05089200
H	-6.16806900	-1.04840100	1.18791100	H	-1.88261400	5.36698300	-1.34241000
H	-5.32672400	0.10401500	3.29454100	C	-0.67391400	2.28195900	0.71400000
H	-5.71621700	-1.74534900	-1.17054800	H	-2.47370700	2.55848500	1.85202800
N	-2.78210900	-0.24609700	-0.51298500	C	0.13010600	2.79382400	-0.32823200
Co	-0.69216200	-0.16661100	-0.88735100	H	0.30257200	4.29173400	-1.83793700
C	3.31288000	-2.97482700	0.07777600	C	-0.31965500	1.10292200	1.55983800
C	3.74116000	-2.32113900	1.24561600	C	1.53210400	2.34165000	-0.69177900
C	3.37149300	-0.98635700	1.46135100	C	-1.13955400	0.01719800	1.68837600
C	2.59060400	-0.31737100	0.52519900	C	0.84503000	1.31158200	2.52907400
C	2.15370700	-0.95026800	-0.65516200	O	2.28376400	3.19838600	-1.17620000
C	2.53364100	-2.30199800	-0.84296600	N	1.86400000	1.03889400	-0.44297400
H	3.60059500	-4.00951700	-0.07588500	C	-2.43460900	-0.30390500	1.06661300
H	3.68127200	-0.46096900	2.35620600	H	-0.84095300	-0.69773800	2.45313400
H	2.31088600	0.70469700	0.73128900	C	1.38255000	0.09664300	3.19826400
H	2.19688700	-2.82217400	-1.73519100	H	0.49868100	2.03548300	3.28063800
C	1.30682900	-0.36620600	-1.68201800	H	1.64938700	1.82775400	1.98426900
C	0.97670800	0.99907000	-1.94046700	C	3.18783800	0.59503900	-0.53474800
C	-0.79717000	1.27635500	-2.53292300	C	-2.93043700	0.24399800	-0.12779900
C	0.47161200	1.39220600	-3.30200400	C	-3.22868200	-1.27400100	1.71087700
H	-1.22640000	2.17446600	-2.10483100	H	1.63901800	-0.78551600	2.62055900
H	-1.49805000	0.51658700	-2.87256300	H	1.69789700	0.13278500	4.23500600
H	0.61350500	0.64470300	-4.08028900	C	3.40364100	-0.79494500	-0.22325700
H	0.76477600	2.38990700	-3.61941500	C	4.31969900	1.34785000	-0.85228100
H	1.10547700	-1.03546100	-2.51289800	C	-4.17015600	-0.12958200	-0.64192900
C	-0.96182300	-2.65258400	-1.25997900	H	-2.34220000	0.95786400	-0.68652700
O	-1.07235200	-1.96239100	-2.31618600	C	-4.46821500	-1.64873800	1.21847000
O	-0.70122900	-2.09744000	-0.14215700	H	-2.85649300	-1.74029800	2.61856400
C	-1.17355100	-4.14771800	-1.29211200	C	4.71060500	-1.36661000	-0.22763300
H	-0.49750800	-4.64272600	-0.59117300	N	2.31063200	-1.55776000	0.07731700
H	-2.20049100	-4.36440600	-0.97552400	C	5.61010200	0.77358800	-0.85227500
				H	4.19282600	2.38776500	-1.10657600

C	-4.95389500	-1.07412000	0.03433000	C	5.44505100	1.14376700	-1.02295500
H	-4.50747400	0.31413100	-1.57035000	H	3.94393100	2.68909100	-0.91968800
H	-5.07485400	-2.39115500	1.72613300	C	2.62450100	-2.73360400	0.21086400
C	4.82246200	-2.74029300	0.09639900	C	4.93706800	-2.50187200	-0.40686600
C	5.82348700	-0.55152700	-0.54924700	C	5.75715600	-0.19554400	-0.92420100
C	2.44310800	-2.84523200	0.36789700	H	6.22077400	1.85633400	-1.28834200
H	6.45289700	1.41061400	-1.10519900	C	3.88733500	-3.30827100	-0.02775800
O	-6.17622000	-1.50198700	-0.37858500	H	1.77499500	-3.32153200	0.53277700
C	3.69824200	-3.47958400	0.39387000	H	5.92452600	-2.91886600	-0.58256400
H	5.80713400	-3.19937000	0.10323700	H	6.76203600	-0.56052900	-1.11072000
H	6.81904900	-0.98394600	-0.55421100	H	4.01259700	-4.37708900	0.10343800
H	1.52085000	-3.37715200	0.57296000	N	2.41336400	-1.43254900	0.06078300
C	-6.69282900	-0.97543200	-1.59501400	Co	0.82294000	-0.48886400	0.50208800
H	3.76139200	-4.53331400	0.64108700	C	-4.62129800	-1.73855300	0.88515200
H	-7.66388800	-1.45168900	-1.74043500	C	-4.96049300	-1.18826900	-0.36090400
H	-6.82995500	0.11142200	-1.53903900	C	-4.10552300	-0.24904600	-0.95706900
H	-6.04325200	-1.21468200	-2.44607800	C	-2.94286400	0.14603400	-0.30377900
Co	0.57952600	-0.46875700	-0.14241700	C	-2.59490000	-0.37922400	0.95281900
O	-0.57708100	-1.10385300	-1.65360300	C	-3.45196500	-1.34649400	1.51647000
C	-0.96680400	-2.17418800	-1.05630200	H	-5.28292600	-2.47510800	1.32838400
O	-0.52874200	-2.43332900	0.09635200	H	-4.33070300	0.17131800	-1.92916300
C	-1.97662400	-3.06619200	-1.72570900	H	-2.28801400	0.85109600	-0.79632700
H	-2.97273800	-2.77068900	-1.37921600	H	-3.18729400	-1.79357600	2.47048900
H	-1.94005700	-2.95531600	-2.81093400	C	-1.37342600	-0.05089700	1.68888300
H	-1.81422200	-4.10795100	-1.44122500	C	-0.53779000	1.02953500	1.60468600
				C	1.47473200	-0.16208500	2.28835600
				C	0.65675200	1.09111200	2.57214200
16_S				H	2.55445100	-0.00887300	2.32110800
C	-2.56151800	3.97304700	0.43772000	H	1.19449600	-1.02933800	2.89466500
C	-1.81010400	4.45769800	-0.63464200	H	0.29935600	1.17380100	3.60817700
C	-0.60215700	3.85141100	-0.95575000	H	1.23895100	1.98678100	2.35182200
C	-0.11916600	2.74011800	-0.24344600	H	-1.13697900	-0.77676700	2.46228000
C	-0.90043500	2.22637500	0.80622300	C	-0.57673400	-2.14704900	-0.53301500
C	-2.10482900	2.86744200	1.14504200	O	-0.14031300	-2.21117500	0.67863400
H	-3.49774100	4.44721500	0.71704800	O	-0.24404000	-1.15282200	-1.23384900
H	-2.15670700	5.31253000	-1.20760100	C	-1.48795300	-3.22127800	-1.05175200
H	0.01465600	4.23029000	-1.76115100	H	-2.52050500	-2.94433200	-0.81412900
H	-2.69072900	2.46907300	1.96693200	H	-1.39376300	-3.30738300	-2.13591600
C	1.25619300	2.26933700	-0.65768600	H	-1.27218100	-4.17836500	-0.57182100
O	1.89153000	3.01987800	-1.41311400	O	-6.11892900	-1.63182000	-0.91017900
N	1.75923400	1.08580800	-0.17970500	C	-6.50124400	-1.11650200	-2.18152300
C	3.09712000	0.77505800	-0.45663800	H	-7.44776600	-1.60004400	-2.42833300
C	3.42720300	-0.60548400	-0.32588900	H	-6.64910500	-0.03041200	-2.14784100
C	4.14109700	1.63635800	-0.80201800	H	-5.76080900	-1.35875500	-2.95340300
C	4.73834200	-1.10854200	-0.56346200				

## 16\_T

C	-2.50997800	3.98615600	0.24885900
C	-1.71312300	4.42351500	-0.81009400
C	-0.49575800	3.80130600	-1.05012200
C	-0.03975700	2.71475800	-0.28010500
C	-0.87476100	2.23820600	0.75722700
C	-2.08658700	2.90897000	1.01499600
H	-3.45285400	4.47550200	0.47438400
H	-2.02889200	5.25520400	-1.43271200
H	0.15578400	4.15361300	-1.83974000
H	-2.70588600	2.55099500	1.83028800
C	1.36601900	2.26467200	-0.64677300
O	2.03810200	3.05476300	-1.32215500
N	1.83206100	1.04378600	-0.22497700
C	3.19209600	0.72966500	-0.38363000
C	3.54516600	-0.66284400	-0.30017800
C	4.24445700	1.62701900	-0.56764000
C	4.89340600	-1.10536900	-0.44712100
C	5.57931100	1.18513000	-0.69423700
H	4.02884100	2.68082400	-0.64106600
C	2.79165400	-2.85116500	0.01834900
C	5.13169900	-2.50006000	-0.36934100
C	5.91675400	-0.14906200	-0.65225800
H	6.35381500	1.93259400	-0.84013400
C	4.08954400	-3.37307800	-0.14718100
H	1.93555900	-3.48518300	0.22471000
H	6.14812800	-2.86640600	-0.48377200
H	6.94367900	-0.48036000	-0.77047100
H	4.25062300	-4.44346400	-0.08432500
N	2.54381600	-1.55402600	-0.05605700
Co	0.79797400	-0.54484200	0.34711800
C	-4.76727100	-1.60802000	1.04479500
C	-5.08876500	-1.11706100	-0.22988200
C	-4.21046900	-0.22937200	-0.86746800
C	-3.04018200	0.17081200	-0.22954300
C	-2.70818600	-0.29418000	1.05466700
C	-3.59307700	-1.20777500	1.66301000
H	-5.44707100	-2.30555100	1.52258200
H	-4.42005200	0.14473600	-1.86182600
H	-2.36662500	0.83145400	-0.75658100
H	-3.34638800	-1.60847200	2.64244500
C	-1.47520100	0.03753600	1.77343600
C	-0.59708600	1.06982300	1.63395400

C	1.43284000	-0.19445500	2.25532700
C	0.65291900	1.07389700	2.53185800
H	2.51769100	-0.12256200	2.26233800
H	1.06448900	-1.10135200	2.73925100
H	0.35125200	1.14781800	3.58652700
H	1.26130400	1.94849700	2.30002300
H	-1.24138300	-0.67998500	2.55770300
C	-0.75257700	-2.16012200	-0.61501900
O	-0.24702000	-2.38047600	0.53546800
O	-0.40577900	-1.10920400	-1.24401600
C	-1.76641500	-3.10774000	-1.19235500
H	-2.71762100	-2.95963900	-0.67078800
H	-1.91275100	-2.92004900	-2.25690400
H	-1.45276300	-4.14206900	-1.02837500
O	-6.25518500	-1.56484200	-0.76310300
C	-6.61126800	-1.11802200	-2.06645800
H	-7.56669500	-1.59273800	-2.29602500
H	-6.73320000	-0.02855600	-2.10058000
H	-5.86879100	-1.42320000	-2.81390400

## TS11\_Q

C	1.19026800	4.44487300	0.84860800
C	-0.13704700	4.63314100	1.25691800
C	-1.13996700	3.83569500	0.70676900
C	-0.86929100	2.84989200	-0.24626300
C	0.47648300	2.69302400	-0.72828800
C	1.48449300	3.49927300	-0.11305600
H	1.98792800	5.04219500	1.27968100
H	-0.38517900	5.38200200	2.00272100
H	-2.16782800	3.95134700	1.03379900
H	2.50815800	3.36923600	-0.44772900
C	-2.06845200	1.97854000	-0.56633100
O	-3.13786500	2.52834400	-0.86242900
N	-1.87238000	0.64802800	-0.34946600
C	-2.90097300	-0.27879800	-0.32029200
C	-2.50243600	-1.63080900	-0.01804100
C	-4.26249800	-0.04726900	-0.53110200
C	-3.46423700	-2.68068700	0.08163400
C	-5.20264300	-1.09379100	-0.42885100
H	-4.58183000	0.95612300	-0.76791100
C	-0.75253500	-3.09942000	0.44330300
C	-2.98165200	-3.97828400	0.38517900
C	-4.83370800	-2.38722200	-0.12780500

H	-6.25048900	-0.86022400	-0.59620200	C	-1.16871900	2.69845400	-0.15828800
C	-1.63380700	-4.19157200	0.56730200	C	0.13751700	2.54794100	-0.71958200
H	0.31837500	-3.22531300	0.56894700	C	1.15187100	3.41078800	-0.22971800
H	-3.69069300	-4.79727100	0.46874000	H	1.72609300	4.99151700	1.09363500
H	-5.56744300	-3.18372300	-0.05300200	H	-0.58577600	5.28097900	2.00662800
H	-1.24119000	-5.17560200	0.79858900	H	-2.40552900	3.79367900	1.18566500
N	-1.17226500	-1.87625900	0.16555500	H	2.13332700	3.34519000	-0.68511300
Co	-0.03822000	-0.14494400	-0.12610200	C	-2.34887500	1.77251300	-0.34773800
C	4.51867000	-1.41911700	-1.28015900	O	-3.50582100	2.20938000	-0.37232900
C	3.82978200	-2.05925700	-0.21888000	N	-2.00101500	0.46083000	-0.33899900
C	2.68008900	-1.46883600	0.31470700	C	-2.86293400	-0.60138700	-0.18667100
C	2.15511200	-0.26391900	-0.19103800	C	-2.17879400	-1.84714200	-0.03536000
C	2.83208200	0.35092000	-1.31257100	C	-4.25581100	-0.61031600	-0.14683300
C	4.04362600	-0.24150500	-1.79820700	C	-2.87536500	-3.07276900	0.13885100
H	5.42179000	-1.88402800	-1.66218200	C	-4.94467800	-1.82845300	0.04124200
H	2.20553300	-1.91141000	1.18466000	H	-4.78844000	0.32315400	-0.25723700
H	1.87986000	0.56539000	0.87712800	C	-0.09871500	-2.91174900	0.01596700
H	4.56802400	0.23670600	-2.62156600	C	-2.09003800	-4.24709100	0.25683900
C	2.28035700	1.44114200	-2.00244000	C	-4.29179200	-3.03780300	0.18065400
C	0.88785000	1.85287100	-1.80565600	H	-6.03024000	-1.80402400	0.07159200
C	-0.10829800	-0.31829300	-2.18527400	C	-0.71604700	-4.16626000	0.19286300
C	-0.06072900	1.09763700	-2.72554300	H	0.97648500	-2.80548300	-0.05327500
H	-1.04908400	-0.84181200	-2.34568000	H	-2.58355500	-5.20521300	0.39117800
H	0.75675500	-0.92375900	-2.45344200	H	-4.84314000	-3.96204800	0.31993400
H	0.32074100	1.13964100	-3.75434500	H	-0.09427200	-5.05092600	0.27109800
H	-1.05465700	1.54819800	-2.72582100	N	-0.81060000	-1.79927000	-0.08136800
H	2.80862300	1.80921600	-2.88309500	Co	-0.18101900	-0.03523500	-0.33027800
C	0.71660600	0.93130000	2.48151900	C	4.64084700	-0.84060100	-1.17804500
O	1.85549800	1.19653400	1.96597100	C	4.09269500	-1.49146600	-0.05648600
O	-0.15690900	0.22085400	1.90880200	C	2.83144800	-1.10792200	0.40649000
C	0.40125700	1.53543000	3.82563800	C	2.07483100	-0.10915500	-0.23789600
H	-0.06995600	2.50919400	3.65243400	C	2.64416000	0.53829600	-1.37523200
H	-0.30419200	0.90608100	4.37091200	C	3.92739500	0.15227200	-1.82435900
H	1.31152900	1.69315800	4.40668100	H	5.62709200	-1.13907900	-1.51925700
O	4.39319300	-3.21053300	0.22202400	H	2.42771800	-1.55200600	1.31055100
C	3.77251600	-3.89004100	1.30846800	H	1.64514800	0.66071600	0.74789000
H	4.37925600	-4.77747600	1.49391300	H	4.35313700	0.62959300	-2.70328800
H	3.75321400	-3.26936700	2.21204800	C	1.77480200	1.32153600	-2.22923300
H	2.75037200	-4.19847400	1.05643900	C	0.50177400	1.76126100	-1.92176100
				C	-0.48851300	-0.28812000	-2.28876500
				C	-0.54132300	1.14889300	-2.83622200
TS11_S				H	-1.40863500	-0.85647300	-2.43975500
C	0.91396800	4.35804400	0.75063400	H	0.36821200	-0.83223700	-2.69555400
C	-0.37709300	4.52019000	1.26075800	H	-0.23557300	1.21290900	-3.88869400
C	-1.39799200	3.69847600	0.79625400				

H -1.52821100 1.60603600 -2.74071500  
H 1.95362900 1.15625700 -3.29364500  
C 0.47526800 0.92595200 2.37693100  
O 1.59647800 1.29534300 1.89962000  
O -0.35489900 0.23263600 1.72701000  
C 0.11724400 1.37320900 3.77324600  
H -0.37733700 2.34772000 3.69826500  
H -0.57814100 0.67018100 4.23506000  
H 1.01295200 1.49089800 4.38599700  
O 4.86693700 -2.46336400 0.49772600  
C 4.38055900 -3.11467400 1.66439900  
H 5.14837300 -3.83542200 1.95012300  
H 4.22586400 -2.40615900 2.48725600  
H 3.44194200 -3.64880300 1.46789500

TS11\_T

C 0.48862100 -4.39020300 0.27003000  
C -0.57389700 -4.53867900 -0.62596200  
C -1.56157000 -3.56061800 -0.69404900  
C -1.50470000 -2.42204800 0.11772100  
C -0.44022000 -2.27279300 1.04892200  
C 0.54425500 -3.28055500 1.10385900  
H 1.26703900 -5.14478500 0.32571400  
H -0.62834500 -5.41179100 -1.26934800  
H -2.38846900 -3.65193400 -1.39072300  
H 1.34623100 -3.18156900 1.82782100  
C -2.53855100 -1.34281600 -0.11762300  
O -3.74319000 -1.60160900 -0.21855700  
N -1.93797800 -0.13299100 -0.23759700  
C -2.56366200 1.08452600 -0.39950200  
C -1.65096600 2.18752900 -0.40970600  
C -3.92519900 1.34915100 -0.51099000  
C -2.11353000 3.52681300 -0.52360000  
C -4.37657700 2.68263500 -0.63091900  
H -4.61971500 0.52079500 -0.50375000  
C 0.57266600 2.86689900 -0.27013000  
C -1.13232200 4.54941200 -0.51011400  
C -3.50907300 3.75591600 -0.63887500  
H -5.44481400 2.85923400 -0.71897700  
C 0.19981600 4.22188800 -0.38236300  
H 1.61096800 2.57284700 -0.16481000  
H -1.44450300 5.58629000 -0.59781400  
H -3.87469400 4.77364800 -0.73234100  
H 0.96943800 4.98560700 -0.36486200

N -0.31824800 1.88534700 -0.28866100  
Co -0.04575800 -0.10900400 -0.21918700  
C 3.92967800 1.18638100 1.92894600  
C 4.09255200 1.10083800 0.53717400  
C 3.11101200 0.45873700 -0.22541400  
C 1.97381700 -0.11860200 0.36658700  
C 1.82098000 -0.03387400 1.77414100  
C 2.80601700 0.63989300 2.52704600  
H 4.69063700 1.69210200 2.51451700  
H 3.22528100 0.37560200 -1.30069900  
H 1.71678200 -1.15331500 -0.52903200  
H 2.67519100 0.74312000 3.60146300  
C 0.59378900 -0.42922200 2.47979200  
C -0.43661500 -1.24625300 2.14086000  
C -2.67503200 -0.21320100 2.74461800  
C -1.66855500 -1.26740700 3.06628200  
H -3.60520800 -0.45372200 2.24480300  
H -2.40093400 0.83249200 2.84425300  
H -1.29806600 -1.12617500 4.09208600  
H -2.13052100 -2.25762500 3.02113500  
H 0.46371900 0.09435200 3.42724100  
C 0.94621000 -1.65570700 -2.34291500  
O 1.83965000 -1.97921400 -1.48715500  
O 0.06784900 -0.77529100 -2.12305500  
C 0.93503700 -2.39218100 -3.65706800  
H 0.39158800 -3.33267600 -3.51577300  
H 0.42168400 -1.80692300 -4.42124200  
H 1.95185500 -2.63423300 -3.97270000  
O 5.21936900 1.67376700 0.03353300  
C 5.42070200 1.62028400 -1.37375700  
H 6.36589900 2.13207200 -1.56241700  
H 5.49255500 0.58626500 -1.73233800  
H 4.61791100 2.13522900 -1.91642400

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C -2.82857300 3.48227900 -0.62350800  
C -1.95075900 3.92220600 -1.61652100  
C -0.62193000 3.51147900 -1.58839100  
C -0.14990500 2.64623800 -0.59282400  
C -1.02944300 2.21514900 0.42690100  
C -2.36562000 2.64843500 0.38901900  
H -3.86748100 3.79804000 -0.62928100  
H -2.29936000 4.58251700 -2.40489200  
H 0.07878300 3.84916600 -2.34447100

H	-3.03893000	2.32443400	1.17495500				
C	1.29844500	2.22504400	-0.71791000	17_S			
O	2.14220600	3.07483400	-1.02808900	C	3.33681200	-3.49544700	-0.86443300
N	1.51588000	0.88986900	-0.52269600	C	2.40091800	-4.03242800	-1.74847900
C	2.77981500	0.31080400	-0.59288400	C	1.05271400	-3.71752300	-1.59942200
C	2.82388000	-1.09001800	-0.26425600	C	0.61540800	-2.85472800	-0.58697300
C	3.98611400	0.92345700	-0.92969000	C	1.55483100	-2.33275800	0.32354400
C	4.04715500	-1.82159400	-0.28857800	C	2.91042300	-2.66353900	0.16786600
C	5.19385100	0.19076800	-0.94938300	H	4.39138800	-3.73338900	-0.96676600
H	3.97902200	1.97437600	-1.17596900	H	2.71834000	-4.69275900	-2.54986600
C	1.62670500	-2.98570700	0.39755800	H	0.30772000	-4.12310900	-2.27419500
C	3.99053300	-3.19463600	0.05407000	H	3.62565800	-2.27714800	0.88640800
C	5.24461700	-1.15081000	-0.64140100	C	-0.85642000	-2.52344100	-0.60066100
H	6.10672500	0.71423800	-1.21898800	O	-1.63408700	-3.36111100	-1.07812000
C	2.78951500	-3.77820800	0.39577800	N	-1.21074500	-1.26939300	-0.17594100
H	0.65888800	-3.40329800	0.65888500	C	-2.49714200	-0.78117800	-0.39743500
H	4.90719500	-3.77770400	0.04438100	C	-2.64214200	0.61690200	-0.12263500
H	6.17926800	-1.70238000	-0.65897600	C	-3.62965800	-1.45468100	-0.86105700
H	2.72405000	-4.82713800	0.66177900	C	-3.87781000	1.30094400	-0.30463200
N	1.64806600	-1.69780100	0.08185300	C	-4.84990000	-0.77019900	-1.05401000
Co	0.05123600	-0.39109800	-0.07051300	H	-3.55669200	-2.50797700	-1.07827300
C	-4.43402200	-1.49278200	1.00126200	C	-1.60278000	2.55294100	0.67113900
C	-4.07656200	-1.90780000	-0.29301700	C	-3.91662300	2.67511600	0.03390100
C	-2.79719500	-1.62845300	-0.79213800	C	-4.99299900	0.57454600	-0.78955100
C	-1.86929800	-0.90558100	-0.02730800	H	-5.70142600	-1.33796300	-1.41824300
C	-2.26345300	-0.46232200	1.25993300	C	-2.78874200	3.29523100	0.52513000
C	-3.52767000	-0.78528200	1.77921500	H	-0.69799800	3.00159300	1.05888700
H	-5.42622300	-1.73576000	1.36810300	H	-4.84536600	3.22459800	-0.08967900
H	-2.51720100	-1.98005100	-1.77993200	H	-5.94057300	1.08390800	-0.93282100
H	-3.81213000	-0.46442700	2.77895600	H	-2.79400300	4.34291400	0.80378500
C	-1.25620100	0.30146600	2.03873800	N	-1.53214800	1.26582000	0.34585200
C	-0.58913300	1.40861800	1.60964800	Co	-0.06982000	0.09229000	0.69506700
C	1.26849000	1.05128000	3.31564400	C	4.00910300	2.09062600	-0.20819800
C	0.53415300	2.00902700	2.44718900	C	2.92155900	2.86263400	-0.65292200
H	1.72839900	1.38579300	4.23918900	C	1.60469000	2.52557600	-0.29464900
H	1.54219800	0.07127500	2.93622400	C	1.39355400	1.40356600	0.51863600
H	0.11081800	2.82752400	3.04789200	C	2.49410200	0.65386700	0.94006200
H	1.24047400	2.51056500	1.76619800	C	3.80470600	0.97378700	0.60135900
H	-0.97858300	-0.08484200	3.02082400	H	5.00663200	2.38756600	-0.51529800
O	-5.04360900	-2.59192300	-0.97204000	H	0.77275300	3.11354800	-0.66543100
C	-4.74950000	-3.02261100	-2.29275000	H	4.64924900	0.38169300	0.94334700
H	-3.91511800	-3.73551500	-2.31183800	C	1.85847200	-0.35361500	1.83478200
H	-5.65087500	-3.51984300	-2.65652200	C	1.17345000	-1.49063400	1.47863000
H	-4.51374300	-2.17778000	-2.95211200	C	-0.81238300	-0.54633100	2.38880500



C	0.02213900	-1.83316000	2.43987600
H	-1.88916700	-0.69637400	2.30819500
H	-0.57544000	0.18195000	3.16772600
H	0.39847500	-2.07852200	3.44142000
H	-0.54172200	-2.69287800	2.07676000
H	1.67203300	0.02187700	2.84075000
O	3.25256000	3.92812600	-1.44072700
C	2.20007900	4.74029100	-1.93898900
H	1.62963100	5.21001800	-1.12709600
H	2.67662300	5.52000100	-2.53621800
H	1.51334600	4.16932800	-2.57690800

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C	4.13414900	-2.42464600	-0.83233700
C	3.38352500	-3.06380200	-1.81943200
C	1.99509100	-3.07152300	-1.73016600
C	1.32632500	-2.43736500	-0.67366100
C	2.08391100	-1.81438900	0.33719900
C	3.48489800	-1.81470600	0.23676200
H	5.21852600	-2.40913900	-0.88684400
H	3.87620600	-3.55198700	-2.65485800
H	1.39334500	-3.56182600	-2.48668400
H	4.06221300	-1.34269900	1.02488600
C	-0.17934200	-2.45567900	-0.76795800
O	-0.71382800	-3.43178500	-1.31016200
N	-0.83254300	-1.33474200	-0.32216100
C	-2.17779500	-1.11909200	-0.62391300
C	-2.74552600	0.07558100	-0.05908400
C	-3.01669300	-1.88470300	-1.43732900
C	-4.08327800	0.48181900	-0.33773100
C	-4.34258800	-1.48053200	-1.70614000
H	-2.63230700	-2.79752100	-1.86357200
C	-2.39532100	1.94521800	1.30444800
C	-4.53740900	1.68423900	0.25658100
C	-4.88248700	-0.32654700	-1.18271600
H	-4.94787000	-2.11121800	-2.35106000
C	-3.69918800	2.41603900	1.07017800
H	-1.70181400	2.48807700	1.93794500
H	-5.55219700	2.01851400	0.06070500
H	-5.90330200	-0.02769700	-1.39847700
H	-4.02326200	3.34097000	1.53354000
N	-1.94840700	0.81969800	0.76174700
Co	-0.19998600	0.01041500	1.01356900
C	3.30718900	2.99077800	-0.00723800

C	2.16172100	3.24298600	-0.78693700
C	1.00526800	2.46112700	-0.63474500
C	1.02696300	1.39762000	0.27227600
C	2.18062100	1.15280600	1.02669200
C	3.31947300	1.95349700	0.92038500
H	4.17346200	3.62841200	-0.15105400
H	0.11633700	2.66693400	-1.22181600
H	4.20198400	1.77590500	1.53025700
C	1.83523400	0.05405600	1.97245100
C	1.50316100	-1.22208000	1.56739000
C	-0.64526900	-1.08918100	2.62352200
C	0.56814100	-2.01894300	2.49273200
H	-1.61898100	-1.56188800	2.48833600
H	-0.63668600	-0.46297400	3.52073500
H	1.06065300	-2.26286600	3.44280000
H	0.29886100	-2.96177500	2.01277900
H	1.64280300	0.32181200	3.01318300
O	2.27947700	4.28297900	-1.66281600
C	1.16525700	4.58274100	-2.49109900
H	0.28774700	4.87670100	-1.90090200
H	1.47146500	5.42289200	-3.11739400
H	0.89770800	3.73399100	-3.13291100

TS12\_Q

C	1.94859400	4.13016400	1.94610800
C	0.99114000	3.13943900	2.12956800
C	0.29368800	2.60289800	1.03858500
C	0.54862800	3.07845700	-0.26490400
C	1.49886400	4.09290300	-0.43059100
C	2.19453600	4.61360400	0.65944400
H	2.49307700	4.52771000	2.79676000
H	0.75880500	2.76285800	3.11917500
H	1.71638200	4.46563500	-1.42506800
H	2.93422500	5.39296900	0.50092800
C	-0.19886300	2.47669700	-1.41575400
C	-0.28264400	0.99105500	-1.38188100
C	-0.78634600	1.62142100	1.35203300
O	-1.32844700	1.62999300	2.45216900
N	-1.14123600	0.66675700	0.37469500
Co	-0.07687900	-1.16306400	0.72367300
C	1.91860700	-2.06169400	1.74812800
O	1.68436700	-0.80671600	1.72206100
O	1.02302600	-2.85890200	1.31999600
C	3.23925200	-2.59271900	2.22978400

H	3.74209100	-3.08123400	1.38891600	C	-0.37020900	3.77443400	-1.49243000
H	3.86666100	-1.79218000	2.62291800	C	0.08071800	2.87359500	-0.52520800
H	3.07556200	-3.35242300	2.99950300	C	-0.58558500	2.75633600	0.70664000
C	-1.42216600	3.21667600	-1.93893600	C	-1.71674200	3.54249900	0.93826300
C	-0.19141400	3.12692300	-2.79106900	C	-2.18143300	4.42259100	-0.04034000
H	-1.64753700	4.17192500	-1.47569900	H	-1.86894400	5.22726400	-2.01790100
H	-2.29073700	2.62112200	-2.20044800	H	0.17899700	3.85676400	-2.42393500
H	-0.20264000	2.45405500	-3.64258700	H	-2.24509300	3.45895800	1.88224300
H	0.39644600	4.02559200	-2.94340300	H	-3.06882300	5.01860200	0.15173200
C	-2.50512400	0.36097900	0.24625900	C	-0.00151600	1.82199300	1.72211700
C	-2.84894400	-1.00555500	0.05429200	C	0.21006600	0.41134700	1.25071000
C	-3.51824200	1.33601100	0.16405600	C	1.34374000	2.12446700	-0.76693400
C	-4.20226300	-1.38542600	-0.23122800	O	2.27828600	2.62233300	-1.38379900
C	-4.83507400	0.96117400	-0.09998500	N	1.39689900	0.82121000	-0.24207200
H	-3.26583400	2.37815100	0.32485000	Co	0.22184300	-0.46621600	-1.09418900
C	-2.12492900	-3.24575900	-0.02440100	C	-1.75022700	-0.56287600	-2.32342500
C	-4.44943900	-2.76979700	-0.42768200	O	-1.28256300	0.54984000	-1.91323700
C	-5.18654200	-0.37428000	-0.30311000	O	-1.06983400	-1.61235900	-2.07887200
H	-5.60300400	1.72821600	-0.14689800	C	-3.07489500	-0.63128000	-3.02681400
C	-3.41029500	-3.69043900	-0.32190900	H	-3.17720200	0.20474200	-3.72329300
H	-1.28543300	-3.92424400	0.08183200	H	-3.18633800	-1.58043400	-3.55369900
H	-5.45814800	-3.09876000	-0.65923300	H	-3.87167000	-0.54482900	-2.27990500
H	-6.21490700	-0.65170700	-0.51327900	C	1.04818500	2.38042300	2.66570100
H	-3.58842500	-4.75086800	-0.46561100	C	-0.30146800	1.97442300	3.19549000
N	-1.85474200	-1.93418000	0.15199600	H	1.26716400	3.44064800	2.58970300
C	0.90857900	0.14999300	-1.44034300	H	1.90407500	1.75197200	2.89260000
C	0.75970700	-1.23391700	-1.75211100	H	-0.37153400	1.06257600	3.78034400
C	2.21812400	0.59741600	-1.15399300	H	-0.98879100	2.75462900	3.50389000
C	1.83753300	-2.10725000	-1.72910600	C	2.66011700	0.24719800	0.02766500
H	-0.21800200	-1.60727000	-2.04332000	C	2.70454200	-1.15771200	-0.15153200
C	3.30108400	-0.27295600	-1.13725600	C	3.77780600	0.89367300	0.52818200
H	2.39419100	1.64029800	-0.92959600	C	3.85677600	-1.91712000	0.17692500
C	3.11766700	-1.63905200	-1.39370200	C	4.93517700	0.14685500	0.84589300
H	1.70607900	-3.16023600	-1.95252800	H	3.77130100	1.96836700	0.65907100
H	4.28204700	0.11885100	-0.89801900	C	1.53864100	-3.03146500	-0.88318700
H	-1.12648500	0.58419000	-1.93247600	C	3.78923000	-3.31647600	-0.05068000
O	4.10313400	-2.57714400	-1.33956500	C	4.98467800	-1.22456700	0.68622600
C	5.42180200	-2.13936000	-1.03164100	H	5.80414800	0.67357500	1.22833500
H	5.47058200	-1.66694100	-0.04317000	C	2.63729700	-3.86129800	-0.57803100
H	6.04372100	-3.03589800	-1.03214400	H	0.61745200	-3.42617800	-1.29658600
H	5.79909800	-1.43857700	-1.78663500	H	4.64573800	-3.94056700	0.18617400
				H	5.88227500	-1.78151500	0.93653600
TS12_S				H	2.55785300	-4.92614300	-0.76766100
C	-1.50907400	4.54015700	-1.25841100	N	1.56711800	-1.71838300	-0.67256500

C	-0.97033000	-0.47425600	1.16092300	H	-1.93627200	2.37554500	-2.67454000
C	-0.82553300	-1.83662500	1.52465500	H	0.25122600	1.80043300	-3.82752600
C	-2.27504400	-0.01196900	0.89817000	H	0.95216700	3.39250200	-3.28446200
C	-1.90283100	-2.70154300	1.53566700	C	-2.62540200	0.39861000	0.06090800
H	0.16150900	-2.21183400	1.77770100	C	-2.82928500	-1.01364200	0.12070200
C	-3.36511400	-0.87896300	0.89981700	C	-3.71510000	1.21062200	-0.21984600
H	-2.43539000	1.02509200	0.63846000	C	-4.12344900	-1.57170000	-0.09623500
C	-3.18587700	-2.23516200	1.20214700	C	-4.99525000	0.65828100	-0.43324500
H	-1.78158300	-3.74604100	1.80403900	H	-3.57826400	2.28481800	-0.25568400
H	-4.34910300	-0.48509700	0.67483600	C	-1.89862000	-3.10887300	0.50371700
H	1.01725900	-0.08144600	1.78568600	C	-4.24560800	-2.98155700	-0.00139900
O	-4.18192200	-3.16436200	1.22435300	C	-5.20700100	-0.70417000	-0.37964600
C	-5.49015800	-2.74366600	0.86597600	H	-5.82464900	1.32614300	-0.64522800
H	-5.51978400	-2.34172200	-0.15476400	C	-3.14133600	-3.74610000	0.30161800
H	-6.11953500	-3.63395700	0.91772900	H	-1.00461600	-3.67542600	0.74560000
H	-5.87921000	-1.98909200	1.56162800	H	-5.21633200	-3.44177200	-0.16253800
				H	-6.19407800	-1.12462100	-0.54555700
				H	-3.20766100	-4.82485700	0.38948300
TS12_T				N	-1.74665600	-1.79708200	0.40787700
C	1.87839200	4.20562200	1.68101600	C	0.88649600	-0.23782200	-1.34426300
C	0.73895900	3.42663300	1.85917900	C	0.61439200	-1.62700600	-1.58124000
C	0.16545000	2.75051300	0.77869700	C	2.25069700	0.12066100	-1.11692600
C	0.71983400	2.87764200	-0.50764100	C	1.63946700	-2.57434700	-1.57622600
C	1.85284200	3.67812600	-0.67969100	H	-0.38352200	-1.92677000	-1.88256200
C	2.43402500	4.33274400	0.40674800	C	3.25145100	-0.82716800	-1.09774300
H	2.32859200	4.71398200	2.52804000	H	2.50521000	1.15584200	-0.93708500
H	0.27570700	3.32615300	2.83417300	C	2.95274900	-2.19425800	-1.31094000
H	2.29430500	3.77999200	-1.66551000	H	1.42650700	-3.61957000	-1.77422900
H	3.32071800	4.94151200	0.25571800	H	4.26977300	-0.50883100	-0.91094000
C	0.03728600	2.17072200	-1.63967200	H	-1.06409700	0.33236400	-1.97277400
C	-0.20810200	0.71464800	-1.42243100	O	3.88229700	-3.18916100	-1.30306300
C	-1.10657800	2.00083800	1.01135400	C	5.22813800	-2.84744600	-1.00136800
O	-1.90249300	2.37409500	1.87244300	H	5.31832400	-2.40209900	-0.00279100
N	-1.31514500	0.87426300	0.22777300	H	5.78902500	-3.78339800	-1.02600300
Co	0.02286300	-0.75637600	0.62891400	H	5.65016300	-2.15854000	-1.74403400
C	1.86256200	-1.14619500	2.23025300				
O	1.57448300	0.04783800	1.90765100				
O	1.17980700	-2.12223700	1.78266700	18_Q			
C	3.05427500	-1.40515100	3.12365200	C	2.50778000	3.80922400	1.96039900
H	3.96989800	-1.22679600	2.54865200	C	1.35864300	3.03693800	2.08554500
H	3.05515800	-0.70496700	3.96337900	C	0.68501600	2.58911800	0.94398300
H	3.06016500	-2.43298800	3.48999600	C	1.15307300	2.91920400	-0.34067000
C	-1.04194500	2.92478200	-2.39558900	C	2.30146500	3.70921300	-0.45334800
C	0.25328500	2.58859600	-3.08101900	C	2.97428900	4.14751700	0.68706600
H	-1.21062300	3.95734000	-2.10774900	H	3.03645000	4.14870200	2.84534600

H	0.96254900	2.76501300	3.05712200	H	2.49360700	0.86165600	-0.75264800
H	2.68136800	3.97688000	-1.43330500	C	2.33946300	-2.40975000	-1.63846500
H	3.86981800	4.75254600	0.58011900	H	0.57433800	-3.43202300	-2.31754600
C	0.36407100	2.42028800	-1.50376200	H	3.92579300	-1.10075200	-0.95308800
C	-0.26372700	1.05883700	-1.27444900	H	-1.05034300	0.92063600	-2.01677500
C	-0.56954400	1.81708000	1.13034200	O	3.04249800	-3.55904200	-1.75903100
O	-1.21261300	1.85272000	2.16856600	C	4.40944900	-3.55831700	-1.35872300
N	-0.98681600	0.99046300	0.05495400	H	4.51467500	-3.28728400	-0.30147000
Co	-0.13108100	-1.03555100	0.80317200	H	4.76436800	-4.57927600	-1.50485800
C	1.82975300	-1.69148400	2.05801700	H	5.00932500	-2.87688000	-1.97382800
O	1.50115500	-0.46228500	1.91992200				
O	1.08633100	-2.58799400	1.55071200	18_S			
C	3.08916800	-2.04735100	2.79646500	C	1.85063400	3.51004800	2.35320000
H	3.23461900	-3.12746600	2.82760300	C	0.66745900	2.82213300	2.10495900
H	3.94178500	-1.56923100	2.30401400	C	0.38950900	2.33902700	0.82290400
H	3.03854600	-1.64976700	3.81475800	C	1.28277900	2.57553700	-0.23427200
C	-0.45166600	3.42823600	-2.30348500	C	2.46835900	3.26884300	0.02646700
C	0.73268200	2.74664600	-2.92784700	C	2.75676000	3.72742100	1.31162400
H	-0.34894700	4.47110600	-2.02123700	H	2.06800700	3.87552400	3.35244100
H	-1.44923100	3.13326700	-2.61413100	H	-0.05165100	2.63750300	2.89604600
H	0.54786100	1.97193800	-3.66592800	H	3.17469400	3.45255400	-0.77669200
H	1.62788400	3.32904600	-3.11607900	H	3.68597600	4.25783600	1.49820800
C	-2.41753400	0.73985200	-0.04829200	C	0.85570600	2.12866300	-1.59612600
C	-2.87590900	-0.57052900	0.13876700	C	0.19060700	0.76500500	-1.62735200
C	-3.29236300	1.78619800	-0.38182700	C	-0.89536300	1.61813700	0.59961900
C	-4.27068100	-0.85748300	-0.05311200	O	-1.97119200	2.00540300	1.07488800
C	-4.64594300	1.51289900	-0.55323200	N	-0.87824700	0.66707000	-0.55803200
H	-2.90220300	2.79250900	-0.49295200	Co	-0.45413900	-0.40446100	1.06800100
C	-2.43126300	-2.85671300	0.63668700	C	1.27274800	-0.94016900	2.52416100
C	-4.69734000	-2.20580800	0.11243800	O	1.49758900	-0.23480800	1.49463200
C	-5.12798800	0.20975500	-0.40009000	O	0.06502300	-1.31897300	2.71967200
H	-5.33098800	2.31618900	-0.80792200	C	2.37073200	-1.29029500	3.48536200
C	-3.75278100	-3.19357200	0.45356900	H	2.05970600	-2.09056000	4.15868100
H	-1.67773500	-3.58740300	0.91024100	H	3.26605300	-1.58583500	2.93227600
H	-5.74371100	-2.45579600	-0.02853800	H	2.62235400	-0.40265800	4.07646800
H	-6.18453000	-0.00043100	-0.54214900	C	0.27858400	3.18804200	-2.52556400
H	-4.05725800	-4.22775800	0.58110200	C	1.59690700	2.53844000	-2.84166700
N	-1.97905400	-1.56105300	0.49054100	H	0.28811000	4.21078200	-2.16349100
C	0.69027500	-0.12497000	-1.40767100	H	-0.58755300	2.92859100	-3.12750400
C	0.17343900	-1.36012800	-1.86673400	H	1.63279800	1.81393300	-3.64950800
C	2.05745700	-0.06624400	-1.09922300	H	2.49985600	3.13087300	-2.74323600
C	0.97904000	-2.48500600	-1.97862000	C	-2.20176400	0.32435500	-1.00943300
H	-0.87540500	-1.42907600	-2.13672100	C	-2.91527900	-0.54607400	-0.15410000
C	2.87812300	-1.18857100	-1.21148600	C	-2.81059700	0.79826700	-2.15028900

C	-4.24498700	-0.94096400	-0.44859100	O	1.02332500	-2.06073000	-2.21519800
C	-4.13021700	0.39302400	-2.46744900	N	0.37025200	-1.59248800	-0.07521100
H	-2.29434500	1.49183200	-2.80361200	Co	-0.39539000	0.67448000	-0.86065600
C	-2.87134300	-1.78456100	1.81159500	C	0.10507300	2.81984800	-2.02284300
C	-4.88281900	-1.80615300	0.47780400	O	0.90264000	1.81874800	-1.92816100
C	-4.83814700	-0.45246400	-1.64143400	O	-1.06291800	2.77575300	-1.55299200
H	-4.58881000	0.77179700	-3.37529800	C	0.62688200	4.07903900	-2.68073200
C	-4.19686900	-2.21800100	1.59911000	H	-0.18584800	4.77406300	-2.89802600
H	-2.29999200	-2.09243800	2.67985700	H	1.34060700	4.56565200	-2.00582700
H	-5.90278300	-2.12986900	0.29391100	H	1.16560400	3.83098700	-3.59916300
H	-5.85209900	-0.75080000	-1.88933300	C	2.67013100	-2.64284100	2.26231300
H	-4.65685800	-2.87479000	2.32903700	C	2.62702900	-1.35306800	3.03378100
N	-2.24668500	-0.97712500	0.96178900	H	3.64088800	-3.02679500	1.96554100
C	1.12825400	-0.42722700	-1.54295300	H	1.92358000	-3.40282100	2.47503400
C	0.58605700	-1.71823700	-1.66270900	H	1.83837500	-1.21938000	3.76809700
C	2.50103300	-0.30709100	-1.35036300	H	3.56402400	-0.88007400	3.30525900
C	1.38642800	-2.84641600	-1.56928300	C	-0.83472900	-2.35766400	-0.23691200
H	-0.48051400	-1.84059300	-1.82793300	C	-2.06063100	-1.68781000	-0.48245000
C	3.32544600	-1.43215800	-1.25998400	C	-0.80778900	-3.73014400	-0.07931900
H	2.94782100	0.67261600	-1.23980200	C	-3.27066400	-2.44679500	-0.51084500
C	2.76787400	-2.70929100	-1.35911000	C	-1.99740500	-4.48301600	-0.14640100
H	0.96793800	-3.84366000	-1.65733000	H	0.14399000	-4.22043800	0.09728200
H	4.38794300	-1.29733100	-1.09904000	C	-3.23440800	0.29980300	-0.82507600
H	-0.34177100	0.68718700	-2.57714200	C	-4.49187700	-1.74620600	-0.68990800
O	3.47432300	-3.87211400	-1.27690500	C	-3.20693500	-3.85310900	-0.34722100
C	4.87060700	-3.78206600	-1.03283300	H	-1.95452800	-5.56096100	-0.02792700
H	5.08322800	-3.28035100	-0.08016900	C	-4.46585300	-0.37495200	-0.82960500
H	5.23684300	-4.80925900	-0.98576700	H	-3.17674000	1.37337400	-0.96805200
H	5.39076500	-3.25274500	-1.84145900	H	-5.42578700	-2.29936800	-0.70844300
				H	-4.13033100	-4.42385400	-0.38141900
				H	-5.37891000	0.19634200	-0.95773700
				N	-2.05825000	-0.32262400	-0.67437900
				C	0.11086600	0.12902400	1.68153700
				C	-1.09168700	0.19740900	2.40452400
				C	0.68586600	1.33062800	1.22500100
				C	-1.74195800	1.40593100	2.61017800
				H	-1.53956900	-0.71917000	2.77881900
				C	0.03692100	2.55647000	1.43675700
				H	1.66159700	1.33115800	0.75349700
				C	-1.19866900	2.59178500	2.08634000
				H	-2.68811600	1.45369400	3.13874300
				H	0.48933100	3.45980900	1.05019800
				H	0.20700200	-1.96790100	1.96168600
				O	-1.94051400	3.71879400	2.24962400
18_T							
C	4.62020500	0.09179600	-1.66316700				
C	3.39063700	-0.51674800	-1.89356000				
C	2.61281300	-0.95478000	-0.81808400				
C	3.06514900	-0.79942800	0.50492800				
C	4.30236700	-0.18729500	0.72343300				
C	5.07254400	0.25724900	-0.35209300				
H	5.21978700	0.44153900	-2.49757100				
H	3.00535600	-0.65373500	-2.89713700				
H	4.66843500	-0.04768000	1.73481400				
H	6.02804400	0.73785500	-0.16321700				
C	2.20499000	-1.35733500	1.58939600				
C	0.70954700	-1.22286800	1.34065300				
C	1.30115400	-1.59157200	-1.11529000				

C -1.55385300 4.86661000 1.49540700  
H -2.35411600 5.59683900 1.62837800  
H -0.61572800 5.29723200 1.86858000  
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C -3.31881200 1.50207100 -1.92938800  
C -3.07166200 2.83874600 -1.57232000  
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C -0.85048500 2.20362700 -0.89198500  
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H -4.29482400 1.22691500 -2.32233400  
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C 0.47323400 2.58482600 -0.35398900  
O 0.77869900 3.71688200 0.01604800  
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C 2.66393000 1.54164700 -0.02862800  
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C 3.44337900 2.69353700 0.22505200  
C 4.72229000 0.15782100 0.25008700  
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C 5.29774800 -1.13407000 0.25324800  
C 5.45666900 1.35142400 0.49798800  
H 5.38835500 3.48323600 0.66953100  
C 4.50265700 -2.23398000 -0.00004800  
H 2.47146200 -2.87728500 -0.45237100  
H 6.35891600 -1.24580000 0.45558000  
H 6.52109900 1.28286000 0.70023000  
H 4.91227600 -3.23771100 -0.00238500  
N 2.56972200 -0.83841000 -0.26468000  
Co 0.47533400 -0.36325400 -0.69504700  
C -0.53303200 0.05156600 2.20116600  
C 0.31303900 -0.95636800 2.43465900  
C 0.54536800 -2.39913600 2.52308100  
C 1.62114900 -1.38237300 2.94269300  
H 0.68878200 -2.94254700 1.59167500  
H 0.04024300 -2.96547400 3.30444500  
H 1.81921400 -1.26602400 4.00731700  
H 2.50357400 -1.28323000 2.31676400

C 0.26843600 -2.48020100 -1.97901900  
O -0.04134600 -2.37301700 -0.73445400  
O 0.78163500 -1.51044900 -2.59508100  
C -0.02576000 -3.78531500 -2.68107000  
H -1.10229100 -3.84719800 -2.87592900  
H 0.50723200 -3.84800200 -3.63109400  
H 0.23951800 -4.63005600 -2.03937500  
H -0.17414500 1.06604500 2.37224200  
C -1.93542800 -0.06257900 1.79067600  
C -2.74929600 1.08540400 1.81397600  
C -2.50923600 -1.26679600 1.36196900  
C -4.07995100 1.03343400 1.43056200  
H -2.32122200 2.03355300 2.12598100  
C -3.83902000 -1.33083000 0.95848200  
H -1.89440300 -2.15669200 1.29905300  
C -4.63446900 -0.17731900 0.99172200  
H -4.70336800 1.92092300 1.43702300  
H -4.24254500 -2.27499300 0.61358900  
O -5.94147200 -0.13046400 0.61067900  
C -6.53737800 -1.32706900 0.12963100  
H -7.56691500 -1.07033000 -0.12642100  
H -6.02661700 -1.70132100 -0.76660900  
H -6.54397300 -2.11332600 0.89516900

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C 2.58107000 2.70254100 1.40129000  
C 2.00153800 3.89957300 0.96418000  
C 0.74344500 3.87894800 0.36485200  
C 0.08109900 2.65831000 0.20469400  
C 0.66657300 1.45149300 0.61644300  
C 1.92006400 1.48195500 1.22550000  
H 3.56102800 2.71802100 1.87204900  
H 2.52899100 4.83976500 1.09748600  
H 0.25578100 4.78910200 0.02746500  
H 2.40029500 0.55967100 1.53832000  
C -1.29239600 2.56494600 -0.35955500  
O -1.94447700 3.52877500 -0.77391900  
N -1.72251400 1.25820800 -0.31154400  
C -3.02421600 0.84790100 -0.50233500  
C -3.26346700 -0.51464200 -0.12925700  
C -4.10502400 1.59019700 -0.97952500  
C -4.55771900 -1.10062000 -0.22129000  
C -5.38317900 0.99965400 -1.07602400  
H -3.94461500 2.62106900 -1.25958100

C	-2.33458600	-2.47580300	0.71802700	C	4.81025400	1.06734100	0.05583000
C	-4.68175000	-2.45007200	0.19531500	C	5.13226700	-0.14332900	-0.56892200
C	-5.62665200	-0.30980200	-0.71113200	C	4.12332200	-0.94806100	-1.09697000
H	-6.20134900	1.60870600	-1.45023000	C	2.79728200	-0.52462500	-0.99891100
C	-3.58186800	-3.13079200	0.67030600	C	2.46986700	0.67845100	-0.36288100
H	-1.44204800	-2.97594300	1.07958300	C	3.47701900	1.48259600	0.16698800
H	-5.65246800	-2.93446200	0.13985600	H	5.60162400	1.68990100	0.46510200
H	-6.61940600	-0.74161500	-0.78746600	H	6.17022600	-0.45420100	-0.64202200
H	-3.65515900	-4.16038400	1.00246100	H	4.34214000	-1.89231700	-1.58658400
N	-2.18399800	-1.22231200	0.32065500	H	3.23921300	2.41354600	0.67173200
Co	-0.54394200	-0.04524700	0.38962700	C	1.65251400	-1.29301000	-1.55737300
C	0.92750400	0.01988800	-1.58767200	O	1.74201400	-2.36794600	-2.14512000
C	-0.10686700	-0.88256900	-1.59019300	N	0.47980400	-0.59019700	-1.32224600
C	-0.23810500	-2.31313400	-1.92986400	C	-0.78755100	-0.98181200	-1.73426000
C	-1.15232700	-1.25552300	-2.56521300	C	-1.82265600	-0.06751400	-1.36839700
H	-0.70497400	-2.99509300	-1.22733900	C	-1.14784300	-2.12928400	-2.43188700
H	0.54992100	-2.76021600	-2.53243500	C	-3.17988600	-0.29258500	-1.72024700
H	-0.98561600	-0.97963700	-3.60386500	C	-2.50274600	-2.35767100	-2.76952200
H	-2.19457100	-1.27042600	-2.27057300	H	-0.38104400	-2.83870700	-2.70618200
C	-0.02471200	-0.82728900	2.52143100	C	-2.33942500	1.92307200	-0.27080900
O	0.51934300	-1.32180100	1.47538700	C	-4.11733100	0.68751000	-1.31602200
O	-0.87440300	0.10232800	2.33451000	C	-3.50673600	-1.47323500	-2.43633300
C	0.34830500	-1.28466200	3.89646600	H	-2.74831900	-3.26471800	-3.31406800
H	1.22708900	-0.71683400	4.22307500	C	-3.70111300	1.79066100	-0.59921800
H	-0.46565000	-1.09411600	4.59812200	H	-1.97039400	2.76164100	0.30987200
H	0.60924100	-2.34507200	3.88851100	H	-5.16510600	0.55602500	-1.57040800
H	0.71537500	1.01928500	-1.95762500	H	-4.53959300	-1.66293100	-2.71002800
C	2.32266400	-0.26433000	-1.29827800	H	-4.40292900	2.55067400	-0.27560100
C	3.28619100	0.73167400	-1.56013800	N	-1.43893400	1.02738800	-0.64617000
C	2.75986400	-1.48767300	-0.76440400	Co	0.56755200	1.01945200	-0.35943100
C	4.62969700	0.50746300	-1.32434200	C	-2.83948700	-1.37712900	1.53870500
H	2.96078800	1.69505900	-1.94089900	C	-3.55191500	-0.40793700	2.10777100
C	4.10633400	-1.72065800	-0.50692900	C	-3.59663800	0.80106200	2.93597800
H	2.03337500	-2.25150900	-0.51951600	C	-4.87358400	0.17515400	2.35010400
C	5.05172600	-0.72269200	-0.79138900	H	-3.25227400	1.74218700	2.51184800
H	5.37420800	1.26973300	-1.52664800	H	-3.42977600	0.71346100	4.00875200
H	4.41036300	-2.67099900	-0.08622500	H	-5.55404100	-0.32371700	3.03868400
O	6.38472100	-0.84813300	-0.58273000	H	-5.37298500	0.70437900	1.54025500
C	6.87002000	-2.06564800	-0.02552500	C	0.75125600	3.44004900	-0.17287600
H	7.95117100	-1.94622600	0.05890500	O	0.57906000	2.61950700	0.80749600
H	6.44825600	-2.24765700	0.97021500	O	0.84287000	2.97972900	-1.33946100
H	6.65117600	-2.92097500	-0.67595700	C	0.86648100	4.91220800	0.11480300
				H	1.91231900	5.14232600	0.34815400
				H	0.57516700	5.49560000	-0.76015600

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H 0.25976800 5.18749000 0.97998900  
H -3.37302100 -2.13244900 0.96284900  
C -1.38728800 -1.55776800 1.61730000  
C -0.80887000 -2.71912600 1.07334300  
C -0.52596200 -0.62062600 2.21103000  
C 0.55603400 -2.95216100 1.14157400  
H -1.44843600 -3.44857400 0.58480700  
C 0.85001500 -0.84142500 2.29126300  
H -0.93444300 0.29382700 2.62599300  
C 1.39793600 -2.02114500 1.76399300  
H 0.99717300 -3.84470500 0.71200100  
H 1.47947300 -0.09774300 2.76321700  
O 2.71633200 -2.34395000 1.80039400  
C 3.60359200 -1.45683300 2.47171200  
H 4.59894000 -1.88998800 2.36479100  
H 3.59597000 -0.46142000 2.02101300  
H 3.35529100 -1.38082400 3.53847700

TS13\_S

C 2.30258600 2.82707200 1.59066200  
C 1.58178000 3.98154600 1.26278000  
C 0.41124600 3.88022500 0.51278400  
C -0.02987000 2.62732000 0.08236900  
C 0.71320700 1.46426400 0.37272400  
C 1.88060800 1.57919900 1.13224700  
H 3.20646300 2.90270900 2.18871600  
H 1.92908200 4.95313600 1.60172400  
H -0.19012100 4.75175500 0.27328700  
H 2.47579600 0.69784200 1.34611500  
C -1.37565200 2.47252800 -0.54865100  
O -2.01745800 3.41008600 -1.03518800  
N -1.78856700 1.17645700 -0.42419700  
C -3.06577900 0.72042900 -0.67231100  
C -3.28554100 -0.60912000 -0.19523800  
C -4.12719500 1.37734700 -1.29086000  
C -4.53878100 -1.26316700 -0.33972200  
C -5.37121300 0.72345100 -1.43437100  
H -3.98235200 2.38748800 -1.64624700  
C -2.34138700 -2.44414300 0.89219200  
C -4.63845600 -2.57802200 0.18062500  
C -5.59204800 -0.56193600 -0.98003500  
H -6.17965700 1.26116300 -1.92156200  
C -3.55129000 -3.16072400 0.79587600  
H -1.45738700 -2.86491600 1.35790800

H -5.57833900 -3.11503400 0.09077500  
H -6.55796500 -1.04238400 -1.09821200  
H -3.60579800 -4.16369200 1.20404600  
N -2.21915300 -1.21659200 0.40971600  
Co -0.64219800 -0.07826100 0.41222600  
C 4.74101000 0.41475700 -1.59309600  
C 5.16185100 -0.74327000 -0.91717700  
C 4.20901700 -1.59650800 -0.34381600  
C 2.85312800 -1.29500500 -0.45659900  
C 2.42071800 -0.14480700 -1.13031100  
C 3.39180900 0.70921700 -1.68543600  
H 5.49235800 1.06574800 -2.02727600  
H 4.51053900 -2.48937700 0.18958500  
H 2.12242300 -1.94010200 0.01364100  
H 3.07444100 1.61847500 -2.18838700  
C 0.99912400 0.21067300 -1.26228300  
C -0.04124800 -0.77873300 -1.28195000  
C -0.84828600 -1.22500000 -2.44764500  
C 0.02714100 -2.20973100 -1.67756600  
H -0.52104600 -0.92198500 -3.44027900  
H -1.92474800 -1.31858000 -2.34600300  
H -0.47478700 -2.95055600 -1.06185100  
H 0.93724900 -2.56826300 -2.15298600  
H 0.81775800 1.07369400 -1.89602200  
C -0.03633800 -0.64925300 2.64191600  
O 0.40266300 -1.25611900 1.59563100  
O -0.86420700 0.28957100 2.47907300  
C 0.47272600 -1.03695100 4.00034500  
H 1.43343300 -0.53618200 4.16723200  
H -0.22405400 -0.71743100 4.77701500  
H 0.64000800 -2.11525600 4.05555700  
O 6.50320300 -0.94481600 -0.86991600  
C 6.98652700 -2.09336300 -0.18184400  
H 6.62138800 -3.02077800 -0.63963400  
H 8.07389900 -2.05703700 -0.26441000  
H 6.70483400 -2.07597800 0.87807900

TS13\_T

C 2.28926800 2.75482600 1.74478400  
C 1.56113200 3.92261100 1.49802700  
C 0.38665500 3.86351400 0.74857000  
C -0.05885100 2.64282600 0.23549400  
C 0.71294600 1.48070900 0.43094600  
C 1.87751300 1.53975900 1.19369400



H	3.19281200	2.79138700	2.34678000	O	0.46547500	-1.73481700	1.49408900
H	1.90009100	4.87098200	1.90419600	O	-0.59880100	-0.08263400	2.48022000
H	-0.22527900	4.74427100	0.57907500	C	0.58225500	-1.62071500	3.90464000
H	2.48172600	0.65061400	1.33755800	H	1.53317200	-1.12987300	4.14282600
C	-1.43270700	2.54321700	-0.35982300	H	-0.13791300	-1.35641100	4.68163700
O	-2.03763200	3.51668800	-0.82195300	H	0.74958900	-2.69969800	3.88916800
N	-1.89115100	1.26364400	-0.22150300	O	6.58276000	-0.80011700	-0.90436800
C	-3.16616900	0.82704900	-0.51217900	C	7.06918700	-1.97936200	-0.27279100
C	-3.39046800	-0.56205700	-0.21150600	H	8.15701000	-1.92947900	-0.34143100
C	-4.23218300	1.55980900	-1.02924800	H	6.77627100	-2.02069600	0.78337400
C	-4.66280900	-1.16660900	-0.41597500	H	6.71733800	-2.88428000	-0.78297300
C	-5.48955900	0.94939600	-1.23508700				
H	-4.07709400	2.60492900	-1.25817600	20_Q			
C	-2.48346600	-2.55688200	0.59614200	C	-1.98824300	3.54991400	1.53490600
C	-4.79118900	-2.53487400	-0.07140700	C	-2.12570900	2.36370300	0.81663200
C	-5.71940600	-0.37785600	-0.93984300	C	-1.26422700	1.27898500	1.02075100
H	-6.29719500	1.55560400	-1.63545100	C	-0.23932000	1.41935100	1.98142500
C	-3.71310900	-3.22561900	0.43957000	C	-0.13322400	2.59895700	2.72900100
H	-1.60075600	-3.05607400	0.98273100	C	-0.98992200	3.66977600	2.50176300
H	-5.74910900	-3.02766600	-0.21213600	H	-2.67281800	4.37248700	1.34865200
H	-6.69381300	-0.83000700	-1.09541800	H	-2.93609600	2.27857000	0.10489200
H	-3.79101900	-4.27115800	0.71580700	H	0.64152900	2.66275400	3.48596900
N	-2.33218900	-1.28067800	0.27646700	H	-0.88474100	4.58541400	3.07584600
Co	-0.65597900	-0.13654200	0.41911100	C	0.76332600	0.33884300	2.30527500
C	4.81618600	0.58178700	-1.57165600	O	0.90501500	-0.02490000	3.47648000
C	5.24014800	-0.60712400	-0.95455600	N	1.47340800	-0.12077600	1.22410000
C	4.28880700	-1.49676400	-0.43615600	C	-1.40225000	-0.02741800	0.22821600
C	2.93138800	-1.20152700	-0.54612100	C	-2.82532700	-0.54186400	0.03019500
C	2.49634100	-0.02156700	-1.16616800	C	-3.18846800	-1.73782700	0.67391500
C	3.46522200	0.86950800	-1.66415300	C	-3.79687600	0.06907700	-0.77166700
H	5.56610200	1.26168500	-1.96179300	C	-4.45428700	-2.29027900	0.53743300
H	4.59264900	-2.41229900	0.05598000	H	-2.45919400	-2.24283100	1.30156200
H	2.20269400	-1.87275200	-0.10824700	C	-5.07638300	-0.47110400	-0.92395200
H	3.14536300	1.80043300	-2.12399000	H	-3.57494100	0.98766300	-1.30004600
C	1.07471500	0.32979200	-1.29305200	C	-5.41289000	-1.65883500	-0.26668800
C	0.05338900	-0.66494700	-1.36837200	H	-4.72261100	-3.21137900	1.04443600
C	-0.82475300	-1.04093900	-2.50625000	H	-5.79342700	0.04093300	-1.55384200
C	0.08666900	-2.06901800	-1.83910000	C	2.35807800	-1.19177200	1.30595600
H	-0.54882200	-0.66365300	-3.48883400	C	3.07554200	-1.47256600	0.09388800
H	-1.89352800	-1.14276900	-2.35111100	C	2.61345100	-2.01586600	2.40139200
H	-0.38851200	-2.83716600	-1.23751500	C	4.00861300	-2.54546300	0.00797700
H	0.97936000	-2.39916300	-2.36549900	C	3.53566900	-3.08232800	2.30797700
H	0.88148500	1.23105100	-1.86768200	H	2.10225600	-1.81563800	3.33071500
C	0.11747600	-1.13309400	2.55599100	C	3.47254700	-0.85359600	-2.12672600

C	4.66974800	-2.73037000	-1.23023800	N	1.36356700	-0.41443900	0.98009200
C	4.22797600	-3.35708700	1.14905800	C	-1.52150800	-0.20142900	0.30287100
H	3.69978000	-3.69613400	3.18894900	C	-2.94889200	-0.62754300	0.01073800
C	4.40857700	-1.88998000	-2.29247500	C	-3.43072400	-1.81978000	0.57283500
H	3.23557700	-0.15847800	-2.92503300	C	-3.83250200	0.10985000	-0.78684400
H	5.38711600	-3.54028200	-1.32877300	C	-4.73236400	-2.25482600	0.35876000
H	4.93811100	-4.17594500	1.09356700	H	-2.77036400	-2.41561500	1.19763300
H	4.90835000	-2.01211500	-3.24662900	C	-5.14562600	-0.30877100	-1.01413700
N	2.83316800	-0.66355600	-0.97925200	H	-3.49765200	1.03054000	-1.25317900
C	-0.57743100	0.04656200	-1.05259200	C	-5.60309500	-1.49925800	-0.43779200
C	-0.99782000	0.47003100	-2.42332400	H	-5.09677200	-3.17725000	0.79906200
C	-0.59102600	-0.97196600	-2.14421800	H	-5.79359900	0.29486800	-1.63792800
H	-0.30960300	1.06961700	-3.01335000	C	2.47120700	-1.27151000	1.01267400
H	-2.04568200	0.67952200	-2.61335100	C	3.42292400	-1.07440000	-0.03519100
H	-1.37209900	-1.72885200	-2.10294600	C	2.74324900	-2.26762700	1.94591400
H	0.34493800	-1.31924200	-2.57638500	C	4.61982500	-1.84110500	-0.12029300
H	-0.91183900	-0.79779900	0.82703600	C	3.92190700	-3.04118700	1.84996200
C	1.98649500	2.88617000	-1.51806500	H	2.05545600	-2.43180900	2.76133200
O	1.71725900	2.68241200	-0.28393200	C	3.97297300	0.16052300	-1.93217700
O	1.95098200	1.90263100	-2.32074000	C	5.50160000	-1.53948900	-1.18794600
C	2.31468800	4.27497400	-1.98825500	C	4.85331300	-2.84423600	0.85214300
H	2.70732300	4.26025000	-3.00556100	H	4.09266300	-3.81052900	2.59745100
H	1.40212700	4.88048000	-1.96192100	C	5.18631300	-0.54118100	-2.08420500
H	3.03464000	4.73824700	-1.30873200	H	3.67433000	0.94019100	-2.62514900
Co	1.36271400	0.70817800	-0.59717400	H	6.42514600	-2.10295600	-1.28697900
O	-6.62571600	-2.27238100	-0.34659900	H	5.75784800	-3.44175500	0.79783300
C	-7.62660800	-1.66472600	-1.15200200	H	5.84752100	-0.29076800	-2.90622100
H	-7.88405300	-0.66145000	-0.78976000	N	3.12791400	-0.10257200	-0.94731900
H	-7.31700200	-1.60051800	-2.20290400	C	-0.63935600	0.09644900	-0.91274600
H	-8.50545600	-2.30762100	-1.07763600	C	-1.10039700	-0.03827500	-2.31177300
				C	-0.09056500	-1.06242300	-1.77810700
20_S				H	-0.70823100	0.63574800	-3.06492500
C	-2.18987200	3.08021800	2.21033000	H	-2.11026900	-0.39134500	-2.49198300
C	-2.35136000	1.99982700	1.34340500	H	-0.39310800	-2.06524800	-1.49217200
C	-1.39244300	0.98522800	1.26174000	H	0.88496100	-1.02632300	-2.27267800
C	-0.25936300	1.06428800	2.09215200	H	-1.04916600	-1.04702400	0.80986800
C	-0.12307500	2.13113100	2.98890600	C	1.46429400	2.63445000	-1.44657300
C	-1.06944600	3.14952700	3.03799400	O	1.49374200	2.28660000	-0.21968300
H	-2.94944700	3.85600000	2.24898200	O	1.28058900	1.69384300	-2.29029500
H	-3.25011000	1.93747700	0.74292500	C	1.60245900	4.06478500	-1.85944700
H	0.73932400	2.14415300	3.64655700	H	2.05833100	4.13198400	-2.84925100
H	-0.94183700	3.98033800	3.72564700	H	0.60320400	4.51218100	-1.90933600
C	0.81057300	0.00823700	2.16389500	H	2.19060800	4.61895700	-1.12579400
O	1.17043300	-0.38645100	3.27963100	Co	1.18639700	0.45672300	-0.72335100

O	-6.85947200	-2.00254800	-0.59432000	H	5.69205400	-3.35099600	0.93460500
C	-7.77743200	-1.26295100	-1.38734000	H	4.92029300	-1.47279900	-3.46980800
H	-7.95989300	-0.26423200	-0.97073700	N	2.80361400	-0.40775300	-1.08999400
H	-7.42978300	-1.16326000	-2.42355800	C	-0.41832700	-0.57107200	-0.61095300
H	-8.71028100	-1.82944000	-1.37746600	C	-0.76246800	-1.04450000	-1.98980200
				C	-0.09365800	-1.97943700	-1.00500700
20_T				H	-0.16428100	-0.66743100	-2.81266400
C	-1.98852300	3.46226300	1.27333900	H	-1.80480700	-1.21758200	-2.23520100
C	-2.13039200	2.18016200	0.74389500	H	-0.69802900	-2.75828900	-0.54303600
C	-1.23511400	1.15441900	1.07043200	H	0.93657600	-2.26635000	-1.19004100
C	-0.18013700	1.45529700	1.96171000	H	-1.03798200	-0.92334500	1.36979200
C	-0.06876700	2.73192100	2.52422500	C	1.29668200	2.62394100	-1.89452900
C	-0.96058000	3.74073700	2.17429400	O	1.76933600	2.65716800	-0.71930900
H	-2.69738800	4.23713100	0.99638200	O	0.72338200	1.54600500	-2.28154800
H	-2.96909400	1.97093100	0.09284100	C	1.36338200	3.81658300	-2.80535000
H	0.73542100	2.92262200	3.22745600	H	1.39953500	3.50204400	-3.85040100
H	-0.85703000	4.73303600	2.60250000	H	0.45814700	4.41732100	-2.66097100
C	0.88857800	0.45439300	2.33063200	H	2.22782500	4.43645400	-2.56045100
O	1.13803100	0.18017700	3.50551000	Co	1.10116500	0.66838900	-0.48702600
N	1.55979900	-0.00155500	1.22695500	O	-6.76354800	-2.00019300	-0.26651300
C	-1.38603200	-0.28701300	0.55001600	C	-7.54979400	-1.51178200	-1.34491300
C	-2.81956100	-0.70603400	0.27571100	H	-8.52503400	-1.99228000	-1.24913300
C	-3.43908700	-1.62824000	1.13297500	H	-7.67923200	-0.42347900	-1.29143700
C	-3.56910300	-0.22193600	-0.80324400	H	-7.11389300	-1.77598700	-2.31667100
C	-4.74992100	-2.04181000	0.93272500				
H	-2.88222700	-2.02520700	1.97755600	TS14_Q			
C	-4.88873400	-0.62351800	-1.02058300	C	2.31059000	3.87438400	0.19857300
H	-3.12127600	0.47931200	-1.49918200	C	2.37903900	2.58589100	-0.32847200
C	-5.48755900	-1.53958200	-0.14782900	C	1.22886300	1.90772100	-0.74325400
H	-5.22299000	-2.75361000	1.60126700	C	-0.00526400	2.57825400	-0.65238500
H	-5.43151400	-0.22247100	-1.86768900	C	-0.06580700	3.88621000	-0.14932900
C	2.62226500	-0.90119300	1.24872200	C	1.08307600	4.52995600	0.29658700
C	3.28341400	-1.09674600	-0.01227400	H	3.22152500	4.36910600	0.52294000
C	3.10059300	-1.60414500	2.34952300	H	3.34275900	2.10015600	-0.41975600
C	4.39341000	-1.98031000	-0.13111100	H	-1.02950900	4.38350900	-0.11959000
C	4.20245300	-2.48046200	2.22084200	H	1.02417200	5.53619300	0.69974300
H	2.62543500	-1.45487500	3.30807100	C	-1.30227600	1.99579500	-1.11712200
C	3.37821500	-0.54234200	-2.27414400	O	-2.12785100	2.68407100	-1.70192300
C	4.98228600	-2.10733100	-1.41357700	N	-1.54336200	0.66950100	-0.71984500
C	4.84595200	-2.67630200	1.01877200	C	1.31547100	0.54232400	-1.42461400
H	4.54468500	-3.00866600	3.10593000	C	2.62960100	-0.18950500	-1.20670400
C	4.48325500	-1.39162400	-2.48090500	C	3.35887000	-0.68068100	-2.29748700
H	2.94529700	0.03643200	-3.08465100	C	3.10644000	-0.46094300	0.08217700
H	5.83018500	-2.77455600	-1.54075700	C	4.52597800	-1.41414800	-2.11370600

H	3.00925200	-0.48294700	-3.30745500	TS14_S		
C	4.27783200	-1.19087400	0.28362300	C	2.45076500	3.87717700 0.35209700
H	2.55132800	-0.08973100	0.93835000	C	2.38973900	2.60334700 -0.21127100
C	4.99444500	-1.67536500	-0.81935100	C	1.16330900	1.99115100 -0.48878200
H	5.09248000	-1.79130400	-2.95880500	C	-0.00851900	2.71407600 -0.22190900
H	4.62006900	-1.37574700	1.29469100	C	0.05357900	4.00089200 0.32727300
C	-2.70292800	0.03229000	-1.17193600	C	1.27903000	4.58109800 0.63191900
C	-3.38223500	-0.78200900	-0.21788500	H	3.41915000	4.32041900 0.56621900
C	-3.18266400	0.07510700	-2.49796700	H	3.31087600	2.08102500 -0.43709600
C	-4.54454300	-1.53183700	-0.59610600	H	-0.87736900	4.52675900 0.50700800
C	-4.31138500	-0.65854300	-2.85703100	H	1.32145100	5.57351900 1.07006800
H	-2.67291900	0.69277000	-3.22575500	C	-1.35606900	2.19578700 -0.55653800
C	-3.50602600	-1.56977600	1.99945000	O	-2.28327100	2.95247900 -0.83189900
C	-5.15961800	-2.31142000	0.41751400	N	-1.52857200	0.80199800 -0.50802900
C	-4.99327500	-1.45357100	-1.93388200	C	1.09955600	0.65373000 -1.22190600
H	-4.67048900	-0.60419200	-3.88079900	C	2.40863500	-0.11116400 -1.16362700
C	-4.63954000	-2.32346800	1.70846900	C	3.06435000	-0.49556200 -2.33835700
H	-3.05612500	-1.54998100	2.98555800	C	2.97752700	-0.48096400 0.06113700
H	-6.03840200	-2.89961500	0.17033500	C	4.24627900	-1.22890900 -2.29907000
H	-5.87361400	-2.01609200	-2.22897500	H	2.64678500	-0.21362300 -3.30139700
H	-5.10139900	-2.91686600	2.49024200	C	4.16198500	-1.21321700 0.12031900
N	-2.89516600	-0.82182600	1.05485900	H	2.48128400	-0.17993600 0.97744500
C	0.15023600	-0.37807700	-1.10620200	C	4.80324400	-1.59447900 -1.06746500
C	0.17440500	-1.69407100	-0.38159500	H	4.75615500	-1.52453300 -3.21006100
C	-0.18020800	-1.59809100	-1.85507100	H	4.57482900	-1.47868100 1.08612300
H	-0.63854000	-1.97675200	0.28347300	C	-2.75568700	0.28676100 -1.00177400
H	1.13988000	-2.09739800	-0.09121700	C	-3.29648800	-0.77039900 -0.23488500
H	0.54225200	-1.95301400	-2.58793600	C	-3.40543000	0.67432600 -2.16031600
H	-1.22196100	-1.77795200	-2.11537500	C	-4.49545400	-1.42938300 -0.61089300
H	1.24092300	0.74811800	-2.50124600	C	-4.60056100	0.02527800 -2.54463400
C	0.35037000	0.25960800	3.17479900	H	-3.00978800	1.48280800 -2.76066500
O	0.65872000	0.76478300	2.04119900	C	-3.04407600	-2.07737500 1.66964000
O	-0.81493100	-0.22693600	3.32377900	C	-4.95585200	-2.46363400 0.24477600
C	1.36716500	0.21346300	4.27868600	C	-5.14281600	-1.00237600 -1.79725800
H	1.94724600	1.13892000	4.29410800	H	-5.09964900	0.35018000 -3.45222700
H	0.88772000	0.04527500	5.24374300	C	-4.23528200	-2.77474800 1.37785500
H	2.06082000	-0.61174300	4.08096700	H	-2.44563300	-2.30460300 2.54450300
Co	-1.19154700	0.24989000	1.29000700	H	-5.87098900	-2.99463100 0.00041400
O	6.14477100	-2.40030300	-0.73507700	H	-6.06387000	-1.48785200 -2.10454900
C	6.65202300	-2.69663000	0.55890700	H	-4.56400300	-3.55590800 2.05427300
H	6.90121700	-1.78442900	1.11565500	N	-2.58194000	-1.10929600 0.88371900
H	5.94283000	-3.29462200	1.14537300	C	-0.09811700	-0.27503500 -0.88022800
H	7.56245200	-3.27728500	0.40051800	C	0.10840000	-1.78547500 -0.65344700
				C	-0.45078600	-1.26640800 -1.94633300

H	-0.56813300	-2.32029500	-0.00121800	C	-2.80680300	0.34768300	-1.02622600
H	1.13381800	-2.13494500	-0.61487100	C	-3.38108200	-0.72349500	-0.28038000
H	0.18949700	-1.25919900	-2.82511600	C	-3.45951200	0.79079300	-2.16502900
H	-1.49173300	-1.47692500	-2.16503600	C	-4.61857300	-1.30531500	-0.67982200
H	0.94293700	0.92640100	-2.27444200	C	-4.68378300	0.21087800	-2.56303300
C	0.49260400	-0.05817800	2.94374500	H	-3.03608300	1.60591100	-2.73753600
O	0.57662900	0.79502100	2.00207500	C	-3.20033300	-2.14313600	1.54816900
O	-0.45232800	-0.91106400	2.87556900	C	-5.12906700	-2.35401100	0.12716700
C	1.49106000	-0.08677200	4.06485300	C	-5.26215100	-0.81329000	-1.84248300
H	0.99673700	-0.33515600	5.00713500	H	-5.17402100	0.58748500	-3.45538200
H	2.23384900	-0.86728200	3.86180100	C	-4.42950400	-2.76567300	1.23940700
H	2.00476400	0.87253800	4.14587700	H	-2.60740100	-2.44635000	2.40582600
Co	-1.01225700	-0.08716200	1.15258700	H	-6.07186600	-2.82093400	-0.14329200
O	5.96073100	-2.31017300	-1.12461200	H	-6.20521600	-1.25198200	-2.15346100
C	6.56401300	-2.70064900	0.10143400	H	-4.79919100	-3.56152700	1.87639100
H	7.46533200	-3.25379600	-0.16851400	N	-2.69292800	-1.16666200	0.81252800
H	6.84543400	-1.83183100	0.70965400	C	-0.08002300	-0.19095700	-0.84166500
H	5.90507800	-3.35345500	0.68778100	C	0.14546100	-1.74057000	-0.51088300
				C	-0.37451300	-1.24400500	-1.83951300
TS14_T				H	-0.56029000	-2.30555500	0.08975800
C	2.35106600	3.85278600	0.71644900	H	1.17564200	-2.05542300	-0.40851400
C	2.32625500	2.63611300	0.03660500	H	0.28207100	-1.28012700	-2.70553100
C	1.11943600	2.04273600	-0.34411200	H	-1.40867900	-1.48886500	-2.06140700
C	-0.07430400	2.73008500	-0.06473500	H	0.88904900	1.08524900	-2.20414700
C	-0.04472900	3.96098500	0.60300300	C	0.62185500	-0.40743600	3.06320700
C	1.16151600	4.51814100	1.01141100	O	0.83698500	0.53701300	2.24308700
H	3.30502800	4.28105300	1.01038300	O	-0.32054000	-1.23904200	2.86455500
H	3.26089900	2.14207900	-0.19647500	C	1.53001000	-0.57499400	4.26045200
H	-0.98656600	4.46578100	0.78641500	H	1.86885900	0.39730000	4.62485600
H	1.17491700	5.46572500	1.54115400	H	1.02941900	-1.12690900	5.05833400
C	-1.41685500	2.24579100	-0.49489000	H	2.41543500	-1.14432000	3.95300100
O	-2.33397800	3.03412200	-0.72126700	Co	-0.80678200	-0.27281900	1.01584200
N	-1.58596500	0.86992300	-0.55580300	O	5.99486200	-2.12010600	-1.42165700
C	1.09144700	0.76205500	-1.17391300	C	6.64532100	-2.57962400	-0.24419000
C	2.41297600	0.01740100	-1.20141900	H	7.54220900	-3.10304000	-0.58011200
C	3.03513000	-0.27862600	-2.42000900	H	6.93843100	-1.74706600	0.40753700
C	3.02778100	-0.41916800	-0.02065700	H	6.01408800	-3.27613200	0.32189100
C	4.22780600	-0.99300400	-2.46704300				
H	2.58222100	0.05928600	-3.34852400	21_Q			
C	4.22501700	-1.13310000	-0.05009300	C	-1.95157200	-4.13304000	-0.83218500
H	2.55821900	-0.18942400	0.93147600	C	-2.48410800	-2.84235500	-0.84870500
C	4.83099100	-1.42766200	-1.28017600	C	-1.64793000	-1.72641100	-0.80647700
H	4.71076100	-1.22079000	-3.41156000	C	-0.25315200	-1.93094500	-0.78859700
H	4.67377800	-1.45231900	0.88276400	C	0.27885100	-3.22827400	-0.77749100

C	-0.56971800	-4.32942500	-0.78532000	O	3.90228100	-2.12688900	1.33991400
H	-2.62126300	-4.98766200	-0.85556100	O	5.12430300	-1.33767400	-0.31297700
H	-3.55815900	-2.70345900	-0.88740500	C	6.02914600	-3.19718500	0.93599600
H	1.35537500	-3.35313000	-0.76993000	H	5.77464800	-4.11534500	0.39410500
H	-0.15847700	-5.33355300	-0.76636600	H	7.00683100	-2.85537100	0.59298300
C	0.67317300	-0.78799200	-0.88978700	H	6.05300400	-3.42955400	2.00234800
O	1.88773300	-0.98768800	-1.22382900	Co	3.25542700	-0.57859500	0.13253300
N	0.20087400	0.44786800	-0.67544600	O	-7.51464600	0.72628700	0.78271700
C	-2.15624300	-0.29257900	-0.84790800	C	-8.05494800	0.16713400	1.97335700
C	-3.58701600	-0.09519800	-0.39165600	H	-9.07510500	0.54721800	2.04855500
C	-4.43582500	0.74544500	-1.12769800	H	-8.08237600	-0.92890200	1.92955100
C	-4.09756100	-0.67670400	0.77345200	H	-7.48873000	0.47957600	2.85962000
C	-5.73647400	1.00293500	-0.71630400				
H	-4.06546400	1.20972000	-2.03773400	21_S			
C	-5.40282400	-0.43044500	1.20396700	C	-1.91215100	3.26168400	2.29267800
H	-3.47646800	-1.34867300	1.35642400	C	-2.26684800	2.01978800	1.76548300
C	-6.23046200	0.41742300	0.45821900	C	-1.28848700	1.12071200	1.32855100
H	-6.38959100	1.65272300	-1.28924600	C	0.06182400	1.47864600	1.47392900
H	-5.75955000	-0.90262800	2.11104800	C	0.41684700	2.71655400	2.01749700
C	0.97275700	1.63885300	-0.91797800	C	-0.56685200	3.61728900	2.41173400
C	2.03922900	2.01988200	-0.07863400	H	-2.68901800	3.94817000	2.61670900
C	0.49148000	2.49940700	-1.92388500	H	-3.31358600	1.74733500	1.69955800
C	2.53687200	3.36850000	-0.18714200	H	1.47007000	2.95360900	2.12727400
C	1.03064400	3.77058900	-2.07200900	H	-0.28873300	4.58292900	2.82347900
H	-0.31698900	2.15512800	-2.56008500	C	1.14853600	0.49072800	1.19911400
C	3.44756700	1.63794000	1.80627900	O	2.00367100	0.21978000	2.05602400
C	3.50216200	3.80349300	0.76513700	N	0.80522000	-0.51007400	0.11741700
C	2.02443200	4.21072800	-1.19700500	C	-1.59553500	-0.26802700	0.77435400
H	0.66525900	4.42675500	-2.85607900	C	-3.03586200	-0.51984600	0.37908400
C	3.90649400	2.93471200	1.79156700	C	-3.66267200	-1.71010900	0.77883700
H	3.76855200	0.92228900	2.55730900	C	-3.77349700	0.36252400	-0.41811500
H	3.87594000	4.82070400	0.71168300	C	-4.96197100	-2.01459600	0.39424000
H	2.42099000	5.21866000	-1.27982900	H	-3.11907400	-2.41186600	1.40613200
H	4.58874800	3.26910300	2.56665000	C	-5.08120300	0.07596400	-0.81500800
N	2.58415000	1.13437600	0.84296400	H	-3.33257200	1.30380900	-0.72786700
C	-1.14820800	0.58237500	-0.09369300	C	-5.68249900	-1.12162100	-0.41094100
C	-1.18989900	0.74250100	1.40796800	H	-5.44118300	-2.93570800	0.70914500
C	-1.52776000	1.90170900	0.50471200	H	-5.61562000	0.78923800	-1.43036600
H	-0.22750400	0.76593600	1.90883000	C	1.50606600	-1.75242100	0.28578000
H	-1.98988500	0.26180100	1.95882900	C	2.89154100	-1.68454200	0.01562900
H	-2.57004500	2.18644300	0.41100700	C	0.95131600	-2.94086700	0.70458600
H	-0.82225100	2.71988600	0.43842400	C	3.72786800	-2.81670300	0.18618100
H	-2.10721400	0.03442300	-1.89742000	C	1.77384600	-4.08378000	0.85705900
C	4.97600200	-2.16607500	0.64760200	H	-0.11031500	-3.00555700	0.91121100

C	4.66278700	-0.34528300	-0.66890100	O	-2.13181400	-0.53804300	1.80574900
C	5.10875900	-2.64608800	-0.09331600	N	-0.66744200	0.56372900	0.36739200
C	3.12948800	-4.03071400	0.61266300	C	1.75687300	0.31591900	0.85518300
H	1.31961800	-5.01462500	1.18146100	C	3.16904900	0.48983300	0.33457000
C	5.56767700	-1.41734900	-0.51325000	C	3.84480900	1.69826800	0.56264500
H	4.98948500	0.63410400	-1.00060100	C	3.82529700	-0.48659900	-0.42247500
H	5.78767000	-3.48468300	0.02917400	C	5.11456500	1.93005300	0.05007800
H	3.75169900	-4.91114200	0.74036100	H	3.36278900	2.47316900	1.15321000
H	6.61741900	-1.25361000	-0.72966900	C	5.10217900	-0.27403500	-0.94557800
N	3.36676500	-0.47294600	-0.41704300	H	3.34320500	-1.44190700	-0.60067600
C	-0.59415600	-0.56254900	-0.35760200	C	5.75352300	0.94317900	-0.71371000
C	-0.84196900	-0.08975000	-1.76505200	H	5.63249700	2.86617600	0.23091300
C	-0.89148300	-1.55835100	-1.44692800	H	5.57422100	-1.05857100	-1.52401700
H	0.02233300	0.28559500	-2.29910200	C	-1.40786900	1.78008400	0.48697500
H	-1.76859200	0.42921500	-1.97572300	C	-2.76767700	1.80746200	0.05796600
H	-1.85805000	-2.04991900	-1.41324100	C	-0.81997300	2.94115100	0.94746100
H	-0.07595200	-2.18142100	-1.79637100	C	-3.50943900	3.02271300	0.14789700
H	-1.36148300	-0.98773800	1.57202600	C	-1.55110200	4.14798000	1.01732900
C	2.00211400	3.01335400	-1.48185500	H	0.21901500	2.92482400	1.25514400
O	0.91296200	2.40534800	-1.23463500	C	-4.58886000	0.68438000	-0.85161600
O	3.08790400	2.36631300	-1.28153900	C	-4.86170800	2.99940200	-0.27896200
C	2.01820100	4.44107700	-1.94082900	C	-2.87267300	4.19163300	0.63634000
H	1.98775900	5.09248800	-1.05968700	H	-1.05890100	5.04194600	1.38677600
H	2.93118900	4.65730700	-2.49877800	C	-5.40103800	1.83500800	-0.77315300
H	1.13696100	4.65509000	-2.54924100	H	-4.97576200	-0.25200900	-1.24190000
Co	2.01996000	0.84668500	-0.64672200	H	-5.45367000	3.90748300	-0.21137400
O	-6.94822900	-1.50095600	-0.73831500	H	-3.44148300	5.11447400	0.69674300
C	-7.71668500	-0.62252000	-1.55006100	H	-6.43139600	1.78376000	-1.10666000
H	-8.68345000	-1.10922200	-1.68997100	N	-3.32594100	0.66676700	-0.45371600
H	-7.87065200	0.34829100	-1.06244900	C	0.67865300	0.58035800	-0.20964000
H	-7.24922200	-0.46413700	-2.53008400	C	0.81012900	0.01628700	-1.60360800
				C	0.89441300	1.50223200	-1.37358000
21_T				H	-0.09163000	-0.38875800	-2.04741000
C	2.11511200	-3.07497800	2.64107700	H	1.72023200	-0.51458700	-1.85537100
C	2.44409000	-1.86321700	2.03235100	H	1.86546400	1.97976400	-1.44928300
C	1.45354200	-1.03324700	1.50018600	H	0.05962800	2.11790300	-1.68939700
C	0.10750200	-1.42831300	1.63224800	H	1.61214000	1.08095800	1.63192800
C	-0.22118400	-2.64072200	2.25367800	C	-2.64179700	-3.03194100	-1.66728400
C	0.77974700	-3.47126800	2.74427800	O	-1.52871200	-2.39808200	-1.72313300
H	2.90410900	-3.70722700	3.03762700	O	-3.56565900	-2.63706400	-0.89945900
H	3.48314200	-1.56130200	1.96827800	C	-2.81604300	-4.26577800	-2.51970900
H	-1.26865900	-2.90472400	2.35173700	H	-2.16028900	-5.05676600	-2.13993500
H	0.52135900	-4.41386500	3.21693500	H	-3.84902300	-4.61558600	-2.49874300
C	-1.00371000	-0.53479500	1.22460600	H	-2.50982100	-4.05547800	-3.54837600

Co	-2.19471800	-1.03577600	-0.32584400	H	-2.02853700	0.64824500	-2.30831800
O	6.99474500	1.25678500	-1.17562000	H	-1.50927200	-0.04031600	-3.91624600
C	7.67776600	0.28795700	-1.96085800	C	-0.08235300	-1.76537500	2.65971600
H	8.63504400	0.73805500	-2.22921200	O	0.33732700	-2.05193500	1.49418400
H	7.86078900	-0.63483100	-1.39621800	O	-0.73518900	-0.67718500	2.82169300
H	7.12455400	0.04678800	-2.87715000	C	0.20458100	-2.65672000	3.83309300
22_Q				H	1.12759300	-2.31129700	4.31287100
C	2.84549200	2.51808500	1.17138600	H	-0.60121800	-2.59680600	4.56716500
C	2.16504000	3.74057300	1.20372600	H	0.35191300	-3.68714400	3.50509400
C	0.78419800	3.78278600	1.01324600	H	0.23633500	-2.03381400	-1.58844700
C	0.08646400	2.59136200	0.79375300	C	2.17902900	-1.06305500	-1.47337600
C	0.77074500	1.36871900	0.76245800	C	2.72280500	-2.06663900	-0.64980900
C	2.15344200	1.32435600	0.93236200	C	3.03721900	-0.04362300	-1.91228200
H	3.92142300	2.49151400	1.32382000	C	4.05494100	-2.04012400	-0.26335600
H	2.71673500	4.66080900	1.37325700	H	2.07614900	-2.85564800	-0.28129800
H	0.23507900	4.71965900	1.02480700	C	4.37940100	-0.00852300	-1.54096000
H	2.69457200	0.38520300	0.89361000	H	2.64877800	0.74400700	-2.54709100
C	-1.39308800	2.58140400	0.56431700	C	4.89548200	-1.00674800	-0.70343400
O	-2.06172300	3.60880700	0.43805600	H	4.46827700	-2.80737400	0.38319000
N	-1.86063300	1.28624500	0.48039100	H	5.00708600	0.79829600	-1.89881400
C	-3.10847400	0.93022800	0.02027100	O	6.18488600	-1.06190200	-0.26996000
C	-3.25690000	-0.47851000	-0.22148300	C	7.06358200	-0.01470600	-0.65868000
C	-4.19681400	1.75686400	-0.25707200	H	8.02489700	-0.23877800	-0.19302100
C	-4.47321800	-1.01794000	-0.72454500	H	7.19244700	0.02348400	-1.74761300
C	-5.40280500	1.21120300	-0.75017400	H	6.71055400	0.96166300	-0.30303800
H	-4.09911000	2.81887400	-0.08354800	22_S			
C	-2.23880400	-2.57224100	-0.19504200	C	2.85696800	2.13902100	1.52107600
C	-4.51437000	-2.41496000	-0.94839500	C	2.35677100	3.42283300	1.27916600
C	-5.55727200	-0.13910900	-0.98261400	C	1.04599100	3.58183900	0.82971400
H	-6.22981700	1.88678200	-0.94821200	C	0.25558400	2.44952100	0.61953400
C	-3.40504600	-3.19060500	-0.68242400	C	0.75770900	1.15453900	0.83088700
H	-1.34435300	-3.14127800	0.03510200	C	2.06167100	1.00693500	1.30210100
H	-5.42593900	-2.86355700	-1.33301300	H	3.87694400	2.01574400	1.87752200
H	-6.49122600	-0.54262300	-1.36049600	H	2.98500800	4.29258900	1.44992400
H	-3.41324900	-4.26239500	-0.84533600	H	0.61958900	4.56464600	0.64939900
N	-2.16811700	-1.26440200	0.01839400	H	2.47258100	0.01813100	1.48041500
Co	-0.54488200	-0.20101800	0.85062200	C	-1.16849800	2.53571000	0.19135900
C	0.75140500	-1.10140800	-1.81198000	O	-1.78077200	3.59020500	-0.00662800
C	0.05134900	-0.10665400	-2.36428600	N	-1.68378000	1.26729100	0.05792800
C	0.05375100	1.25237900	-2.91441900	C	-3.00160700	0.94622600	-0.18319400
C	-1.20238700	0.36912500	-2.95487800	C	-3.26257800	-0.46469900	-0.20310300
H	0.57932500	1.44593600	-3.84821500	C	-4.07054200	1.81036800	-0.42249300
H	0.05785200	2.08799900	-2.21697400	C	-4.56435700	-0.97835000	-0.46087600



C	-5.35960400	1.29107100	-0.66962900			
H	-3.88923500	2.87548900	-0.41707000	22_T		
C	-2.36242200	-2.60054800	0.02535800	C	-3.95663000	0.49104200 1.64965600
C	-4.70714300	-2.38909100	-0.46454200	C	-3.79517400	-0.68113400 2.39783300
C	-5.62205200	-0.06437400	-0.69484700	C	-2.53496900	-1.26666700 2.51877600
H	-6.16862200	1.99368300	-0.84880100	C	-1.44568800	-0.66114900 1.89145200
C	-3.61629800	-3.19555100	-0.22310800	C	-1.60587000	0.50988200 1.13976100
H	-1.48130500	-3.19856100	0.23569500	C	-2.86307400	1.09146600 1.01338800
H	-5.68488700	-2.82174400	-0.65715600	H	-4.94287900	0.93643000 1.55111400
H	-6.62082700	-0.44187800	-0.88935800	H	-4.65449900	-1.13475300 2.88338000
H	-3.70390400	-4.27631600	-0.21833000	H	-2.38094800	-2.18027400 3.08565400
N	-2.19546700	-1.28746400	0.02793200	H	-3.00533700	1.98169900 0.41012700
Co	-0.54876900	-0.18604100	0.46087700	C	-0.06580300	-1.20932400 1.94209800
C	0.69971400	-1.11034400	-1.45729600	O	0.26866400	-2.24234200 2.52169600
C	-0.07742900	-0.09943800	-1.92234900	N	0.77634000	-0.37846300 1.22150500
C	-0.02269800	1.14204800	-2.70326800	C	2.15102700	-0.53224200 1.10329300
C	-1.20125200	0.16585300	-2.83351200	C	2.75867500	0.38069300 0.18570400
H	0.70731200	1.20656200	-3.50765700	C	2.97512500	-1.42814700 1.77516400
H	-0.23626900	2.08551500	-2.21092400	C	4.15697400	0.37197600 -0.06097600
H	-2.15195700	0.50971900	-2.44455600	C	4.37077000	-1.42356800 1.53880800
H	-1.27433100	-0.45632000	-3.72327700	H	2.53619700	-2.12461300 2.47447500
C	-0.17939500	-1.30997800	2.45729100	C	2.40939500	2.13699700 -1.30883100
O	0.40389100	-1.68264900	1.38578200	C	4.64703900	1.31254100 -0.99885600
O	-0.96516700	-0.31009500	2.35104900	C	4.96465700	-0.55917200 0.64381500
C	0.07076500	-1.97408600	3.77315100	H	4.98421000	-2.13457500 2.08416800
H	0.98215500	-1.54892800	4.20865200	C	3.78065100	2.18796600 -1.62186000
H	-0.75922600	-1.79433100	4.45848500	H	1.69065800	2.81348000 -1.76008400
H	0.22818600	-3.04580300	3.63275800	H	5.71076100	1.33783300 -1.21755600
H	0.22907500	-2.08175900	-1.31861800	H	6.03611300	-0.57308500 0.47249900
C	2.13580800	-1.07111500	-1.20944300	H	4.13701500	2.91685900 -2.34073200
C	2.76635000	-2.19925300	-0.64865200	N	1.92239100	1.26277700 -0.44011400
C	2.93083600	0.04642800	-1.51170300	Co	0.03373700	1.08013100 0.30096700
C	4.12835100	-2.21120800	-0.40002100	C	0.89516600	-1.54062600 -2.05425200
H	2.16669100	-3.06723900	-0.39461700	C	1.56008400	-2.55811800 -1.51428900
C	4.30043000	0.04621100	-1.27572600	C	1.55159600	-3.72129700 -0.62267600
H	2.46906600	0.93821800	-1.91576700	C	2.83766100	-3.24759800 -1.32178300
C	4.90802600	-1.08477200	-0.71096500	H	1.10186700	-4.65053900 -0.97035100
H	4.61564200	-3.07640100	0.03678700	H	1.44832100	-3.54557800 0.44680600
H	4.87884400	0.92996600	-1.51298700	H	3.60302600	-2.77332800 -0.71214400
O	6.23130100	-1.18432100	-0.42957400	H	3.22742700	-3.86684900 -2.12873000
C	7.06052800	-0.05736600	-0.69427800	C	-0.44759800	3.46444100 0.29214500
H	8.06618600	-0.34549500	-0.38433600	O	-0.67459300	2.64332300 -0.67684000
H	7.07072300	0.19336800	-1.76183100	O	0.07048400	3.02672000 1.35144100
H	6.74226600	0.81975400	-0.11786800	C	-0.84289400	4.90656200 0.13200100

H	-1.92481900	4.99097700	0.28430500	C	-4.82596700	-1.08216800	1.01788600
H	-0.33580600	5.52827300	0.87101100	H	-3.87220800	0.83674700	1.46140400
H	-0.62148100	5.25564300	-0.87933300	H	-5.44474900	-3.04619800	0.41136300
H	1.44290800	-0.84006600	-2.68389500	H	-3.93888100	-4.55523700	-1.04891300
C	-0.53230800	-1.25384100	-1.87927100	H	-5.73518200	-0.84960800	1.56083700
C	-1.07574700	-0.07417700	-2.42515300	N	-2.65880200	-0.35812200	0.32268900
C	-1.41390400	-2.12774700	-1.22034000	Co	-1.09553100	0.79190700	0.18001900
C	-2.43131600	0.21270200	-2.33318500	C	0.88198600	0.79738300	1.49676300
H	-0.42121200	0.62188500	-2.94190300	C	-0.32228500	0.07511900	1.79803200
C	-2.77404900	-1.85561000	-1.12626600	C	-0.51181900	-1.23906500	2.46363900
H	-1.02790700	-3.03878800	-0.77812300	C	-1.04806600	0.04185600	3.09640700
C	-3.29338400	-0.67936200	-1.68544800	H	0.35225200	-1.71112700	2.92528600
H	-2.83897700	1.12865600	-2.74648600	H	-1.23417300	-1.94058700	2.05660900
H	-3.41679400	-2.55198300	-0.60307800	H	-2.12313000	0.19331800	3.10194200
O	-4.60595400	-0.32027600	-1.64297400	H	-0.53986700	0.42571500	3.97916700
C	-5.52578400	-1.23549900	-1.06232400	C	-2.34942300	2.78246700	-0.15719100
H	-6.50825000	-0.76661200	-1.14313600	O	-1.94942000	2.36920700	0.99264900
H	-5.53803000	-2.18975000	-1.60435700	O	-2.08757400	2.07077500	-1.16789400
H	-5.30014400	-1.42002700	-0.00636200	C	-3.06431700	4.09796600	-0.27591200
TS15_S				H	-2.31538200	4.89579200	-0.34128300
C	1.80955400	3.73846800	-1.04489600	H	-3.67385900	4.12262900	-1.18093400
C	2.32407800	3.04407500	-2.14505700	H	-3.68051300	4.28321900	0.60691300
C	1.98354500	1.70572000	-2.34794900	C	2.17681900	0.14147300	1.24428600
C	1.14813800	1.05878700	-1.44038700	C	3.35919500	0.89470800	1.37247900
C	0.65269000	1.73907200	-0.30670000	C	2.28315300	-1.19846900	0.84730700
C	0.98435400	3.08660800	-0.12678100	C	4.59785100	0.33087200	1.12521200
H	2.06318000	4.78442300	-0.89596400	H	3.29339200	1.94211000	1.65285100
H	2.98135800	3.54965000	-2.84628400	C	3.52235500	-1.77510600	0.58090100
H	2.34156200	1.15216300	-3.21039500	H	1.38758600	-1.79182900	0.71982500
H	0.61185700	3.62278900	0.74197300	C	4.68883200	-1.01158200	0.71873600
C	0.67454500	-0.33502000	-1.69316900	H	5.51151700	0.90717700	1.22454100
O	1.18421200	-1.09438500	-2.52374900	H	3.56680700	-2.80847800	0.26123500
N	-0.41823900	-0.59363500	-0.91357100	H	0.96684200	1.75631800	1.99910200
C	-1.23590100	-1.69731100	-1.02720500	O	5.94290600	-1.47383100	0.48543100
C	-2.47578100	-1.54612500	-0.33179300	C	6.08840500	-2.81067800	0.01761700
C	-1.01263200	-2.88569400	-1.71890800	H	7.15931500	-2.96345600	-0.12530800
C	-3.46512500	-2.56550600	-0.32869300	H	5.71603900	-3.53678500	0.75056500
C	-1.99624900	-3.89997900	-1.70840800	H	5.57093300	-2.96017300	-0.93745000
H	-0.08925500	-3.00681900	-2.26719200	TS15_T			
C	-3.79119200	-0.12594100	0.96903400	C	1.68210400	3.83908900	-1.13689700
C	-4.66192900	-2.29367800	0.38141400	C	2.25053200	3.13594400	-2.20249600
C	-3.19542300	-3.76469800	-1.03667000	C	1.98703400	1.77395800	-2.35926600
H	-1.79413700	-4.81638900	-2.25568500	C	1.17222600	1.10642100	-1.44623300

C	0.64477700	1.80404600	-0.33977400	C	4.61357100	0.39458500	1.10297500
C	0.88930400	3.17139700	-0.19960700	H	3.35646900	2.05635000	1.58911900
H	1.87055100	4.90291500	-1.02240100	C	3.48230100	-1.71098800	0.68469800
H	2.88506500	3.65187600	-2.91687300	H	1.35195100	-1.67500800	0.86843200
H	2.38003700	1.21255200	-3.20134400	C	4.66712600	-0.96694900	0.75847500
H	0.47906600	3.71271600	0.64824900	H	5.54085300	0.95542800	1.15154900
C	0.76057100	-0.31304900	-1.70480900	H	3.49761900	-2.75806500	0.41007700
O	1.36213300	-1.05610400	-2.48679500	H	1.02066400	1.94241300	1.97773200
N	-0.38257800	-0.58795700	-1.00778100	O	5.90519500	-1.46654200	0.51655900
C	-1.11861200	-1.75039300	-1.08124400	C	6.01010500	-2.82467100	0.10238200
C	-2.36174400	-1.69933000	-0.35768000	H	5.46612200	-3.00187600	-0.83306200
C	-0.80868200	-2.92683400	-1.75969800	H	7.07361100	-3.00759200	-0.05923100
C	-3.25527700	-2.80659400	-0.34530100	H	5.64030400	-3.51104800	0.87399700
C	-1.69712200	-4.02534300	-1.73186600				
H	0.11648000	-2.97212800	-2.31739900				
C	-3.80167200	-0.41880500	0.96180000	23_Q			
C	-4.46823000	-2.65017800	0.37057900	C	-1.79886400	3.65007100	1.97993600
C	-2.89459500	-3.98499700	-1.04901100	C	-1.86317300	2.93418100	0.79044100
H	-1.42206900	-4.92483300	-2.27539300	C	-1.30543900	1.65209300	0.66080300
C	-4.74703100	-1.46200000	1.01152700	C	-0.66670000	1.09023300	1.78237400
H	-3.96860700	0.53314900	1.45572200	C	-0.62864700	1.80866700	2.98828300
H	-5.17486000	-3.47489600	0.39990400	C	-1.17693000	3.08107200	3.09257200
H	-3.57120600	-4.83371400	-1.04685700	H	-2.23488100	4.64288900	2.04014500
H	-5.67363600	-1.31702800	1.55546400	H	-2.36556700	3.36917700	-0.06954600
N	-2.65444000	-0.54165000	0.31247300	H	-0.14791100	1.35216000	3.84813500
Co	-1.14247400	0.80292200	0.15775300	H	-1.12080100	3.62305600	4.03173800
C	0.91970100	0.95676700	1.53454000	C	-0.01108000	-0.27216000	1.84892400
C	-0.28808800	0.27353100	1.87392300	O	-0.54267000	-1.16660700	2.51600500
C	-0.53177200	-0.99695200	2.60498900	N	1.18514800	-0.34905300	1.19216100
C	-1.08484100	0.32565100	3.12600700	C	-1.51976100	0.96692600	-0.69135500
H	0.31664300	-1.44098400	3.12050800	C	1.97544400	-1.49213700	1.20254600
H	-1.24095100	-1.71719300	2.20964700	C	2.99659600	-1.52813100	0.19359700
H	-2.15554600	0.48601800	3.05698700	C	1.91048300	-2.56983400	2.08456600
H	-0.61949000	0.77619900	4.00038000	C	3.92855200	-2.60201700	0.11278300
C	-2.59034700	2.79156500	-0.14109900	C	2.83742300	-3.63220400	1.99952200
O	-2.30224300	2.46429800	1.05046600	H	1.13570200	-2.57984500	2.83661500
O	-2.14229200	2.09817200	-1.11101700	C	3.94158400	-0.47004500	-1.66672000
C	-3.41866700	4.01919000	-0.42517300	C	4.89725400	-2.54102200	-0.91815800
H	-2.74308500	4.87208400	-0.55874700	C	3.83376000	-3.66338200	1.04754600
H	-3.99016800	3.89483100	-1.34738200	H	2.75374000	-4.44538000	2.71465400
H	-4.08542100	4.23840500	0.41129500	C	4.90985100	-1.48115200	-1.80115400
C	2.19362800	0.26257800	1.29160100	H	3.89875600	0.38103800	-2.33838400
C	3.39361600	0.99613400	1.35517700	H	5.62657100	-3.34152800	-1.00483700
C	2.26228000	-1.09557100	0.95210600	H	4.54048400	-4.48535500	0.99530600
				H	5.64332700	-1.41668200	-2.59678600

N	3.02521000	-0.49994800	-0.70669200	C	0.25201700	-0.41273800	1.74943000
C	-0.36968200	0.08802500	-1.18019500	O	0.69230200	0.04588200	2.81328000
C	-0.27397400	-0.43780400	-2.57883200	N	-0.32434200	0.34271600	0.77010400
C	-0.41855100	-1.38500800	-1.39840600	C	1.15723800	-1.81134600	-0.91106000
H	0.68099600	-0.42302200	-3.09910100	C	-0.48415300	1.71869400	0.97355200
H	-1.13319000	-0.27843700	-3.22886200	C	-1.68698700	2.27451100	0.44187700
H	-1.36782300	-1.89112100	-1.24801500	C	0.39033800	2.57838400	1.62836000
H	0.44921100	-1.98529400	-1.13627300	C	-2.00895900	3.65301500	0.59321900
C	2.22297700	3.07792200	-0.91992800	C	0.08076700	3.95040800	1.76083800
O	1.80817600	2.69930000	0.22991200	H	1.30346200	2.18556600	2.04991900
O	2.25633400	2.22979800	-1.86457600	C	-3.66009100	1.84438300	-0.71758600
C	2.65361600	4.50349400	-1.12091800	C	-3.24172700	4.08721400	0.04461200
H	2.99380300	4.66950000	-2.14346700	C	-1.08883500	4.49225200	1.26841600
H	1.81332300	5.16782900	-0.89606300	H	0.79177500	4.59082300	2.27474100
H	3.45557100	4.74486700	-0.41659400	C	-4.06634900	3.18981200	-0.59904600
Co	1.47756700	0.80736800	-0.42521600	H	-4.26649900	1.10963000	-1.23738900
H	-1.59222600	1.78320500	-1.41782700	H	-3.52464300	5.13193700	0.13849100
C	-2.85203400	0.22530800	-0.73316300	H	-1.31467900	5.54734500	1.38655300
C	-3.70502700	0.38067400	-1.83492300	H	-5.01482300	3.49942300	-1.02352900
C	-3.23806100	-0.65589800	0.28201900	N	-2.51394300	1.41016000	-0.21748400
C	-4.90548200	-0.31486100	-1.92235400	C	-0.12492000	-1.20821600	-1.51624100
H	-3.42798700	1.06376100	-2.63374300	C	-0.36125800	-1.32368000	-2.97401300
C	-4.43954400	-1.36163200	0.20924300	C	-0.15754900	0.07054700	-2.36856400
H	-2.59754400	-0.80537300	1.14564900	H	-1.35638900	-1.52187400	-3.35603600
C	-5.28111900	-1.19409000	-0.89806800	H	0.44797300	-1.73427900	-3.57620000
H	-5.56924400	-0.18897000	-2.77157200	H	0.76123600	0.63435900	-2.47586800
H	-4.70681500	-2.03242700	1.01651200	H	-1.05379100	0.70106500	-2.41253300
O	-6.47286500	-1.83301800	-1.06697600	C	-3.30167900	-1.73224000	-0.61501200
C	-6.89132200	-2.73754100	-0.05368600	O	-2.56592900	-1.53196100	0.40860300
H	-7.02203300	-2.23265500	0.91168900	O	-2.98765400	-1.08048100	-1.66617200
H	-7.85365600	-3.13431000	-0.38221300	C	-4.43972900	-2.70152300	-0.58385300
H	-6.18331700	-3.56726900	0.06668200	H	-5.22927500	-2.38052600	-1.26637900
				H	-4.07499800	-3.68000400	-0.91656900
23_S				H	-4.82668900	-2.80512300	0.43137900
C	0.55467600	-4.69996000	1.48932500	Co	-1.48096600	-0.30815300	-0.59773600
C	0.89788200	-3.93825600	0.37480800	H	1.45185300	-2.60120300	-1.61101600
C	0.79272700	-2.54053100	0.37220600	C	2.36938400	-0.88052400	-0.84278200
C	0.33336500	-1.90270600	1.54081600	C	2.97232800	-0.48802900	-2.05237600
C	0.02274600	-2.67408600	2.66974900	C	2.96088200	-0.42914800	0.33738600
C	0.11067300	-4.06171700	2.64729400	C	4.07228200	0.35734200	-2.08459600
H	0.64173800	-5.78207200	1.45418800	H	2.57699300	-0.86031300	-2.99380100
H	1.25997800	-4.43503000	-0.52144500	C	4.07051200	0.42229800	0.32709300
H	-0.28801700	-2.15625900	3.57027400	H	2.57657700	-0.73388900	1.30067600
H	-0.15510100	-4.63843400	3.52825500	C	4.62657100	0.83159600	-0.88708600

H 4.52602700 0.65401900 -3.02473100  
H 4.48765800 0.74768000 1.27230400  
O 5.70047200 1.66206100 -1.01153200  
C 6.29517000 2.15528500 0.18084500  
H 6.68992100 1.34233700 0.80335400  
H 7.12045800 2.79610900 -0.13510500  
H 5.58587800 2.74847700 0.77191800

23\_T

C -1.87560300 3.67861300 1.87502800  
C -1.87924800 2.92982200 0.70434600  
C -1.30253200 1.65069800 0.63824100  
C -0.70200600 1.13028300 1.80159200  
C -0.73195900 1.88058100 2.98980600  
C -1.30148300 3.14678600 3.03200200  
H -2.32411700 4.66747700 1.88757900  
H -2.35064400 3.33077900 -0.18867500  
H -0.28811400 1.45103900 3.88209400  
H -1.29762700 3.71459300 3.95736400  
C 0.00042300 -0.20367100 1.92784100  
O -0.41187100 -1.03623200 2.73939100  
N 1.13932100 -0.30313500 1.17411800  
C -1.47129300 0.90543700 -0.68651700  
C 2.00110900 -1.39746800 1.22431800  
C 2.94629200 -1.47863500 0.14664700  
C 2.05598600 -2.38041700 2.20801100  
C 3.92779000 -2.50981100 0.09959300  
C 3.03177000 -3.40087000 2.15305400  
H 1.34030500 -2.35184800 3.01582200  
C 3.70230300 -0.55593600 -1.85334600  
C 4.81821200 -2.50346300 -1.00260800  
C 3.95645400 -3.47778800 1.13453400  
H 3.04361700 -4.14274200 2.94622700  
C 4.71196400 -1.53156700 -1.97347500  
H 3.58135100 0.22446600 -2.59921900  
H 5.58146900 -3.27354800 -1.06980400  
H 4.70064200 -4.26739700 1.10590800  
H 5.38375100 -1.50562200 -2.82406900  
N 2.85472800 -0.53810900 -0.83763000  
C -0.30419600 -0.00890200 -1.06678200  
C -0.14841500 -0.55863800 -2.45218100  
C -0.38921800 -1.48231800 -1.27184700  
H 0.83501500 -0.57940200 -2.91311200  
H -0.96361200 -0.37164200 -3.14846300

H -1.36158900 -1.95320300 -1.16805500  
H 0.44332600 -2.10120300 -0.95264900  
C 2.36665700 2.93230600 -0.95312000  
O 2.84296400 2.36612600 0.06367900  
O 1.39648600 2.35906200 -1.58819000  
C 2.87238700 4.25716200 -1.45173900  
H 3.09789000 4.19203500 -2.52017200  
H 2.08677500 5.01002000 -1.32815200  
H 3.75994700 4.56489000 -0.89779000  
Co 1.32927500 0.81118400 -0.37584400  
H -1.49801900 1.68369700 -1.45512400  
C -2.81043900 0.17984600 -0.73747100  
C -3.63304400 0.30510700 -1.86518700  
C -3.23648100 -0.65306100 0.30165200  
C -4.84293300 -0.37387700 -1.95437700  
H -3.32388200 0.95043200 -2.68329700  
C -4.44774100 -1.34130400 0.22872200  
H -2.61958000 -0.77628900 1.18637100  
C -5.25939200 -1.20366900 -0.90499300  
H -5.48324000 -0.27197100 -2.82451900  
H -4.74649400 -1.97412700 1.05530000  
O -6.45850300 -1.82712400 -1.07681600  
C -6.92334200 -2.67374300 -0.03395300  
H -7.06652100 -2.12095400 0.90301000  
H -7.88602700 -3.06409400 -0.36897100  
H -6.23814200 -3.51232200 0.14351700

TS16\_Q

C -0.62410800 -4.70260200 -0.51222000  
C -0.96733500 -3.73804500 0.43252100  
C -0.78452000 -2.37650900 0.17321500  
C -0.25257600 -1.99010800 -1.06893700  
C 0.05680500 -2.96208200 -2.03037700  
C -0.11195200 -4.31353800 -1.75204100  
H -0.76448900 -5.75531500 -0.28498600  
H -1.39200400 -4.03994400 1.38595100  
H 0.43739400 -2.63549800 -2.99210800  
H 0.15058800 -5.05949500 -2.49574500  
C -0.06084900 -0.56050300 -1.46622200  
O -0.30050500 -0.19317500 -2.61122600  
N 0.49102200 0.28954800 -0.49292200  
C -1.23861600 -1.34647200 1.18880300  
C 0.40200500 1.67160100 -0.68224500  
C 1.56217900 2.43193900 -0.35624600

C	-0.78012500	2.34699800	-1.04086200	H	-6.31941100	1.85751100	-1.44050000
C	1.53388500	3.86492700	-0.40761000				
C	-0.79907900	3.74007100	-1.09204200	TS16_S			
H	-1.66923200	1.77348700	-1.27109600	C	0.59093700	-4.72182600	0.61205700
C	3.81257400	2.42695200	0.33803600	C	0.80129600	-3.73567500	-0.35071000
C	2.73170600	4.53960100	-0.05972000	C	0.58843300	-2.38879800	-0.05079200
C	0.32908500	4.50146200	-0.78501000	C	0.17076100	-2.04241300	1.24110100
H	-1.71854000	4.24331500	-1.37761300	C	-0.01617800	-3.02824800	2.21537200
C	3.86295400	3.81843500	0.31040200	C	0.18201000	-4.36848700	1.90076000
H	4.66651800	1.82023500	0.61865900	H	0.75122100	-5.76575000	0.35864600
H	2.75114600	5.62528500	-0.07959600	H	1.13886200	-4.01083300	-1.34624600
H	0.29661200	5.58564300	-0.83014500	H	-0.32188200	-2.72329600	3.21020300
H	4.78313300	4.32478700	0.58131500	H	0.02204300	-5.13433000	2.65346700
N	2.68812900	1.75593800	0.01153400	C	-0.00278200	-0.61983000	1.62699200
C	-0.21516500	-0.25420600	1.35676400	O	0.20332700	-0.22488900	2.77064800
C	0.72457600	-0.13347300	2.51190400	N	-0.39688400	0.25145400	0.59675400
C	-0.32712500	0.92972200	2.20962600	C	0.89717700	-1.31579300	-1.07030300
H	1.76634200	0.16261400	2.38715100	C	-0.26968700	1.64569700	0.81256600
H	0.57460100	-0.81596800	3.34897200	C	-1.39392600	2.40054400	0.41122600
H	-1.19494300	1.03222900	2.85719000	C	0.84414100	2.30106500	1.30236800
H	0.03982100	1.87650700	1.81251800	C	-1.41493300	3.81562800	0.50595200
C	3.93596500	-2.12410700	0.37338200	C	0.83147800	3.70995800	1.41026300
O	2.72235600	-2.29792600	0.01882900	H	1.71759400	1.73832200	1.60426300
O	4.36072600	-0.93011200	0.52173100	C	-3.54014900	2.31241900	-0.47407600
C	4.84978200	-3.29799700	0.57720600	C	-2.59873100	4.46964100	0.07510100
H	5.37129900	-3.50199100	-0.36507100	C	-0.26350400	4.45983100	1.02451200
H	5.60006000	-3.07173100	1.33711900	H	1.71091800	4.20935500	1.80478700
H	4.27866000	-4.18626300	0.85186200	C	-3.64978500	3.71738700	-0.40457500
Co	2.44625600	-0.25240000	-0.01169700	H	-4.34561400	1.69236300	-0.85108800
C	-2.63516800	-0.79226000	0.91076200	H	-2.66484500	5.55207600	0.13040700
C	-3.14367800	-0.58608700	-0.37285000	H	-0.25519800	5.54172700	1.11388600
C	-3.44242800	-0.42279100	1.99880300	H	-4.56847500	4.18756400	-0.73753500
C	-4.40087800	-0.00998200	-0.57846600	N	-2.44261500	1.66927000	-0.08518400
H	-2.57349100	-0.88027500	-1.24529400	C	-0.18733300	-0.22332700	-1.13909400
C	-4.69399600	0.14846900	1.81515800	C	-0.98291100	-0.16163300	-2.45892700
H	-3.08358600	-0.59264400	3.01065700	C	0.02794200	0.89899900	-2.09235900
C	-5.18197900	0.36635600	0.51853000	H	-2.02731400	0.12313400	-2.48288800
H	-4.75496700	0.13068500	-1.59230100	H	-0.71618200	-0.92444700	-3.18888700
H	-5.31427200	0.42949200	2.66002400	H	0.98311400	0.94543400	-2.60414900
H	-1.29822700	-1.86506700	2.15745300	H	-0.37424200	1.87475200	-1.84607600
O	-6.41759100	0.93327300	0.43331100	C	-3.61033500	-1.98088300	-0.50567000
C	-6.95040900	1.17035200	-0.86289000	O	-2.42193700	-2.18008100	-0.09905400
H	-7.07620100	0.23699000	-1.42611900	O	-3.97353000	-0.76957000	-0.68440700
H	-7.92885700	1.62860700	-0.70815800	C	-4.56171000	-3.12074000	-0.73011400

H	-5.13018400	-3.29548300	0.19081100	C	4.51905500	-2.96796300	0.60529900
H	-5.27028400	-2.87778000	-1.52498500	H	3.78545100	-3.94266800	2.36049700
H	-4.01368000	-4.03344900	-0.97195500	C	4.91747800	-0.58629900	-2.25069800
Co	-2.16347200	-0.19750400	-0.08454100	H	3.60530700	1.12436100	-2.58151500
C	2.31159400	-0.75610300	-0.90824400	H	5.99456900	-2.33548700	-1.62318900
C	2.91600400	-0.50938400	0.32670900	H	5.33470700	-3.66608500	0.44383400
C	3.05741100	-0.46057200	-2.06175100	H	5.53277000	-0.38655300	-3.12087900
C	4.19386100	0.04861800	0.42134800	N	3.04404600	0.08051600	-0.91013900
H	2.41100200	-0.76474000	1.24966300	C	-0.19087600	-0.62567600	-0.05145600
C	4.32906400	0.09191400	-1.98989500	C	0.06036700	-1.55176800	-1.18739500
H	2.63405500	-0.67816800	-3.03899800	C	-0.40567900	-2.09097400	0.14694800
C	4.90599300	0.36139100	-0.74116200	H	1.08806400	-1.74962800	-1.47323900
H	4.62142200	0.21917300	1.40184600	H	-0.63490400	-1.50671700	-2.02143400
H	4.89729700	0.31488200	-2.88703400	H	-1.43059500	-2.43249700	0.24117900
H	0.87876300	-1.80146200	-2.05134500	H	0.31546100	-2.65409800	0.73043400
O	6.15362300	0.90669300	-0.76390400	C	0.90677300	2.79643000	-2.09199300
C	6.78190100	1.17869500	0.48171300	O	0.59289500	1.59863500	-2.35406700
H	6.92823600	0.26379800	1.06948700	O	1.43096700	3.09464600	-0.96601400
H	7.75595100	1.60824900	0.24109700	C	0.63023400	3.89873700	-3.08866300
H	6.20755400	1.90078200	1.07577200	H	-0.33552100	4.35809900	-2.84749300
TS16_T				H	1.39384500	4.67721700	-3.02520500
C	-2.54647300	2.83250400	2.64806500	H	0.57559400	3.50010800	-4.10350900
C	-2.40755200	2.08871100	1.48225100	Co	1.36513800	1.12773500	-0.31478100
C	-1.36326700	1.16687800	1.31669700	C	-2.64149100	-0.18948900	-0.40332300
C	-0.43262800	1.01075800	2.36192600	C	-3.45791800	-0.86133200	0.51069700
C	-0.60053600	1.74724900	3.54997000	C	-3.06301500	-0.11362600	-1.73845200
C	-1.63915200	2.65467200	3.69623100	C	-4.66078200	-1.44891600	0.11662000
H	-3.36266100	3.54271800	2.74178200	H	-3.15955500	-0.92035600	1.55298300
H	-3.12807500	2.20701400	0.67921900	C	-4.25812800	-0.69207100	-2.14824200
H	0.11566300	1.58696900	4.34718300	H	-2.44391400	0.41120600	-2.46104100
H	-1.74143700	3.22176600	4.61627400	C	-5.06597000	-1.36673800	-1.22230700
C	0.76238900	0.10130600	2.35652300	H	-5.26953500	-1.95758600	0.85410400
O	1.26161600	-0.26848700	3.41757100	H	-4.58925900	-0.62886800	-3.17959300
N	1.31531100	-0.21439700	1.11415500	H	-1.06639000	1.15209800	-0.78419500
C	-1.29961400	0.41559800	-0.00592500	O	-6.21876400	-1.89871900	-1.71441400
C	2.37836300	-1.14510300	1.02868900	C	-7.07446900	-2.58683200	-0.81189900
C	3.26918100	-0.97765600	-0.07817200	H	-7.43291000	-1.92768400	-0.01122600
C	2.58411500	-2.22108900	1.88280100	H	-7.92667500	-2.92582300	-1.40343500
C	4.34110700	-1.88925000	-0.29608500	H	-6.57759300	-3.45805200	-0.36665500
C	3.65402600	-3.11731500	1.66770100	24_Q			
H	1.93250100	-2.35889100	2.73293800	C	-1.25910600	4.84260100	-0.86748500
C	3.83508800	0.26907600	-1.95343300	C	-1.92690700	3.71213300	-1.34010600
C	5.16889900	-1.65829600	-1.42428300	C	-1.42492000	2.43730300	-1.08442400

C	-0.24511500	2.30425700	-0.32745100	C	-3.11766300	0.84556800	0.76011200
C	0.41837500	3.44152400	0.15636600	C	-5.12093300	-0.77431900	-0.28513400
C	-0.08379000	4.70788600	-0.12190500	H	-4.27177600	-0.33277000	-2.19768900
H	-1.65474700	5.83074300	-1.08224900	C	-4.03705700	0.24377700	1.62339200
H	-2.84339000	3.81803400	-1.91346800	H	-2.34824500	1.47928200	1.18738500
H	1.31967200	3.31484900	0.74493400	C	-5.04140900	-0.57871700	1.10249000
H	0.43490800	5.58877800	0.24254800	H	-5.91256900	-1.40411600	-0.67753500
C	0.25463500	0.96455100	0.04183300	H	-3.95581700	0.42122000	2.68854500
O	1.07724000	0.84318200	1.00771700	H	-2.58559500	1.39051900	-2.53460500
N	-0.20948900	-0.10204500	-0.62586600	O	-5.98258600	-1.21869700	1.84802400
C	-2.11068400	1.18076100	-1.57087600	C	-5.92362100	-1.07209900	3.26144900
C	0.03996800	-1.46374700	-0.22617600	H	-6.06510000	-0.02756300	3.56621300
C	1.30417000	-2.06570700	-0.38880900	H	-6.74116700	-1.67437500	3.66122500
C	-1.08613000	-2.21473200	0.16396300	H	-4.97296200	-1.44120800	3.66581500
C	1.38883300	-3.50013800	-0.27038200				
C	-0.97515200	-3.58652400	0.34971000	24_S			
H	-2.03367400	-1.70587200	0.29277800	C	0.64336300	-4.64562100	-1.07692100
C	3.58559500	-1.97709200	-1.07596800	C	-0.11829900	-4.01266300	-0.09677900
C	2.62789000	-4.12662500	-0.58851200	C	-0.10811300	-2.62003400	0.02397900
C	0.24143200	-4.22680300	0.11194000	C	0.67382300	-1.86313000	-0.85882000
H	-1.84244900	-4.16100100	0.66079400	C	1.42287000	-2.49778800	-1.85596000
C	3.70347300	-3.34719200	-1.04337300	C	1.41609000	-3.88450700	-1.96038500
H	4.40733500	-1.33696800	-1.38316500	H	0.63358700	-5.72880900	-1.15509300
H	2.70631000	-5.20677300	-0.52173200	H	-0.73172000	-4.59983200	0.58174900
H	0.32364600	-5.30527800	0.21417000	H	2.00729600	-1.88838300	-2.53763900
H	4.63313400	-3.81104400	-1.35755500	H	2.00729500	-4.37412700	-2.72863600
N	2.43471700	-1.30994500	-0.67734300	C	0.63399300	-0.36737200	-0.83669600
C	-1.01886900	0.14665900	-1.82615600	O	0.37878700	0.28175400	-1.86464400
C	-0.27996200	0.16507800	-3.14423200	N	0.31901200	0.21320500	0.53843700
C	-1.22260800	-0.96437700	-2.80551000	C	-0.93886400	-1.90431100	1.06628300
H	0.78331700	-0.04838800	-3.10704300	C	-0.29068800	1.51232300	0.46656100
H	-0.57936300	0.90559400	-3.87990900	C	0.56895300	2.53577600	0.00328200
H	-2.18833900	-1.00459500	-3.29873800	C	-1.60000800	1.81343600	0.77133500
H	-0.79344800	-1.93248700	-2.57928500	C	0.10020000	3.86163300	-0.18256600
C	4.81517300	1.27603200	1.41038100	C	-2.06966100	3.14025100	0.61344000
O	4.33152600	1.59219400	0.27035600	H	-2.27206000	1.04363800	1.12558000
O	4.25713600	0.34534600	2.08398200	C	2.71385200	3.08530800	-0.70823600
C	5.99830200	2.01592100	1.96583400	C	1.03166800	4.81289100	-0.67276500
H	5.63698400	2.91467400	2.47874300	C	-1.25202900	4.14394600	0.14086200
H	6.53373100	1.39870100	2.68877800	H	-3.10392000	3.35622100	0.86211600
H	6.66312800	2.33149800	1.15946800	C	2.32588700	4.42273200	-0.93658000
Co	2.87094000	0.15559800	0.56730900	H	3.72499100	2.74299900	-0.89927700
C	-3.17318600	0.64586200	-0.62025400	H	0.71284700	5.83815900	-0.83565600
C	-4.19940600	-0.16765400	-1.12637600	H	-1.62719900	5.15483100	0.01387500



H 3.05897000 5.12549900 -1.31634500  
 N 1.86661800 2.17357000 -0.25065200  
 C -0.12225900 -0.72054100 1.59191900  
 C 0.82549600 -0.98375900 2.73354900  
 C -0.41242800 -0.15540500 2.95402400  
 H 1.77862000 -0.47019900 2.70589300  
 H 0.86614000 -1.99749600 3.11983500  
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 H -0.28455700 0.91168000 3.09750400  
 C 4.19905400 -0.91562800 0.20325500  
 O 3.12483100 -1.35905600 0.71930400  
 O 4.16324600 0.26548000 -0.28906900  
 C 5.43877100 -1.75607900 0.13085800  
 H 5.35685500 -2.42595200 -0.73287200  
 H 6.32475800 -1.13120400 0.00610900  
 H 5.52896500 -2.37483600 1.02654700  
 Co 2.25618600 0.36295400 0.17647800  
 C -2.31840000 -1.47816100 0.58186000  
 C -3.37085100 -1.38960500 1.50739200  
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 C -3.81184600 -0.56148400 -1.11157100  
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 H -6.25618100 -0.33206500 -2.48550700  
 H -7.38978900 0.82967000 -1.74752300  
 H -5.69687300 1.30742400 -2.04236900

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C -0.16295400 -4.82763900 -0.82497600  
 C -0.80597400 -4.03780400 0.12742600  
 C -0.57442900 -2.66235100 0.18598900  
 C 0.31018700 -2.07753500 -0.73747800  
 C 0.94150700 -2.87042200 -1.70731300  
 C 0.71197300 -4.24117100 -1.74525500  
 H -0.34532500 -5.89777500 -0.85229200  
 H -1.49840100 -4.48872000 0.83316800  
 H 1.60378500 -2.39168500 -2.42059400

H 1.20964500 -4.85280000 -2.49153600  
 C 0.55145100 -0.61147900 -0.75424100  
 O 0.87137400 0.01620000 -1.80937500  
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 C -1.28119100 -1.77556200 1.18829000  
 C -0.20761200 1.50820700 0.26146300  
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 C 0.49348300 3.83270700 -0.17636900  
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 C -0.84033900 4.25718900 0.04883200  
 H -2.82770800 3.65457200 0.56534500  
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 H 1.31647500 5.78698400 -0.61380200  
 H -1.07850400 5.31278400 -0.04089100  
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 C -0.31928100 -0.64426600 1.55864400  
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 H -1.25184400 -0.21756700 3.52217700  
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 O 3.63836300 -1.10066700 1.02193500  
 O 4.44125300 -0.32865600 -0.88701700  
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 H 5.83656000 -2.69507400 0.42743100  
 H 6.71384700 -1.26224500 -0.16282000  
 H 6.21239700 -1.39035300 1.55278500  
 Co 2.39534500 -0.01311400 -0.22388400  
 C -2.61985900 -1.24433900 0.69762600  
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 C -4.06703800 -0.38750500 -1.06751900  
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 C -5.01989900 -0.00373200 -0.11814900

H	-5.53564700	0.02494400	1.96575100
H	-4.22862200	-0.21194400	-2.12384300
H	-1.46033600	-2.35315600	2.10087400
O	-6.20009100	0.60974800	-0.40841800
C	-6.48015900	0.89890900	-1.77224500
H	-6.53231500	-0.01484900	-2.37713000
H	-7.45464800	1.39021000	-1.78220400
H	-5.73146700	1.57499100	-2.20382900

4s\_AQ\_S

C	0.33924	0.74841	2.13334
C	0.01632	2.02961	1.68092
C	0.43504	2.45087	0.41444
C	1.17533	1.59379	-0.39471
C	1.48506	0.30176	0.0492
C	1.06945	-0.11497	1.31792
H	0.01904	0.42029	3.11796
H	-0.55973	2.70015	2.31249
H	0.18193	3.44626	0.06136
H	1.50887	1.89866	-1.37978
H	1.31917	-1.11658	1.64177
C	2.34404	-0.56939	-0.80276
N	2.30822	-1.95445	-0.57646
O	3.14081	-0.07174	-1.5956
C	3.5035	-2.62855	-0.46611
C	3.41792	-4.04729	-0.55677
C	4.76872	-2.07694	-0.23714
C	4.57091	-4.8796	-0.448
C	5.89695	-2.90287	-0.08816
H	4.88391	-1.00258	-0.18999
C	2.0466	-5.85305	-1.05674
C	4.38125	-6.26887	-0.64719
C	5.82452	-4.27961	-0.18854
H	6.85678	-2.4298	0.09927
C	3.13357	-6.74614	-0.97338
H	1.07319	-6.2134	-1.34678
H	5.23266	-6.93846	-0.56589
H	6.70739	-4.90302	-0.09424
H	2.96075	-7.79824	-1.17023
N	2.17551	-4.55669	-0.81538
Co	0.78883	-3.13201	-0.7601
O	0.73455	-3.32992	1.13686
O	-1.49983	-3.09366	1.42275
C	-0.33681	-3.17648	1.85145

O	-0.48649	-1.74939	-0.70235
O	-0.1113	-0.47582	-2.54685
C	-0.7404	-0.77101	-1.5344
C	-1.97182	0.00827	-1.09871
H	-1.86964	0.31017	-0.05382
H	-2.10575	0.88538	-1.73342
H	-2.85474	-0.63611	-1.1708
C	-0.08754	-3.17726	3.34749
H	-0.86569	-2.60456	3.85595
H	-0.14182	-4.21327	3.70152
H	0.90123	-2.78512	3.59319
C	-2.5734	-6.25649	2.70072
C	-1.71025	-7.24089	3.1842
C	-0.65684	-7.69961	2.38906
C	-0.47166	-7.17666	1.11275
C	-1.31121	-6.15745	0.64021
C	-2.37067	-5.70574	1.43645
H	-3.40156	-5.90868	3.30987
H	-1.86159	-7.65533	4.17645
H	0.01258	-8.46966	2.75944
H	0.33015	-7.54386	0.48285
H	-3.03573	-4.93347	1.0732
C	-1.11053	-5.67454	-0.75468
N	-1.06874	-4.26652	-0.9859
H	-1.45104	-3.69342	-0.18635
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C	-1.47163	-3.89357	-2.32651
C	-0.47904	-3.39178	-3.20047
C	-2.75415	-4.08543	-2.78668
C	-0.78812	-3.14342	-4.56508
C	-3.07955	-3.80462	-4.13427
H	-3.5115	-4.47553	-2.1144
C	1.71312	-2.65106	-3.48073
C	0.25972	-2.67124	-5.39427
C	-2.11529	-3.36347	-5.01273
H	-4.09789	-3.9595	-4.47476
C	1.5065	-2.44917	-4.85975
H	2.6502	-2.38534	-3.00905
H	0.05971	-2.47892	-6.44408
H	-2.35759	-3.16825	-6.05265
H	2.32547	-2.07771	-5.46419
N	0.75824	-3.10798	-2.69089

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C	2.69719	0.18624	3.86601	H	-0.44541	-1.63553	3.84653
C	3.86796	0.93302	4.01304	C	-4.7726	0.63199	2.86567
C	4.79073	1.00276	2.96411	C	-5.51855	-0.50905	2.56673
C	4.54186	0.32823	1.77223	C	-5.43657	-1.08137	1.29443
C	3.35897	-0.40536	1.61389	C	-4.60405	-0.51783	0.33214
C	2.44196	-0.47862	2.66809	C	-3.82173	0.60434	0.63825
H	1.98024	0.12827	4.6794	C	-3.92663	1.18849	1.90647
H	4.06324	1.4592	4.94313	H	-4.84881	1.09246	3.84591
H	5.70077	1.58429	3.07817	H	-6.17046	-0.94469	3.31829
H	5.24315	0.36818	0.94644	H	-6.026	-1.96082	1.05309
H	1.53286	-1.05059	2.53442	H	-4.55242	-0.93406	-0.66729
C	3.14397	-1.15432	0.34226	H	-3.35017	2.07208	2.14693
N	1.81841	-1.48348	0.01094	C	-2.95429	1.16969	-0.44376
O	4.09628	-1.52476	-0.33689	N	-1.79889	1.79432	-0.0515
C	1.55812	-2.75193	-0.49155	H	-1.47557	1.73941	0.93495
C	0.23531	-2.92623	-0.98896	O	-3.26689	1.05165	-1.63307
C	2.39968	-3.86393	-0.51349	C	-1.10556	2.60982	-0.98729
C	-0.22994	-4.16681	-1.50473	C	-0.22616	2.04145	-1.95129
C	1.93401	-5.1031	-1.00141	C	-1.34537	3.96836	-1.01012
H	3.42066	-3.77347	-0.16999	C	0.30072	2.87308	-2.98549
C	-1.77393	-1.85126	-1.48952	C	-0.76613	4.80449	-1.99041
C	-1.55126	-4.19198	-2.01476	H	-2.02093	4.38327	-0.26932
C	0.65428	-5.27321	-1.49175	C	0.87971	0.18752	-2.83746
H	2.61966	-5.94534	-0.99504	C	1.09701	2.26861	-3.98815
C	-2.31044	-3.04211	-2.01769	C	0.01958	4.26263	-2.9794
H	-2.33056	-0.92363	-1.51519	H	-0.976	5.86887	-1.97529
H	-1.94833	-5.12045	-2.4148	C	1.35704	0.92115	-3.93686
H	0.3191	-6.23088	-1.87614	H	1.15243	-0.8543	-2.71832
H	-3.31523	-3.02895	-2.42417	H	1.49631	2.88579	-4.78746
N	-0.5536	-1.81432	-0.97606	H	0.43788	4.88282	-3.76604
Co	0.30107	-0.27382	-0.11203	H	1.96029	0.42339	-4.68657
O	-0.74494	-0.72691	1.44967	N	0.13187	0.71971	-1.88003
O	-1.09002	1.22305	2.54545				
C	-0.97161	-0.00895	2.51274	4s_AQ_Q			
O	1.02529	1.22936	0.68004	C	2.80392	0.30362	3.74821
O	2.70015	1.57613	-0.80106	C	4.07503	0.85265	3.92035
C	2.04866	1.89359	0.18828	C	5.05301	0.68926	2.93188
C	2.33918	3.14279	0.99797	C	4.75823	-0.02102	1.77387
H	2.42339	2.88854	2.05709	C	3.47754	-0.5636	1.59387
H	3.26087	3.608	0.64628	C	2.50199	-0.40178	2.5846
H	1.50689	3.84614	0.89022	H	2.04139	0.43684	4.50912
C	-1.17935	-0.82914	3.772	H	4.30644	1.41176	4.82239
H	-1.13639	-0.18885	4.65454	H	6.03982	1.12156	3.06681
H	-2.17197	-1.29071	3.72065	H	5.49598	-0.15413	0.99056

H	1.51143	-0.81202	2.43336	H	-4.34033	-1.06789	-0.98691
C	3.19808	-1.31496	0.34959	H	-3.51484	1.79049	2.0999
N	1.82458	-1.54938	0.04714	C	-2.94671	1.14032	-0.5393
O	4.06667	-1.72075	-0.4074	N	-1.8903	1.86206	-0.05028
C	1.41218	-2.78901	-0.22644	H	-1.60117	1.76856	0.94726
C	0.10167	-2.91068	-0.84217	O	-3.2066	1.07562	-1.74549
C	2.1348	-3.98285	0.04464	C	-1.22324	2.7857	-0.90031
C	-0.42047	-4.1856	-1.17377	C	-0.36477	2.32248	-1.93826
C	1.58822	-5.23015	-0.25731	C	-1.44047	4.13859	-0.75417
H	3.11683	-3.91391	0.49469	C	0.16671	3.25946	-2.87328
C	-1.7082	-1.81798	-1.77135	C	-0.85438	5.07399	-1.63852
C	-1.67177	-4.22189	-1.83249	H	-2.09373	4.47678	0.04358
C	0.33895	-5.34687	-0.85571	C	0.7018	0.56338	-3.01044
H	2.15546	-6.12505	-0.02345	C	0.94467	2.7522	-3.94391
C	-2.30762	-3.03705	-2.1407	C	-0.08852	4.64375	-2.69654
H	-2.17499	-0.86565	-2.00261	H	-1.04282	6.13285	-1.49294
H	-2.10843	-5.17954	-2.1	C	1.18403	1.40227	-4.03491
H	-0.06826	-6.32402	-1.0957	H	0.95948	-0.49116	-2.99726
H	-3.25889	-3.0269	-2.66077	H	1.34782	3.44363	-4.67842
N	-0.54735	-1.76312	-1.12638	H	0.33336	5.34979	-3.40563
Co	0.33214	-0.01052	-0.1189	H	1.77419	0.9805	-4.84041
O	-0.6359	-0.71626	1.50833	N	-0.03159	0.99696	-1.99866
O	-1.21664	1.21386	2.53088				
C	-1.01342	-0.01443	2.52502	TS2s_AQ_S			
O	1.11268	1.63208	0.68299	C	2.95934	-0.09144	3.84657
O	2.71167	1.22355	-0.82069	C	4.16619	0.60952	3.89755
C	2.21877	1.92291	0.08425	C	4.92551	0.77877	2.73527
C	2.8967	3.19604	0.5523	C	4.48085	0.24458	1.52943
H	3.07206	3.14334	1.63082	C	3.26172	-0.44303	1.47113
H	3.84258	3.34902	0.03035	C	2.50432	-0.61155	2.63511
H	2.23252	4.04774	0.36975	H	2.37511	-0.23476	4.75113
C	-1.26046	-0.81593	3.79309	H	4.51681	1.0213	4.83975
H	-1.38073	-0.15454	4.65284	H	5.86271	1.32614	2.77303
H	-2.18096	-1.39597	3.6623	H	5.05464	0.3623	0.61779
H	-0.44888	-1.527	3.97295	H	1.5651	-1.14514	2.57103
C	-4.82661	0.17943	2.64177	C	2.85168	-1.07825	0.18519
C	-5.45328	-0.99618	2.22596	N	1.49267	-1.36613	0.00036
C	-5.27318	-1.45437	0.91823	O	3.7035	-1.42494	-0.63219
C	-4.46138	-0.74341	0.03929	C	1.15421	-2.59276	-0.52925
C	-3.79384	0.41393	0.46276	C	-0.15588	-2.68924	-1.08134
C	-4.00082	0.88392	1.76546	C	1.93939	-3.75037	-0.54763
H	-4.9804	0.55274	3.64969	C	-0.63974	-3.89314	-1.67366
H	-6.08971	-1.54629	2.9131	C	1.43937	-4.95205	-1.08043
H	-5.77171	-2.35939	0.5836	H	2.9505	-3.71678	-0.16449

C	-2.04211	-1.49955	-1.74116	C	-0.93161	4.49083	-2.16637
C	-1.90817	-3.83456	-2.30139	H	-2.20815	3.95403	-0.49757
C	0.17881	-5.04534	-1.64067	C	1.47139	0.16955	-2.63266
H	2.08213	-5.82758	-1.06171	C	1.48425	2.21387	-3.89907
C	-2.58872	-2.64009	-2.35969	C	0.00279	4.06576	-3.08579
H	-2.56212	-0.55594	-1.79663	H	-1.30647	5.50854	-2.20498
H	-2.31704	-4.73153	-2.75752	C	1.94218	0.92923	-3.72186
H	-0.18158	-5.97142	-2.07586	H	1.89541	-0.79817	-2.39862
H	-3.54345	-2.55269	-2.86537	H	1.87149	2.83783	-4.69918
N	-0.89265	-1.53684	-1.0792	H	0.37241	4.73377	-3.85736
Co	0.03595	-0.08156	-0.1119	H	2.69704	0.50122	-4.37077
O	-0.52507	-0.6849	1.64855	N	0.54642	0.63559	-1.81283
O	-1.31926	1.32416	2.29115				
C	-0.93882	0.13467	2.52857	5s_AQ_S			
O	0.94605	1.29931	0.79487	C	-1.7671	2.08159	0.97582
O	2.67463	1.90345	-0.54967	C	-2.31806	3.33607	1.23793
C	1.98003	2.02709	0.45471	C	-3.64549	3.46129	1.69635
C	2.25268	3.10611	1.49172	C	-4.46133	2.367	1.90477
H	2.37033	2.64936	2.4776	C	-3.95305	1.07279	1.6399
H	3.15422	3.66099	1.22848	C	-2.61628	0.95258	1.16433
H	1.39865	3.78957	1.54303	N	-2.07927	-0.26457	0.85072
C	-0.99997	-0.34003	3.95442	C	-2.78716	-1.37259	1.02348
H	-0.25386	0.2101	4.53719	C	-4.10767	-1.33928	1.50781
H	-1.9838	-0.11333	4.37283	C	-4.68806	-0.12596	1.80651
H	-0.79778	-1.40908	4.02066	N	-0.44962	1.79313	0.62155
C	-5.58619	0.54928	2.20918	H	-4.02919	4.45889	1.88941
C	-5.32449	-0.74367	2.66753	H	-5.48132	2.48009	2.25696
C	-4.25501	-1.46197	2.13316	H	-5.71023	-0.07454	2.17014
C	-3.43291	-0.8893	1.16169	H	-4.64813	-2.27117	1.62716
C	-3.68074	0.41214	0.71104	H	-2.30472	-2.30553	0.76159
C	-4.78087	1.11562	1.22499	C	0.29025	2.79759	-0.00383
H	-6.42144	1.11377	2.61246	C	1.76604	2.82623	0.23095
H	-5.95555	-1.1904	3.43006	C	2.57987	3.45285	-0.7216
H	-4.05331	-2.47416	2.47082	C	2.34062	2.33566	1.40733
H	-2.60124	-1.45673	0.7745	C	3.95052	3.57014	-0.50641
H	-4.9907	2.11277	0.85269	C	3.70955	2.46777	1.63314
C	-2.90457	1.12413	-0.36521	C	4.5181	3.08169	0.67391
N	-1.51288	1.33621	-0.18261	H	1.70726	1.8584	2.14283
H	-1.33759	1.47471	1.07754	H	4.57737	4.04303	-1.25648
O	-3.51674	1.58493	-1.32148	H	4.1457	2.09122	2.5539
C	-0.98613	2.31242	-1.10077	H	5.58643	3.1791	0.84466
C	0.02099	1.88495	-1.99715	O	-0.22875	3.68055	-0.69034
C	-1.43775	3.61302	-1.18012	H	-1.7249	4.22516	1.07526
C	0.50706	2.74313	-3.01999	C	0.4349	-2.84421	0.20756

C	0.77065	-4.16678	-0.06464
C	1.43592	-4.94098	0.91428
C	1.75786	-4.446	2.16169
C	1.41928	-3.10766	2.48623
C	0.77669	-2.32315	1.49262
N	0.41699	-1.02475	1.73987
C	0.61593	-0.47524	2.92784
C	1.23218	-1.19787	3.96784
C	1.64474	-2.49423	3.74341
N	-0.24532	-1.92787	-0.58294
H	1.6902	-5.96751	0.66734
H	2.2523	-5.06507	2.90307
H	2.13485	-3.06101	4.52954
H	1.38051	-0.7146	4.92653
H	0.28999	0.55002	3.05027
C	-1.00234	-2.26914	-1.67509
C	-1.85782	-1.13125	-2.15207
C	-3.19586	-1.39191	-2.46128
C	-1.3983	0.1975	-2.12633
C	-4.07639	-0.33325	-2.68336
C	-2.28892	1.25714	-2.33631
C	-3.63034	0.99161	-2.60435
H	-0.32018	0.41456	-2.08335
H	-5.11998	-0.53945	-2.90333
H	-1.92016	2.27621	-2.27662
H	-4.3278	1.80916	-2.75963
O	-1.08632	-3.40356	-2.1534
H	0.50715	-4.59106	-1.0221
Co	-0.2253	-0.14602	0.17247
C	2.15552	0.26804	-1.43548
O	1.63453	-0.06025	-0.28516
O	1.54531	0.70663	-2.41212
C	3.65634	0.03945	-1.47309
H	2.12053	3.83304	-1.62654
H	-3.53904	-2.42084	-2.49046
H	4.08806	0.52462	-2.34933
H	3.84948	-1.03792	-1.52489
H	4.12232	0.42026	-0.56223

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C	-1.37806	2.18146	0.72165
C	-1.91691	3.46446	0.78085
C	-3.24019	3.66662	1.23763

C	-4.05117	2.62978	1.64701
C	-3.54657	1.30552	1.60026
C	-2.2278	1.10812	1.11276
N	-1.69491	-0.13872	0.98723
C	-2.37296	-1.20594	1.39123
C	-3.6679	-1.09201	1.92318
C	-4.2583	0.15345	2.00762
N	-0.07155	1.78866	0.40326
H	-3.61896	4.68402	1.26406
H	-5.06149	2.80653	2.00086
H	-5.27016	0.26131	2.3873
H	-4.19123	-1.98801	2.23593
H	-1.89051	-2.16693	1.2623
C	0.8178	2.75271	-0.09188
C	2.26048	2.57818	0.24791
C	3.21708	3.17253	-0.58427
C	2.67299	1.90136	1.40028
C	4.57216	3.0631	-0.28184
C	4.02698	1.80276	1.71089
C	4.97981	2.37695	0.86571
H	1.9251	1.45725	2.04463
H	5.31136	3.51027	-0.9397
H	4.34019	1.27565	2.6074
H	6.03667	2.29347	1.10216
O	0.45006	3.73626	-0.72936
H	-1.32594	4.31075	0.46513
C	0.60638	-2.76701	-0.4908
C	0.90892	-3.90788	-1.22375
C	1.83472	-4.85389	-0.72976
C	2.46076	-4.69548	0.48839
C	2.17883	-3.5484	1.27234
C	1.25854	-2.58489	0.77247
N	0.95263	-1.45689	1.47491
C	1.48617	-1.25724	2.66642
C	2.39599	-2.16512	3.24779
C	2.74809	-3.29686	2.54554
N	-0.28845	-1.75855	-0.84641
H	2.04821	-5.73076	-1.33362
H	3.16039	-5.43687	0.86147
H	3.45746	-4.00849	2.95843
H	2.80944	-1.95507	4.22784
H	1.19923	-0.34612	3.18285
C	-1.40114	-2.01182	-1.62578
C	-2.25994	-0.81364	-1.896

C	-3.64959	-0.96452	-1.79423	C	3.92111	2.31029	1.5412
C	-1.71781	0.44513	-2.18733	C	4.78462	3.10254	0.78169
C	-4.48356	0.14259	-1.92555	H	1.90513	1.57861	1.75195
C	-2.56118	1.54983	-2.33266	H	4.98126	4.39827	-0.93258
C	-3.93997	1.40504	-2.18754	H	4.29314	1.77436	2.40885
H	-0.64636	0.56917	-2.33568	H	5.8313	3.18301	1.06005
H	-5.55821	0.02487	-1.81982	O	0.17354	3.59951	-1.14369
H	-2.1288	2.52169	-2.54712	H	-1.2406	4.26317	0.63931
H	-4.59184	2.26854	-2.28091	C	0.34916	-3.1528	-0.44685
O	-1.73054	-3.13218	-2.02106	C	0.39127	-4.44288	-0.9773
H	0.41789	-4.07388	-2.17165	C	1.12617	-5.46708	-0.34523
Co	0.02135	-0.11079	0.07437	C	1.8218	-5.25131	0.82521
C	2.08426	0.30083	-1.84201	C	1.8039	-3.96246	1.4134
O	1.76574	-0.10242	-0.6421	C	1.0781	-2.91202	0.77455
O	1.32929	0.85251	-2.64151	N	1.03186	-1.65658	1.3132
C	3.53239	-0.00502	-2.18199	C	1.65029	-1.40677	2.45417
H	2.88029	3.70155	-1.46861	C	2.38421	-2.38455	3.1552
H	-4.05752	-1.94864	-1.58872	C	2.46538	-3.65343	2.62784
H	3.84281	0.57317	-3.05354	N	-0.33698	-2.06449	-0.96379
H	3.62043	-1.07331	-2.41046	H	1.13519	-6.45302	-0.80153
H	4.18193	0.21144	-1.33162	H	2.37848	-6.04883	1.30755
5s_AQ_Q				H	3.02951	-4.43202	3.13392
C	-1.30124	2.10305	0.7771	H	2.87414	-2.12398	4.08693
C	-1.82083	3.41013	0.96305	H	1.57172	-0.39414	2.83859
C	-3.07473	3.604	1.54802	C	-1.42602	-2.21338	-1.77599
C	-3.85659	2.53616	1.96684	C	-2.13381	-0.91252	-2.05108
C	-3.38831	1.20188	1.80941	C	-3.53211	-0.89709	-1.96069
C	-2.11869	0.98762	1.21594	C	-1.4485	0.28423	-2.30429
N	-1.61488	-0.24459	1.0134	C	-4.23019	0.30398	-2.0618
C	-2.31747	-1.30656	1.393	C	-2.15292	1.48616	-2.41968
C	-3.5799	-1.19669	1.99996	C	-3.54004	1.50192	-2.28055
C	-4.11966	0.05815	2.20346	H	-0.36884	0.30215	-2.45281
N	-0.10051	1.78844	0.26225	H	-5.31254	0.30978	-1.96577
H	-3.44131	4.61748	1.67444	H	-1.60264	2.40551	-2.58825
H	-4.82976	2.70558	2.41648	H	-4.08497	2.43894	-2.35187
H	-5.09841	0.17952	2.658	O	-1.91223	-3.27887	-2.17917
H	-4.11444	-2.09444	2.28865	H	-0.16321	-4.64811	-1.8807
H	-1.86967	-2.27327	1.19137	Co	0.24532	-0.29102	-0.13863
C	0.67368	2.8205	-0.34607	C	2.40514	0.48814	-1.88054
C	2.09855	2.88605	0.05706	O	2.08547	-0.18731	-0.81782
C	2.96721	3.68533	-0.69929	O	1.60244	1.11164	-2.58677
C	2.58166	2.19846	1.17665	C	3.88811	0.46784	-2.20718
C	4.30651	3.78907	-0.3393	H	2.57562	4.20033	-1.56881
				H	-4.05239	-1.83358	-1.78877

H	4.10457	1.10123	-3.06876	N	-0.37294	1.98288	0.43889
H	4.20182	-0.55983	-2.41996	H	0.95012	6.06586	-1.32243
H	4.46028	0.81078	-1.34038	H	1.37635	5.03466	-3.53201
TS3s_AQ_S				H	1.31748	2.90325	-4.98214
C	-1.65518	-2.14571	-0.98924	H	0.8005	0.46436	-5.11966
C	-2.09503	-3.42604	-1.33083	H	0.04533	-0.7394	-3.0416
C	-3.41766	-3.64686	-1.76183	C	-0.94661	2.30198	1.63792
C	-4.34126	-2.62449	-1.86025	C	-1.53163	1.07287	2.2594
C	-3.9495	-1.31162	-1.5094	C	-2.58707	1.1674	3.16134
C	-2.61155	-1.09279	-1.06945	C	-1.0738	-0.18372	1.79314
N	-2.18114	0.14688	-0.69052	C	-3.22672	0.00147	3.58936
C	-3.0001	1.18621	-0.75449	C	-1.7388	-1.34302	2.23066
C	-4.33186	1.05547	-1.19312	C	-2.8095	-1.24867	3.12016
C	-4.80493	-0.18342	-1.56136	H	0.19764	-0.35045	1.89599
N	-0.35687	-1.76197	-0.66302	H	-4.0584	0.06688	4.28528
H	-3.71058	-4.6597	-2.02312	H	-1.39755	-2.3167	1.8904
H	-5.35742	-2.80885	-2.1932	H	-3.31558	-2.14909	3.45628
H	-5.83093	-0.31119	-1.89423	O	-1.05993	3.43626	2.11494
H	-4.96253	1.93651	-1.22544	H	0.11368	4.71939	0.59045
H	-2.60141	2.1432	-0.44745	Co	-0.32375	0.16577	-0.13049
C	0.46191	-2.72328	-0.08538	C	2.11471	-0.01198	1.29397
C	1.94052	-2.61601	-0.3013	O	1.57407	0.25244	0.17413
C	2.79189	-3.21957	0.63433	O	1.46827	-0.43122	2.29642
C	2.48951	-2.03394	-1.44857	C	3.59549	0.22671	1.4124
C	4.16998	-3.22601	0.43307	H	-2.91139	2.14773	3.49633
C	3.86703	-2.05562	-1.66122	H	2.35287	-3.67937	1.51249
C	4.71079	-2.64847	-0.71907	H	3.75558	1.29615	1.59052
H	1.83299	-1.56944	-2.17108	H	4.00993	-0.33704	2.24799
H	4.82254	-3.68525	1.16967	H	4.09303	-0.045	0.48096
H	4.2821	-1.60962	-2.56041	6s_AQ_S			
H	5.78469	-2.66112	-0.88176	C	-2.54153	-1.37411	-0.83847
O	0.03204	-3.68965	0.55519	C	-3.40882	-2.36886	-1.29526
H	-1.41351	-4.26209	-1.25622	C	-4.80129	-2.15762	-1.32694
C	0.10832	2.87902	-0.49508	C	-5.37764	-0.97757	-0.90065
C	0.32024	4.24825	-0.35995	C	-4.54369	0.05495	-0.41148
C	0.78744	5.00094	-1.46126	C	-3.13512	-0.16039	-0.38358
C	1.03105	4.43449	-2.69635	N	-2.2808	0.79321	0.09403
C	0.81166	3.04537	-2.88034	C	-2.75018	1.95216	0.53417
C	0.36707	2.28039	-1.7686	C	-4.1276	2.24447	0.52619
N	0.13216	0.93791	-1.87285	C	-5.01765	1.3039	0.06069
C	0.27027	0.32071	-3.03321	N	-1.14829	-1.38995	-0.85498
C	0.6959	1.00874	-4.18801	H	-5.43376	-2.95889	-1.69839
C	0.97806	2.35542	-4.10779				



H	-6.45235	-0.82979	-0.92627	O	0.70858	2.77077	2.96062
H	-6.08531	1.50334	0.05161	H	1.38006	4.29439	1.42264
H	-4.46102	3.20763	0.89526	Co	-0.44298	0.26259	0.03488
H	-2.02318	2.6609	0.90525	C	2.30709	-0.77781	0.53651
C	-0.52204	-2.62194	-0.84996	O	1.47857	-0.16901	-0.15052
C	0.8631	-2.71292	-1.42049	O	2.00894	-1.47797	1.60916
C	1.72289	-3.70116	-0.92192	C	3.76363	-0.73077	0.20523
C	1.28201	-1.92574	-2.49836	H	4.19758	0.13664	0.71643
C	2.98931	-3.88013	-1.47451	H	4.27174	-1.63033	0.55236
C	2.53991	-2.11869	-3.06818	H	3.8899	-0.60451	-0.86912
C	3.39907	-3.09225	-2.55389	H	-0.03166	1.09223	4.85372
H	0.61898	-1.16615	-2.88793	H	1.37973	-4.32191	-0.10171
H	3.65292	-4.63965	-1.0717				
H	2.84933	-1.50917	-3.9123	6s_AQ_T			
H	4.38163	-3.23909	-2.99302	C	-0.25529	2.44248	-1.46059
O	-1.04558	-3.66553	-0.43829	C	-0.80867	3.5026	-2.17825
H	-3.00721	-3.31717	-1.62207	C	-0.01635	4.58202	-2.61977
C	0.60384	2.85986	0.04352	C	1.33523	4.65605	-2.35553
C	1.19123	4.07859	0.38074	C	1.94619	3.61378	-1.61915
C	1.5198	5.01057	-0.6282	C	1.14885	2.51431	-1.18052
C	1.26637	4.77536	-1.96456	N	1.68994	1.49753	-0.46018
C	0.66114	3.55268	-2.3509	C	2.97257	1.50068	-0.14739
C	0.35339	2.59525	-1.34401	C	3.83724	2.54021	-0.54908
N	-0.21991	1.39248	-1.64651	C	3.32273	3.5881	-1.27917
C	-0.55649	1.1172	-2.89443	N	-0.9276	1.27577	-1.07385
C	-0.3003	2.01209	-3.95414	H	-0.49879	5.37722	-3.18097
C	0.31728	3.21372	-3.68434	H	1.93388	5.49545	-2.69492
N	0.18525	1.85245	0.88731	H	3.95959	4.40819	-1.59893
H	1.97972	5.94854	-0.32983	H	4.88554	2.50167	-0.27445
H	1.51307	5.5118	-2.72272	H	3.32765	0.66173	0.44317
H	0.53502	3.91727	-4.48301	C	-2.29652	1.35099	-0.88264
H	-0.58857	1.73928	-4.96328	C	-3.06489	0.06738	-0.95079
H	-1.04032	0.16025	-3.05884	C	-4.19169	-0.07882	-0.13139
C	0.27333	1.854	2.25395	C	-2.7388	-0.94713	-1.85545
C	-0.26025	0.56634	2.78976	C	-4.95119	-1.24491	-0.18355
C	-0.35578	0.32235	4.15948	C	-3.51377	-2.10331	-1.92869
C	-0.65625	-0.39723	1.83639	C	-4.61386	-2.26036	-1.08434
C	-0.8607	-0.90105	4.60358	H	-1.87821	-0.82575	-2.49918
C	-1.16637	-1.61727	2.29617	H	-5.81075	-1.36086	0.47018
C	-1.26259	-1.86353	3.6754	H	-3.2555	-2.88313	-2.63918
H	1.04215	-1.38452	1.79737	H	-5.21211	-3.16579	-1.13133
H	-0.93845	-1.10551	5.66742	O	-2.91692	2.39824	-0.66139
H	-1.47929	-2.38668	1.59681	H	-1.86739	3.50273	-2.39401
H	-1.65518	-2.81666	4.01986	C	1.8542	-2.16409	0.60034

C	2.58616	-3.19419	1.18504	C	1.75132	3.63518	-1.64624
C	3.05947	-4.26728	0.39548	C	0.98341	2.51749	-1.21327
C	2.83808	-4.33751	-0.96393	N	1.56804	1.4386	-0.63116
C	2.10519	-3.30337	-1.60158	C	2.8799	1.3989	-0.45431
C	1.60406	-2.2351	-0.80819	C	3.7176	2.45248	-0.86646
N	0.88366	-1.21093	-1.35588	C	3.15319	3.56442	-1.45637
C	0.68254	-1.16873	-2.66269	N	-1.0737	1.30679	-0.96
C	1.14977	-2.18067	-3.5242	H	-0.81108	5.54916	-2.79928
C	1.84457	-3.24682	-2.9931	H	1.65913	5.59489	-2.57052
N	1.33577	-1.03142	1.20337	H	3.77257	4.39785	-1.77567
H	3.62358	-5.05521	0.88629	H	4.78738	2.37893	-0.70714
H	3.2201	-5.16345	-1.55543	H	3.27036	0.51407	0.03751
H	2.20888	-4.04555	-3.63305	C	-2.4434	1.3482	-0.70384
H	0.95302	-2.10786	-4.58794	C	-3.22026	0.1082	-1.00663
H	0.13211	-0.31057	-3.03327	C	-4.4202	-0.11372	-0.31743
C	1.50626	-0.68108	2.52088	C	-2.81001	-0.80161	-1.98658
C	0.72805	0.55867	2.80198	C	-5.18282	-1.24751	-0.5861
C	0.72068	1.16537	4.05808	C	-3.58165	-1.92713	-2.26872
C	-0.0247	1.08698	1.73643	C	-4.76515	-2.15601	-1.56377
C	-0.04624	2.31297	4.25865	H	-1.88631	-0.62156	-2.52085
C	-0.78686	2.24054	1.93883	H	-6.10421	-1.42293	-0.03878
C	-0.7971	2.84254	3.20595	H	-3.25827	-2.62673	-3.03372
H	-1.72395	-0.08343	2.26608	H	-5.3631	-3.03733	-1.77698
H	-0.06398	2.79304	5.23262	O	-3.01912	2.33294	-0.23448
H	-1.38041	2.67241	1.13982	H	-2.12943	3.6305	-2.01867
H	-1.39817	3.73388	3.36421	C	2.01048	-2.19982	0.73097
O	2.18312	-1.28127	3.36002	C	2.78536	-3.17519	1.36453
H	2.79279	-3.15193	2.24479	C	3.28776	-4.28014	0.64515
Co	0.20311	0.07107	0.08917	C	3.05783	-4.4492	-0.70447
C	-2.00491	-1.82319	1.58452	C	2.2854	-3.48401	-1.39696
O	-1.28855	-1.64774	0.60645	C	1.75393	-2.37387	-0.67533
O	-2.24931	-0.88039	2.49316	N	1.00054	-1.4217	-1.29446
C	-2.66055	-3.13364	1.90364	C	0.78295	-1.49254	-2.59786
H	-2.06813	-3.63783	2.6758	C	1.2747	-2.54846	-3.39027
H	-3.66607	-2.97767	2.29824	C	2.01167	-3.5433	-2.78616
H	-2.69127	-3.75676	1.01115	N	1.458	-1.0623	1.27687
H	1.31109	0.72356	4.85555	H	3.88228	-5.01468	1.1818
H	-4.45092	0.72603	0.54767	H	3.46085	-5.29938	-1.24596
6s_AQ_Q				H	2.39924	-4.377	-3.36536
C	-0.44245	2.48525	-1.34881	H	1.06456	-2.56467	-4.45403
C	-1.05304	3.6035	-1.9177	H	0.20262	-0.68638	-3.03606
C	-0.29049	4.70601	-2.35515	C	1.65107	-0.6753	2.5691
C	1.08321	4.73967	-2.23171	C	0.89089	0.58272	2.8831
				C	1.05555	1.22177	4.11523

C	0.0136	1.10916	1.92667	C	-5.12056	-1.93382	-1.84055
C	0.35324	2.39745	4.38205	H	-1.96761	-0.8279	-2.44127
C	-0.68332	2.2911	2.18832	H	-6.52447	-0.97569	-0.51154
C	-0.51319	2.93115	3.42448	H	-3.52564	-2.63326	-3.11212
H	-1.54931	-0.05776	2.24799	H	-5.80652	-2.72631	-2.12502
H	0.47945	2.89937	5.33732	O	-2.99743	2.28836	-0.29201
H	-1.36853	2.70873	1.45521	H	-2.05482	3.43722	-2.1607
H	-1.06176	3.84552	3.63613	C	2.14576	-2.06256	0.30669
O	2.35566	-1.22866	3.42626	C	3.12972	-2.95218	0.73591
H	2.99811	-3.05879	2.41699	C	3.72868	-3.84571	-0.178
Co	0.1566	0.04026	0.04584	C	3.39199	-3.87142	-1.51552
C	-2.04211	-1.69589	1.43932	C	2.40939	-2.97192	-1.99886
O	-1.27671	-1.5501	0.48528	C	1.77473	-2.09094	-1.07724
O	-2.19234	-0.79774	2.39701	N	0.80934	-1.20775	-1.47258
C	-2.85924	-2.93629	1.63076	C	0.50229	-1.10619	-2.75627
H	-2.31591	-3.60215	2.31122	C	1.08019	-1.93655	-3.737
H	-3.823	-2.69936	2.08356	C	2.01475	-2.87539	-3.35566
H	-2.99513	-3.43833	0.674	N	1.48273	-1.10451	1.04843
H	1.73595	0.78478	4.84005	H	4.48287	-4.53274	0.19532
H	-4.73288	0.60895	0.42814	H	3.87149	-4.55911	-2.20473
7s_AQ_S				H	2.47047	-3.53529	-4.08854
C	-0.43082	2.29138	-1.34483	H	0.78267	-1.82305	-4.77351
C	-0.98457	3.38654	-2.01473	H	-0.21195	-0.33347	-3.0161
C	-0.1742	4.43103	-2.49652	C	1.76706	-0.77414	2.35213
C	1.19661	4.43777	-2.32655	C	0.99509	0.43832	2.74096
C	1.80543	3.36332	-1.63816	C	1.1213	1.02259	4.00299
C	0.98182	2.30567	-1.15123	C	0.12538	0.96688	1.76869
N	1.51521	1.25311	-0.46018	C	0.37685	2.16295	4.3047
C	2.82161	1.19212	-0.23625	C	-0.59893	2.12094	2.07154
C	3.69941	2.18929	-0.70156	C	-0.47561	2.70745	3.339
C	3.19719	3.26729	-1.39277	H	0.46136	2.62937	5.28203
N	-1.09199	1.1405	-0.93157	H	-1.27228	2.56175	1.34268
H	-0.65353	5.2553	-3.01704	H	-1.05209	3.59972	3.57055
H	1.8113	5.24974	-2.70086	O	2.5597	-1.36195	3.09726
H	3.854	4.05395	-1.7526	H	3.41703	-2.94358	1.7765
H	4.75886	2.08963	-0.49525	Co	0.20938	-0.02347	0.12485
H	3.1843	0.34412	0.32508	H	1.79762	0.57298	4.72443
C	-2.46029	1.25914	-0.71617	H	-4.94897	0.84994	0.11572
C	-3.34298	0.10451	-1.08896	C	-1.40796	-2.13519	0.62564
C	-4.64608	0.0679	-0.57089	C	-1.76684	-1.25562	1.58519
C	-2.9587	-0.86923	-2.01602	C	-1.92152	-1.1216	3.04034
C	-5.52343	-0.94976	-0.93191	C	-2.83987	-0.37742	2.06615
C	-3.84005	-1.8844	-2.39093	H	-1.21548	-0.51646	3.59885
				H	-2.30773	-1.98531	3.57927

H	-3.85915	-0.72723	1.92845	C	-1.90279900	1.13789600	3.11458200
H	-2.71919	0.69885	2.01297	H	-0.08202500	-0.05381100	3.25141400
H	-1.83815	-2.0152	-0.36172	H	-3.67107600	2.24847700	2.61466500
C	-0.61216	-3.34291	0.82827	H	-4.34716900	2.70574700	0.17453000
C	-0.40414	-4.20926	-0.26132	H	-2.02128100	1.23226200	4.18807800
C	-0.0276	-3.68099	2.05778	N	-0.60873600	0.28219300	1.29784400
C	0.36703	-5.3534	-0.13669	Co	0.83812500	-0.72950900	0.32131800
H	-0.84549	-3.96242	-1.22294	C	-0.62920600	-2.48021900	0.75423200
C	0.75501	-4.82135	2.19707	C	0.38626200	-2.76078400	-0.14522500
H	-0.14966	-3.02318	2.9086	C	0.45725800	-3.48128700	-1.43161800
C	0.96785	-5.65908	1.09278	C	1.34078400	-3.88484600	-0.24492600
H	0.54477	-6.01027	-0.98112	H	0.96752400	-3.01801100	-2.26821600
H	1.21411	-5.0336	3.15435	H	-0.38541700	-4.11309300	-1.70314300
O	1.74397	-6.77465	1.11332	H	1.09402100	-4.78899200	0.30689200
C	2.44082	-7.07973	2.31526	H	2.39933500	-3.68321400	-0.34297600
H	3.02343	-7.97847	2.10563	C	2.58729900	-0.65691600	2.56096300
H	3.11934	-6.26751	2.60333	O	1.72391900	-1.35259100	1.93990700
H	1.75079	-7.2848	3.14293	O	2.94869200	0.51415800	2.24791600

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C	4.56142400	-1.56649100	-1.58886800	H	2.66290400	-2.11800200	4.14731500
C	4.25701300	-1.15891900	-2.89098600	H	-0.37819700	-2.58321000	1.80796300
C	2.97740800	-0.68993600	-3.18979600	C	-2.01307500	-2.18235500	0.46789700
C	2.01684700	-0.64064200	-2.18050400	C	-2.90422100	-1.99669700	1.54946100
C	2.30668100	-1.05571200	-0.86867400	C	-2.50803800	-1.99476200	-0.83651900
C	3.59077300	-1.52080600	-0.58024700	C	-4.21229800	-1.61153100	1.34235000
H	5.56031900	-1.92550400	-1.35502500	H	-2.54002100	-2.13487300	2.56279500
H	5.01768200	-1.20182600	-3.66466000	C	-3.81926400	-1.59995000	-1.05735600
H	2.70998800	-0.34487000	-4.18393400	H	-1.83823400	-2.10553400	-1.67933400
H	3.84401900	-1.85463900	0.42127100	C	-4.67371900	-1.38014100	0.03360400
C	0.65442500	-0.08223300	-2.39897700	H	-4.89477000	-1.44667900	2.16838700
O	0.21437900	0.29285100	-3.48475900	H	-4.15481400	-1.42519900	-2.07086100
N	-0.01273800	-0.02091800	-1.19137700	O	-5.94850900	-0.94442900	-0.06994800
C	-1.16554400	0.69799300	-0.96931100	C	-6.42605200	-0.55963700	-1.35453400
C	-1.47840000	0.85565300	0.41563800	H	-7.43693000	-0.18168000	-1.19602300
C	-2.00957100	1.29272600	-1.90512500	H	-5.80299300	0.23267200	-1.78507600
C	-2.62007400	1.57990900	0.84588500	H	-6.46691000	-1.41262200	-2.04254800
C	-3.14962300	2.00331800	-1.47196800	C	0.54591800	3.42708700	-0.60297900
H	-1.76931800	1.20234200	-2.95440300	O	1.53531600	2.68133900	-1.00278900
C	-0.80609200	0.42464900	2.60132000	O	0.12653300	3.46365100	0.56147200
C	-2.81087700	1.70079000	2.24082500	C	-0.06170200	4.28734600	-1.69703600
C	-3.47181900	2.14524000	-0.13693700	H	-0.18670600	3.70157500	-2.61039900
H	-3.78632400	2.46003300	-2.22464000	H	-1.01964200	4.69497400	-1.37185600

H	0.62157300	5.11332500	-1.92383200	O	-3.01093100	-0.20975200	2.45676500
Ag	2.15916200	1.53023100	0.59621300	C	-2.81475500	1.70403900	3.86067600
5s_AgOAc_T				H	-3.49209100	2.49329300	3.51494000
C	-4.33571200	1.86526700	-1.55650900	H	-3.33864900	1.09269300	4.59607400
C	-4.10009800	1.40760600	-2.85828100	H	-1.94472400	2.18687000	4.31041400
C	-2.91045000	0.74688500	-3.16264600	H	0.64644500	3.12749400	1.56739600
C	-1.96615500	0.55369100	-2.15420100	C	2.24326500	2.32550500	0.32984700
C	-2.19150200	1.01310400	-0.84844100	C	3.05260700	2.05176500	1.44782100
C	-3.38599500	1.66989400	-0.54612600	C	2.72627800	1.95205100	-0.93317000
H	-5.26574900	2.37704800	-1.32458700	C	4.27859000	1.41965300	1.31484100
H	-4.84816300	1.56440200	-3.62938100	H	2.70099800	2.33160100	2.43708200
H	-2.70483500	0.37072600	-4.16027600	C	3.95644300	1.31798900	-1.08295500
H	-3.58538500	2.03344300	0.45609300	H	2.11841600	2.13386300	-1.81185200
C	-0.68722200	-0.16944300	-2.36544600	C	4.73526100	1.03391900	0.04614300
O	-0.31157800	-0.65258200	-3.43109600	H	4.89338400	1.19510800	2.17984300
N	0.01483100	-0.21044400	-1.16963100	H	4.28166100	1.02310300	-2.07231900
C	1.19916500	-0.91270500	-0.96368000	O	5.93043200	0.38443400	0.01657800
C	1.59426400	-0.97537100	0.40440000	C	6.42485500	-0.03953400	-1.24774900
C	1.99361400	-1.54794500	-1.90812400	H	7.37170900	-0.54398700	-1.04717400
C	2.75636800	-1.67612600	0.81395400	H	5.73633700	-0.74138700	-1.73176400
C	3.16346800	-2.23270300	-1.49990700	H	6.60638300	0.81167900	-1.91581100
H	1.70575700	-1.51799400	-2.94830800	C	-1.13179300	-3.30174100	-0.66393900
C	1.05781500	-0.39351300	2.59493100	O	-2.24038400	-2.65837800	-0.87491000
C	3.03066900	-1.70842600	2.20040100	O	-0.51741200	-3.30053900	0.41446800
C	3.55273200	-2.30319600	-0.17994900	C	-0.61121000	-4.05820400	-1.87361900
H	3.76257300	-2.72186500	-2.26232100	H	-0.42474700	-3.34711400	-2.68394100
C	2.18090800	-1.07944100	3.08838400	H	0.30923700	-4.59080500	-1.63116400
H	0.37530600	0.13113500	3.25436400	H	-1.36857300	-4.76517400	-2.22693900
H	3.91090700	-2.23634400	2.55521300	Ag	-2.59108700	-1.45839400	0.79714600
H	4.45017600	-2.83647900	0.11556000	5s_AgOAc_Q			
H	2.36708000	-1.09773900	4.15606900	C	4.50747000	-1.26407500	-2.01302900
N	0.78423600	-0.33812200	1.29880300	C	4.01626100	-0.94429200	-3.28689500
Co	-0.74770400	0.56892600	0.34742500	C	2.68457300	-0.57353900	-3.43652900
C	0.93719300	2.96051800	0.53134300	C	1.85366100	-0.52947400	-2.30732500
C	0.11067900	3.39731800	-0.42706500	C	2.31525000	-0.85259000	-1.00923600
C	-0.09335200	3.67918100	-1.84981700	C	3.66803500	-1.21475700	-0.89607700
C	-1.03733100	4.23884400	-0.77289600	H	5.55011400	-1.55012200	-1.89640600
H	-0.49054700	2.88978100	-2.48394000	H	4.67510600	-0.98025600	-4.14941400
H	0.59535600	4.35744200	-2.35090100	H	2.27854000	-0.30944200	-4.40835500
H	-0.97792400	5.30043100	-0.53793800	H	4.07911100	-1.46498000	0.08024200
H	-2.03951400	3.82282500	-0.73129600	C	0.44327900	-0.10569300	-2.45327100
C	-2.40440900	0.87142700	2.67101300	O	-0.12381600	0.11359700	-3.52026200
O	-1.46516600	1.35151300	1.94330400	N	-0.17502800	0.00971800	-1.18660700

C	-1.24205300	0.76526900	-0.92419100	C	-6.36394300	-0.20592100	-1.32557800
C	-1.54201600	0.89185700	0.49318400	H	-7.32269100	0.28957100	-1.16413500
C	-2.06994200	1.45555600	-1.84650200	H	-5.68325700	0.48182200	-1.84135900
C	-2.65826700	1.64120800	0.93040500	H	-6.52016800	-1.09594300	-1.94724500
C	-3.17755200	2.17656400	-1.39427600	C	0.73024700	3.35046600	-0.66631000
H	-1.84034900	1.37999600	-2.89944200	O	1.84238800	2.73440300	-0.90519200
C	-0.89496800	0.42352500	2.66277400	O	0.09801800	3.29677400	0.40141900
C	-2.86718600	1.74803600	2.32259600	C	0.21584900	4.18285500	-1.83414000
C	-3.48665500	2.26641900	-0.04277900	H	0.15403900	3.56506300	-2.73508400
H	-3.80801900	2.68031300	-2.11999500	H	-0.76279900	4.60863400	-1.60789800
C	-1.97879600	1.14352300	3.19021800	H	0.92389600	4.99106000	-2.04633900
H	-0.17447600	-0.06958000	3.30639200	Ag	2.38549400	1.49901000	0.71199800
H	-3.71574000	2.31366400	2.69504900				
H	-4.35171900	2.83196600	0.28850300	TS1_AgOAc_S			
H	-2.10081300	1.21724200	4.26476300	C	4.15468700	-1.97949800	-1.55943300
N	-0.69025400	0.29635400	1.35499000	C	3.86478500	-1.47392200	-2.83044500
Co	0.85862000	-0.86675900	0.42670900	C	2.59815600	-0.95075600	-3.10211500
C	-0.78202500	-2.85031700	0.68474700	C	1.62425300	-0.95034000	-2.10694800
C	0.11881900	-3.23887500	-0.23714400	C	1.90541300	-1.47606200	-0.82951600
C	0.34501100	-3.66678200	-1.62240100	C	3.17391100	-1.99462300	-0.56251200
C	1.30938400	-4.05897300	-0.49112200	H	5.14514300	-2.36936600	-1.34274600
H	0.72102400	-2.94850000	-2.34531200	H	4.62891300	-1.47513000	-3.60174500
H	-0.32089700	-4.42227500	-2.03544900	H	2.35855200	-0.50856800	-4.06396300
H	1.30551800	-5.08506600	-0.12846800	H	3.40074400	-2.40778800	0.41428600
H	2.28528300	-3.58254500	-0.50710300	C	0.32288000	-0.23843500	-2.28247000
C	2.62519000	-0.78107700	2.74605900	O	-0.12616900	0.12672600	-3.37225600
O	1.69815400	-1.44501100	2.17534500	N	-0.22878200	-0.01046900	-1.05373100
O	3.03093100	0.36546100	2.40235300	C	-1.26683000	0.86303700	-0.79644200
C	3.30870300	-1.44223300	3.92343800	C	-1.38862800	1.18021200	0.58668400
H	3.99332700	-2.20911100	3.54369900	C	-2.14942400	1.45492900	-1.69157400
H	3.87969300	-0.71734500	4.50459700	C	-2.37902300	2.07648700	1.06275500
H	2.57261800	-1.94466000	4.55591900	C	-3.13828200	2.34629900	-1.21559800
H	-0.50603800	-2.96025000	1.73314500	H	-2.05935200	1.23116300	-2.74460900
C	-2.13049200	-2.33472600	0.43171600	C	-0.52332100	0.84283000	2.72413700
C	-2.95972700	-2.02079200	1.52509000	C	-2.39663400	2.33005600	2.45390900
C	-2.62152800	-2.07916000	-0.85718300	C	-3.26740900	2.65829400	0.12189400
C	-4.20690300	-1.44574500	1.34279500	H	-3.81352900	2.79816100	-1.93649200
H	-2.60161700	-2.21150900	2.53265000	C	-1.47228000	1.72012000	3.27819200
C	-3.87219800	-1.50119500	-1.05655300	H	0.20781200	0.33427600	3.34061100
H	-2.00180300	-2.30018000	-1.71839700	H	-3.13784900	3.01085700	2.86221500
C	-4.66529400	-1.16111100	0.04752700	H	-4.03067600	3.34780000	0.46753300
H	-4.83608200	-1.18482200	2.18702100	H	-1.46180400	1.90438700	4.34642200
H	-4.20433800	-1.29649700	-2.06630700	N	-0.48558900	0.58278000	1.42296600
O	-5.87624600	-0.54815200	-0.03354400	Co	0.66236100	-0.68074100	0.46357200

C	-0.61854100	-2.20271100	0.82450700	C	1.74670400	-0.54754500	-2.15169500
C	0.35119000	-2.73754200	-0.06808900	C	1.87481200	-1.35734500	-1.00616500
C	0.17317500	-3.68903800	-1.19048900	C	3.11669300	-1.90603200	-0.67226700
C	1.01385000	-4.06194800	0.03307200	H	5.18725000	-2.08253600	-1.22955000
H	0.71738200	-3.53652900	-2.11492800	H	4.93842300	-0.73621100	-3.30408400
H	-0.81469900	-4.12552700	-1.30892100	H	2.72130900	0.29974400	-3.85231200
H	0.59721700	-4.74582600	0.76829900	H	3.22109900	-2.52141500	0.21474600
H	2.07841200	-4.16375800	-0.12860700	C	0.48342000	0.23311600	-2.33024400
C	-2.02986800	-1.95658400	0.53379000	O	0.13702200	0.74232900	-3.40093600
C	-2.89021100	-1.68335300	1.61793700	N	-0.15312100	0.32192100	-1.12324200
C	-2.57904300	-1.92703500	-0.75861900	C	-1.29606700	1.05472700	-0.86665800
C	-4.22447000	-1.37431700	1.42305900	C	-1.67920100	1.06861100	0.51542500
H	-2.48689100	-1.69607000	2.62650400	C	-2.09650400	1.73686000	-1.77570400
C	-3.91867800	-1.62081300	-0.97050700	C	-2.84413200	1.75380100	0.95119200
H	-1.94254800	-2.09938100	-1.61662700	C	-3.26318700	2.40413500	-1.33767000
C	-4.74841600	-1.32584000	0.12075900	H	-1.81182800	1.74255300	-2.81796300
H	-4.88015800	-1.14941000	2.25742800	C	-1.15434900	0.40694100	2.68934800
H	-4.29796000	-1.58597800	-1.98388500	C	-3.12176200	1.73771100	2.33863100
H	-0.40907500	-2.35843800	1.88040400	C	-3.64751000	2.41744800	-0.01349200
O	-6.05647900	-0.98374700	0.02027500	H	-3.86656800	2.92544400	-2.07552300
C	-6.60768000	-0.82252500	-1.28306200	C	-2.27402900	1.08230700	3.20761600
H	-6.59572200	-1.76385600	-1.84575900	H	-0.47330300	-0.14478400	3.32911500
H	-7.64182000	-0.50792100	-1.13471500	H	-4.00329600	2.25372800	2.70821600
H	-6.07116500	-0.05185500	-1.84927700	H	-4.53995600	2.94390500	0.30956500
C	2.64961900	-0.63909000	2.52169500	H	-2.45923200	1.07036500	4.27576500
O	1.63975100	-1.25392100	2.05146300	N	-0.88113600	0.39139600	1.39363000
O	3.14075200	0.43007700	2.05763800	Co	0.54791200	-0.67950800	0.39621700
C	3.33447300	-1.25585400	3.71812600	C	-4.05113600	-1.73698000	1.23847700
H	4.20803700	-1.81715900	3.36716000	C	-4.58903900	-1.26532000	0.02575800
H	3.69175400	-0.47597500	4.39376300	C	-3.81321000	-1.31278100	-1.14218200
H	2.66805200	-1.94221900	4.24227000	C	-2.50822400	-1.78284100	-1.08656700
C	0.94528500	3.23215500	-1.16454000	C	-1.93702600	-2.22691900	0.12380800
O	1.87696800	2.36001300	-1.41568100	C	-2.75416700	-2.20419300	1.28116800
O	0.55220900	3.53113200	-0.02816800	H	-4.66795700	-1.69976800	2.12973900
C	0.35673200	3.87672700	-2.40836200	H	-4.20402100	-0.95087700	-2.08399500
H	0.05474200	3.09676700	-3.11219000	H	-1.90591000	-1.75957800	-1.98537400
H	-0.49840500	4.50325000	-2.15166000	H	-2.33474200	-2.53664700	2.22614100
H	1.12162400	4.48723600	-2.90073500	C	-0.55516800	-2.63762700	0.26504700
Ag	2.40310300	1.39219800	0.34178700	C	0.38215300	-2.84710700	-0.76932200
				C	0.18528500	-3.39629100	-2.13112800
				C	1.08112400	-4.11203700	-1.11765500
TS1_AgOAc_T				H	0.68749100	-2.92823800	-2.97021800
C	4.21987100	-1.66642600	-1.49572900	H	-0.79064600	-3.81604100	-2.36071400
C	4.07913300	-0.90802800	-2.66321900	H	0.71158700	-5.01742400	-0.64268000
C	2.84338600	-0.34503600	-2.98757900				

H	2.14493900	-4.10488300	-1.32145900	C	-2.83372700	2.12468200	2.21101200
H	-0.27049200	-2.99625700	1.25243200	C	-3.31608400	2.77774300	-0.17363800
O	-5.85188400	-0.78617400	0.08897400	H	-3.50420000	3.21542800	-2.25303300
C	-6.40898500	-0.20014100	-1.08601300	C	-2.04275700	1.40198300	3.08132000
H	-6.51390700	-0.93708400	-1.89087700	H	-0.38047500	-0.01476300	3.21360600
H	-7.39806000	0.15995800	-0.79942300	H	-3.64430100	2.74254700	2.58622200
H	-5.79876200	0.64105900	-1.43244100	H	-4.14033800	3.41705200	0.12573200
C	1.19016500	3.25972100	-0.64015900	H	-2.20868700	1.43651100	4.15183500
O	0.60303600	3.29470800	0.45203400	N	-0.76778800	0.51944500	1.27377100
O	2.26004300	2.56370800	-0.88114100	Co	0.52466000	-0.55245100	0.40549600
C	0.67719800	4.04026200	-1.83959000	C	-0.55074300	-2.18350900	0.09108700
H	1.45862900	4.71186200	-2.20991000	C	0.22822600	-2.70184200	-1.10515000
H	0.43938000	3.33845100	-2.64447300	C	-0.43175000	-3.17020800	-2.38166100
H	-0.21162700	4.61600100	-1.57781400	C	0.14385400	-4.18183400	-1.42829700
C	2.47688900	-0.94800400	2.68238700	H	0.09673100	-2.98275400	-3.31081600
O	3.12761100	0.09415200	2.38845600	H	-1.50986000	-3.11686900	-2.45887200
O	1.47399000	-1.39923800	2.04295400	H	-0.55343500	-4.77401100	-0.84310800
C	2.94637400	-1.75647800	3.87163200	H	1.05387800	-4.70160800	-1.71058500
H	3.60150900	-1.16541200	4.51235000	C	-2.00492100	-1.94868400	0.06995500
H	2.09117800	-2.12900600	4.44051300	C	-2.73437400	-2.16396700	1.25924500
H	3.50334900	-2.62618900	3.50463300	C	-2.70430700	-1.39635700	-1.01601300
Ag	2.61988800	1.32969900	0.75994800	C	-4.07147800	-1.82409600	1.36903100

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C	4.02011300	-2.20507800	-0.94271100	H	-2.18032200	-1.18077800	-1.93643600
C	4.19090800	-1.03092000	-1.68645100	C	-4.73968200	-1.24808600	0.27704700
C	3.08343700	-0.34970300	-2.17929400	H	-4.62148700	-1.97948800	2.29095800
C	1.78967300	-0.83647600	-1.93967400	H	-4.53629200	-0.60304600	-1.78116100
C	1.60389000	-2.05728300	-1.23700900	H	-0.25938600	-2.72331000	0.99413400
C	2.74506400	-2.71484900	-0.73464500	O	-6.03999700	-0.91043600	0.48463100
H	4.88376700	-2.72308200	-0.53781500	C	-6.72204300	-0.23006300	-0.55778600
H	5.18717700	-0.63497600	-1.85681500	H	-6.81742800	-0.85305500	-1.45629300
H	3.19056700	0.59063800	-2.70720400	H	-7.71877400	-0.00882900	-0.17235000
H	2.61120400	-3.64579400	-0.19305700	H	-6.21826000	0.70891800	-0.82045500
C	0.61814300	0.05342900	-2.29297000	C	2.42629100	-1.09843000	2.50316200
O	0.41898100	0.53386700	-3.40625200	O	1.28025000	-1.36487100	2.01122900
N	-0.08499800	0.27774400	-1.15121100	O	3.18817200	-0.15969300	2.14368400
C	-1.14909000	1.13800500	-0.97673300	C	2.91613800	-2.01834000	3.59772500
C	-1.51562500	1.25125800	0.39377800	H	3.33298200	-2.91865700	3.13232000
C	-1.86976500	1.85301600	-1.92163000	H	3.69759900	-1.53787800	4.18715800
C	-2.58750500	2.07040400	0.81944900	H	2.08756900	-2.33008100	4.23703800
C	-2.95087800	2.66238600	-1.49971900	C	1.34132900	3.25004600	-0.66074800
H	-1.59015000	1.78273200	-2.96392000	O	2.38514300	2.53117100	-0.94925700
C	-1.00969700	0.59335900	2.57550800	O	0.75053000	3.21803200	0.42861900



C	0.86976200	4.14304100	-1.79517100
H	0.64140100	3.52265400	-2.66666000
H	-0.01407300	4.70931400	-1.50011600
H	1.67199900	4.82945300	-2.08412900
Ag	2.71170400	1.22272800	0.63706100